



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 10:03 AM JST

PDB ID : 7E82
EMDB ID : EMD-31008
Title : Cryo-EM structure of the flagellar rod with partial hook from Salmonella
Authors : Tan, J.X.; Chang, S.H.; Wang, X.F.; Xu, C.H.; Zhou, Y.; Zhang, X.; Zhu, Y.Q.
Deposited on : 2021-02-28
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

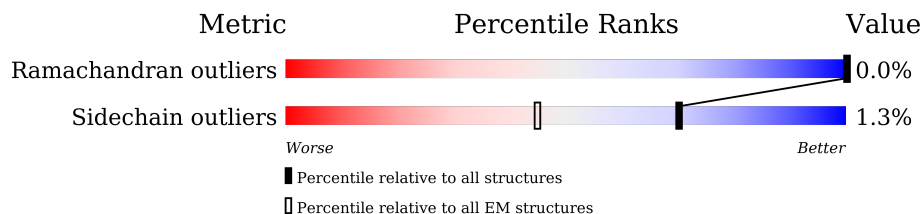
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	260	<div> <div>13%</div> <div>98%</div> </div>
1	B	260	<div> <div>24%</div> <div>99%</div> </div>
1	C	260	<div> <div>14%</div> <div>99%</div> </div>
1	D	260	<div> <div>12%</div> <div>100%</div> </div>
1	E	260	<div> <div>12%</div> <div>98%</div> </div>
1	F	260	<div> <div>11%</div> <div>100%</div> </div>
1	G	260	<div> <div>11%</div> <div>98%</div> </div>
1	H	260	<div> <div>10%</div> <div>99%</div> </div>
1	I	260	<div> <div>8%</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	260	9% 99% .
1	K	260	8% 99% .
1	L	260	8% 98% .
1	M	260	10% 99% .
1	N	260	7% 96% .
1	O	260	11% 97% .
1	P	260	8% 95% 5%
1	Q	260	8% 93% 5%
1	R	260	9% 94% .
1	S	260	9% 94% 5%
1	T	260	8% 97% .
1	U	260	8% 99% .
1	V	260	8% 98% .
1	W	260	11% 98% .
1	X	260	18% 98% .
2	a	251	10% 97% ..
2	b	251	25% 97% ..
2	c	251	11% 97% ..
2	d	251	13% 98% ..
2	e	251	27% 98% ..
3	0	15	40% 100%
3	1	15	67% 100%
3	2	15	33% 100%
3	3	15	40% 100%
3	4	15	60% 100%

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Mol	Chain	Length	Quality of chain
4	5	21	14% 100%
4	6	21	86% 100%
4	7	21	14% 100%
4	8	21	38% 100%
4	9	21	86% 100%
5	f	134	13% 93% • •
5	g	134	30% 95% • •
5	h	134	7% 95% • •
5	i	134	11% 95% • •
5	j	134	13% 94% • 5%
5	p	134	31% 96% •
6	k	138	14% 75% • 22%
6	l	138	22% 75% • 23%
6	m	138	16% 76% • 23%
6	n	138	20% 75% • 22%
6	o	138	40% 76% • 21%
7	q	104	30% 67% • 32%
7	r	104	37% 67% 33%
7	s	104	28% 69% 31%
7	t	104	25% 69% 31%
7	u	104	48% 69% 31%
7	v	104	31% 36% • 63%
8	DA	403	58% 98% •
8	DB	403	55% 99% •
8	DC	403	55% 99%

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Mol	Chain	Length	Quality of chain
8	DD	403	<div> <div>56%</div> <div>99%</div> </div>
8	DE	403	<div> <div>62%</div> <div>99%</div> </div>
8	DF	403	<div> <div>67%</div> <div>99%</div> </div>
8	DG	403	<div> <div>70%</div> <div>99%</div> </div>
8	DH	403	<div> <div>72%</div> <div>98%</div> </div>
8	DI	403	<div> <div>73%</div> <div>98%</div> </div>
8	DJ	403	<div> <div>81%</div> <div>98%</div> </div>
8	DK	403	<div> <div>84%</div> <div>99%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 101606 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 basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	B	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	C	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	D	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	E	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	F	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	G	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	H	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	I	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	J	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	K	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	L	259	Total 1941	C 1197	N 340	O 399	S 5	0	0
1	M	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	N	251	Total 1887	C 1167	N 330	O 384	S 6	0	0
1	O	252	Total 1894	C 1172	N 331	O 385	S 6	0	0
1	P	248	Total 1862	C 1151	N 327	O 379	S 5	0	0
1	Q	247	Total 1858	C 1149	N 326	O 378	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	250	Total	C	N	O	S	0	0
			1875	1159	329	382	5		
1	S	247	Total	C	N	O	S	0	0
			1858	1149	326	378	5		
1	T	253	Total	C	N	O	S	0	0
			1902	1176	333	388	5		
1	U	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	V	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	W	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	X	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	b	248	Total	C	N	O	S	0	0
			1804	1106	324	367	7		
2	c	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	d	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	e	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

- Molecule 3 is a protein called Flagellar MS ring L2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	0	15	Total	C	N	O	0	0
			75	45	15	15		
3	1	15	Total	C	N	O	0	0
			75	45	15	15		
3	2	15	Total	C	N	O	0	0
			75	45	15	15		
3	3	15	Total	C	N	O	0	0
			75	45	15	15		
3	4	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 4 is a protein called Flagellar MS ring L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	21	Total	C	N	O	0	0
			140	88	24	28		
4	6	21	Total	C	N	O	0	0
			140	88	24	28		
4	7	21	Total	C	N	O	0	0
			140	88	24	28		
4	9	21	Total	C	N	O	0	0
			140	88	24	28		
4	8	21	Total	C	N	O	0	0
			140	88	24	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	128	Total	C	N	O	S	0	0
			936	585	160	186	5		
5	g	130	Total	C	N	O	S	0	0
			949	592	163	189	5		
5	h	128	Total	C	N	O	S	0	0
			935	584	160	186	5		
5	j	127	Total	C	N	O	S	0	0
			931	582	159	185	5		
5	p	129	Total	C	N	O	S	0	0
			940	587	161	187	5		
5	i	129	Total	C	N	O	S	0	0
			944	589	162	188	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	106	Total	C	N	O	S	0	0
			833	515	150	163	5		
6	m	106	Total	C	N	O	S	0	0
			833	515	150	163	5		
6	o	109	Total	C	N	O	S	0	0
			856	529	156	166	5		
6	k	108	Total	C	N	O	S	0	0
			852	527	155	165	5		
6	n	107	Total	C	N	O	S	0	0
			844	521	154	164	5		

- Molecule 7 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	71	Total	C	N	O	S	0	0
			536	330	98	102	6		
7	r	70	Total	C	N	O	S	0	0
			526	323	97	100	6		
7	s	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	t	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	u	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	v	38	Total	C	N	O	S	0	0
			289	178	50	55	6		

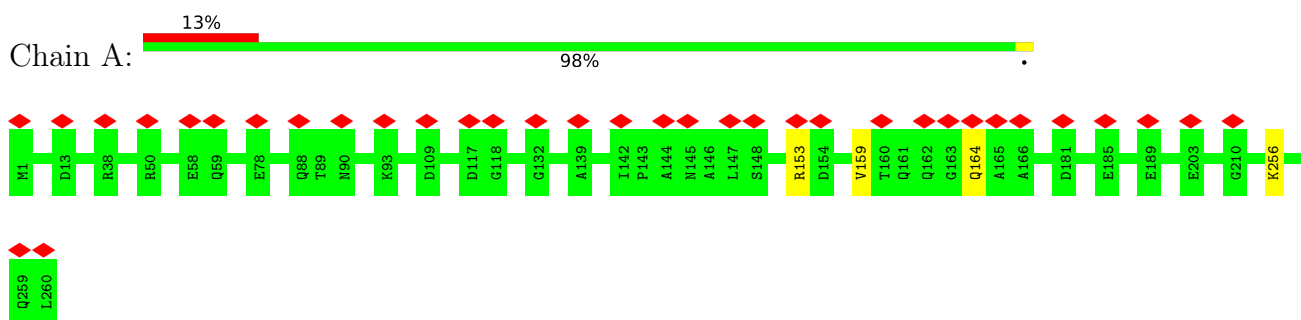
- Molecule 8 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DA	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DB	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DC	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DD	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DE	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DH	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DI	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DJ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DK	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

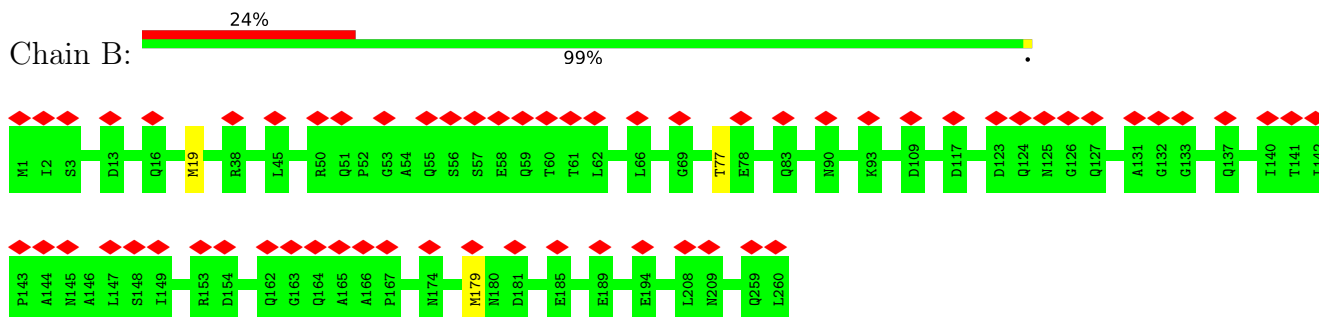
3 Residue-property plots [i](#)

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.

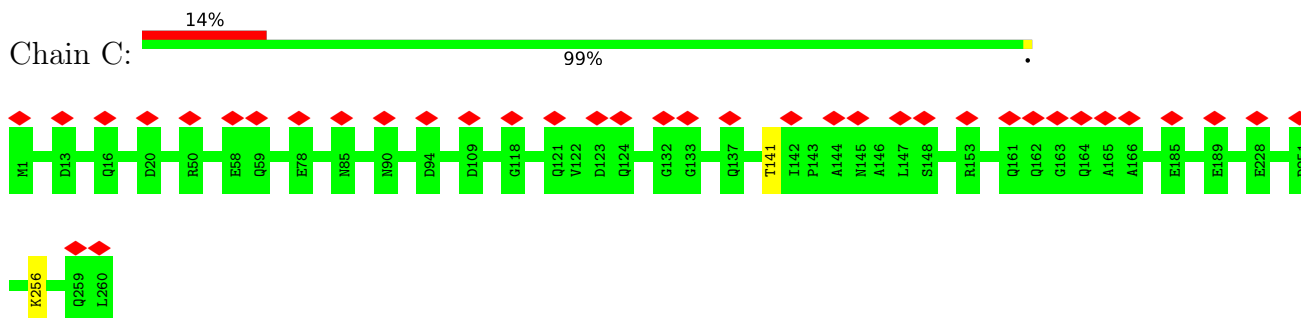
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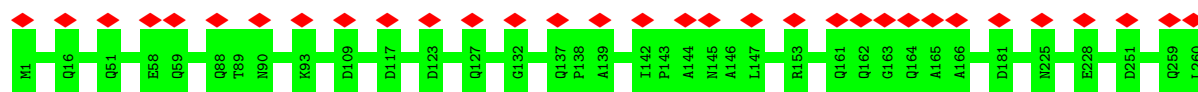


- Molecule 1: Flagellar basal-body rod protein FlgG

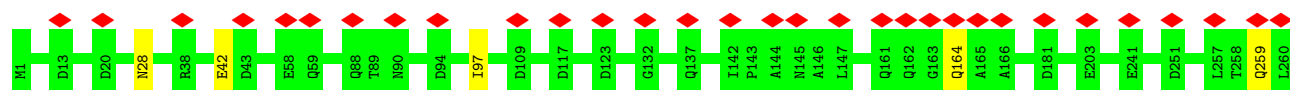


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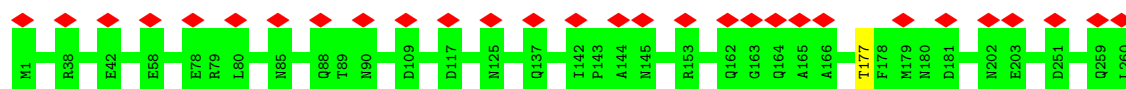




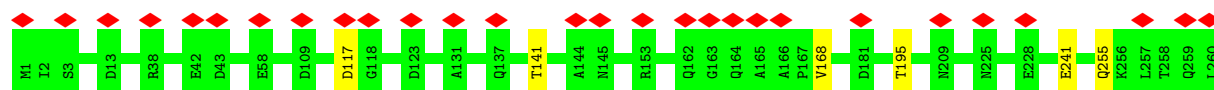
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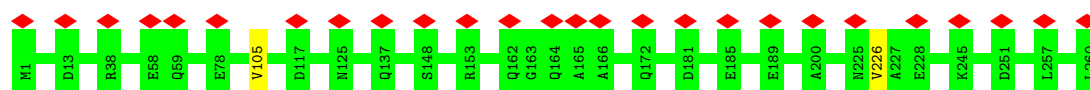
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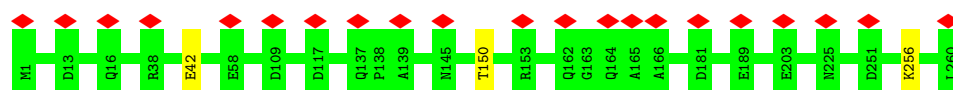
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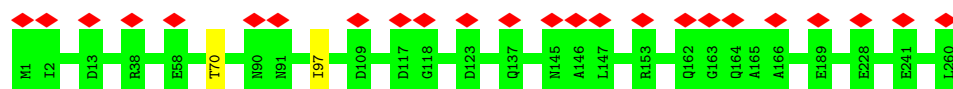
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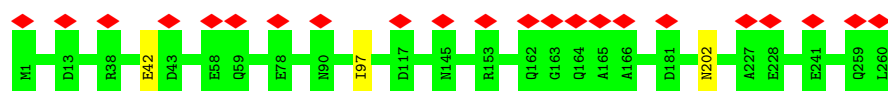
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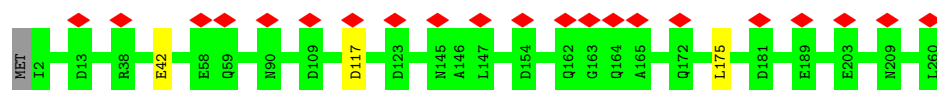
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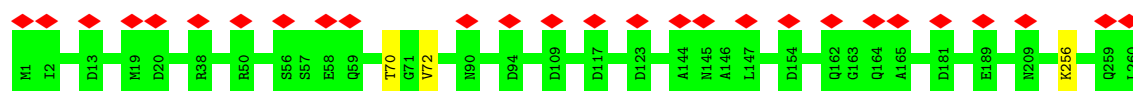
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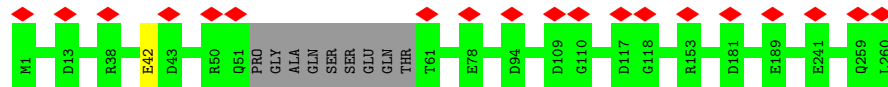
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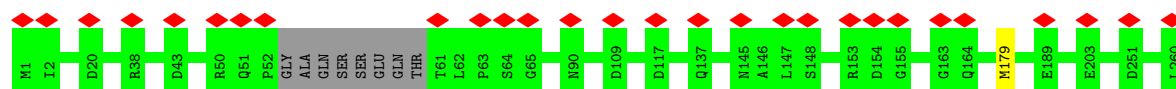
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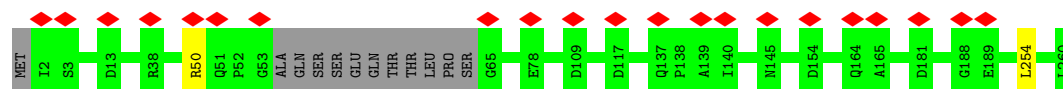
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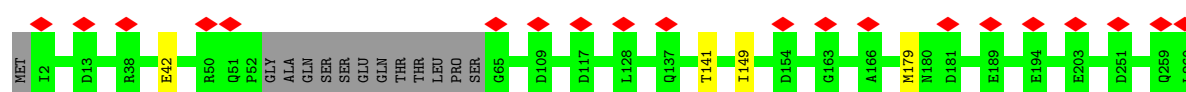
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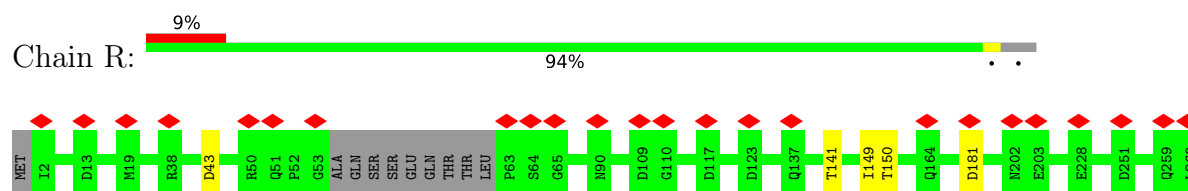
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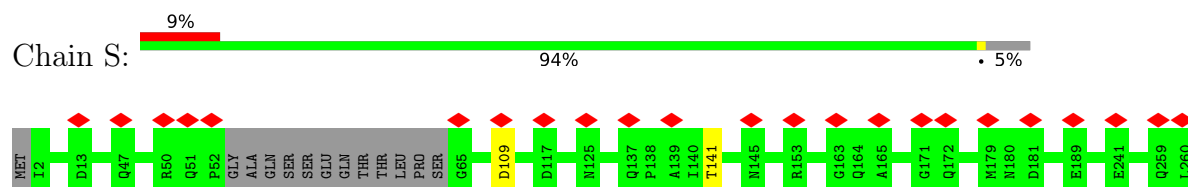
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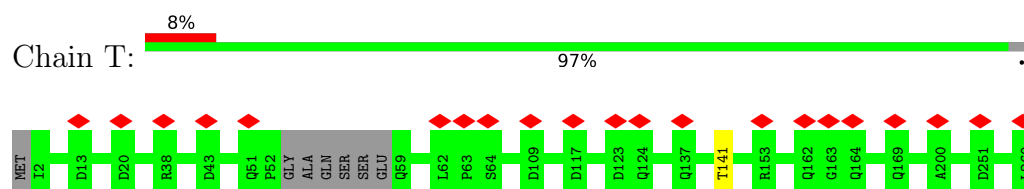
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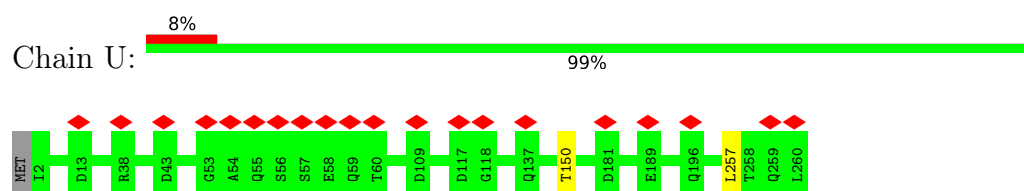
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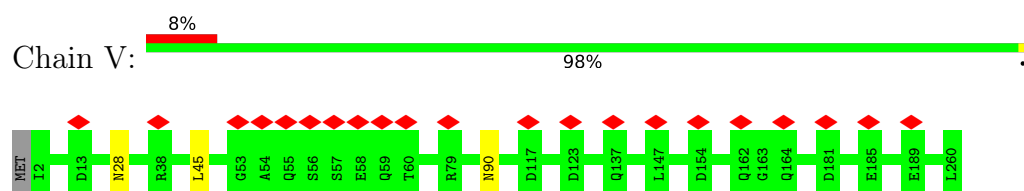
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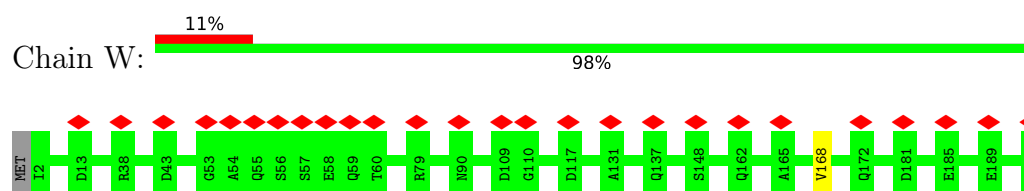
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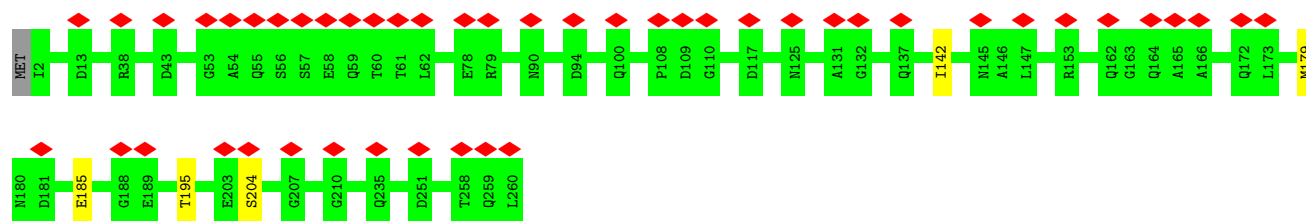


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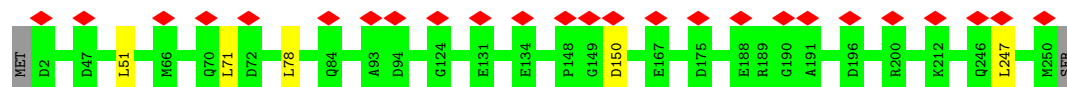


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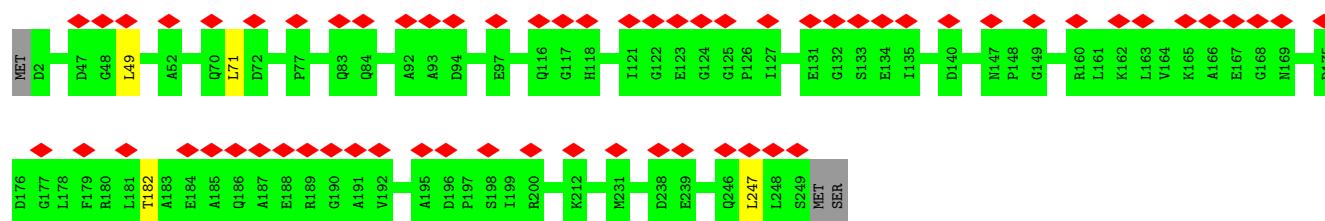




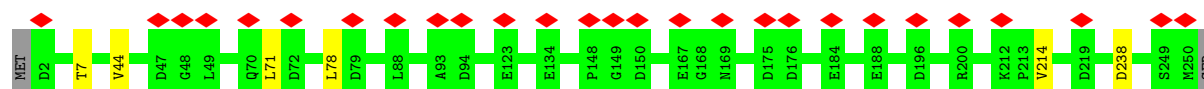
- Molecule 2: Flagellar basal-body rod protein FlgF



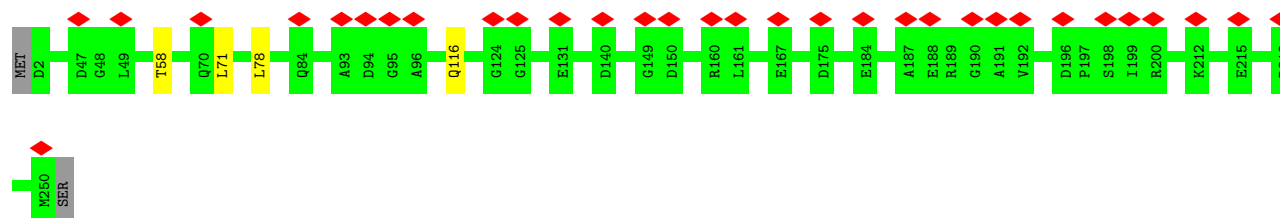
- Molecule 2: Flagellar basal-body rod protein FlgF



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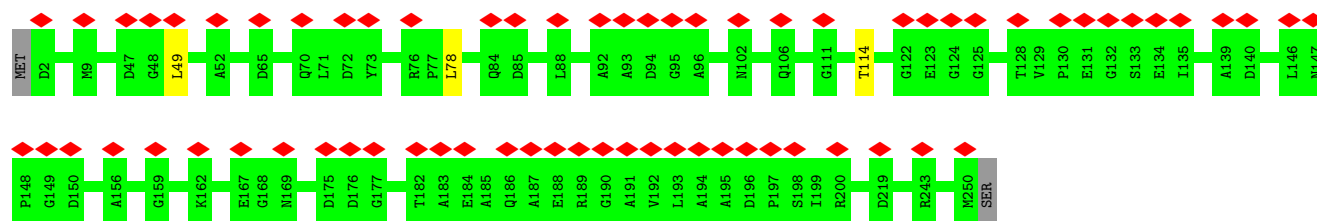


- Molecule 2: Flagellar basal-body rod protein FlgF

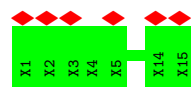
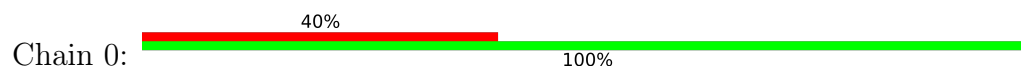


- Molecule 2: Flagellar basal-body rod protein FlgF

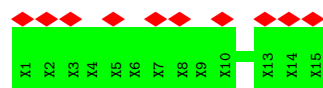




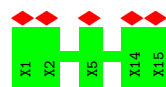
- Molecule 3: Flagellar MS ring L2



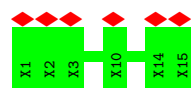
- Molecule 3: Flagellar MS ring L2



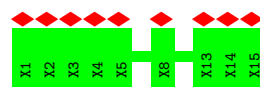
- Molecule 3: Flagellar MS ring L2



- Molecule 3: Flagellar MS ring L2

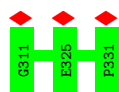


- Molecule 3: Flagellar MS ring L2

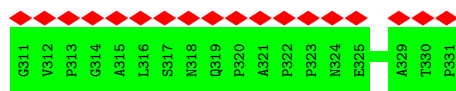
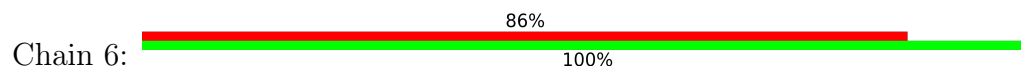


- Molecule 4: Flagellar MS ring L1

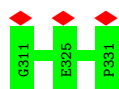




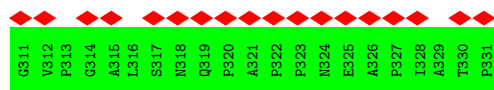
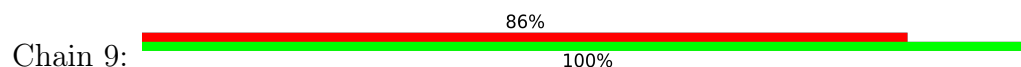
- Molecule 4: Flagellar MS ring L1



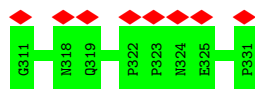
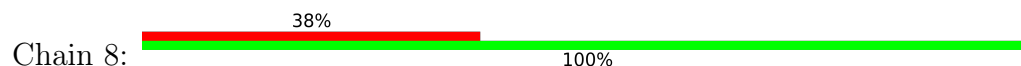
- Molecule 4: Flagellar MS ring L1



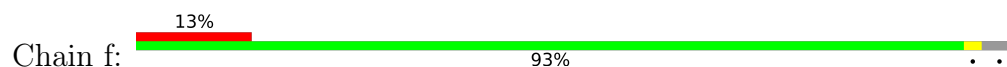
- Molecule 4: Flagellar MS ring L1



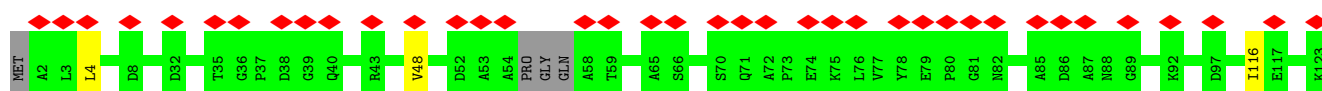
- Molecule 4: Flagellar MS ring L1



- Molecule 5: Flagellar basal-body rod protein FlgC

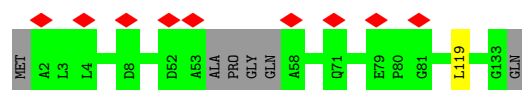


- Molecule 5: Flagellar basal-body rod protein FlgC

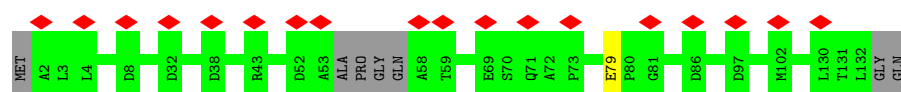




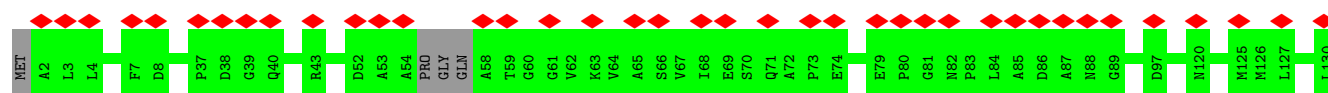
- Molecule 5: Flagellar basal-body rod protein FlgC



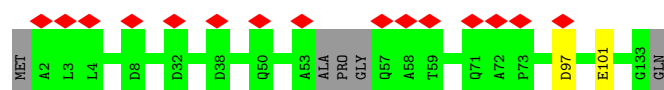
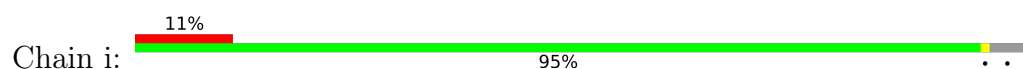
- Molecule 5: Flagellar basal-body rod protein FlgC



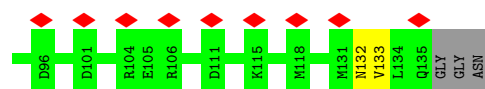
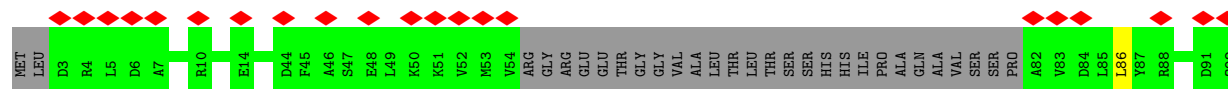
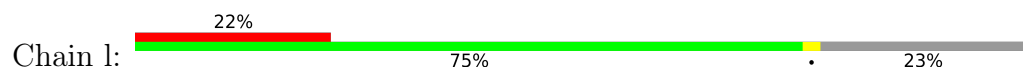
- Molecule 5: Flagellar basal-body rod protein FlgC



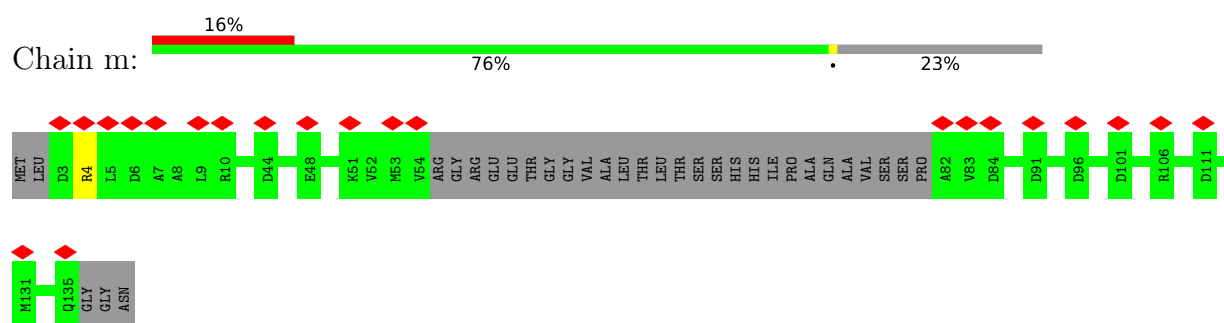
- Molecule 5: Flagellar basal-body rod protein FlgC



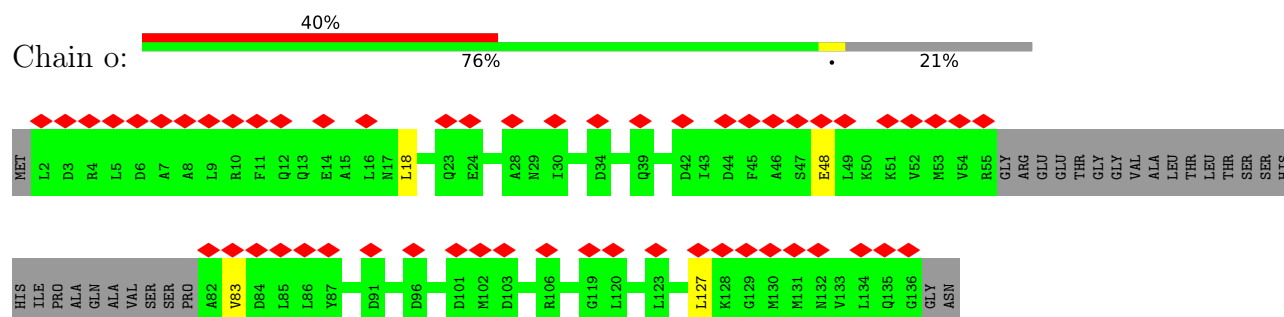
- Molecule 6: Flagellar basal body rod protein FlgB



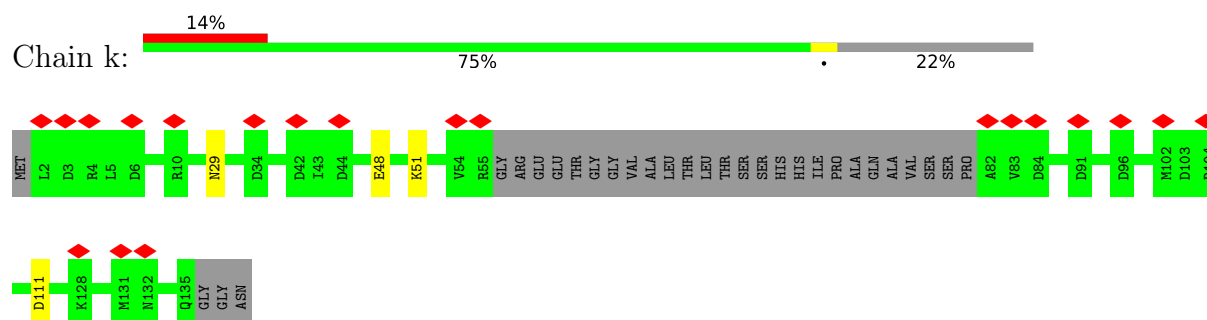
- Molecule 6: Flagellar basal body rod protein FlgB



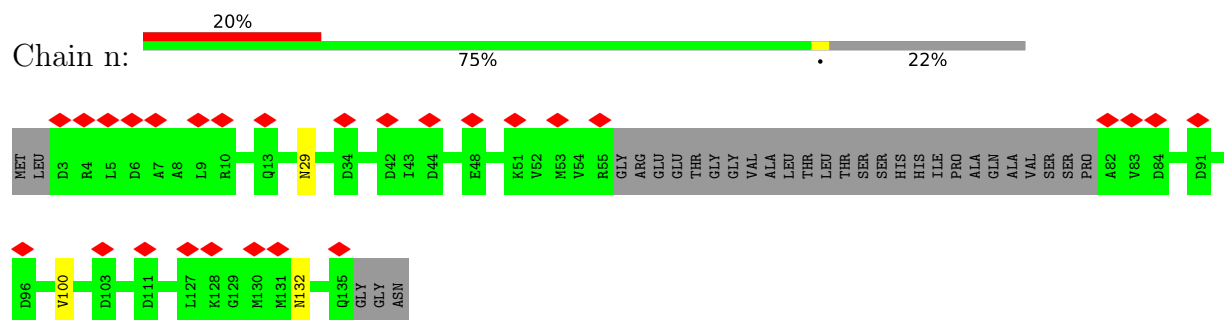
- Molecule 6: Flagellar basal body rod protein FlgB



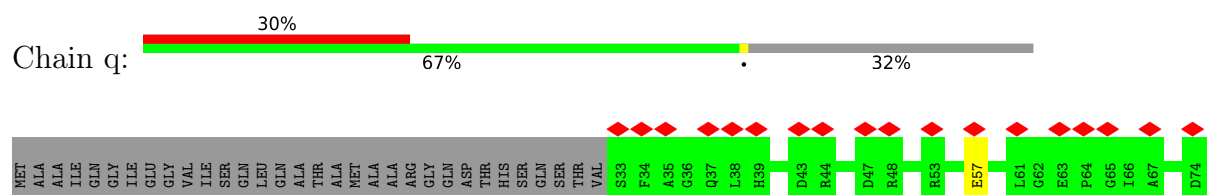
- Molecule 6: Flagellar basal body rod protein FlgB

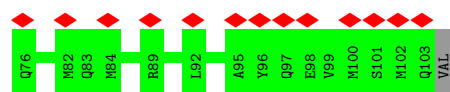


- Molecule 6: Flagellar basal body rod protein FlgB

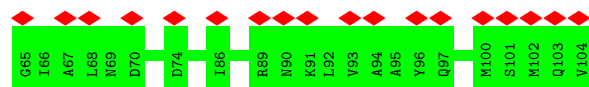


- Molecule 7: Flagellar hook-basal body complex protein FliE

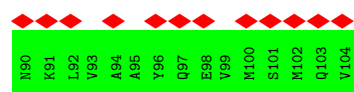
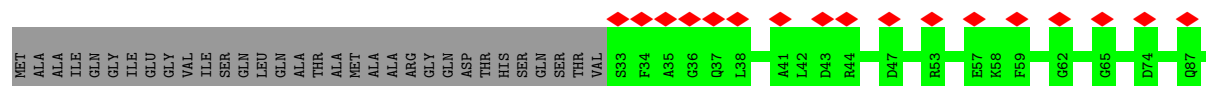




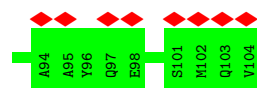
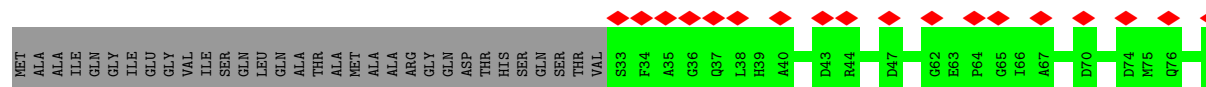
- Molecule 7: Flagellar hook-basal body complex protein FliE



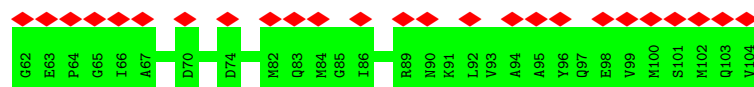
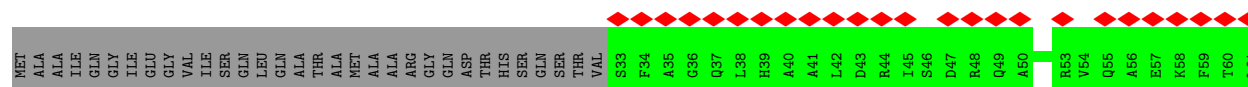
- Molecule 7: Flagellar hook-basal body complex protein FliE



- Molecule 7: Flagellar hook-basal body complex protein FliE



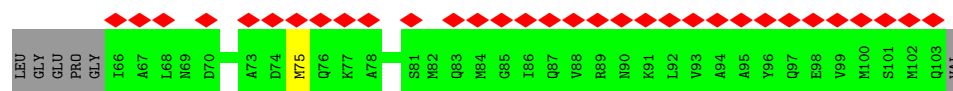
- Molecule 7: Flagellar hook-basal body complex protein FliE



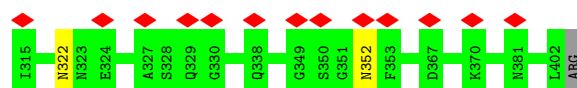
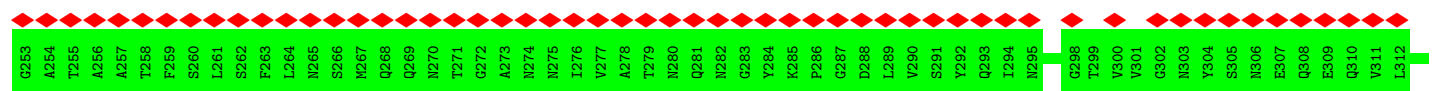
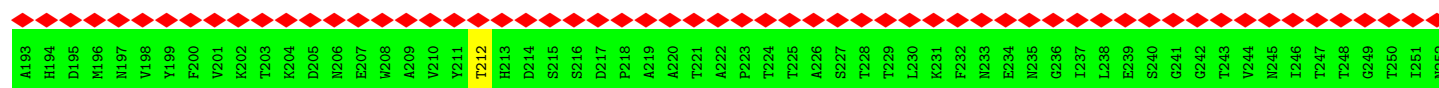
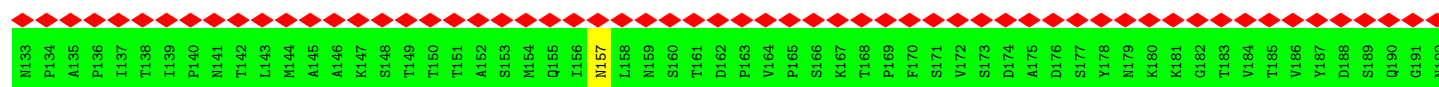
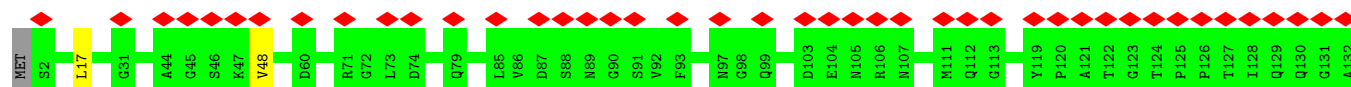
- Molecule 7: Flagellar hook-basal body complex protein FliE



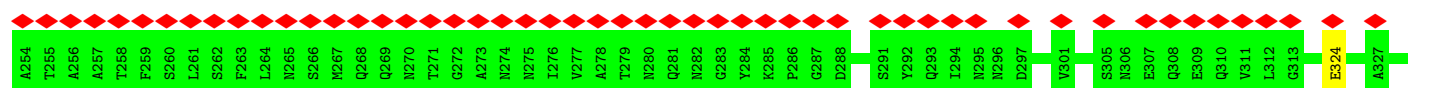
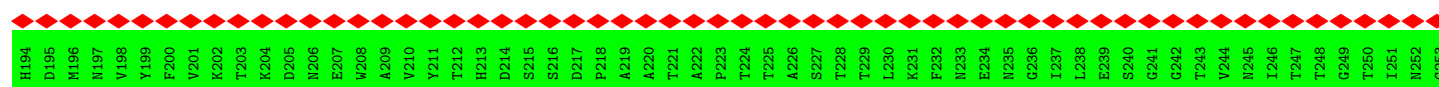
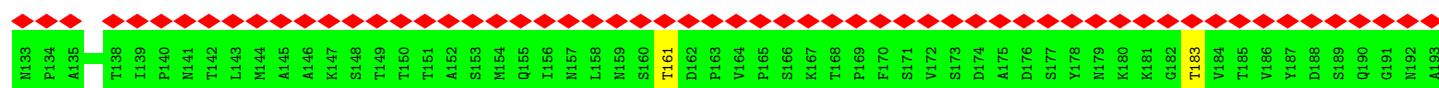
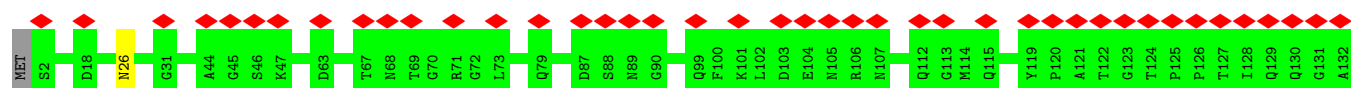
MET ALA ILE GLN ILE GLU VAL ILE SER GLN LEU GLN ALA THR MET ALA ARG GLN ASP THR HIS SER GLN SER THR VAL SER PHE ALA GLY LEU HIS ALA ALA LEU ASP ARG ILE SER ASP ARG GLN ALA ALA ARG VAL GLN ALA GLU LYS PHE THR

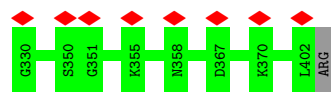


• Molecule 8: Flagellar hook protein FlgE

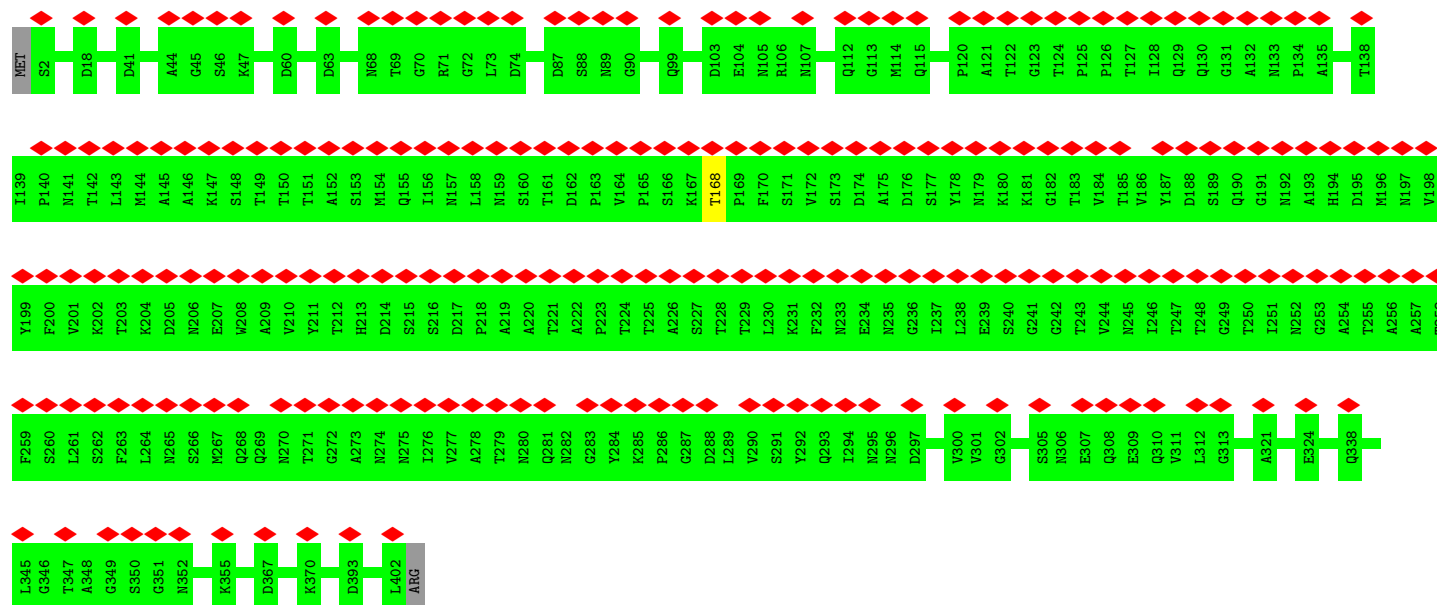


• Molecule 8: Flagellar hook protein FlgE





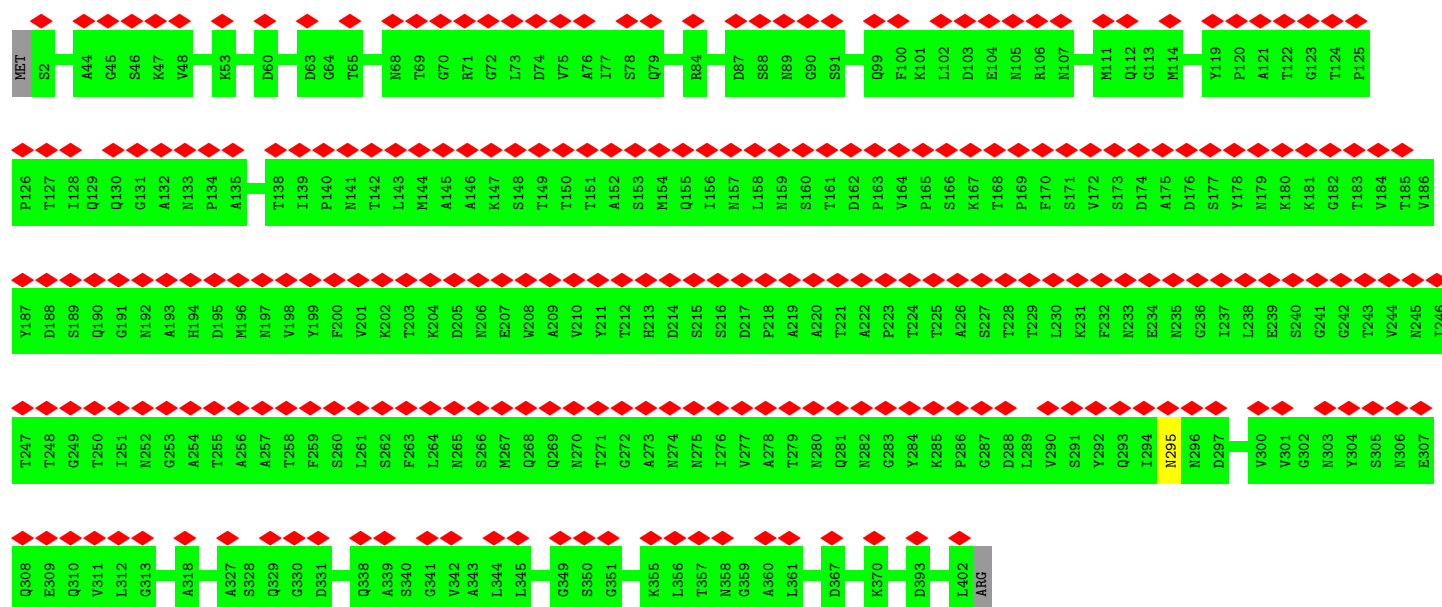
• Molecule 8: Flagellar hook protein FlgE



• Molecule 8: Flagellar hook protein FlgE



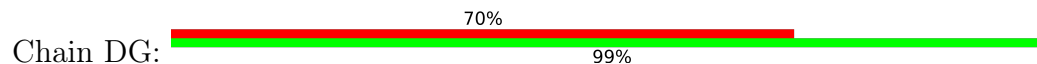
• Molecule 8: Flagellar hook protein FlgE



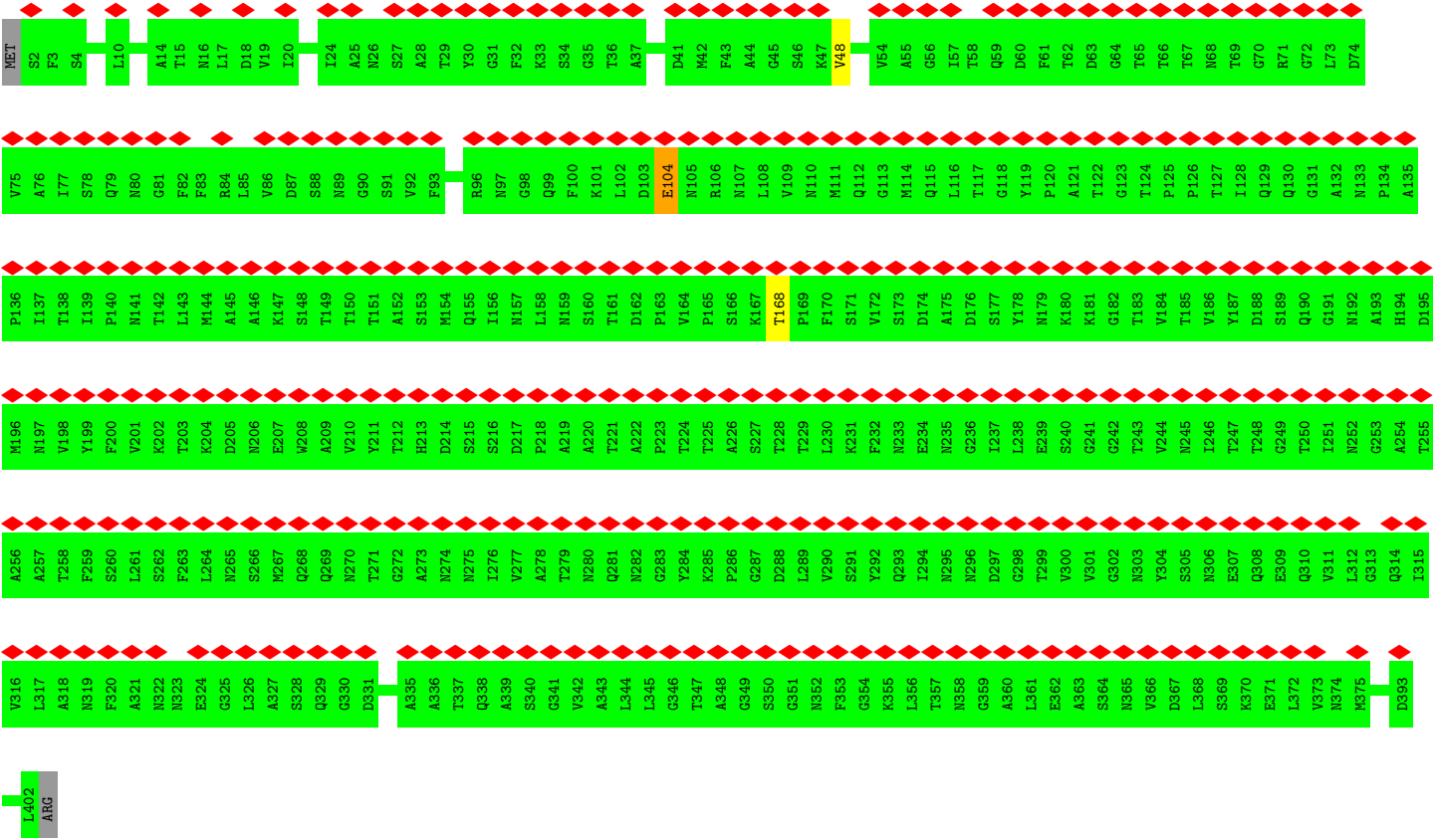
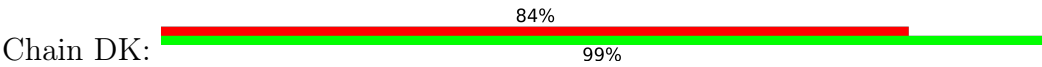
• Molecule 8: Flagellar hook protein FlgE



• Molecule 8: Flagellar hook protein FlgE







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102044	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.722	Depositor
Minimum map value	-1.395	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	669.184, 669.184, 669.184	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	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	A	0.27	0/1973	0.48	0/2682
1	B	0.27	0/1973	0.48	0/2682
1	C	0.27	0/1973	0.48	0/2682
1	D	0.28	0/1973	0.48	0/2682
1	E	0.28	0/1973	0.49	0/2682
1	F	0.28	0/1973	0.48	0/2682
1	G	0.28	0/1973	0.48	0/2682
1	H	0.28	0/1973	0.48	0/2682
1	I	0.28	0/1973	0.48	0/2682
1	J	0.28	0/1973	0.48	0/2682
1	K	0.28	0/1973	0.48	0/2682
1	L	0.28	0/1965	0.47	0/2672
1	M	0.28	0/1973	0.48	0/2682
1	N	0.28	0/1909	0.47	0/2593
1	O	0.28	0/1917	0.48	0/2605
1	P	0.28	0/1884	0.48	0/2559
1	Q	0.29	0/1880	0.48	0/2554
1	R	0.28	0/1898	0.48	0/2578
1	S	0.28	0/1880	0.48	0/2554
1	T	0.28	0/1925	0.47	0/2617
1	U	0.28	0/1965	0.48	0/2672
1	V	0.28	0/1965	0.47	0/2672
1	W	0.29	0/1965	0.49	0/2672
1	X	0.28	0/1965	0.49	1/2672 (0.0%)
2	a	0.27	0/1836	0.50	0/2502
2	b	0.27	0/1828	0.49	0/2492
2	c	0.27	0/1836	0.49	0/2502
2	d	0.27	0/1836	0.50	0/2502
2	e	0.26	0/1836	0.50	0/2502
4	5	0.28	0/145	0.42	0/203
4	6	0.26	0/145	0.43	0/203
4	7	0.40	0/145	0.55	0/203
4	8	0.27	0/145	0.42	0/203
4	9	0.26	0/145	0.44	0/203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	f	0.27	0/946	0.44	0/1285
5	g	0.27	0/959	0.45	0/1302
5	h	0.28	0/945	0.45	0/1283
5	i	0.28	0/954	0.46	0/1295
5	j	0.28	0/941	0.46	0/1278
5	p	0.27	0/950	0.43	0/1290
6	k	0.27	0/859	0.49	0/1156
6	l	0.26	0/840	0.48	0/1131
6	m	0.26	0/840	0.47	0/1131
6	n	0.26	0/851	0.49	0/1145
6	o	0.25	0/863	0.50	0/1161
7	q	0.26	0/540	0.44	0/723
7	r	0.26	0/529	0.47	0/709
7	s	0.26	0/547	0.44	0/733
7	t	0.25	0/547	0.44	0/733
7	u	0.25	0/547	0.46	0/733
7	v	0.24	0/289	0.39	0/385
8	DA	0.26	0/2991	0.45	0/4076
8	DB	0.26	0/2991	0.45	0/4076
8	DC	0.26	0/2991	0.45	0/4076
8	DD	0.26	0/2991	0.45	0/4076
8	DE	0.26	0/2991	0.45	0/4076
8	DF	0.25	0/2991	0.46	0/4076
8	DG	0.25	0/2991	0.45	0/4076
8	DH	0.26	0/2991	0.45	0/4076
8	DI	0.26	0/2991	0.46	0/4076
8	DJ	0.28	0/2991	0.48	1/4076 (0.0%)
8	DK	0.26	0/2991	0.47	1/4076 (0.0%)
All	All	0.27	0/102539	0.47	3/139428 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	204	SER	C-N-CA	5.83	136.28	121.70
8	DJ	383	GLN	CB-CA-C	-5.62	99.15	110.40
8	DK	104	GLU	CB-CA-C	5.38	121.16	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/260 (99%)	249 (96%)	9 (4%)	0	100	100
1	B	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	C	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	D	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	E	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	F	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	G	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	H	258/260 (99%)	245 (95%)	13 (5%)	0	100	100
1	I	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	J	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
1	K	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	L	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
1	M	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	N	247/260 (95%)	240 (97%)	7 (3%)	0	100	100
1	O	248/260 (95%)	240 (97%)	8 (3%)	0	100	100
1	P	244/260 (94%)	236 (97%)	8 (3%)	0	100	100
1	Q	243/260 (94%)	237 (98%)	6 (2%)	0	100	100
1	R	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
1	S	243/260 (94%)	235 (97%)	8 (3%)	0	100	100
1	T	249/260 (96%)	241 (97%)	8 (3%)	0	100	100
1	U	257/260 (99%)	243 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	257/260 (99%)	249 (97%)	8 (3%)	0	100	100
1	W	257/260 (99%)	242 (94%)	15 (6%)	0	100	100
1	X	257/260 (99%)	244 (95%)	13 (5%)	0	100	100
2	a	247/251 (98%)	236 (96%)	11 (4%)	0	100	100
2	b	246/251 (98%)	236 (96%)	10 (4%)	0	100	100
2	c	247/251 (98%)	237 (96%)	10 (4%)	0	100	100
2	d	247/251 (98%)	232 (94%)	15 (6%)	0	100	100
2	e	247/251 (98%)	231 (94%)	16 (6%)	0	100	100
4	5	19/21 (90%)	19 (100%)	0	0	100	100
4	6	19/21 (90%)	19 (100%)	0	0	100	100
4	7	19/21 (90%)	19 (100%)	0	0	100	100
4	8	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
4	9	19/21 (90%)	19 (100%)	0	0	100	100
5	f	124/134 (92%)	120 (97%)	4 (3%)	0	100	100
5	g	126/134 (94%)	121 (96%)	5 (4%)	0	100	100
5	h	124/134 (92%)	120 (97%)	4 (3%)	0	100	100
5	i	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
5	j	123/134 (92%)	119 (97%)	4 (3%)	0	100	100
5	p	125/134 (93%)	120 (96%)	5 (4%)	0	100	100
6	k	104/138 (75%)	99 (95%)	5 (5%)	0	100	100
6	l	102/138 (74%)	101 (99%)	1 (1%)	0	100	100
6	m	102/138 (74%)	99 (97%)	3 (3%)	0	100	100
6	n	103/138 (75%)	99 (96%)	4 (4%)	0	100	100
6	o	105/138 (76%)	103 (98%)	2 (2%)	0	100	100
7	q	69/104 (66%)	68 (99%)	1 (1%)	0	100	100
7	r	68/104 (65%)	64 (94%)	4 (6%)	0	100	100
7	s	70/104 (67%)	70 (100%)	0	0	100	100
7	t	70/104 (67%)	69 (99%)	1 (1%)	0	100	100
7	u	70/104 (67%)	70 (100%)	0	0	100	100
7	v	36/104 (35%)	36 (100%)	0	0	100	100
8	DA	399/403 (99%)	377 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	DB	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
8	DC	399/403 (99%)	375 (94%)	24 (6%)	0	100	100
8	DD	399/403 (99%)	378 (95%)	21 (5%)	0	100	100
8	DE	399/403 (99%)	380 (95%)	19 (5%)	0	100	100
8	DF	399/403 (99%)	376 (94%)	23 (6%)	0	100	100
8	DG	399/403 (99%)	382 (96%)	17 (4%)	0	100	100
8	DH	399/403 (99%)	379 (95%)	18 (4%)	2 (0%)	29	61
8	DI	399/403 (99%)	381 (96%)	18 (4%)	0	100	100
8	DJ	399/403 (99%)	375 (94%)	23 (6%)	1 (0%)	41	71
8	DK	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
All	All	13465/14151 (95%)	12899 (96%)	563 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	DJ	332	ASN
8	DH	270	ASN
8	DH	71	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/215 (100%)	211 (98%)	4 (2%)	57	77
1	B	215/215 (100%)	212 (99%)	3 (1%)	67	82
1	C	215/215 (100%)	213 (99%)	2 (1%)	78	87
1	D	215/215 (100%)	215 (100%)	0	100	100
1	E	215/215 (100%)	210 (98%)	5 (2%)	50	73
1	F	215/215 (100%)	214 (100%)	1 (0%)	88	93
1	G	215/215 (100%)	209 (97%)	6 (3%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	215/215 (100%)	213 (99%)	2 (1%)	78	87
1	I	215/215 (100%)	212 (99%)	3 (1%)	67	82
1	J	215/215 (100%)	213 (99%)	2 (1%)	78	87
1	K	215/215 (100%)	212 (99%)	3 (1%)	67	82
1	L	214/215 (100%)	211 (99%)	3 (1%)	67	82
1	M	215/215 (100%)	212 (99%)	3 (1%)	67	82
1	N	208/215 (97%)	207 (100%)	1 (0%)	88	93
1	O	209/215 (97%)	208 (100%)	1 (0%)	88	93
1	P	204/215 (95%)	202 (99%)	2 (1%)	76	86
1	Q	204/215 (95%)	200 (98%)	4 (2%)	55	76
1	R	206/215 (96%)	201 (98%)	5 (2%)	49	73
1	S	204/215 (95%)	202 (99%)	2 (1%)	76	86
1	T	210/215 (98%)	209 (100%)	1 (0%)	88	93
1	U	214/215 (100%)	212 (99%)	2 (1%)	78	87
1	V	214/215 (100%)	211 (99%)	3 (1%)	67	82
1	W	214/215 (100%)	211 (99%)	3 (1%)	67	82
1	X	214/215 (100%)	210 (98%)	4 (2%)	57	77
2	a	191/193 (99%)	186 (97%)	5 (3%)	46	71
2	b	190/193 (98%)	186 (98%)	4 (2%)	53	75
2	c	191/193 (99%)	185 (97%)	6 (3%)	40	67
2	d	191/193 (99%)	187 (98%)	4 (2%)	53	75
2	e	191/193 (99%)	188 (98%)	3 (2%)	62	79
4	5	15/15 (100%)	15 (100%)	0	100	100
4	6	15/15 (100%)	15 (100%)	0	100	100
4	7	15/15 (100%)	15 (100%)	0	100	100
4	8	15/15 (100%)	15 (100%)	0	100	100
4	9	15/15 (100%)	15 (100%)	0	100	100
5	f	101/105 (96%)	98 (97%)	3 (3%)	41	68
5	g	102/105 (97%)	99 (97%)	3 (3%)	42	69
5	h	101/105 (96%)	100 (99%)	1 (1%)	76	86
5	i	102/105 (97%)	100 (98%)	2 (2%)	55	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	j	101/105 (96%)	100 (99%)	1 (1%)	76	86
5	p	101/105 (96%)	101 (100%)	0	100	100
6	k	91/113 (80%)	87 (96%)	4 (4%)	28	59
6	l	89/113 (79%)	86 (97%)	3 (3%)	37	65
6	m	89/113 (79%)	88 (99%)	1 (1%)	73	85
6	n	90/113 (80%)	87 (97%)	3 (3%)	38	66
6	o	91/113 (80%)	87 (96%)	4 (4%)	28	59
7	q	55/79 (70%)	54 (98%)	1 (2%)	59	78
7	r	54/79 (68%)	54 (100%)	0	100	100
7	s	56/79 (71%)	56 (100%)	0	100	100
7	t	56/79 (71%)	56 (100%)	0	100	100
7	u	56/79 (71%)	56 (100%)	0	100	100
7	v	32/79 (40%)	31 (97%)	1 (3%)	40	67
8	DA	321/323 (99%)	315 (98%)	6 (2%)	57	77
8	DB	321/323 (99%)	317 (99%)	4 (1%)	71	83
8	DC	321/323 (99%)	320 (100%)	1 (0%)	92	96
8	DD	321/323 (99%)	319 (99%)	2 (1%)	86	91
8	DE	321/323 (99%)	320 (100%)	1 (0%)	92	96
8	DF	321/323 (99%)	318 (99%)	3 (1%)	78	87
8	DG	321/323 (99%)	320 (100%)	1 (0%)	92	96
8	DH	321/323 (99%)	316 (98%)	5 (2%)	62	79
8	DI	321/323 (99%)	316 (98%)	5 (2%)	62	79
8	DJ	321/323 (99%)	318 (99%)	3 (1%)	78	87
8	DK	321/323 (99%)	318 (99%)	3 (1%)	78	87
All	All	11022/11422 (96%)	10874 (99%)	148 (1%)	70	82

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	159	VAL
1	A	164	GLN
1	A	256	LYS
1	B	19	MET

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Mol	Chain	Res	Type
1	B	77	THR
1	B	179	MET
1	C	141	THR
1	C	256	LYS
1	E	28	ASN
1	E	42	GLU
1	E	97	ILE
1	E	164	GLN
1	E	259	GLN
1	F	177	THR
1	G	117	ASP
1	G	141	THR
1	G	168	VAL
1	G	195	THR
1	G	241	GLU
1	G	255	GLN
1	H	105	VAL
1	H	226	VAL
1	I	42	GLU
1	I	150	THR
1	I	256	LYS
1	J	70	THR
1	J	97	ILE
1	K	42	GLU
1	K	97	ILE
1	K	202	ASN
1	L	42	GLU
1	L	117	ASP
1	L	175	LEU
1	M	70	THR
1	M	72	VAL
1	M	256	LYS
1	N	42	GLU
1	O	179	MET
1	P	50	ARG
1	P	254	LEU
1	Q	42	GLU
1	Q	141	THR
1	Q	149	ILE
1	Q	179	MET
1	R	43	ASP
1	R	141	THR

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Mol	Chain	Res	Type
1	R	149	ILE
1	R	150	THR
1	R	181	ASP
1	S	109	ASP
1	S	141	THR
1	T	141	THR
1	U	150	THR
1	U	257	LEU
2	a	51	LEU
2	a	71	LEU
2	a	78	LEU
2	a	150	ASP
2	a	247	LEU
2	b	49	LEU
2	b	71	LEU
2	b	182	THR
2	b	247	LEU
2	c	7	THR
2	c	44	VAL
2	c	71	LEU
2	c	78	LEU
2	c	214	VAL
2	c	238	ASP
2	d	58	THR
2	d	71	LEU
2	d	78	LEU
2	d	116	GLN
2	e	49	LEU
2	e	78	LEU
2	e	114	THR
5	f	119	LEU
5	f	125	MET
5	f	132	LEU
5	g	4	LEU
5	g	48	VAL
5	g	116	ILE
5	h	119	LEU
5	j	79	GLU
6	l	86	LEU
6	l	132	ASN
6	l	133	VAL
6	m	4	ARG

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Mol	Chain	Res	Type
6	o	18	LEU
6	o	48	GLU
6	o	83	VAL
6	o	127	LEU
5	i	97	ASP
5	i	101	GLU
6	k	29	ASN
6	k	48	GLU
6	k	51	LYS
6	k	111	ASP
6	n	29	ASN
6	n	100	VAL
6	n	132	ASN
1	V	28	ASN
1	V	45	LEU
1	V	90	ASN
1	W	168	VAL
1	W	257	LEU
1	W	260	LEU
1	X	142	ILE
1	X	179	MET
1	X	185	GLU
1	X	195	THR
7	q	57	GLU
7	v	75	MET
8	DA	17	LEU
8	DA	48	VAL
8	DA	157	ASN
8	DA	212	THR
8	DA	322	ASN
8	DA	352	ASN
8	DB	26	ASN
8	DB	161	THR
8	DB	183	THR
8	DB	324	GLU
8	DC	168	THR
8	DD	80	ASN
8	DD	295	ASN
8	DE	295	ASN
8	DF	250	THR
8	DF	332	ASN
8	DF	344	LEU

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Mol	Chain	Res	Type
8	DG	395	ILE
8	DH	97	ASN
8	DH	161	THR
8	DH	279	THR
8	DH	322	ASN
8	DH	355	LYS
8	DI	17	LEU
8	DI	60	ASP
8	DI	119	TYR
8	DI	168	THR
8	DI	185	THR
8	DJ	48	VAL
8	DJ	295	ASN
8	DJ	331	ASP
8	DK	48	VAL
8	DK	104	GLU
8	DK	168	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	255	GLN
1	C	259	GLN
1	E	164	GLN
1	F	145	ASN
1	F	161	GLN
1	F	255	GLN
1	J	255	GLN
1	J	259	GLN
1	K	25	ASN
1	M	47	GLN
1	T	135	GLN
1	T	172	GLN
5	g	82	ASN
6	m	29	ASN
6	o	29	ASN
1	W	169	GLN
8	DA	97	ASN
8	DB	107	ASN
8	DB	129	GLN
8	DB	352	ASN
8	DC	352	ASN

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Mol	Chain	Res	Type
8	DD	107	ASN
8	DE	107	ASN
8	DF	22	ASN
8	DF	26	ASN
8	DF	338	GLN
8	DF	365	ASN
8	DG	129	GLN
8	DH	80	ASN
8	DH	197	ASN
8	DH	213	HIS
8	DH	310	GLN
8	DH	319	ASN
8	DH	365	ASN
8	DI	129	GLN
8	DJ	252	ASN
8	DJ	310	GLN
8	DJ	352	ASN
8	DK	97	ASN
8	DK	105	ASN
8	DK	332	ASN
8	DK	383	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 monosaccharides 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.

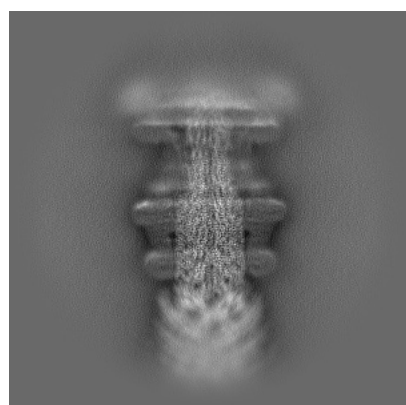
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31008. These allow visual inspection of the internal detail of the map and identification of artifacts.

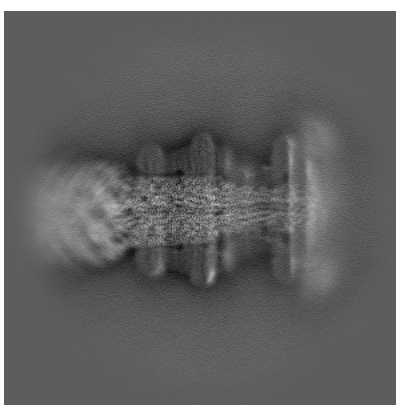
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

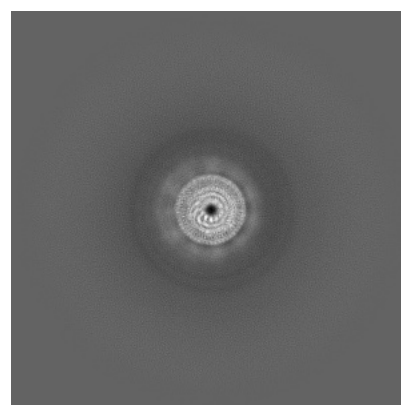
6.1.1 Primary map



X



Y

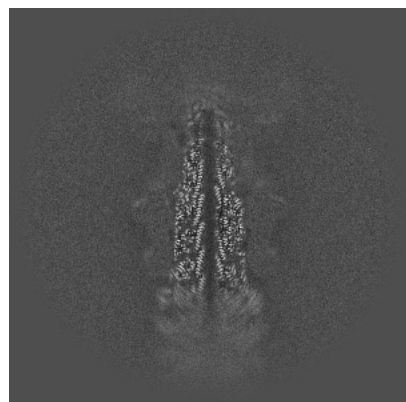


Z

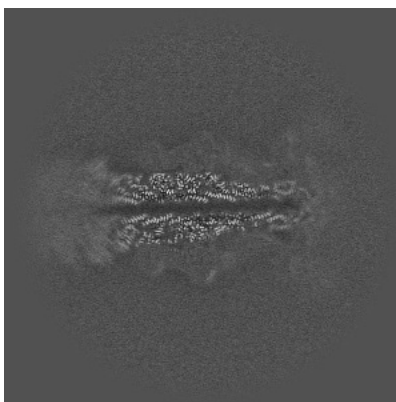
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

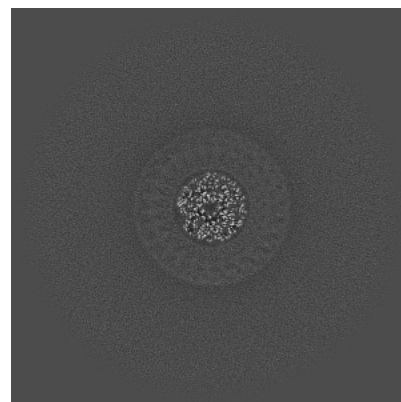
6.2.1 Primary map



X Index: 256



Y Index: 256

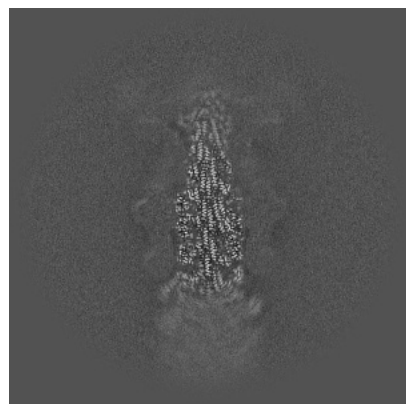


Z Index: 256

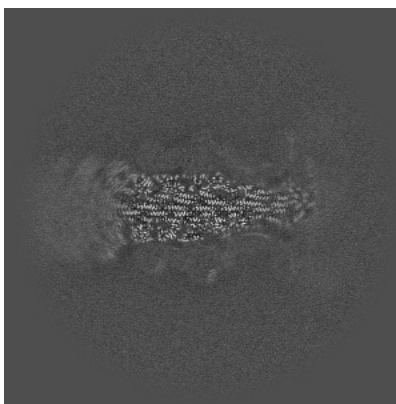
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

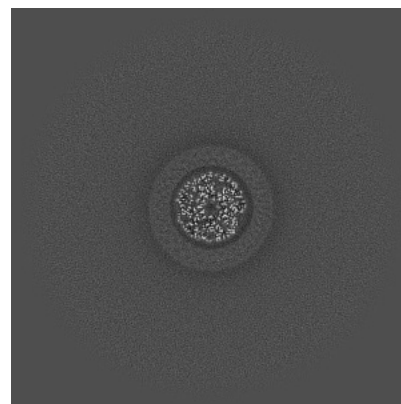
6.3.1 Primary map



X Index: 269



Y Index: 243

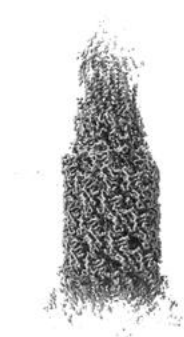


Z Index: 224

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

6.4 Orthogonal surface views [i](#)

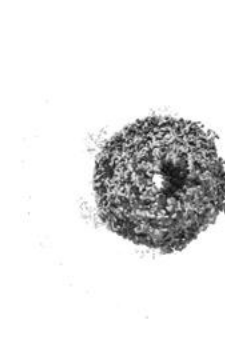
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

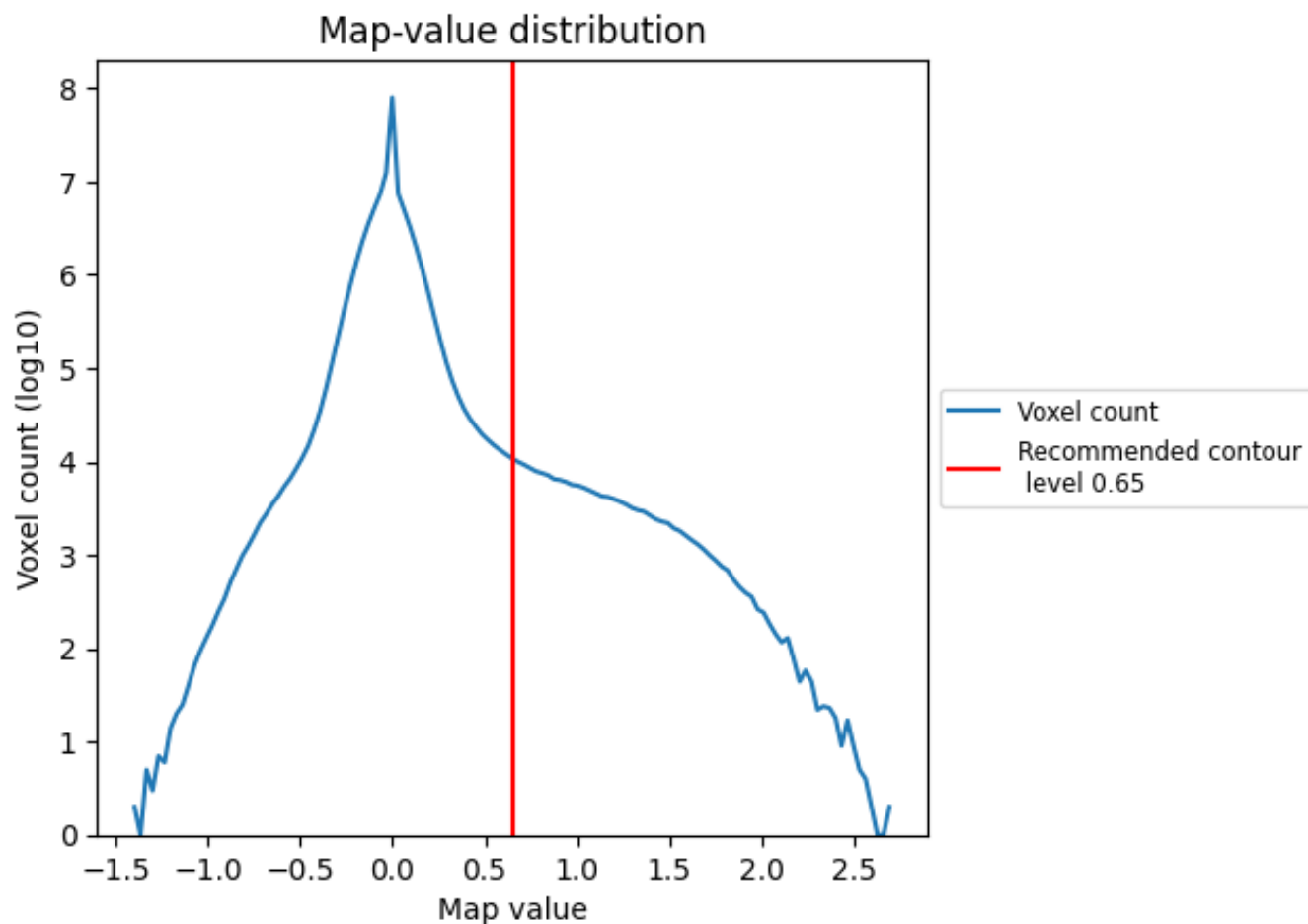
6.5 Mask visualisation

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

7 Map analysis [i](#)

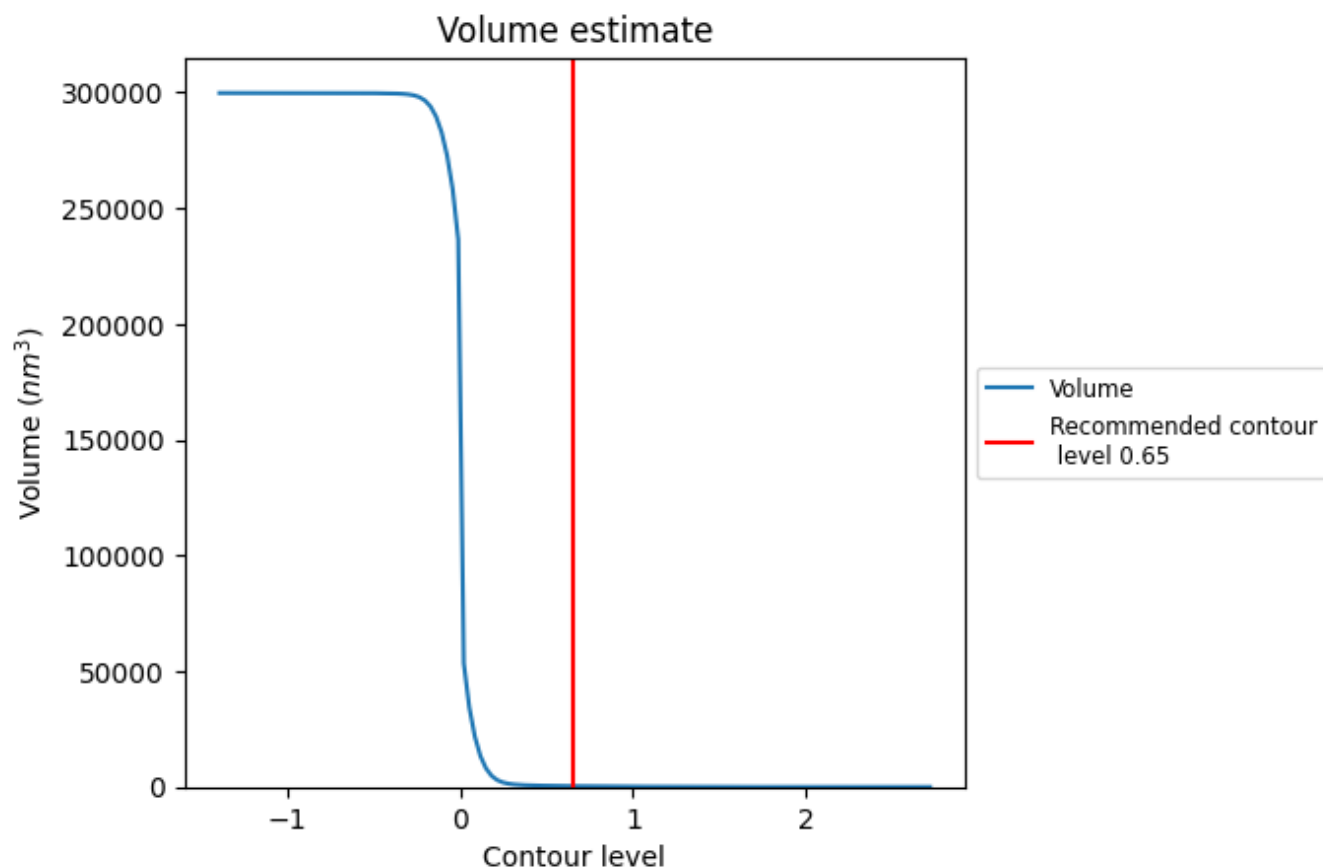
This section contains the results of statistical analysis of the map.

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.

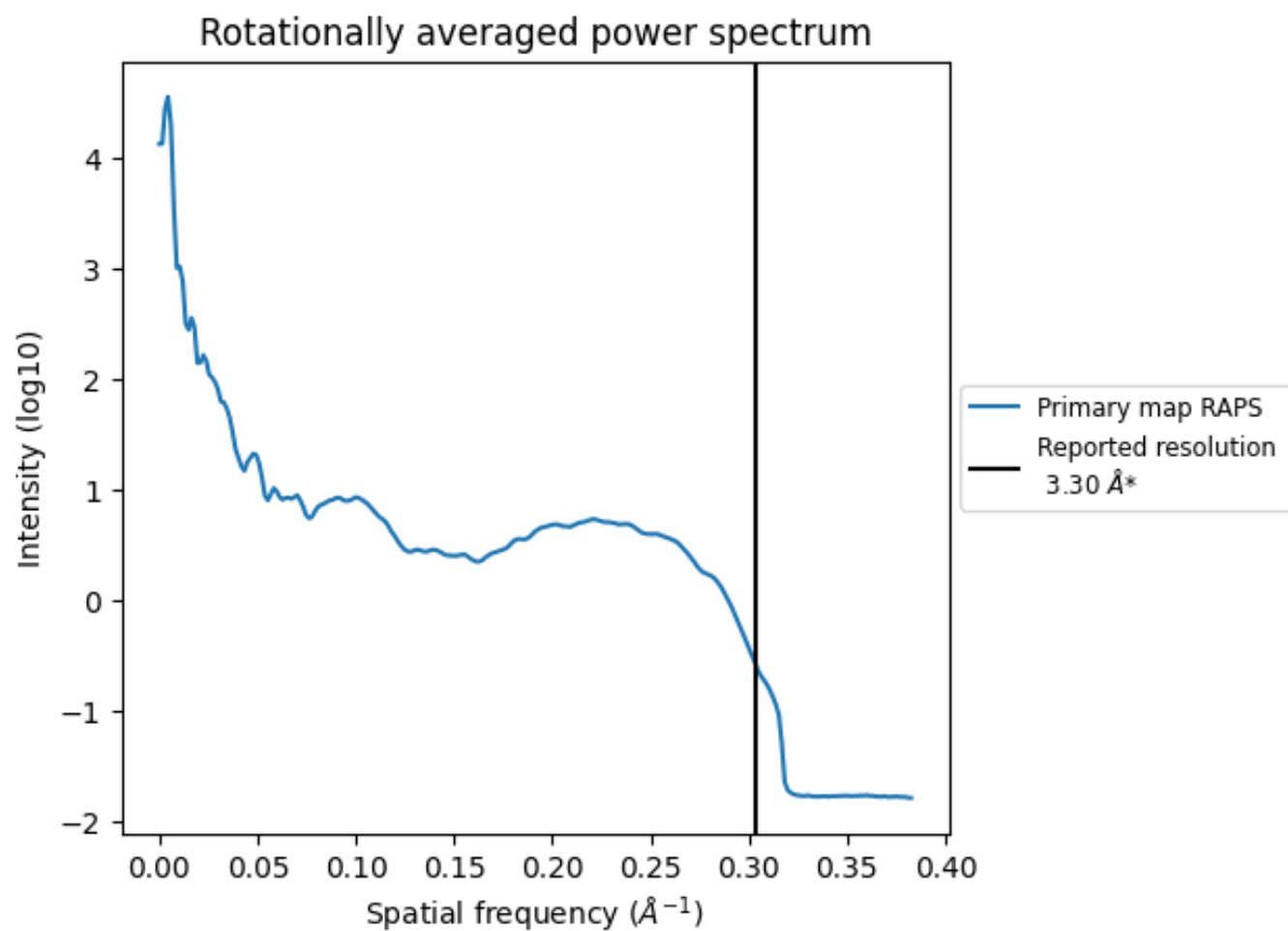
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm^3 ; this corresponds to an approximate mass of 321 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

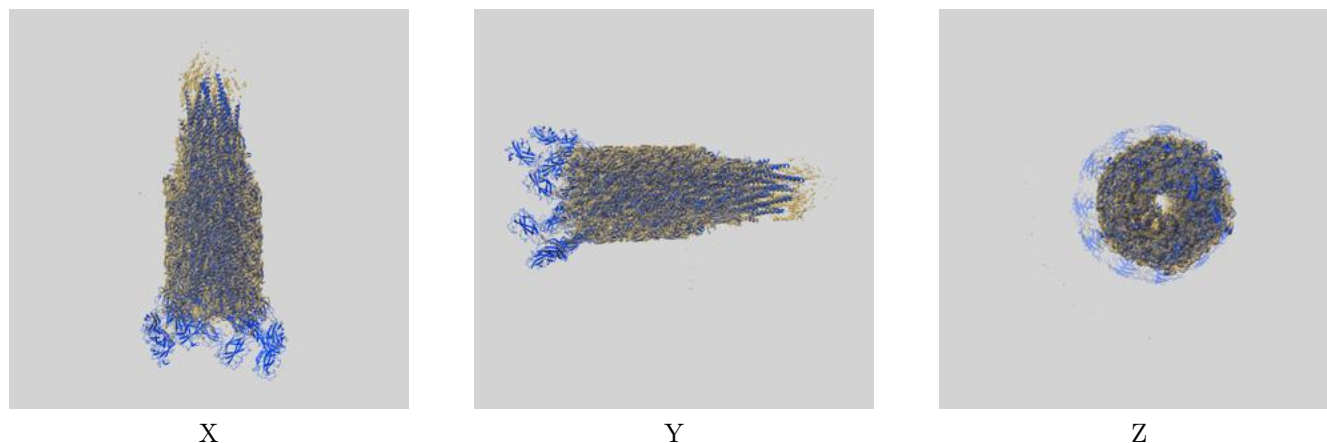
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

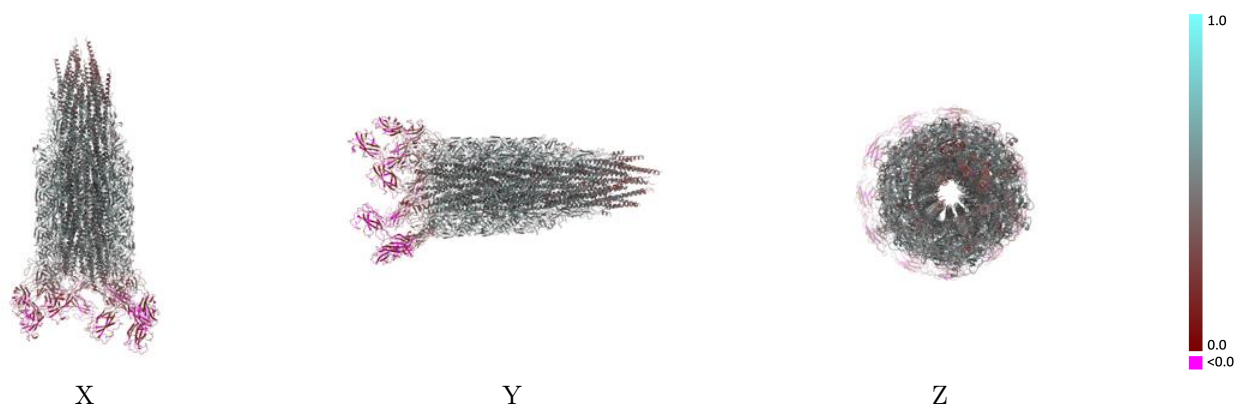
This section contains information regarding the fit between EMDB map EMD-31008 and PDB model 7E82. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



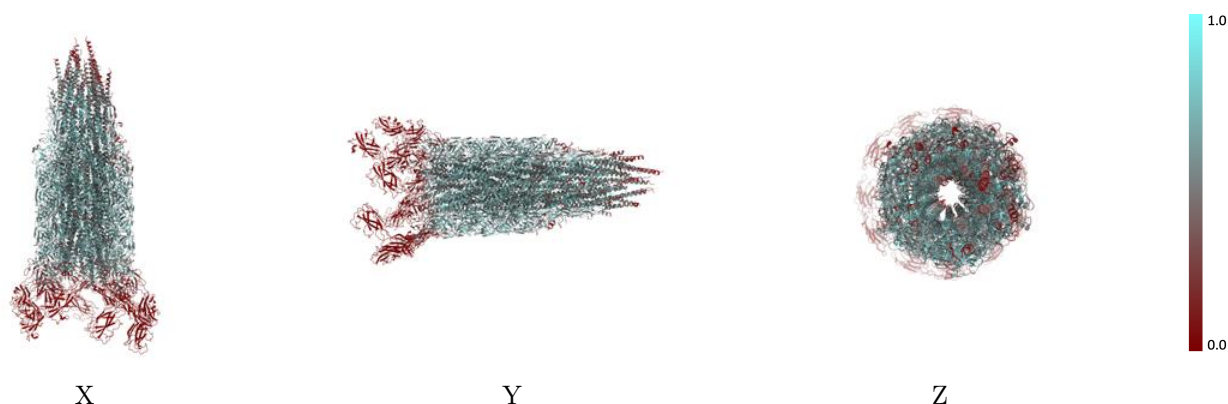
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



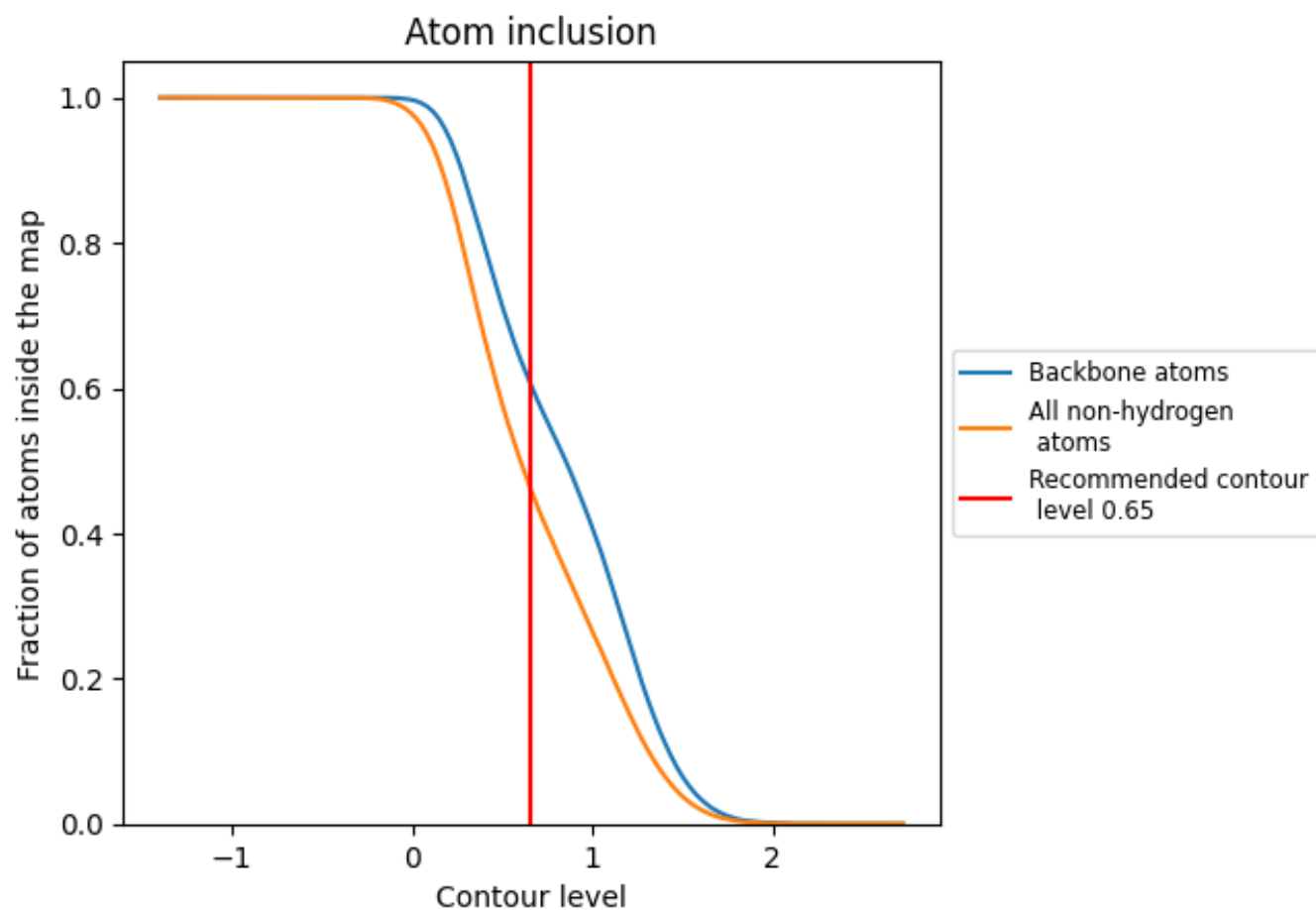
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.65).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 47% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4661	 0.4240
0	 0.5467	 0.4520
1	 0.3733	 0.4130
2	 0.5600	 0.5110
3	 0.5467	 0.4350
4	 0.4133	 0.4530
5	 0.5643	 0.5040
6	 0.1929	 0.4650
7	 0.5143	 0.4840
8	 0.4000	 0.4600
9	 0.1143	 0.4370
A	 0.5784	 0.4880
B	 0.5119	 0.4690
C	 0.5706	 0.4810
D	 0.5846	 0.4880
DA	 0.2965	 0.3420
DB	 0.3235	 0.3580
DC	 0.3338	 0.3520
DD	 0.3092	 0.3200
DE	 0.2835	 0.3180
DF	 0.2555	 0.3140
DG	 0.2329	 0.3020
DH	 0.2155	 0.2900
DI	 0.1956	 0.2680
DJ	 0.1460	 0.1970
DK	 0.1252	 0.2390
E	 0.5846	 0.4860
F	 0.5955	 0.4880
G	 0.6064	 0.4920
H	 0.5976	 0.4970
I	 0.5919	 0.4980
J	 0.6002	 0.5010
K	 0.6101	 0.5000
L	 0.6074	 0.5020
M	 0.5971	 0.5010



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Chain	Atom inclusion	Q-score
N	 0.6164	 0.5060
O	 0.5847	 0.4900
P	 0.5965	 0.4940
Q	 0.6076	 0.4980
R	 0.6010	 0.4990
S	 0.5880	 0.4940
T	 0.5902	 0.4980
U	 0.5985	 0.4970
V	 0.6053	 0.4960
W	 0.5892	 0.5000
X	 0.5401	 0.4830
a	 0.6235	 0.4960
b	 0.5321	 0.4680
c	 0.6150	 0.5000
d	 0.6038	 0.4940
e	 0.5079	 0.4750
f	 0.5821	 0.4740
g	 0.4952	 0.4310
h	 0.6162	 0.4860
i	 0.6039	 0.4810
j	 0.5928	 0.4790
k	 0.5848	 0.4640
l	 0.4853	 0.4440
m	 0.5627	 0.4550
n	 0.5383	 0.4540
o	 0.4180	 0.4250
p	 0.4839	 0.4490
q	 0.4023	 0.4140
r	 0.3830	 0.3380
s	 0.4176	 0.4050
t	 0.4419	 0.4180
u	 0.3202	 0.3950
v	 0.2238	 0.3270