



# wwPDB EM Validation Summary Report ⓘ

Mar 18, 2025 – 10:45 PM JST

PDB ID : 8WKK  
EMDB ID : EMD-37601  
Title : Cryo-EM structure of the whole rod with export apparatus and hook within the flagellar motor-hook complex in the CW state.  
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2023-09-28  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

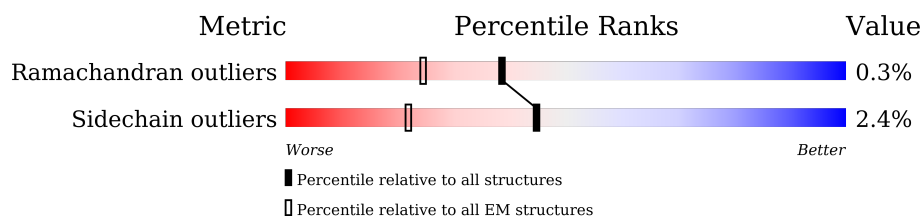
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	89	<div> <div>89%</div> <div>99%</div> </div>
1	B	89	<div> <div>75%</div> <div>99%</div> </div>
1	C	89	<div> <div>71%</div> <div>100%</div> </div>
1	D	89	<div> <div>87%</div> <div>99%</div> </div>
2	E	264	<div> <div>77%</div> <div>91%</div> </div>
3	F	245	<div> <div>51%</div> <div>81%</div> <div>16%</div> </div>
3	G	245	<div> <div>33%</div> <div>82%</div> <div>15%</div> </div>
3	H	245	<div> <div>27%</div> <div>83%</div> <div>15%</div> </div>
3	I	245	<div> <div>29%</div> <div>82%</div> <div>15%</div> </div>

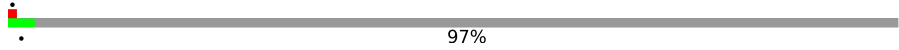
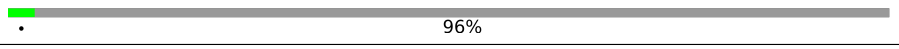
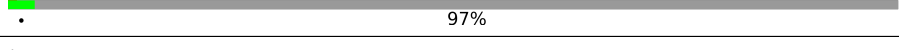
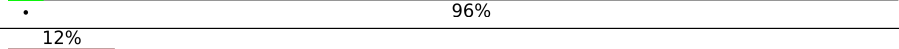
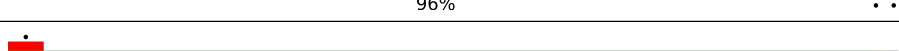
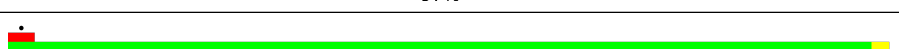
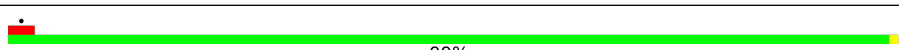

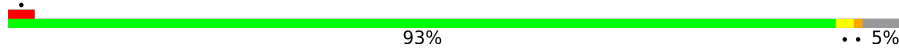
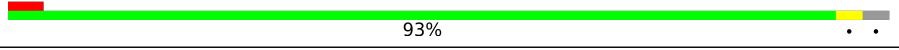
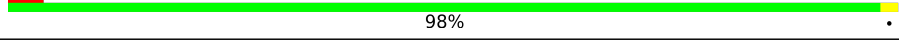
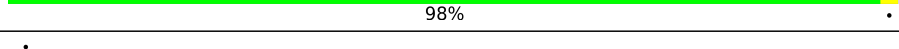
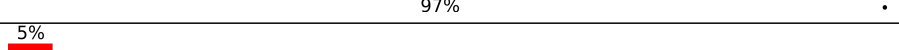
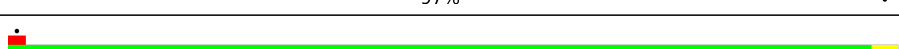
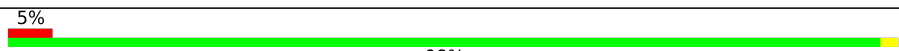
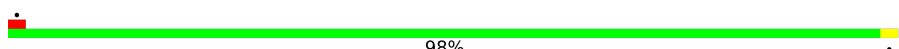
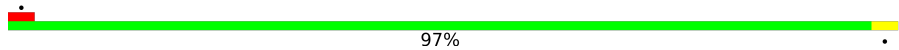
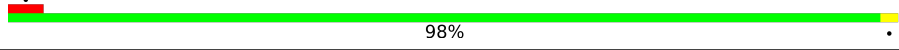
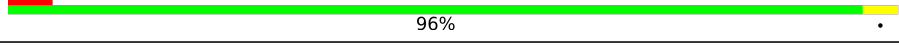
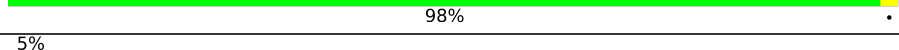
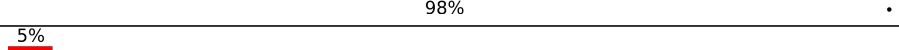
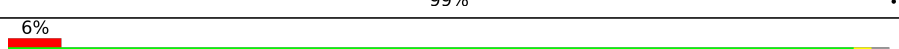



*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	245	
4	K	104	
4	L	104	
4	M	104	
4	N	104	
4	O	104	
4	P	104	
5	Q	138	
5	R	138	
5	S	138	
5	T	138	
5	U	138	
6	V	134	
6	W	134	
6	X	134	
6	Y	134	
6	Z	134	
6	a	134	
7	b	560	
7	c	560	
7	d	560	
7	e	560	
7	f	560	
7	g	560	
7	h	560	

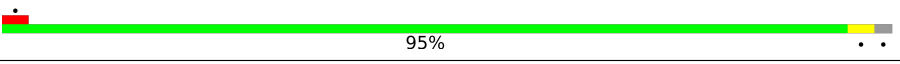
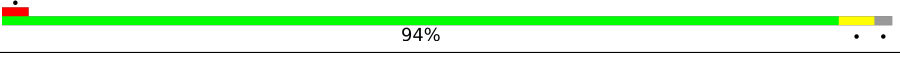
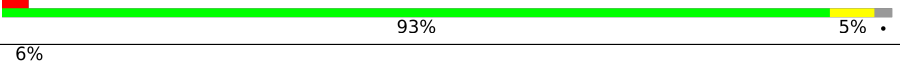
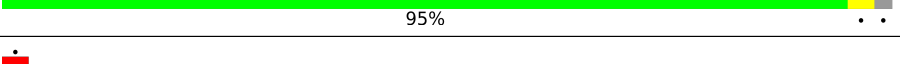
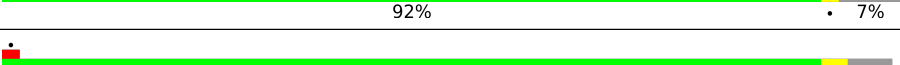
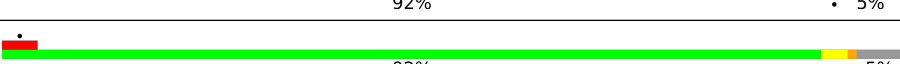
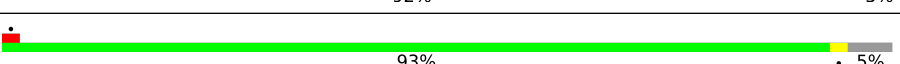
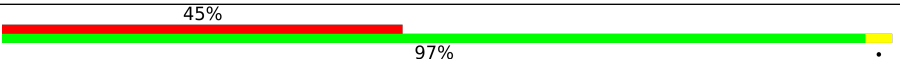
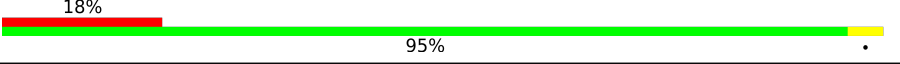
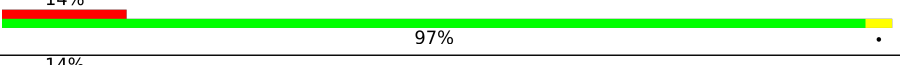
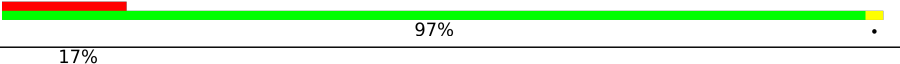
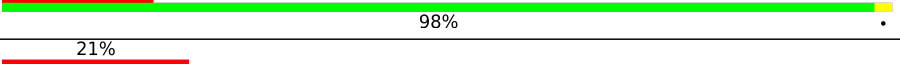
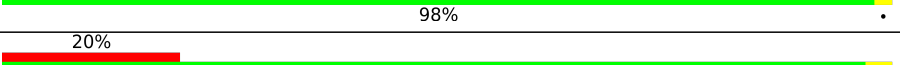
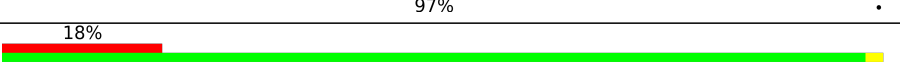
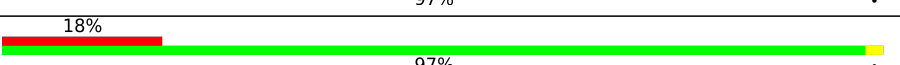
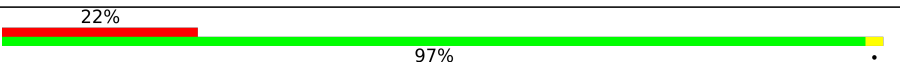
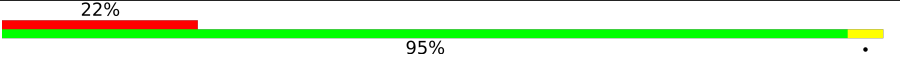
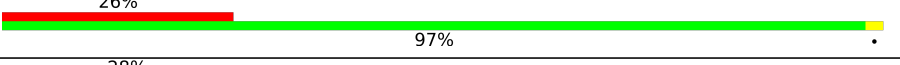
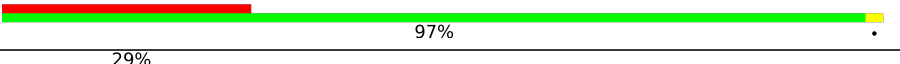
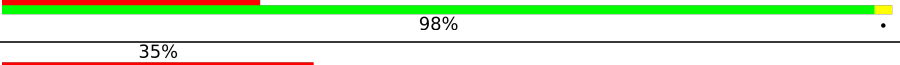
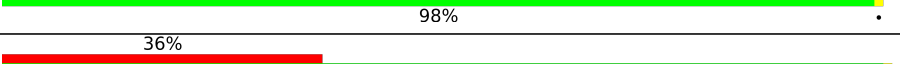
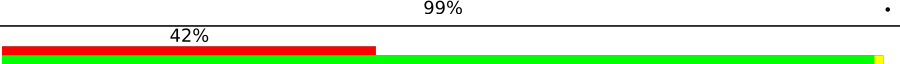
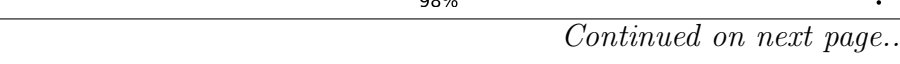


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	i	560	 97%
7	j	560	 96%
7	k	560	 97%
7	l	560	 96%
8	m	251	 12% 96%
8	n	251	 97%
8	o	251	 97%
8	p	251	 99%
8	q	251	 6% 98%
9	0	260	 93% 5%
9	1	260	 93%
9	2	260	 98%
9	3	260	 98%
9	4	260	 97%
9	5	260	 5% 97%
9	6	260	 97%
9	7	260	 5% 98%
9	8	260	 98%
9	9	260	 97%
9	ZA	260	 98%
9	ZB	260	 5% 96%
9	ZC	260	 98%
9	ZD	260	 5% 98%
9	ZE	260	 99%
9	r	260	 6% 95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	s	260	
9	t	260	
9	u	260	
9	v	260	
9	w	260	
9	x	260	
9	y	260	
9	z	260	
10	ZF	403	
10	ZG	403	
10	ZH	403	
10	ZI	403	
10	ZJ	403	
10	ZK	403	
10	ZL	403	
10	ZM	403	
10	ZN	403	
10	ZO	403	
10	ZP	403	
10	ZQ	403	
10	ZR	403	
10	ZS	403	
10	ZT	403	
10	ZU	403	
10	ZV	403	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
10	ZW	403	<div> <div>40%</div> <div>96%</div> </div>
10	ZX	403	<div> <div>42%</div> <div>99%</div> </div>
10	ZY	403	<div> <div>46%</div> <div>98%</div> </div>
10	ZZ	403	<div> <div>49%</div> <div>98%</div> </div>
10	Za	403	<div> <div>52%</div> <div>98%</div> </div>
10	Zb	403	<div> <div>52%</div> <div>98%</div> </div>
10	Zc	403	<div> <div>57%</div> <div>97%</div> </div>
10	Zd	403	<div> <div>61%</div> <div>98%</div> </div>
10	Ze	403	<div> <div>66%</div> <div>97%</div> </div>
10	Zf	403	<div> <div>69%</div> <div>98%</div> </div>
10	Zg	403	<div> <div>72%</div> <div>98%</div> </div>
10	Zh	403	<div> <div>76%</div> <div>98%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 167771 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 biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
1	B	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
1	C	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
1	D	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

- Molecule 2 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	253	Total	C	N	O	S	0	0
			1945	1305	307	318	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	207	Total	C	N	O	S	0	0
			1605	1072	249	272	12		
3	G	209	Total	C	N	O	S	0	0
			1626	1086	252	276	12		
3	H	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
3	I	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
3	J	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		

- Molecule 4 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	40	Total	C	N	O	S	0	0
			300	185	52	57	6		
4	L	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
4	M	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
4	N	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
4	O	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
4	P	73	Total	C	N	O	S	0	0
			550	340	100	104	6		

- Molecule 5 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	119	Total	C	N	O	S	0	0
			922	565	169	183	5		
5	R	108	Total	C	N	O	S	0	0
			848	523	155	165	5		
5	S	108	Total	C	N	O	S	0	0
			848	523	155	165	5		
5	T	110	Total	C	N	O	S	0	0
			863	531	160	167	5		
5	U	106	Total	C	N	O	S	0	0
			832	514	150	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
6	W	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
6	X	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
6	Y	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
6	Z	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
6	a	133	Total	C	N	O	S	0	0
			969	604	167	193	5		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	b	13	Total	C	N	O	0	0
			81	50	15	16		
7	c	16	Total	C	N	O	0	0
			103	64	19	20		
7	d	20	Total	C	N	O	0	0
			133	83	23	27		
7	e	16	Total	C	N	O	0	0
			103	64	19	20		
7	f	21	Total	C	N	O	0	0
			140	88	24	28		
7	g	16	Total	C	N	O	0	0
			103	64	19	20		
7	h	21	Total	C	N	O	0	0
			140	88	24	28		
7	i	16	Total	C	N	O	0	0
			103	64	19	20		
7	j	20	Total	C	N	O	0	0
			133	83	23	27		
7	k	16	Total	C	N	O	0	0
			103	64	19	20		
7	l	21	Total	C	N	O	0	0
			140	88	24	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	248	Total	C	N	O	S	0	0
			1804	1106	324	367	7		
8	n	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
8	o	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
8	p	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
8	q	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
9	1	252	Total	C	N	O	S	0	0
			1894	1172	331	385	6		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	3	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	4	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	5	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	6	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	7	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	8	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	9	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZA	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZB	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZC	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZD	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZE	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	r	254	Total 1903	C 1175	N 334	O 389	S 5	0	0
9	s	255	Total 1911	C 1181	N 335	O 390	S 5	0	0
9	t	256	Total 1919	C 1186	N 336	O 391	S 6	0	0
9	u	254	Total 1903	C 1175	N 334	O 389	S 5	0	0
9	v	255	Total 1911	C 1181	N 335	O 390	S 5	0	0
9	w	243	Total 1823	C 1127	N 318	O 373	S 5	0	0
9	x	248	Total 1866	C 1154	N 327	O 379	S 6	0	0
9	y	248	Total 1866	C 1154	N 327	O 379	S 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
9	z	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		

- Molecule 10 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	ZF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZH	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZI	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZJ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZK	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZL	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZM	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZN	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZO	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZP	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZQ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZR	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZS	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZT	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZU	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZV	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
10	ZW	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

*Continued on next page...*

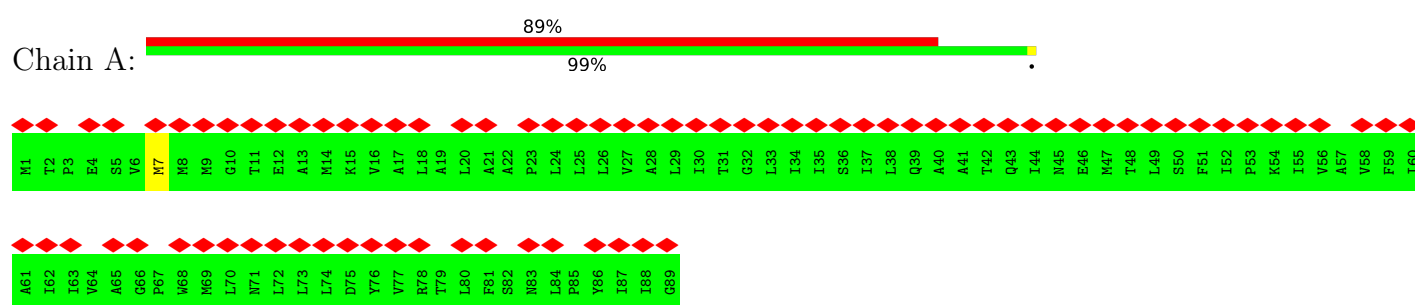
*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
10	ZX	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	ZY	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	ZZ	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Za	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zb	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zc	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zd	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Ze	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zf	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zg	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zh	401	Total 2947	C 1814	N 507	O 618	S 8	0	0

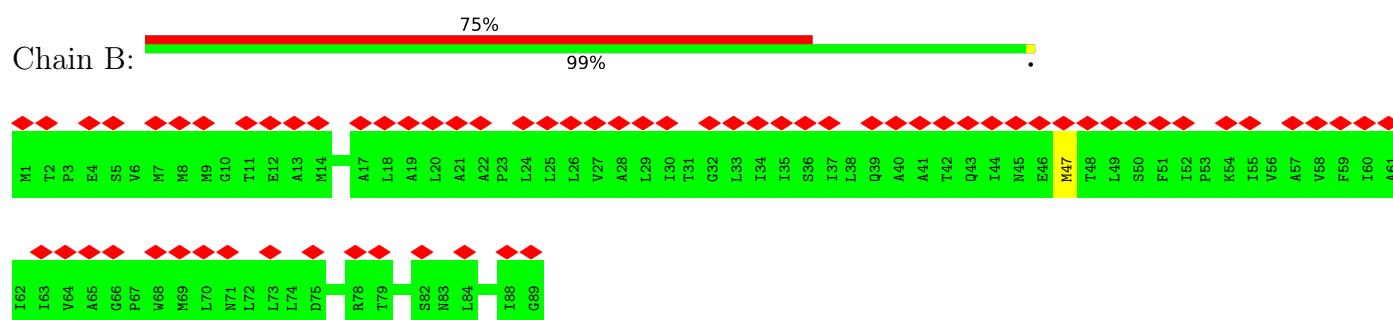
### 3 Residue-property plots

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.

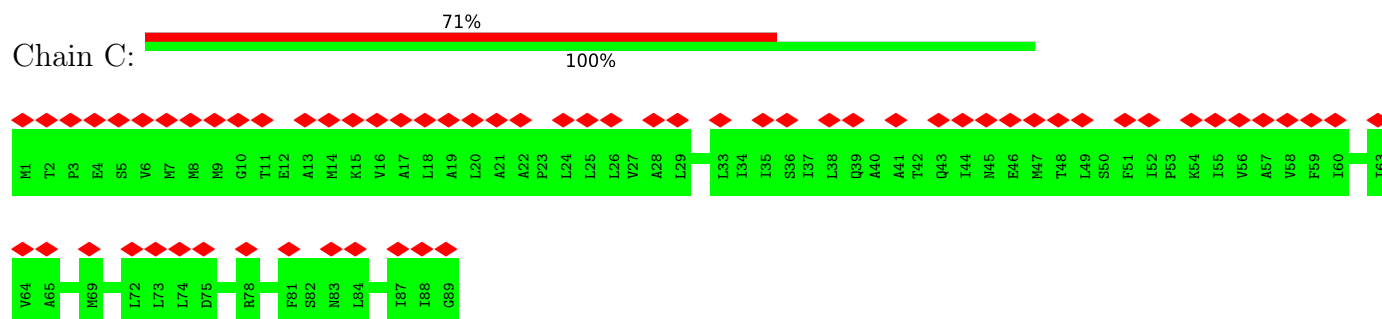
#### • Molecule 1: Flagellar biosynthetic protein FliQ



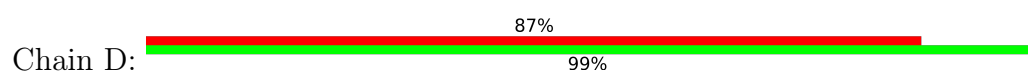
#### • Molecule 1: Flagellar biosynthetic protein FliQ



#### • Molecule 1: Flagellar biosynthetic protein FliQ

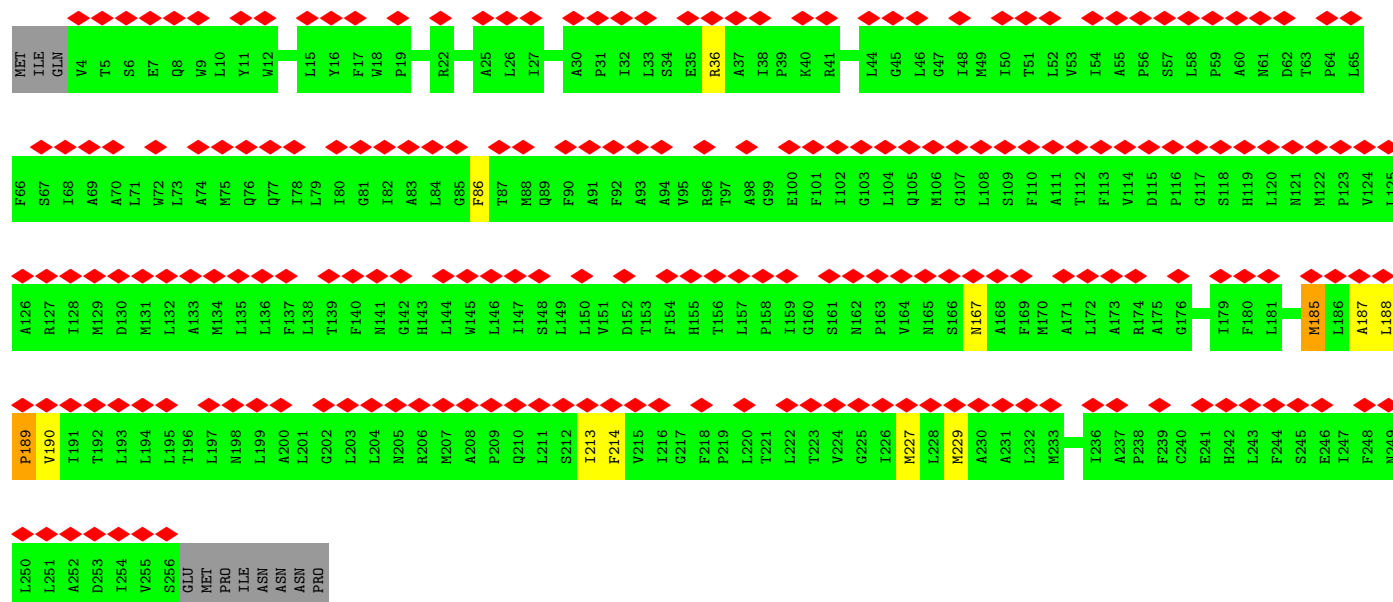
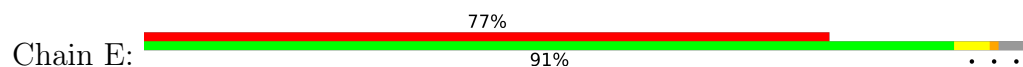


#### • Molecule 1: Flagellar biosynthetic protein FliQ

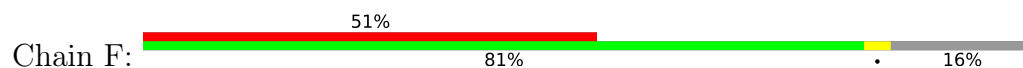




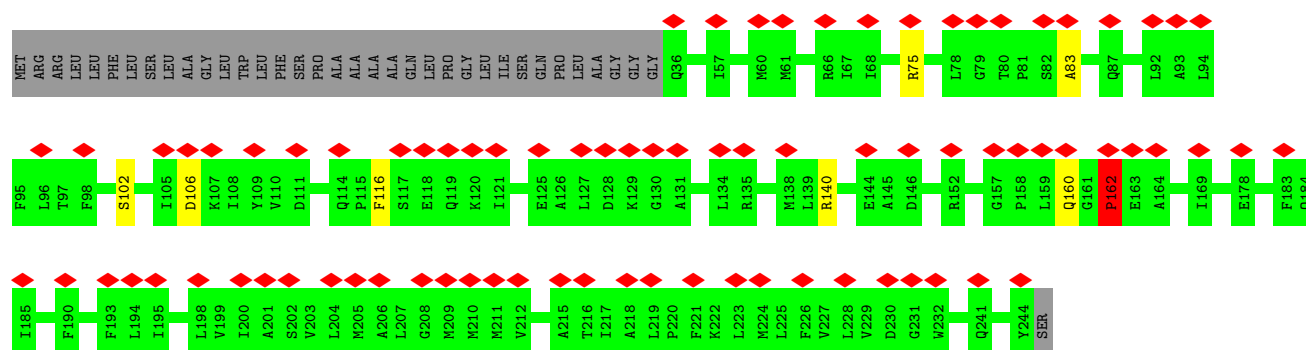
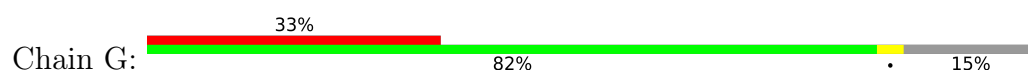
• Molecule 2: Flagellar biosynthetic protein FlIR



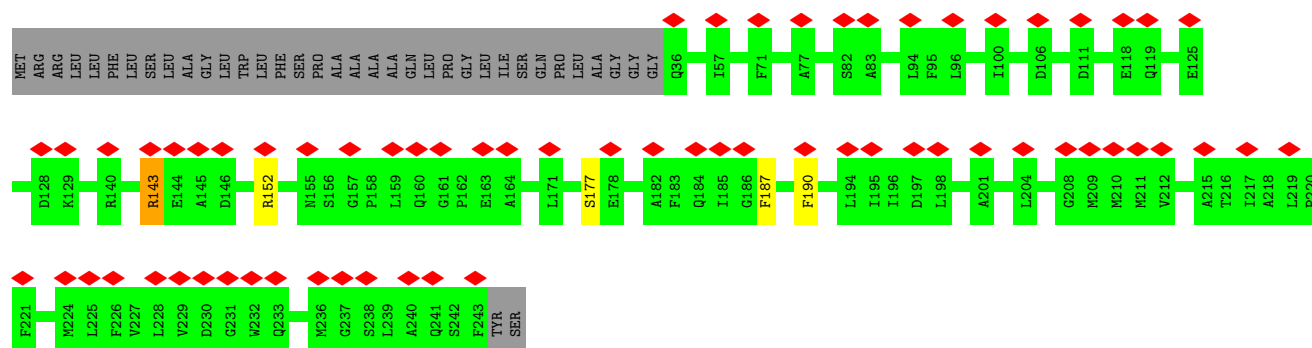
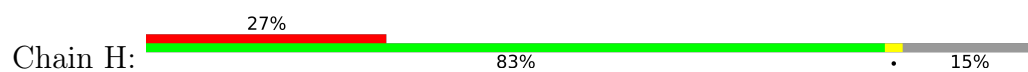
• Molecule 3: Flagellar biosynthetic protein FlIP



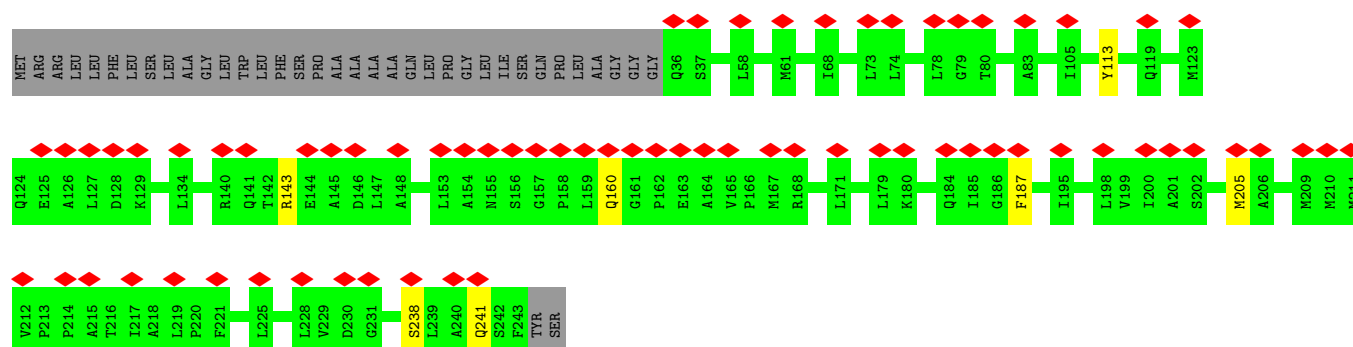
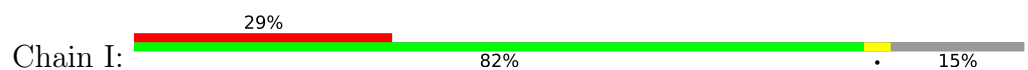
• Molecule 3: Flagellar biosynthetic protein FlIP



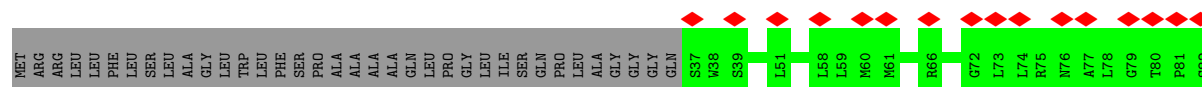
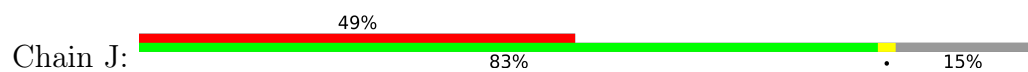
• Molecule 3: Flagellar biosynthetic protein FliP

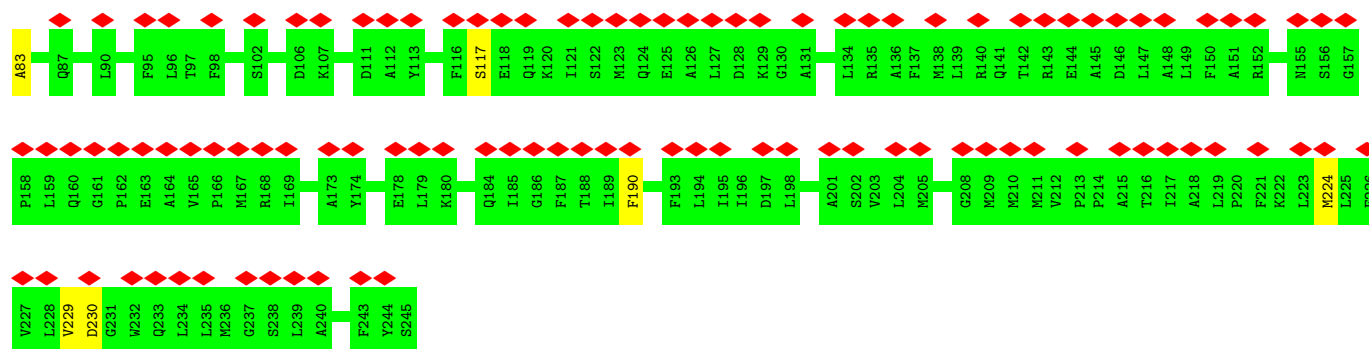


• Molecule 3: Flagellar biosynthetic protein FliP

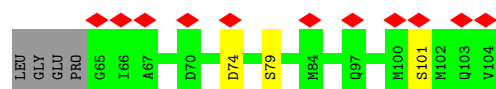
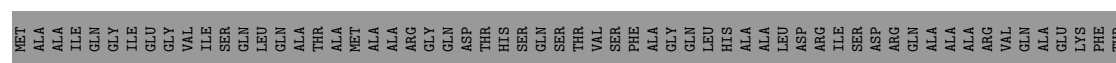


• Molecule 3: Flagellar biosynthetic protein FliP

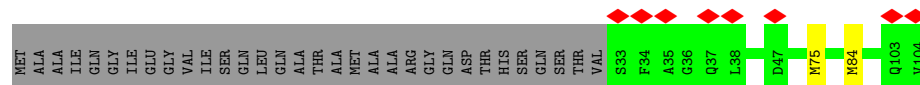




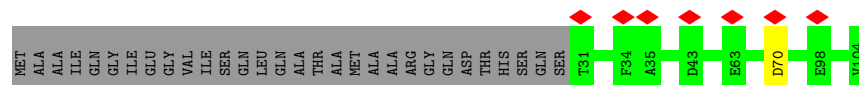
- Molecule 4: Flagellar hook-basal body complex protein FliE



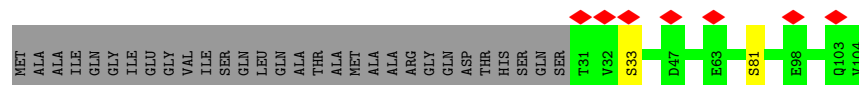
- Molecule 4: Flagellar hook-basal body complex protein FliE



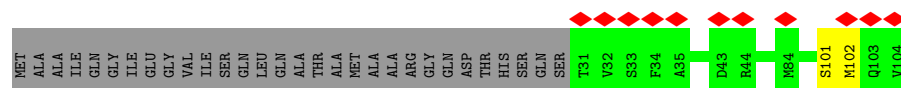
- Molecule 4: Flagellar hook-basal body complex protein FliE



- Molecule 4: Flagellar hook-basal body complex protein FliE

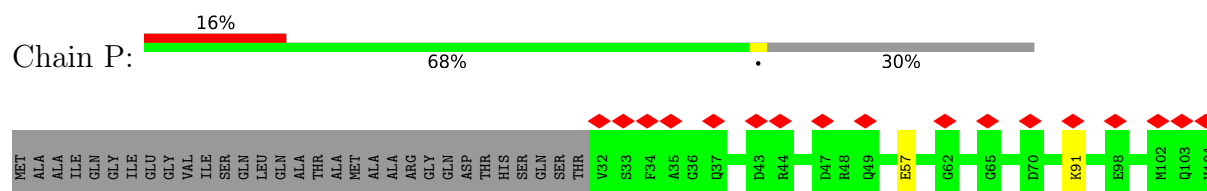


- Molecule 4: Flagellar hook-basal body complex protein FliE

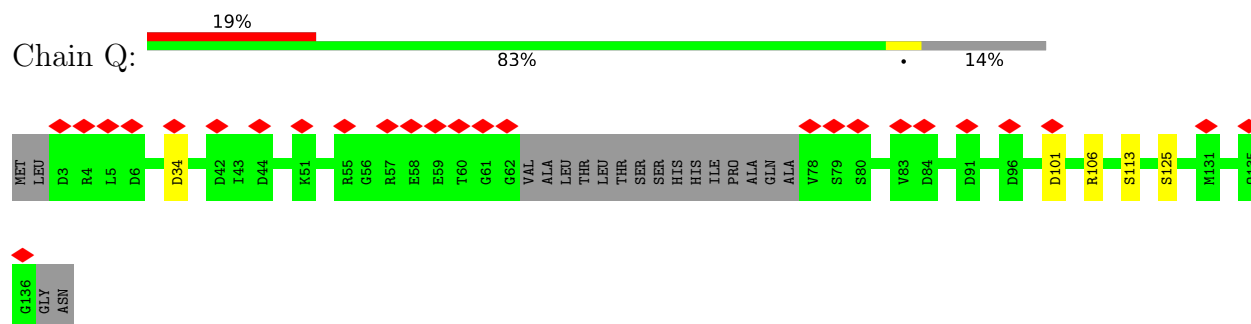




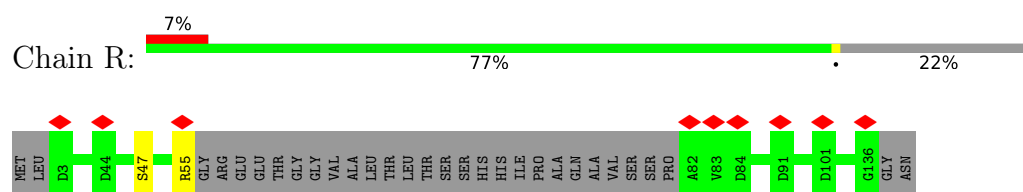
- Molecule 4: Flagellar hook-basal body complex protein FliE



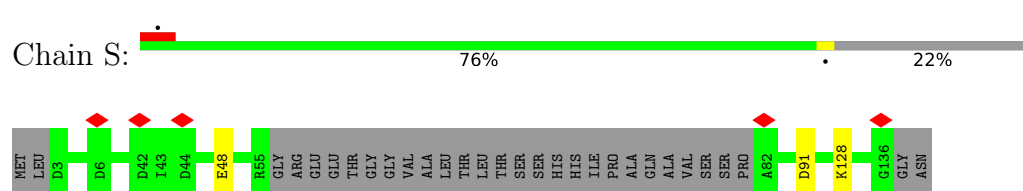
- Molecule 5: Flagellar basal body rod protein FlgB



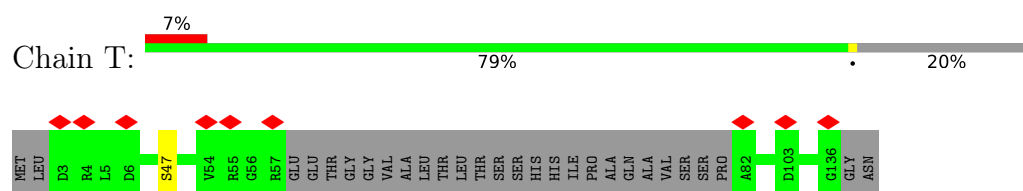
- Molecule 5: Flagellar basal body rod protein FlgB



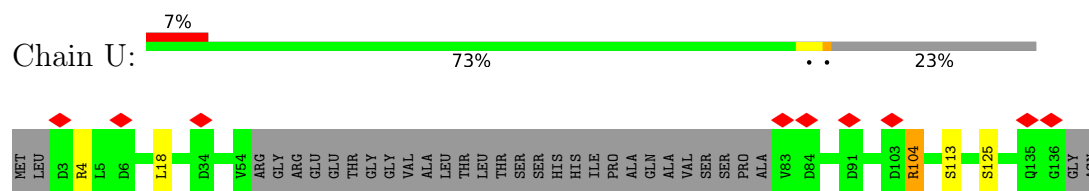
- Molecule 5: Flagellar basal body rod protein FlgB



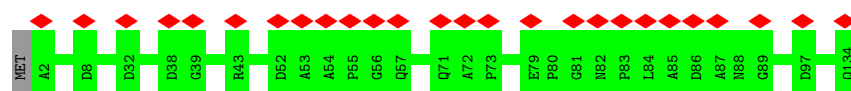
- Molecule 5: Flagellar basal body rod protein FlgB



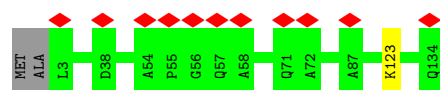
- Molecule 5: Flagellar basal body rod protein FlgB



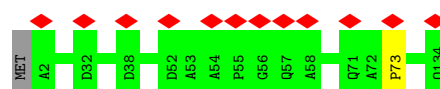
- Molecule 6: Flagellar basal-body rod protein FlgC



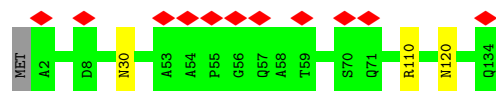
- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 6: Flagellar basal-body rod protein FlgC



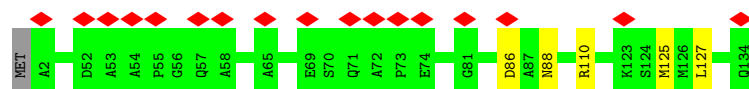
- Molecule 6: Flagellar basal-body rod protein FlgC



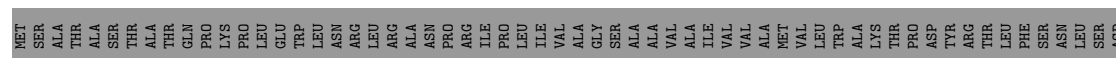
- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 7: Flagellar M-ring protein



[illegible]

- Molecule 7: Flagellar M-ring protein

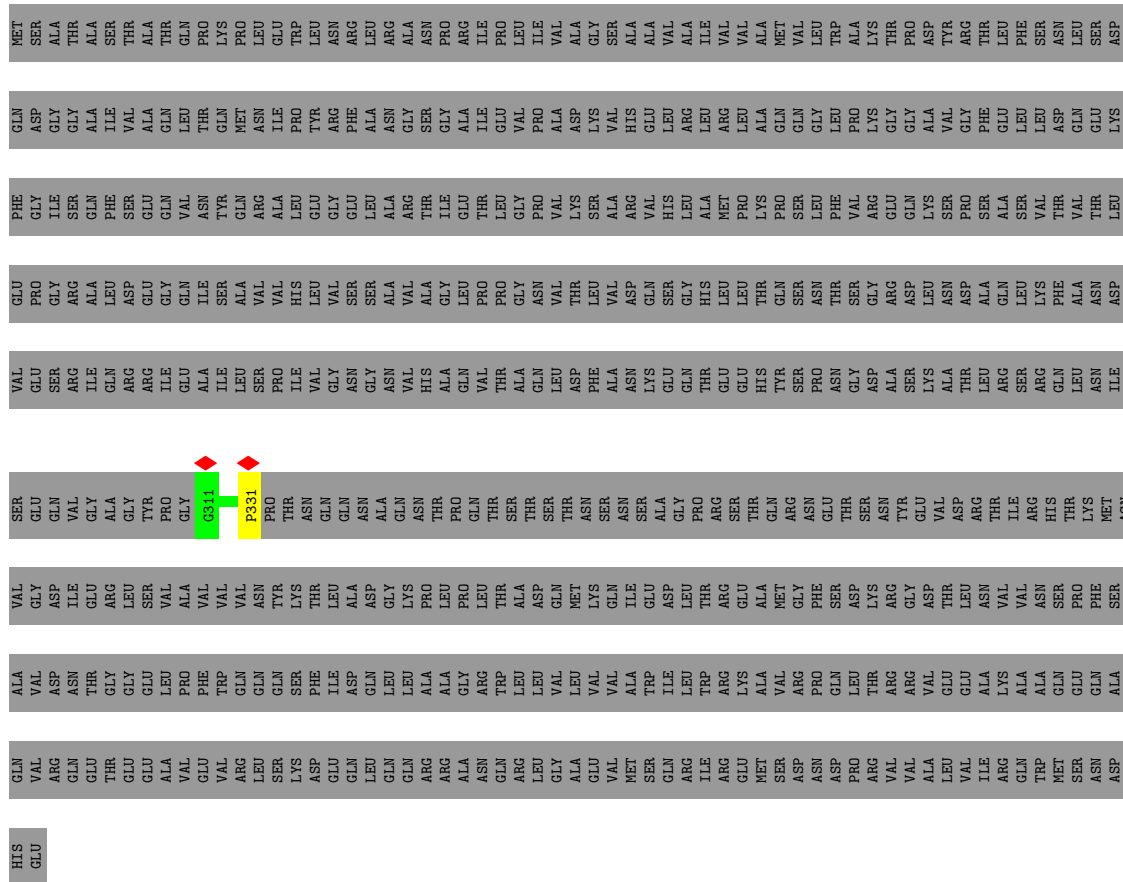
[illegible]





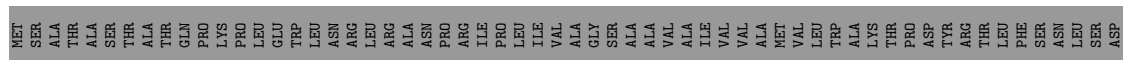
- Molecule 7: Flagellar M-ring protein

Chain f: 96%



- Molecule 7: Flagellar M-ring protein

Chain g:  97%

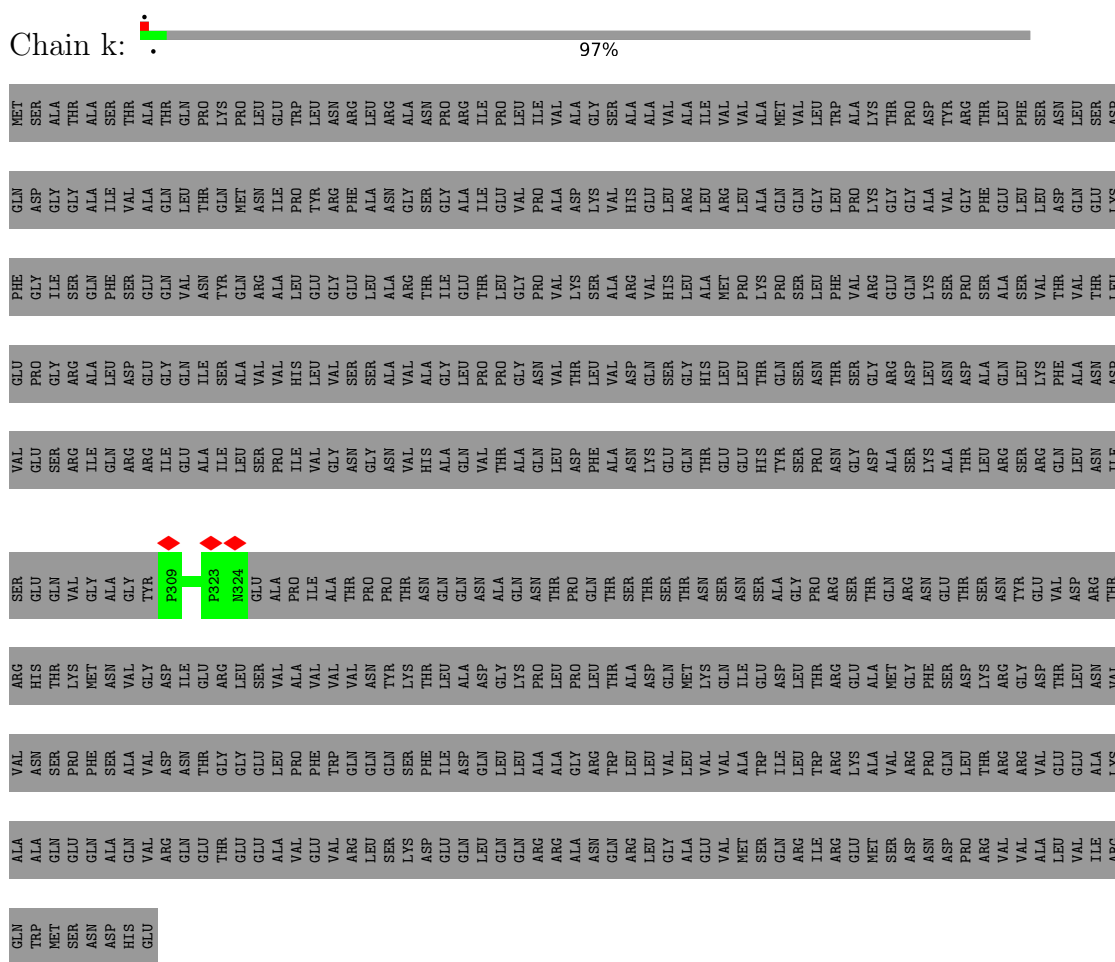




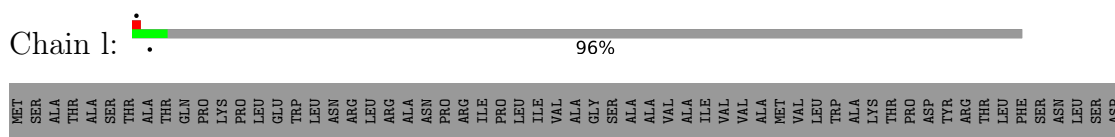




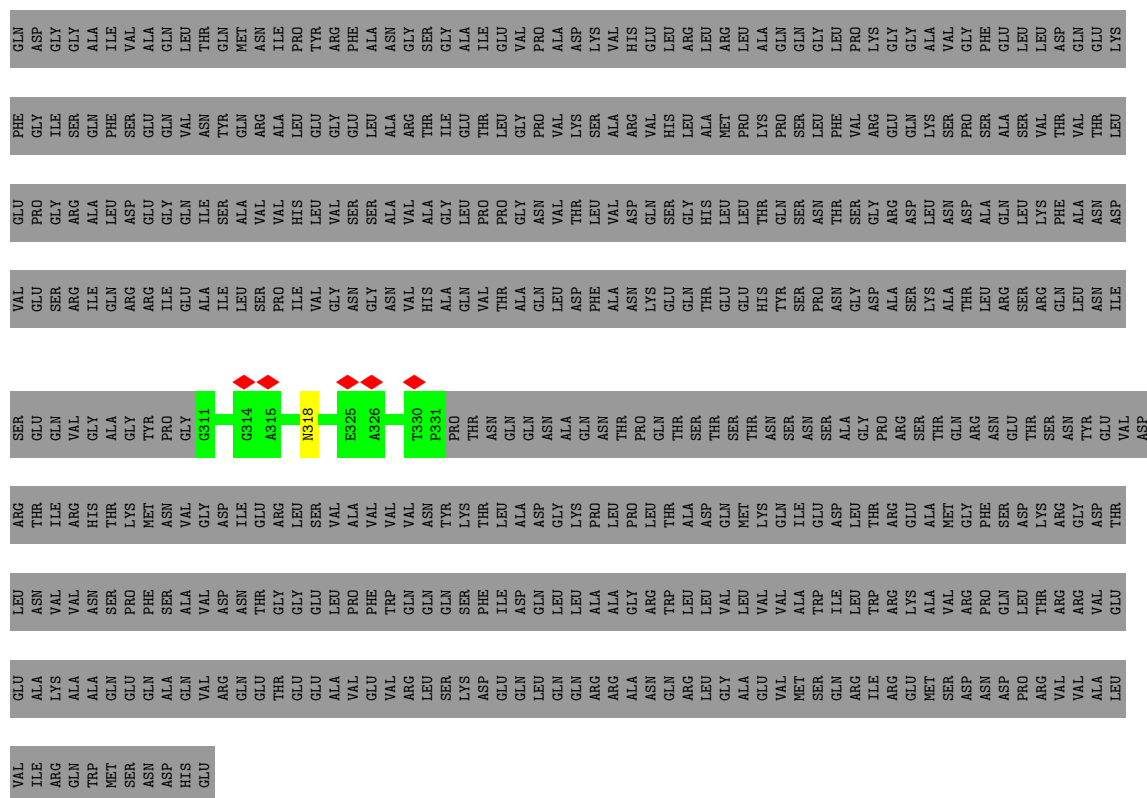
- Molecule 7: Flagellar M-ring protein



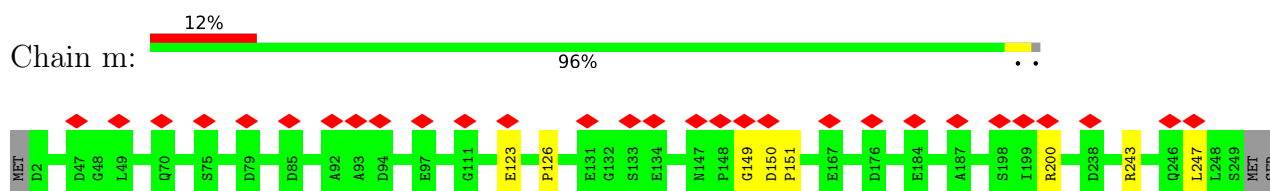
- Molecule 7: Flagellar M-ring protein



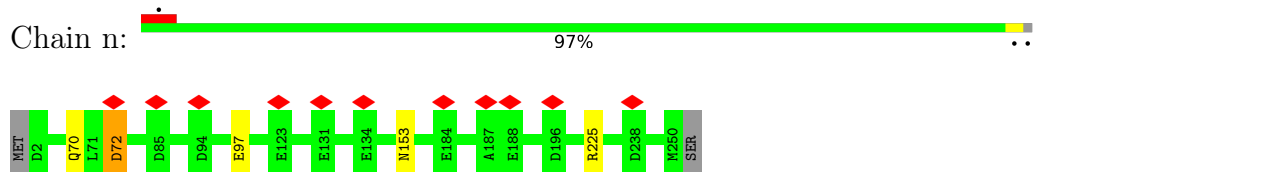




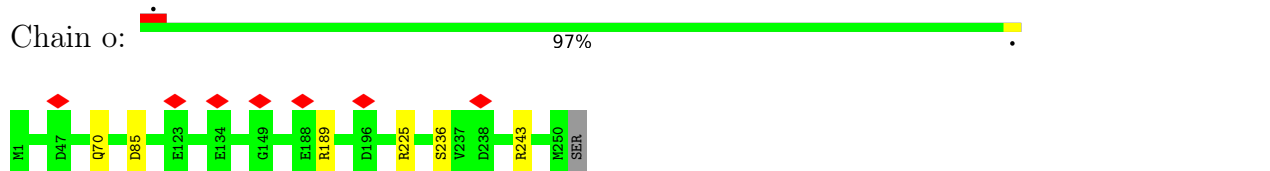
• Molecule 8: Flagellar basal-body rod protein FlgF



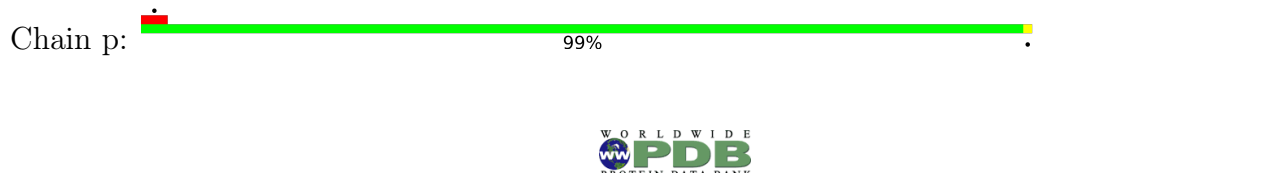
• Molecule 8: Flagellar basal-body rod protein FlgF

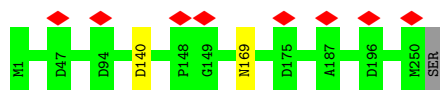


• Molecule 8: Flagellar basal-body rod protein FlgF



• Molecule 8: Flagellar basal-body rod protein FlgF

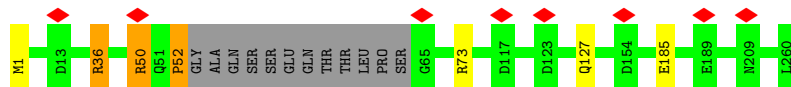




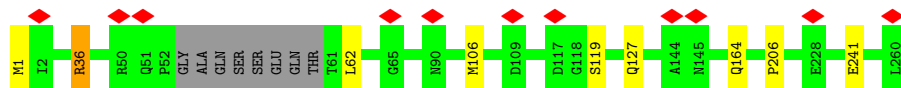
- Molecule 8: Flagellar basal-body rod protein FlgF



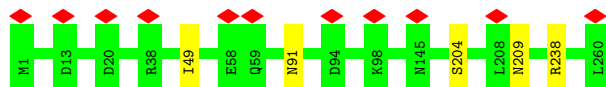
- Molecule 9: Flagellar basal-body rod protein FlgG



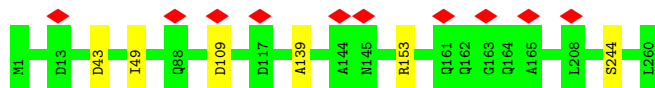
- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG



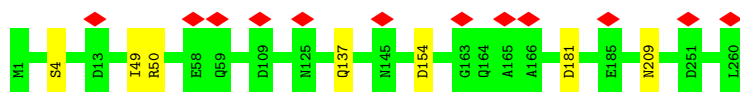
- Molecule 9: Flagellar basal-body rod protein FlgG



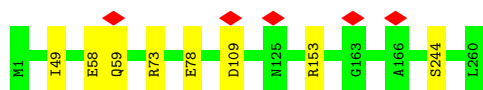
- Molecule 9: Flagellar basal-body rod protein FlgG



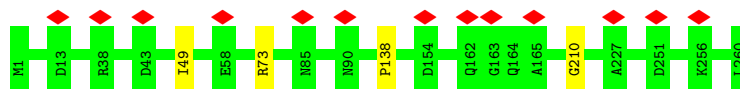
- Molecule 9: Flagellar basal-body rod protein FlgG



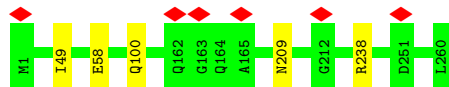
- Molecule 9: Flagellar basal-body rod protein FlgG



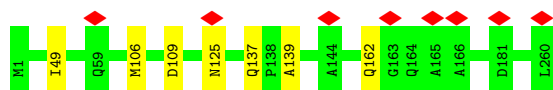
- Molecule 9: Flagellar basal-body rod protein FlgG



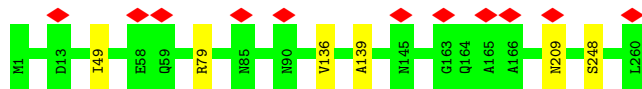
- Molecule 9: Flagellar basal-body rod protein FlgG



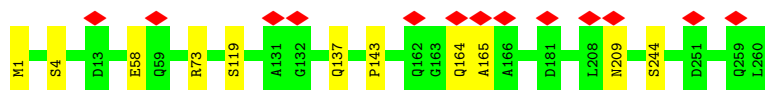
- Molecule 9: Flagellar basal-body rod protein FlgG



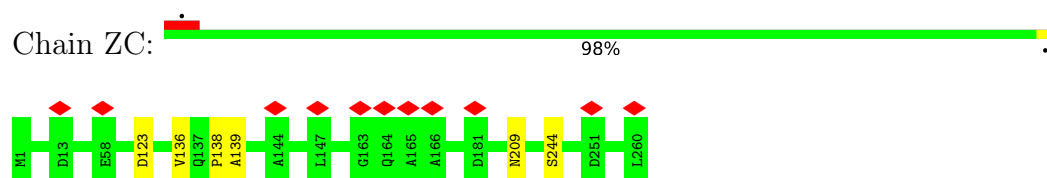
- Molecule 9: Flagellar basal-body rod protein FlgG



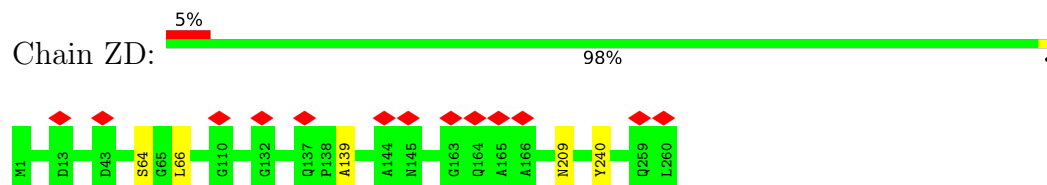
- Molecule 9: Flagellar basal-body rod protein FlgG



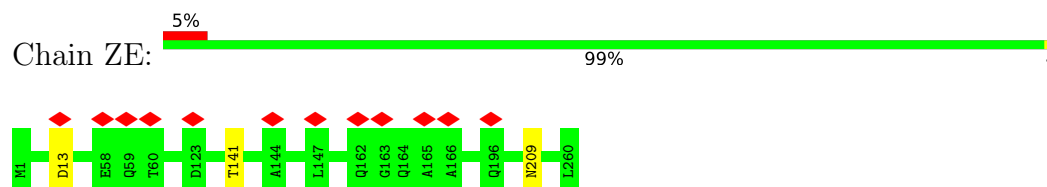
- Molecule 9: Flagellar basal-body rod protein FlgG



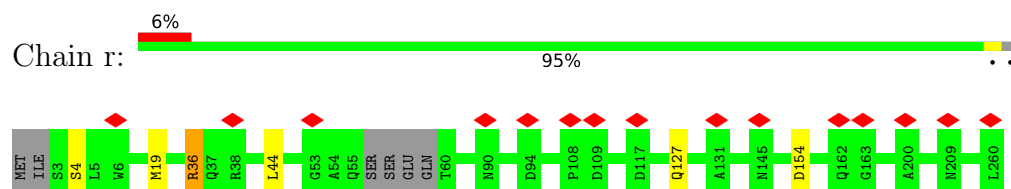
- Molecule 9: Flagellar basal-body rod protein FlgG



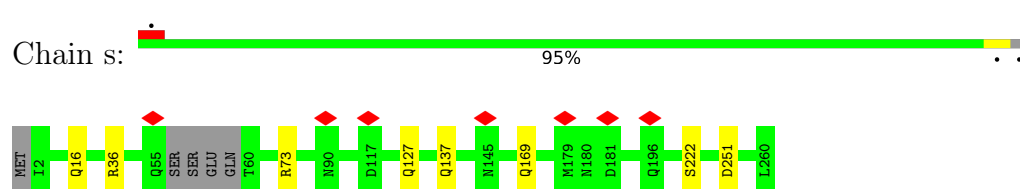
- Molecule 9: Flagellar basal-body rod protein FlgG



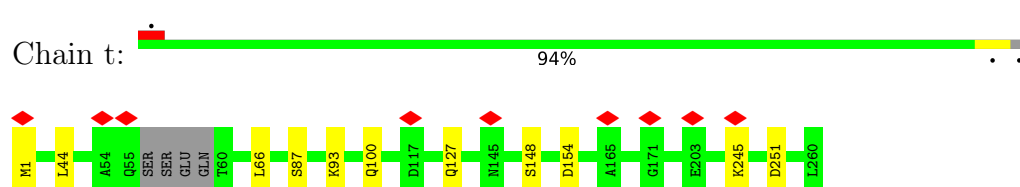
- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG

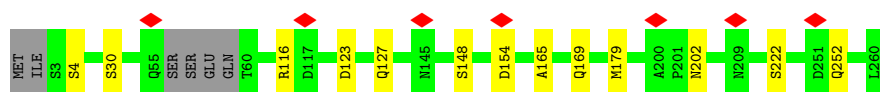


- Molecule 9: Flagellar basal-body rod protein FlgG

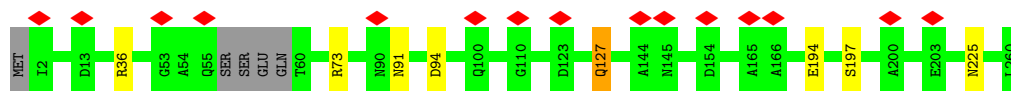


- Molecule 9: Flagellar basal-body rod protein FlgG

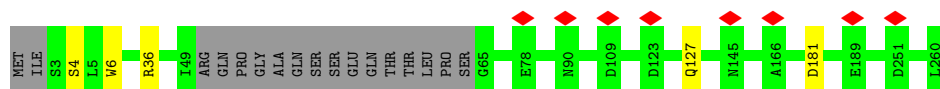




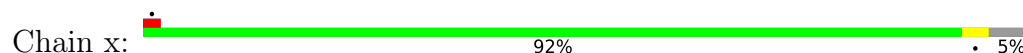
- Molecule 9: Flagellar basal-body rod protein FlgG



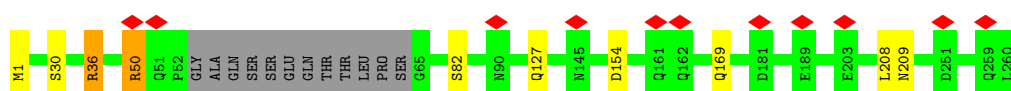
- Molecule 9: Flagellar basal-body rod protein FlgG



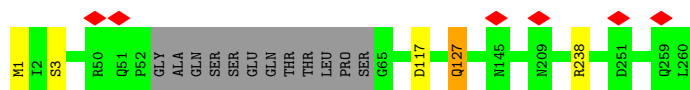
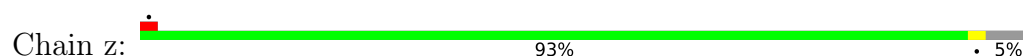
- Molecule 9: Flagellar basal-body rod protein FlgG



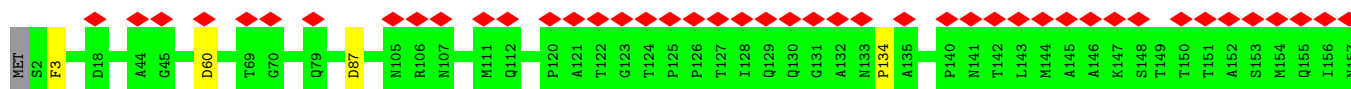
- Molecule 9: Flagellar basal-body rod protein FlgG

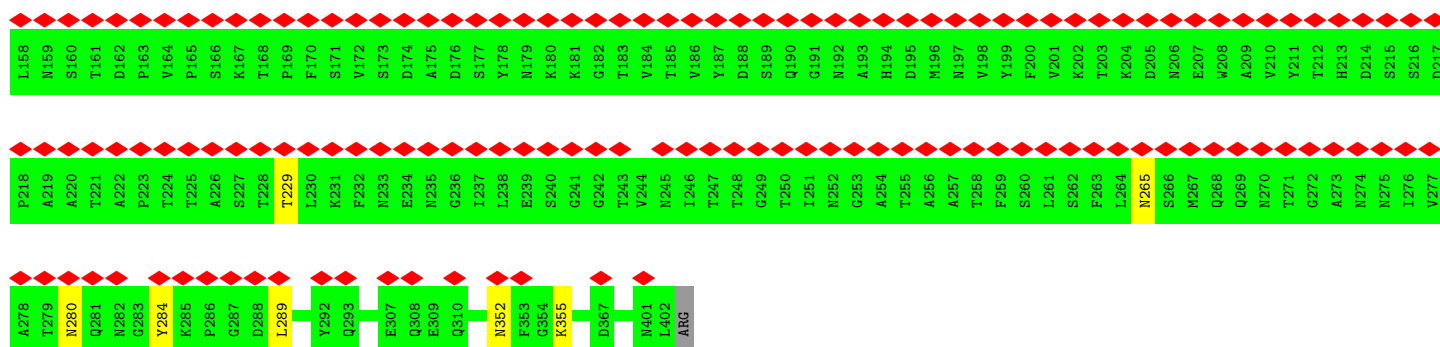


- Molecule 9: Flagellar basal-body rod protein FlgG

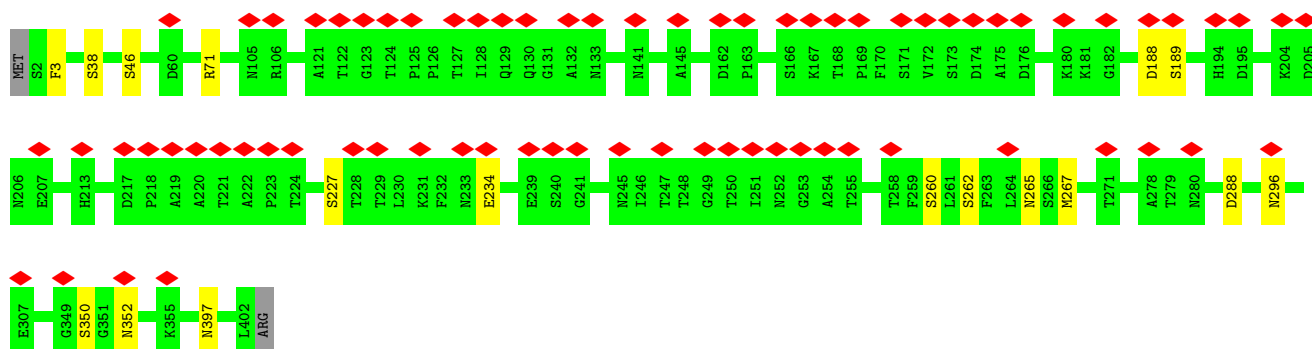


- Molecule 10: Flagellar hook protein FlgE

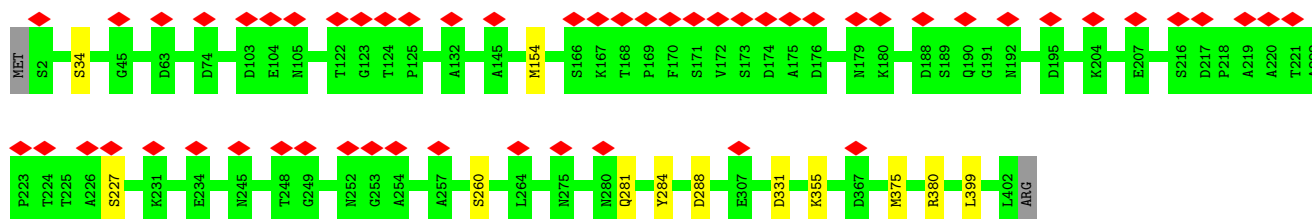




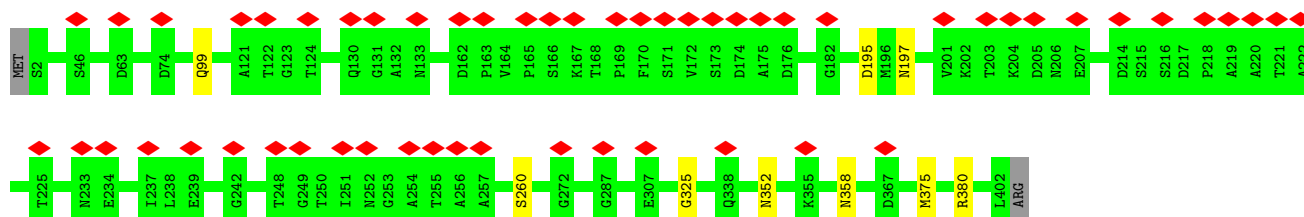
• Molecule 10: Flagellar hook protein FlgE



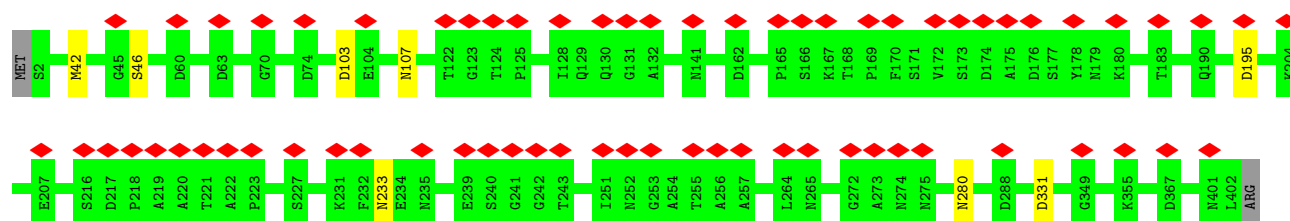
• Molecule 10: Flagellar hook protein FlgE



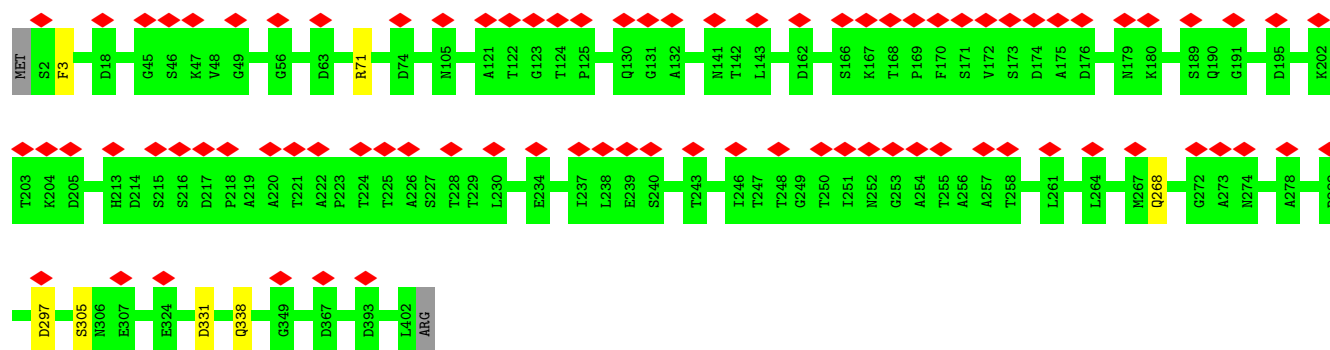
• Molecule 10: Flagellar hook protein FlgE



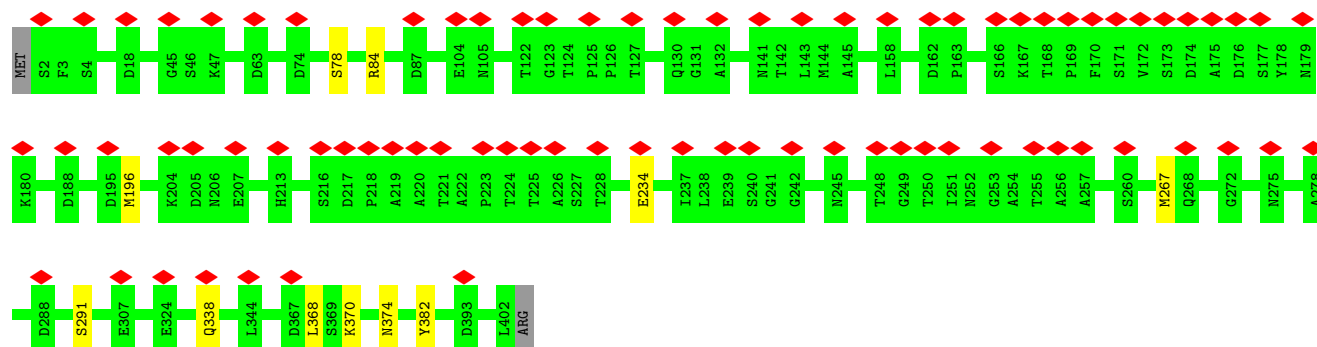
• Molecule 10: Flagellar hook protein FlgE



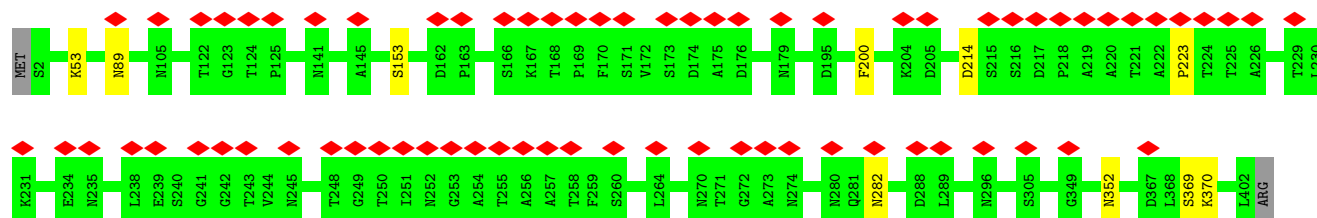
• Molecule 10: Flagellar hook protein FlgE



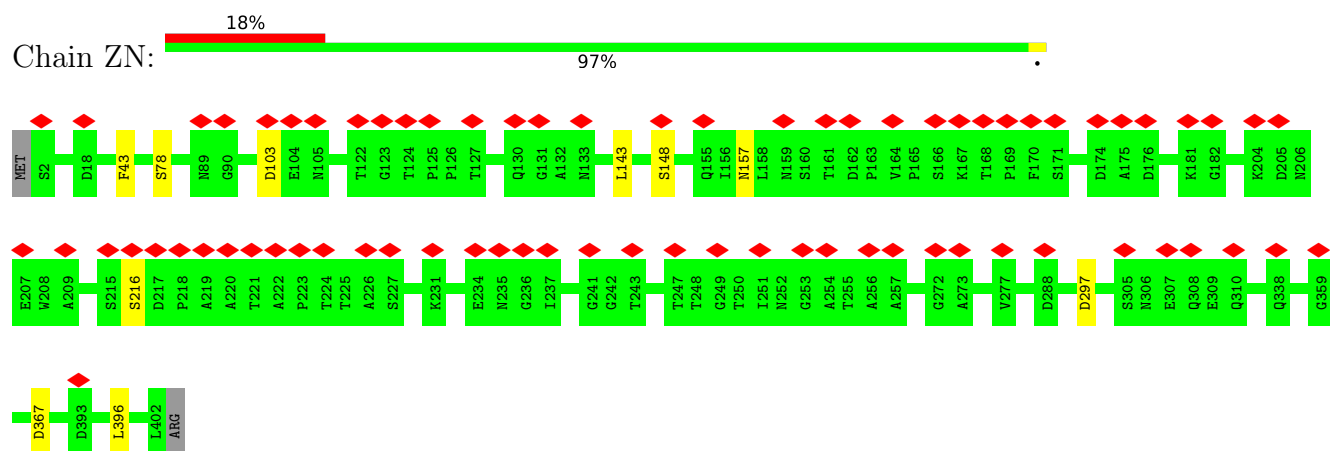
• Molecule 10: Flagellar hook protein FlgE



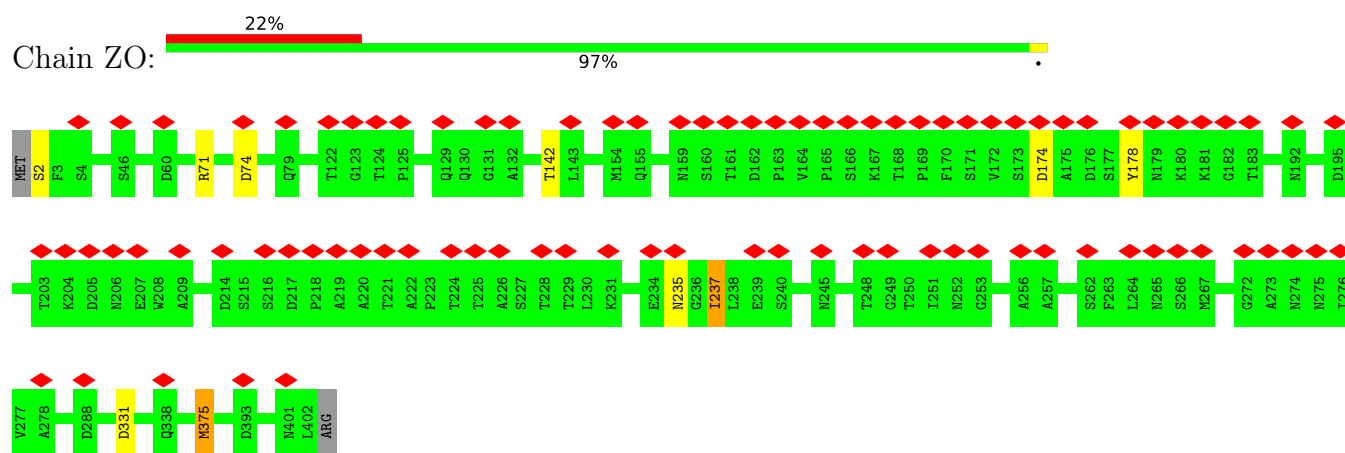
• Molecule 10: Flagellar hook protein FlgE



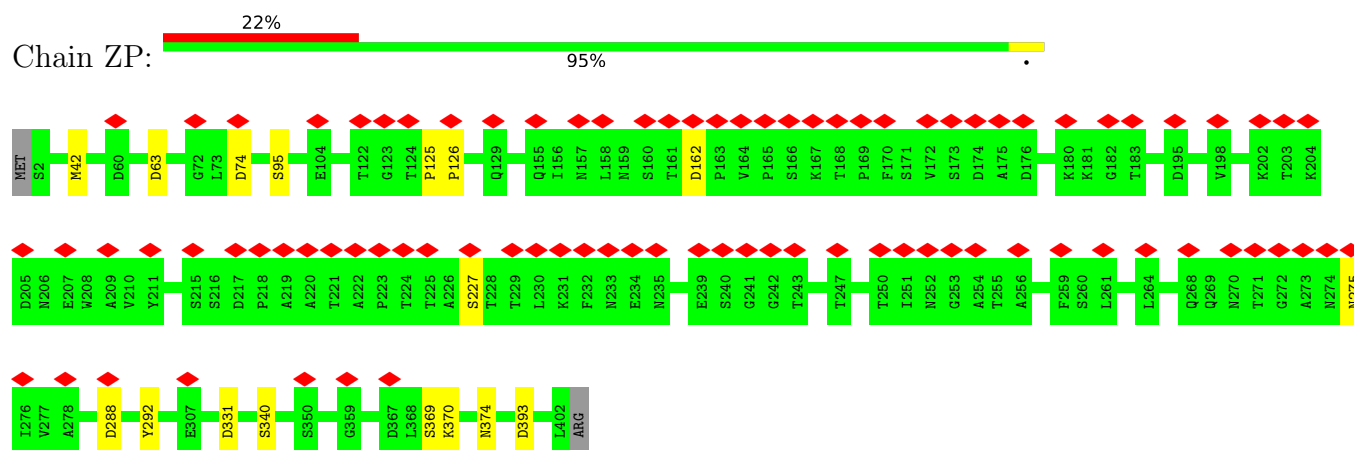
- Molecule 10: Flagellar hook protein FlgE



- Molecule 10: Flagellar hook protein FlgE



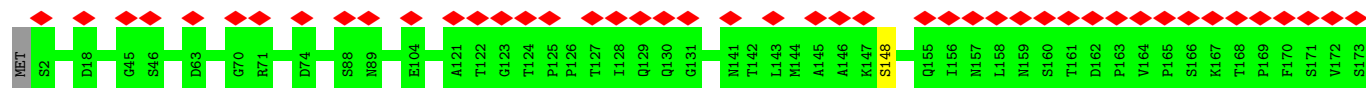
- Molecule 10: Flagellar hook protein FlgE

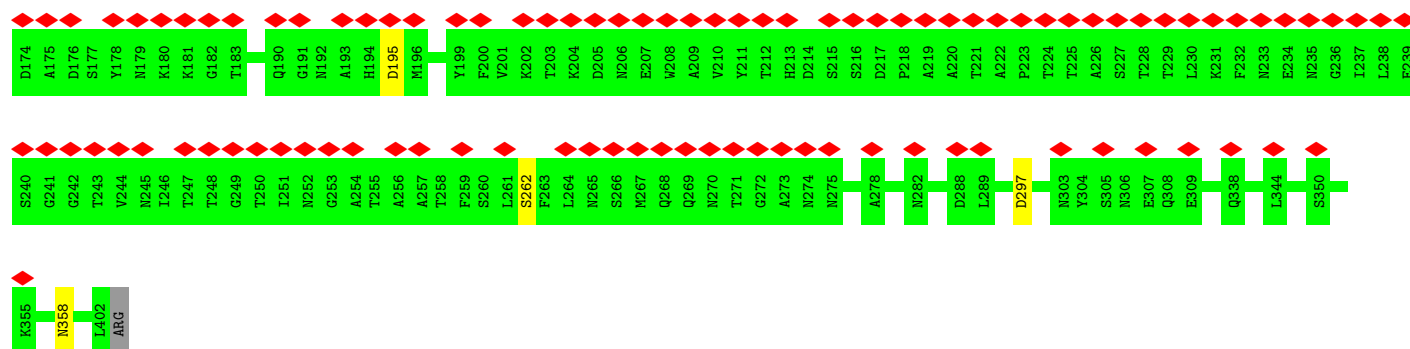


- Molecule 10: Flagellar hook protein FlgE

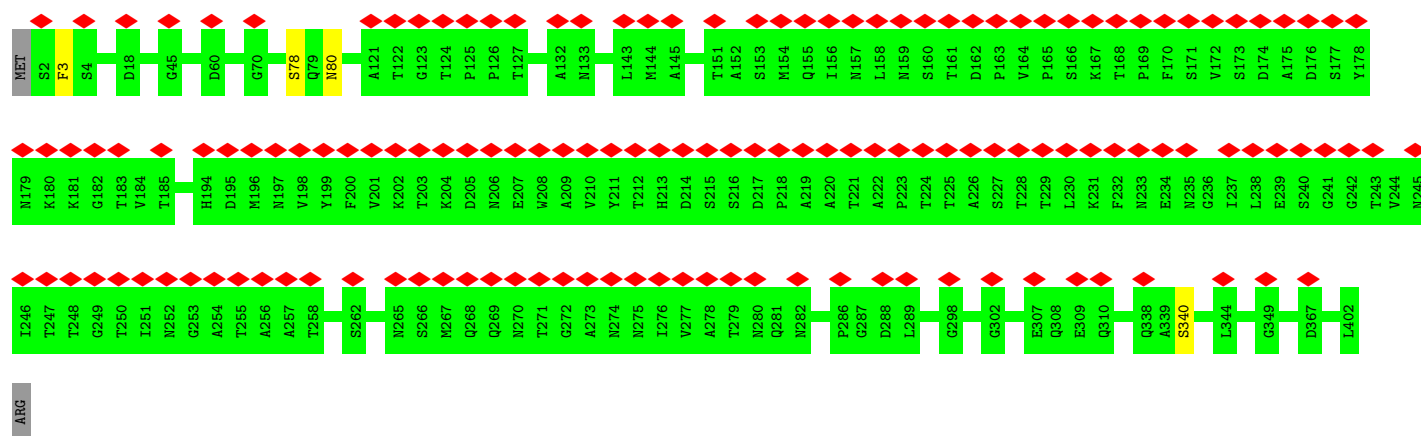




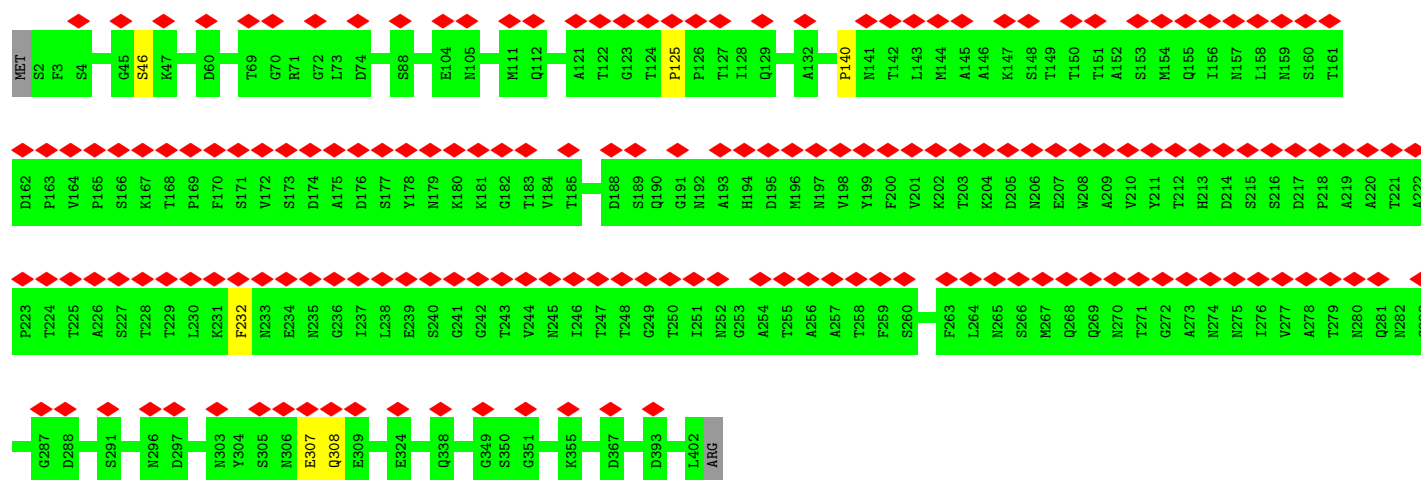




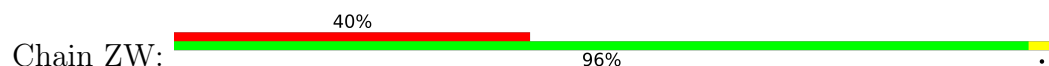
• Molecule 10: Flagellar hook protein FlgE

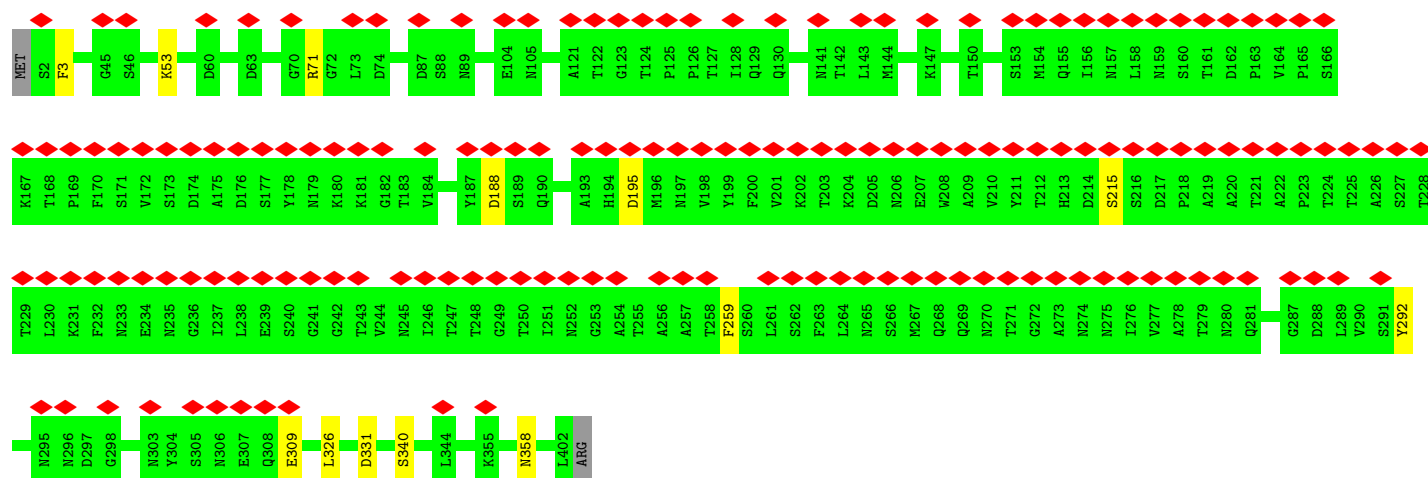


• Molecule 10: Flagellar hook protein FlgE



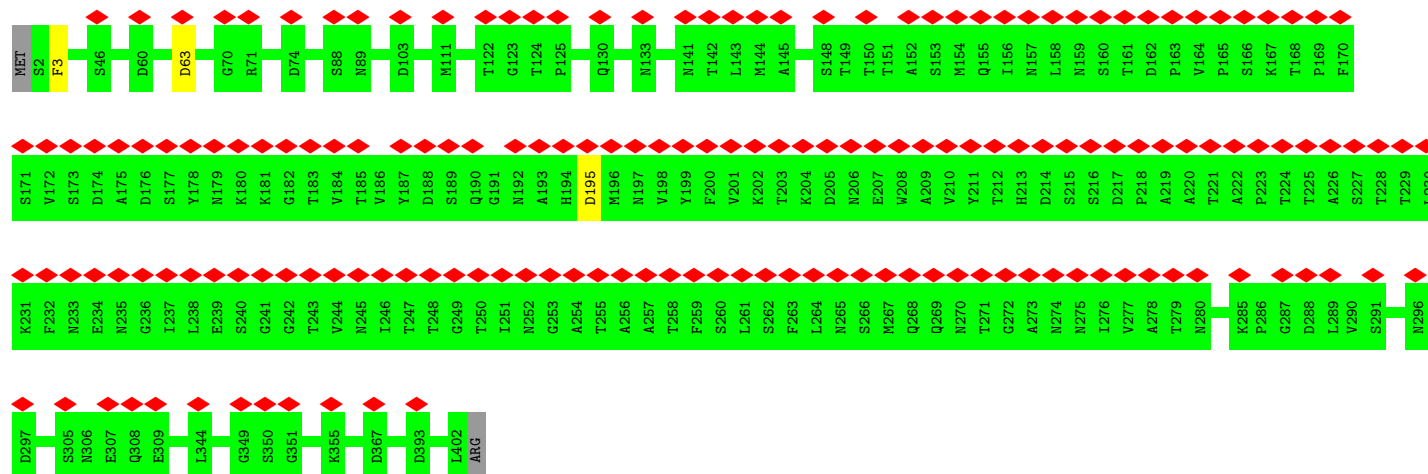
• Molecule 10: Flagellar hook protein FlgE





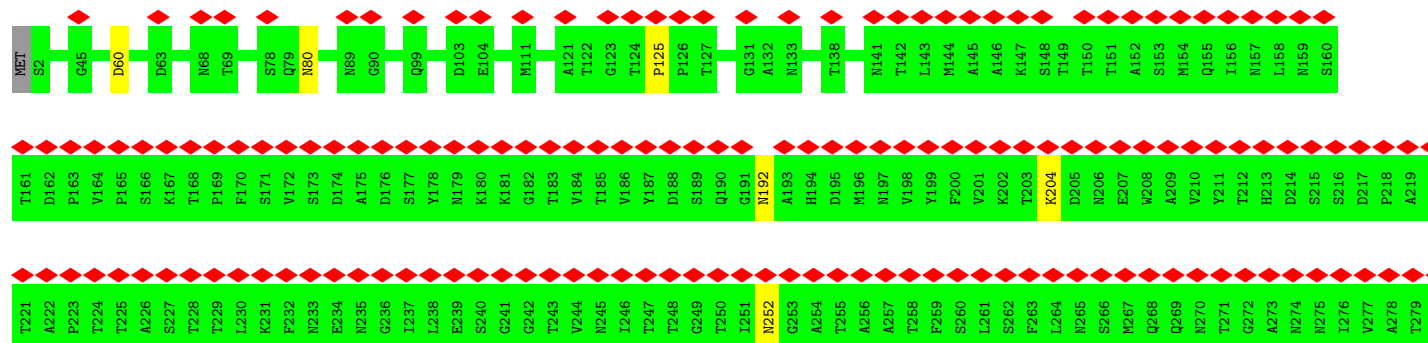
• Molecule 10: Flagellar hook protein FlgE

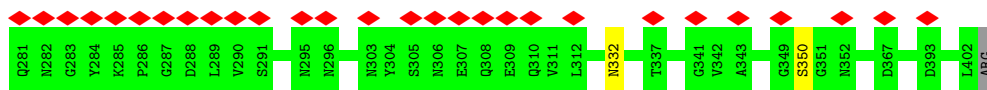
Chain ZX: 42% 99%



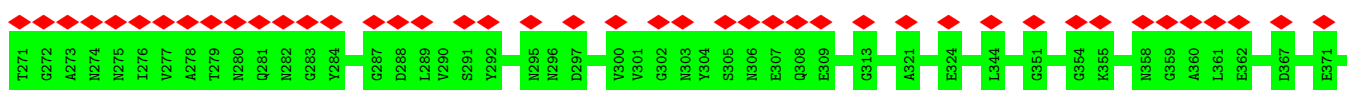
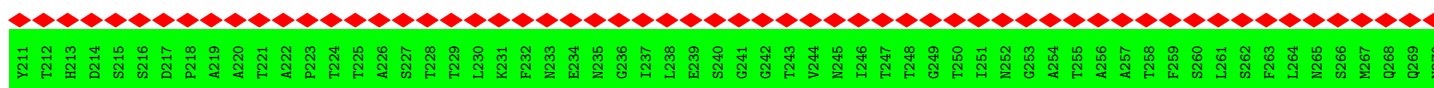
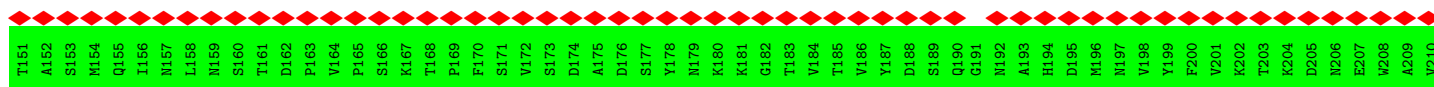
• Molecule 10: Flagellar hook protein FlgE

Chain ZY: 46% 98%

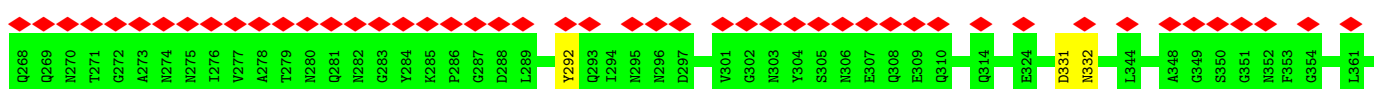
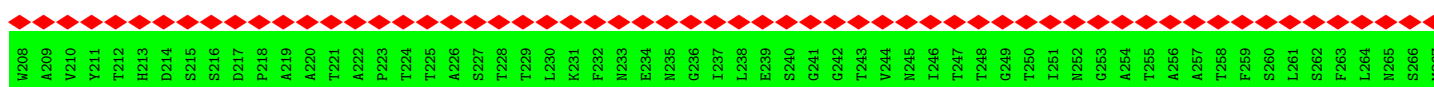
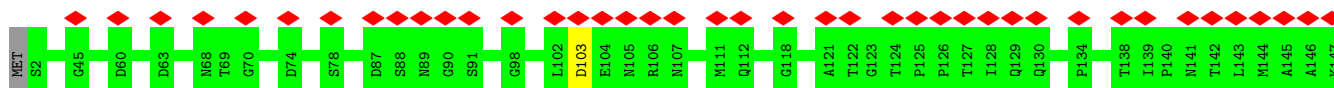




• Molecule 10: Flagellar hook protein FlgE



• Molecule 10: Flagellar hook protein FlgE

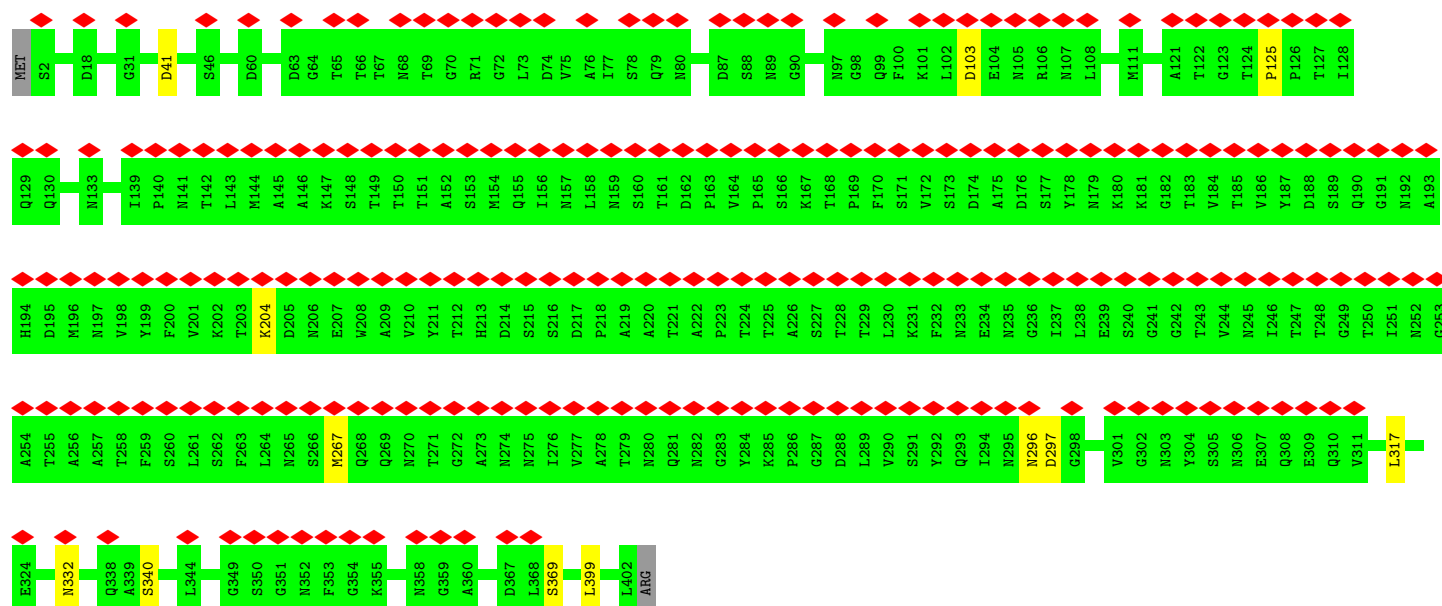


• Molecule 10: Flagellar hook protein FlgE

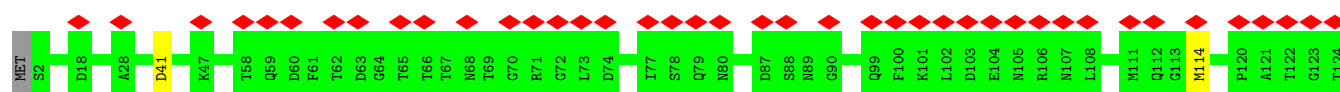


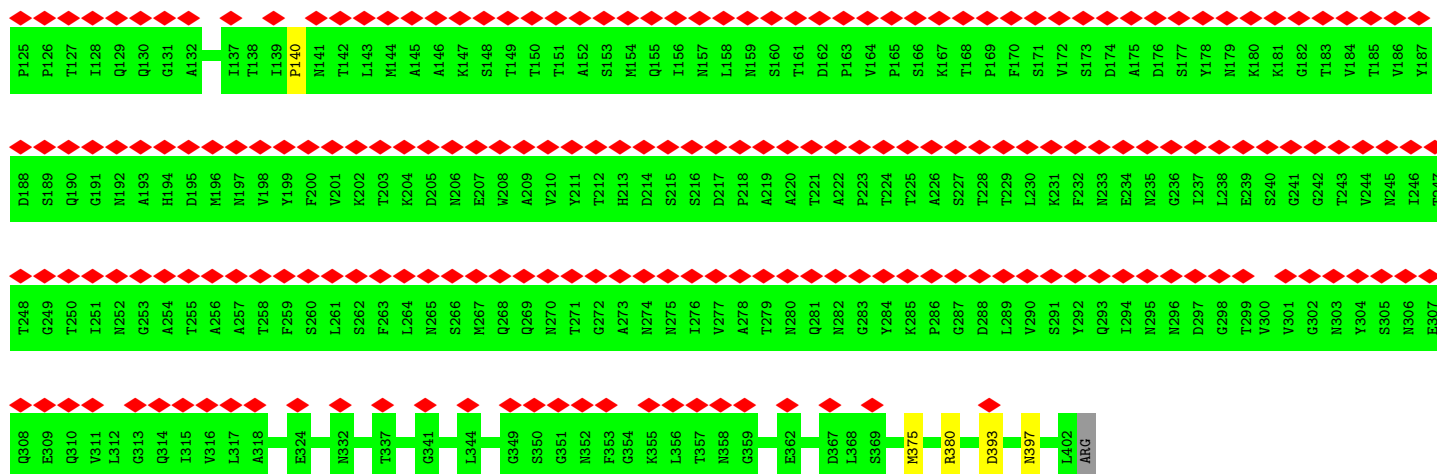


• Molecule 10: Flagellar hook protein FlgE

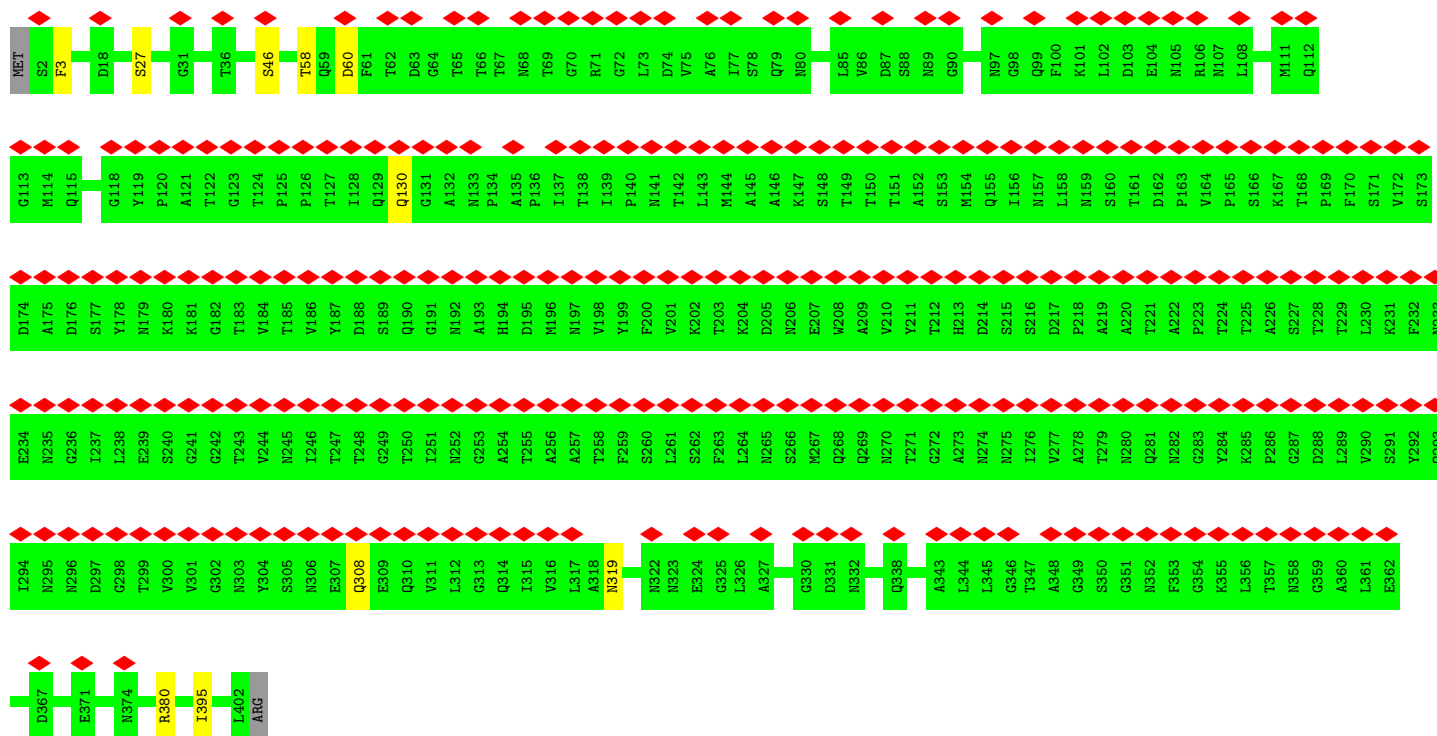


• Molecule 10: Flagellar hook protein FlgE

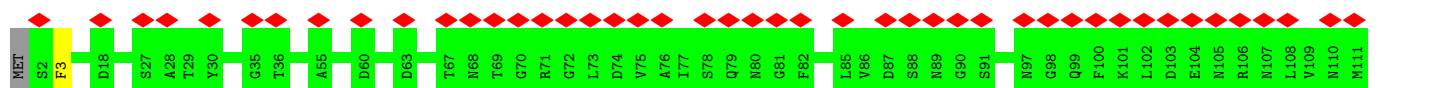


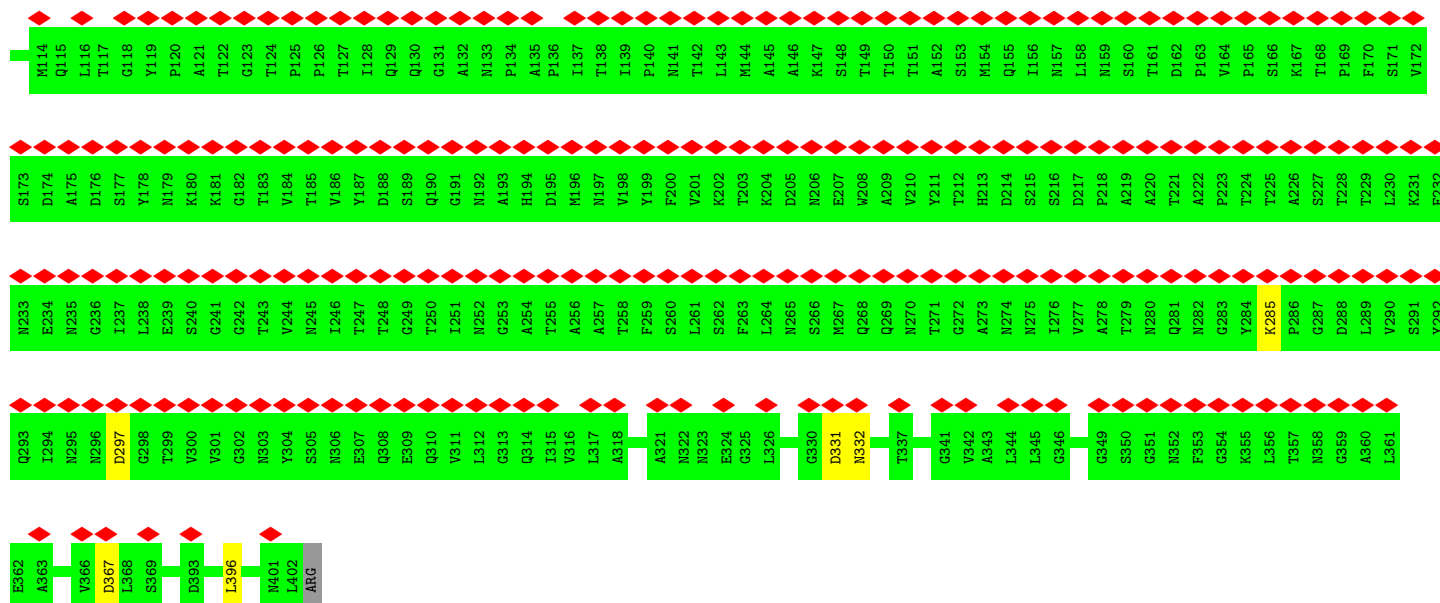


• Molecule 10: Flagellar hook protein FlgE

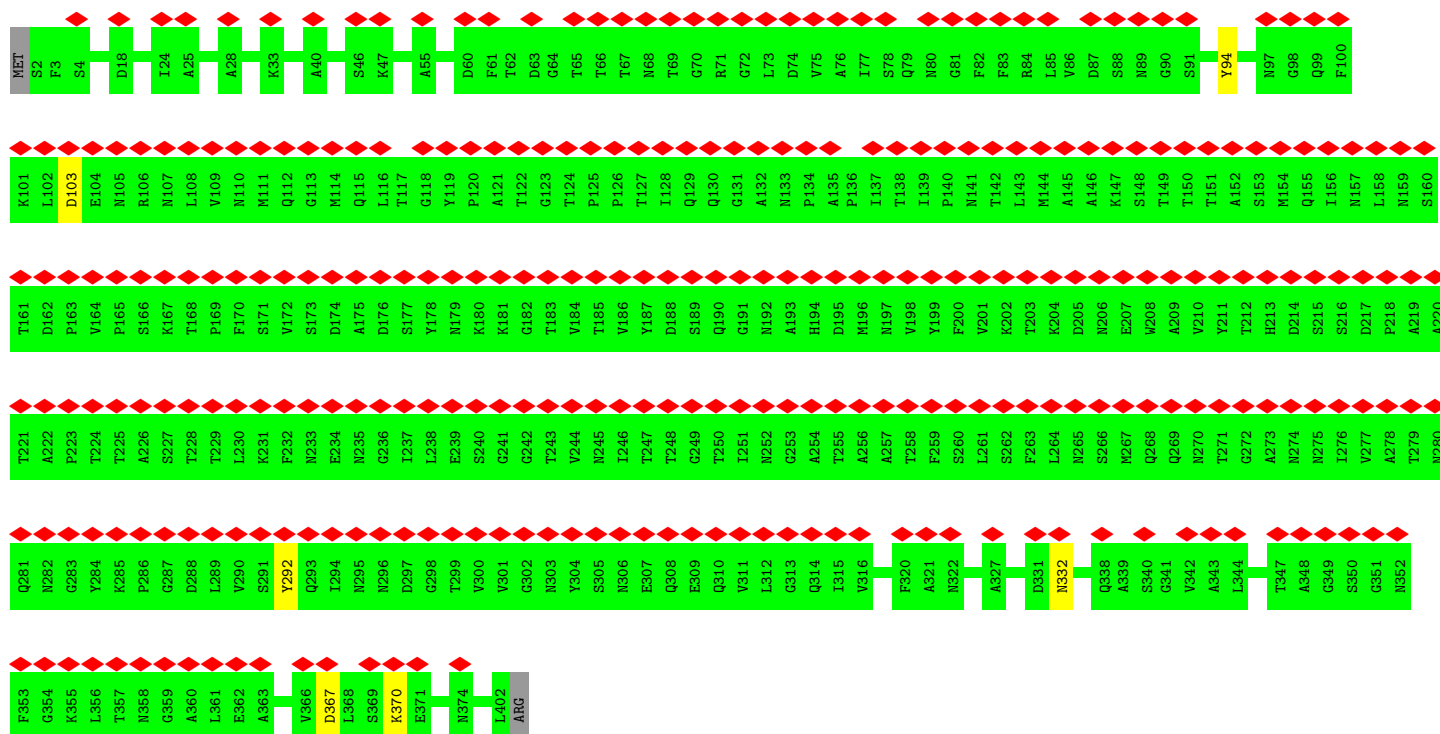
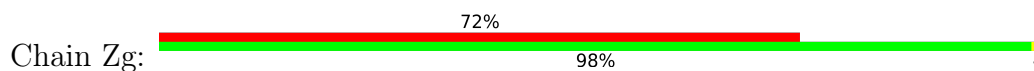


• Molecule 10: Flagellar hook protein FlgE

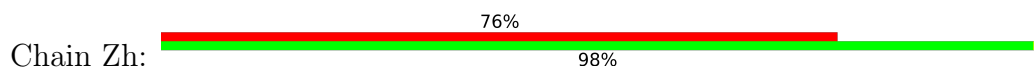


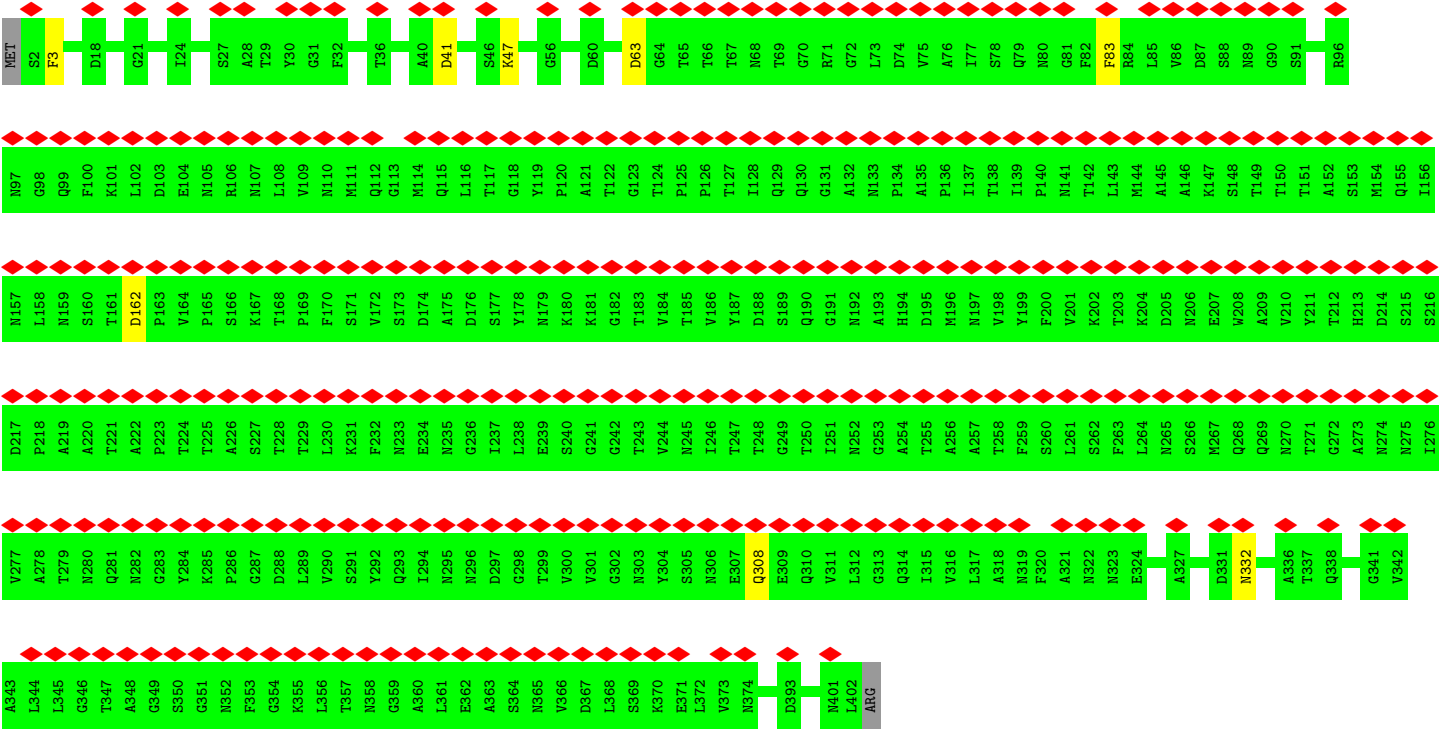


• Molecule 10: Flagellar hook protein FlgE



• Molecule 10: Flagellar hook protein FlgE







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	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	1.715	Depositor
Minimum map value	-1.213	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	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	A	0.29	0/681	0.47	0/930
1	B	0.26	0/681	0.49	0/930
1	C	0.28	0/681	0.48	0/930
1	D	0.28	0/681	0.49	0/930
2	E	0.38	1/1994 (0.1%)	0.56	1/2724 (0.0%)
3	F	0.36	0/1643	0.62	2/2237 (0.1%)
3	G	0.29	0/1665	0.49	1/2267 (0.0%)
3	H	0.29	0/1652	0.48	0/2249
3	I	0.28	0/1652	0.46	0/2249
3	J	0.30	0/1662	0.49	0/2263
4	K	0.26	0/300	0.47	0/400
4	L	0.25	0/547	0.44	0/733
4	M	0.26	0/561	0.44	0/753
4	N	0.25	0/561	0.46	0/753
4	O	0.26	0/561	0.49	0/753
4	P	0.27	0/554	0.46	0/743
5	Q	0.28	0/930	0.54	0/1251
5	R	0.26	0/855	0.48	0/1150
5	S	0.27	0/855	0.54	0/1150
5	T	0.25	0/870	0.49	0/1169
5	U	0.26	0/839	0.47	0/1129
6	V	0.28	0/981	0.44	0/1334
6	W	0.26	0/976	0.46	0/1327
6	X	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
6	Y	0.28	0/981	0.52	0/1334
6	Z	0.26	0/981	0.47	0/1334
6	a	0.28	0/981	0.47	0/1334
7	b	0.52	0/83	0.63	0/114
7	c	0.26	0/107	0.38	0/148
7	d	0.30	0/137	0.49	0/191
7	e	0.28	0/107	0.56	0/148
7	f	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
7	g	0.32	0/107	0.51	0/148
7	h	0.26	0/145	0.43	0/203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	i	0.30	0/107	0.38	0/148
7	j	0.30	0/137	0.57	0/191
7	k	0.30	0/107	0.37	0/148
7	l	0.29	0/145	0.45	0/203
8	m	0.33	0/1828	0.56	0/2492
8	n	0.28	0/1836	0.54	1/2502 (0.0%)
8	o	0.28	0/1844	0.54	0/2512
8	p	0.27	0/1844	0.53	0/2512
8	q	0.31	0/1836	0.55	0/2502
9	0	0.30	0/1888	0.52	1/2564 (0.0%)
9	1	0.31	0/1917	0.50	0/2605
9	2	0.27	0/1973	0.48	0/2682
9	3	0.28	0/1973	0.50	0/2682
9	4	0.28	0/1973	0.50	0/2682
9	5	0.32	0/1973	0.52	0/2682
9	6	0.30	0/1973	0.52	0/2682
9	7	0.28	0/1973	0.50	0/2682
9	8	0.30	0/1973	0.52	0/2682
9	9	0.29	0/1973	0.54	1/2682 (0.0%)
9	ZA	0.29	0/1973	0.52	0/2682
9	ZB	0.29	0/1973	0.49	0/2682
9	ZC	0.28	0/1973	0.51	0/2682
9	ZD	0.28	0/1973	0.51	0/2682
9	ZE	0.28	0/1973	0.50	1/2682 (0.0%)
9	r	0.33	0/1926	0.53	0/2618
9	s	0.36	0/1934	0.56	0/2629
9	t	0.33	0/1942	0.55	0/2639
9	u	0.32	0/1926	0.57	1/2618 (0.0%)
9	v	0.30	0/1934	0.51	0/2629
9	w	0.32	0/1844	0.51	0/2505
9	x	0.31	0/1888	0.51	0/2564
9	y	0.30	0/1888	0.54	1/2564 (0.0%)
9	z	0.30	0/1888	0.51	0/2564
10	ZF	0.27	0/2991	0.49	0/4076
10	ZG	0.31	0/2991	0.50	0/4076
10	ZH	0.28	0/2991	0.50	0/4076
10	ZI	0.29	0/2991	0.51	0/4076
10	ZJ	0.31	0/2991	0.51	0/4076
10	ZK	0.26	0/2991	0.48	0/4076
10	ZL	0.28	0/2991	0.49	0/4076
10	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
10	ZN	0.28	0/2991	0.51	0/4076
10	ZO	0.30	0/2991	0.50	0/4076

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
10	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
10	ZQ	0.28	0/2991	0.51	0/4076
10	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
10	ZS	0.29	0/2991	0.52	1/4076 (0.0%)
10	ZT	0.26	0/2991	0.47	0/4076
10	ZU	0.27	0/2991	0.50	0/4076
10	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
10	ZW	0.25	0/2991	0.48	0/4076
10	ZX	0.28	0/2991	0.48	0/4076
10	ZY	0.29	1/2991 (0.0%)	0.54	2/4076 (0.0%)
10	ZZ	0.25	0/2991	0.46	0/4076
10	Za	0.27	0/2991	0.49	0/4076
10	Zb	0.28	0/2991	0.50	0/4076
10	Zc	0.29	0/2991	0.53	2/4076 (0.0%)
10	Zd	0.29	0/2991	0.50	0/4076
10	Ze	0.27	0/2991	0.48	0/4076
10	Zf	0.27	0/2991	0.48	0/4076
10	Zg	0.27	0/2991	0.49	0/4076
10	Zh	0.26	0/2991	0.48	0/4076
All	All	0.30	10/170184 (0.0%)	0.52	32/231624 (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	H	0	1
5	Q	0	1
5	U	0	1
6	Y	0	1
6	a	0	1
8	m	0	2
8	n	0	1
8	o	0	1
8	q	0	1
9	0	0	2
9	1	0	1
9	5	0	1
9	6	0	1
9	8	0	1
9	ZA	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
9	r	0	1
9	u	0	1
9	y	0	2
9	z	0	1
10	ZG	0	1
10	ZI	0	1
10	ZK	0	1
10	ZO	0	1
10	ZW	0	1
10	Zb	0	1
10	Zd	0	1
10	Ze	0	1
All	All	0	30

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	ZV	140	PRO	CG-CD	-16.10	0.97	1.50
7	f	331	PRO	CG-CD	-14.24	1.03	1.50
6	X	73	PRO	CG-CD	-12.72	1.08	1.50
10	ZV	125	PRO	CG-CD	-10.15	1.17	1.50
10	ZV	140	PRO	N-CD	8.31	1.59	1.47

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	73	PRO	CB-CG-CD	18.81	179.87	106.50
6	X	73	PRO	N-CD-CG	-18.79	75.01	103.20
10	ZV	140	PRO	N-CD-CG	-17.34	77.19	103.20
7	f	331	PRO	N-CD-CG	-16.10	79.05	103.20
6	X	73	PRO	CA-CB-CG	-13.99	77.42	104.00

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	143	ARG	Sidechain
5	Q	106	ARG	Sidechain
5	U	104	ARG	Sidechain
6	Y	110	ARG	Sidechain
6	a	110	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	A	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
1	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
1	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
1	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
2	E	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	5	25
3	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
3	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	42
3	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
3	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	56
3	J	207/245 (84%)	200 (97%)	5 (2%)	2 (1%)	13	42
4	K	38/104 (36%)	36 (95%)	2 (5%)	0	100	100
4	L	70/104 (67%)	70 (100%)	0	0	100	100
4	M	72/104 (69%)	70 (97%)	2 (3%)	0	100	100
4	N	72/104 (69%)	72 (100%)	0	0	100	100
4	O	72/104 (69%)	72 (100%)	0	0	100	100
4	P	71/104 (68%)	71 (100%)	0	0	100	100
5	Q	115/138 (83%)	115 (100%)	0	0	100	100
5	R	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
5	S	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
5	T	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
5	U	102/138 (74%)	101 (99%)	1 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	V	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
6	W	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
6	X	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
6	Y	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
6	Z	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	46
6	a	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
7	b	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
7	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
7	d	18/560 (3%)	18 (100%)	0	0	100	100
7	e	14/560 (2%)	14 (100%)	0	0	100	100
7	f	19/560 (3%)	19 (100%)	0	0	100	100
7	g	14/560 (2%)	13 (93%)	1 (7%)	0	100	100
7	h	19/560 (3%)	19 (100%)	0	0	100	100
7	i	14/560 (2%)	14 (100%)	0	0	100	100
7	j	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
7	k	14/560 (2%)	14 (100%)	0	0	100	100
7	l	19/560 (3%)	19 (100%)	0	0	100	100
8	m	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	11	38
8	n	247/251 (98%)	241 (98%)	6 (2%)	0	100	100
8	o	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
8	p	248/251 (99%)	240 (97%)	8 (3%)	0	100	100
8	q	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	61
9	0	244/260 (94%)	236 (97%)	7 (3%)	1 (0%)	30	61
9	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	61
9	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	46
9	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	46
9	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	11	38
9	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	46
9	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	46
9	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	11	38
9	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	46
9	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	38
9	ZB	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	11	38
9	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	38
9	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	46
9	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	61
9	r	250/260 (96%)	237 (95%)	12 (5%)	1 (0%)	30	61
9	s	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	61
9	t	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	61
9	u	250/260 (96%)	242 (97%)	6 (2%)	2 (1%)	16	46
9	v	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	61
9	w	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	61
9	x	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	11	38
9	y	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	61
9	z	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	61
10	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	37	66
10	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	56
10	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
10	ZK	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	66
10	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	46
10	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	66
10	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	37	66
10	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	ZW	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
10	ZX	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	ZY	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
10	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	Za	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
10	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	Zd	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
10	Ze	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
10	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
10	Zg	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
10	Zh	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
All	All	22393/29305 (76%)	21644 (97%)	680 (3%)	69 (0%)	38	66

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	188	LEU
2	E	190	VAL
3	J	83	ALA
8	m	123	GLU
9	2	209	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	A	74/74 (100%)	73 (99%)	1 (1%)	62	78
1	B	74/74 (100%)	73 (99%)	1 (1%)	62	78
1	C	74/74 (100%)	74 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	74/74 (100%)	73 (99%)	1 (1%)	62	78
2	E	210/221 (95%)	204 (97%)	6 (3%)	37	63
3	F	177/204 (87%)	170 (96%)	7 (4%)	27	55
3	G	179/204 (88%)	172 (96%)	7 (4%)	27	55
3	H	178/204 (87%)	173 (97%)	5 (3%)	38	64
3	I	178/204 (87%)	172 (97%)	6 (3%)	32	59
3	J	179/204 (88%)	175 (98%)	4 (2%)	47	69
4	K	33/79 (42%)	30 (91%)	3 (9%)	7	27
4	L	56/79 (71%)	54 (96%)	2 (4%)	30	57
4	M	58/79 (73%)	57 (98%)	1 (2%)	56	74
4	N	58/79 (73%)	56 (97%)	2 (3%)	32	59
4	O	58/79 (73%)	56 (97%)	2 (3%)	32	59
4	P	57/79 (72%)	55 (96%)	2 (4%)	31	58
5	Q	98/113 (87%)	94 (96%)	4 (4%)	26	54
5	R	90/113 (80%)	88 (98%)	2 (2%)	47	69
5	S	90/113 (80%)	87 (97%)	3 (3%)	33	60
5	T	91/113 (80%)	90 (99%)	1 (1%)	70	82
5	U	89/113 (79%)	84 (94%)	5 (6%)	17	45
6	V	104/105 (99%)	104 (100%)	0	100	100
6	W	104/105 (99%)	103 (99%)	1 (1%)	73	84
6	X	104/105 (99%)	104 (100%)	0	100	100
6	Y	104/105 (99%)	102 (98%)	2 (2%)	52	72
6	Z	104/105 (99%)	101 (97%)	3 (3%)	37	63
6	a	104/105 (99%)	100 (96%)	4 (4%)	28	56
7	b	8/467 (2%)	8 (100%)	0	100	100
7	c	11/467 (2%)	10 (91%)	1 (9%)	7	27
7	d	14/467 (3%)	12 (86%)	2 (14%)	2	12
7	e	11/467 (2%)	11 (100%)	0	100	100
7	f	15/467 (3%)	15 (100%)	0	100	100
7	g	11/467 (2%)	11 (100%)	0	100	100
7	h	15/467 (3%)	15 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	i	11/467 (2%)	11 (100%)	0	100	100
7	j	14/467 (3%)	13 (93%)	1 (7%)	12	37
7	k	11/467 (2%)	11 (100%)	0	100	100
7	l	15/467 (3%)	14 (93%)	1 (7%)	13	39
8	m	190/193 (98%)	187 (98%)	3 (2%)	58	76
8	n	191/193 (99%)	187 (98%)	4 (2%)	48	70
8	o	192/193 (100%)	187 (97%)	5 (3%)	41	66
8	p	192/193 (100%)	190 (99%)	2 (1%)	73	84
8	q	191/193 (99%)	190 (100%)	1 (0%)	86	91
9	0	205/215 (95%)	199 (97%)	6 (3%)	37	63
9	1	209/215 (97%)	201 (96%)	8 (4%)	28	56
9	2	215/215 (100%)	212 (99%)	3 (1%)	62	78
9	3	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	4	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	5	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	6	215/215 (100%)	210 (98%)	5 (2%)	45	68
9	7	215/215 (100%)	214 (100%)	1 (0%)	86	91
9	8	215/215 (100%)	213 (99%)	2 (1%)	75	85
9	9	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	85
9	ZB	215/215 (100%)	207 (96%)	8 (4%)	29	56
9	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	78
9	ZD	215/215 (100%)	212 (99%)	3 (1%)	62	78
9	ZE	215/215 (100%)	214 (100%)	1 (0%)	86	91
9	r	209/215 (97%)	204 (98%)	5 (2%)	44	68
9	s	210/215 (98%)	203 (97%)	7 (3%)	33	60
9	t	211/215 (98%)	201 (95%)	10 (5%)	22	51
9	u	209/215 (97%)	200 (96%)	9 (4%)	25	53
9	v	210/215 (98%)	202 (96%)	8 (4%)	28	56
9	w	200/215 (93%)	196 (98%)	4 (2%)	50	71
9	x	205/215 (95%)	199 (97%)	6 (3%)	37	63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	y	205/215 (95%)	197 (96%)	8 (4%)	27	55
9	z	205/215 (95%)	201 (98%)	4 (2%)	50	71
10	ZF	321/323 (99%)	310 (97%)	11 (3%)	32	59
10	ZG	321/323 (99%)	306 (95%)	15 (5%)	22	51
10	ZH	321/323 (99%)	309 (96%)	12 (4%)	29	56
10	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	67
10	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	61
10	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	64
10	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	61
10	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	67
10	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	51
10	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	64
10	ZR	321/323 (99%)	313 (98%)	8 (2%)	42	67
10	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	ZT	321/323 (99%)	316 (98%)	5 (2%)	58	76
10	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	80
10	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	80
10	ZW	321/323 (99%)	309 (96%)	12 (4%)	29	56
10	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	85
10	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	69
10	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	76
10	Za	321/323 (99%)	316 (98%)	5 (2%)	58	76
10	Zb	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	59
10	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	Ze	321/323 (99%)	312 (97%)	9 (3%)	38	64
10	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	69
10	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	Zh	321/323 (99%)	313 (98%)	8 (2%)	42	67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	18273/23835 (77%)	17828 (98%)	445 (2%)	45 68

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

Mol	Chain	Res	Type
10	ZN	78	SER
9	z	117	ASP
10	ZT	148	SER
9	y	169	GLN
9	t	87	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 449 such sidechains are listed below:

Mol	Chain	Res	Type
10	ZN	129	GLN
9	y	223	ASN
10	ZT	314	GLN
9	y	51	GLN
9	r	172	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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.

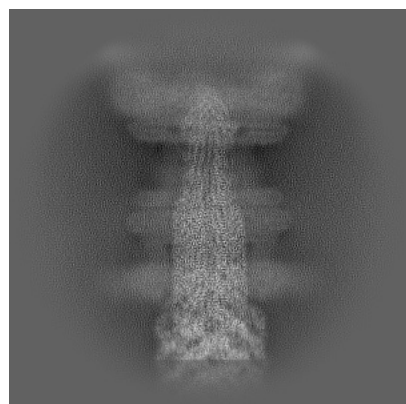
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37601. These allow visual inspection of the internal detail of the map and identification of artifacts.

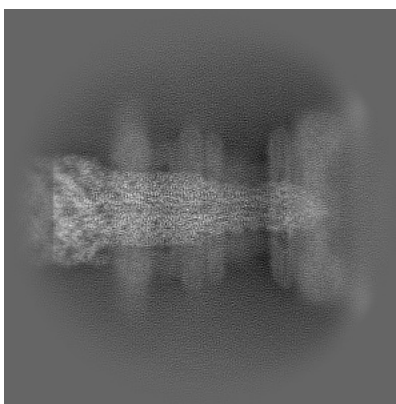
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

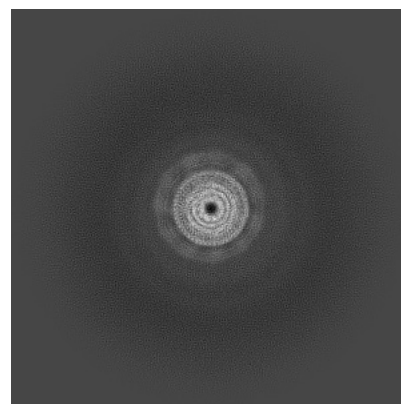
#### 6.1.1 Primary map



X

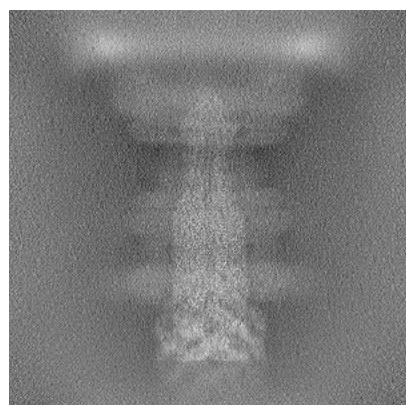


Y

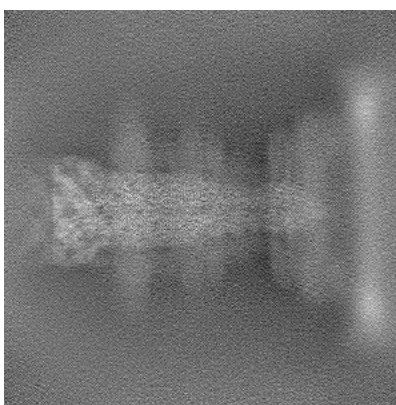


Z

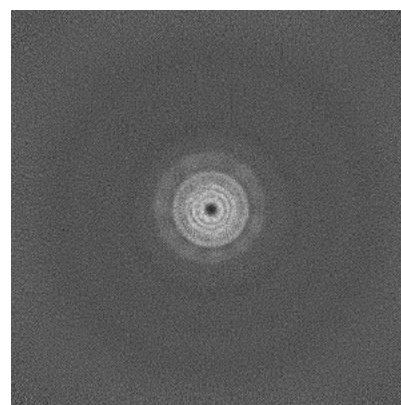
#### 6.1.2 Raw map



X



Y



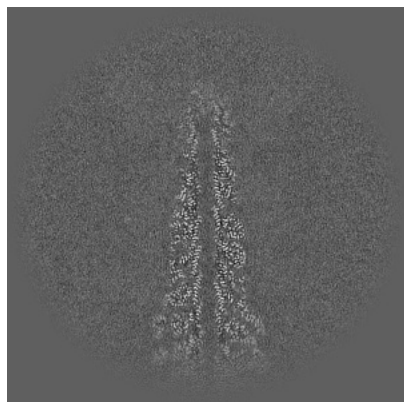
Z

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

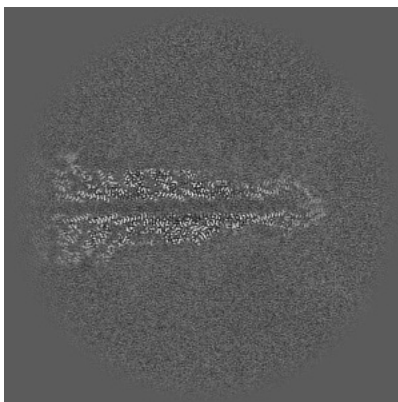


## 6.2 Central slices [i](#)

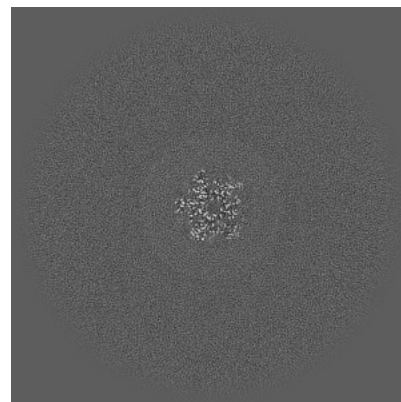
### 6.2.1 Primary map



X Index: 256

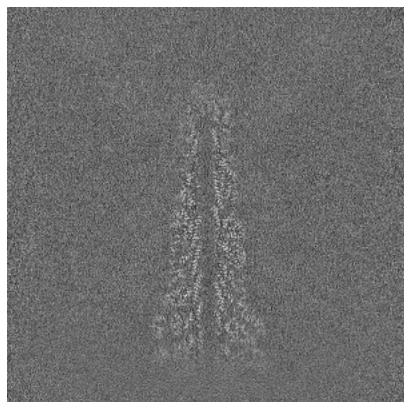


Y Index: 256

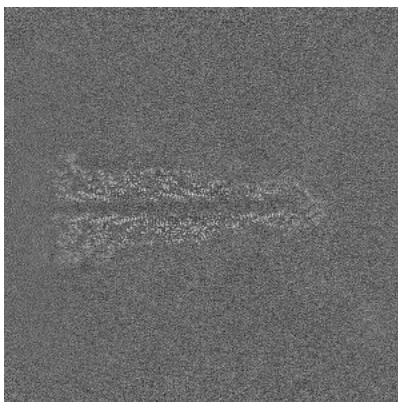


Z Index: 256

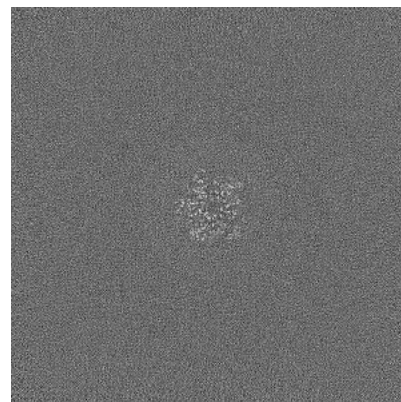
### 6.2.2 Raw map



X Index: 256



Y Index: 256



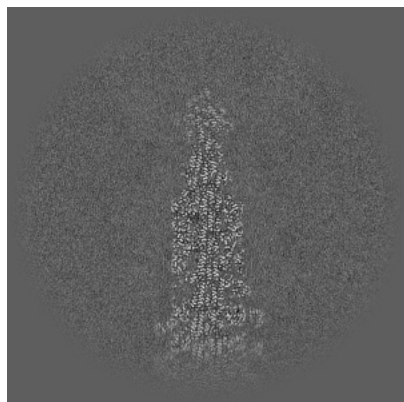
Z Index: 256

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

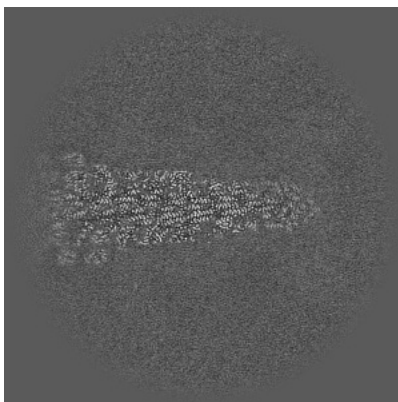


## 6.3 Largest variance slices [i](#)

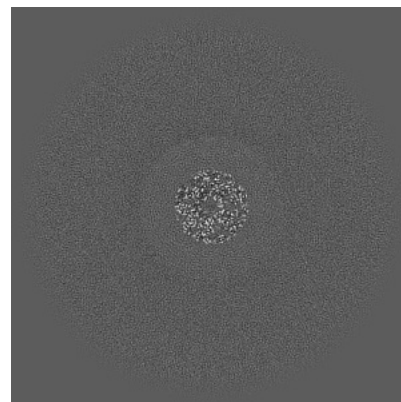
### 6.3.1 Primary map



X Index: 242

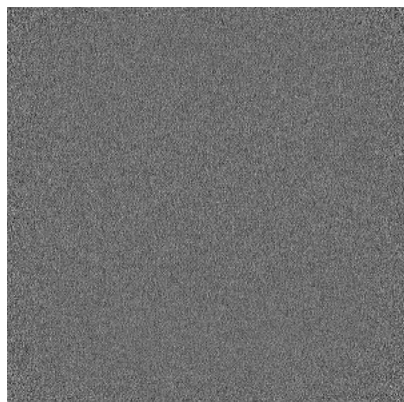


Y Index: 268

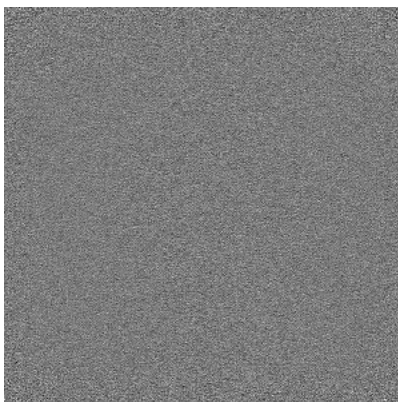


Z Index: 224

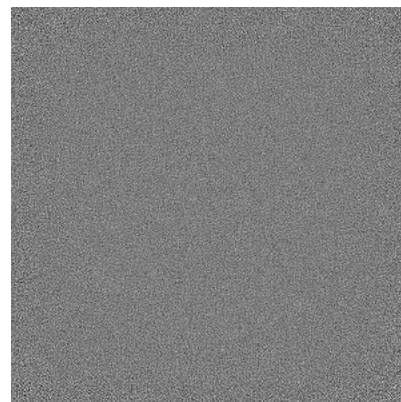
### 6.3.2 Raw map



X Index: 0



Y Index: 0

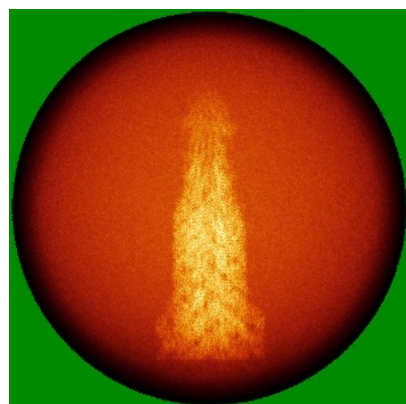


Z Index: 0

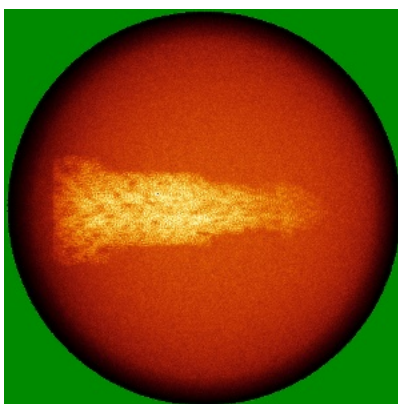
The images above show the largest variance slices of the map in three orthogonal directions.

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

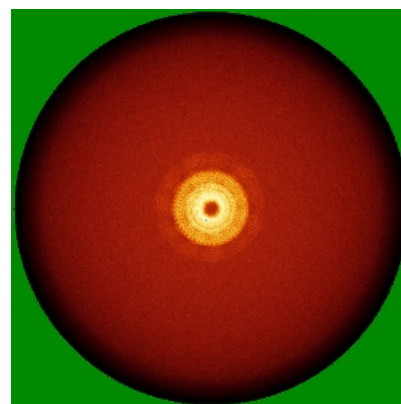
### 6.4.1 Primary map



X

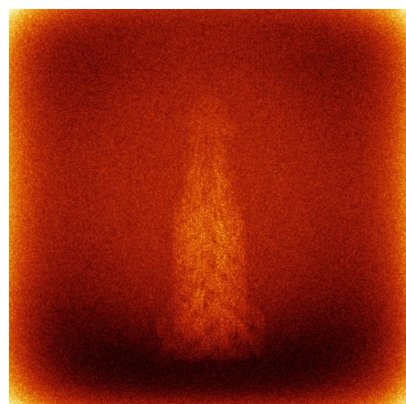


Y

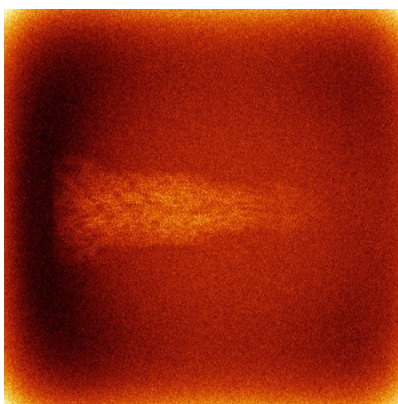


Z

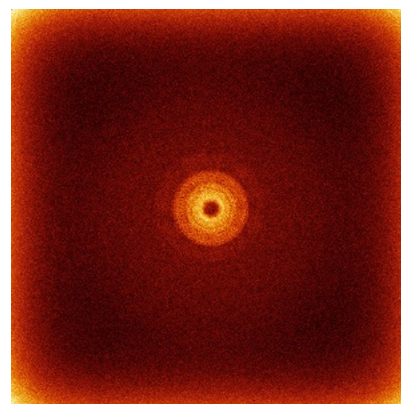
### 6.4.2 Raw map



X



Y

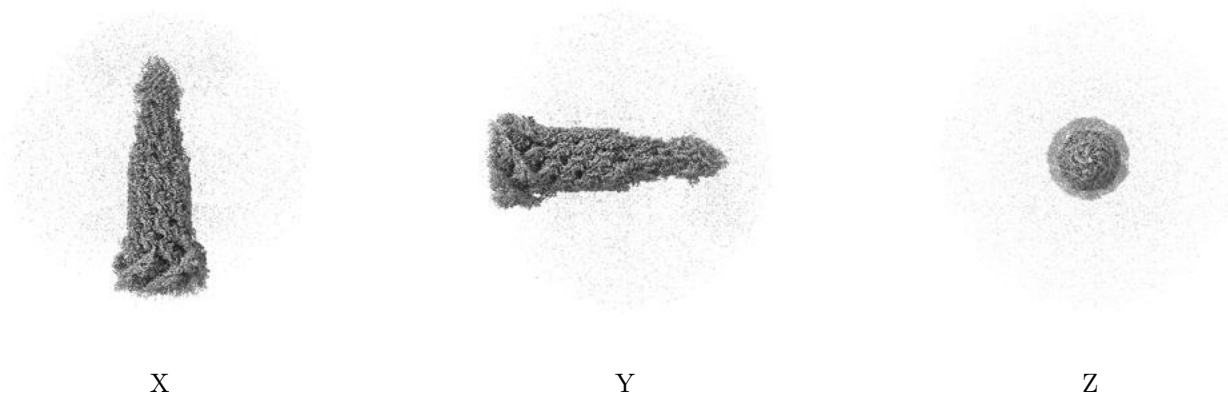


Z

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

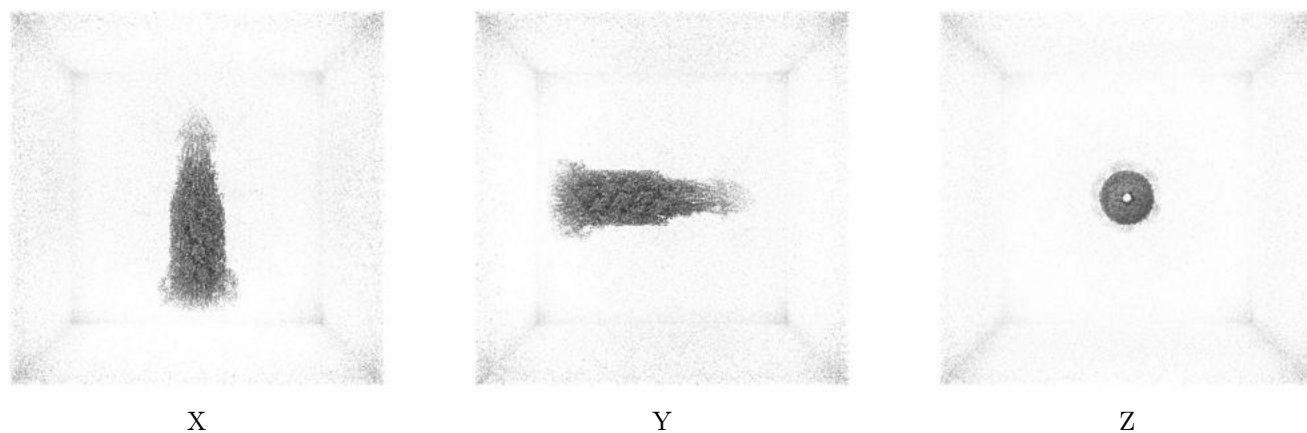
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

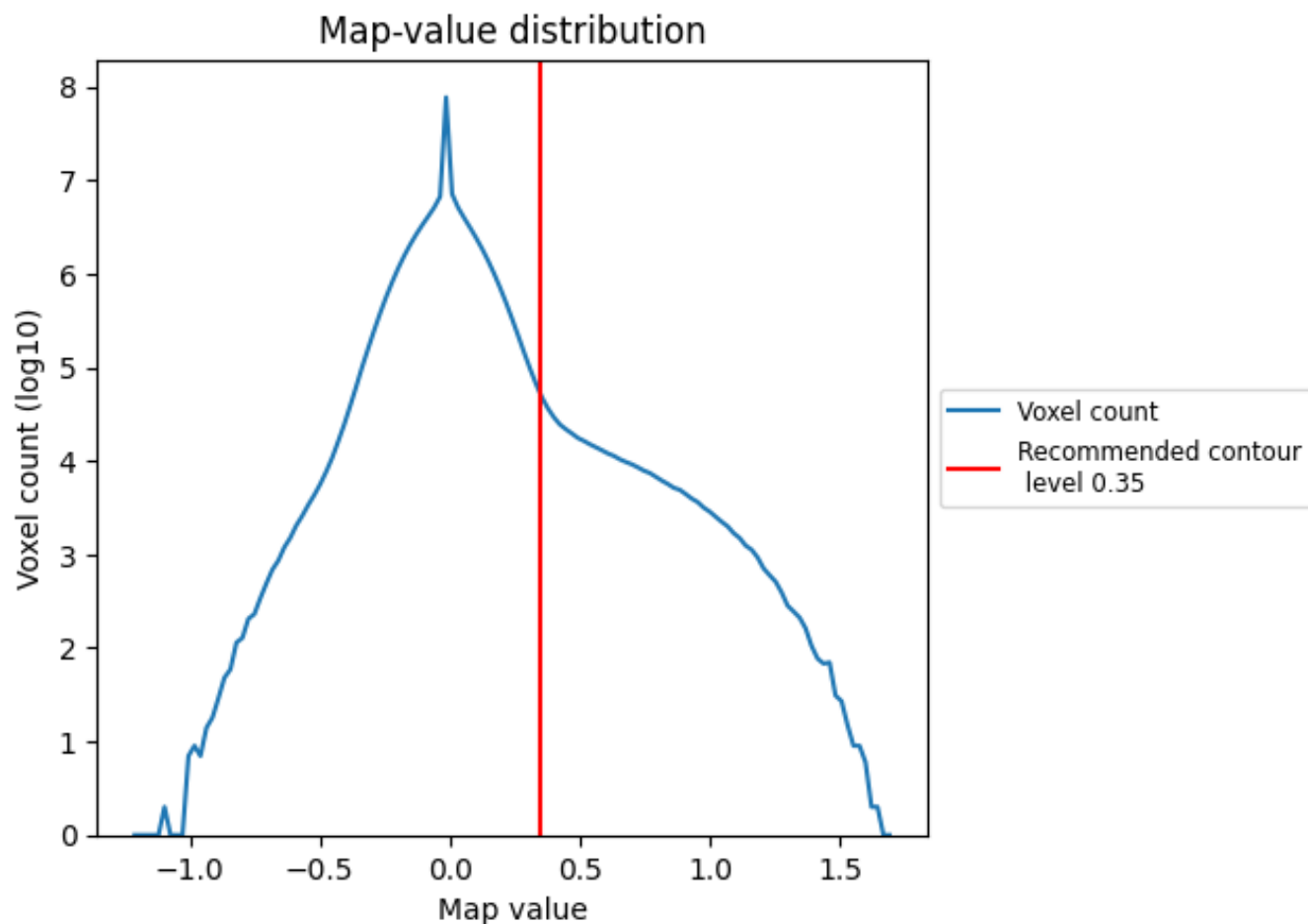
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

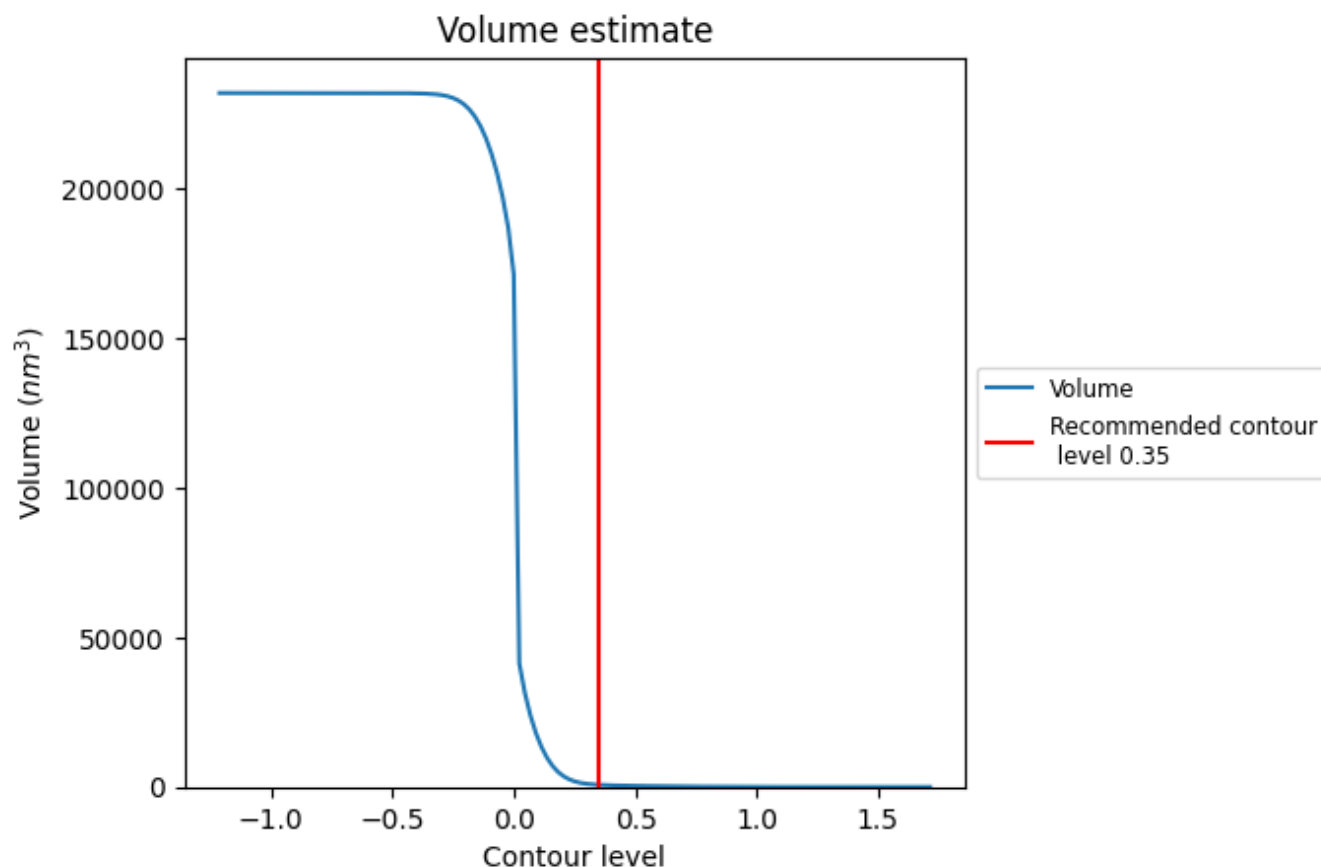
This section contains the results of statistical analysis of the map.

### 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](#)

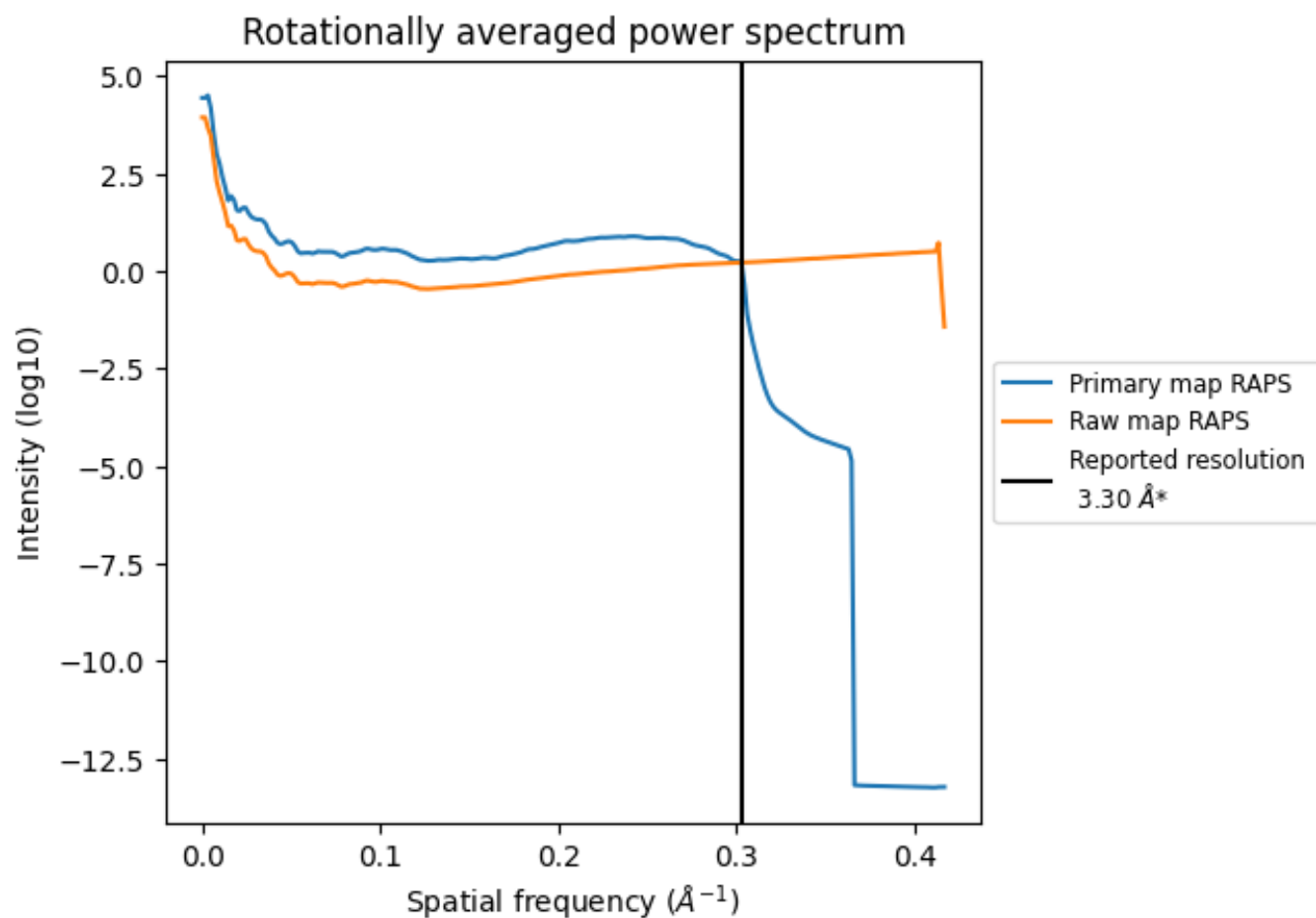


The volume at the recommended contour level is 705  $\text{nm}^3$ ; this corresponds to an approximate mass of 637 kDa.

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 ⓘ

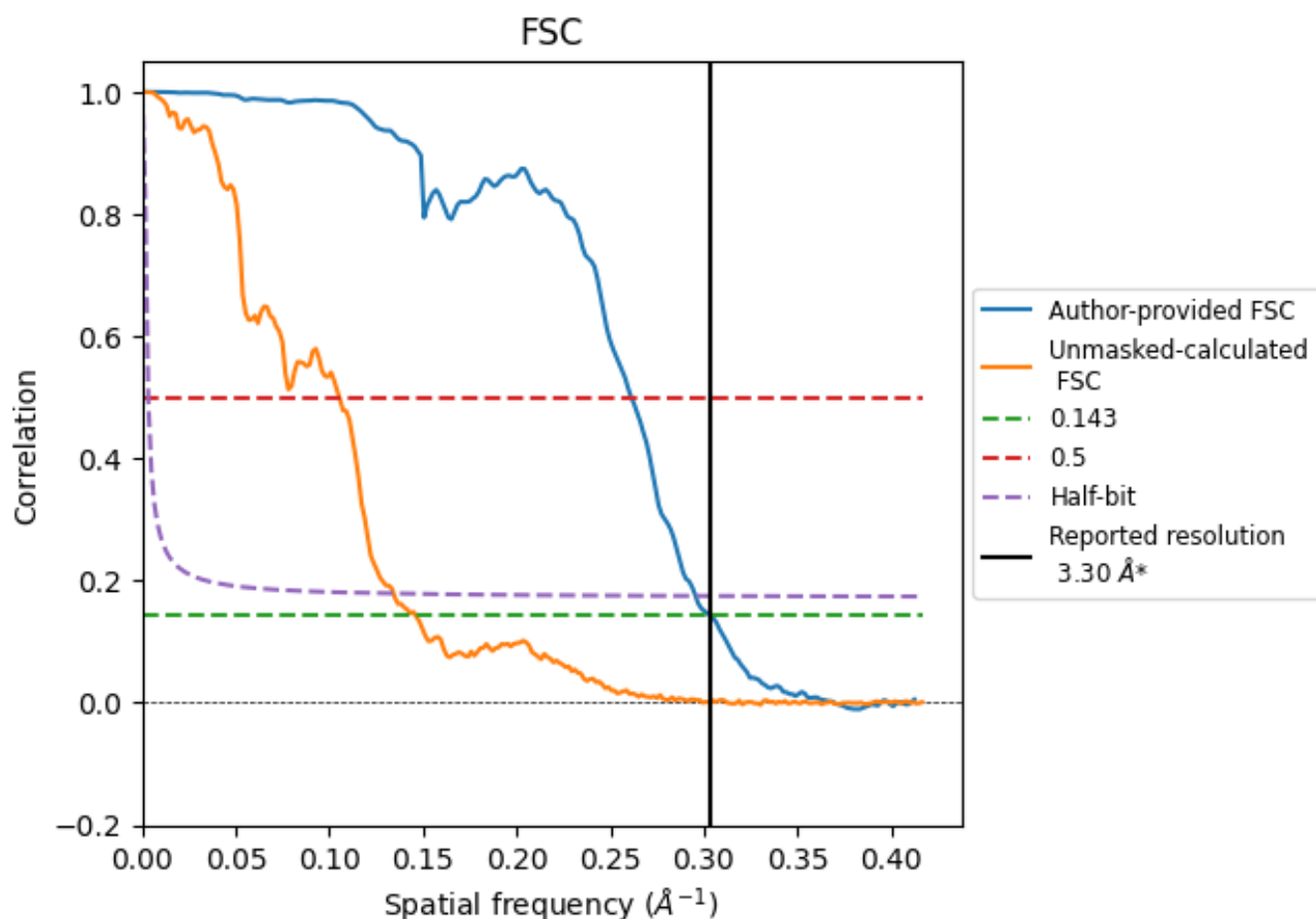


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.83	3.38
Unmasked-calculated*	6.85	9.51	7.45

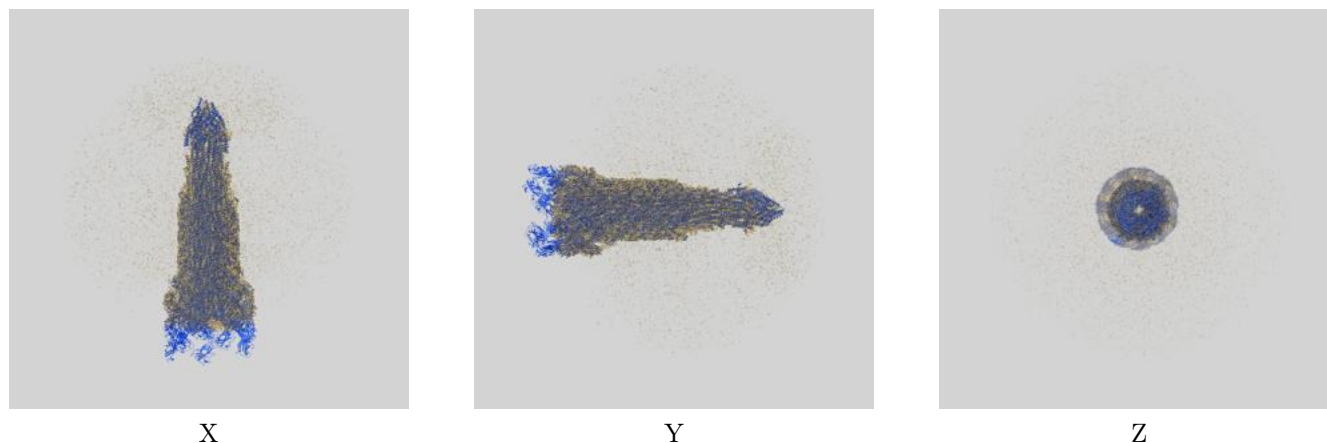
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.85 differs from the reported value 3.3 by more than 10 %



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

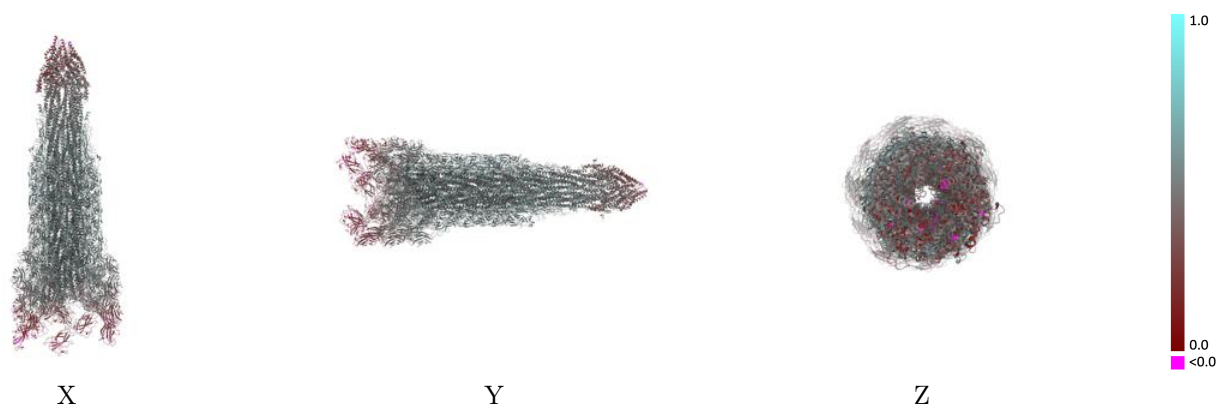
This section contains information regarding the fit between EMDB map EMD-37601 and PDB model 8WKK. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



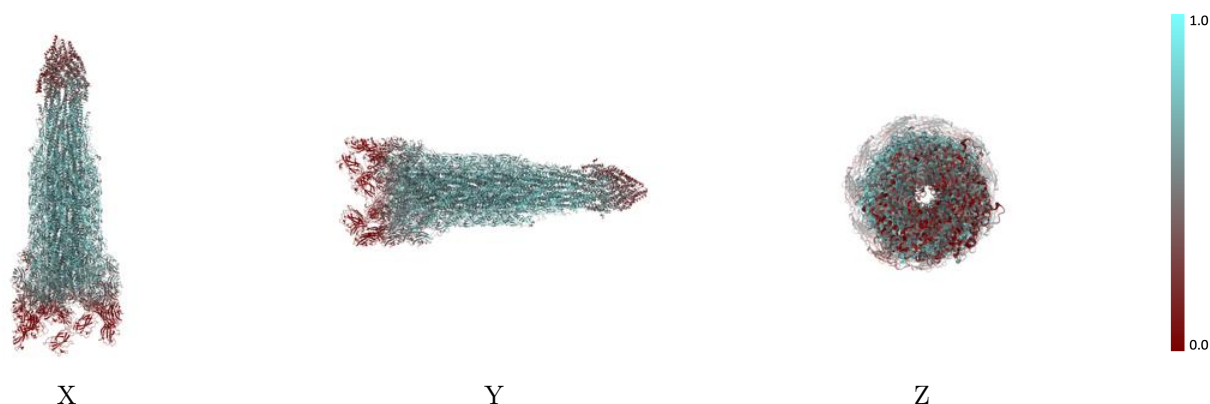
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



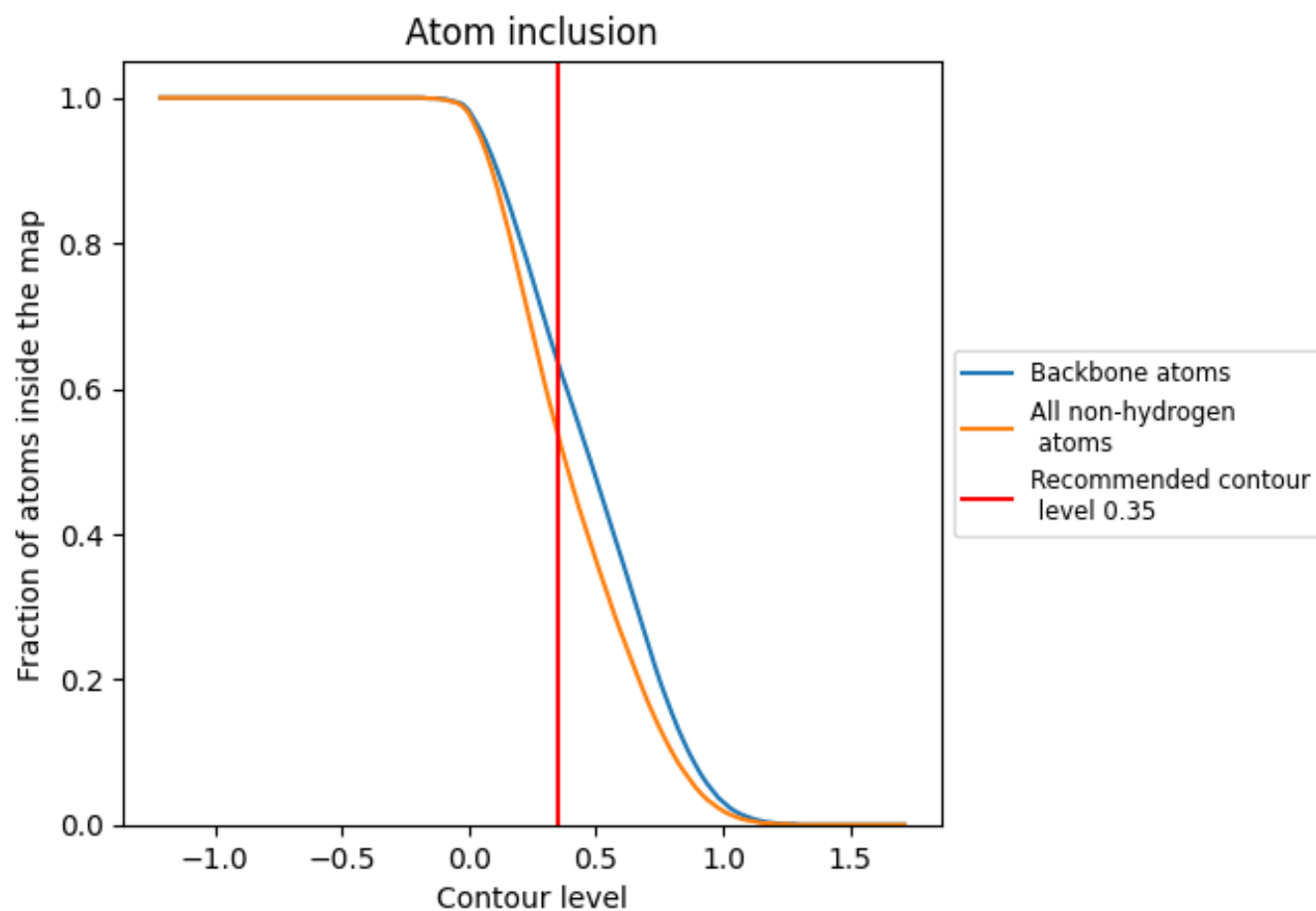
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5380	 0.4710
0	 0.7050	 0.5320
1	 0.6880	 0.5310
2	 0.6930	 0.5370
3	 0.6950	 0.5280
4	 0.6870	 0.5220
5	 0.6760	 0.5240
6	 0.6860	 0.5270
7	 0.6860	 0.5250
8	 0.6940	 0.5250
9	 0.6890	 0.5290
A	 0.1740	 0.2680
B	 0.3050	 0.3490
C	 0.3290	 0.3590
D	 0.2360	 0.3150
E	 0.2560	 0.3370
F	 0.3470	 0.3860
G	 0.4690	 0.4330
H	 0.5000	 0.4440
I	 0.4820	 0.4440
J	 0.3890	 0.4180
K	 0.4950	 0.4730
L	 0.5990	 0.4760
M	 0.6260	 0.4960
N	 0.6280	 0.5020
O	 0.5950	 0.4790
P	 0.5560	 0.4610
Q	 0.5750	 0.4810
R	 0.6770	 0.5040
S	 0.6950	 0.5210
T	 0.6770	 0.5130
U	 0.6510	 0.4950
V	 0.5880	 0.4940
W	 0.6810	 0.5180
X	 0.6760	 0.5290











































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
Y	 0.6770	 0.5160
Z	 0.6570	 0.5150
ZA	 0.6710	 0.5200
ZB	 0.6810	 0.5250
ZC	 0.6810	 0.5230
ZD	 0.6720	 0.5170
ZE	 0.6580	 0.5170
ZF	 0.4120	 0.4580
ZG	 0.5850	 0.5040
ZH	 0.6120	 0.5040
ZI	 0.6150	 0.5040
ZJ	 0.6050	 0.4980
ZK	 0.5810	 0.4940
ZL	 0.5860	 0.4880
ZM	 0.5930	 0.4940
ZN	 0.5990	 0.4910
ZO	 0.5750	 0.4910
ZP	 0.5670	 0.4840
ZQ	 0.5360	 0.4750
ZR	 0.5370	 0.4690
ZS	 0.5260	 0.4690
ZT	 0.4920	 0.4610
ZU	 0.4740	 0.4570
ZV	 0.4360	 0.4420
ZW	 0.4360	 0.4430
ZX	 0.4120	 0.4300
ZY	 0.3940	 0.4240
ZZ	 0.3630	 0.4160
Za	 0.3520	 0.4020
Zb	 0.3390	 0.4000
Zc	 0.3060	 0.3940
Zd	 0.2840	 0.3690
Ze	 0.2500	 0.3670
Zf	 0.2250	 0.3470
Zg	 0.2030	 0.3190
Zh	 0.1840	 0.3290
a	 0.6240	 0.5050
b	 0.3700	 0.4480
c	 0.5630	 0.4860
d	 0.5040	 0.4980
e	 0.5730	 0.5260
f	 0.6430	 0.5100

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
g	 0.5920	 0.4950
h	 0.6570	 0.5050
i	 0.5340	 0.4690
j	 0.6470	 0.4990
k	 0.5630	 0.4830
l	 0.5430	 0.5030
m	 0.6420	 0.5150
n	 0.7010	 0.5350
o	 0.7130	 0.5350
p	 0.7130	 0.5320
q	 0.6710	 0.5170
r	 0.6570	 0.5270
s	 0.6960	 0.5350
t	 0.6940	 0.5340
u	 0.6980	 0.5390
v	 0.6900	 0.5310
w	 0.7100	 0.5340
x	 0.6920	 0.5290
y	 0.6920	 0.5300
z	 0.7000	 0.5370