wwPDB EM Validation Summary Report (i)

Aug 26, 2024 – 08:43 PM JST

PDB ID	:	8WK3
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:

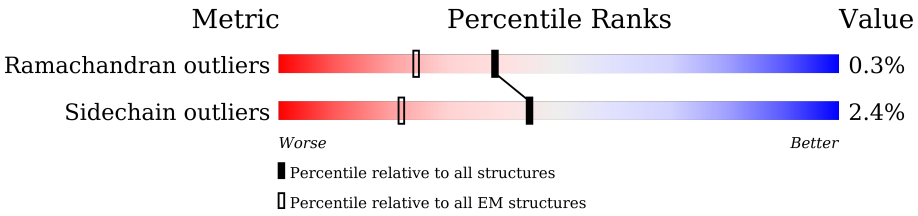
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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%, 36%, 62%
1	L	104	67%, 31%
1	M	104	70%, 29%
1	N	104	69%, 29%
1	O	104	69%, 29%
1	P	104	68%, 30%
2	Q	138	10%, 83%, 14%
2	R	138	77%, 22%
2	S	138	76%, 22%

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Mol	Chain	Length	Quality of chain
2	T	138	79% 20%
2	U	138	73% 23%
3	E	264	23% 91%
4	F	245	10% 81% 16%
4	G	245	82% 15%
4	H	245	83% 15%
4	I	245	6% 82% 15%
4	J	245	9% 83% 15%
5	A	89	34% 99%
5	B	89	15% 99%
5	C	89	17% 100%
5	D	89	26% 99%
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%
6	j	560	96%
6	k	560	97%
6	l	560	96%
7	V	134	13% 99%
7	W	134	98%

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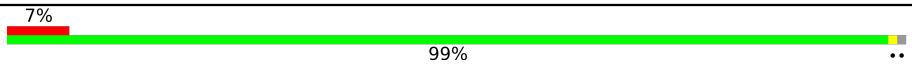
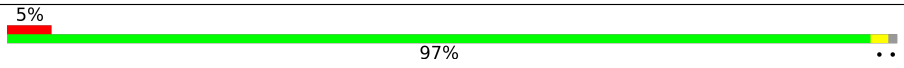
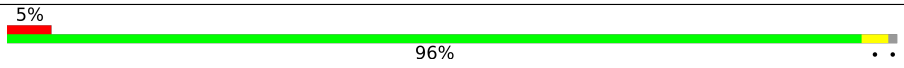
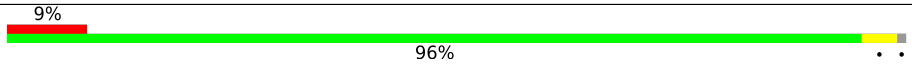
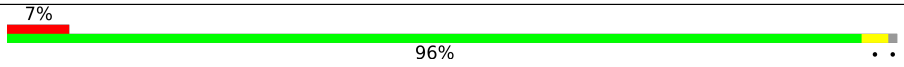
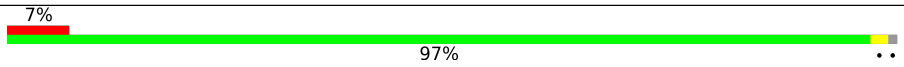
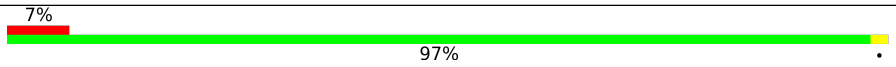
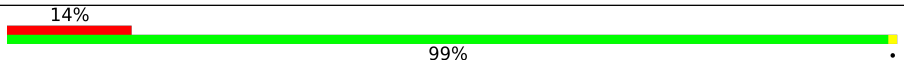
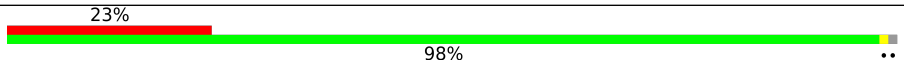
Mol	Chain	Length	Quality of chain
7	X	134	
7	Y	134	
7	Z	134	
7	a	134	
8	m	251	
8	n	251	
8	o	251	
8	p	251	
8	q	251	

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

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

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

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

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

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

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

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

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

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

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

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

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

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

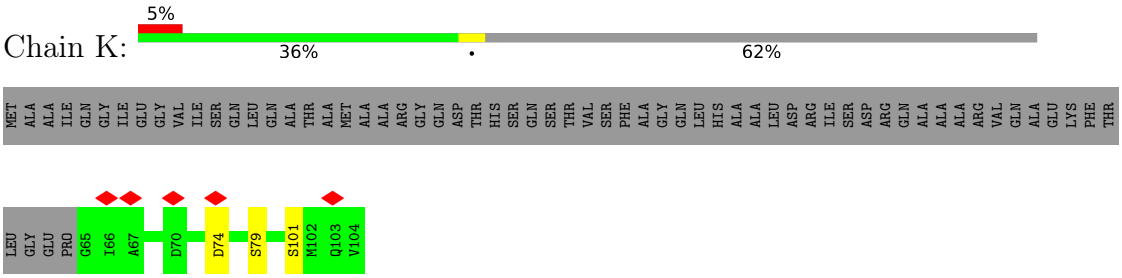
- Molecule 8 is a protein called Flagellar basal-body rod protein FlgF.

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

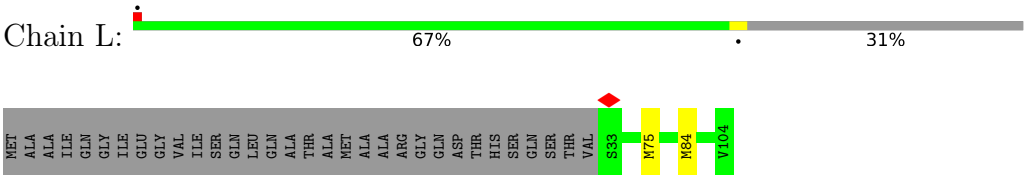
3 Residue-property plots (i)

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.

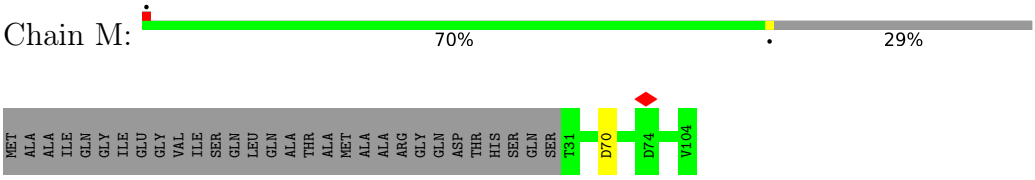
• Molecule 1: Flagellar hook-basal body complex protein FliE



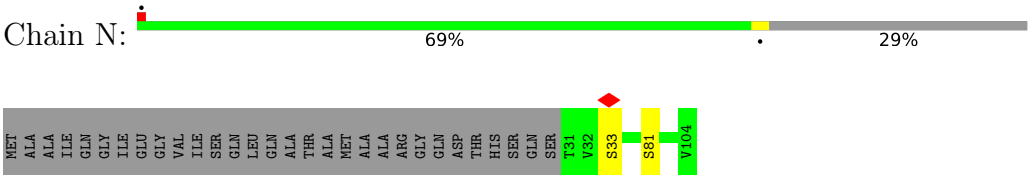
• Molecule 1: Flagellar hook-basal body complex protein FliE



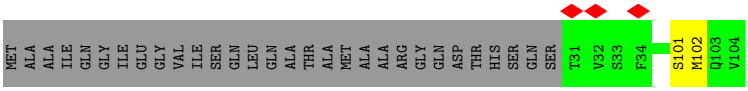
• Molecule 1: Flagellar hook-basal body complex protein FliE



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

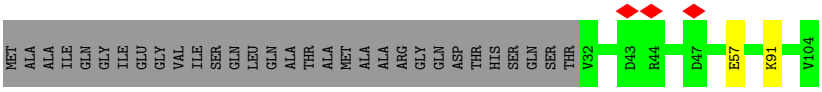


• Molecule 1: Flagellar hook-basal body complex protein FliE



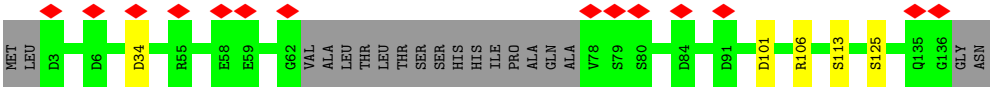
• Molecule 1: Flagellar hook-basal body complex protein FliE

Chain P:



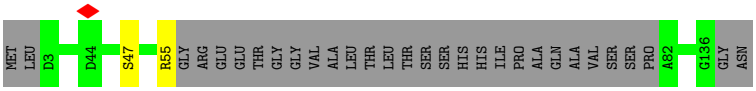
• Molecule 2: Flagellar basal body rod protein FlgB

Chain Q:



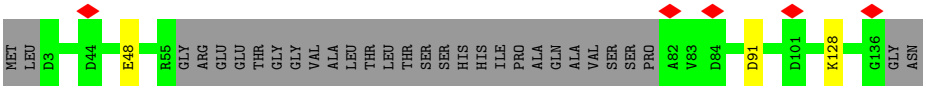
• Molecule 2: Flagellar basal body rod protein FlgB

Chain R:



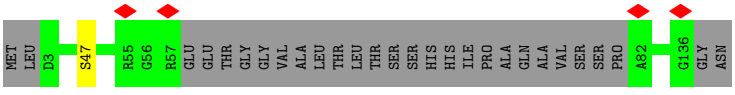
• Molecule 2: Flagellar basal body rod protein FlgB

Chain S:



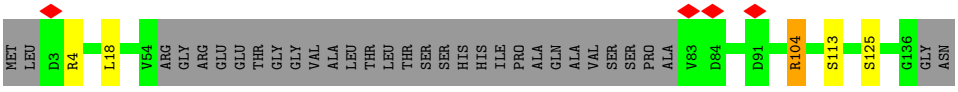
• Molecule 2: Flagellar basal body rod protein FlgB

Chain T:



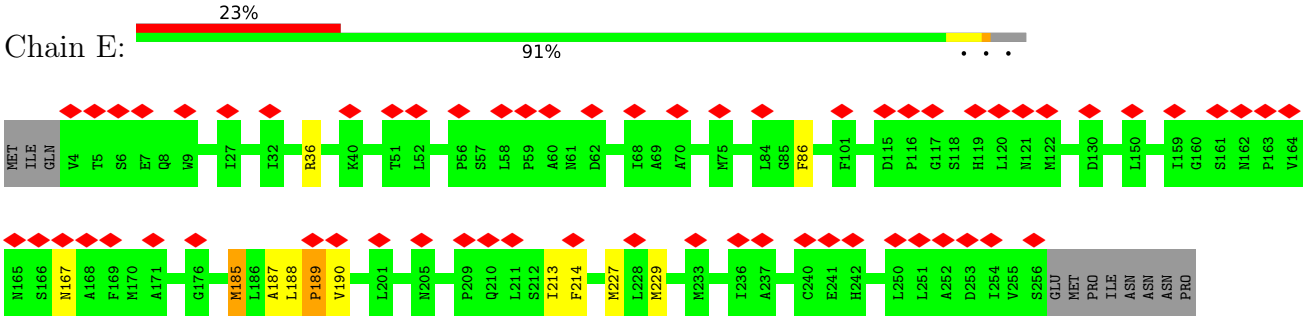
• Molecule 2: Flagellar basal body rod protein FlgB

Chain U:



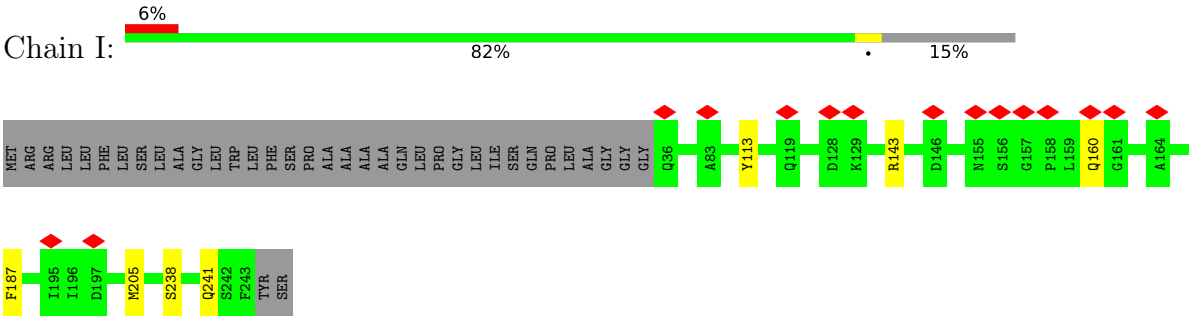
• Molecule 3: Flagellar biosynthetic protein FliR

Chain E:



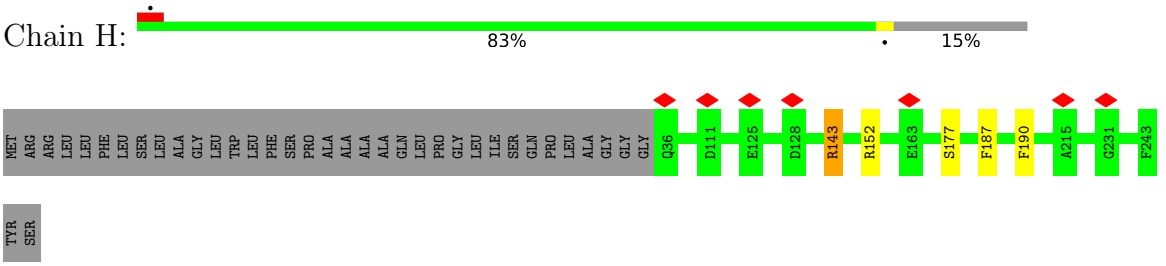
• Molecule 4: Flagellar biosynthetic protein FliP

Chain I:



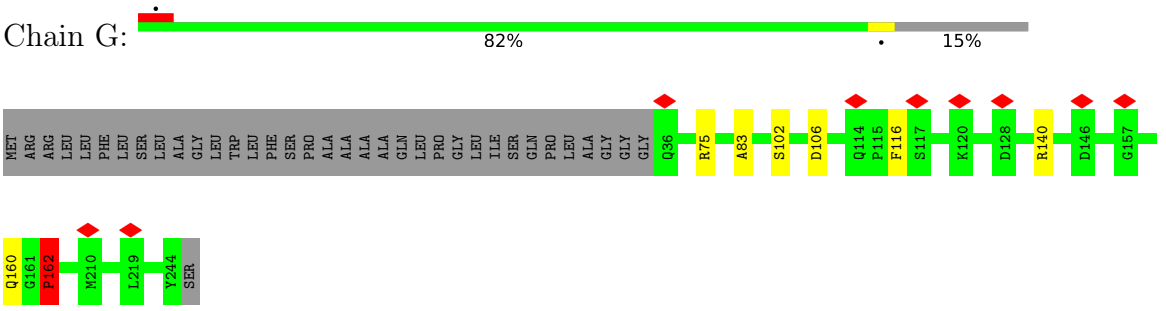
• Molecule 4: Flagellar biosynthetic protein FliP

Chain H:



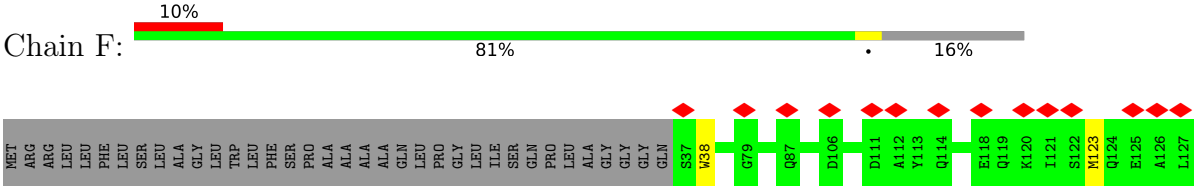
• Molecule 4: Flagellar biosynthetic protein FliP

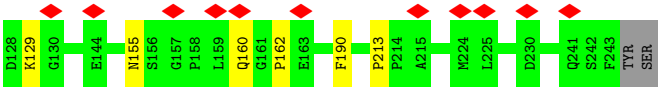
Chain G:



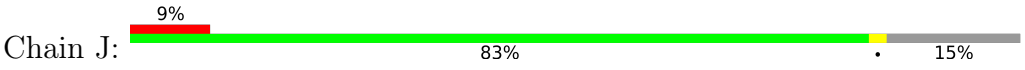
• Molecule 4: Flagellar biosynthetic protein FliP

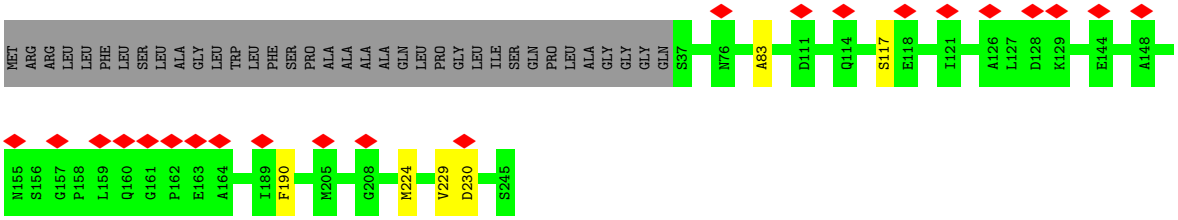
Chain F:



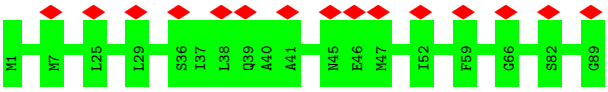


• Molecule 4: Flagellar biosynthetic protein FliP

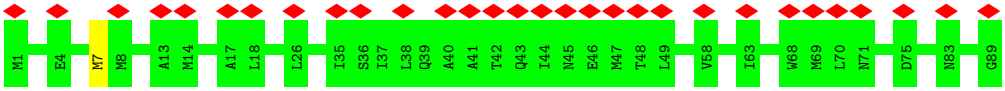




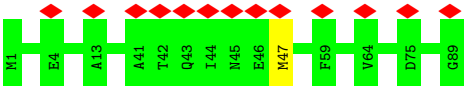
• Molecule 5: Flagellar biosynthetic protein FliQ



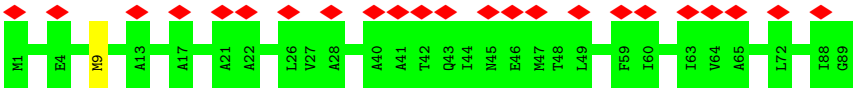
• Molecule 5: Flagellar biosynthetic protein FliQ



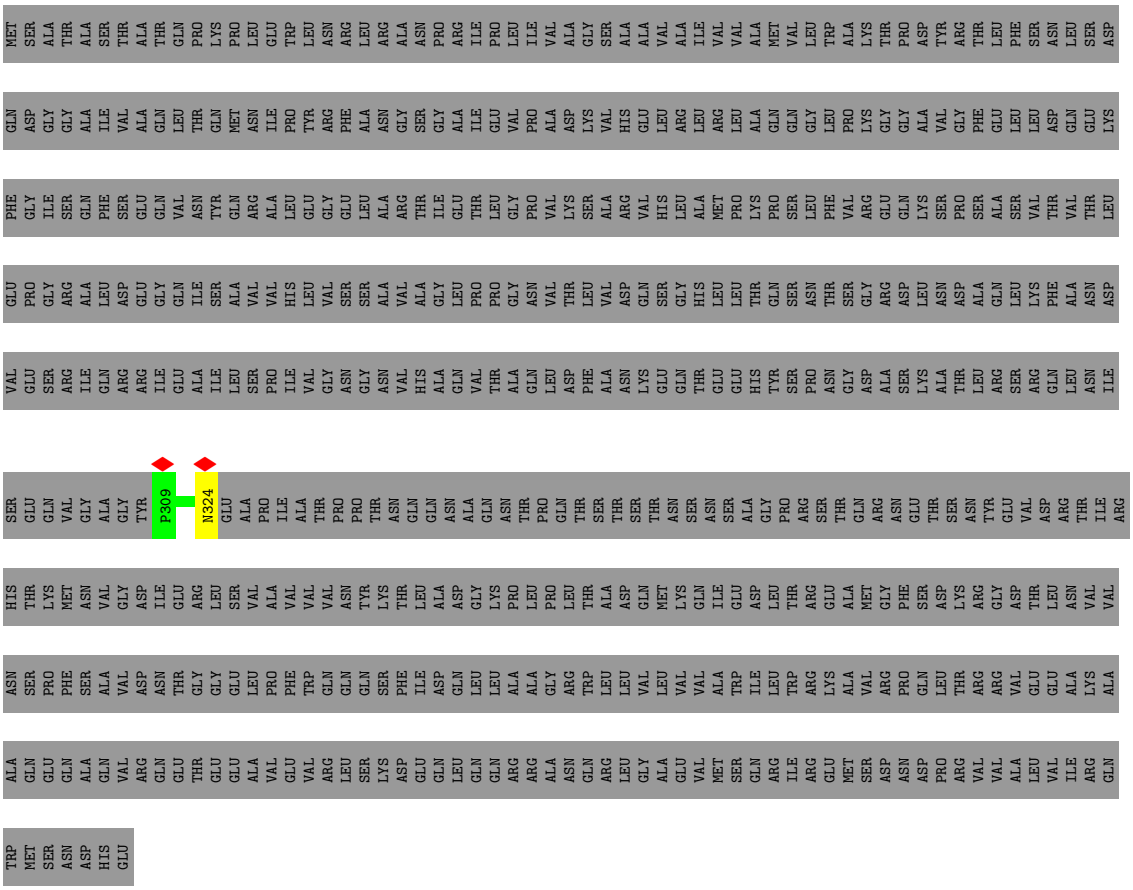
• Molecule 5: Flagellar biosynthetic protein FliQ



• Molecule 5: Flagellar biosynthetic protein FliQ

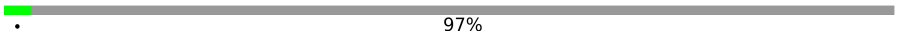


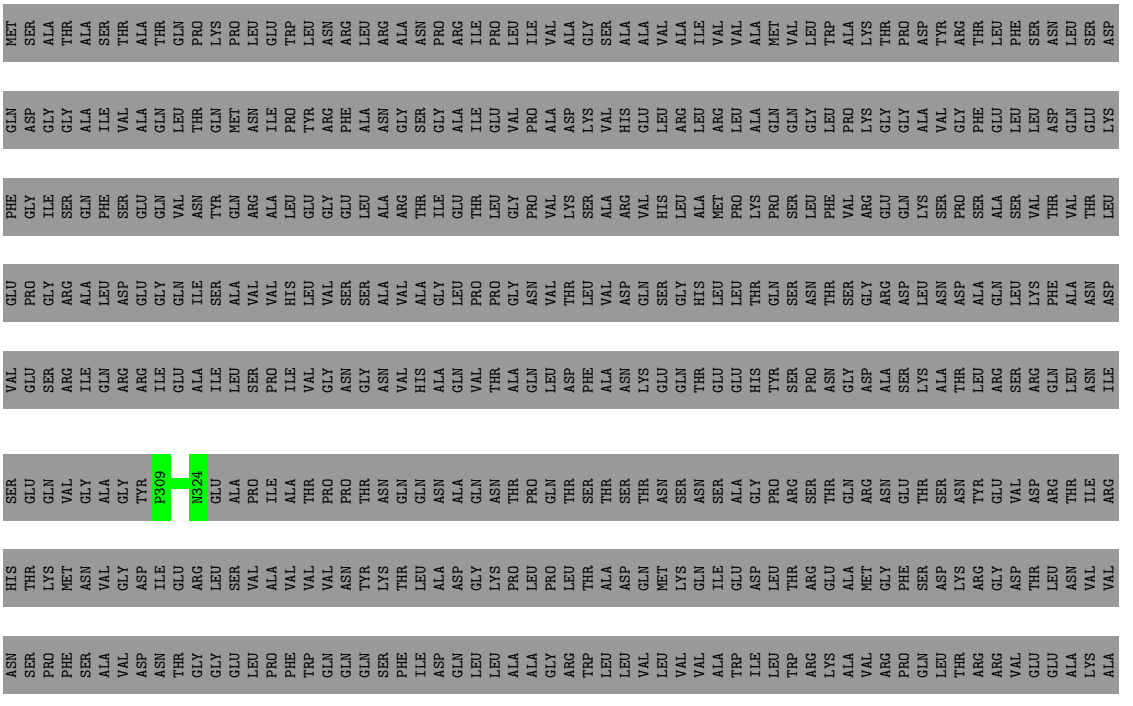
• Molecule 6: Flagellar M-ring protein

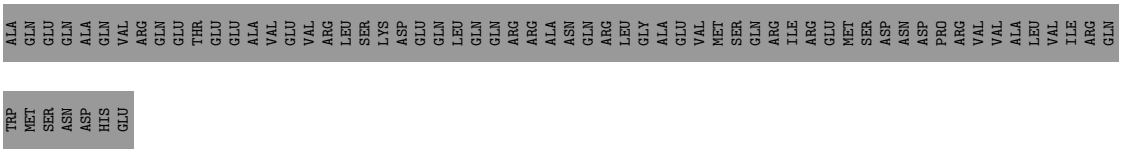


• Molecule 6: Flagellar M-ring protein

Chain e:

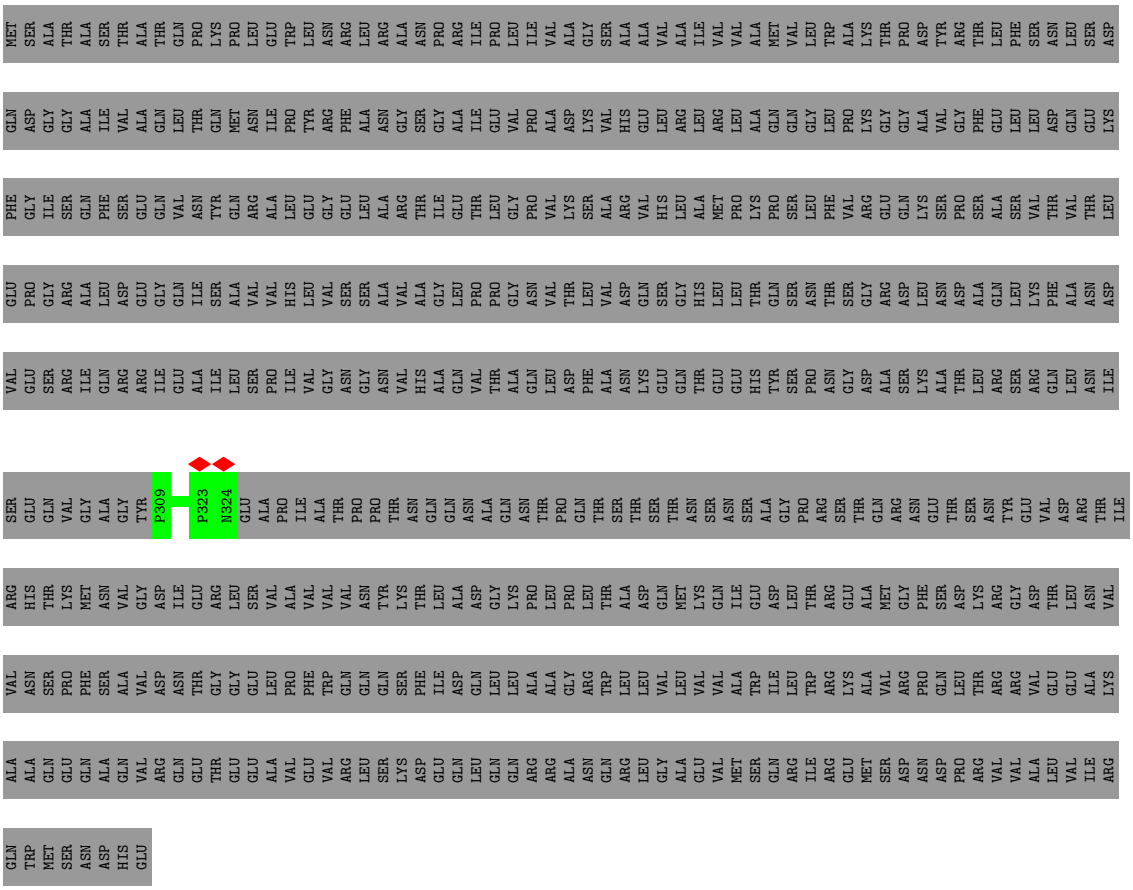






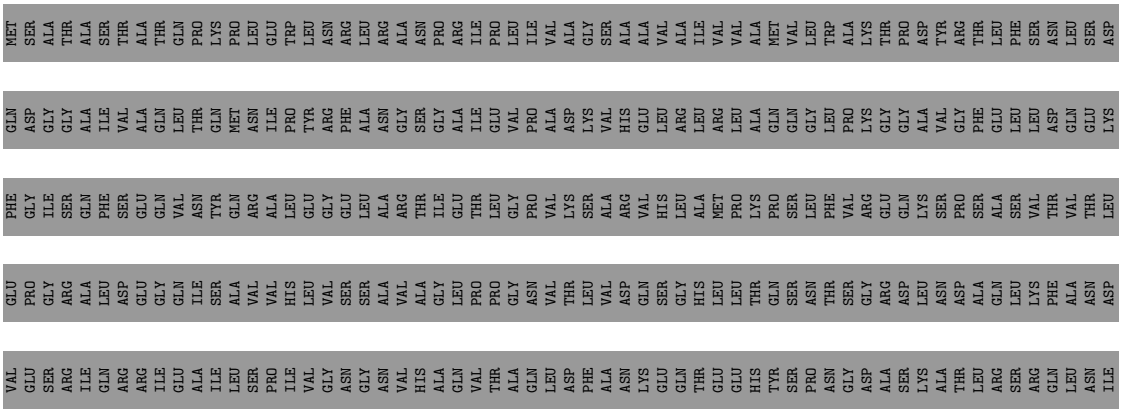
• Molecule 6: Flagellar M-ring protein

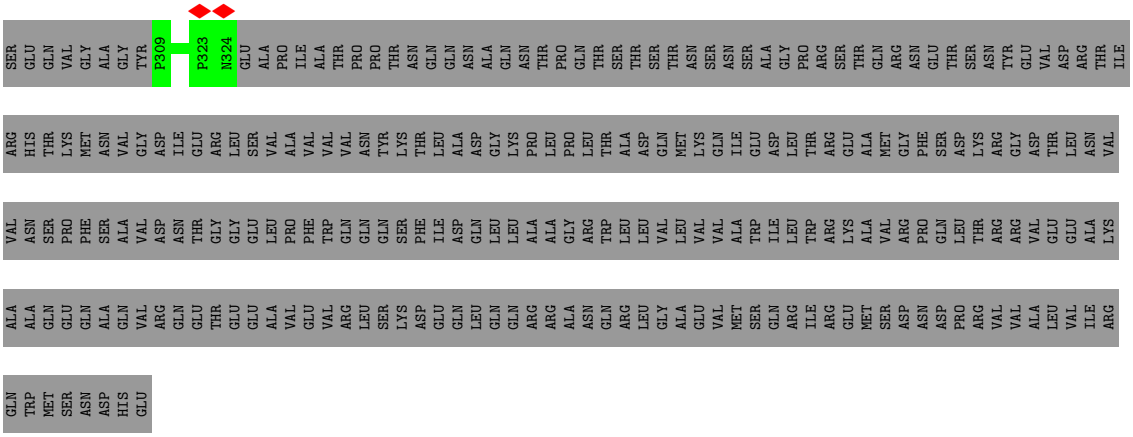
Chain g: 97%



• Molecule 6: Flagellar M-ring protein

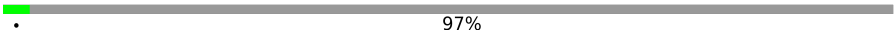
Chain i: 97%

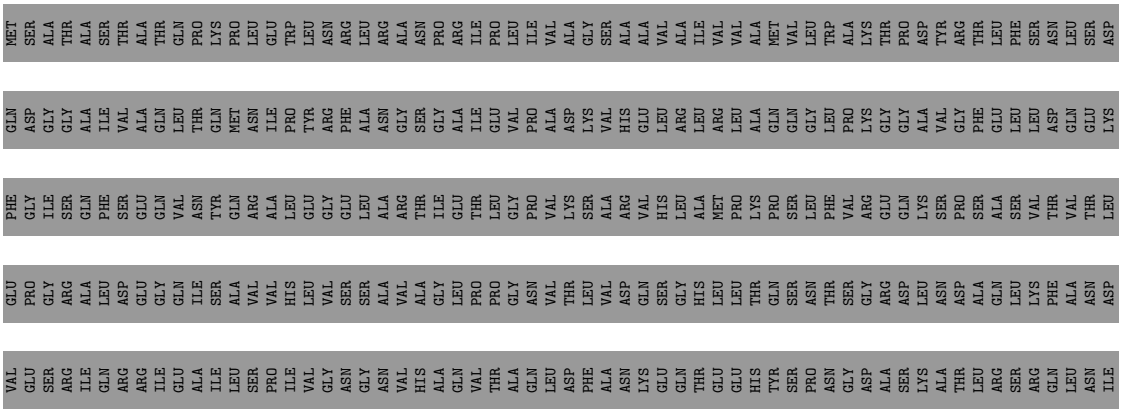


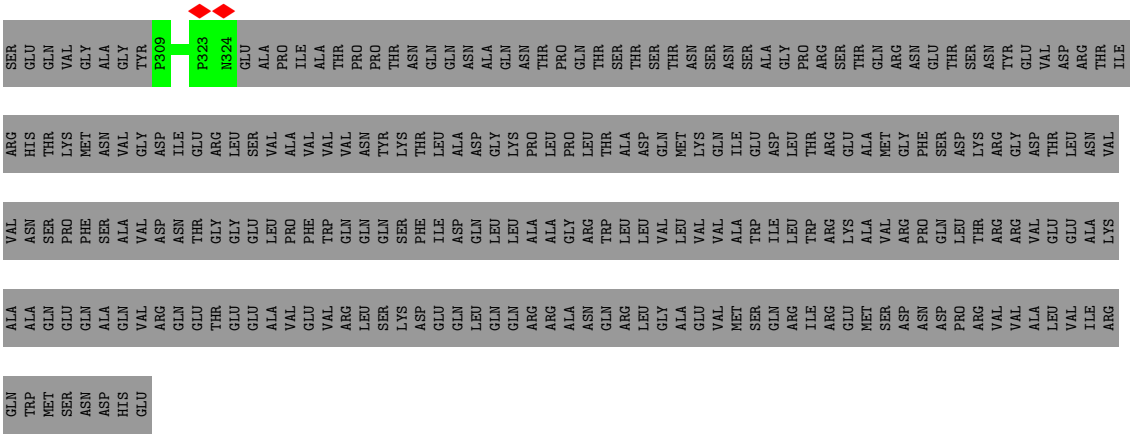


• Molecule 6: Flagellar M-ring protein

Chain k:

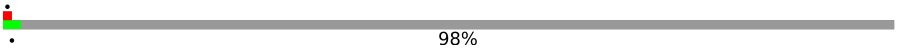


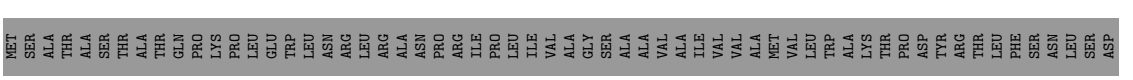


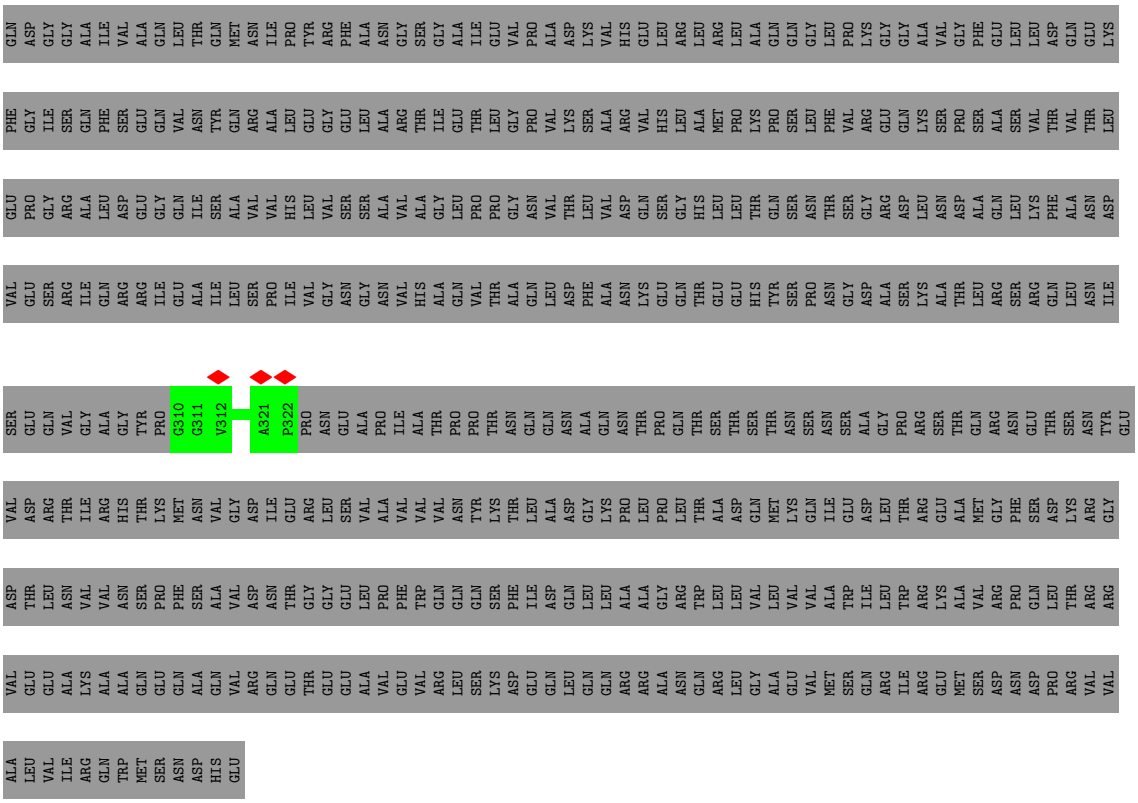


• Molecule 6: Flagellar M-ring protein

Chain b:

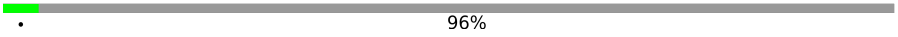


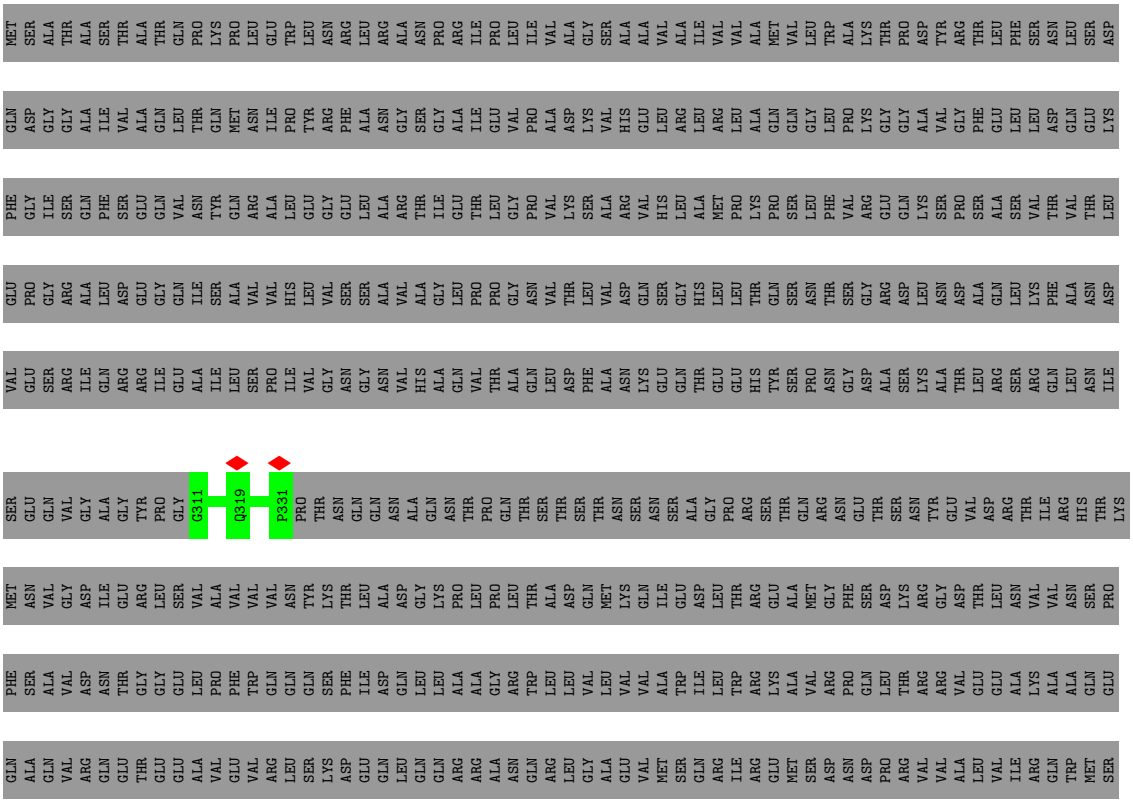




• Molecule 6: Flagellar M-ring protein

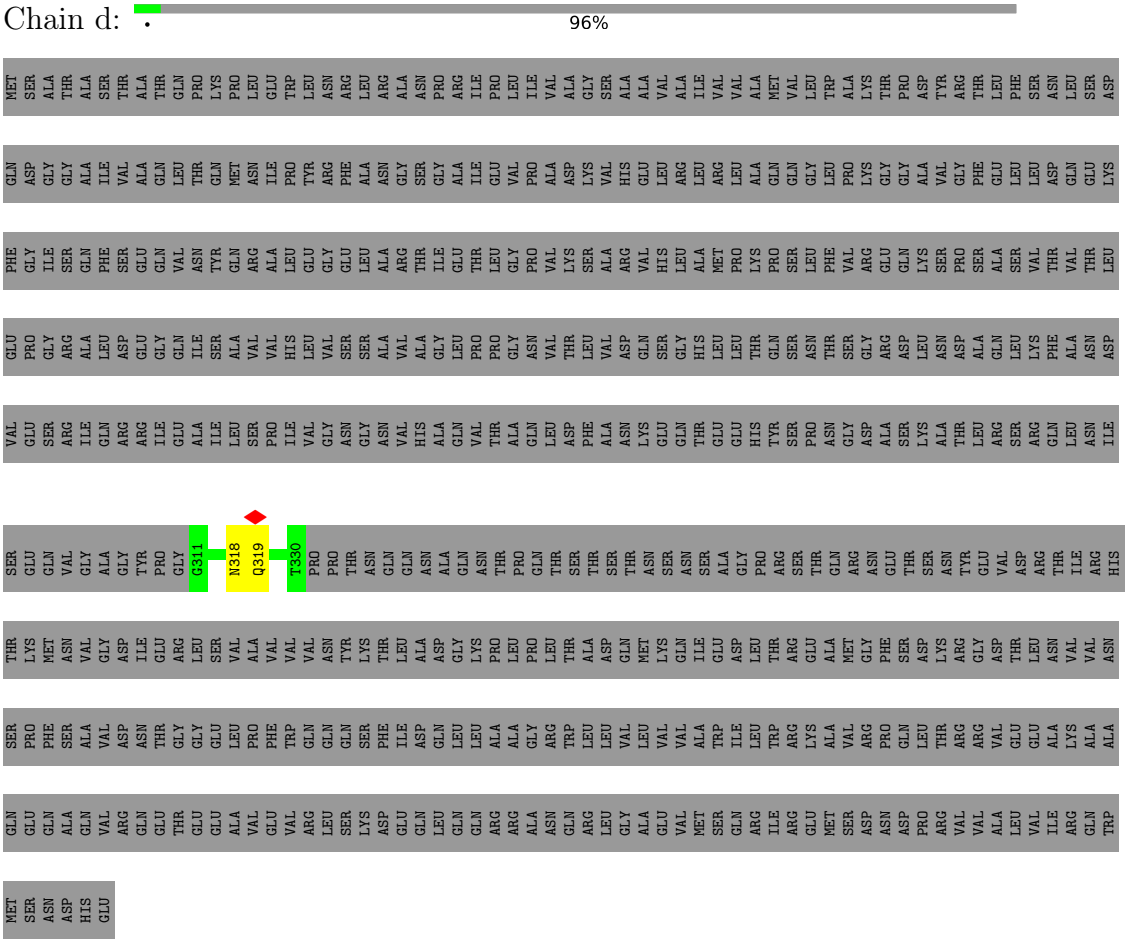
Chain h:





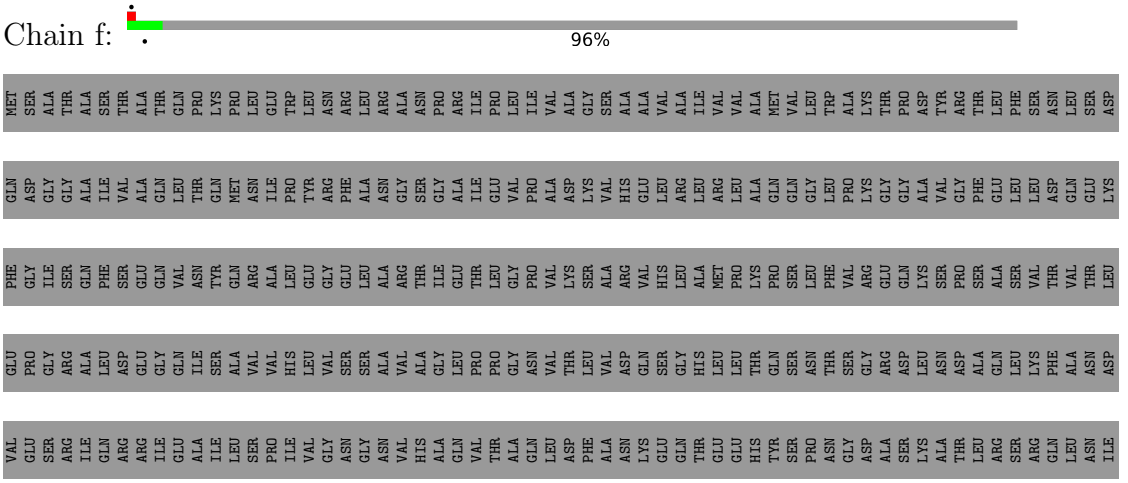
• Molecule 6: Flagellar M-ring protein

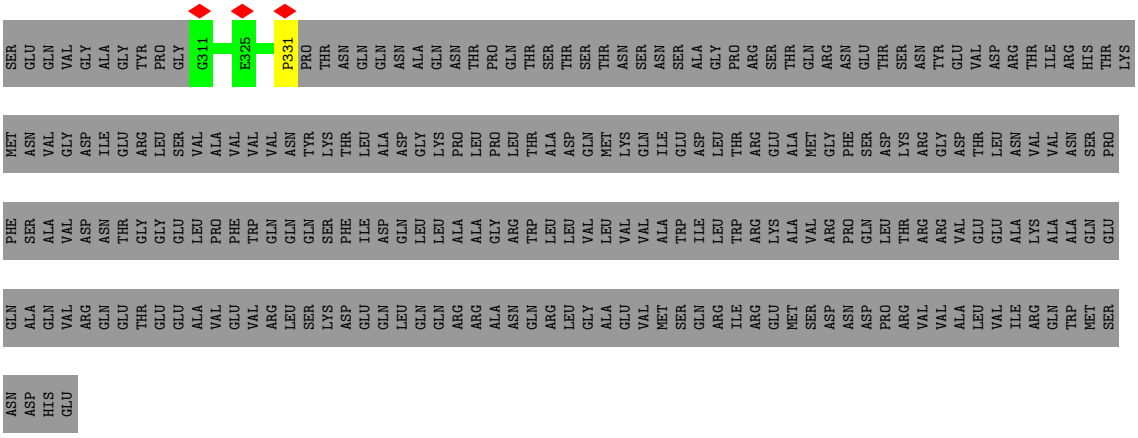
Chain d:



• Molecule 6: Flagellar M-ring protein

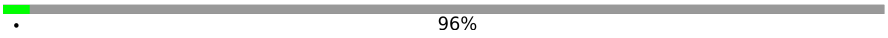
Chain f:

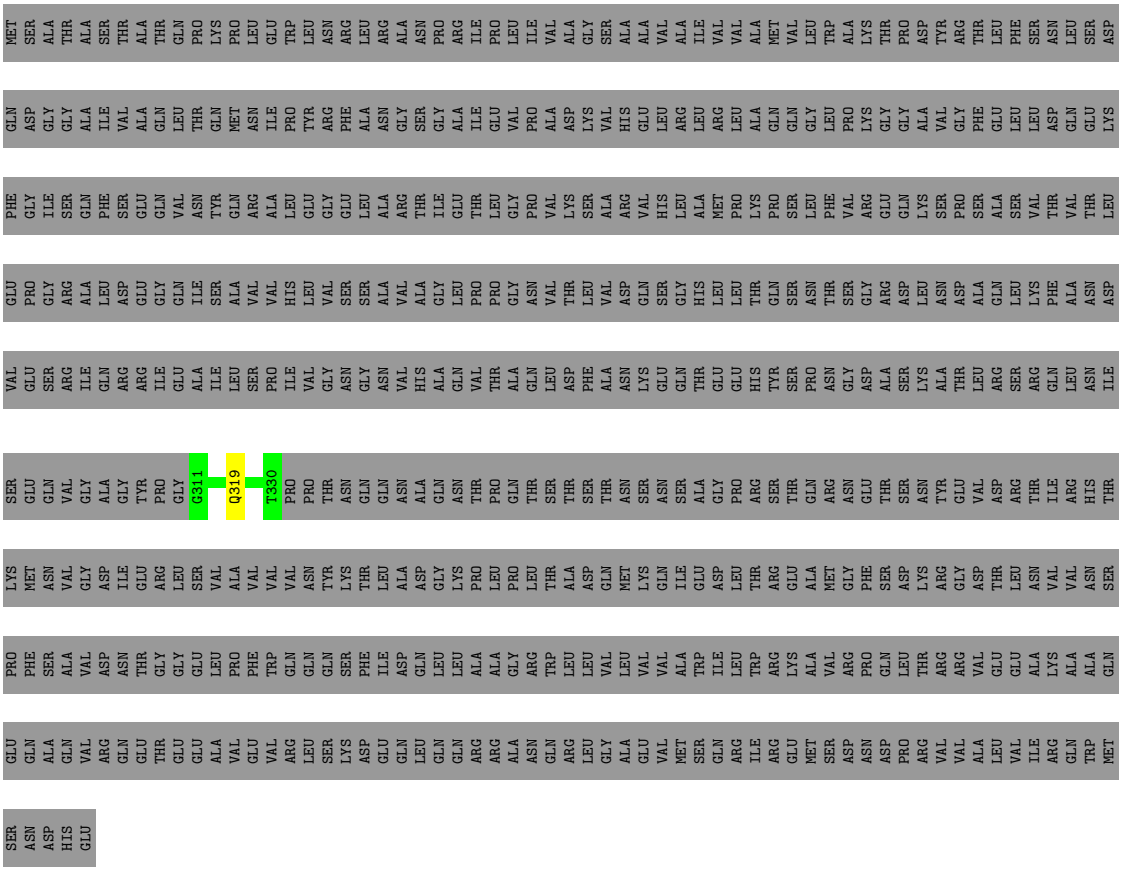




• Molecule 6: Flagellar M-ring protein

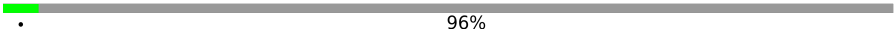
Chain j:

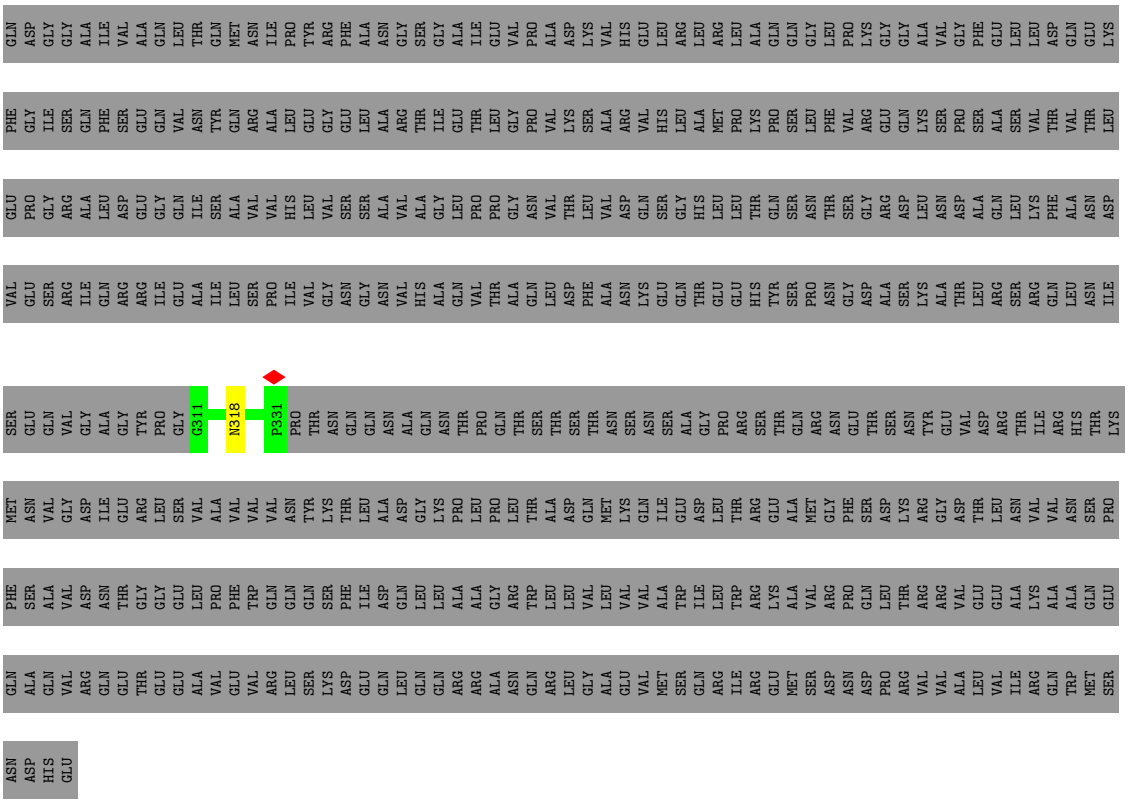




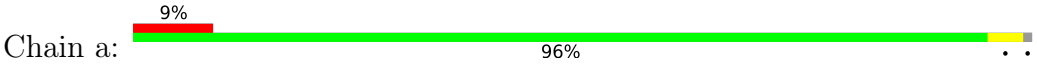
• Molecule 6: Flagellar M-ring protein

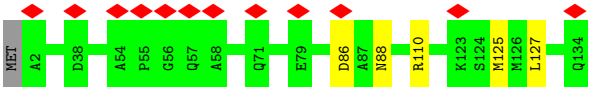
Chain l:



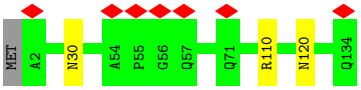


• Molecule 7: Flagellar basal-body rod protein FlgC

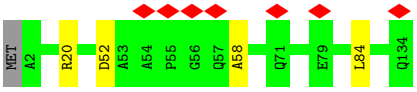




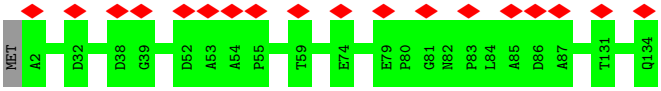
• Molecule 7: Flagellar basal-body rod protein FlgC



• Molecule 7: Flagellar basal-body rod protein FlgC

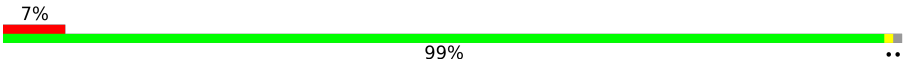


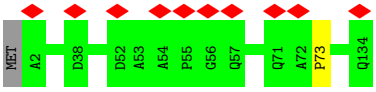
• Molecule 7: Flagellar basal-body rod protein FlgC



• Molecule 7: Flagellar basal-body rod protein FlgC

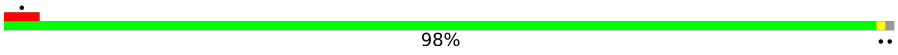
Chain X:

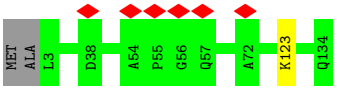




• Molecule 7: Flagellar basal-body rod protein FlgC

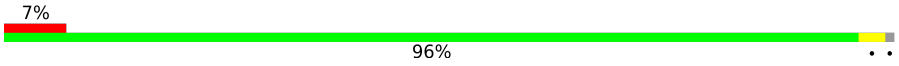
Chain W:

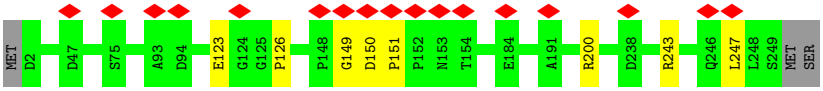




• Molecule 8: Flagellar basal-body rod protein FlgF

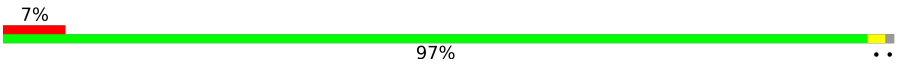
Chain m:

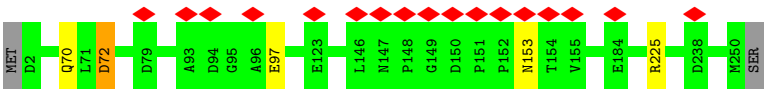




• Molecule 8: Flagellar basal-body rod protein FlgF

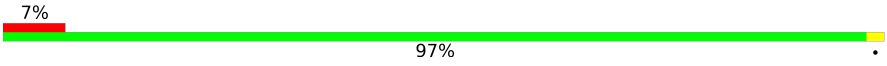
Chain n:

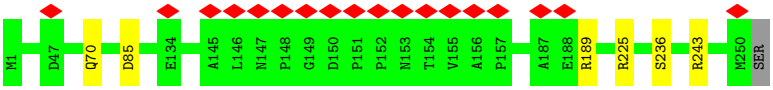




• Molecule 8: Flagellar basal-body rod protein FlgF

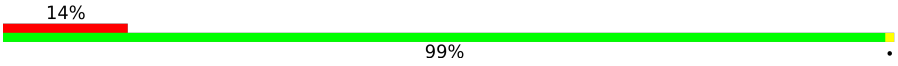
Chain o:

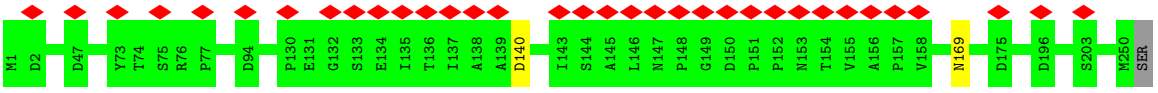




• Molecule 8: Flagellar basal-body rod protein FlgF

Chain p:

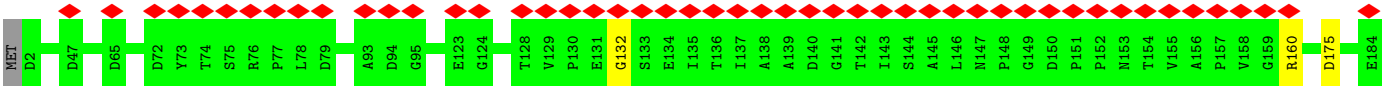


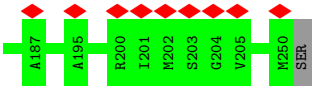


• Molecule 8: Flagellar basal-body rod protein FlgF

Chain q:


23%
98%


MET
D2
D47
D65
D72
Y73
T74
S75
R76
P77
L78
D79
A93
D94
G95
E123
G124
T128
V129
P130
E131
G132
S133
E134
I135
T136
I137
A138
A139
D140
G141
T142
I143
S144
A145
L146
N147
P148
G149
D150
P151
P152
N153
T154
V155
A156
P157
V158
G159
R160
D175
E184


A187
A195
R200
I201
M202
S203
G204
V205
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	0.26	0/300	0.47	0/400
1	L	0.25	0/547	0.44	0/733
1	M	0.26	0/561	0.44	0/753
1	N	0.25	0/561	0.46	0/753
1	O	0.26	0/561	0.49	0/753
1	P	0.27	0/554	0.46	0/743
2	Q	0.28	0/930	0.54	0/1251
2	R	0.26	0/855	0.48	0/1150
2	S	0.27	0/855	0.54	0/1150
2	T	0.25	0/870	0.49	0/1169
2	U	0.26	0/839	0.47	0/1129
3	E	0.38	1/1994 (0.1%)	0.56	1/2724 (0.0%)
4	F	0.36	0/1643	0.62	2/2237 (0.1%)
4	G	0.29	0/1665	0.49	1/2267 (0.0%)
4	H	0.29	0/1652	0.48	0/2249
4	I	0.28	0/1652	0.46	0/2249
4	J	0.30	0/1662	0.49	0/2263
5	A	0.29	0/681	0.47	0/930
5	B	0.26	0/681	0.49	0/930
5	C	0.28	0/681	0.48	0/930
5	D	0.28	0/681	0.49	0/930
6	b	0.52	0/83	0.63	0/114
6	c	0.26	0/107	0.38	0/148
6	d	0.30	0/137	0.49	0/191
6	e	0.28	0/107	0.56	0/148
6	f	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
6	g	0.32	0/107	0.51	0/148
6	h	0.26	0/145	0.43	0/203
6	i	0.30	0/107	0.38	0/148
6	j	0.30	0/137	0.57	0/191
6	k	0.30	0/107	0.37	0/148
6	l	0.29	0/145	0.45	0/203
7	V	0.28	0/981	0.44	0/1334
7	W	0.26	0/976	0.46	0/1327

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	X	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
7	Y	0.28	0/981	0.52	0/1334
7	Z	0.26	0/981	0.47	0/1334
7	a	0.28	0/981	0.47	0/1334
8	m	0.33	0/1828	0.56	0/2492
8	n	0.28	0/1836	0.54	1/2502 (0.0%)
8	o	0.28	0/1844	0.54	0/2512
8	p	0.27	0/1844	0.53	0/2512
8	q	0.31	0/1836	0.55	0/2502
All	All	0.31	4/36821 (0.0%)	0.53	11/50055 (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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	331	PRO	CG-CD	-14.24	1.03	1.50
7	X	73	PRO	CG-CD	-12.72	1.08	1.50
7	X	73	PRO	CB-CG	-7.64	1.11	1.50
3	E	185	MET	C-O	6.30	1.35	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	73	PRO	CB-CG-CD	18.81	179.87	106.50
7	X	73	PRO	N-CD-CG	-18.79	75.01	103.20
6	f	331	PRO	N-CD-CG	-16.10	79.05	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	73	PRO	CA-CB-CG	-13.99	77.42	104.00
4	F	162	PRO	CA-N-CD	-12.03	94.66	111.50

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)

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	5	25
4	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
4	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	42
4	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
4	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	56
4	J	207/245 (84%)	200 (97%)	5 (2%)	2 (1%)	13	42
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
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	46
7	a	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
8	m	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	11	38
8	n	247/251 (98%)	241 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	o	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
8	p	248/251 (99%)	240 (97%)	8 (3%)	0	100	100
8	q	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	61
All	All	4751/11378 (42%)	4588 (97%)	147 (3%)	16 (0%)	38	66

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%)	30 (91%)	3 (9%)	7	27
1	L	56/79 (71%)	54 (96%)	2 (4%)	30	57
1	M	58/79 (73%)	57 (98%)	1 (2%)	56	74
1	N	58/79 (73%)	56 (97%)	2 (3%)	32	59
1	O	58/79 (73%)	56 (97%)	2 (3%)	32	59
1	P	57/79 (72%)	55 (96%)	2 (4%)	31	58
2	Q	98/113 (87%)	94 (96%)	4 (4%)	26	54
2	R	90/113 (80%)	88 (98%)	2 (2%)	47	69
2	S	90/113 (80%)	87 (97%)	3 (3%)	33	60
2	T	91/113 (80%)	90 (99%)	1 (1%)	70	82
2	U	89/113 (79%)	84 (94%)	5 (6%)	17	45
3	E	210/221 (95%)	204 (97%)	6 (3%)	37	63
4	F	177/204 (87%)	170 (96%)	7 (4%)	27	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	G	179/204 (88%)	172 (96%)	7 (4%)	27 55
4	H	178/204 (87%)	173 (97%)	5 (3%)	38 64
4	I	178/204 (87%)	172 (97%)	6 (3%)	32 59
4	J	179/204 (88%)	175 (98%)	4 (2%)	47 69
5	A	74/74 (100%)	73 (99%)	1 (1%)	62 78
5	B	74/74 (100%)	73 (99%)	1 (1%)	62 78
5	C	74/74 (100%)	74 (100%)	0	100 100
5	D	74/74 (100%)	73 (99%)	1 (1%)	62 78
6	b	8/467 (2%)	8 (100%)	0	100 100
6	c	11/467 (2%)	10 (91%)	1 (9%)	7 27
6	d	14/467 (3%)	12 (86%)	2 (14%)	2 12
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%)	12 37
6	k	11/467 (2%)	11 (100%)	0	100 100
6	l	15/467 (3%)	14 (93%)	1 (7%)	13 39
7	V	104/105 (99%)	104 (100%)	0	100 100
7	W	104/105 (99%)	103 (99%)	1 (1%)	73 84
7	X	104/105 (99%)	104 (100%)	0	100 100
7	Y	104/105 (99%)	102 (98%)	2 (2%)	52 72
7	Z	104/105 (99%)	101 (97%)	3 (3%)	37 63
7	a	104/105 (99%)	100 (96%)	4 (4%)	28 56
8	m	190/193 (98%)	187 (98%)	3 (2%)	58 76
8	n	191/193 (99%)	187 (98%)	4 (2%)	48 70
8	o	192/193 (100%)	187 (97%)	5 (3%)	41 66
8	p	192/193 (100%)	190 (99%)	2 (1%)	73 84
8	q	191/193 (99%)	190 (100%)	1 (0%)	86 91
All	All	3891/9308 (42%)	3796 (98%)	95 (2%)	45 68

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	p	169	ASN
4	G	75	ARG
7	Y	30	ASN
4	H	190	PHE
4	G	140	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	155	ASN
5	D	39	GLN
7	W	120	ASN
3	E	162	ASN
2	U	112	ASN

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.

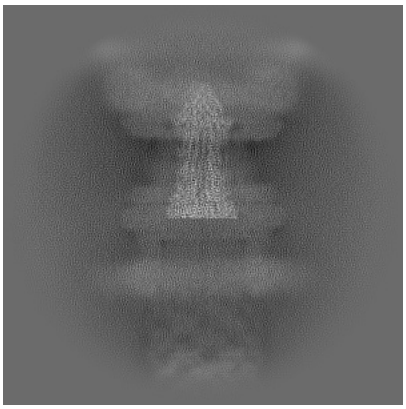
6 Map visualisation

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.

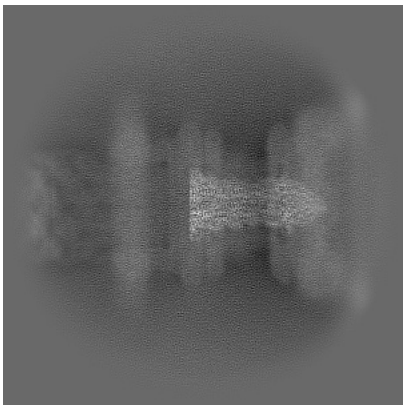
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

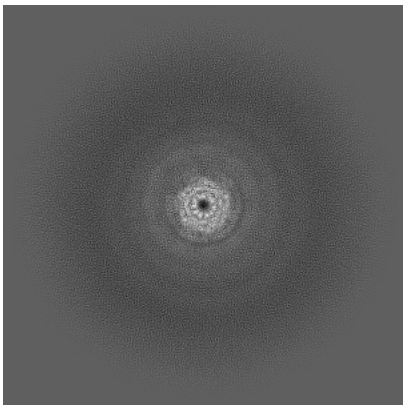
6.1.1 Primary map



X

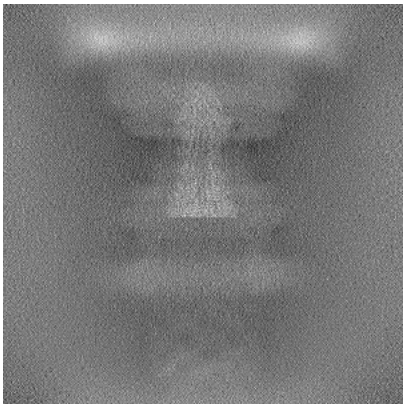


Y

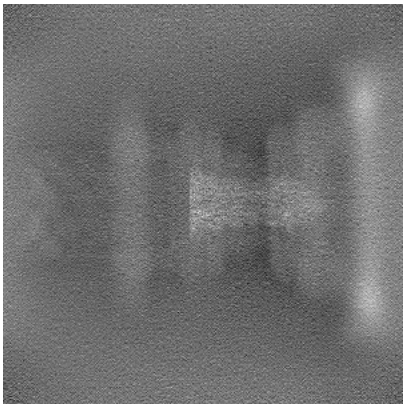


Z

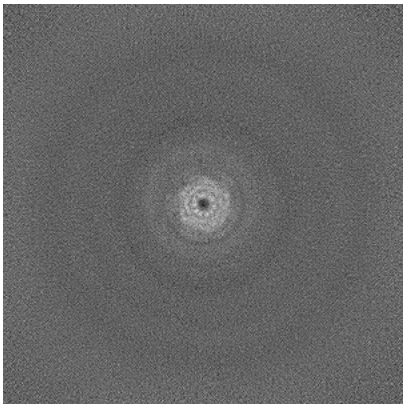
6.1.2 Raw map



X



Y

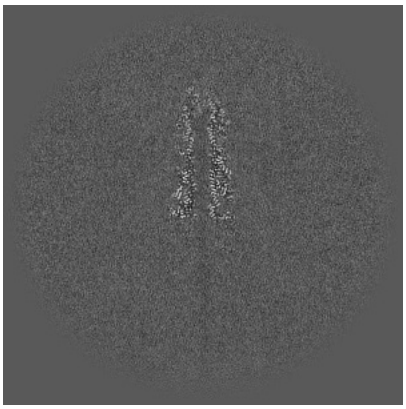


Z

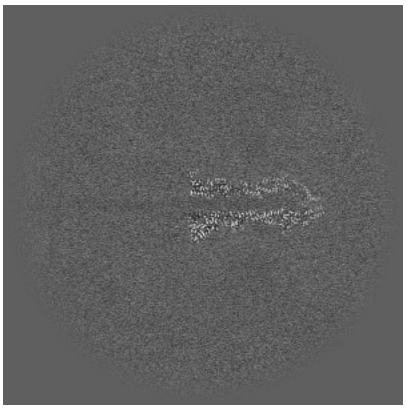
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

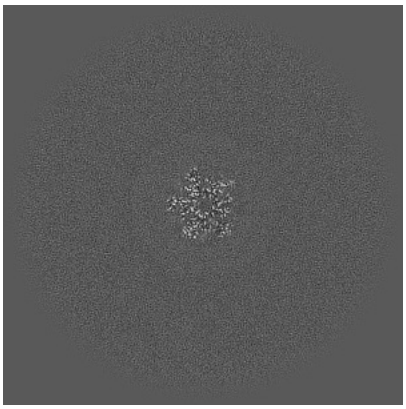
6.2.1 Primary map



X Index: 256

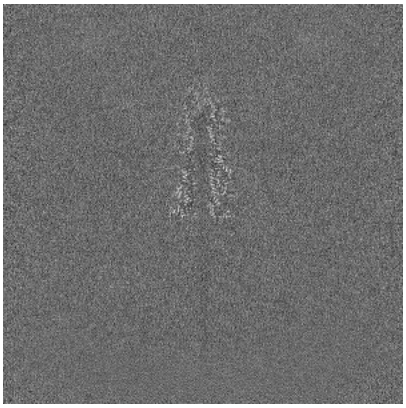


Y Index: 256

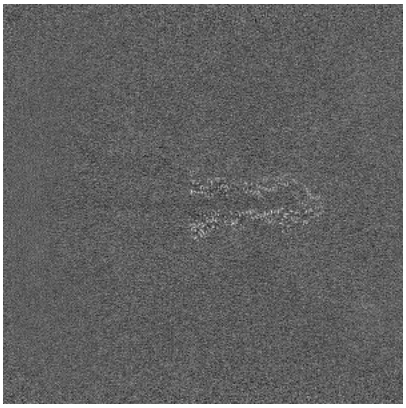


Z Index: 256

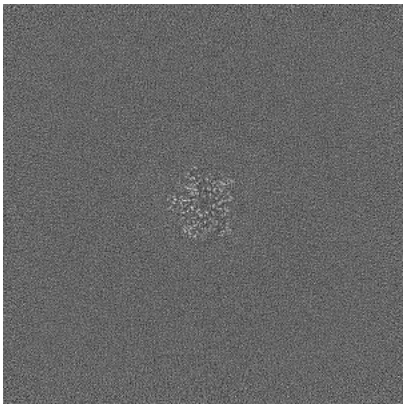
6.2.2 Raw map



X Index: 256



Y Index: 256

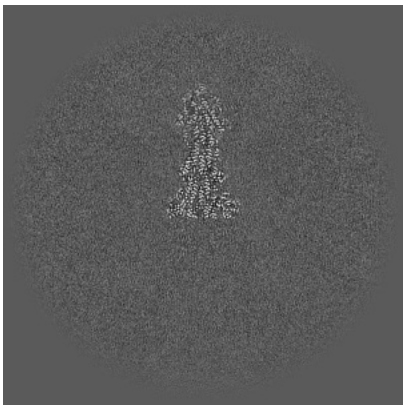


Z Index: 256

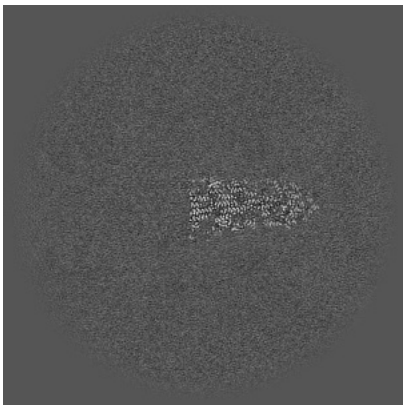
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

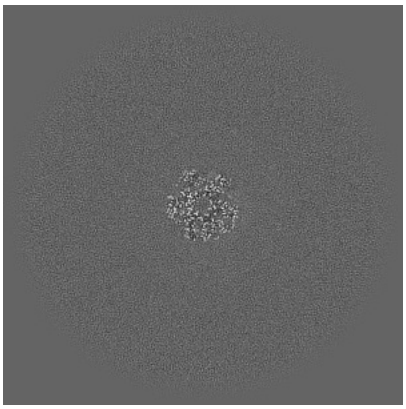
6.3.1 Primary map



X Index: 244

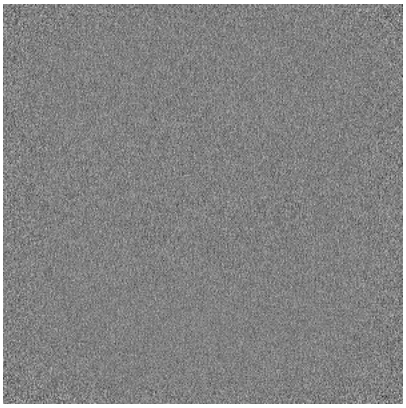


Y Index: 268

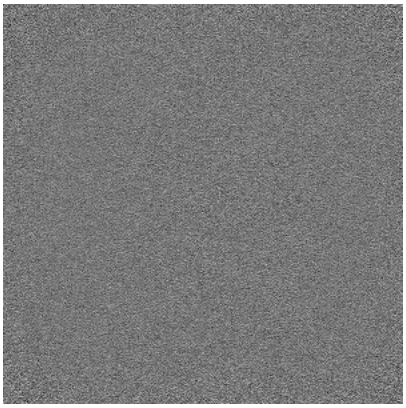


Z Index: 247

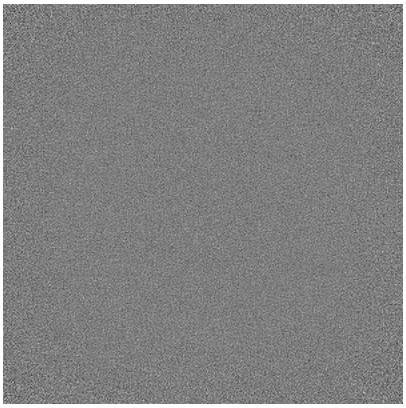
6.3.2 Raw map



X Index: 0



Y Index: 0

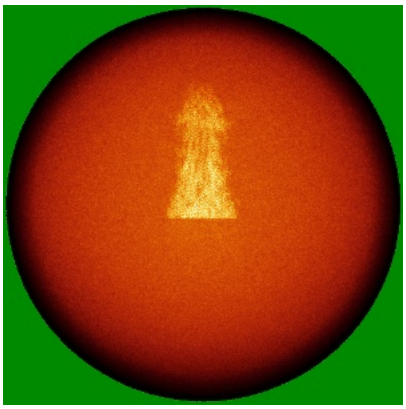


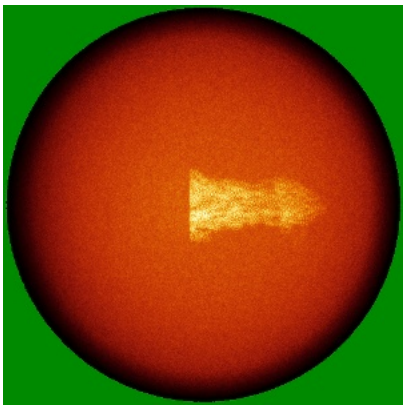
Z Index: 0

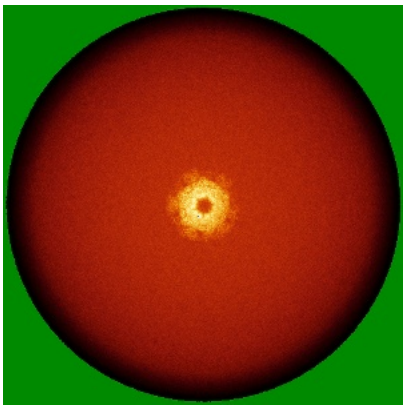
The images above show the largest variance slices of the map in three orthogonal directions.

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

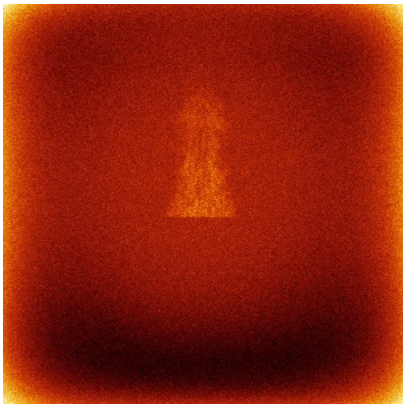
6.4.1 Primary map

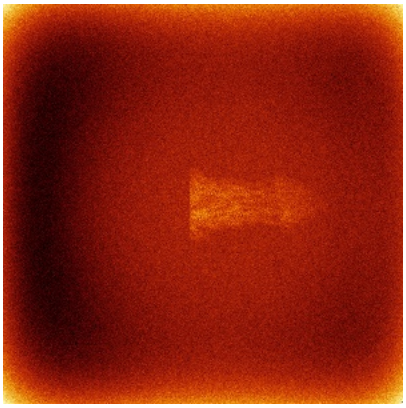

X

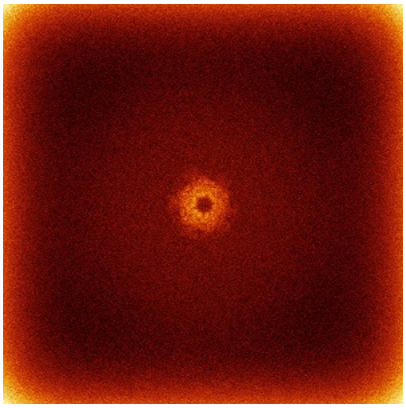

Y


Z

6.4.2 Raw map


X

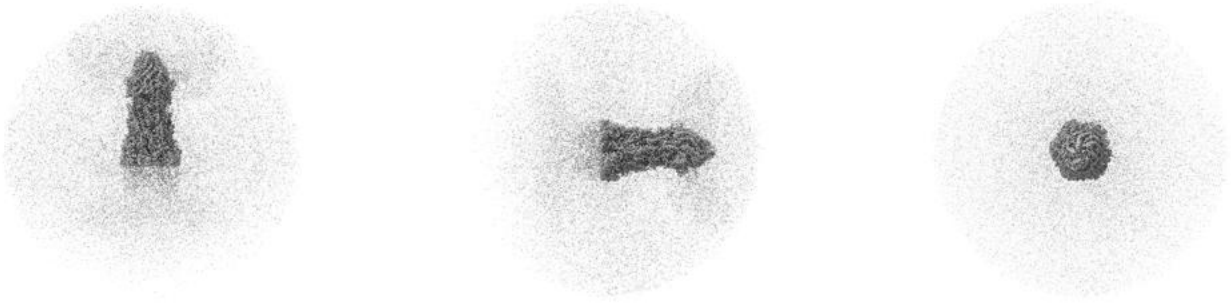

Y


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)

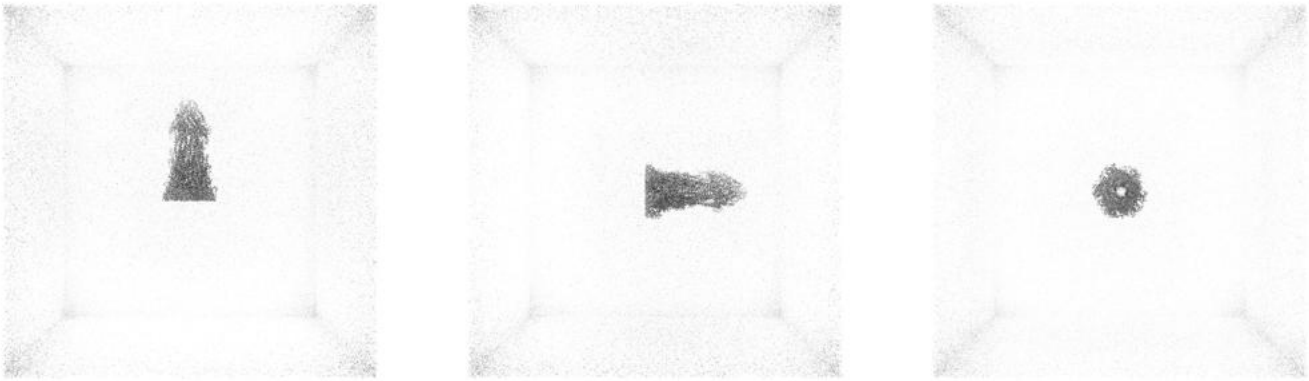
6.5.1 Primary map



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.

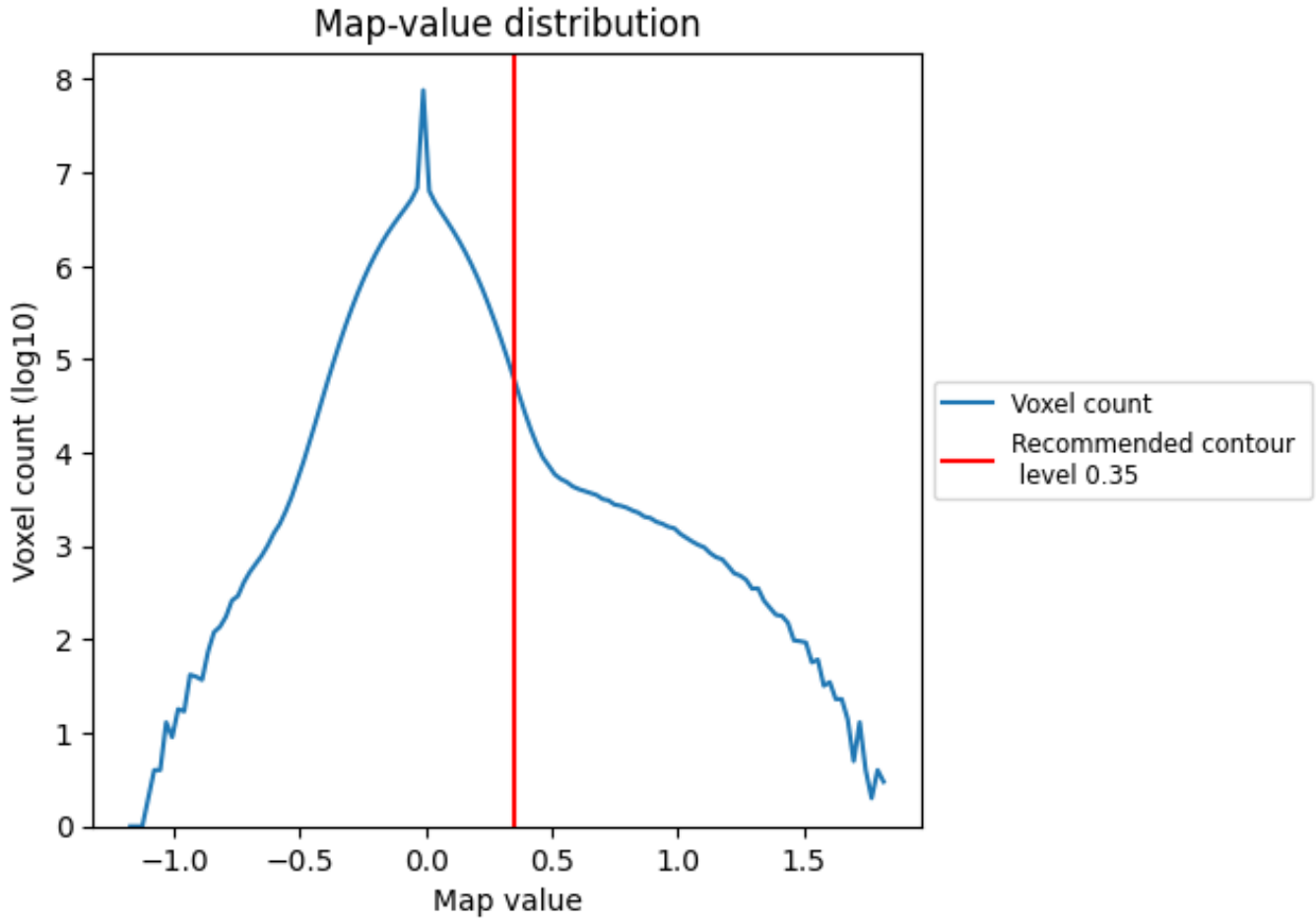
6.6 Mask visualisation (i)

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

7 Map analysis

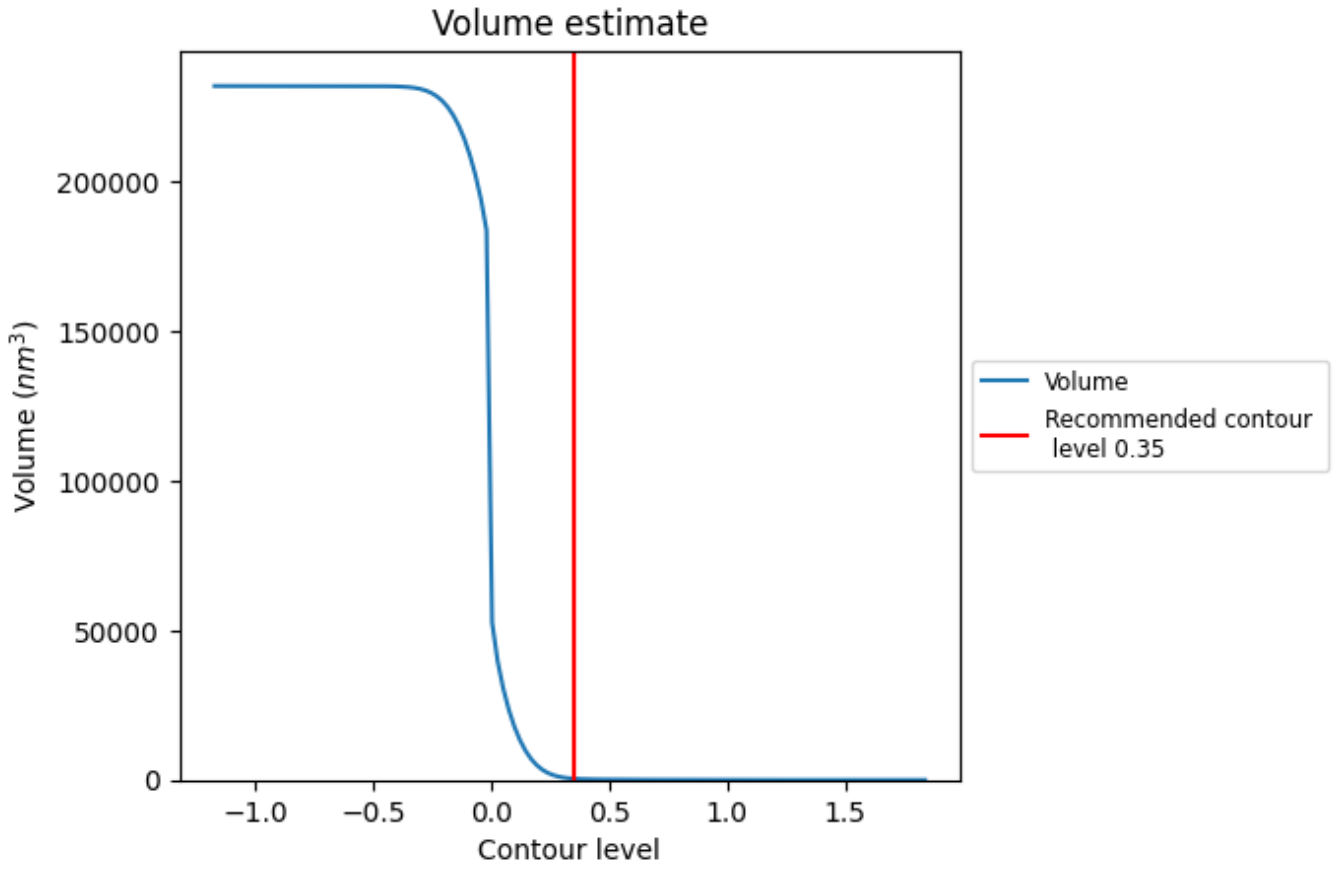
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

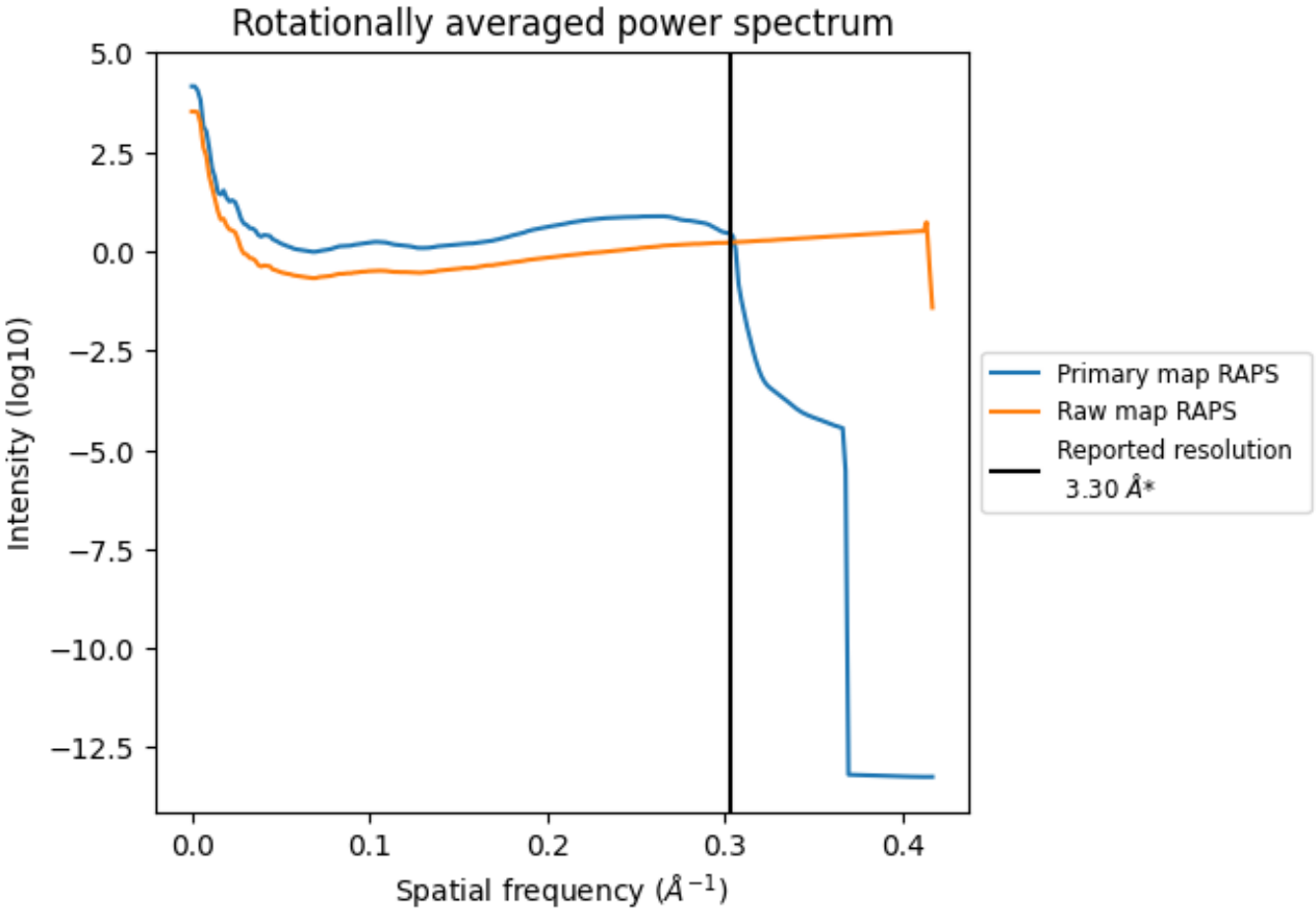
7.2 Volume estimate (i)



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)

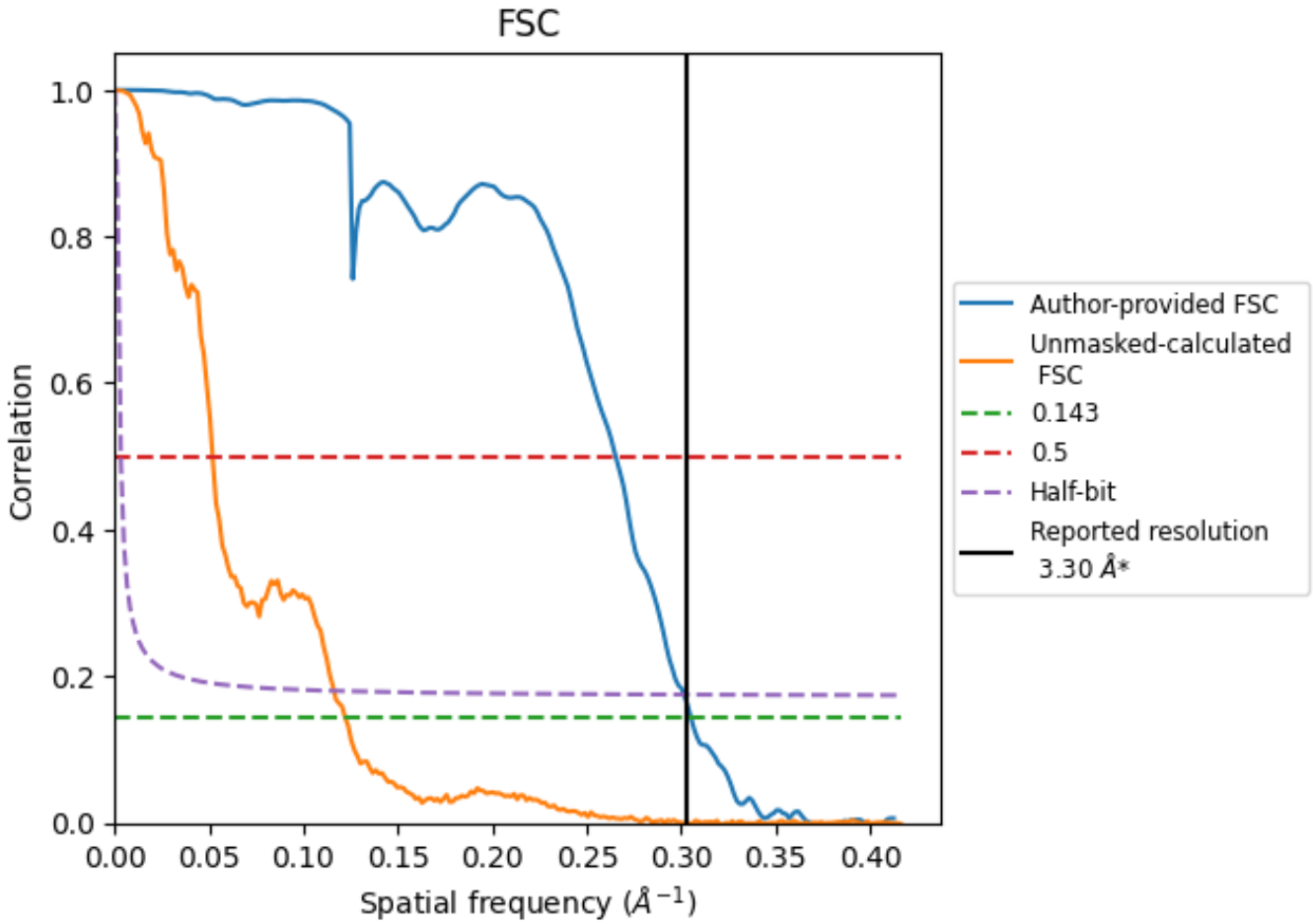


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*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 %

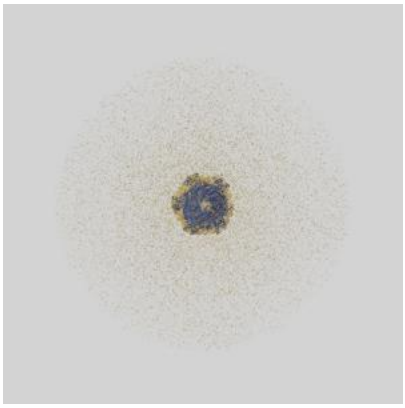
9 Map-model fit

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

X

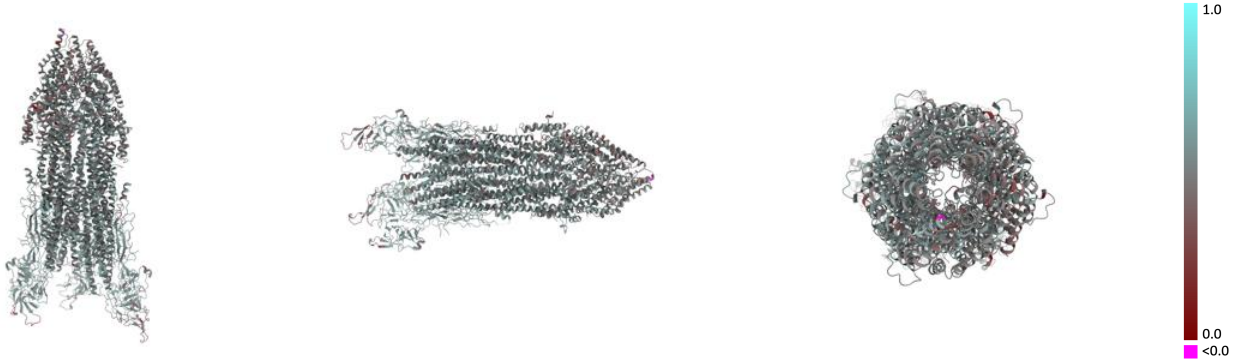
Y



Z

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

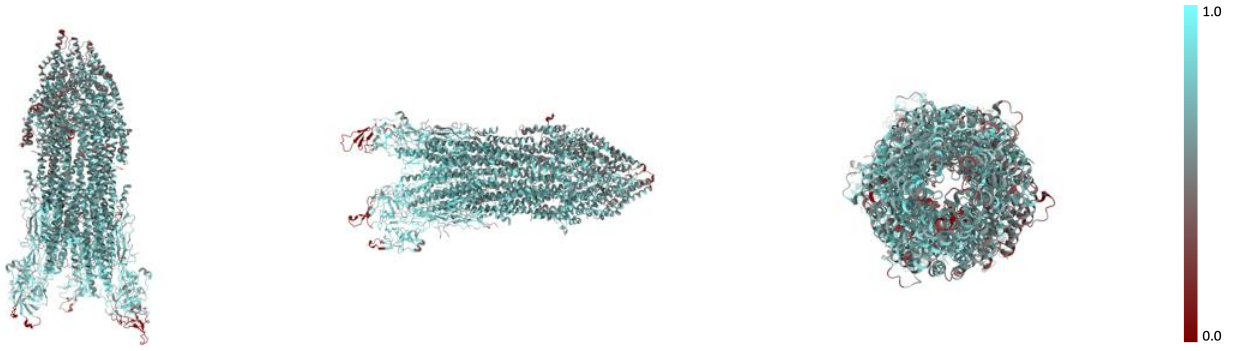
9.2 Q-score mapped to coordinate model (i)



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.

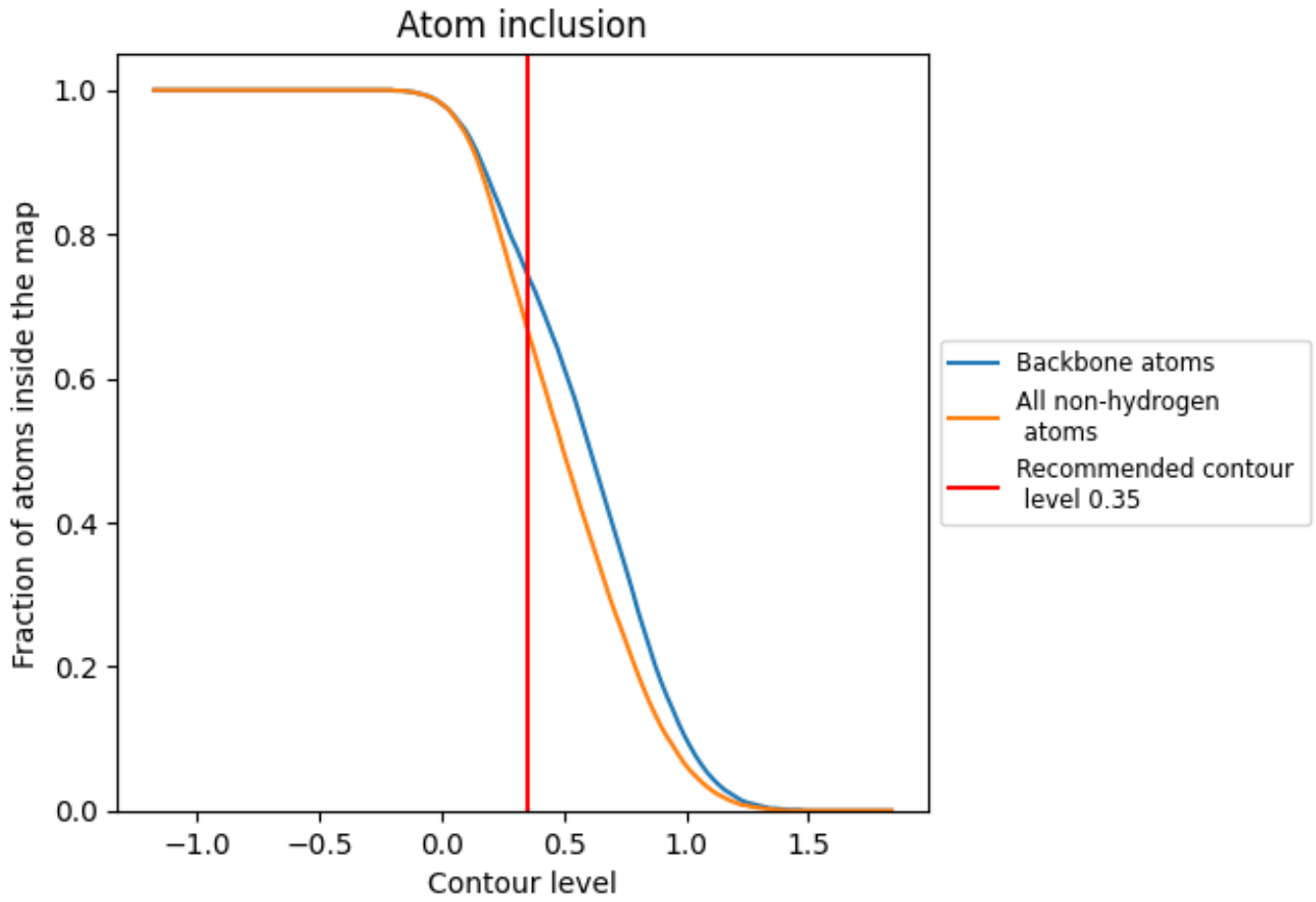
9.3 Atom inclusion mapped to coordinate model (i)



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

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