



wwPDB EM Validation Summary Report ⓘ

Aug 17, 2026 – 11:56 AM EDT

PDB ID : 12DU / pdb_000012du
EMDB ID : EMD-76347
Title : In situ cryo-EM structure of the flagellar export gate in complex with the FlIF
RBM12 ring in *Borrelia burgdorferi*
Authors : Yue, J.; Liu, Y.
Deposited on : 2026-03-30
Resolution : 3.87 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

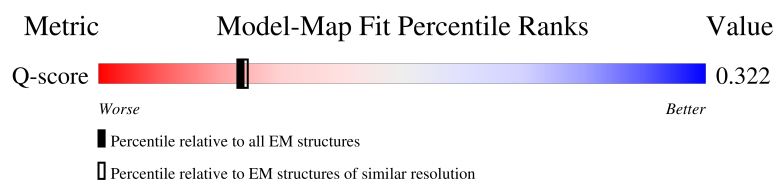
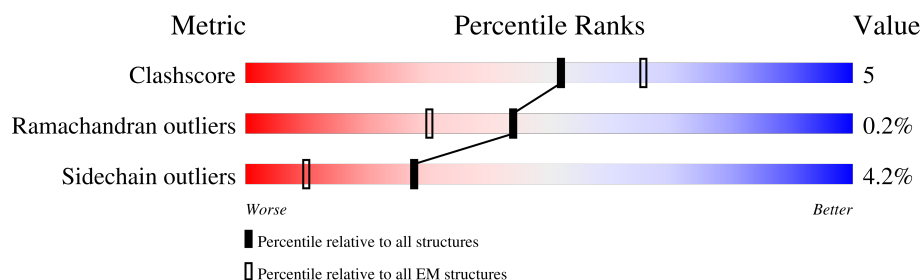
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

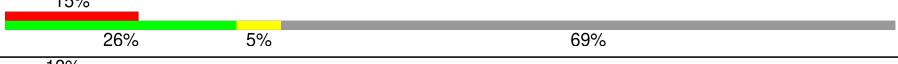
The reported resolution of this entry is 3.87 Å.

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	8831 (3.37 - 4.37)

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	c	569	
1	d	569	
1	e	569	
1	f	569	

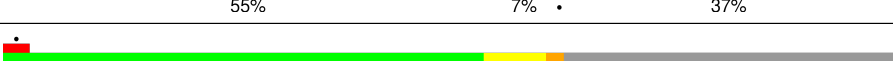
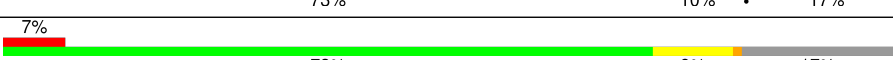
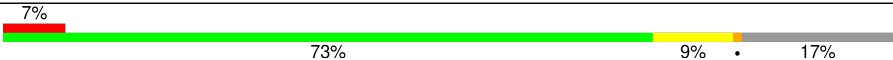
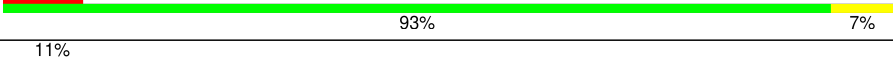
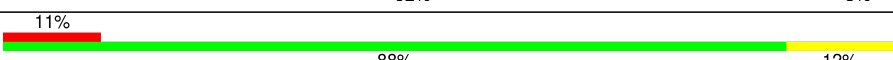
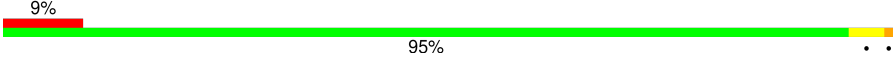
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Mol	Chain	Length	Quality of chain
1	g	569	
1	h	569	
1	i	569	
1	j	569	
1	k	569	
1	l	569	
1	m	569	
1	n	569	
1	o	569	
1	p	569	
1	q	569	
1	r	569	
1	s	569	
1	t	569	
1	u	569	
1	v	569	
1	w	569	
1	x	569	
1	y	569	
2	A	372	
3	F	254	
3	G	254	
3	H	254	
3	I	254	
3	J	254	

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Mol	Chain	Length	Quality of chain
4	K	269	
5	L	111	
5	M	111	
5	N	111	
5	O	111	
5	P	111	
5	Q	111	
6	R	135	
6	S	135	
6	T	135	
6	U	135	
6	V	135	
7	W	152	
7	X	152	
7	Y	152	
7	Z	152	
7	a	152	
7	b	152	
8	1	87	
8	2	87	
8	3	87	
8	z	87	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 61305 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 M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	179	Total	C	N	O	S	0	0
			1397	891	240	264	2		
1	d	179	Total	C	N	O	S	0	0
			1383	880	238	263	2		
1	e	179	Total	C	N	O	S	0	0
			1391	885	240	264	2		
1	f	178	Total	C	N	O	S	0	0
			1390	885	240	263	2		
1	g	177	Total	C	N	O	S	0	0
			1381	879	238	262	2		
1	h	178	Total	C	N	O	S	0	0
			1374	875	238	259	2		
1	i	179	Total	C	N	O	S	0	0
			1392	885	241	264	2		
1	j	179	Total	C	N	O	S	0	0
			1387	884	240	261	2		
1	k	179	Total	C	N	O	S	0	0
			1388	882	240	264	2		
1	l	179	Total	C	N	O	S	0	0
			1385	884	238	261	2		
1	m	179	Total	C	N	O	S	0	0
			1397	892	241	262	2		
1	n	179	Total	C	N	O	S	0	0
			1375	876	238	259	2		
1	o	179	Total	C	N	O	S	0	0
			1387	886	236	263	2		
1	p	179	Total	C	N	O	S	0	0
			1385	882	237	264	2		
1	q	179	Total	C	N	O	S	0	0
			1391	886	240	263	2		
1	r	179	Total	C	N	O	S	0	0
			1401	894	241	264	2		
1	s	179	Total	C	N	O	S	0	0
			1401	894	241	264	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	t	179	Total	C	N	O	S	0	0
			1391	885	240	264	2		
1	u	173	Total	C	N	O	S	0	0
			1347	859	231	255	2		
1	v	173	Total	C	N	O	S	0	0
			1349	860	233	254	2		
1	w	179	Total	C	N	O	S	0	0
			1383	880	238	263	2		
1	x	179	Total	C	N	O	S	0	0
			1372	873	238	259	2		
1	y	179	Total	C	N	O	S	0	0
			1393	889	240	262	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	242	Total	C	N	O	S	0	0
			1988	1325	311	342	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	209	Total	C	N	O	S	0	0
			1665	1118	255	277	15		
3	G	209	Total	C	N	O	S	0	0
			1656	1114	252	275	15		
3	H	209	Total	C	N	O	S	0	0
			1657	1116	252	274	15		
3	I	209	Total	C	N	O	S	0	0
			1666	1119	255	277	15		
3	J	209	Total	C	N	O	S	0	0
			1676	1128	256	277	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	259	Total	C	N	O	S	0	0
			2083	1434	304	340	5		

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	M	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	N	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	O	70	Total	C	N	O	S	0	0
			530	333	91	104	2		
5	P	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	Q	40	Total	C	N	O	S	0	0
			308	193	55	58	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	S	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	T	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	U	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	V	112	Total	C	N	O	S	0	0
			920	577	161	177	5		

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	136	Total	C	N	O	S	0	0
			1030	639	187	200	4		
7	X	152	Total	C	N	O	S	0	0
			1153	724	201	224	4		
7	Y	136	Total	C	N	O	S	0	0
			1034	641	188	201	4		
7	Z	152	Total	C	N	O	S	0	0
			1169	732	208	225	4		
7	a	152	Total	C	N	O	S	0	0
			1169	732	208	225	4		
7	b	152	Total	C	N	O	S	0	0
			1169	732	208	225	4		

- Molecule 8 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	87	Total 678	C 463	N 99	O 112	S 4	0	0
8	1	87	Total 682	C 465	N 100	O 113	S 4	0	0
8	2	87	Total 692	C 471	N 104	O 113	S 4	0	0
8	3	87	Total 692	C 471	N 104	O 113	S 4	0	0

GLY	VAL	ASP	ARG	GLY	ARG	GLY	LEU	LYS
VAL	ASP	ASP	PHE	GLU	PHE	ASP	ASP	GLY
VAL	ASP	ASP	LYS	ASP	LYS	ASP	THR	ALA
VAL	VAL	VAL	PHE	LEU	PHE	LEU	THR	ILE
GLY	GLY	GLY	PHE	THR	PHE	THR	GLY	ILE
GLY	GLY	ILE	ILE	LYS	ILE	LYS	LYS	GLU
ILE	ARG	ASP	ALA	PRO	ASP	ASN	THR	GLN
ARG	ARG	SER	ALA	MET	GLU	GLU	GLN	GLN
GLY	GLY	GLY	ILE	VAL	VAL	GLN	SER	GLN
GLY	ASP	ASP	PHE	GLU	GLU	GLU	ASP	PRO
GLU	GLU	GLU	SER	GLU	GLU	GLU	ILE	LYS
GLN	GLN	GLN	LEU	LEU	LEU	VAL	ASN	SER
SER	SER	ASN	ILE	ILE	ILE	GLU	VAL	THR
ASN	ALA	ALA	VAL	GLU	GLU	GLU	ALA	ASN
ALA	GLU	GLU	PHE	ASP	THR	VAL	LEU	THR
LEU	LEU	LEU	THR	VAL	ILE	VAL	LYS	VAL
LEU	LEU	LEU	ILE	ILE	ILE	GLN	LYS	VAL
ALA	ALA	ALA	PHE	PHE	PHE	SER	SER	SER
ARG	ARG	ARG	ALA	ALA	SER	SER	THR	ASP
GLU	GLU	LYS	ILE	ILE	PHE	SER	SER	THR
PRO	PRO	PRO	SER	GLU	GLU	GLU	ILE	ILE
GLU	GLU	GLU	ARG	THR	THR	GLY	LYS	ILE
ASP	ASP	ASP	GLY	GLY	LYS	GLU	SER	SER
VAL	VAL	VAL	LEU	PRO	PRO	PRO	PRO	SER
ALA	ALA	ALA	GLU	GLU	GLU	ALA	ALA	GLN
LYS	LYS	LYS	ARG	ARG	ARG	ARG	ARG	THR
LEU	LEU	LEU	GLY	GLY	GLY	ILE	ILE	GLN
ILE	ILE	ILE	ARG	ASP	ASP	VAL	VAL	LYS
ARG	ARG	ARG	ARG	SER	SER	GLY	GLY	LYS
THR	THR	THR	LEU	ILE	ILE	VAL	THR	GLU
TRP	TRP	TRP	ARG	THR	THR	VAL	SER	TYR
LEU	LEU	LEU	GLU	VAL	VAL	LEU	GLN	GLN
LEU	LEU	LEU	GLU	ARG	ARG	ILE	GLY	GLY
ASN	ASN	ASN	LEU	LEU	ILE	ASN	ILE	GLN
ALA	ALA	ALA	ALA	SER	SER	PHE	PHE	GLY
			LYS	PHE	PHE	VAL	VAL	TYR
			GLN	ASP	ASP	GLY	ASP	SER
			ALA	ARG	ILE	ILE	TRP	GLY
			HIS	MET	TRP	ASN	PRO	PRO
			LEU	ASN	ASN	PHE	PRO	GLY
			ARG	GLU	PHE	VAL	GLY	GLN
			ARG	PHE	ARG	TYR	GLN	GLY
			GLN	ARG	GLU	ASP	GLY	ASN
			ALA	ILE	ASP	LYS	THR	THR
			LEU	GLU	GLU	GLY	GLY	ASN
			MET	GLU	GLU	LYS	THR	THR
			ASP	ASN	ASN	ASP	PRO	PRO
			GLY	TYR	PHE	VAL	GLU	GLU
			GLY	PHE	ILE	ILE	TYR	TYR
			ASP	ALA	ALA	ILE	ILE	GLN
			ASP	SER	THR	GLY	ASN	ASP
			ASP	THR	THR	ASN	GLY	ASP

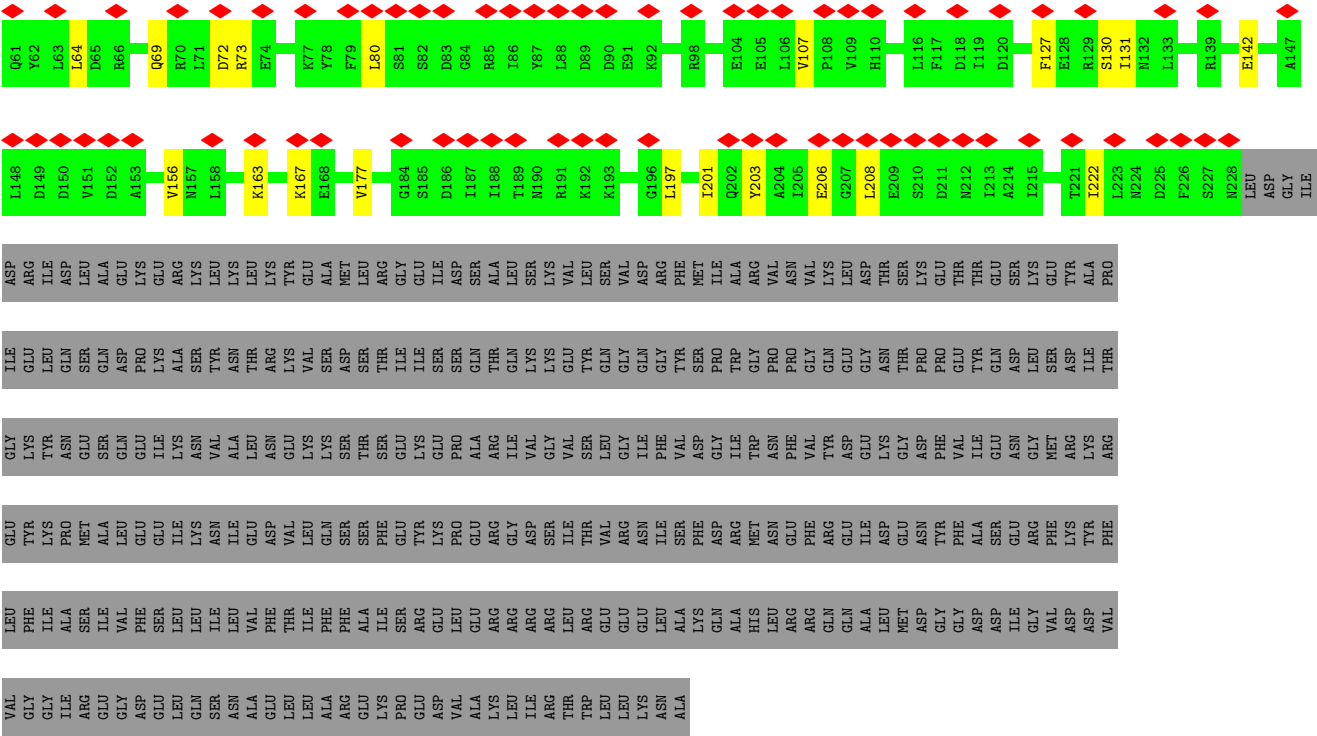
- Molecule 1: Flagellar M-ring protein

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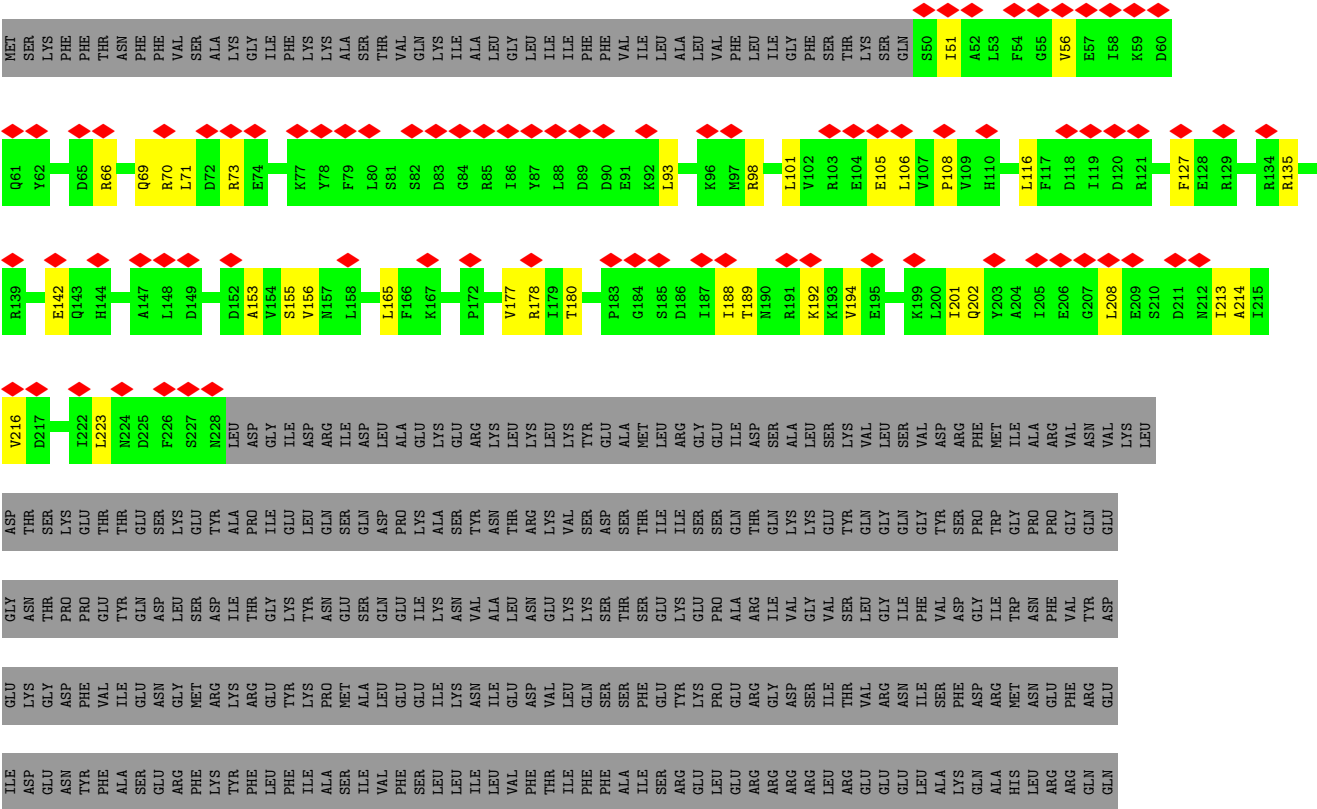
- Molecule 1: Flagellar M-ring protein



MET	SER	LYS	PHE	THR	ASN	PHE	PHE	VAL	SER	ALA	LYS	GLY	ILE	PHE	LYS	LYS	ALA	SER	THR	VAL	GLN	LYS	ILE	ALA	LEU	GLY	LEU	LEU	ALA	ALA	VAL	PHE	LEU	ILE	ILE	GLY	PHE	SER	THR	LYS	SER	GLN	S50	S51	A52	L53	F54	G55	V56	E57	I58	K59	T60
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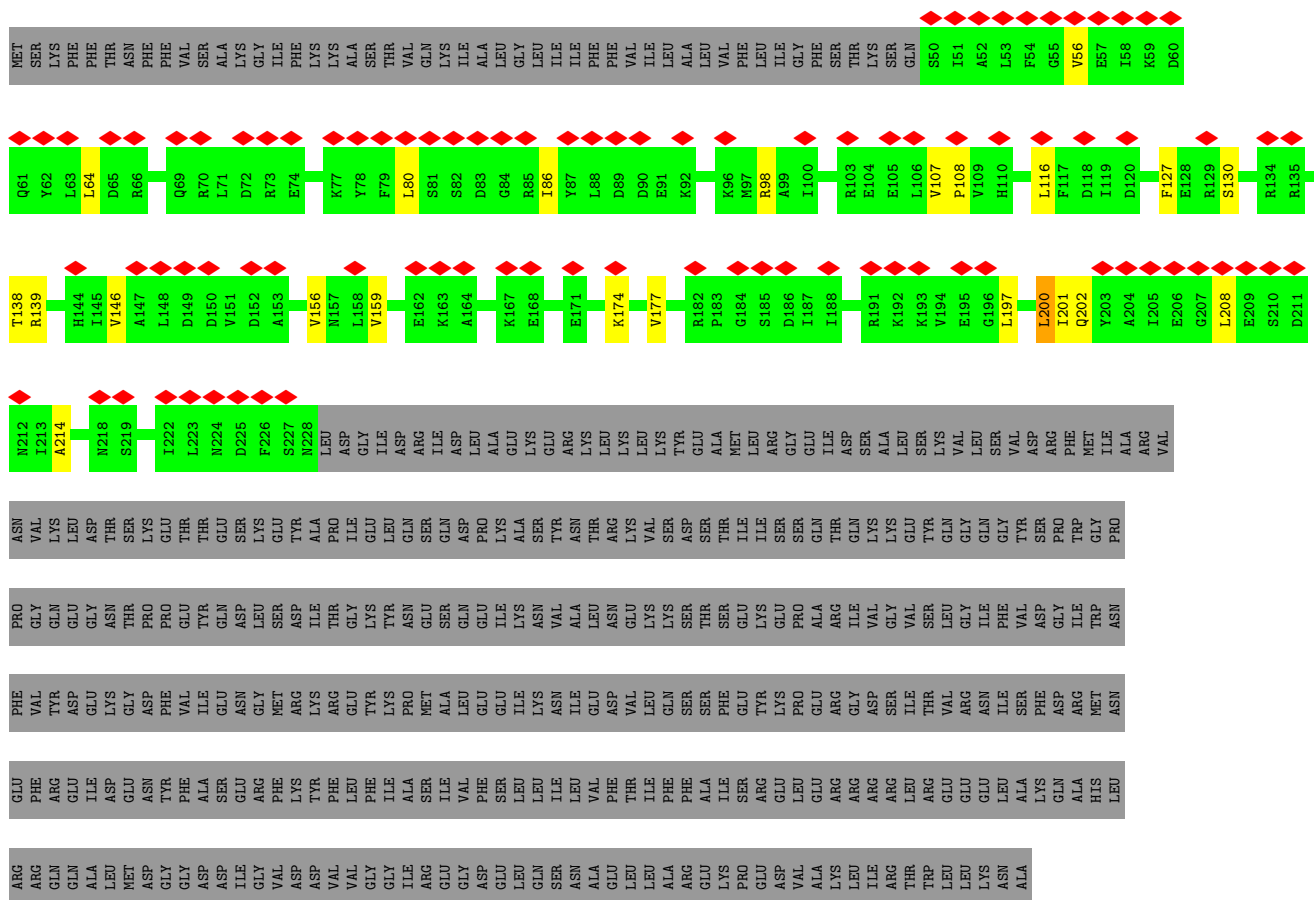


● Molecule 1: Flagellar M-ring protein

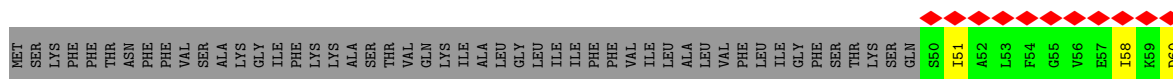


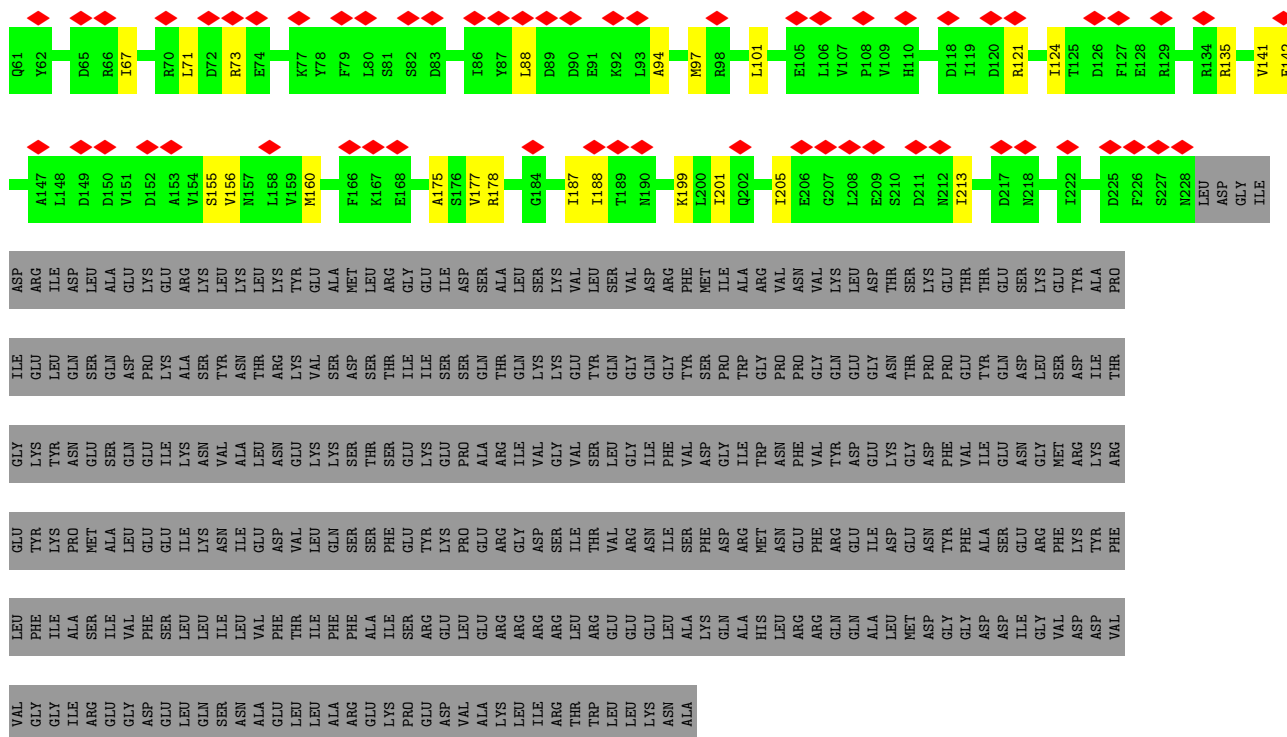


- Molecule 1: Flagellar M-ring protein

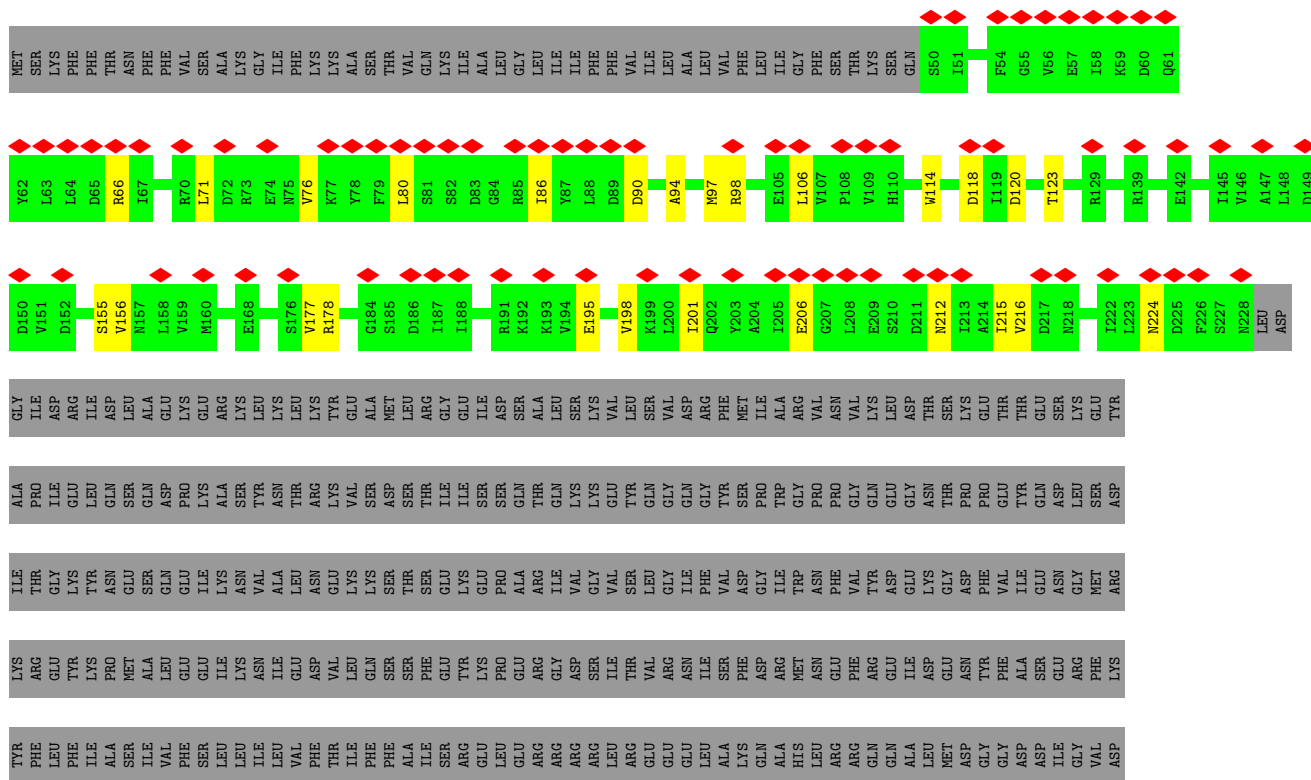


- Molecule 1: Flagellar M-ring protein

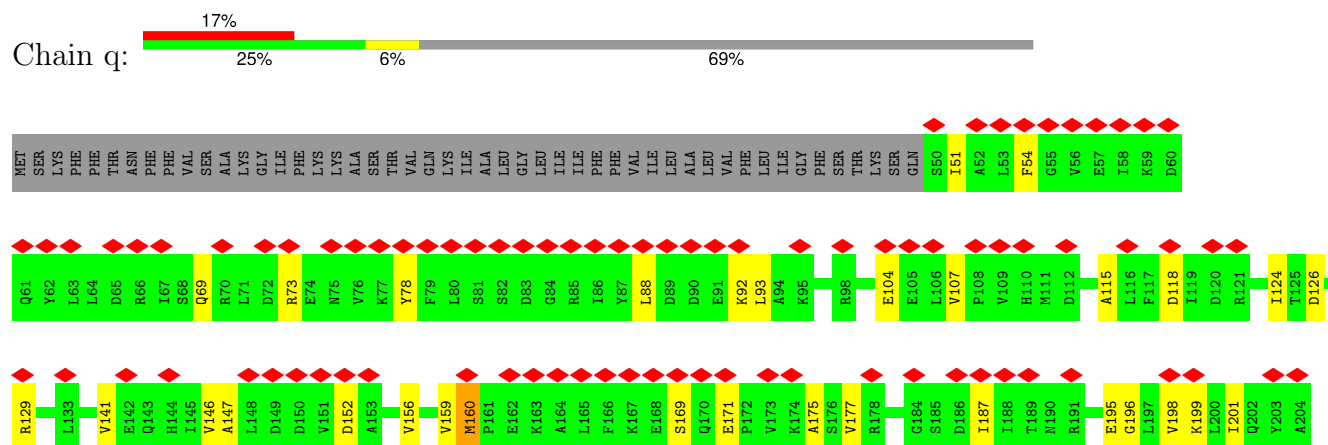
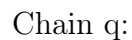




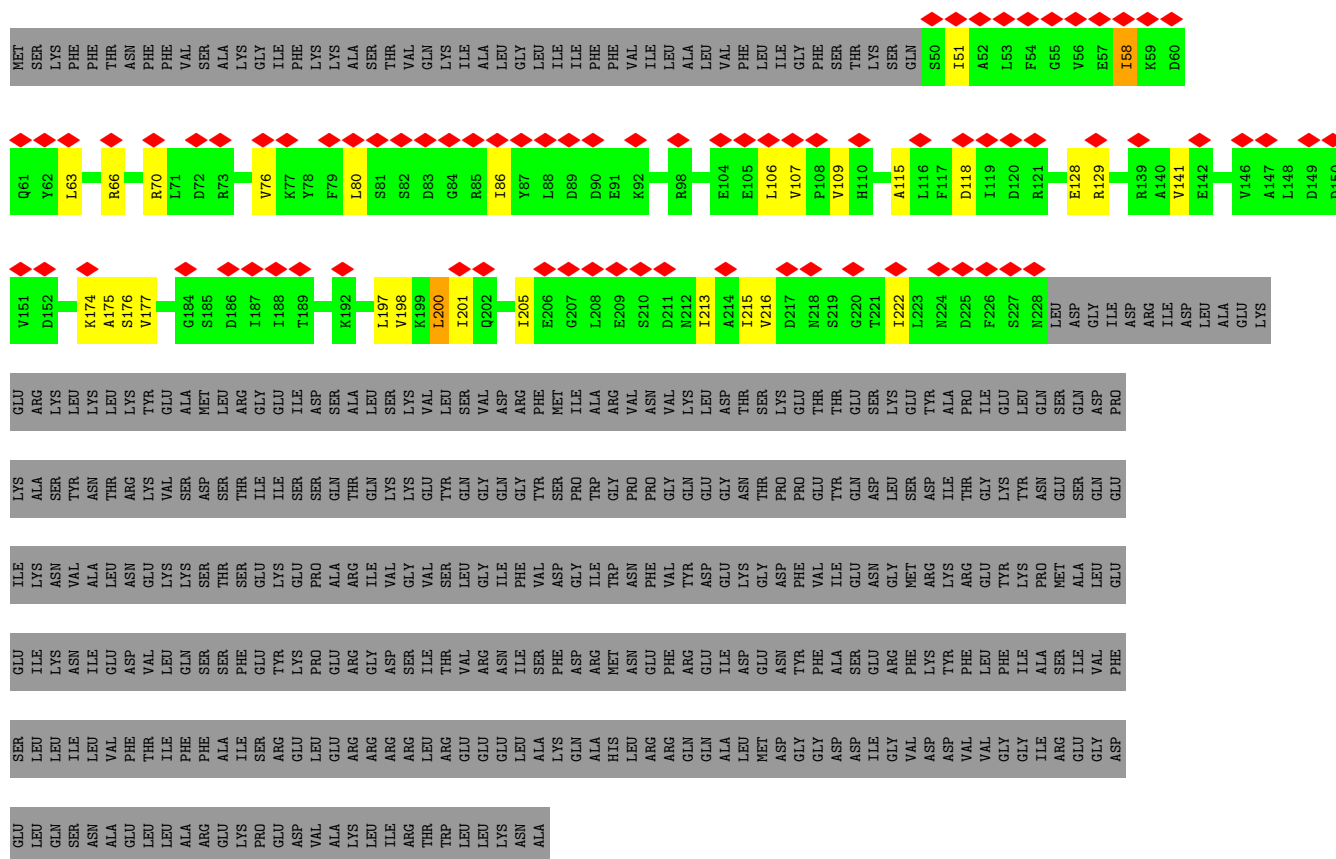
- Molecule 1: Flagellar M-ring protein



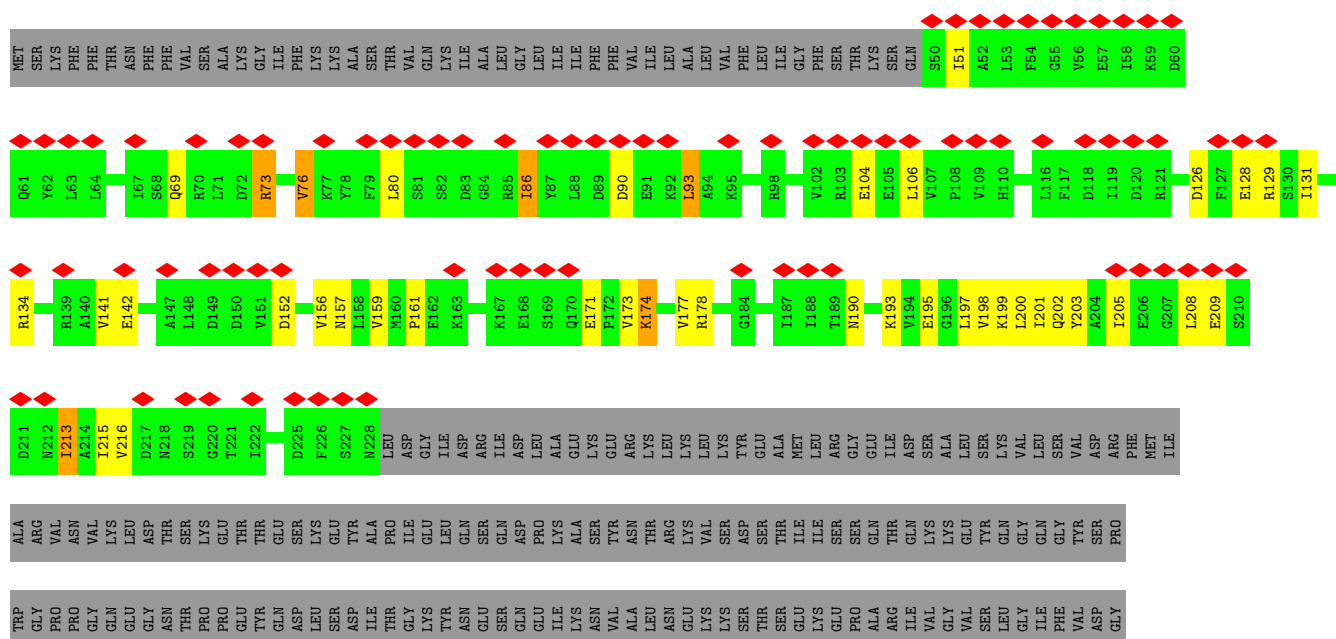
Chain p:







• Molecule 1: Flagellar M-ring protein



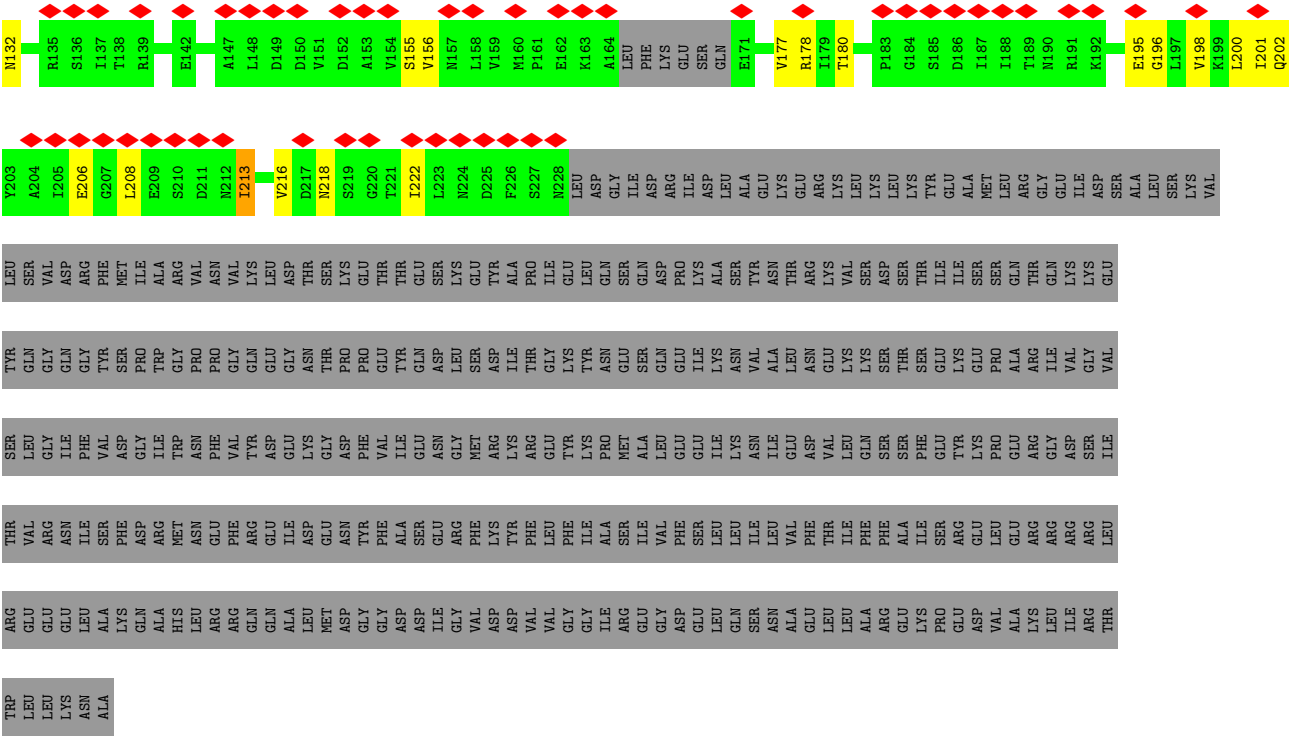
- Molecule 1: Flagellar M-ring protein

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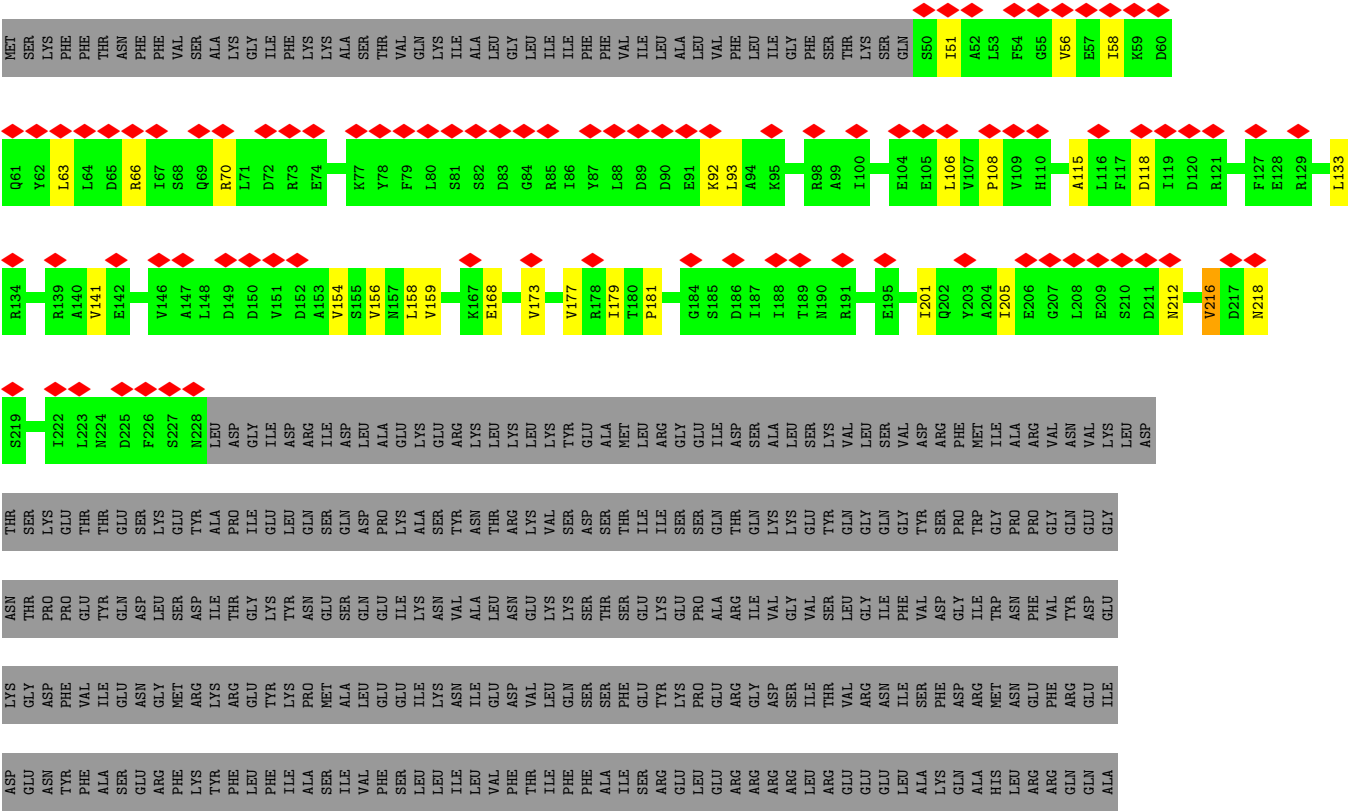
- Molecule 1: Flagellar M-ring protein



Met	Ser	Lys	Phe	Thr	Asn	Phe	Val	Ser	Ala	Lys	Gly	Ile	Phe	Lys	Ala	Ser	Thr	Gln	Lys	Leu	Gly	Ile	Phe	Val	Phe	Leu	Ile	Gly	Phe	Ser	Thr	Lys	Lys	Gln	S50	S51	A52	L53	F54	G55	V56	E57	T58	K59	D60									
Q61	Y62	L63	L64	D65	R66	L67	L71	D72	E73	E74	K77	Y78	F79	L80	S81	S82	D83	G84	R85	T86	Y87	L88	D89	D90	E91	K92	L93	A94	K95	K96	M97	R98	R103	E104	E105	L106	V107	P108	V109	H110	L116	F117	D118	I119	D120	R121	W122	T123	I124	T125	D126	F127	E128	L129



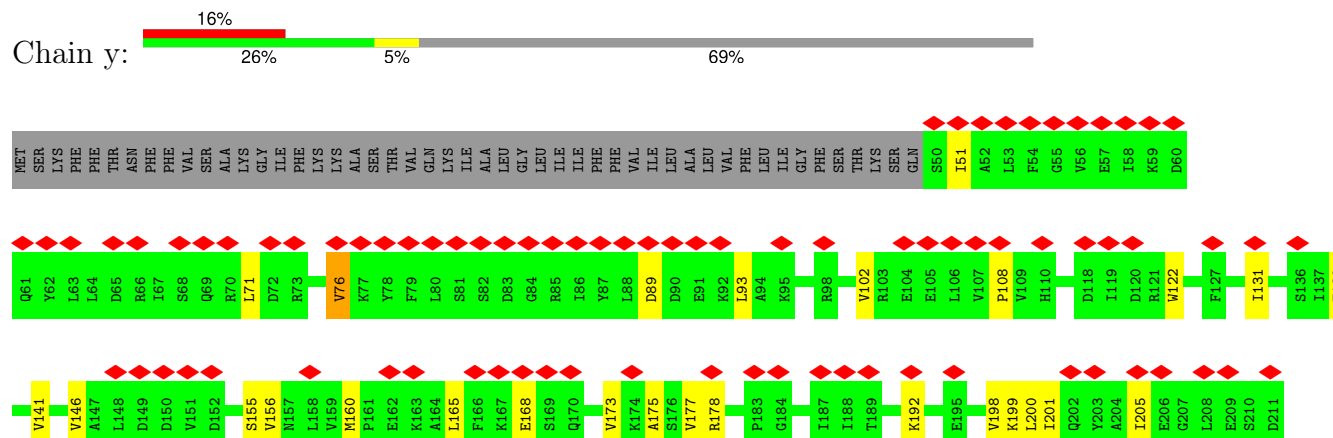
● Molecule 1: Flagellar M-ring protein



Chain x:

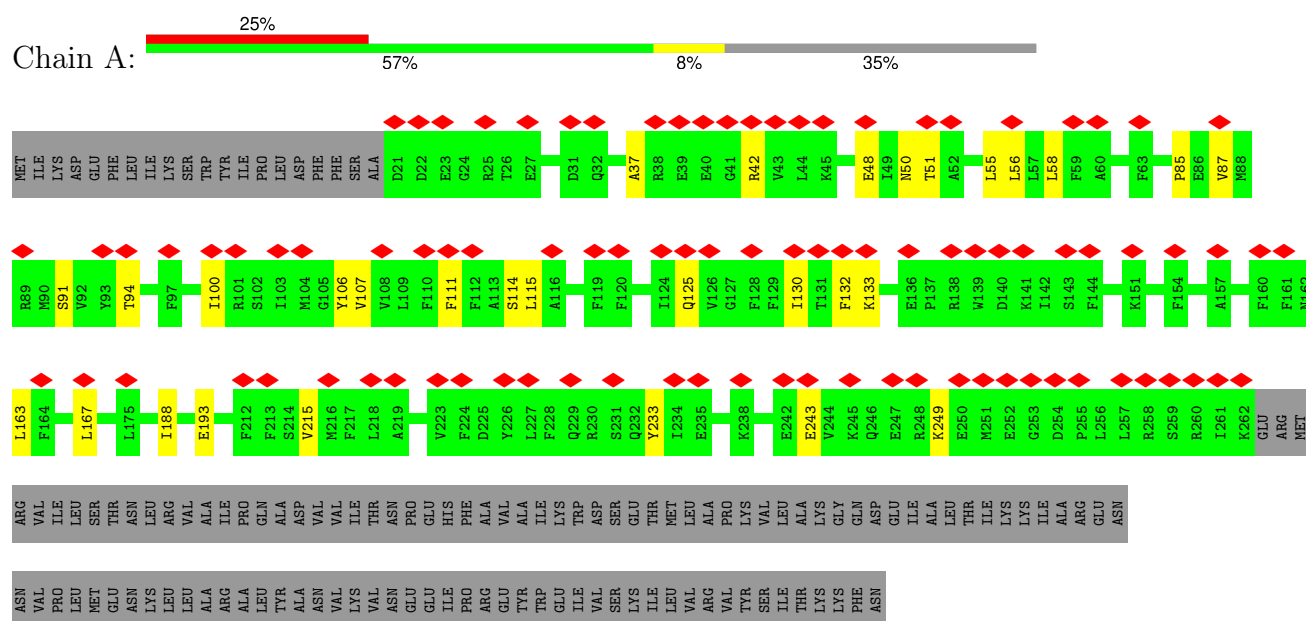


Chain y:

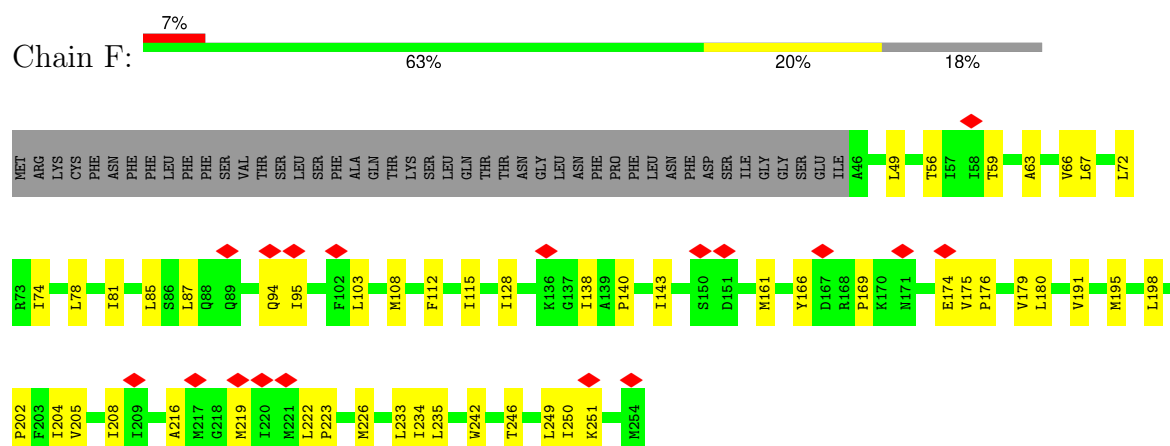




• Molecule 2: Flagellar biosynthetic protein FlhB

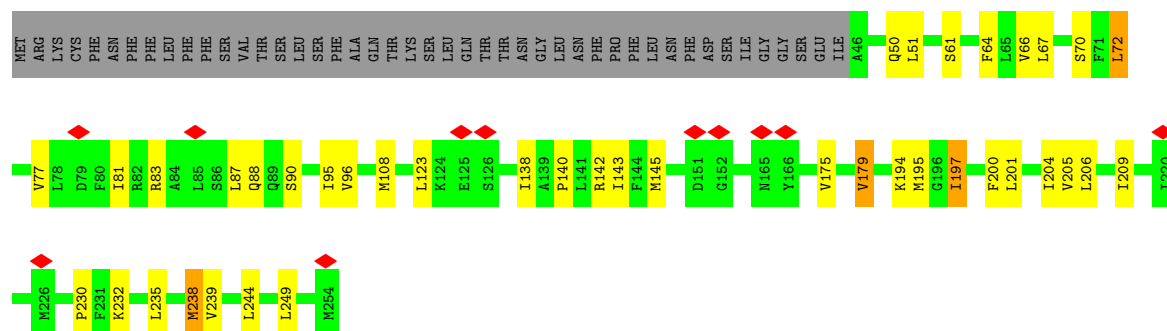


• Molecule 3: Flagellar biosynthetic protein FlhP



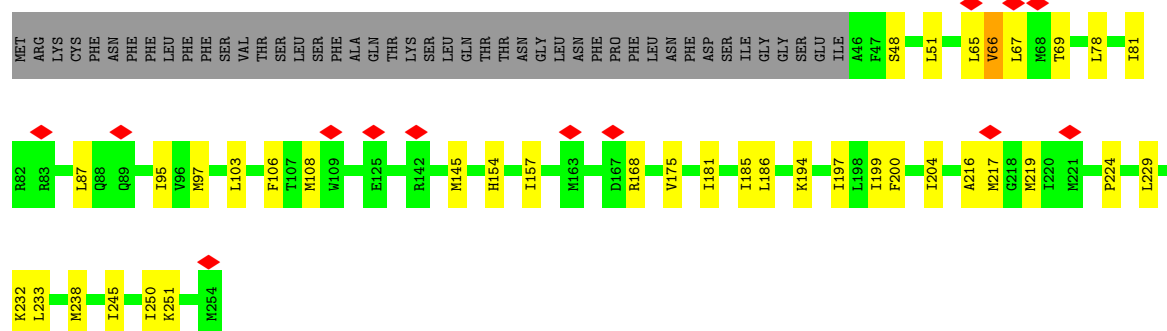
- Molecule 3: Flagellar biosynthetic protein FlIP

Chain G: 



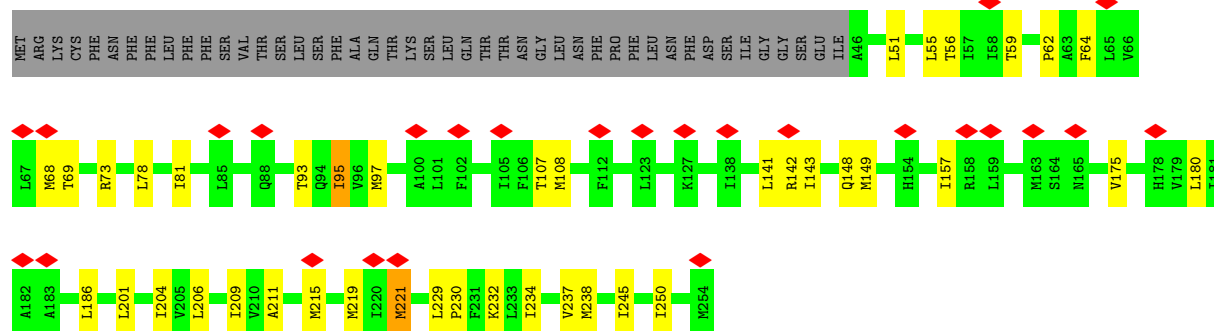
- Molecule 3: Flagellar biosynthetic protein FlIP

Chain H: 



- Molecule 3: Flagellar biosynthetic protein FlIP

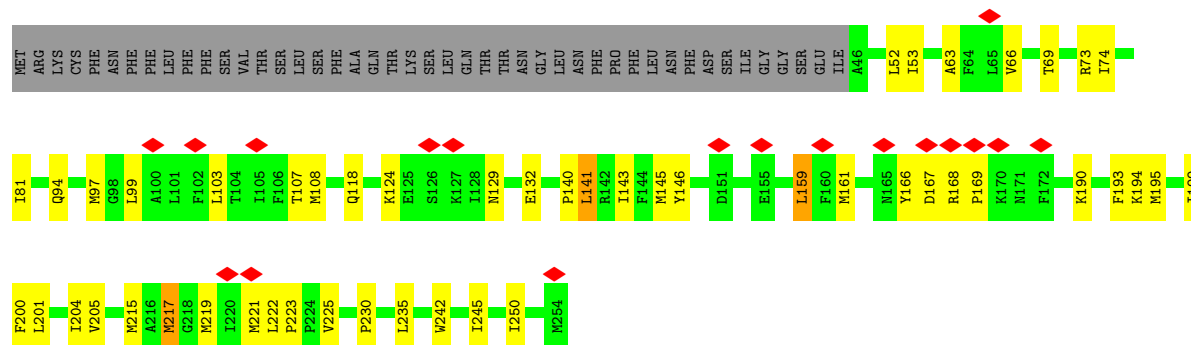
Chain I: 



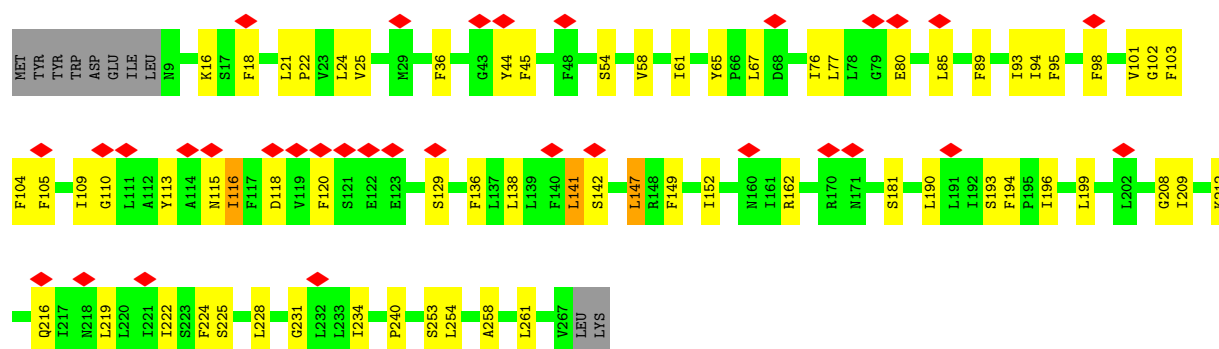
- Molecule 3: Flagellar biosynthetic protein FlIP

Chain J: 

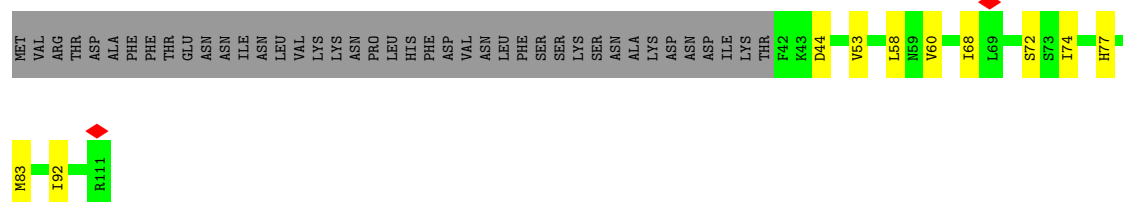




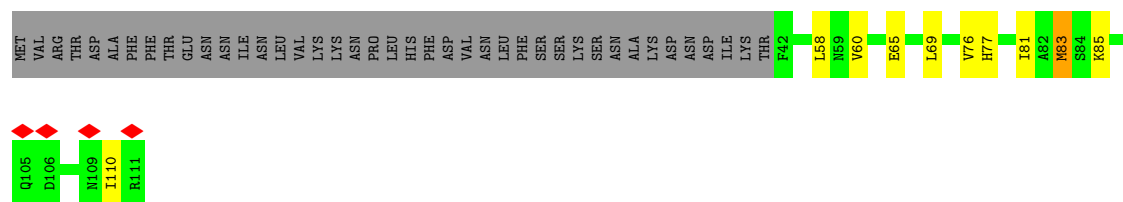
• Molecule 4: Flagellar biosynthetic protein FliR



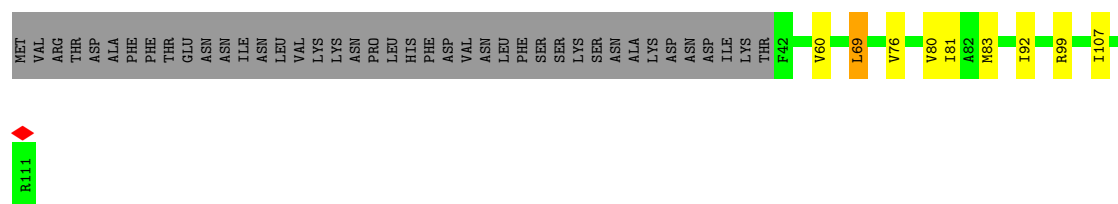
• Molecule 5: Flagellar hook-basal body complex protein FliE



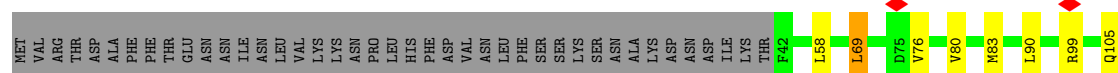
• Molecule 5: Flagellar hook-basal body complex protein FliE



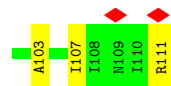
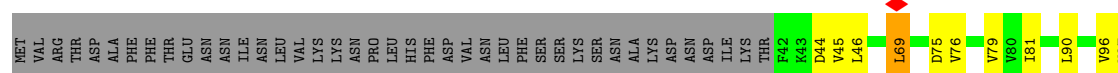
• Molecule 5: Flagellar hook-basal body complex protein FliE



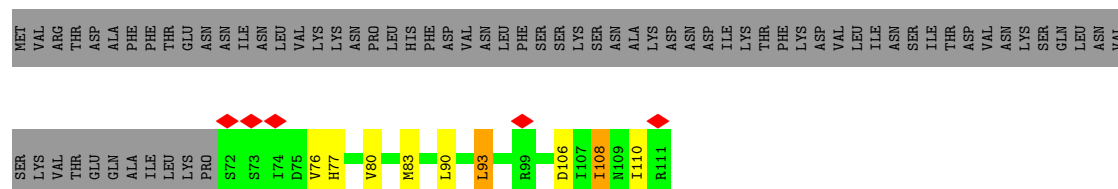
- Molecule 5: Flagellar hook-basal body complex protein FliE



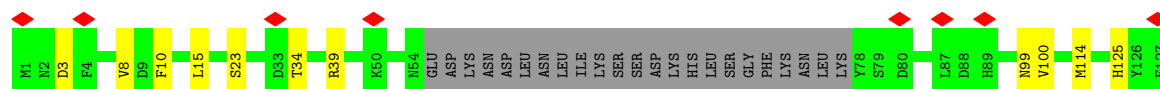
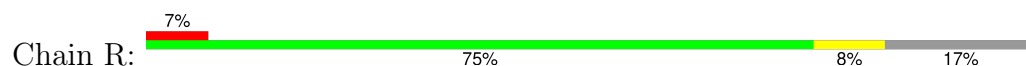
- Molecule 5: Flagellar hook-basal body complex protein FliE



- Molecule 5: Flagellar hook-basal body complex protein FliE

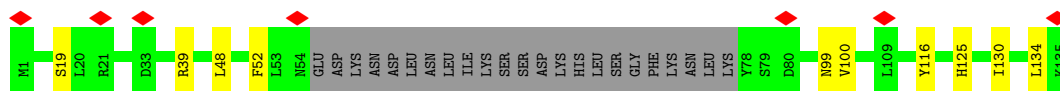
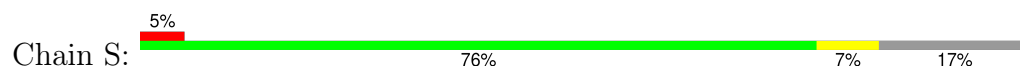


- Molecule 6: Flagellar basal body rod protein FlgB

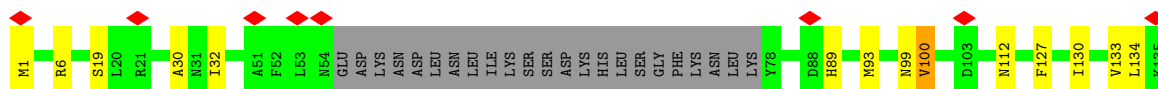




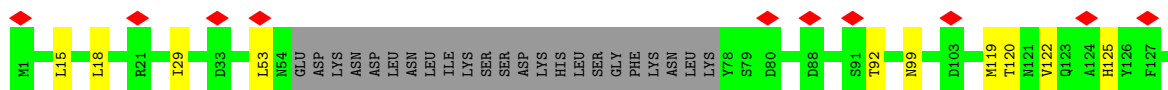
- Molecule 6: Flagellar basal body rod protein FlgB



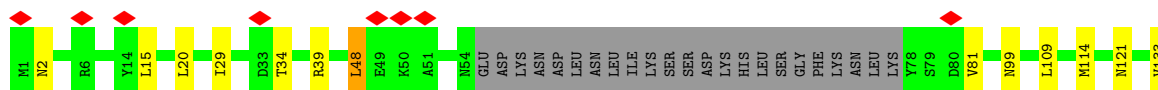
- Molecule 6: Flagellar basal body rod protein FlgB



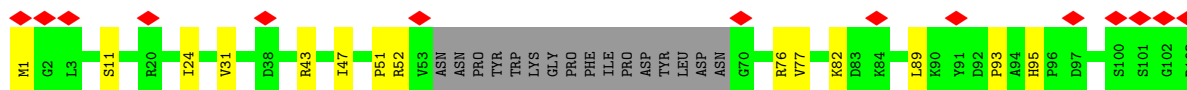
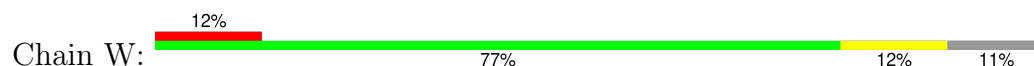
- Molecule 6: Flagellar basal body rod protein FlgB



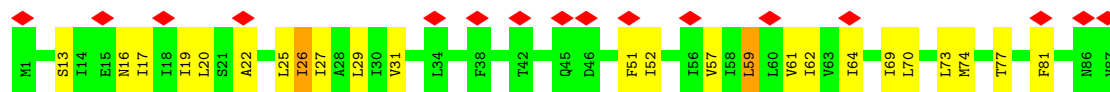
- Molecule 6: Flagellar basal body rod protein FlgB



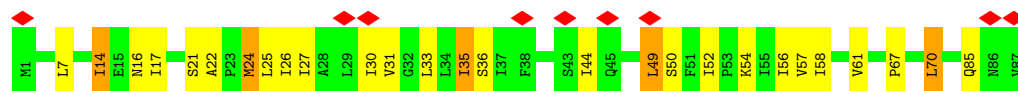
- Molecule 7: Flagellar basal-body rod protein FlgC



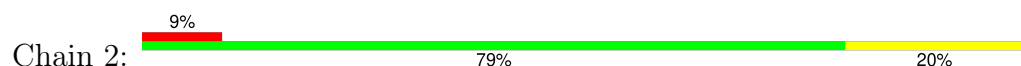




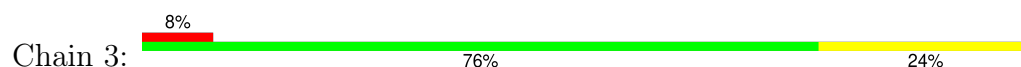
- Molecule 8: Flagellar biosynthetic protein FliQ



- Molecule 8: Flagellar biosynthetic protein FliQ



- Molecule 8: Flagellar biosynthetic protein FliQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.75	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.578	Depositor
Minimum map value	-0.334	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	640.63995, 640.63995, 640.63995	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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	c	0.17	0/1418	0.45	0/1924
1	d	0.17	0/1403	0.44	0/1906
1	e	0.17	0/1411	0.44	0/1915
1	f	0.17	0/1409	0.44	0/1909
1	g	0.16	0/1400	0.48	0/1898
1	h	0.17	0/1393	0.46	0/1891
1	i	0.17	0/1412	0.46	0/1915
1	j	0.18	0/1407	0.48	0/1909
1	k	0.17	0/1408	0.50	2/1911 (0.1%)
1	l	0.17	0/1406	0.47	0/1910
1	m	0.16	0/1418	0.43	0/1923
1	n	0.17	0/1395	0.45	0/1896
1	o	0.16	0/1408	0.43	0/1912
1	p	0.17	0/1405	0.42	0/1908
1	q	0.17	0/1411	0.45	1/1914 (0.1%)
1	r	0.16	0/1422	0.44	0/1928
1	s	0.17	0/1422	0.43	0/1928
1	t	0.16	0/1411	0.45	0/1915
1	u	0.15	0/1366	0.41	0/1853
1	v	0.15	0/1368	0.45	0/1855
1	w	0.16	0/1403	0.46	0/1906
1	x	0.16	0/1392	0.45	0/1892
1	y	0.16	0/1414	0.47	1/1919 (0.1%)
2	A	0.16	0/2033	0.37	0/2734
3	F	0.20	0/1706	0.42	0/2313
3	G	0.20	0/1696	0.43	0/2300
3	H	0.20	0/1697	0.40	0/2300
3	I	0.19	0/1706	0.44	0/2312
3	J	0.19	0/1717	0.40	0/2325
4	K	0.18	0/2135	0.40	0/2892
5	L	0.16	0/545	0.36	0/734
5	M	0.16	0/545	0.34	0/734
5	N	0.16	0/545	0.33	0/734
5	O	0.16	0/532	0.34	0/718

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	P	0.15	0/545	0.35	0/734
5	Q	0.15	0/309	0.32	0/414
6	R	0.17	0/936	0.33	0/1259
6	S	0.15	0/936	0.33	0/1259
6	T	0.16	0/936	0.31	0/1259
6	U	0.16	0/936	0.36	0/1259
6	V	0.16	0/936	0.33	0/1259
7	W	0.16	0/1043	0.33	0/1405
7	X	0.16	0/1175	0.34	0/1593
7	Y	0.15	0/1047	0.35	0/1411
7	Z	0.15	0/1191	0.34	0/1612
7	a	0.15	0/1191	0.35	0/1612
7	b	0.15	0/1191	0.33	0/1612
8	1	0.19	0/694	0.37	0/946
8	2	0.18	0/704	0.40	0/957
8	3	0.19	0/704	0.37	0/957
8	z	0.18	0/690	0.37	0/941
All	All	0.17	0/62323	0.42	4/84422 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	k	170	GLN	CA-C-N	6.57	129.81	120.49
1	k	170	GLN	C-N-CA	6.57	129.81	120.49
1	q	187	ILE	N-CA-C	-5.70	108.29	113.71
1	y	168	GLU	N-CA-C	-5.20	107.95	114.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	1397	0	1402	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	1383	0	1378	19	0
1	e	1391	0	1395	19	0
1	f	1390	0	1403	18	0
1	g	1381	0	1390	14	0
1	h	1374	0	1373	17	0
1	i	1392	0	1397	13	0
1	j	1387	0	1396	19	0
1	k	1388	0	1386	23	0
1	l	1385	0	1381	10	0
1	m	1397	0	1409	14	0
1	n	1375	0	1370	17	0
1	o	1387	0	1385	15	0
1	p	1385	0	1384	24	0
1	q	1391	0	1400	24	0
1	r	1401	0	1413	17	0
1	s	1401	0	1413	18	0
1	t	1391	0	1395	25	0
1	u	1347	0	1352	24	0
1	v	1349	0	1360	16	0
1	w	1383	0	1378	15	0
1	x	1372	0	1361	21	0
1	y	1393	0	1398	17	0
2	A	1988	0	2043	16	0
3	F	1665	0	1752	36	0
3	G	1656	0	1740	28	0
3	H	1657	0	1747	30	0
3	I	1666	0	1755	31	0
3	J	1676	0	1773	31	0
4	K	2083	0	2194	45	0
5	L	542	0	579	8	0
5	M	542	0	579	4	0
5	N	542	0	579	7	0
5	O	530	0	561	10	0
5	P	542	0	579	9	0
5	Q	308	0	327	6	0
6	R	920	0	896	6	0
6	S	920	0	896	6	0
6	T	920	0	896	9	0
6	U	920	0	896	14	0
6	V	920	0	896	8	0
7	W	1030	0	1055	11	0
7	X	1153	0	1150	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Y	1034	0	1058	9	0
7	Z	1169	0	1178	7	0
7	a	1169	0	1178	11	0
7	b	1169	0	1178	5	0
8	1	682	0	749	19	0
8	2	692	0	771	13	0
8	3	692	0	771	18	0
8	z	678	0	743	18	0
All	All	61305	0	62438	669	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 5.

The worst 5 of 669 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:107:VAL:HG22	1:q:69:GLN:HE22	1.52	0.75
1:m:80:LEU:H	1:m:86:ILE:HG23	1.51	0.75
8:1:27:ILE:HG21	8:1:61:VAL:HG21	1.71	0.72
8:2:27:ILE:HG21	8:2:61:VAL:HG21	1.72	0.71
3:J:168:ARG:HE	3:J:169:PRO:HD2	1.57	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	177/569 (31%)	164 (93%)	12 (7%)	1 (1%)	21	55
1	d	177/569 (31%)	160 (90%)	16 (9%)	1 (1%)	21	55
1	e	177/569 (31%)	161 (91%)	16 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	174/569 (31%)	160 (92%)	13 (8%)	1 (1%)	21	55
1	g	173/569 (30%)	162 (94%)	11 (6%)	0	100	100
1	h	174/569 (31%)	158 (91%)	15 (9%)	1 (1%)	21	55
1	i	177/569 (31%)	164 (93%)	13 (7%)	0	100	100
1	j	177/569 (31%)	159 (90%)	18 (10%)	0	100	100
1	k	177/569 (31%)	158 (89%)	19 (11%)	0	100	100
1	l	177/569 (31%)	163 (92%)	12 (7%)	2 (1%)	11	43
1	m	177/569 (31%)	165 (93%)	12 (7%)	0	100	100
1	n	177/569 (31%)	161 (91%)	16 (9%)	0	100	100
1	o	177/569 (31%)	166 (94%)	10 (6%)	1 (1%)	21	55
1	p	177/569 (31%)	161 (91%)	16 (9%)	0	100	100
1	q	177/569 (31%)	162 (92%)	15 (8%)	0	100	100
1	r	177/569 (31%)	160 (90%)	17 (10%)	0	100	100
1	s	177/569 (31%)	164 (93%)	13 (7%)	0	100	100
1	t	177/569 (31%)	167 (94%)	8 (4%)	2 (1%)	11	43
1	u	169/569 (30%)	160 (95%)	8 (5%)	1 (1%)	21	55
1	v	169/569 (30%)	159 (94%)	10 (6%)	0	100	100
1	w	177/569 (31%)	162 (92%)	14 (8%)	1 (1%)	21	55
1	x	177/569 (31%)	162 (92%)	13 (7%)	2 (1%)	11	43
1	y	177/569 (31%)	162 (92%)	15 (8%)	0	100	100
2	A	240/372 (64%)	231 (96%)	8 (3%)	1 (0%)	30	64
3	F	207/254 (82%)	205 (99%)	2 (1%)	0	100	100
3	G	207/254 (82%)	199 (96%)	8 (4%)	0	100	100
3	H	207/254 (82%)	202 (98%)	5 (2%)	0	100	100
3	I	207/254 (82%)	201 (97%)	6 (3%)	0	100	100
3	J	207/254 (82%)	206 (100%)	1 (0%)	0	100	100
4	K	257/269 (96%)	246 (96%)	11 (4%)	0	100	100
5	L	68/111 (61%)	66 (97%)	2 (3%)	0	100	100
5	M	68/111 (61%)	68 (100%)	0	0	100	100
5	N	68/111 (61%)	68 (100%)	0	0	100	100
5	O	68/111 (61%)	68 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	68/111 (61%)	66 (97%)	2 (3%)	0	100	100
5	Q	38/111 (34%)	38 (100%)	0	0	100	100
6	R	108/135 (80%)	108 (100%)	0	0	100	100
6	S	108/135 (80%)	108 (100%)	0	0	100	100
6	T	108/135 (80%)	108 (100%)	0	0	100	100
6	U	108/135 (80%)	106 (98%)	2 (2%)	0	100	100
6	V	108/135 (80%)	103 (95%)	5 (5%)	0	100	100
7	W	132/152 (87%)	132 (100%)	0	0	100	100
7	X	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
7	Y	132/152 (87%)	130 (98%)	2 (2%)	0	100	100
7	Z	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
7	a	150/152 (99%)	148 (99%)	2 (1%)	0	100	100
7	b	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
8	1	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
8	2	85/87 (98%)	85 (100%)	0	0	100	100
8	3	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
8	z	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
All	All	7699/17599 (44%)	7301 (95%)	384 (5%)	14 (0%)	44	74

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	h	76	VAL
1	l	109	VAL
1	c	90	ASP
1	f	110	HIS
1	d	110	HIS

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	c	151/506 (30%)	142 (94%)	9 (6%)	17	44
1	d	148/506 (29%)	141 (95%)	7 (5%)	23	48
1	e	150/506 (30%)	148 (99%)	2 (1%)	61	71
1	f	151/506 (30%)	142 (94%)	9 (6%)	17	44
1	g	150/506 (30%)	145 (97%)	5 (3%)	33	56
1	h	147/506 (29%)	137 (93%)	10 (7%)	14	41
1	i	150/506 (30%)	147 (98%)	3 (2%)	48	65
1	j	149/506 (29%)	143 (96%)	6 (4%)	28	51
1	k	149/506 (29%)	145 (97%)	4 (3%)	39	59
1	l	148/506 (29%)	142 (96%)	6 (4%)	27	51
1	m	151/506 (30%)	147 (97%)	4 (3%)	40	60
1	n	146/506 (29%)	143 (98%)	3 (2%)	47	64
1	o	149/506 (29%)	147 (99%)	2 (1%)	61	71
1	p	149/506 (29%)	140 (94%)	9 (6%)	17	44
1	q	150/506 (30%)	144 (96%)	6 (4%)	28	51
1	r	152/506 (30%)	143 (94%)	9 (6%)	18	44
1	s	152/506 (30%)	146 (96%)	6 (4%)	28	52
1	t	150/506 (30%)	140 (93%)	10 (7%)	15	41
1	u	146/506 (29%)	138 (94%)	8 (6%)	19	46
1	v	146/506 (29%)	141 (97%)	5 (3%)	32	55
1	w	148/506 (29%)	143 (97%)	5 (3%)	32	55
1	x	145/506 (29%)	137 (94%)	8 (6%)	19	46
1	y	150/506 (30%)	143 (95%)	7 (5%)	23	48
2	A	217/335 (65%)	209 (96%)	8 (4%)	30	53
3	F	187/232 (81%)	183 (98%)	4 (2%)	47	64
3	G	185/232 (80%)	175 (95%)	10 (5%)	20	46
3	H	185/232 (80%)	183 (99%)	2 (1%)	65	73
3	I	187/232 (81%)	182 (97%)	5 (3%)	39	59
3	J	189/232 (82%)	172 (91%)	17 (9%)	9	31
4	K	236/249 (95%)	222 (94%)	14 (6%)	18	44
5	L	64/103 (62%)	60 (94%)	4 (6%)	16	42
5	M	64/103 (62%)	57 (89%)	7 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	N	64/103 (62%)	60 (94%)	4 (6%)	16	42
5	O	62/103 (60%)	58 (94%)	4 (6%)	15	42
5	P	64/103 (62%)	58 (91%)	6 (9%)	8	29
5	Q	35/103 (34%)	32 (91%)	3 (9%)	10	33
6	R	107/129 (83%)	103 (96%)	4 (4%)	30	53
6	S	107/129 (83%)	104 (97%)	3 (3%)	38	59
6	T	107/129 (83%)	105 (98%)	2 (2%)	50	66
6	U	107/129 (83%)	103 (96%)	4 (4%)	30	53
6	V	107/129 (83%)	103 (96%)	4 (4%)	30	53
7	W	115/130 (88%)	114 (99%)	1 (1%)	70	75
7	X	127/130 (98%)	125 (98%)	2 (2%)	55	68
7	Y	116/130 (89%)	114 (98%)	2 (2%)	53	67
7	Z	130/130 (100%)	127 (98%)	3 (2%)	44	63
7	a	130/130 (100%)	127 (98%)	3 (2%)	44	63
7	b	130/130 (100%)	128 (98%)	2 (2%)	57	69
8	1	78/80 (98%)	69 (88%)	9 (12%)	5	22
8	2	80/80 (100%)	75 (94%)	5 (6%)	16	42
8	3	80/80 (100%)	77 (96%)	3 (4%)	29	52
8	z	77/80 (96%)	72 (94%)	5 (6%)	15	42
All	All	6764/15745 (43%)	6481 (96%)	283 (4%)	28	50

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	3	ASP
6	T	100	VAL
7	b	149	ILE
1	s	107	VAL
1	s	51	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
6	S	36	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	b	45	GLN
6	V	121	ASN
7	Y	95	HIS
8	1	85	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

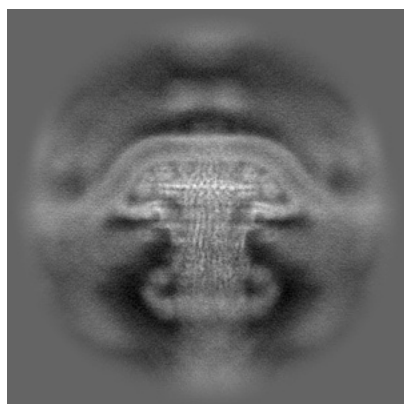
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76347. These allow visual inspection of the internal detail of the map and identification of artifacts.

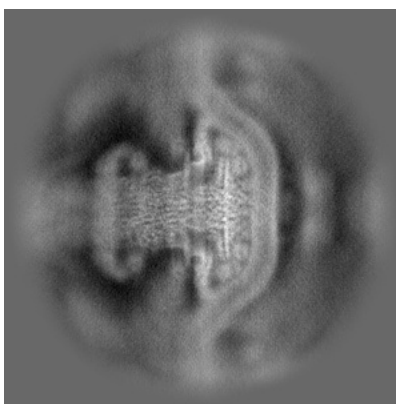
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

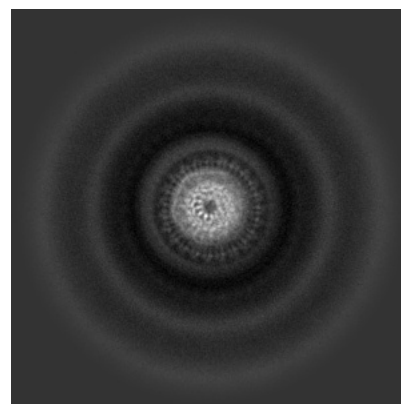
6.1.1 Primary map



X

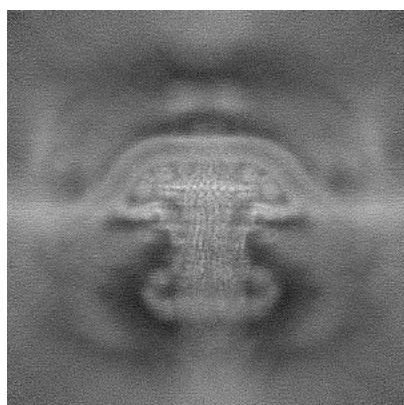


Y

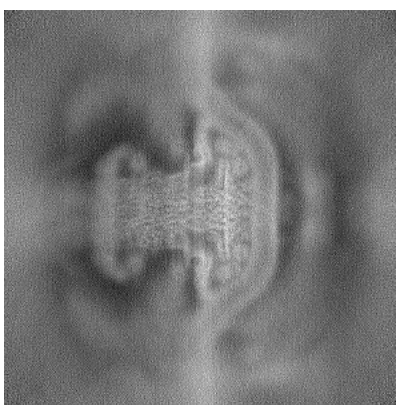


Z

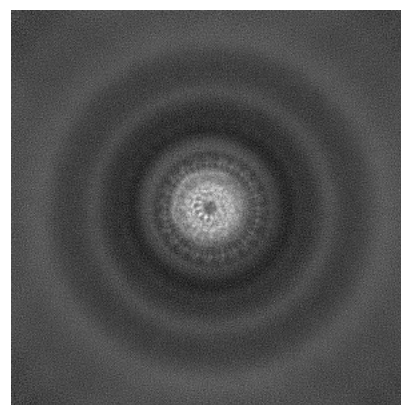
6.1.2 Raw map



X



Y

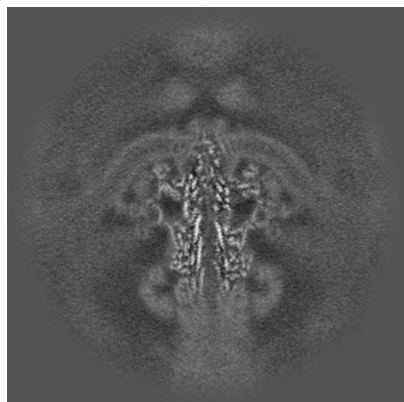


Z

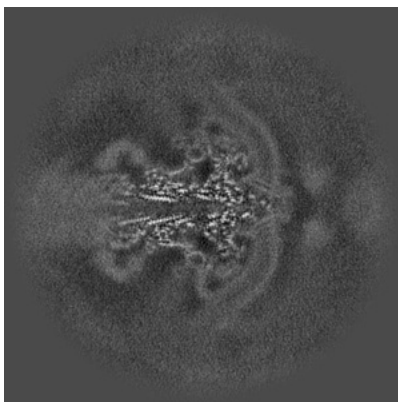
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

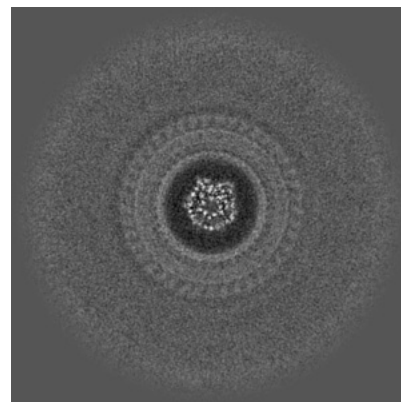
6.2.1 Primary map



X Index: 224

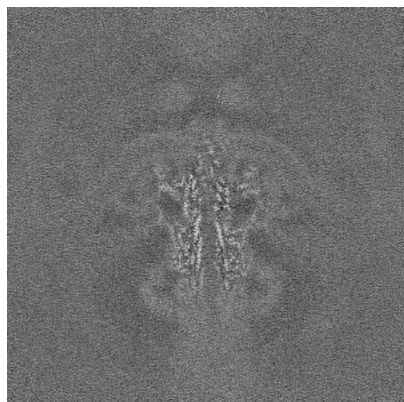


Y Index: 224

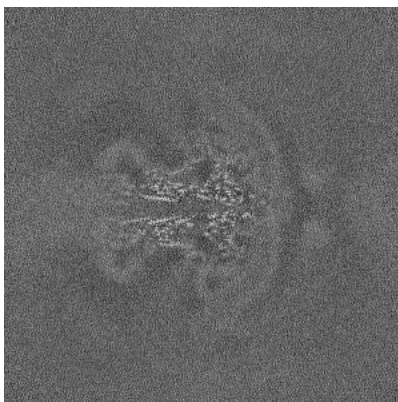


Z Index: 224

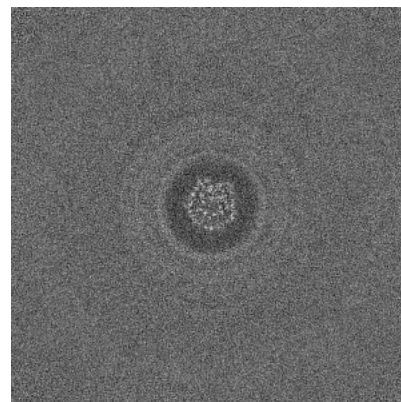
6.2.2 Raw map



X Index: 224



Y Index: 224

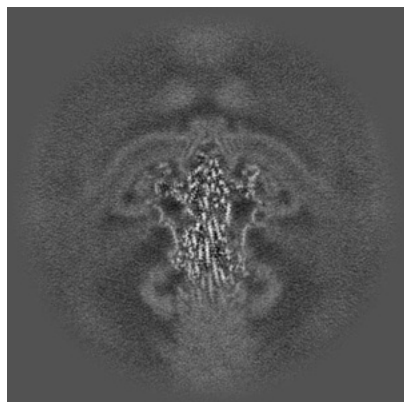


Z Index: 224

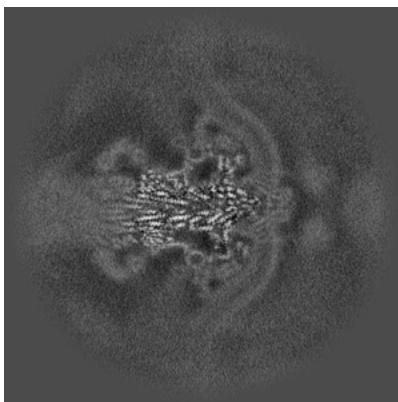
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

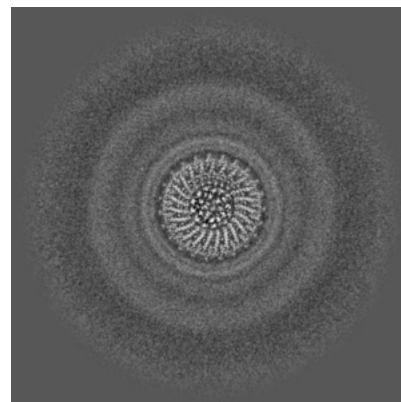
6.3.1 Primary map



X Index: 233

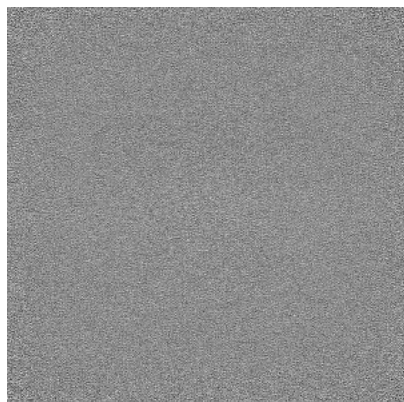


Y Index: 218

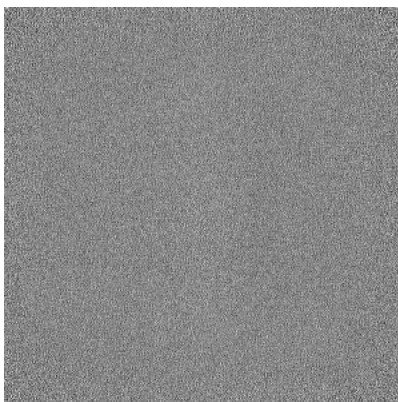


Z Index: 249

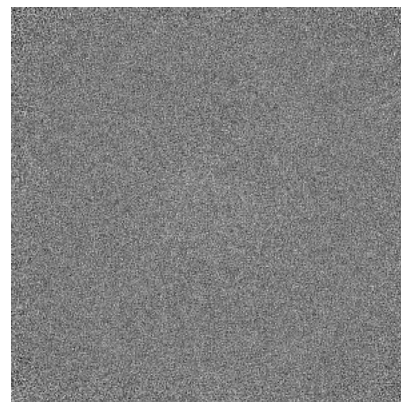
6.3.2 Raw map



X Index: 0



Y Index: 0

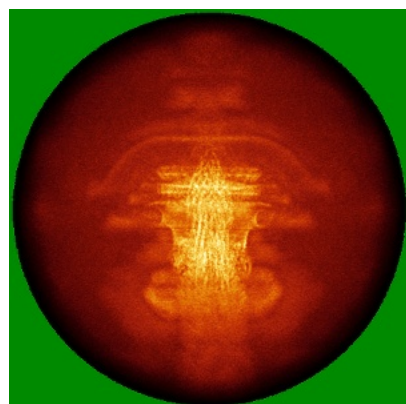


Z Index: 447

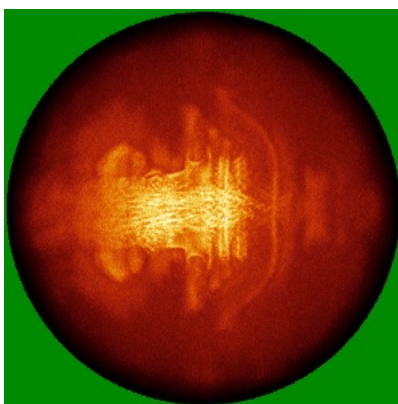
The images above show the largest variance slices of the map in three orthogonal directions.

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

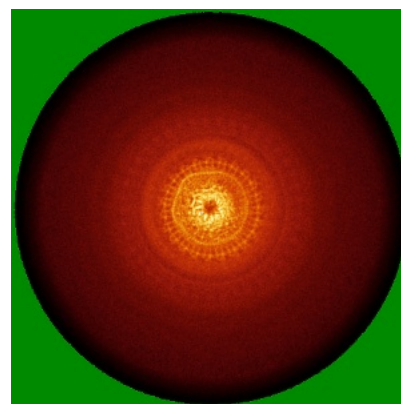
6.4.1 Primary map



X

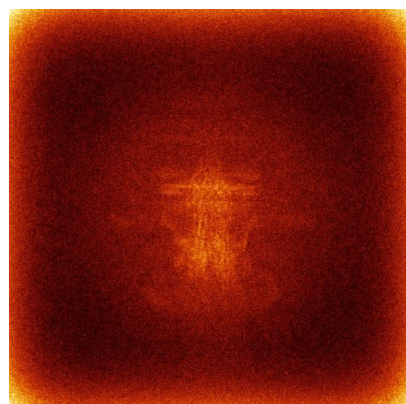


Y

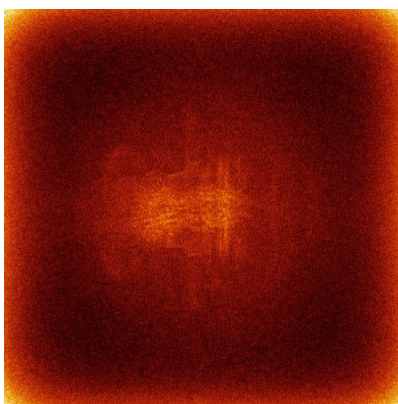


Z

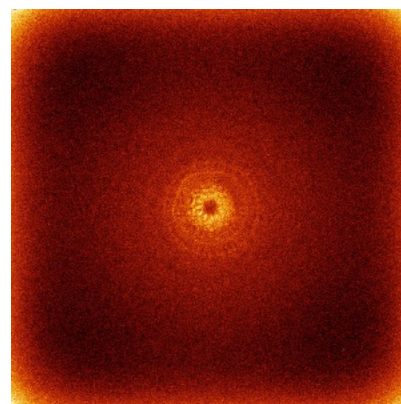
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

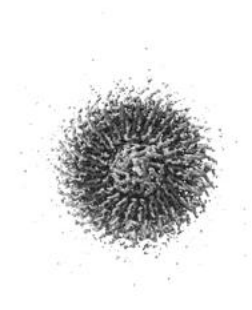
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

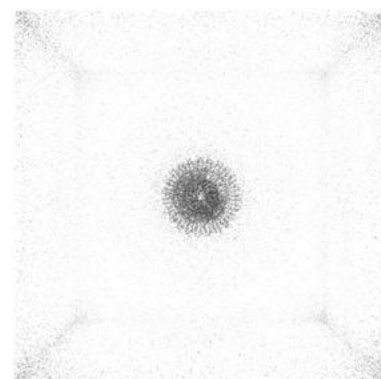
6.5.2 Raw map



X



Y



Z

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

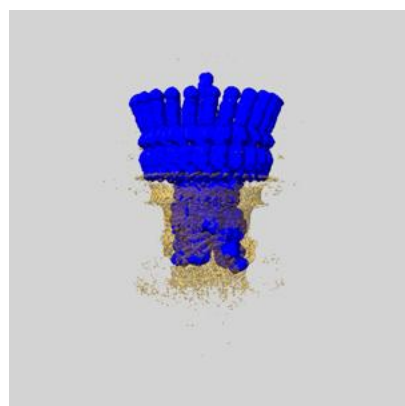
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

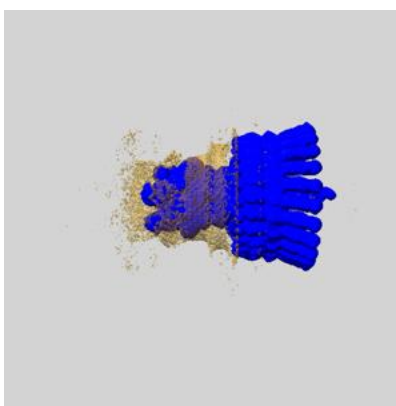
A mask typically either:

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

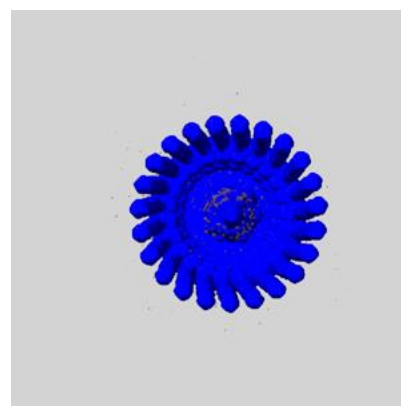
6.6.1 emd_76347_msk_1.map [i](#)



X



Y

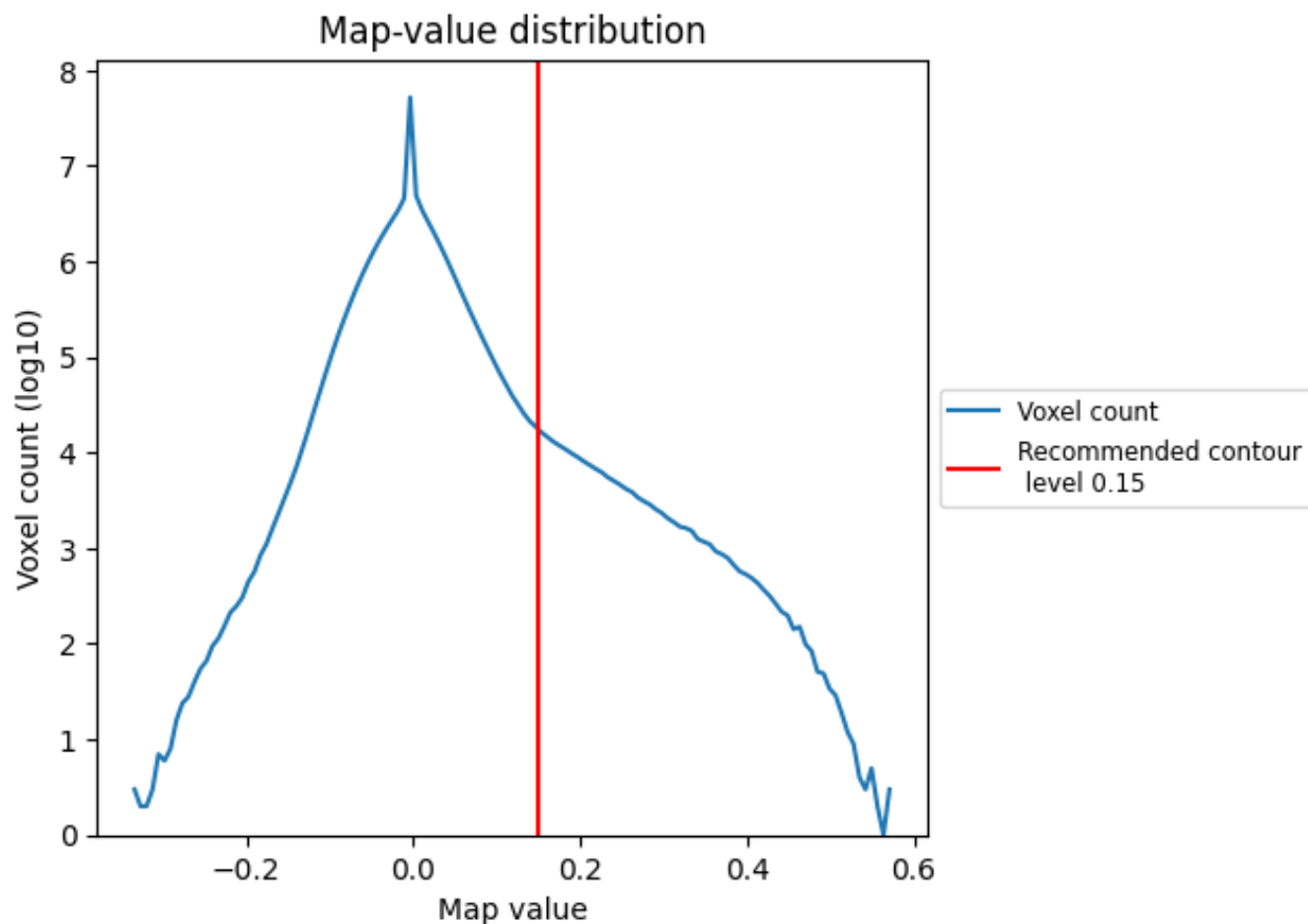


Z

7 Map analysis [i](#)

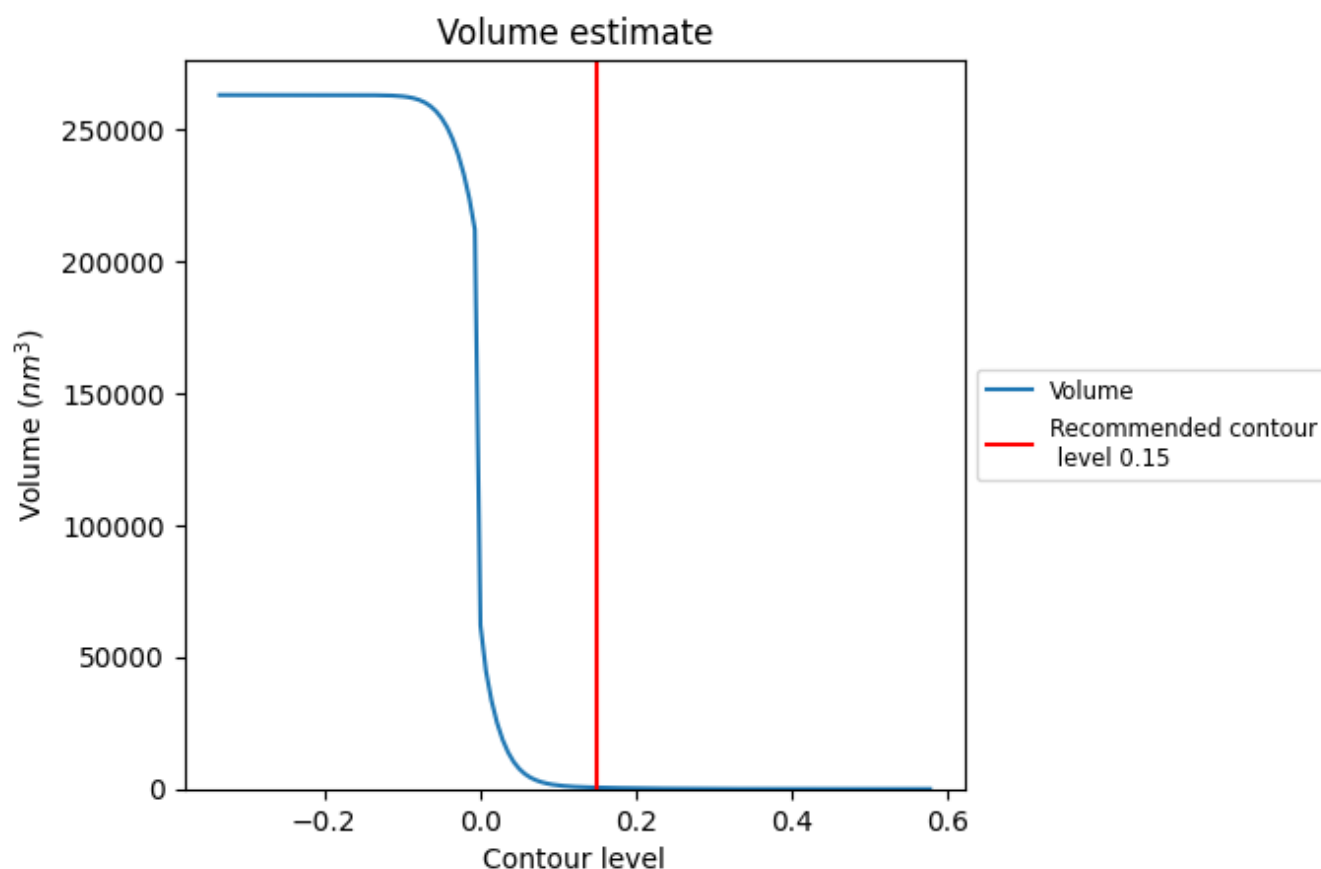
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

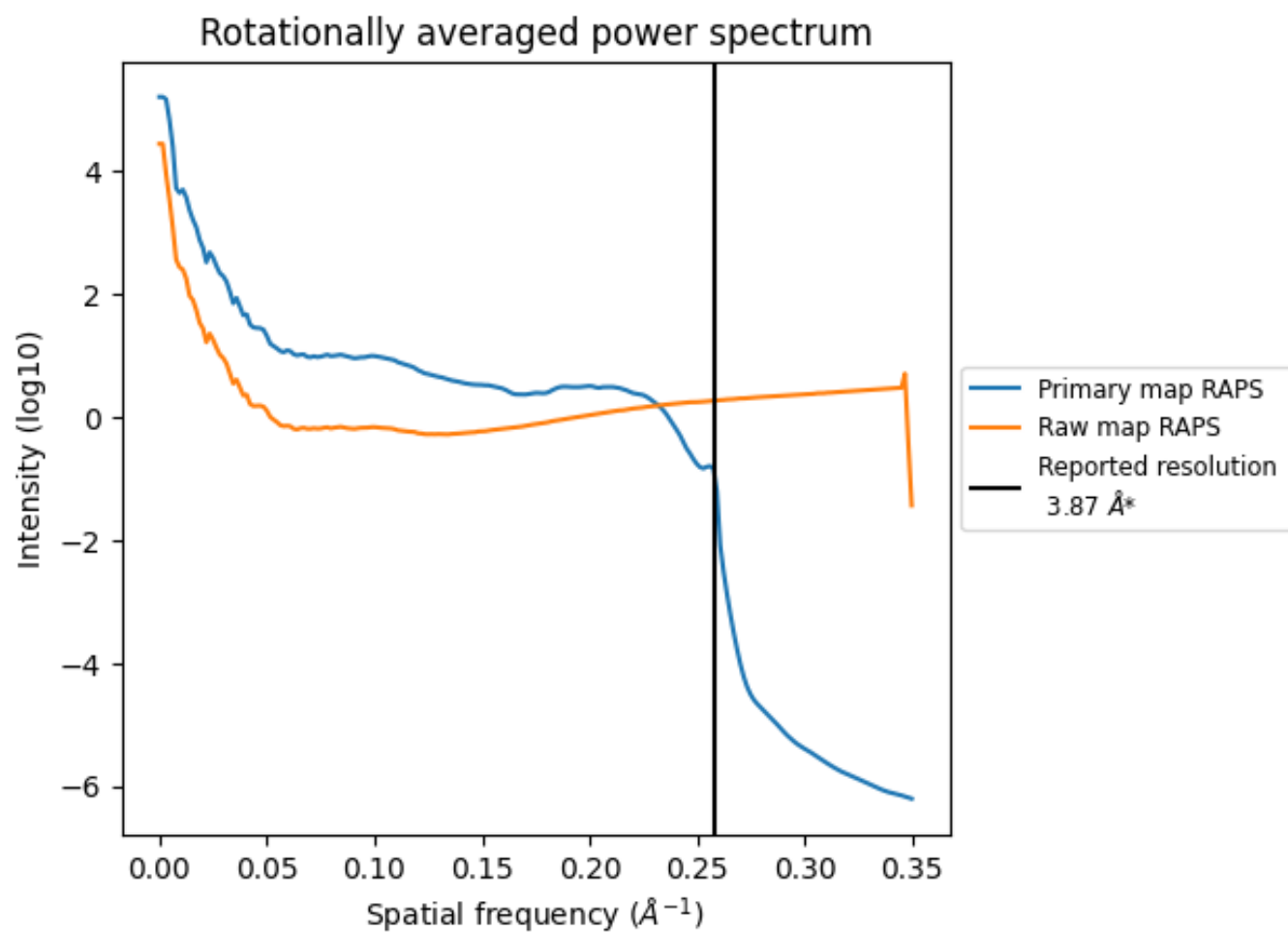
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 529 nm^3 ; this corresponds to an approximate mass of 478 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 ⓘ

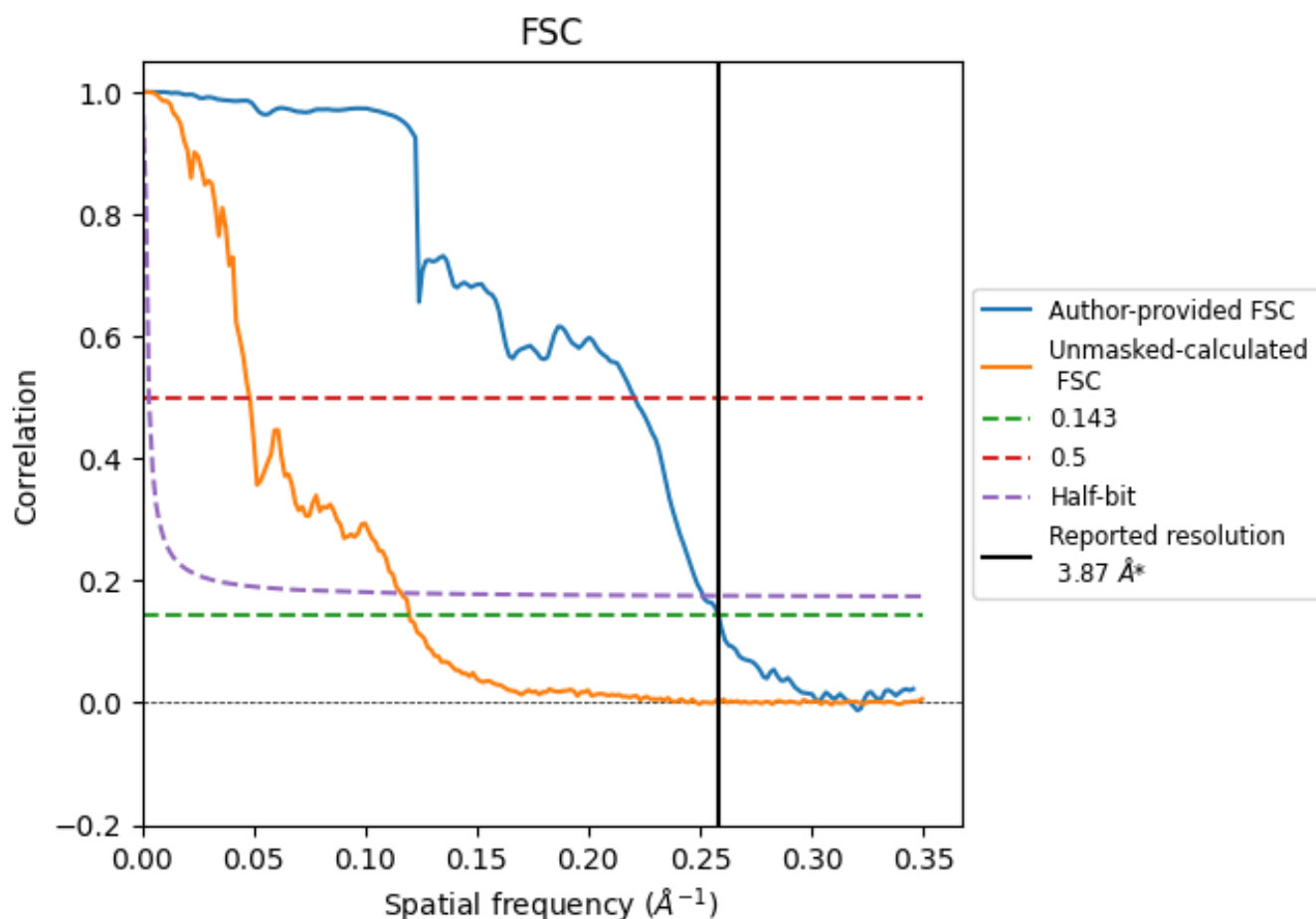


*Reported resolution corresponds to spatial frequency of 0.258 Å⁻¹

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 0.258 Å⁻¹

8.2 Resolution estimates [i](#)

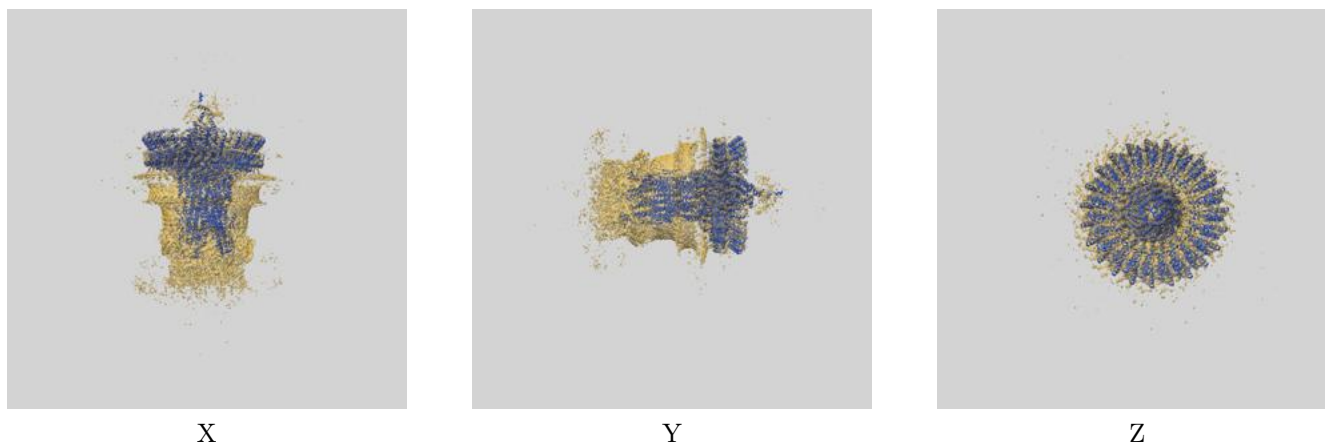
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.87	-	-
Author-provided FSC curve	3.87	4.53	3.98
Unmasked-calculated*	8.35	20.79	8.61

*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 8.35 differs from the reported value 3.87 by more than 10 %

9 Map-model fit [i](#)

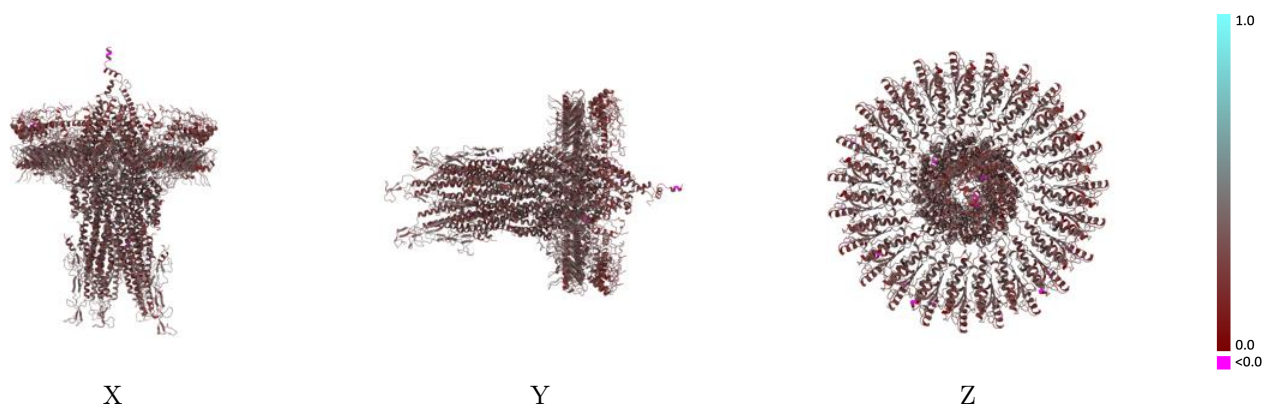
This section contains information regarding the fit between EMDB map EMD-76347 and PDB model 12DU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



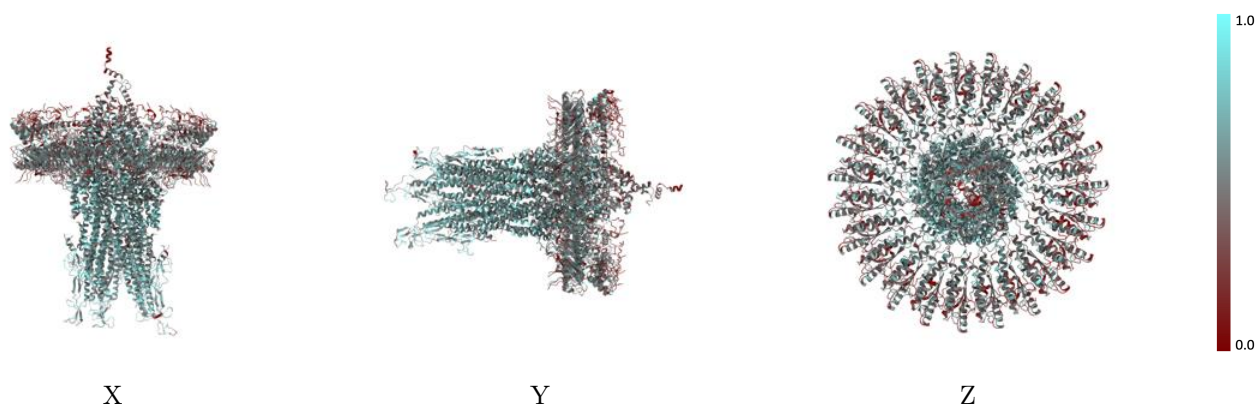
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



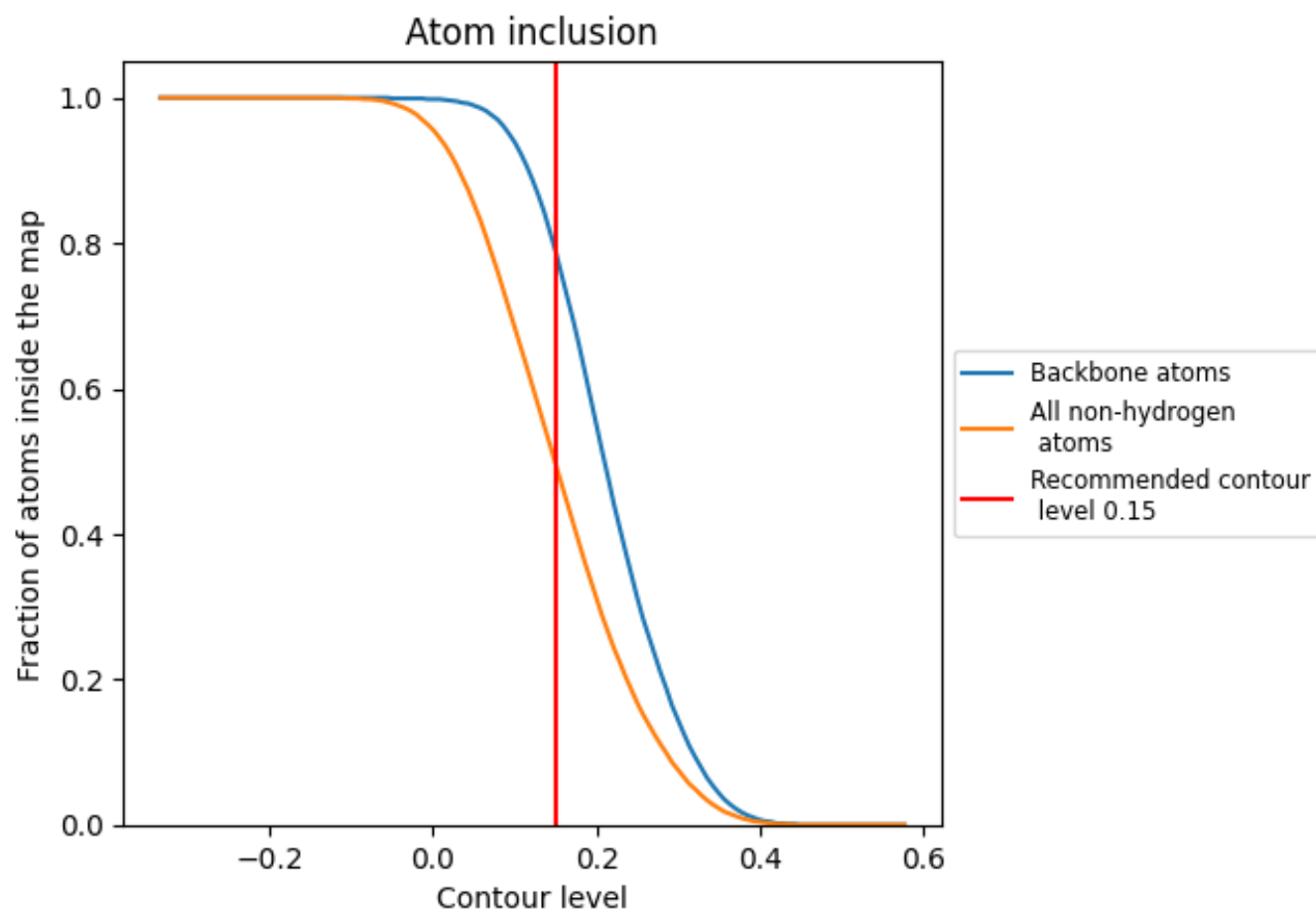
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 50% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4970	 0.3220
1	 0.5690	 0.3240
2	 0.5780	 0.3120
3	 0.5570	 0.3160
A	 0.4470	 0.2770
F	 0.6070	 0.3390
G	 0.6070	 0.3280
H	 0.6100	 0.3430
I	 0.5900	 0.3310
J	 0.5940	 0.3300
K	 0.5610	 0.3140
L	 0.6390	 0.3330
M	 0.6200	 0.3300
N	 0.6350	 0.3320
O	 0.6320	 0.3160
P	 0.6110	 0.3200
Q	 0.5480	 0.3090
R	 0.6160	 0.3330
S	 0.6320	 0.3360
T	 0.5960	 0.3380
U	 0.6100	 0.3280
V	 0.6120	 0.3320
W	 0.6040	 0.3200
X	 0.6430	 0.3540
Y	 0.5820	 0.3210
Z	 0.6300	 0.3520
a	 0.6300	 0.3520
b	 0.6240	 0.3560
c	 0.4190	 0.3230
d	 0.3900	 0.3190
e	 0.3960	 0.3210
f	 0.4210	 0.3180
g	 0.4230	 0.3190
h	 0.4040	 0.3170
i	 0.4160	 0.3160



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Chain	Atom inclusion	Q-score
j	 0.4280	 0.3190
k	 0.4410	 0.3220
l	 0.4210	 0.3220
m	 0.4120	 0.3120
n	 0.4280	 0.3160
o	 0.4400	 0.3210
p	 0.4180	 0.3260
q	 0.3880	 0.3190
r	 0.4050	 0.3090
s	 0.4110	 0.3190
t	 0.4090	 0.3150
u	 0.3830	 0.3160
v	 0.3630	 0.3100
w	 0.3880	 0.3070
x	 0.3820	 0.3050
y	 0.3970	 0.3140
z	 0.5330	 0.3010