wwPDB EM Validation Summary Report (i)

Mar 9, 2026 – 07:01 PM UTC

PDB ID	:	8WK3 / pdb_00008wk3
EMDB ID	:	EMD-37594
Title	:	Cryo-EM structure of the proximal rod-export apparatus and FlgF within the motor-hook complex in the CW state
Authors	:	Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on	:	2023-09-26
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

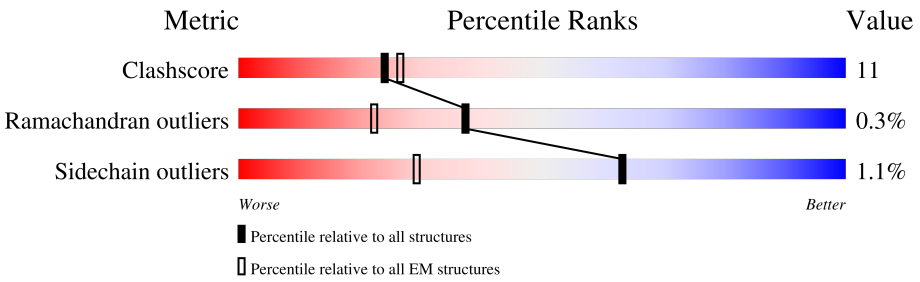
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

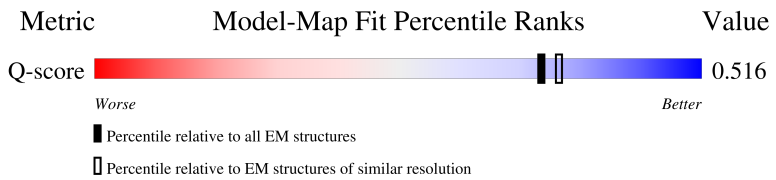
1 Overall quality at a glance (i)

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 <=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	K	104	5% 27% 12% 62%
1	L	104	59% 11% 31%
1	M	104	62% 9% 29%
1	N	104	59% 12% 29%

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Mol	Chain	Length	Quality of chain
1	O	104	56% 15% 29%
1	P	104	55% 15% 30%
2	Q	138	10% 62% 24% 14%
2	R	138	64% 13% 22%
2	S	138	57% 22% 22%
2	T	138	67% 13% 20%
2	U	138	61% 15% 23%
3	E	264	23% 65% 28%
4	F	245	10% 53% 30% 16%
4	G	245	62% 22% 15%
4	H	245	64% 20% 15%
4	I	245	6% 64% 20% 15%
4	J	245	9% 58% 25% 15%
5	A	89	34% 79% 20%
5	B	89	15% 67% 33%
5	C	89	17% 67% 33%
5	D	89	26% 64% 34%
6	b	560	98%
6	c	560	97%
6	d	560	96%
6	e	560	97%
6	f	560	96%
6	g	560	97%
6	h	560	96%
6	i	560	97%

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Mol	Chain	Length	Quality of chain
6	j	560	96%
6	k	560	97%
6	l	560	96%
7	V	134	13% 81% 18%
7	W	134	74% 25%
7	X	134	7% 78% 21%
7	Y	134	5% 77% 22%
7	Z	134	5% 71% 28%
7	a	134	9% 78% 21%
8	m	251	7% 76% 21%
8	n	251	7% 75% 24%
8	o	251	7% 79% 20%
8	p	251	14% 77% 23%
8	q	251	23% 77% 22%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 36243 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar hook-basal body complex protein FliE.

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

- Molecule 2 is a protein called Flagellar basal body rod protein FlgB.

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

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

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

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

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

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

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

- Molecule 6 is a protein called Flagellar M-ring protein.

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	j	20	133	83	23	27	0	0
			Total	C	N	O		
6	l	21	140	88	24	28	0	0

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

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

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

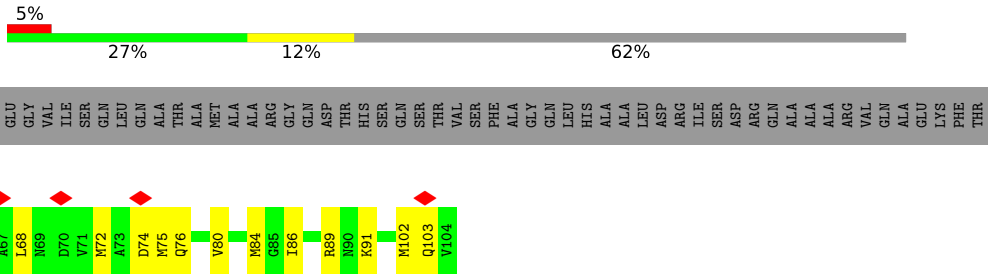
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	m	248	1804	1106	324	367	7	0	0
			Total	C	N	O	S		
8	n	249	1812	1111	325	368	8	0	0
			Total	C	N	O	S		
8	o	250	1820	1116	326	369	9	0	0
			Total	C	N	O	S		
8	p	250	1820	1116	326	369	9	0	0
			Total	C	N	O	S		
8	q	249	1812	1111	325	368	8	0	0

3 Residue-property plots (i)

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

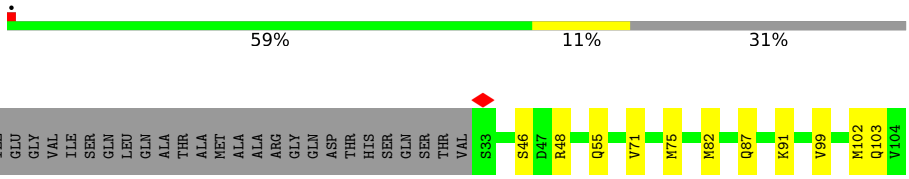
• Molecule 1: Flagellar hook-basal body complex protein FliE

Chain K:



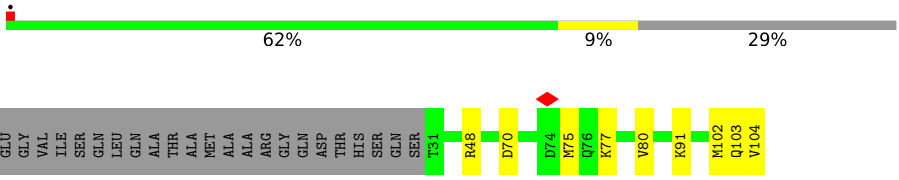
• Molecule 1: Flagellar hook-basal body complex protein FliE

Chain L:



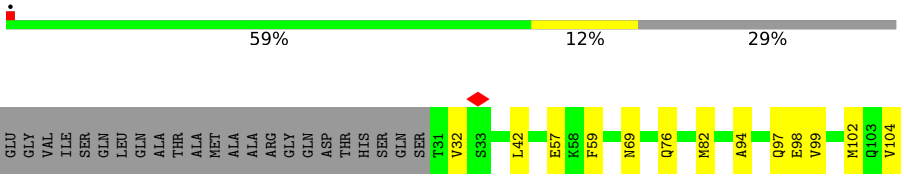
• Molecule 1: Flagellar hook-basal body complex protein FliE

Chain M:



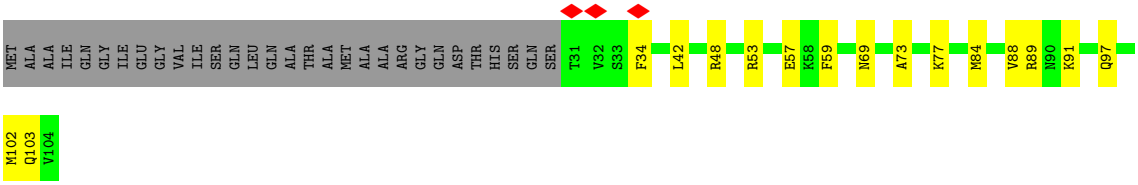
• Molecule 1: Flagellar hook-basal body complex protein FliE

Chain N:



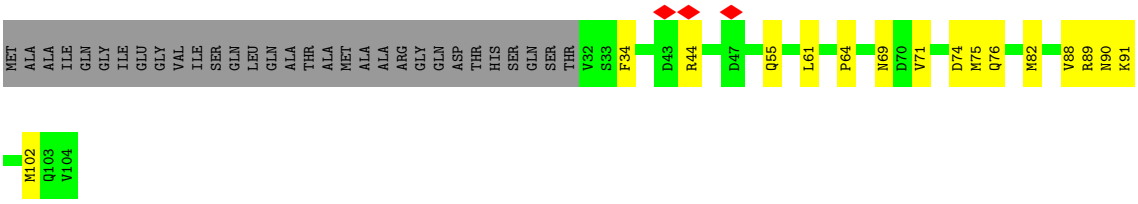
• Molecule 1: Flagellar hook-basal body complex protein FliE

Chain O:



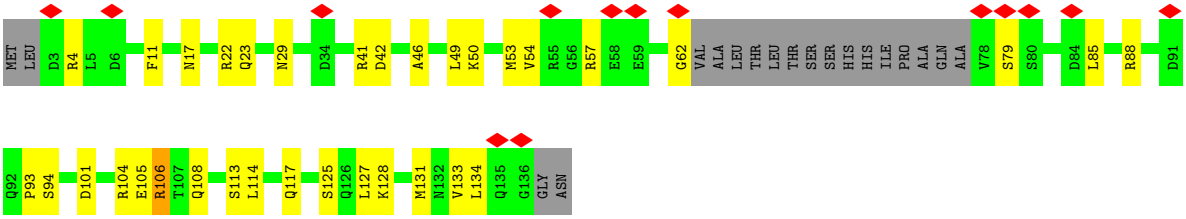
• Molecule 1: Flagellar hook-basal body complex protein FliE

Chain P:



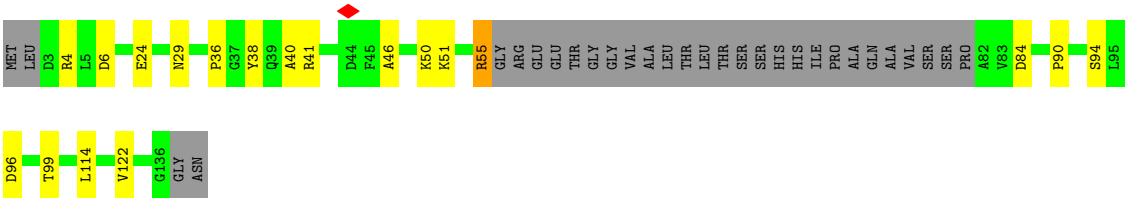
• Molecule 2: Flagellar basal body rod protein FlgB

Chain Q:



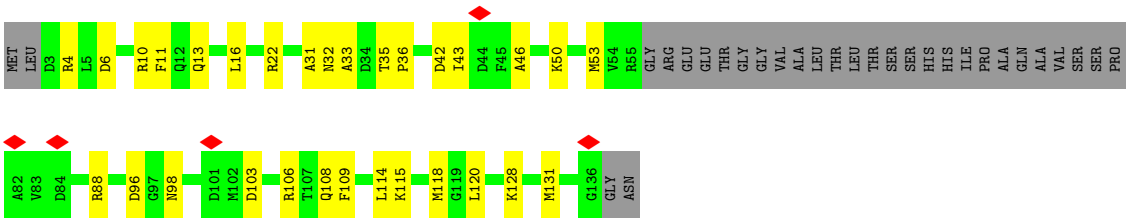
• Molecule 2: Flagellar basal body rod protein FlgB

Chain R:



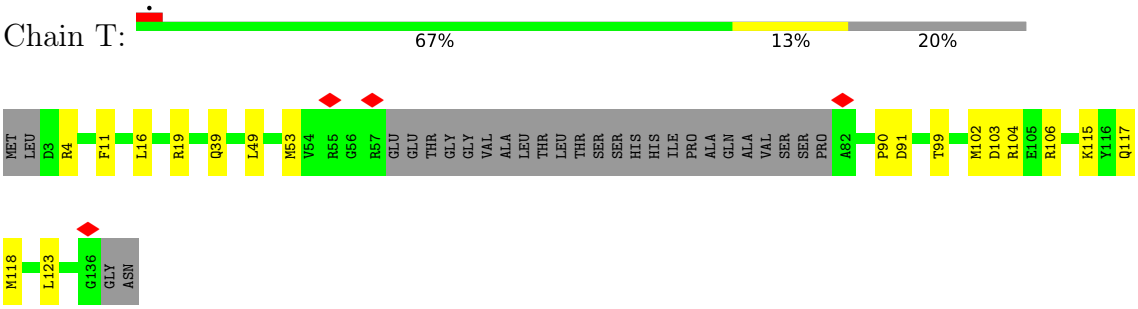
• Molecule 2: Flagellar basal body rod protein FlgB

Chain S:



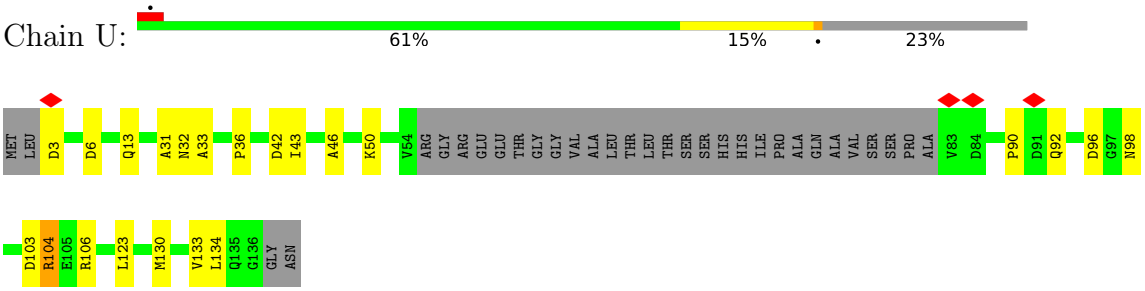
- Molecule 2: Flagellar basal body rod protein FlgB

Chain T:



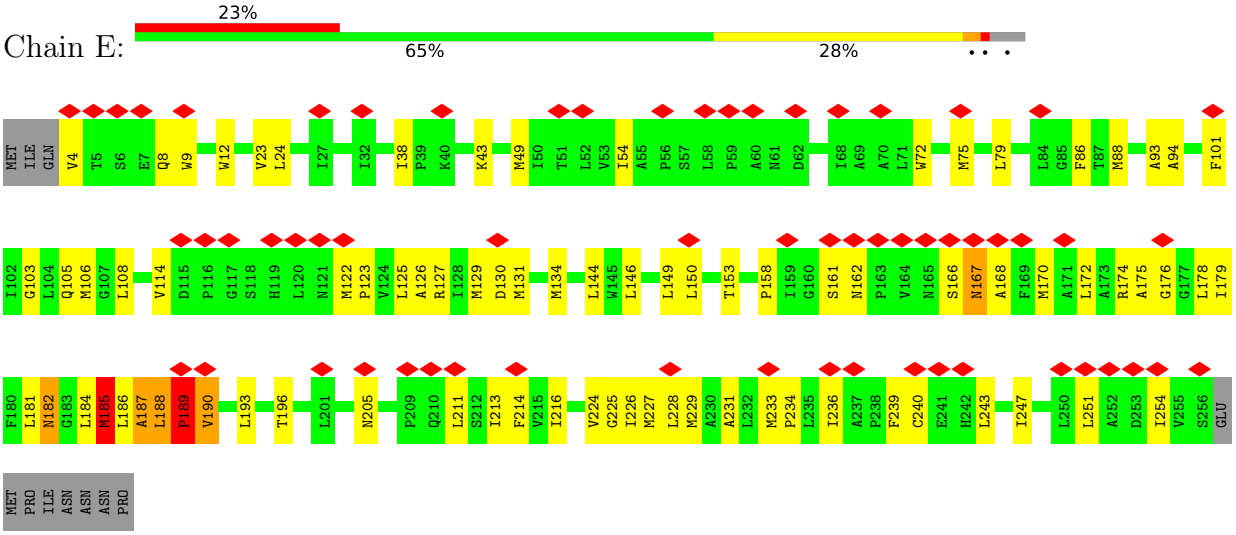
- Molecule 2: Flagellar basal body rod protein FlgB

Chain U:



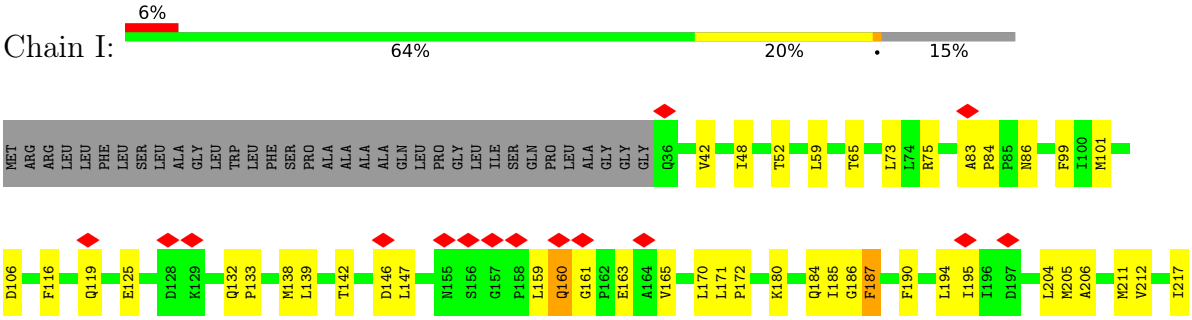
- Molecule 3: Flagellar biosynthetic protein FliR

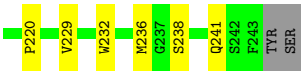
Chain E:



- Molecule 4: Flagellar biosynthetic protein FliP

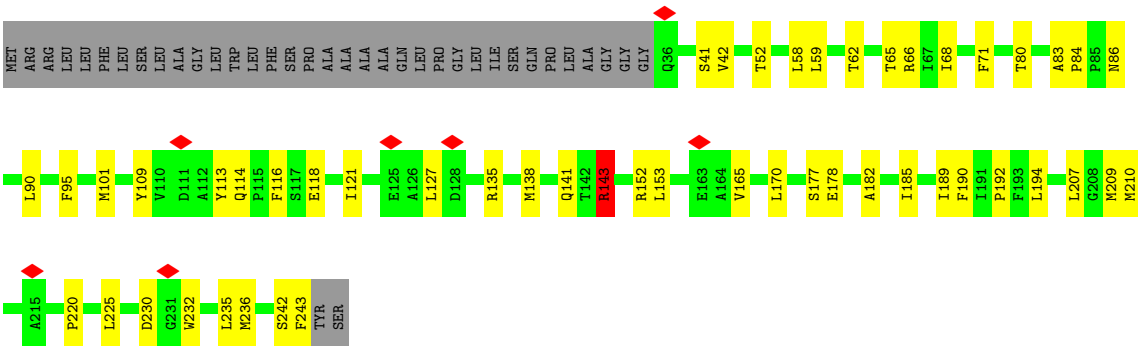
Chain I:





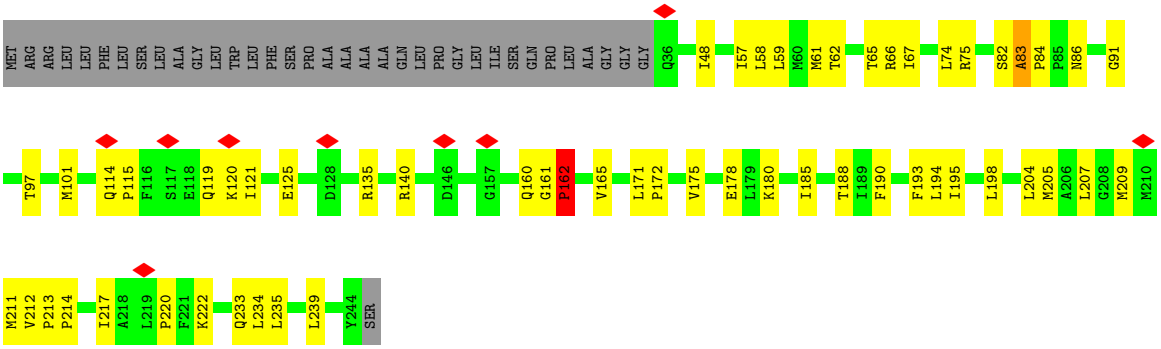
• Molecule 4: Flagellar biosynthetic protein FliP

Chain H:



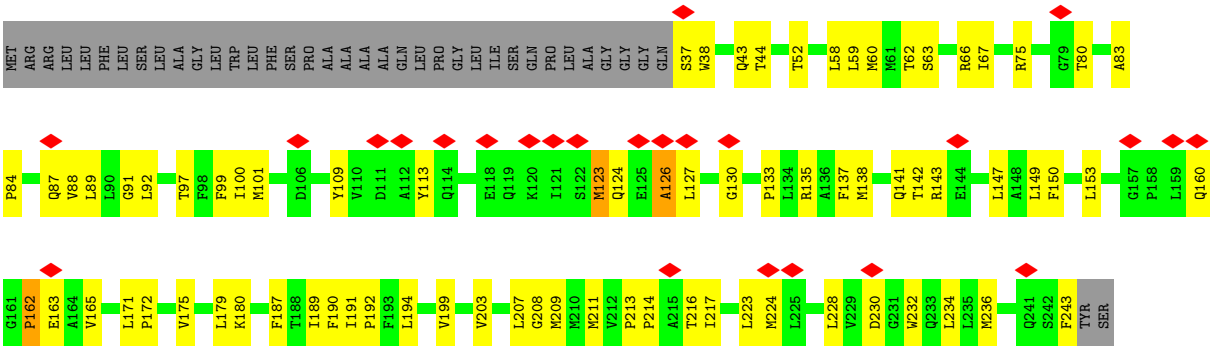
• Molecule 4: Flagellar biosynthetic protein FliP

Chain G:



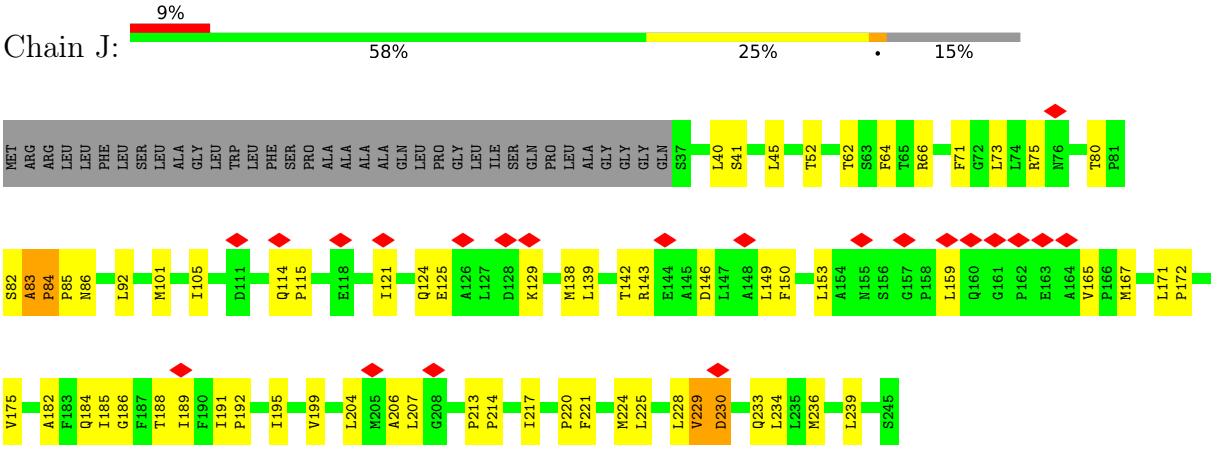
• Molecule 4: Flagellar biosynthetic protein FliP

Chain F:



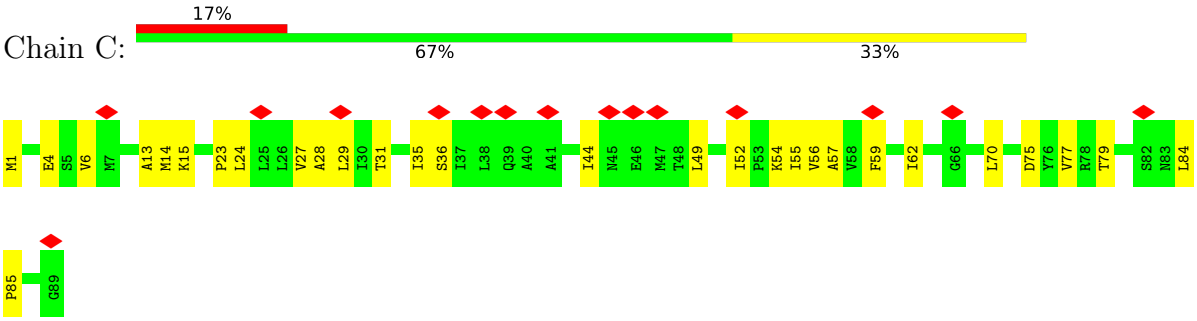
• Molecule 4: Flagellar biosynthetic protein FliP

Chain J:



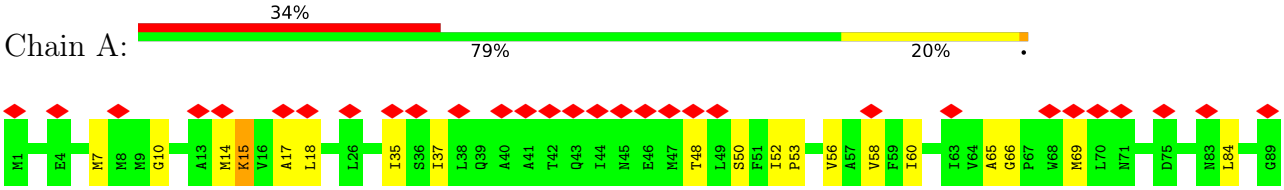
• Molecule 5: Flagellar biosynthetic protein FliQ

Chain C:



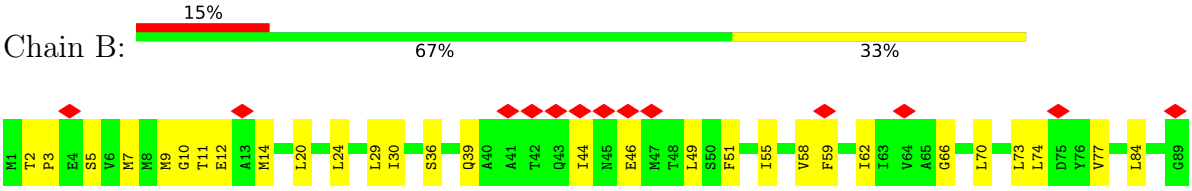
• Molecule 5: Flagellar biosynthetic protein FliQ

Chain A:



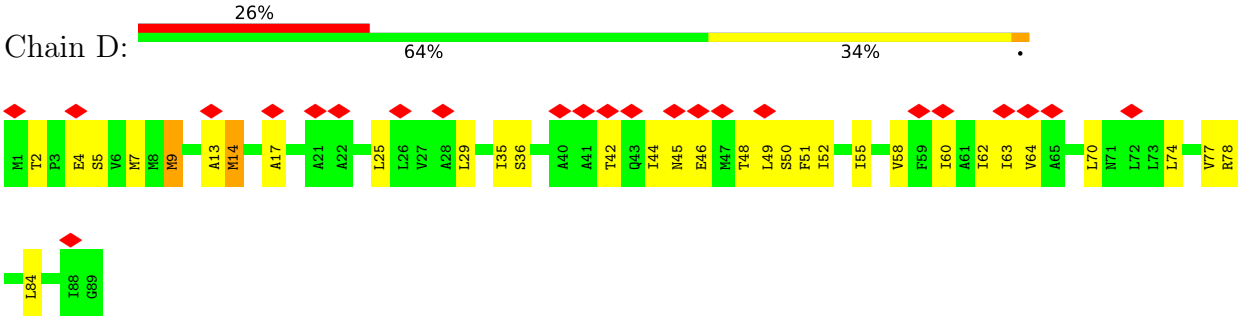
• Molecule 5: Flagellar biosynthetic protein FliQ

Chain B:



• Molecule 5: Flagellar biosynthetic protein FliQ

Chain D:



- Molecule 6: Flagellar M-ring protein

Chain c: 97%

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

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

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR P309 A315 N324 GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG ASN GLU THR SER ASN TYR GLU VAL ASP ARG THR

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

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

LYS ALA ALA GLN GLU GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL MET SER GLN ARG ILE ARG GLU MET SER ASP ASN ASP PRO ARG VAL VAL ALA LEU VAL ILE

ARG GLN TRP MET SER ASN ASP HIS GLU

- Molecule 6: Flagellar M-ring protein

Chain e: 97%

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

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

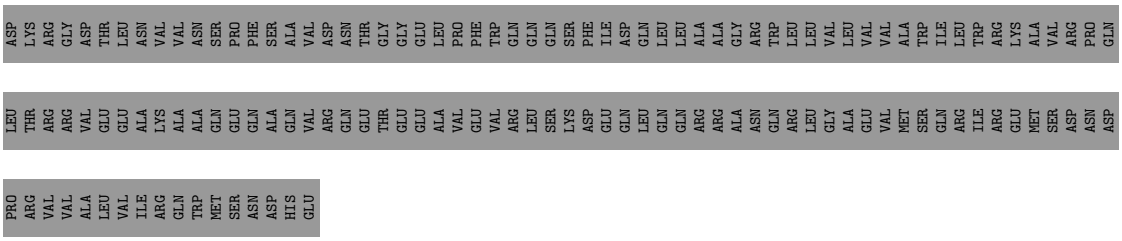
PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU

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

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

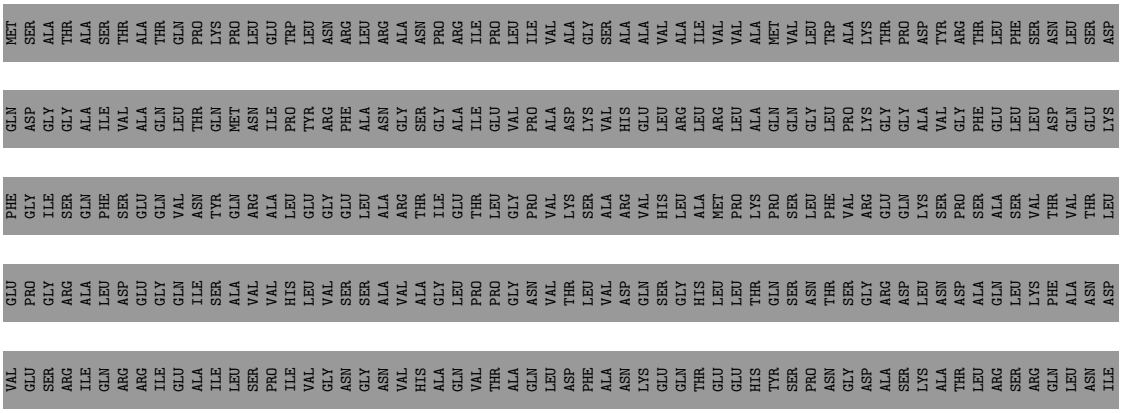
SER GLU GLN VAL GLY ALA GLY TYR P309 G310 G311 V312 P313 G314 A315 L316 S317 P322 P323 N324 GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG ASN GLU THR

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



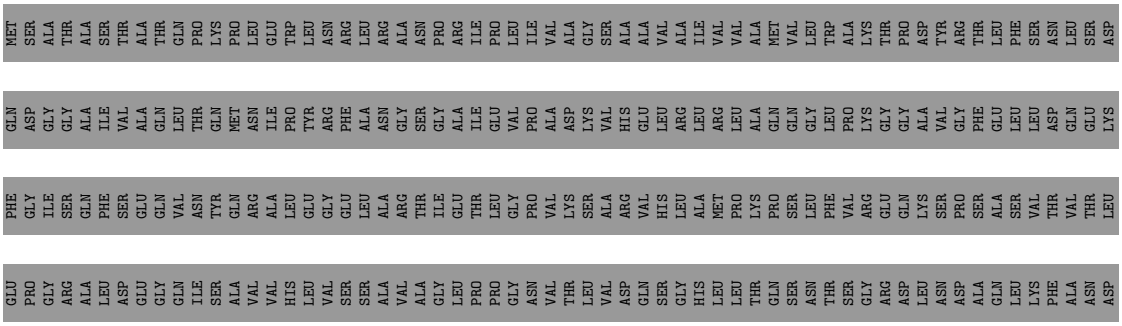
- Molecule 6: Flagellar M-ring protein

Chain g: 97%



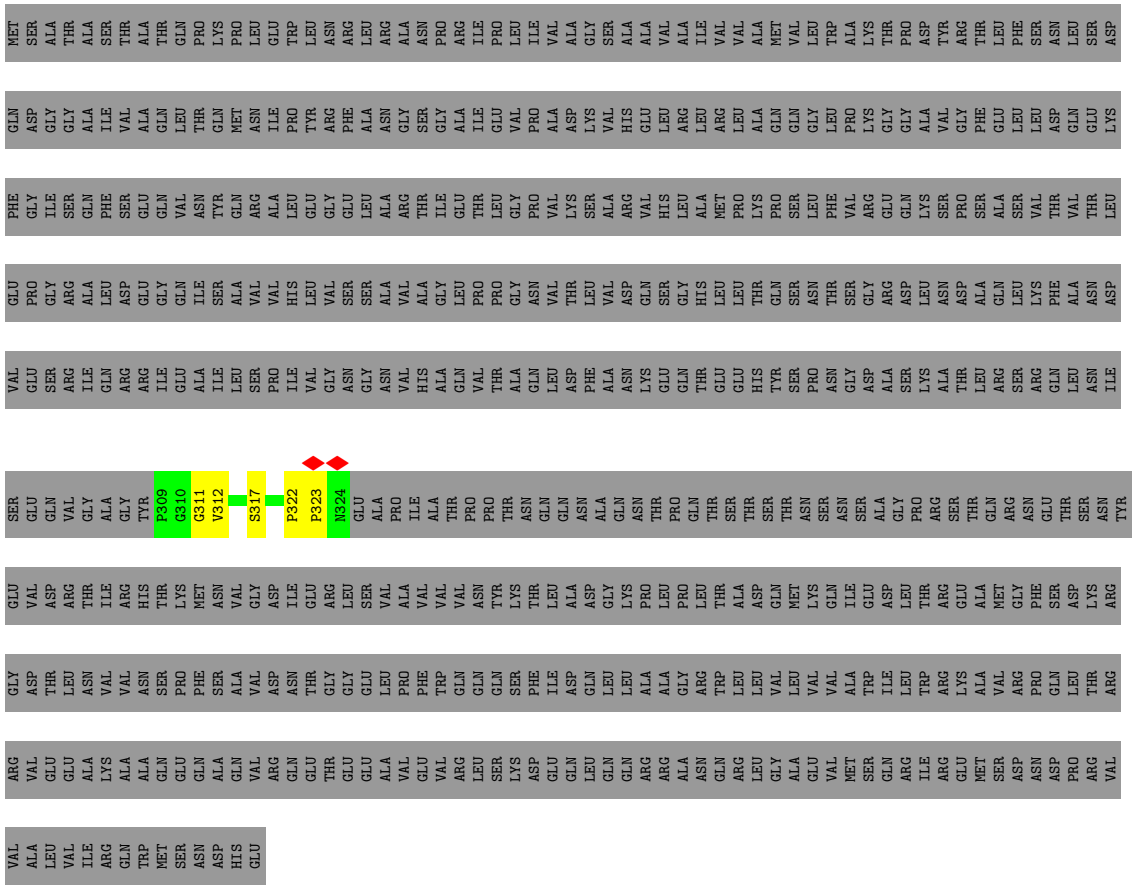
- Molecule 6: Flagellar M-ring protein

Chain i: 97%



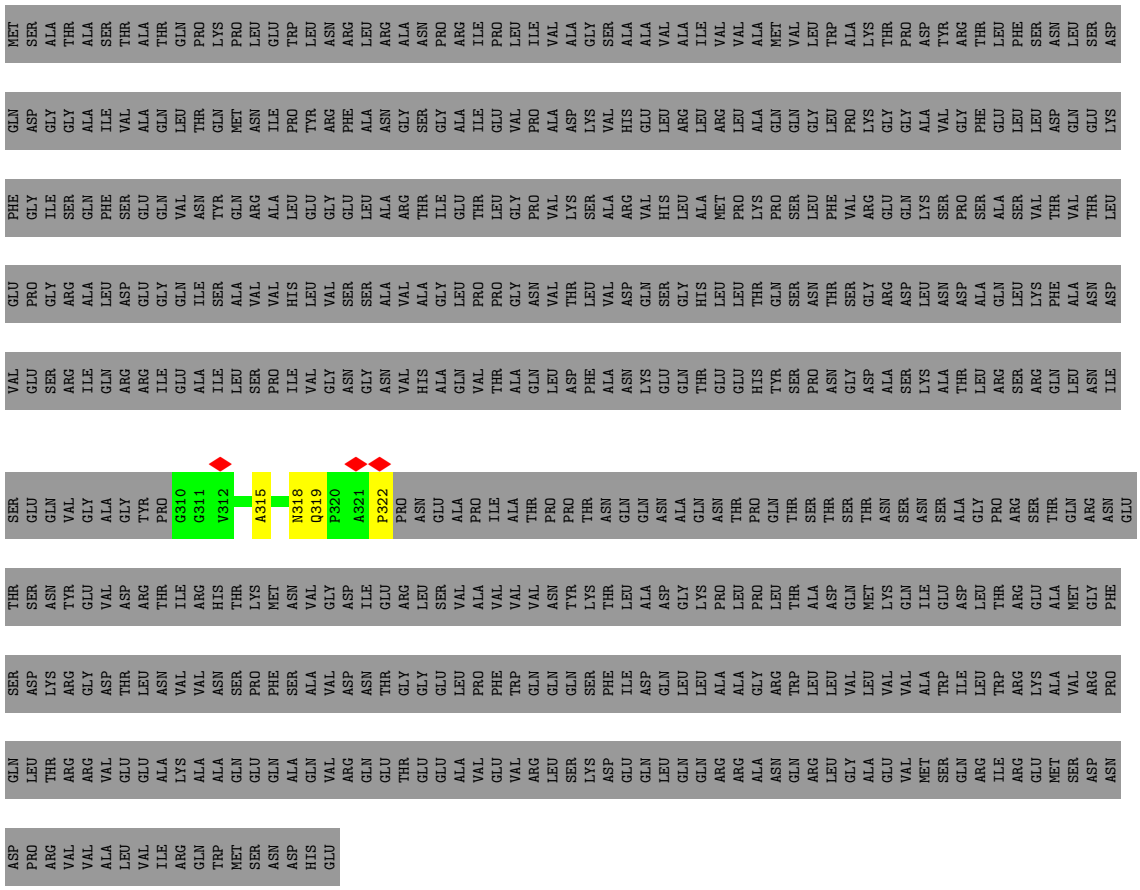
• Molecule 6: Flagellar M-ring protein

Chain k: 97%



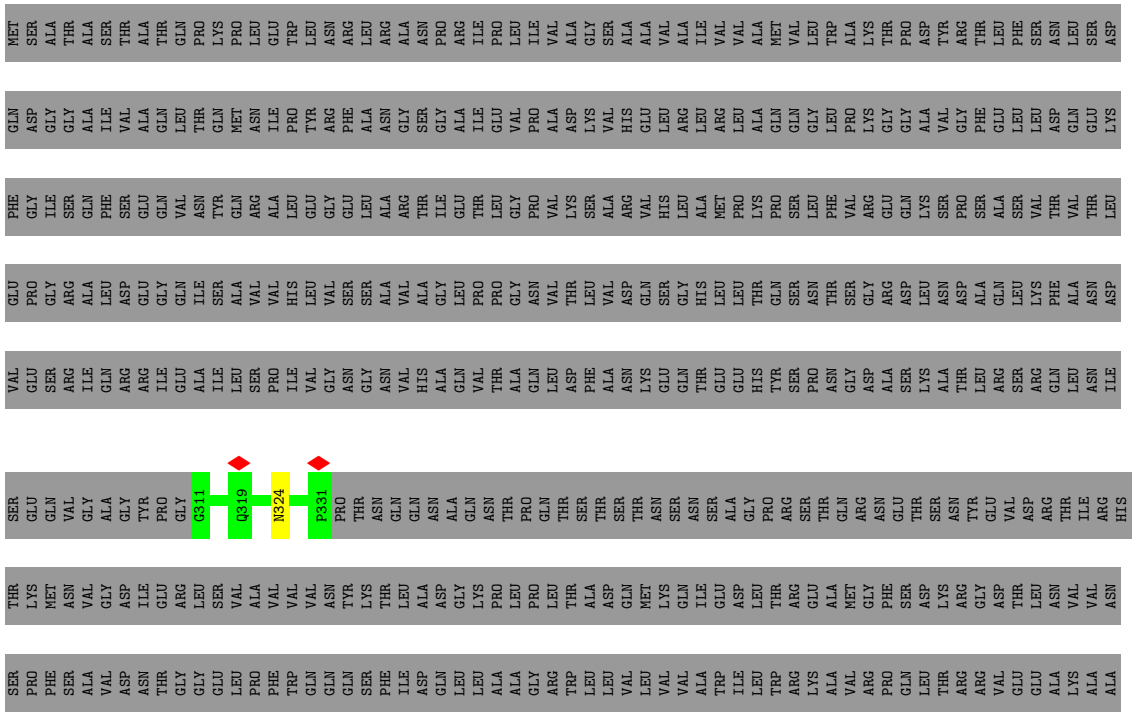
• Molecule 6: Flagellar M-ring protein

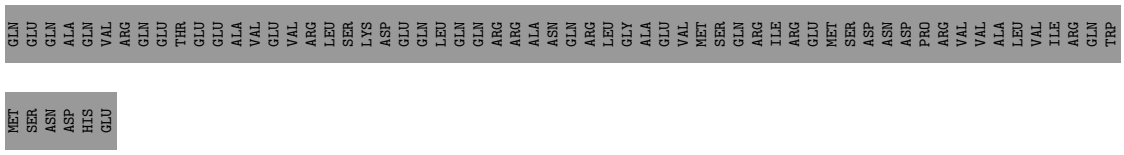
Chain b: 98%



- Molecule 6: Flagellar M-ring protein

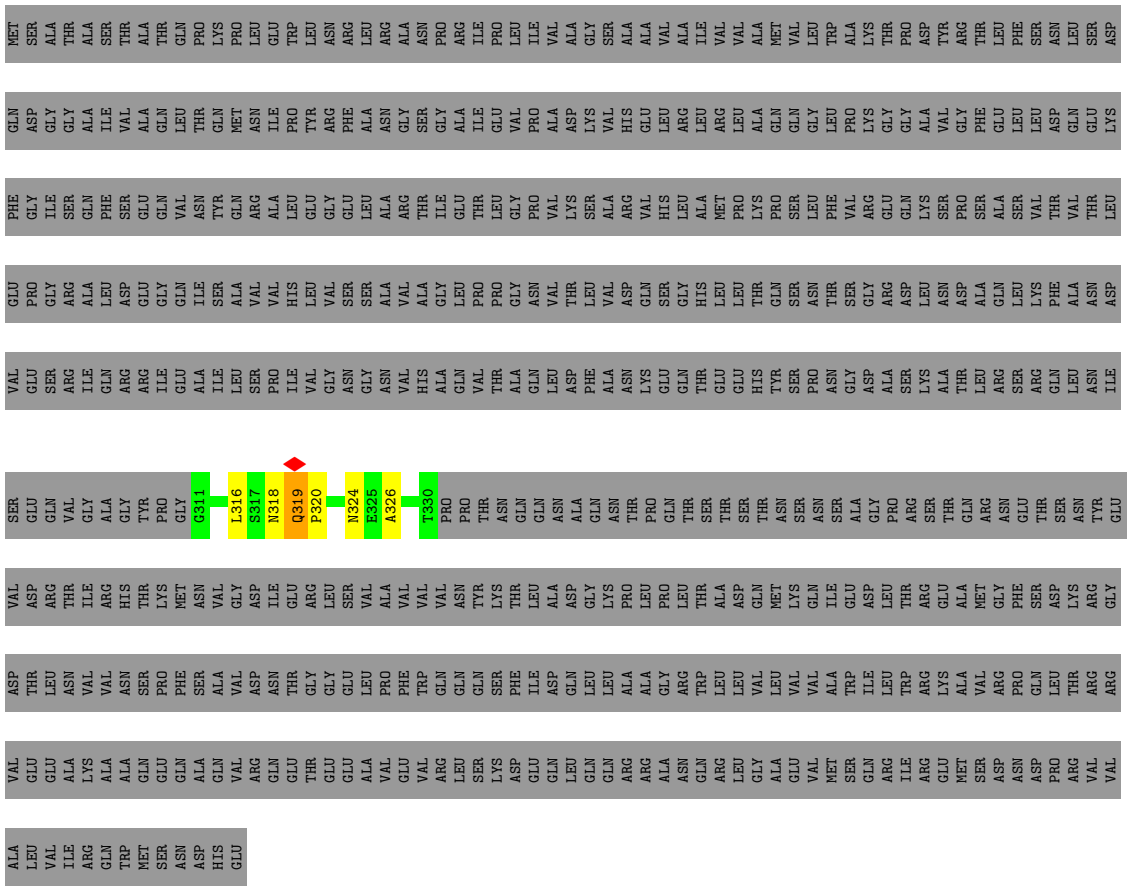
Chain h: 96%





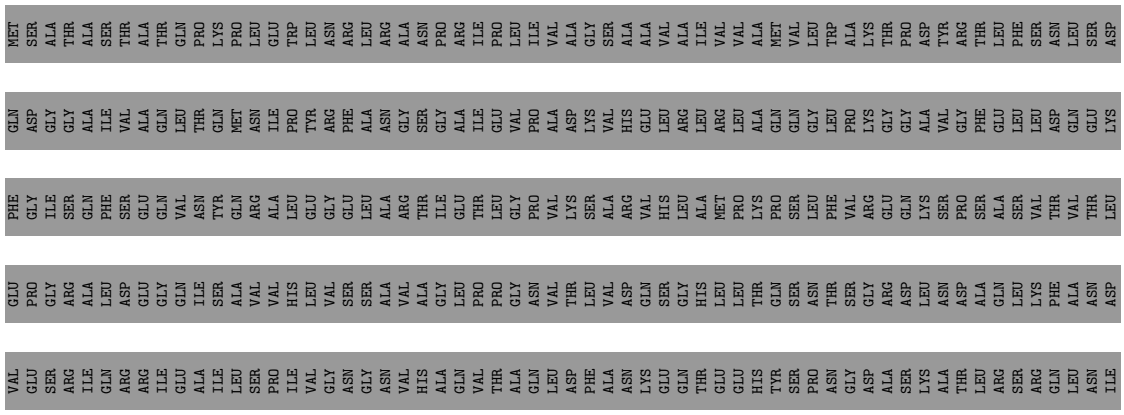
• Molecule 6: Flagellar M-ring protein

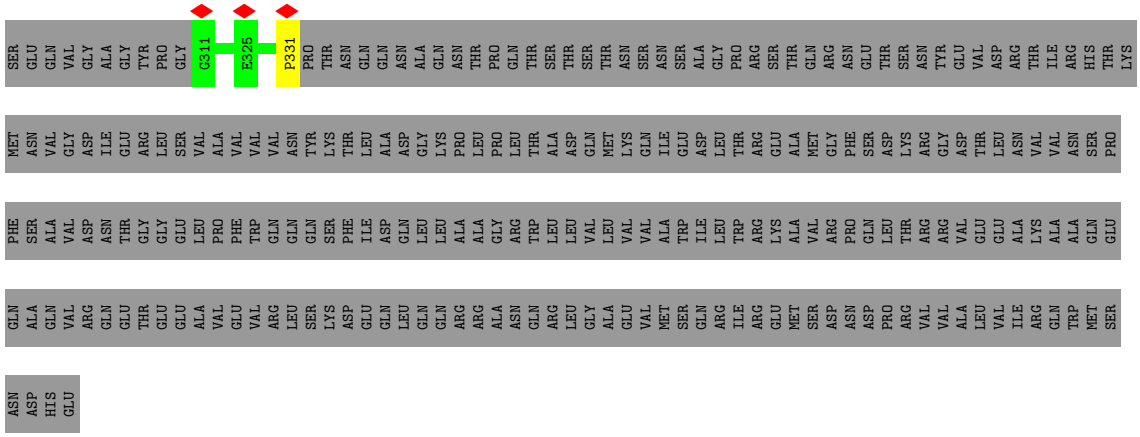
Chain d: 96%



• Molecule 6: Flagellar M-ring protein

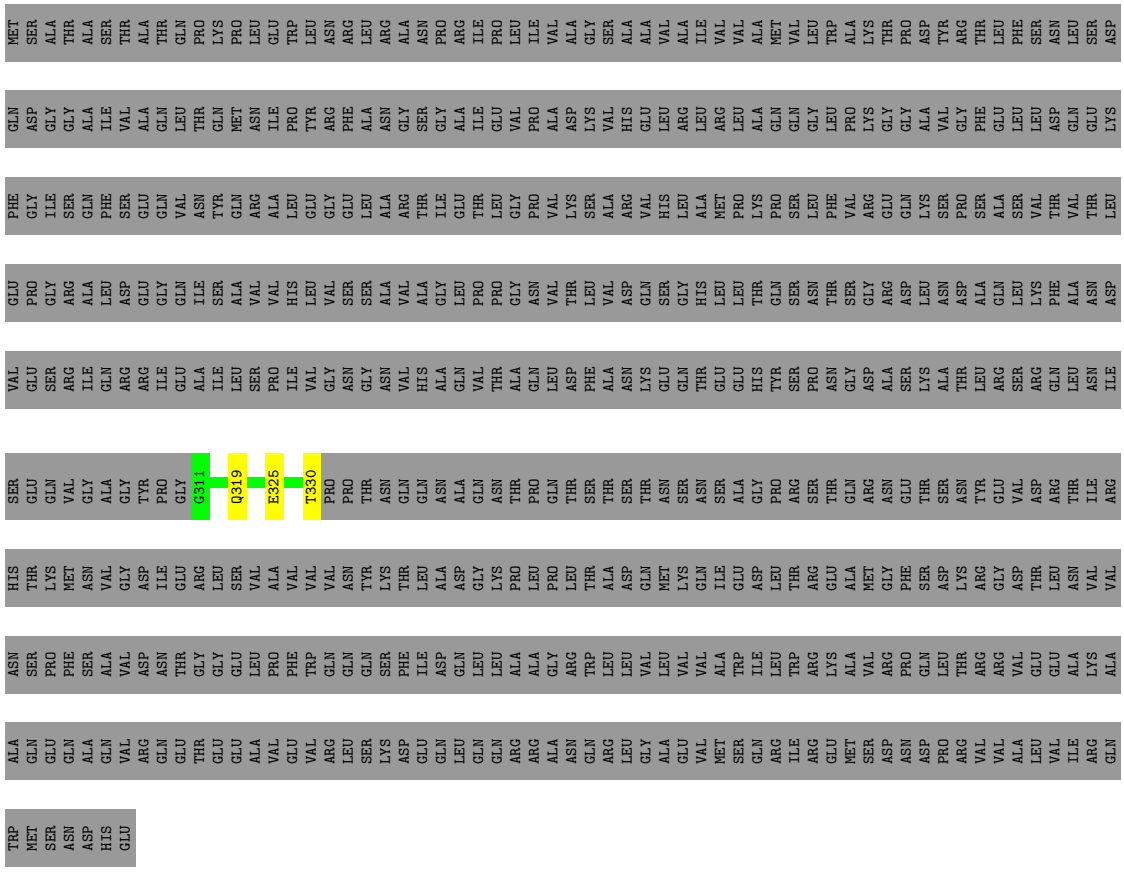
Chain f: 96%





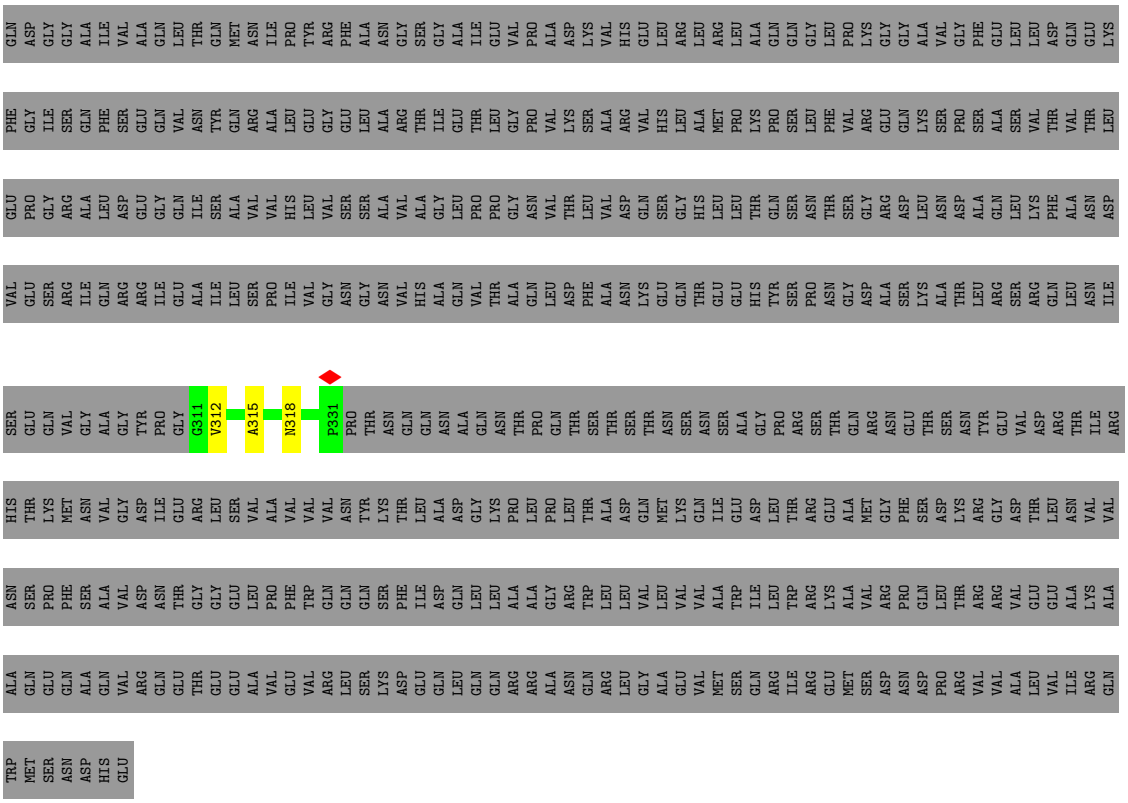
• Molecule 6: Flagellar M-ring protein

Chain j: 96%



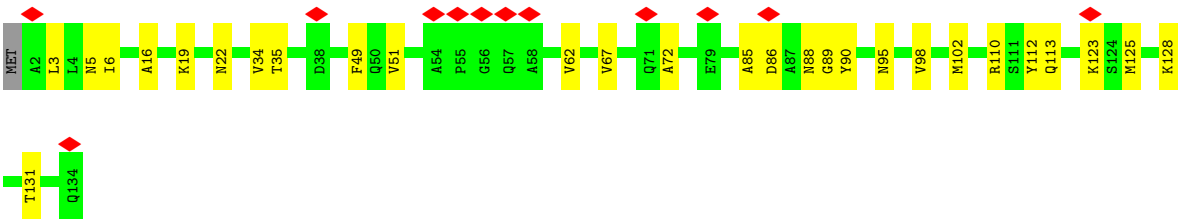
• Molecule 6: Flagellar M-ring protein

Chain l: 96%



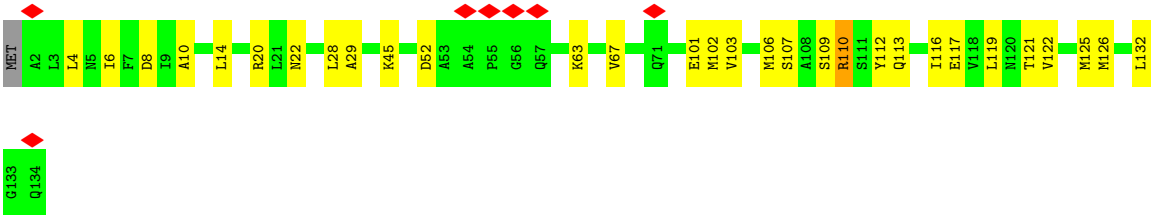
- Molecule 7: Flagellar basal-body rod protein FlgC

Chain a:



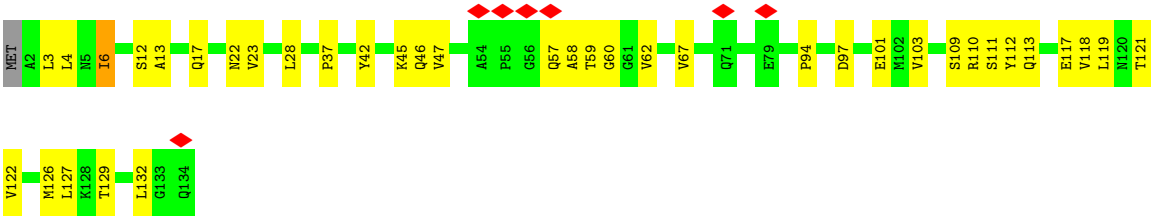
- Molecule 7: Flagellar basal-body rod protein FlgC

Chain Y:



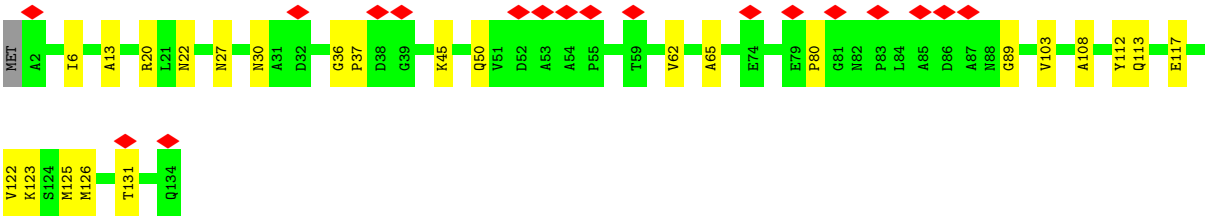
- Molecule 7: Flagellar basal-body rod protein FlgC

Chain Z:



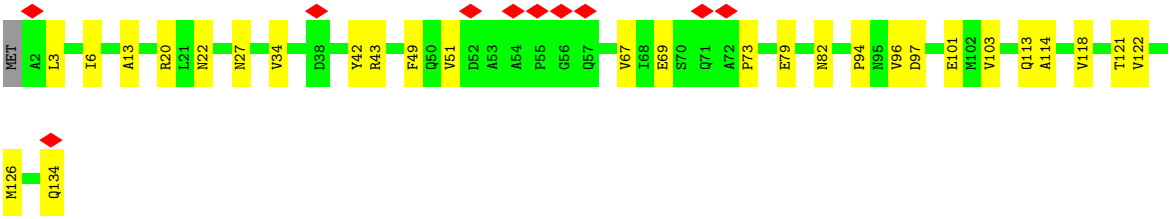
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain V:



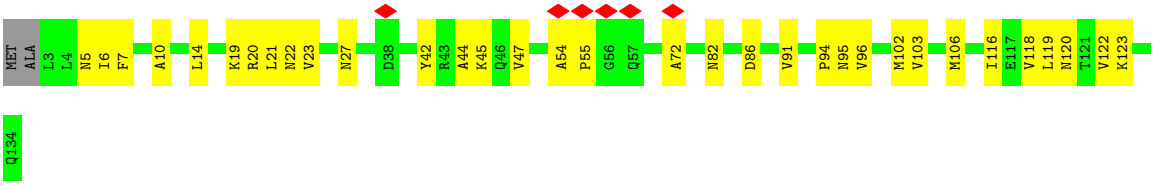
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain X:



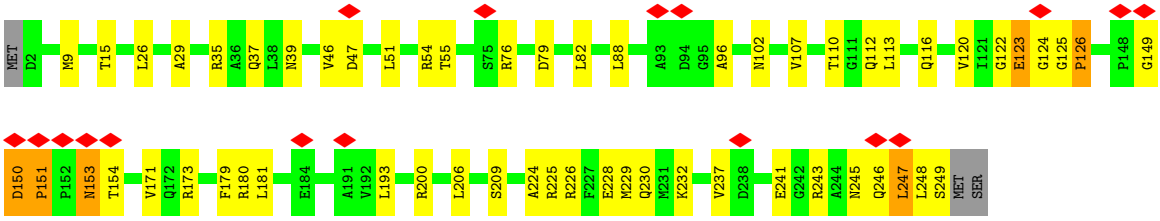
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain W:



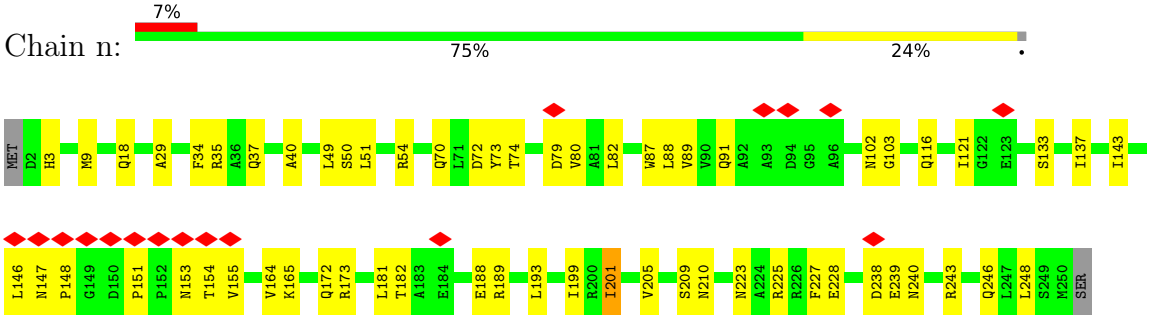
• Molecule 8: Flagellar basal-body rod protein FlgF

Chain m:



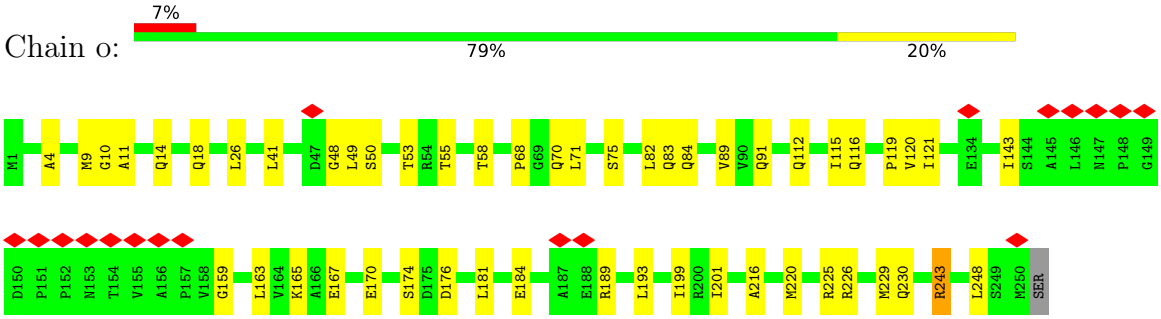
• Molecule 8: Flagellar basal-body rod protein FlgF

Chain n:



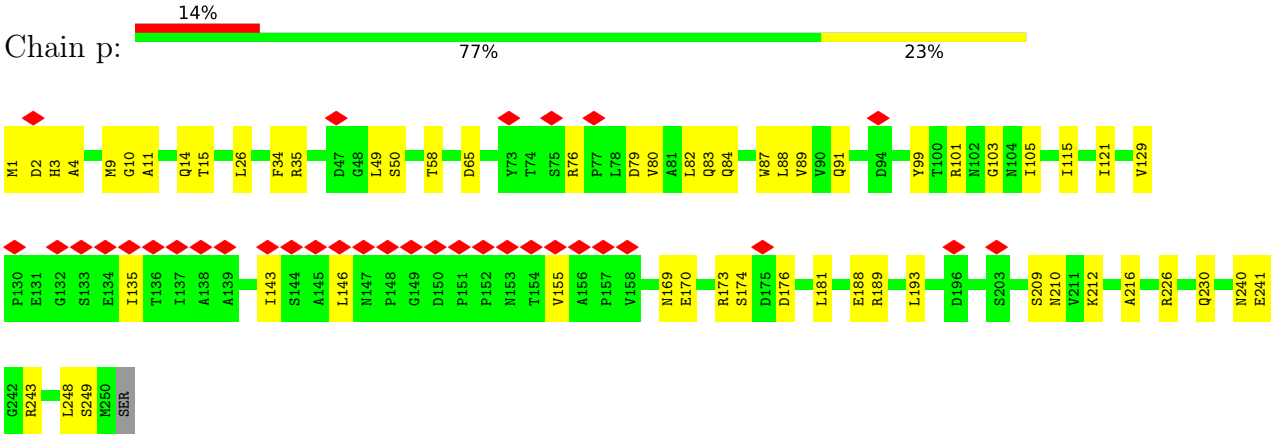
• Molecule 8: Flagellar basal-body rod protein FlgF

Chain o:



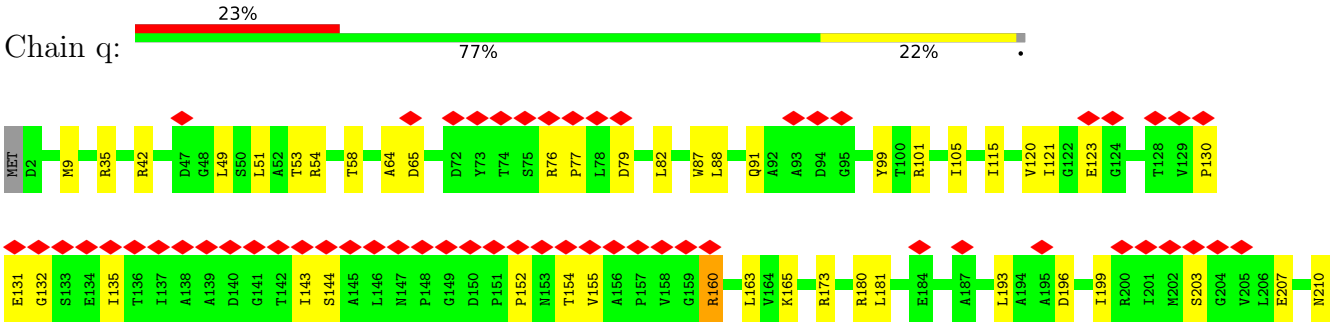
• Molecule 8: Flagellar basal-body rod protein FlgF

Chain p:



• Molecule 8: Flagellar basal-body rod protein FlgF

Chain q:



R226
F227
Q230
M231
D238
E239
N245
Q246
L247
L248
S249
M250
SER

4 Experimental information (i)

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 ($e^-/Å^2$)	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	1.839	Depositor
Minimum map value	-1.172	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.082	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 (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	K	0.17	0/300	0.43	0/400
1	L	0.11	0/547	0.24	0/733
1	M	0.17	0/561	0.29	0/753
1	N	0.13	0/561	0.27	0/753
1	O	0.13	0/561	0.31	0/753
1	P	0.16	0/554	0.32	0/743
2	Q	0.21	0/930	0.46	0/1251
2	R	0.16	0/855	0.34	0/1150
2	S	0.18	0/855	0.39	0/1150
2	T	0.16	0/870	0.33	0/1169
2	U	0.18	0/839	0.35	0/1129
3	E	0.45	3/1994 (0.2%)	0.61	3/2724 (0.1%)
4	F	0.33	0/1643	0.61	4/2237 (0.2%)
4	G	0.26	0/1665	0.46	2/2267 (0.1%)
4	H	0.22	0/1652	0.42	0/2249
4	I	0.22	0/1652	0.40	0/2249
4	J	0.30	0/1662	0.53	1/2263 (0.0%)
5	A	0.26	0/681	0.49	0/930
5	B	0.16	0/681	0.42	0/930
5	C	0.23	0/681	0.44	0/930
5	D	0.26	0/681	0.55	0/930
6	b	0.70	0/83	0.97	0/114
6	c	0.16	0/107	0.37	0/148
6	d	0.27	0/137	0.52	0/191
6	e	0.20	0/107	0.44	0/148
6	f	1.32	1/145 (0.7%)	1.50	3/203 (1.5%)
6	g	0.22	0/107	0.57	0/148
6	h	0.13	0/145	0.29	0/203
6	i	0.14	0/107	0.41	0/148
6	j	0.25	0/137	0.66	0/191
6	k	0.16	0/107	0.30	0/148
6	l	0.26	0/145	0.44	0/203
7	V	0.15	0/981	0.31	0/1334
7	W	0.13	0/976	0.32	0/1327

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	X	0.52	2/981 (0.2%)	0.98	3/1334 (0.2%)
7	Y	0.16	0/981	0.36	0/1334
7	Z	0.15	0/981	0.35	0/1334
7	a	0.19	0/981	0.36	0/1334
8	m	0.36	0/1828	0.56	1/2492 (0.0%)
8	n	0.26	0/1836	0.47	0/2502
8	o	0.22	0/1844	0.44	0/2512
8	p	0.17	0/1844	0.37	0/2512
8	q	0.29	0/1836	0.49	1/2502 (0.0%)
All	All	0.27	6/36821 (0.0%)	0.48	18/50055 (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
2	Q	0	1
2	U	0	1
4	H	0	1
7	Y	0	1
7	a	0	1
8	m	0	2
8	n	0	1
8	o	0	1
8	q	0	1
All	All	0	10

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	331	PRO	CG-CD	-13.86	1.03	1.50
7	X	73	PRO	CG-CD	-12.38	1.08	1.50
3	E	185	MET	C-O	9.78	1.35	1.24
7	X	73	PRO	CB-CG	-7.58	1.11	1.49
3	E	182	ASN	C-O	6.64	1.32	1.24

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	73	PRO	CB-CG-CD	23.05	179.87	106.10
7	X	73	PRO	N-CD-CG	-18.79	75.01	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	331	PRO	N-CD-CG	-16.10	79.05	103.20
7	X	73	PRO	CA-CB-CG	-14.25	77.42	104.50
4	F	162	PRO	CA-N-CD	-12.38	94.66	112.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Q	106	ARG	Sidechain
2	U	104	ARG	Sidechain
7	a	110	ARG	Sidechain
8	m	200	ARG	Sidechain
8	m	243	ARG	Sidechain

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	K	300	0	311	15	0
1	L	543	0	550	10	0
1	M	557	0	566	10	0
1	N	557	0	566	13	0
1	O	557	0	566	18	0
1	P	550	0	559	18	0
2	Q	922	0	914	26	0
2	R	848	0	847	16	0
2	S	848	0	847	25	0
2	T	863	0	863	17	0
2	U	832	0	829	24	0
3	E	1945	0	2063	81	0
4	F	1605	0	1701	63	0
4	G	1626	0	1718	48	0
4	H	1614	0	1709	40	0
4	I	1614	0	1709	43	0
4	J	1623	0	1715	65	0
5	A	670	0	739	15	0
5	B	670	0	739	28	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	670	0	739	28	0
5	D	670	0	739	40	0
6	b	81	0	78	6	0
6	c	103	0	99	1	0
6	d	133	0	129	5	0
6	e	103	0	99	5	0
6	f	140	0	136	0	0
6	g	103	0	99	4	0
6	h	140	0	136	2	0
6	i	103	0	99	2	0
6	j	133	0	129	2	0
6	k	103	0	99	3	0
6	l	140	0	136	1	0
7	V	969	0	981	22	0
7	W	964	0	976	27	0
7	X	969	0	981	24	0
7	Y	969	0	981	30	0
7	Z	969	0	981	33	0
7	a	969	0	981	26	0
8	m	1804	0	1791	42	0
8	n	1812	0	1800	46	0
8	o	1820	0	1812	40	0
8	p	1820	0	1812	45	0
8	q	1812	0	1800	41	0
All	All	36243	0	37124	792	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 792 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:MET:O	3:E:189:PRO:HD2	1.64	0.98
3:E:158:PRO:HG2	3:E:162:ASN:HD21	1.35	0.89
8:m:247:LEU:HB3	7:W:120:ASN:HD21	1.37	0.88
2:Q:88:ARG:NH1	2:Q:105:GLU:OE1	2.10	0.84
3:E:182:ASN:HB3	3:E:239:PHE:HZ	1.43	0.83

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	K	38/104 (36%)	36 (95%)	2 (5%)	0	100	100
1	L	70/104 (67%)	70 (100%)	0	0	100	100
1	M	72/104 (69%)	70 (97%)	2 (3%)	0	100	100
1	N	72/104 (69%)	72 (100%)	0	0	100	100
1	O	72/104 (69%)	72 (100%)	0	0	100	100
1	P	71/104 (68%)	71 (100%)	0	0	100	100
2	Q	115/138 (83%)	115 (100%)	0	0	100	100
2	R	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
2	S	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
2	T	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
2	U	102/138 (74%)	101 (99%)	1 (1%)	0	100	100
3	E	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	4	24
4	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
4	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	12	40
4	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
4	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	24	55
4	J	207/245 (84%)	200 (97%)	5 (2%)	2 (1%)	12	40
5	A	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
5	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
5	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
5	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
6	b	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
6	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	d	18/560 (3%)	18 (100%)	0	0	100	100
6	e	14/560 (2%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	19/560 (3%)	19 (100%)	0	0	100	100
6	g	14/560 (2%)	13 (93%)	1 (7%)	0	100	100
6	h	19/560 (3%)	19 (100%)	0	0	100	100
6	i	14/560 (2%)	14 (100%)	0	0	100	100
6	j	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
6	k	14/560 (2%)	14 (100%)	0	0	100	100
6	l	19/560 (3%)	19 (100%)	0	0	100	100
7	V	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
7	W	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
7	X	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
7	Y	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
7	Z	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	45
7	a	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
8	m	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	10	37
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	60
All	All	4751/11378 (42%)	4588 (97%)	147 (3%)	16 (0%)	37	65

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	188	LEU
3	E	190	VAL
8	m	123	GLU
4	J	83	ALA
3	E	167	ASN

5.3.2 Protein sidechains (i)

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	K	33/79 (42%)	33 (100%)	0	100	100
1	L	56/79 (71%)	56 (100%)	0	100	100
1	M	58/79 (73%)	58 (100%)	0	100	100
1	N	58/79 (73%)	57 (98%)	1 (2%)	53	71
1	O	58/79 (73%)	58 (100%)	0	100	100
1	P	57/79 (72%)	56 (98%)	1 (2%)	51	70
2	Q	98/113 (87%)	96 (98%)	2 (2%)	48	68
2	R	90/113 (80%)	89 (99%)	1 (1%)	65	76
2	S	90/113 (80%)	90 (100%)	0	100	100
2	T	91/113 (80%)	91 (100%)	0	100	100
2	U	89/113 (79%)	88 (99%)	1 (1%)	65	76
3	E	210/221 (95%)	208 (99%)	2 (1%)	68	76
4	F	177/204 (87%)	174 (98%)	3 (2%)	53	71
4	G	179/204 (88%)	174 (97%)	5 (3%)	38	62
4	H	178/204 (87%)	176 (99%)	2 (1%)	65	76
4	I	178/204 (87%)	175 (98%)	3 (2%)	53	71
4	J	179/204 (88%)	178 (99%)	1 (1%)	78	81
5	A	74/74 (100%)	72 (97%)	2 (3%)	39	63
5	B	74/74 (100%)	74 (100%)	0	100	100
5	C	74/74 (100%)	74 (100%)	0	100	100
5	D	74/74 (100%)	72 (97%)	2 (3%)	39	63
6	b	8/467 (2%)	8 (100%)	0	100	100
6	c	11/467 (2%)	11 (100%)	0	100	100
6	d	14/467 (3%)	12 (86%)	2 (14%)	3	14
6	e	11/467 (2%)	11 (100%)	0	100	100
6	f	15/467 (3%)	15 (100%)	0	100	100
6	g	11/467 (2%)	11 (100%)	0	100	100
6	h	15/467 (3%)	15 (100%)	0	100	100
6	i	11/467 (2%)	11 (100%)	0	100	100
6	j	14/467 (3%)	13 (93%)	1 (7%)	13	40
6	k	11/467 (2%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	l	15/467 (3%)	14 (93%)	1 (7%)	15	42
7	V	104/105 (99%)	104 (100%)	0	100	100
7	W	104/105 (99%)	104 (100%)	0	100	100
7	X	104/105 (99%)	104 (100%)	0	100	100
7	Y	104/105 (99%)	103 (99%)	1 (1%)	68	76
7	Z	104/105 (99%)	102 (98%)	2 (2%)	50	68
7	a	104/105 (99%)	104 (100%)	0	100	100
8	m	190/193 (98%)	185 (97%)	5 (3%)	40	64
8	n	191/193 (99%)	189 (99%)	2 (1%)	68	76
8	o	192/193 (100%)	189 (98%)	3 (2%)	55	72
8	p	192/193 (100%)	192 (100%)	0	100	100
8	q	191/193 (99%)	190 (100%)	1 (0%)	81	83
All	All	3891/9308 (42%)	3847 (99%)	44 (1%)	63	76

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Z	127	LEU
4	F	160	GLN
4	G	48	ILE
4	G	162	PRO
6	d	318	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
7	Y	82	ASN
4	J	114	GLN
7	Z	17	GLN
4	F	141	GLN
5	D	39	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.

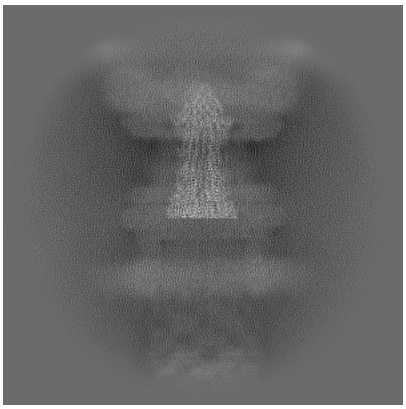
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37594. These allow visual inspection of the internal detail of the map and identification of artifacts.

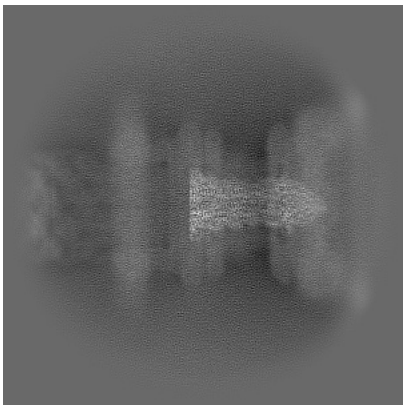
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

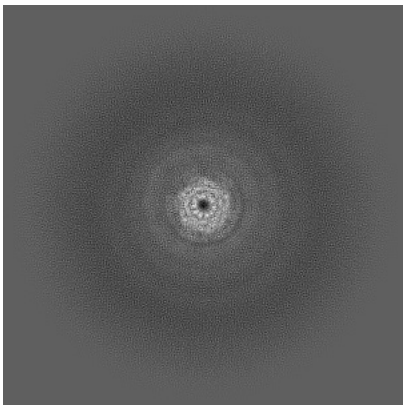
6.1.1 Primary map



X

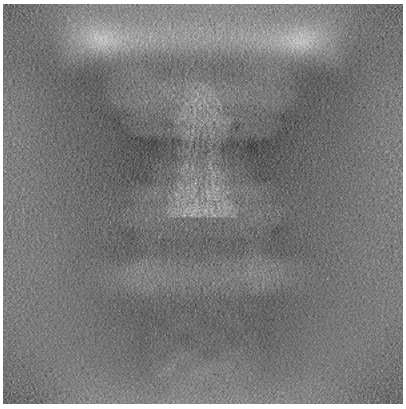


Y

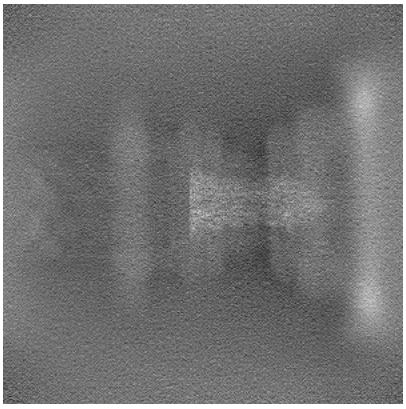


Z

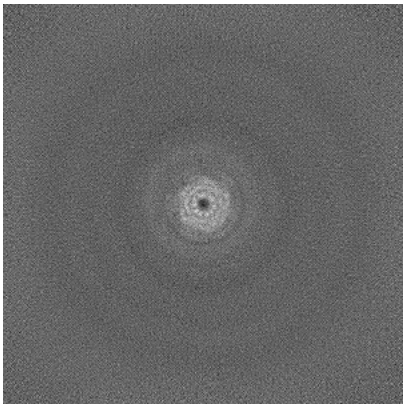
6.1.2 Raw map



X



Y

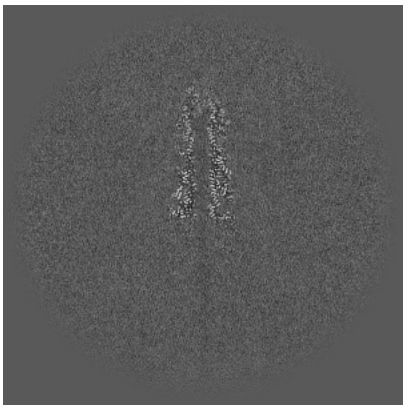


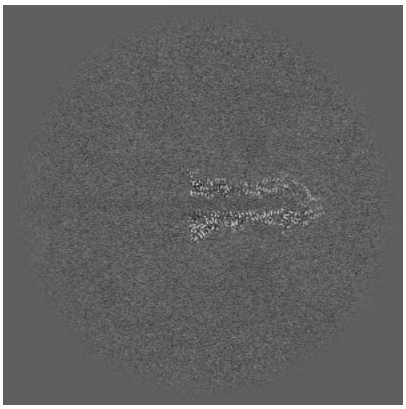
Z

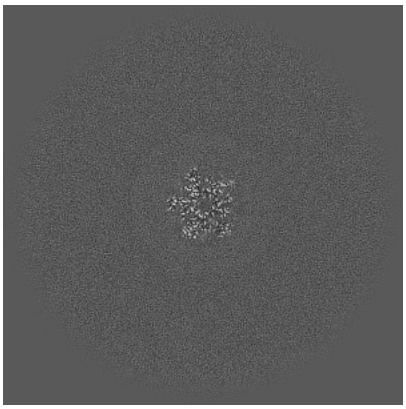
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

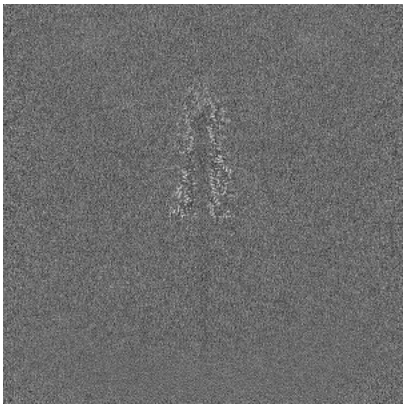
6.2.1 Primary map

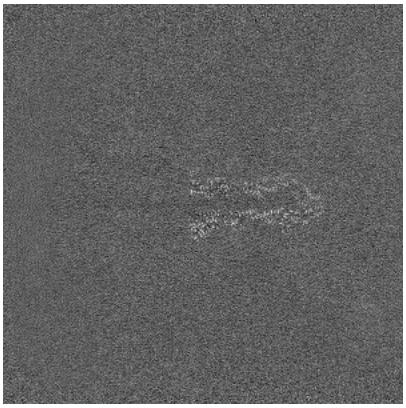

X Index: 256

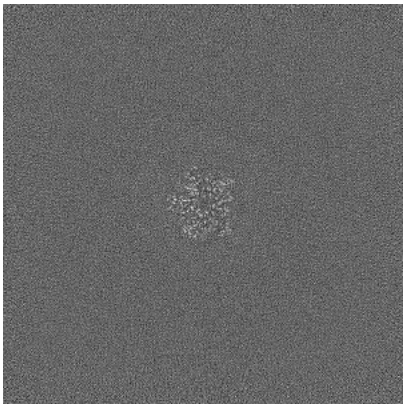

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

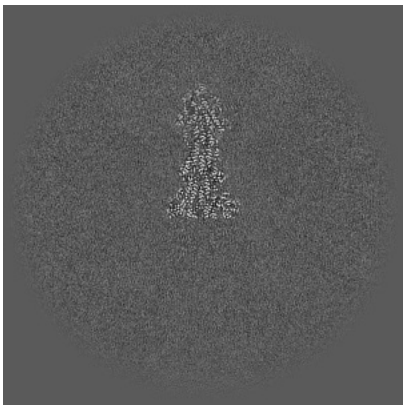

Y Index: 256


Z Index: 256

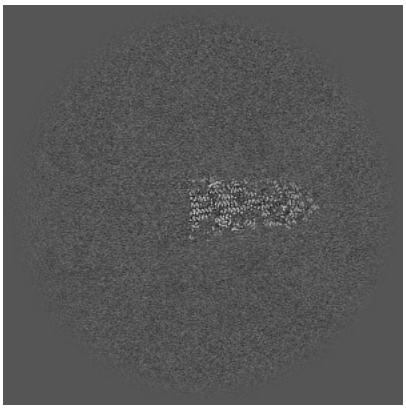
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

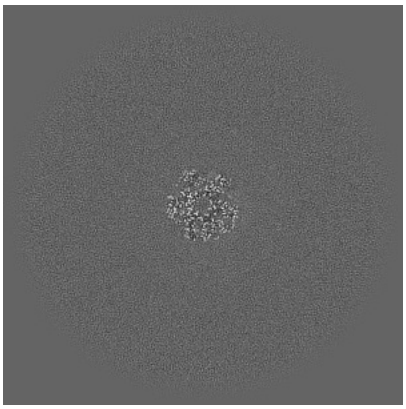
6.3.1 Primary map



X Index: 244

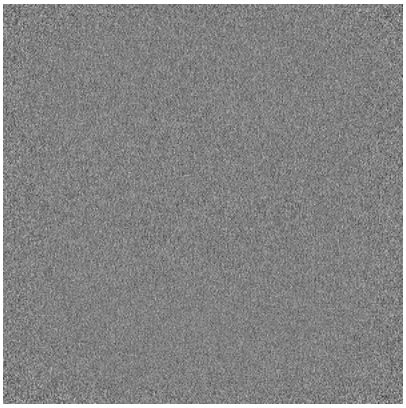


Y Index: 268

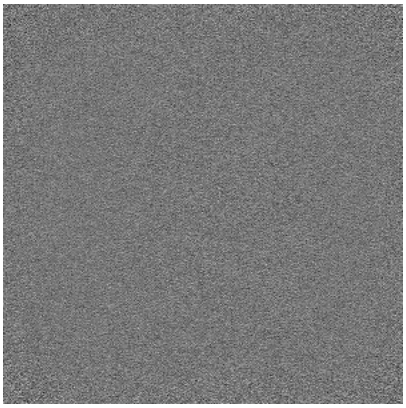


Z Index: 247

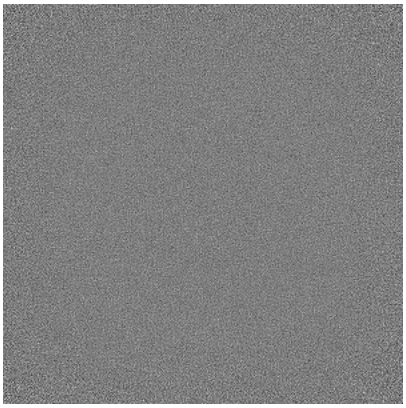
6.3.2 Raw map



X Index: 0



Y Index: 0

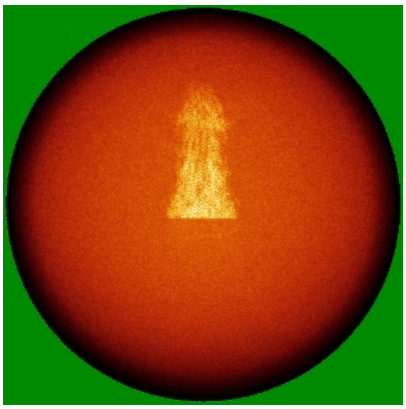


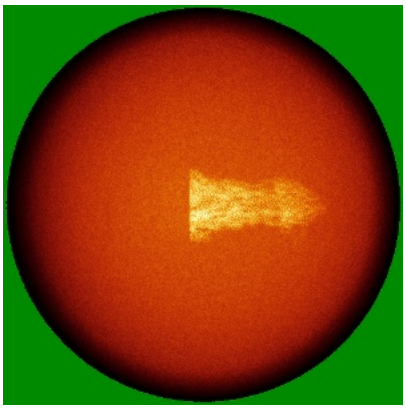
Z Index: 0

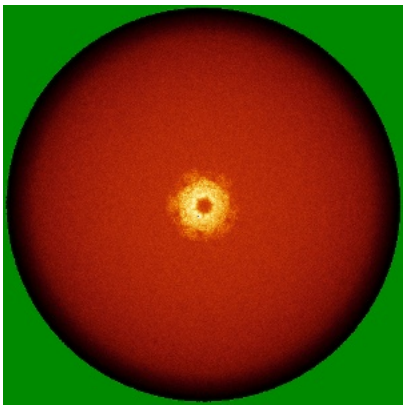
The images above show the largest variance slices of the map in three orthogonal directions.

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

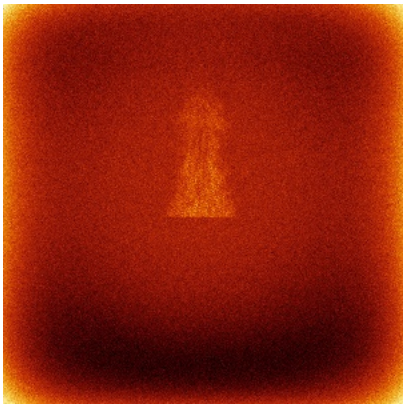
6.4.1 Primary map

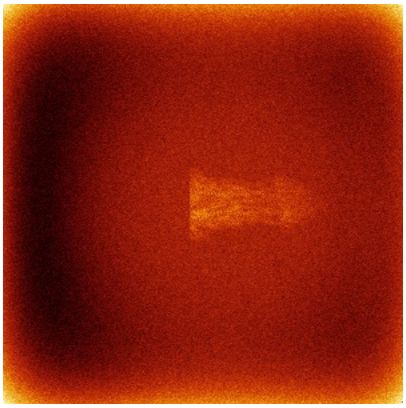

X

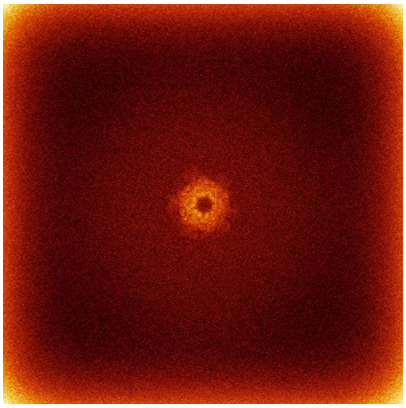

Y


Z

6.4.2 Raw map


X

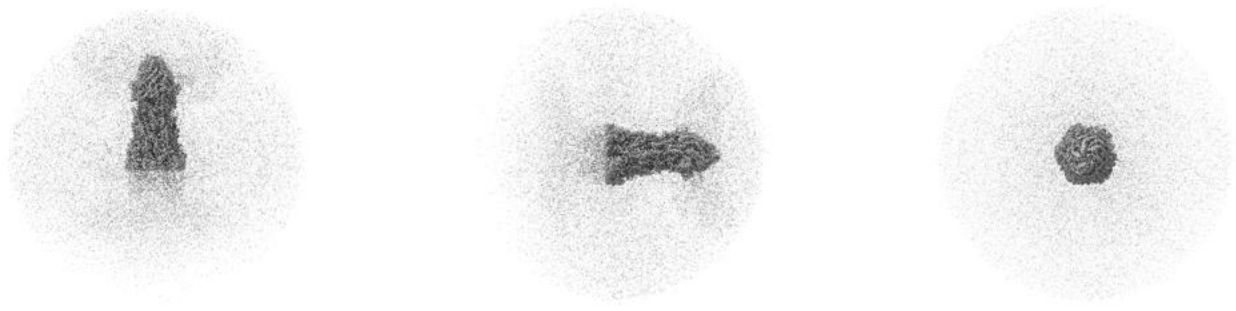

Y


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)

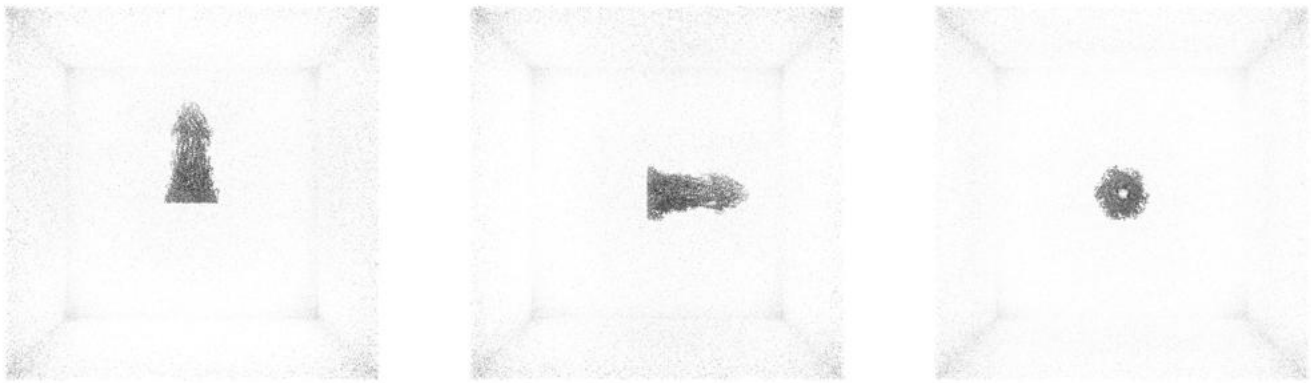
6.5.1 Primary map



X Y Z

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



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.

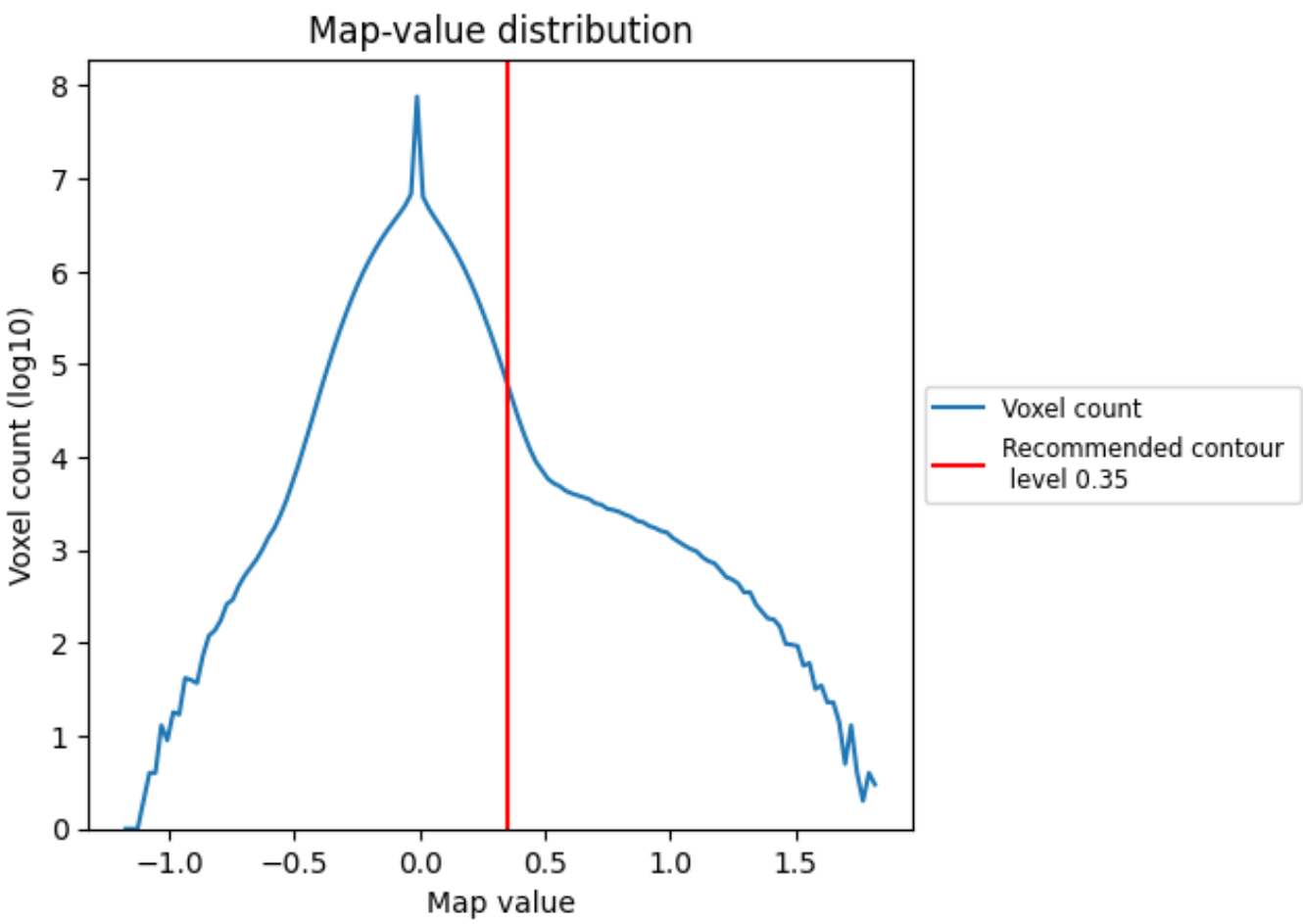
6.6 Mask visualisation (i)

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

7 Map analysis (i)

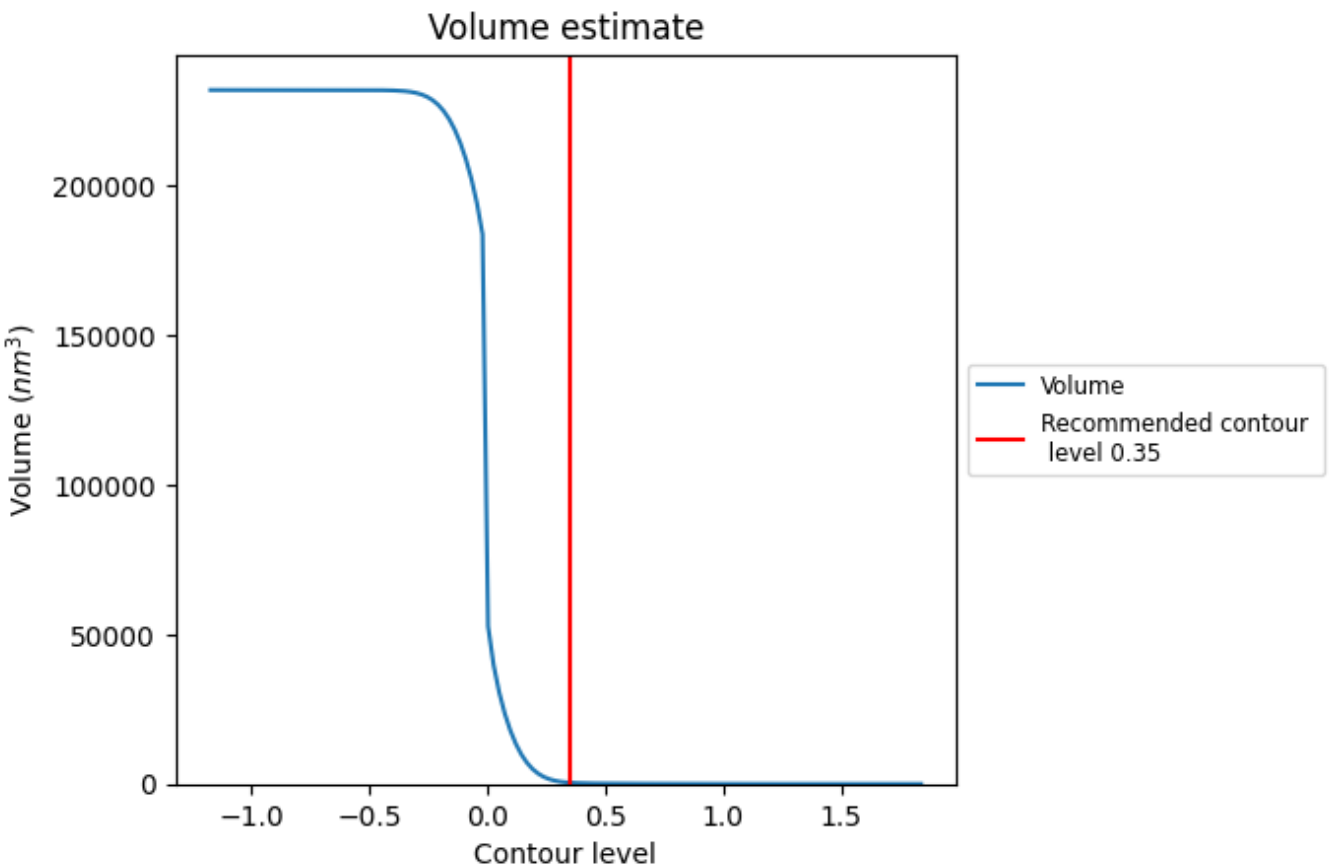
This section contains the results of statistical analysis of the map.

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.

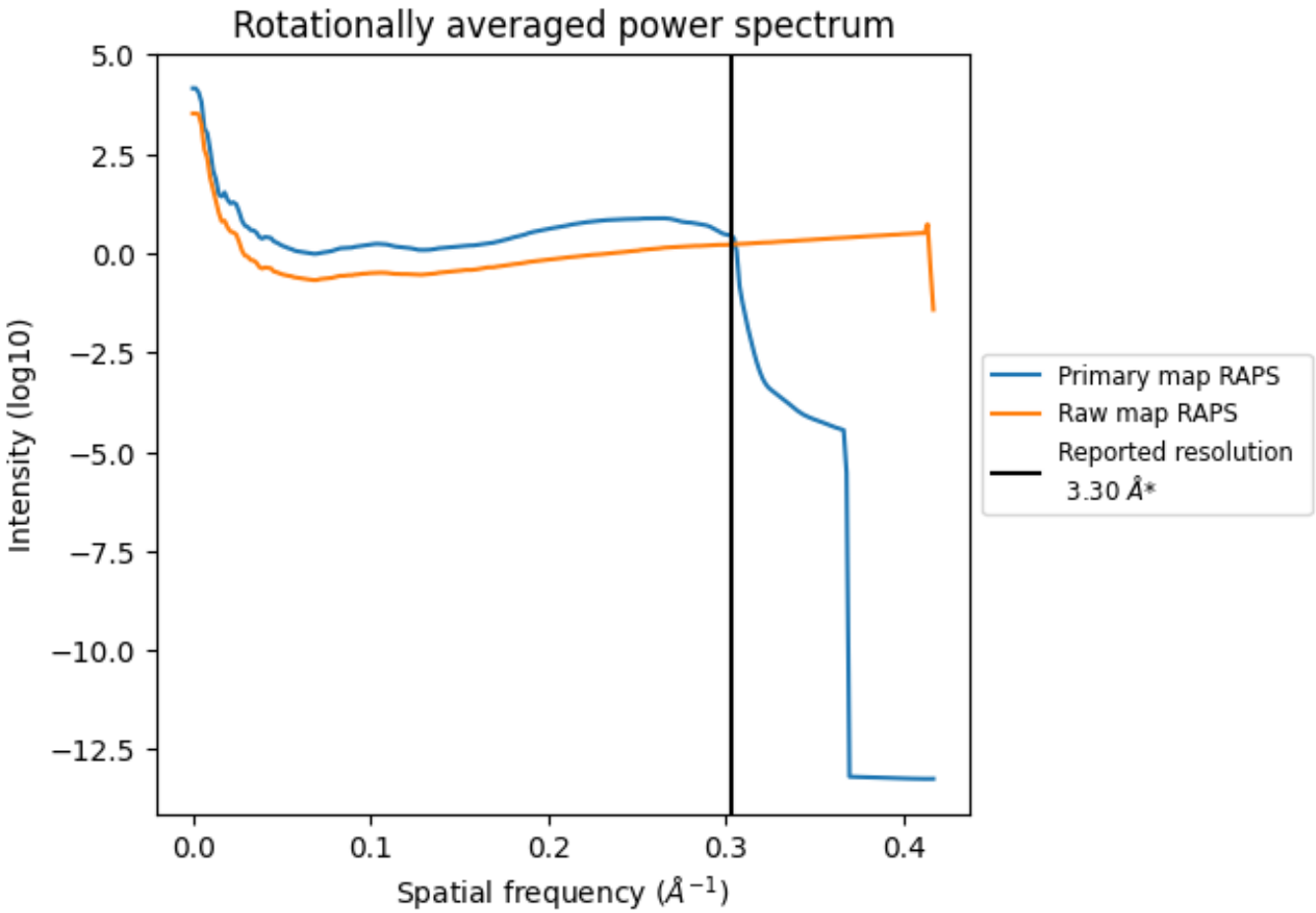
7.2 Volume estimate (i)



The volume at the recommended contour level is 429 nm^3; this corresponds to an approximate mass of 387 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 (i)

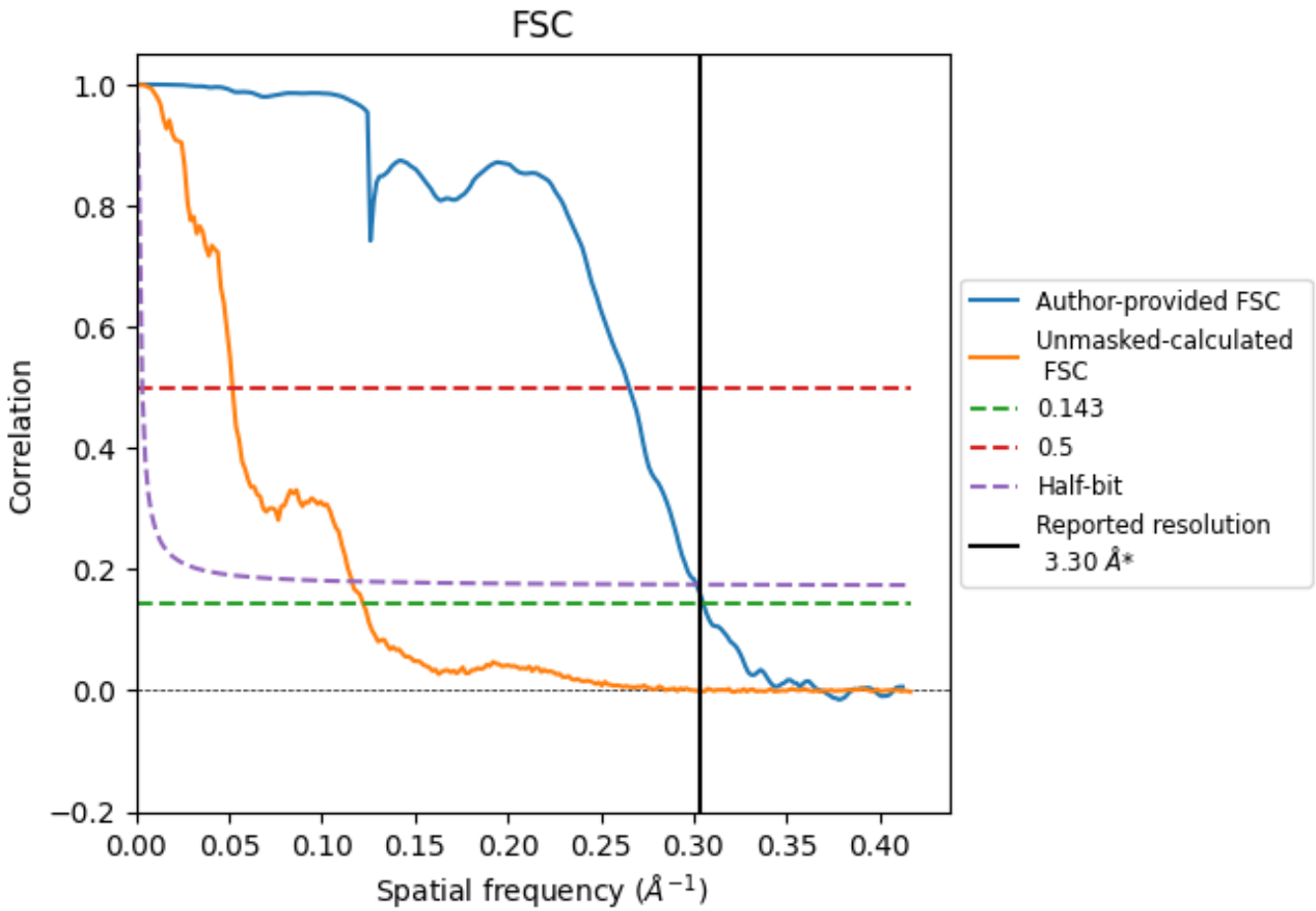


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.77	3.32
Unmasked-calculated*	8.19	19.31	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 8.19 differs from the reported value 3.3 by more than 10 %

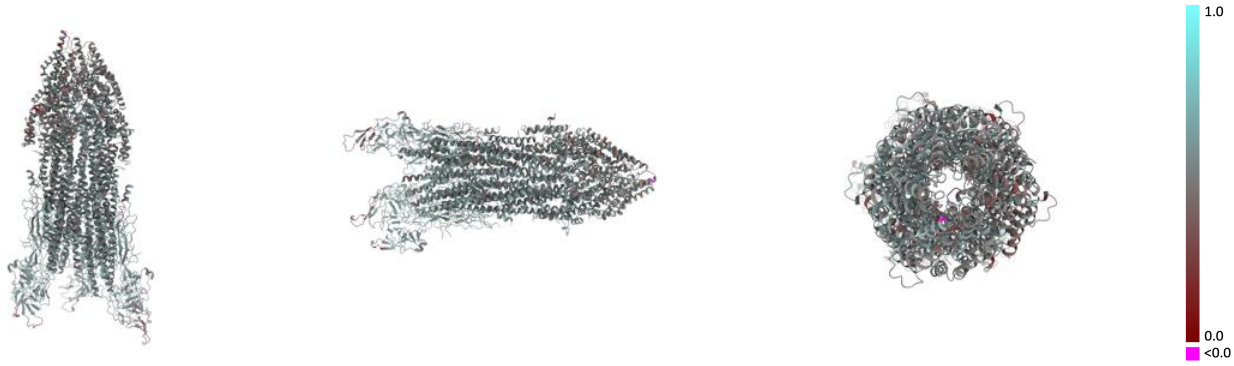
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37594 and PDB model 8WK3. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)

This section was not generated.

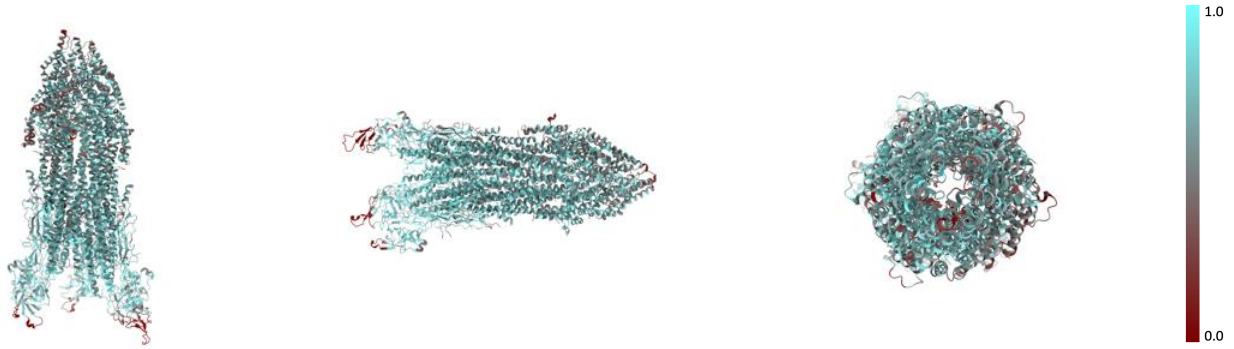
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

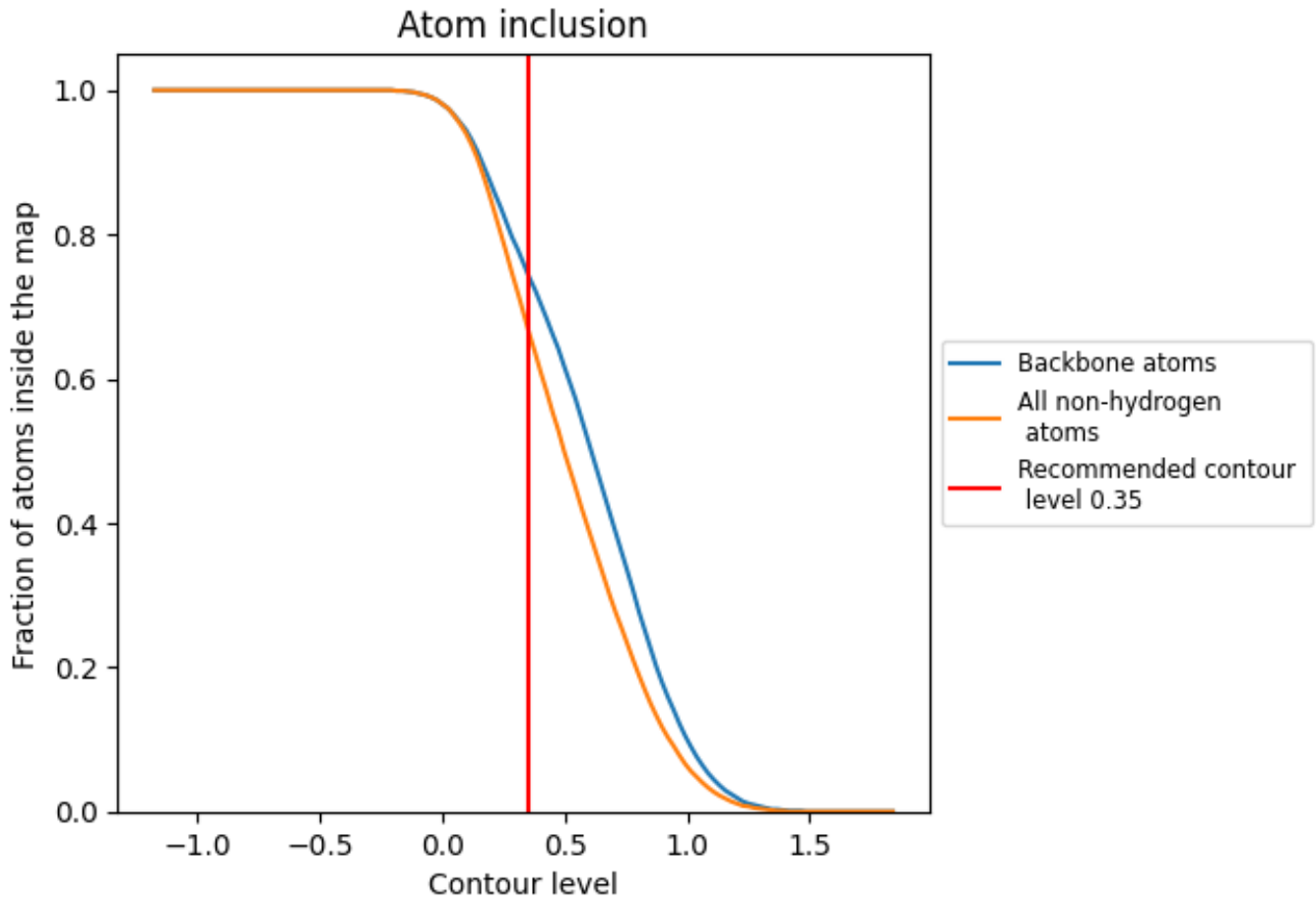
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 75% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.6700	0.5160
A	0.5010	0.4560
B	0.5990	0.4880
C	0.5990	0.4730
D	0.5430	0.4670
E	0.5210	0.4510
F	0.6250	0.4920
G	0.7090	0.5160
H	0.7270	0.5200
I	0.6900	0.5170
J	0.6310	0.5020
K	0.6330	0.5210
L	0.7060	0.5220
M	0.7280	0.5360
N	0.7250	0.5390
O	0.6840	0.5160
P	0.6750	0.5030
Q	0.6710	0.5230
R	0.7420	0.5320
S	0.7510	0.5420
T	0.7290	0.5330
U	0.7120	0.5230
V	0.6750	0.5200
W	0.7320	0.5390
X	0.7400	0.5430
Y	0.7260	0.5310
Z	0.7160	0.5310
a	0.6750	0.5220
b	0.4940	0.4790
c	0.6210	0.5170
d	0.6320	0.5250
e	0.6990	0.5460
f	0.6710	0.5110
g	0.6990	0.5260
h	0.6790	0.5470

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Chain	Atom inclusion	Q-score
i	0.6210	0.5070
j	0.6920	0.5080
k	0.6210	0.5170
l	0.6290	0.5150
m	0.6720	0.5270
n	0.7170	0.5390
o	0.7250	0.5380
p	0.6710	0.5280
q	0.5840	0.5080