



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2024 – 01:50 AM JST

PDB ID : 8WLP
EMDB ID : EMD-37627
Title : Cryo-EM structure of the distal rod-hook within the flagellar motor-hook complex in the CCW state.
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-30
Resolution : 3.80 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 ⓘ 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:

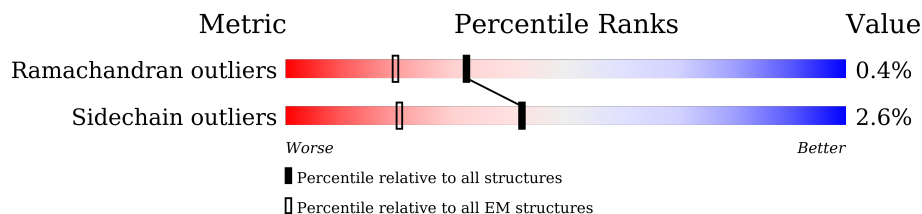
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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 $\leq 5\%$. 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	0	260	
1	1	260	
1	2	260	
1	3	260	
1	4	260	
1	5	260	
1	6	260	
1	7	260	
1	8	260	

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Mol	Chain	Length	Quality of chain
1	9	260	10% 98%
1	ZA	260	8% 98%
1	ZB	260	8% 96%
1	ZC	260	7% 98%
1	ZD	260	8% 97%
1	ZE	260	11% 97%
1	r	260	36% 95%
1	s	260	29% 94%
1	t	260	23% 93%
1	u	260	18% 92%
1	v	260	14% 92%
1	w	260	10% 91%
1	x	260	8% 90%
1	y	260	9% 92%
1	z	260	10% 93%
2	ZF	403	44% 97%
2	ZG	403	17% 95%
2	ZH	403	10% 96%
2	ZI	403	10% 97%
2	ZJ	403	9% 98%
2	ZK	403	9% 98%
2	ZL	403	9% 97%
2	ZM	403	9% 97%
2	ZN	403	10% 97%
2	ZO	403	8% 97%

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Mol	Chain	Length	Quality of chain
2	ZP	403	13% 95%
2	ZQ	403	9% 97%
2	ZR	403	12% 98%
2	ZS	403	13% 98%
2	ZT	403	12% 97%
2	ZU	403	13% 98%
2	ZV	403	14% 98%
2	ZW	403	15% 96%
2	ZX	403	17% 99%
2	ZY	403	22% 98%
2	ZZ	403	25% 98%
2	Za	403	29% 98%
2	Zb	403	33% 98%
2	Zc	403	36% 97%
2	Zd	403	39% 98%
2	Ze	403	43% 97%
2	Zf	403	45% 98%
2	Zg	403	49% 98%
2	Zh	403	51% 98%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 131528 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
			Total	C	N	O	S		
1	0	248	Total 1866	C 1154	N 327	O 379	S 6	0	0
1	1	252	Total 1894	C 1172	N 331	O 385	S 6	0	0
1	2	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	3	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	4	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	5	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	6	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	7	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	8	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	9	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZA	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZB	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZC	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZD	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZE	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	r	254	Total 1903	C 1175	N 334	O 389	S 5	0	0
1	s	255	Total 1911	C 1181	N 335	O 390	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	t	256	Total	C	N	O	S	0	0
			1919	1186	336	391	6		
1	u	254	Total	C	N	O	S	0	0
			1903	1175	334	389	5		
1	v	255	Total	C	N	O	S	0	0
			1911	1181	335	390	5		
1	w	243	Total	C	N	O	S	0	0
			1823	1127	318	373	5		
1	x	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
1	y	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
1	z	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		

- Molecule 2 is a protein called Flagellar hook protein FlgE.

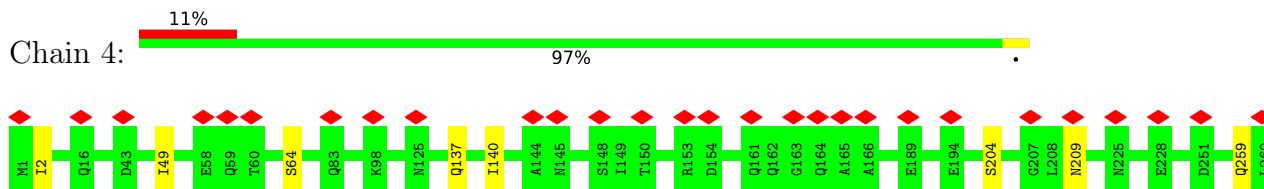
Mol	Chain	Residues	Atoms					AltConf	Trace
2	ZF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZH	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZI	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZJ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZK	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZL	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZM	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZN	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZO	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZP	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZQ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

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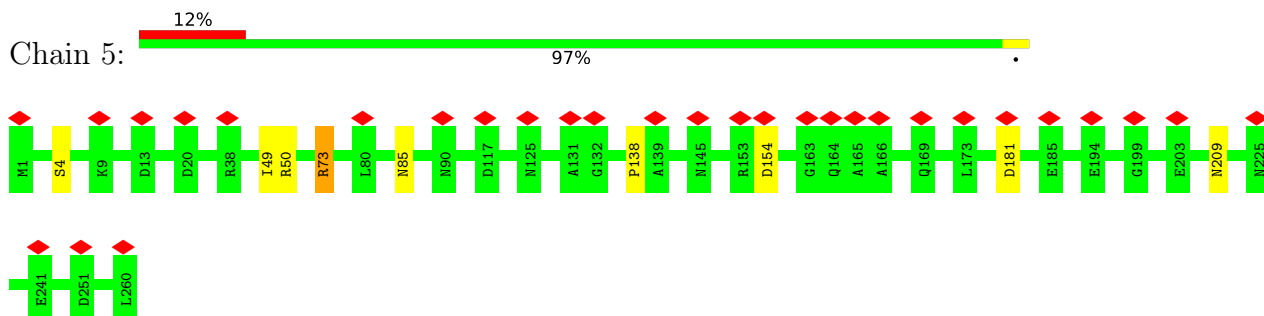
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Mol	Chain	Residues	Atoms					AltConf	Trace
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2	ZS	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
2	ZT	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
2	ZU	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
2	ZV	401	Total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

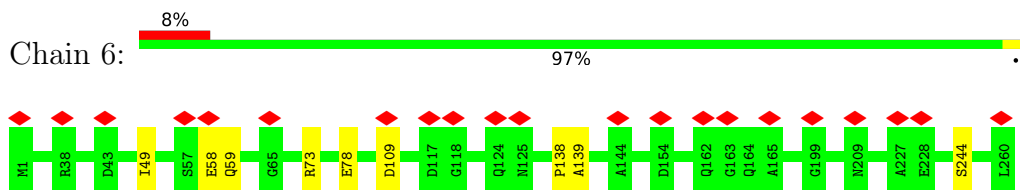
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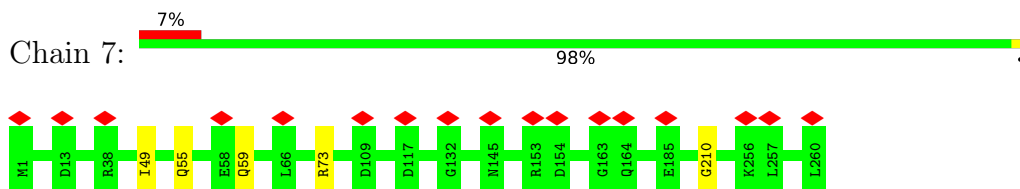
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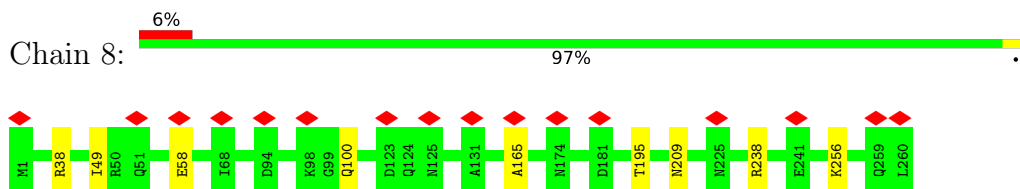
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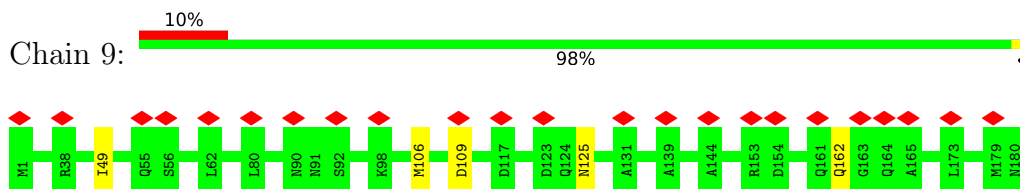
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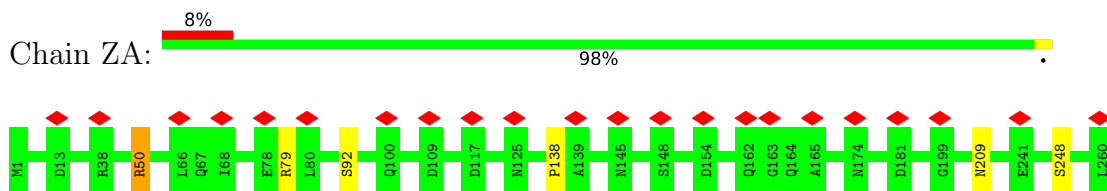
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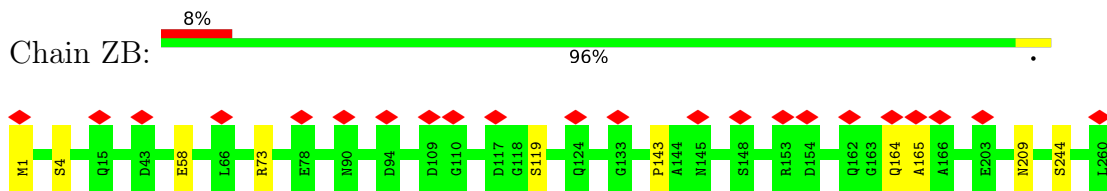
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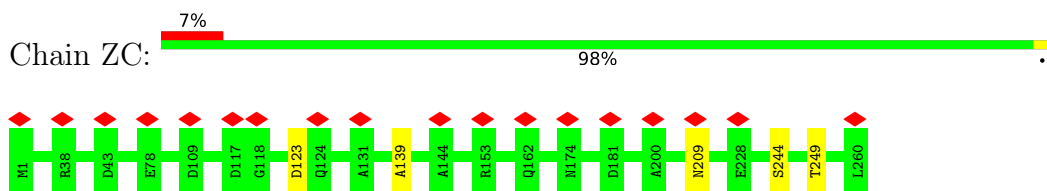
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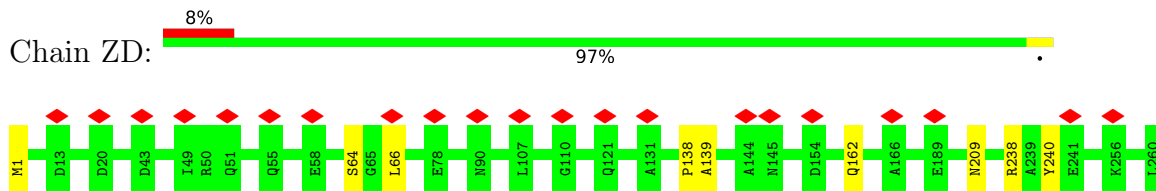
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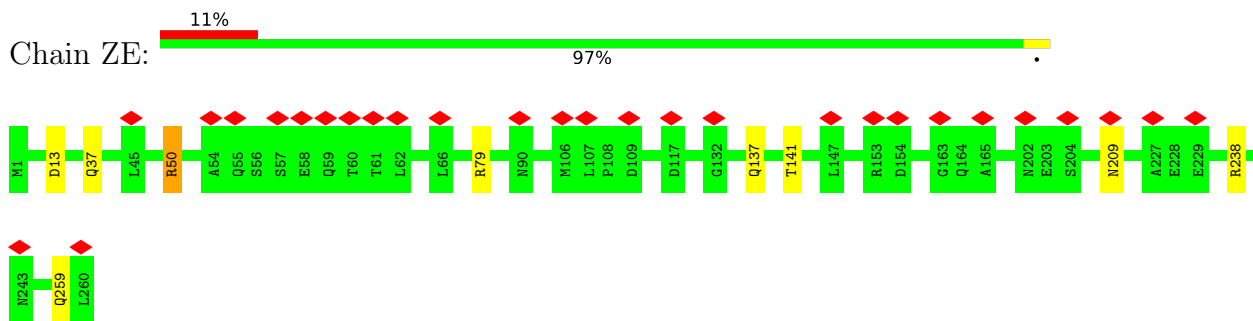
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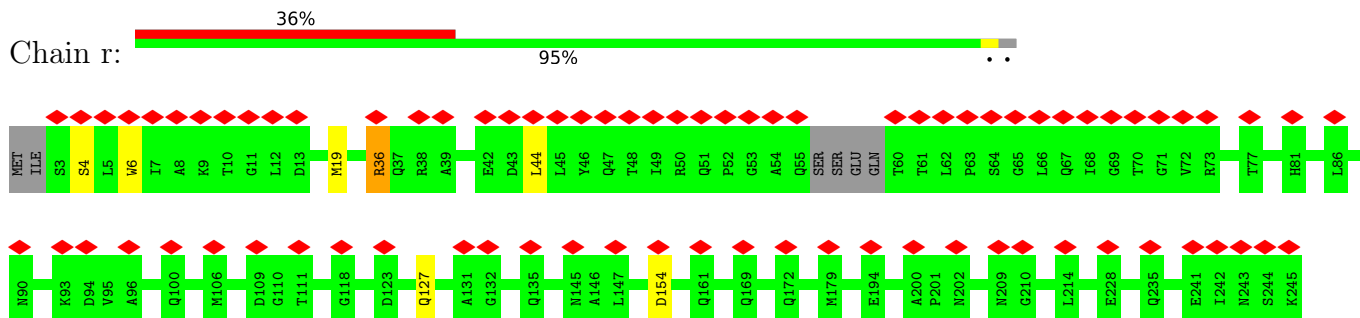
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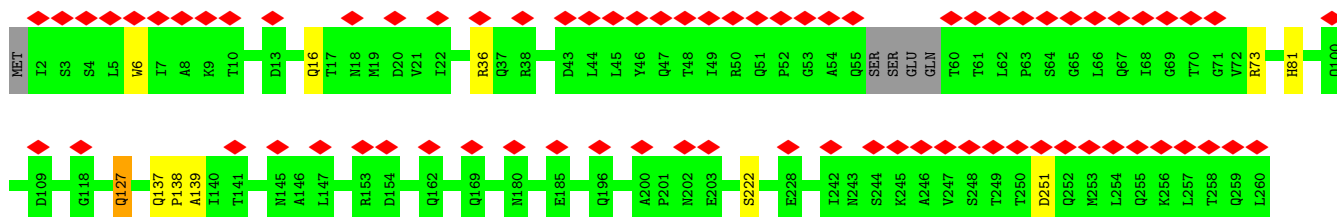
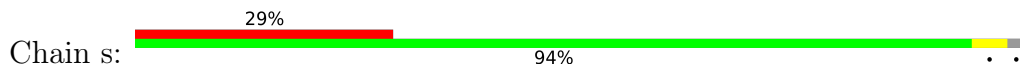


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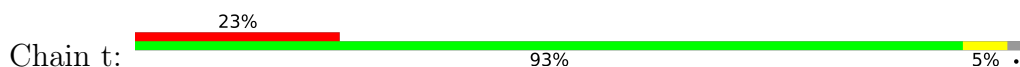




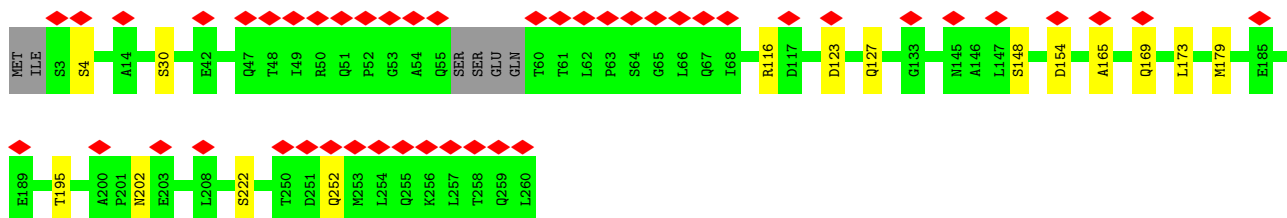
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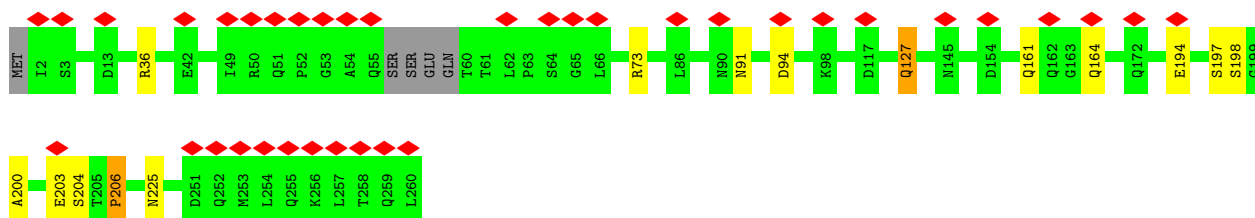
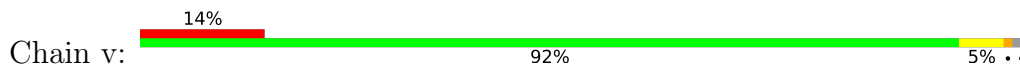
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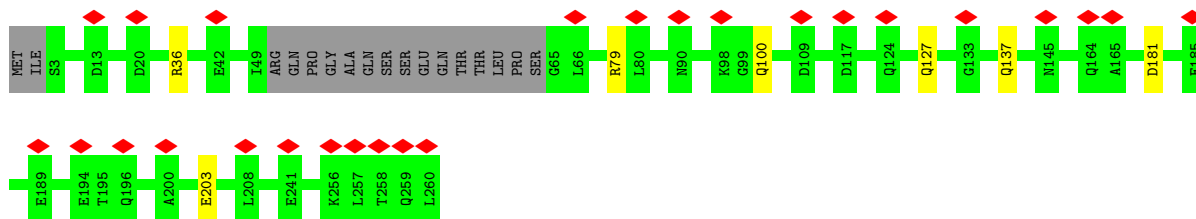
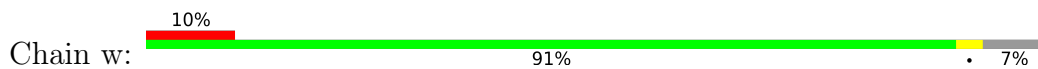
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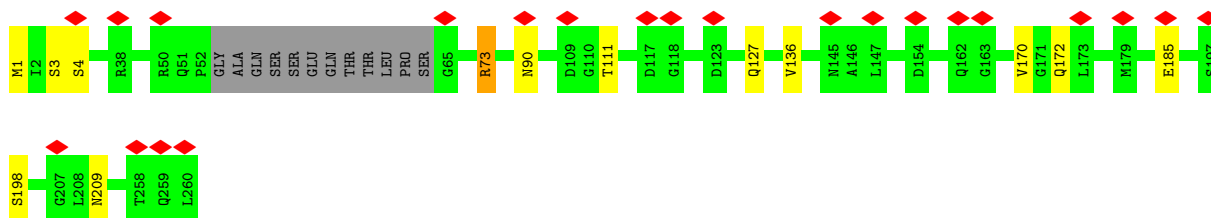
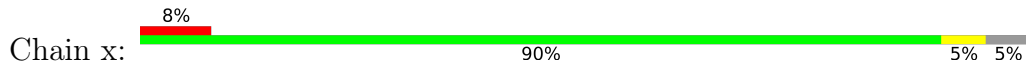
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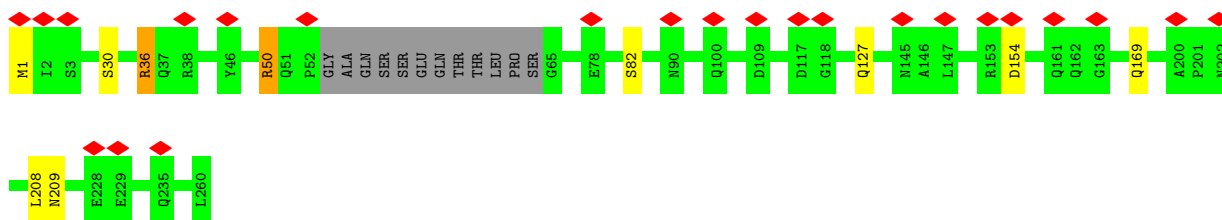
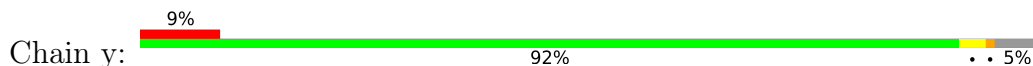
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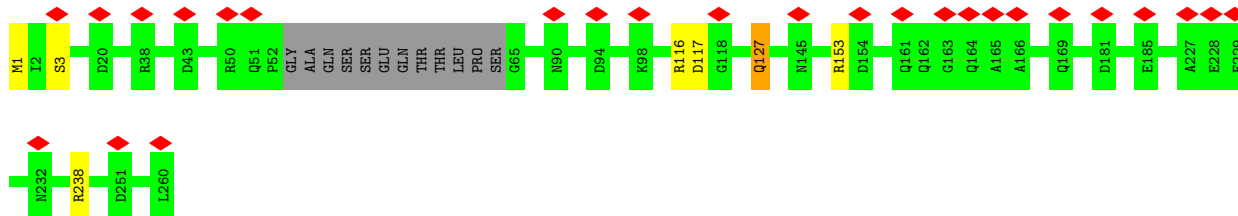
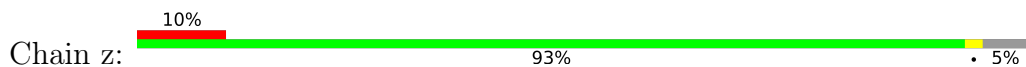
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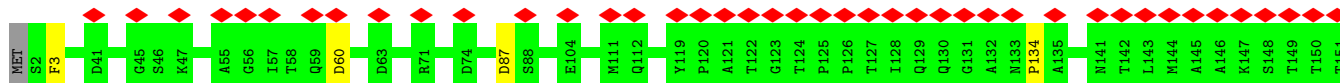
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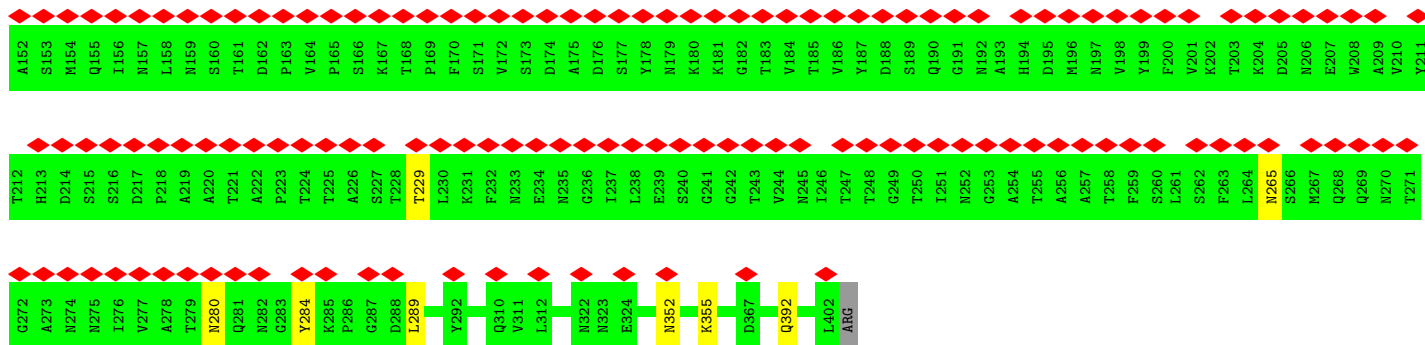


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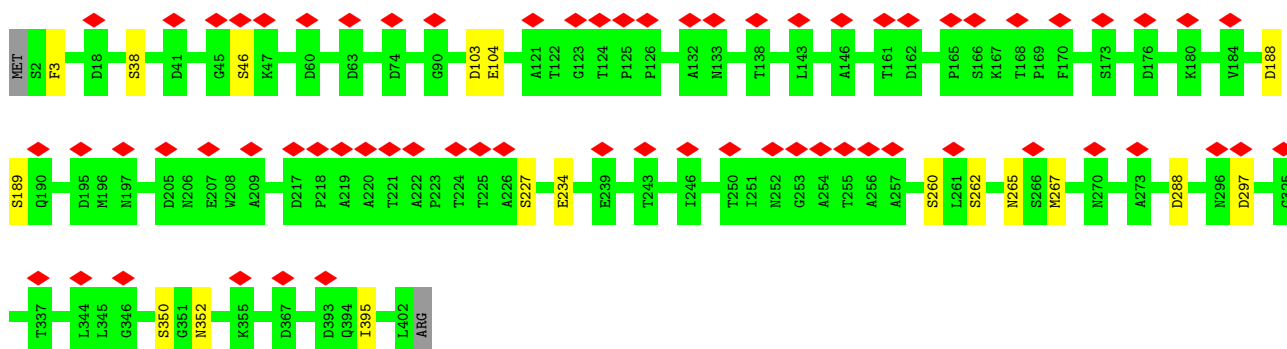


• Molecule 2: Flagellar hook protein FlgE

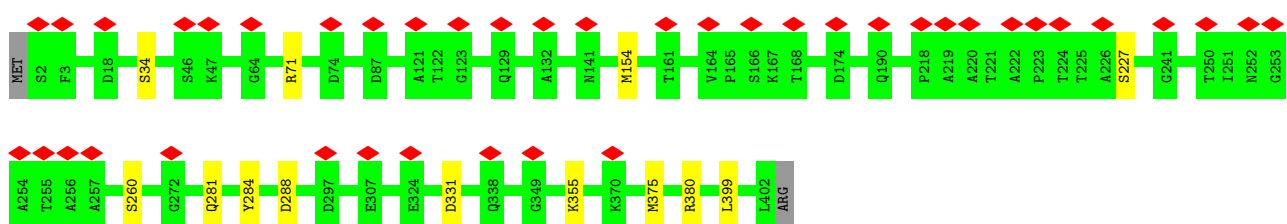




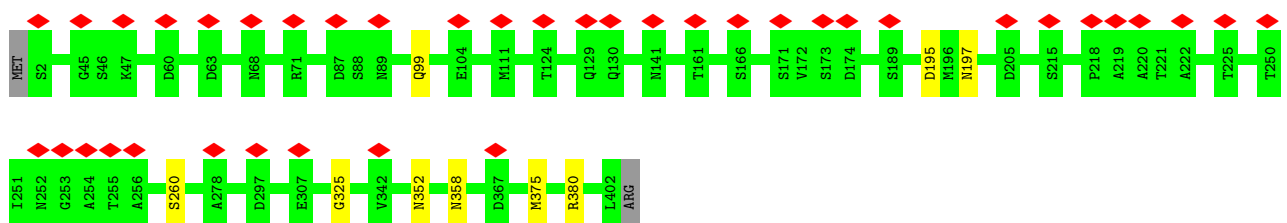
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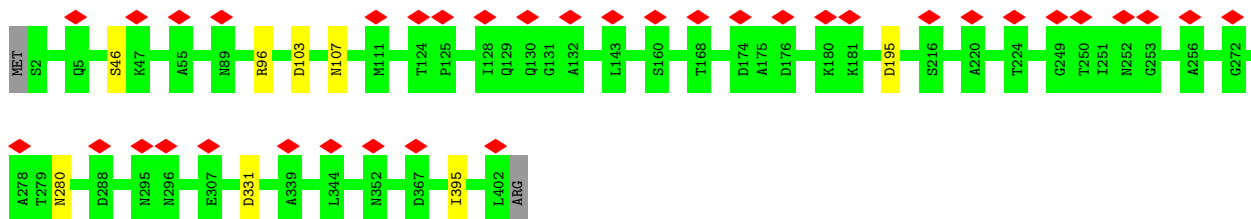
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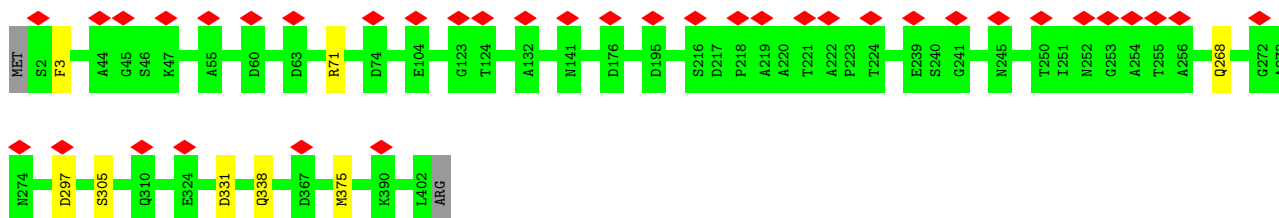
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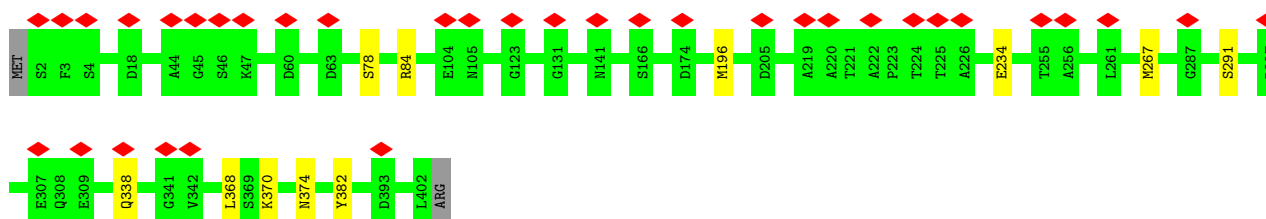
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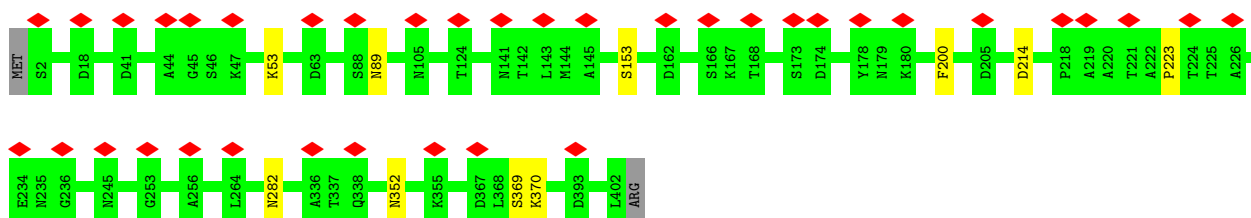
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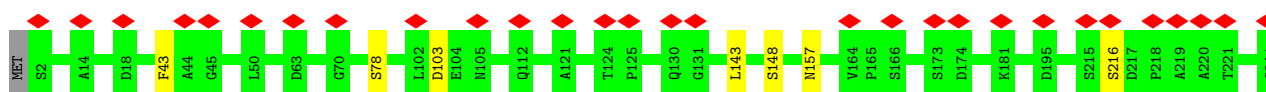
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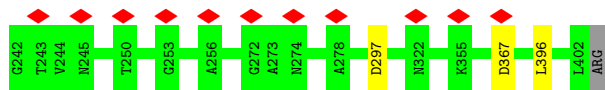


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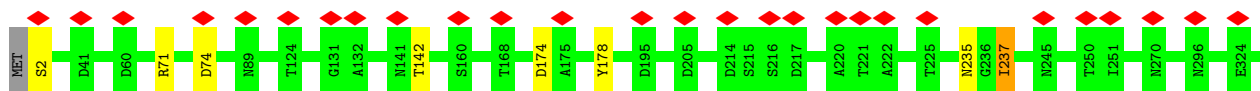


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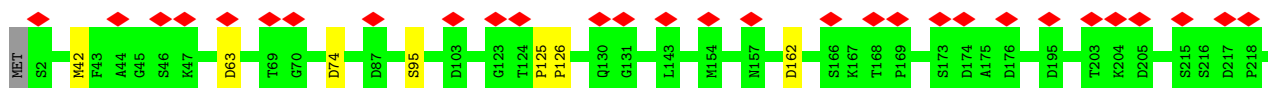




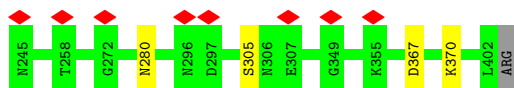
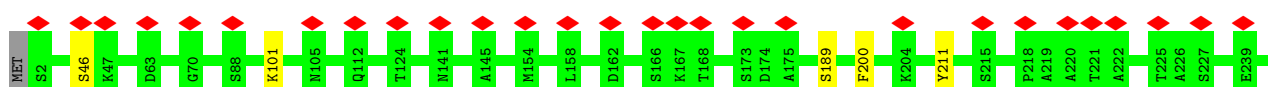
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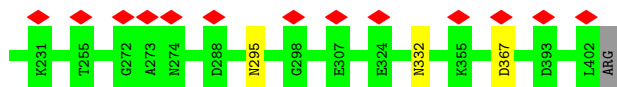
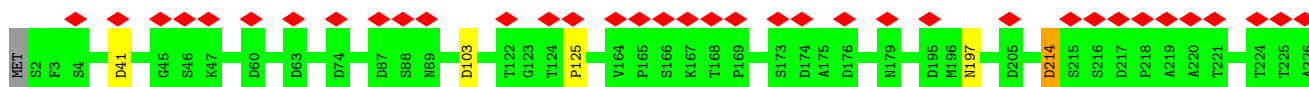
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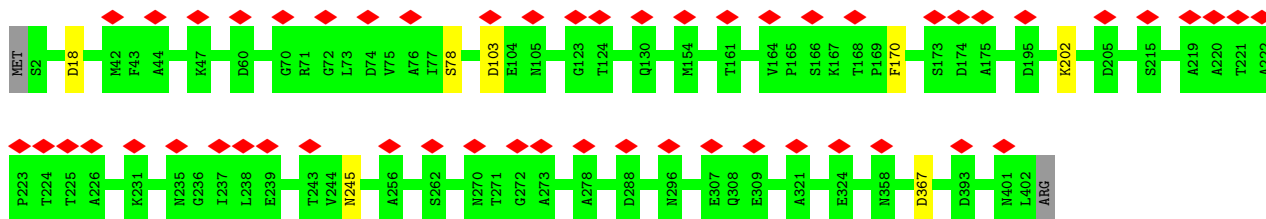
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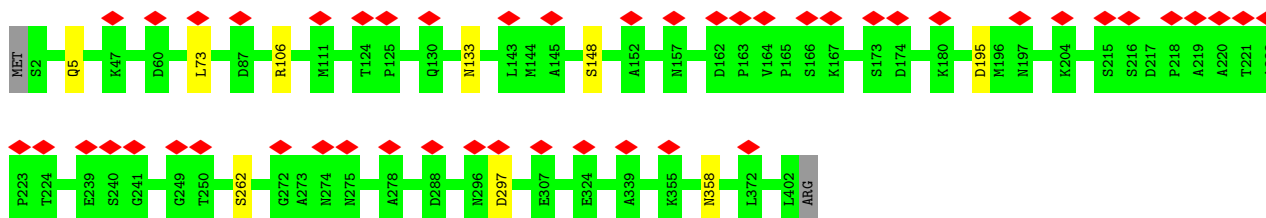
- Molecule 2: Flagellar hook protein FlgE



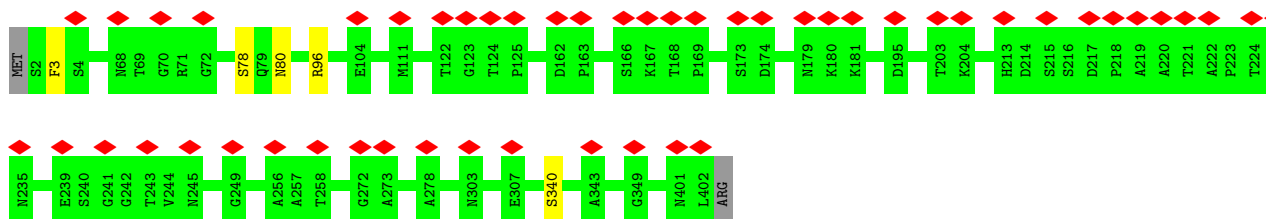
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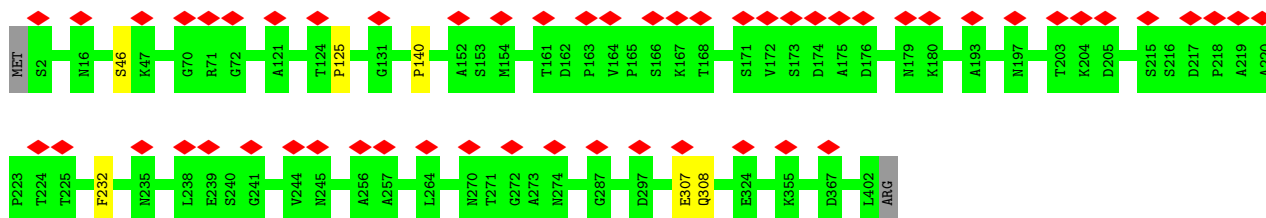
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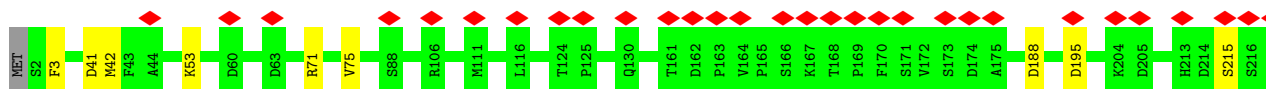
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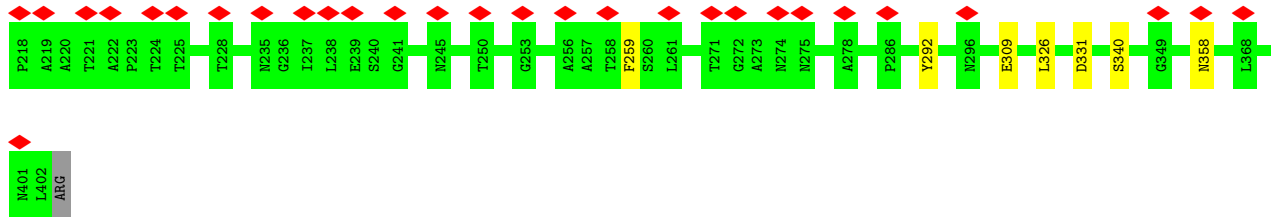


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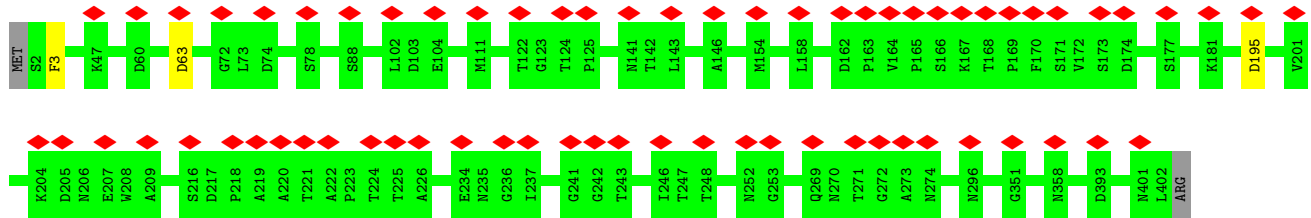


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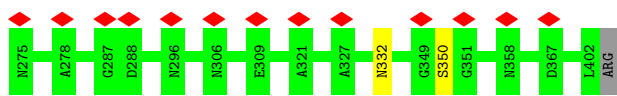
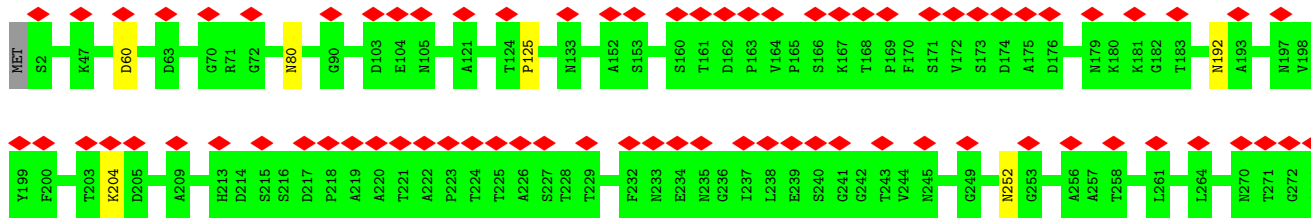




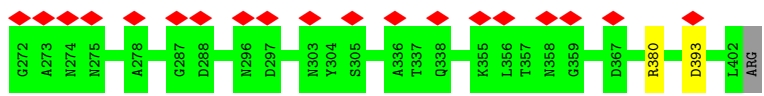
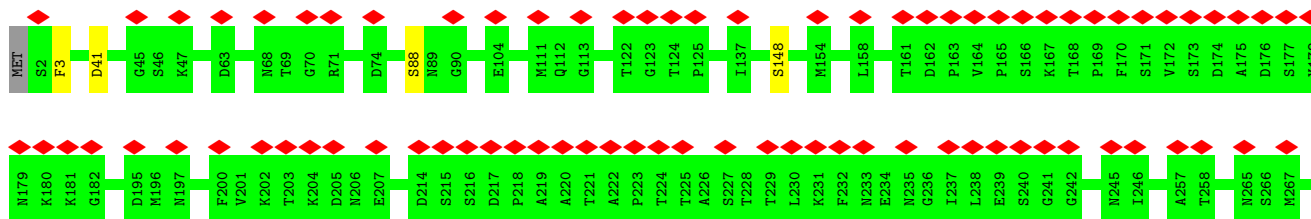
• Molecule 2: Flagellar hook protein FlgE



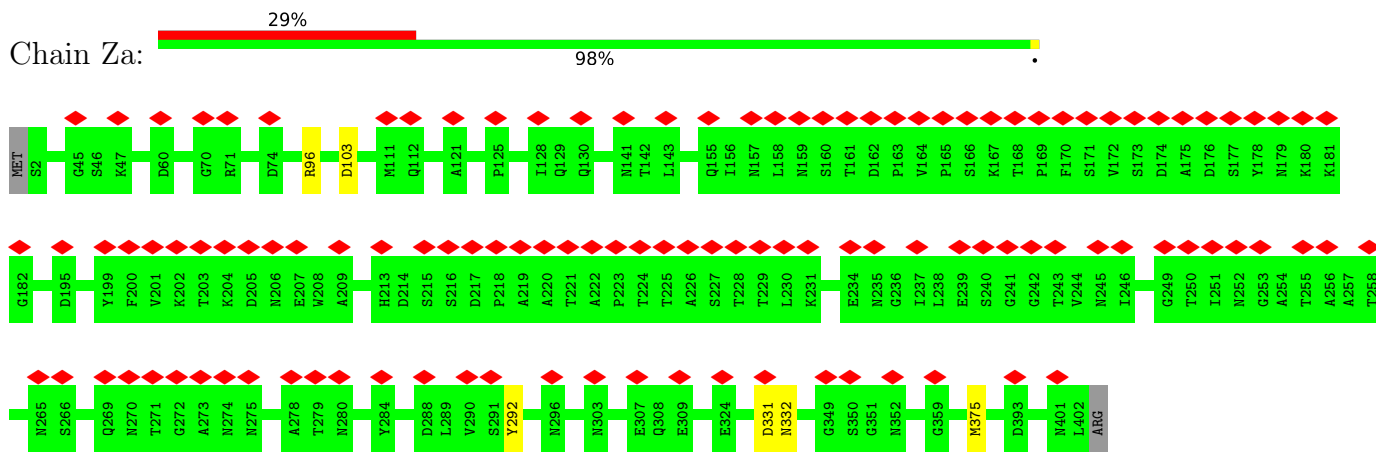
• Molecule 2: Flagellar hook protein FlgE



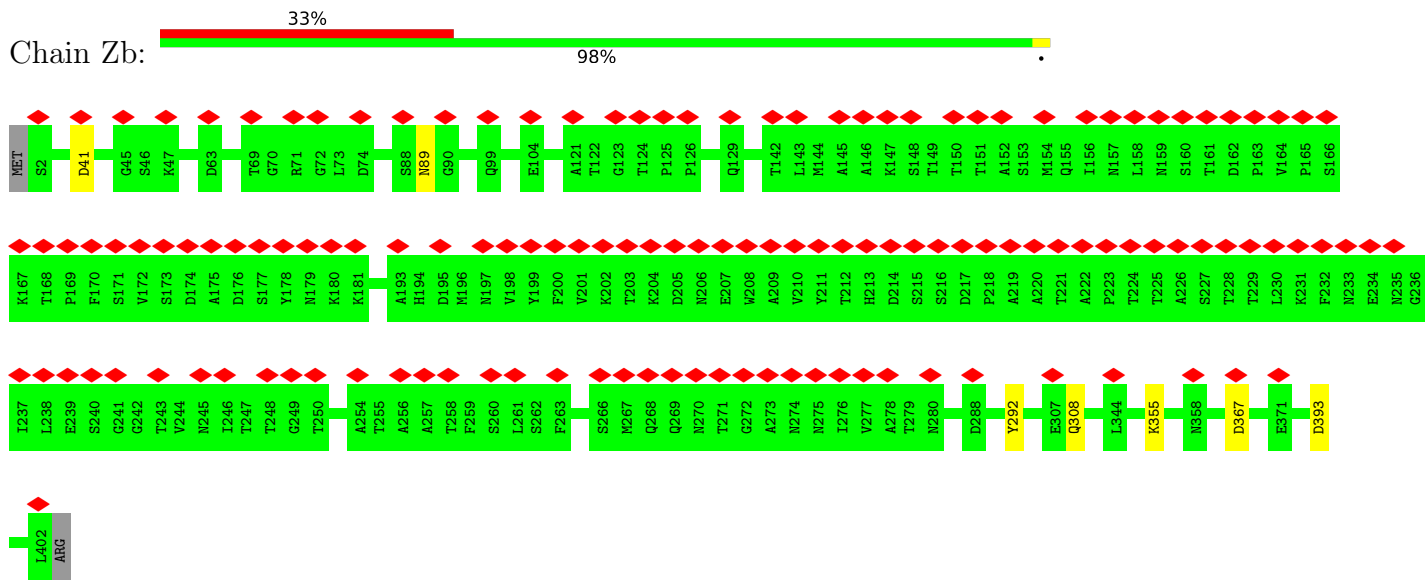
• Molecule 2: Flagellar hook protein FlgE



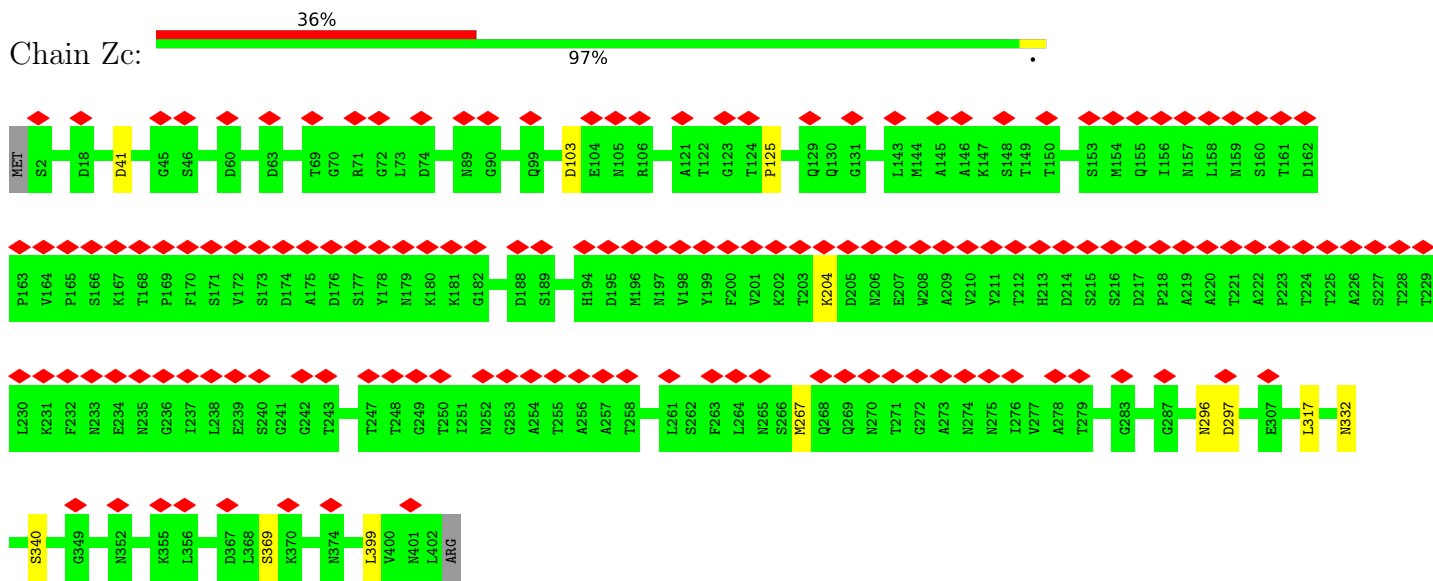
• Molecule 2: Flagellar hook protein FlgE



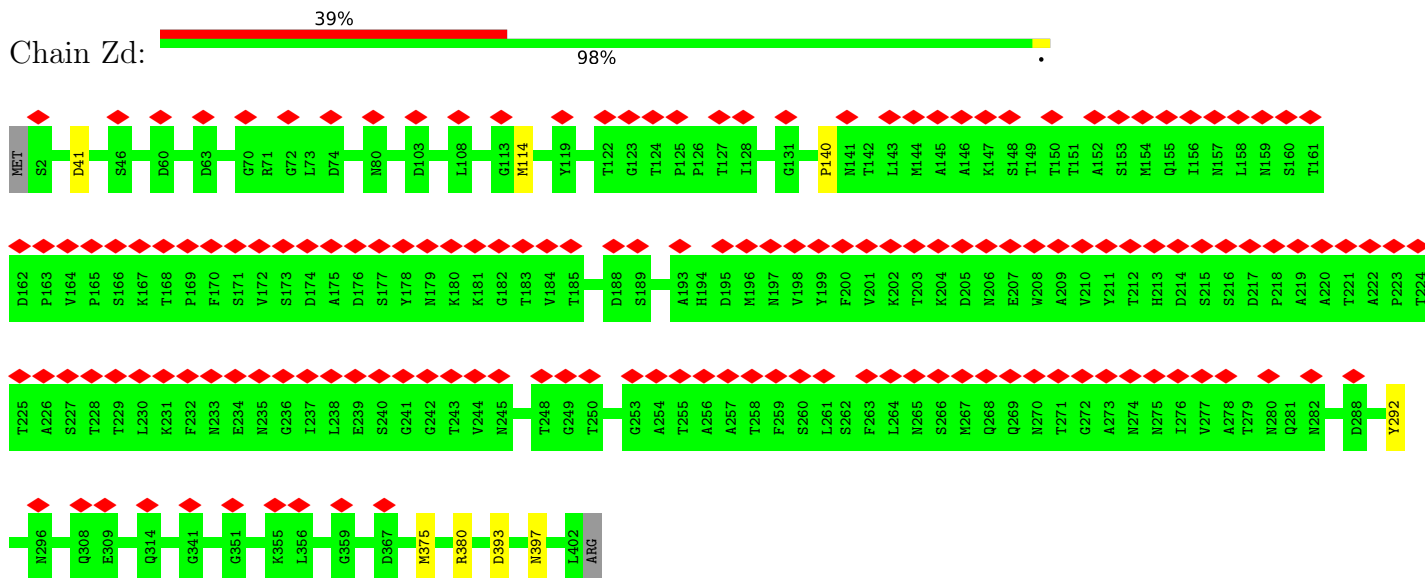
• Molecule 2: Flagellar hook protein FlgE



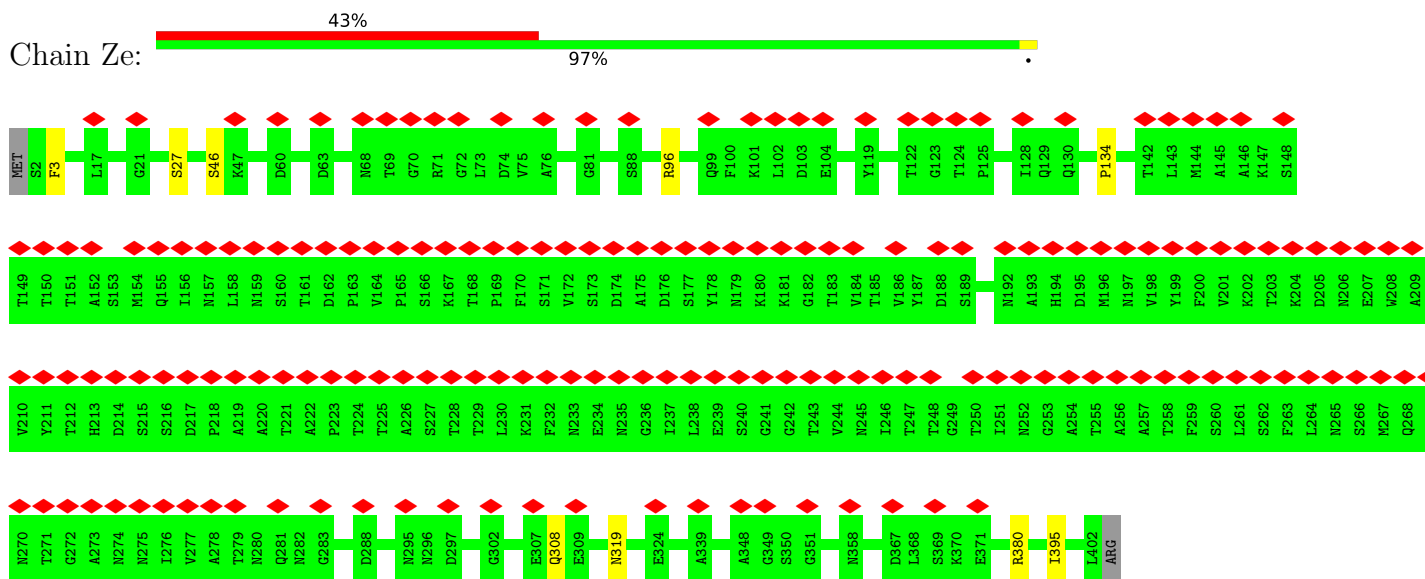
• Molecule 2: Flagellar hook protein FlgE



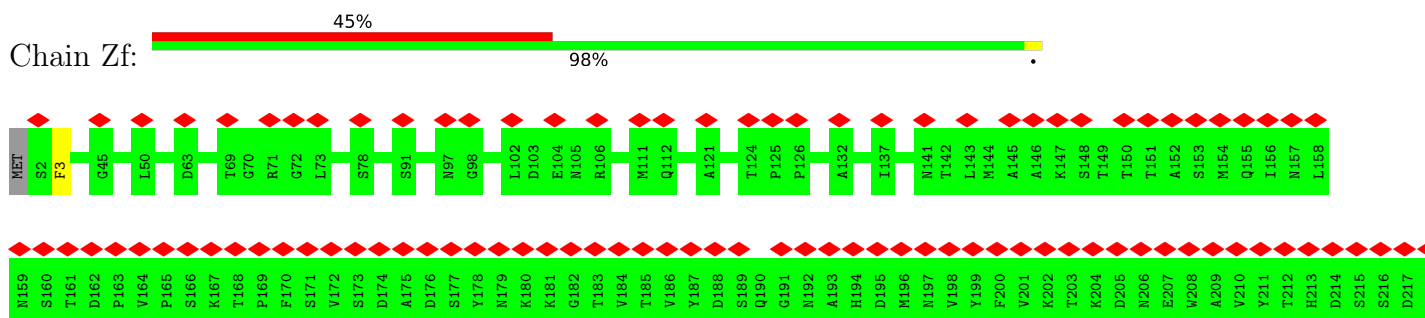
• Molecule 2: Flagellar hook protein FlgE

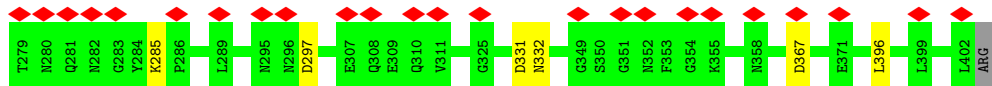
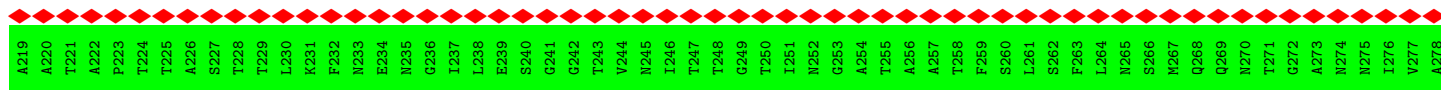


• Molecule 2: Flagellar hook protein FlgE

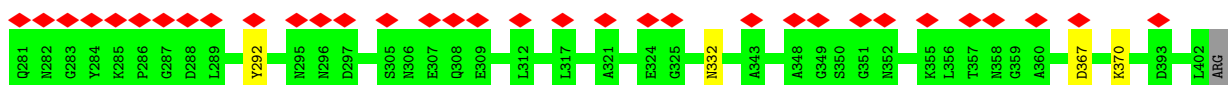
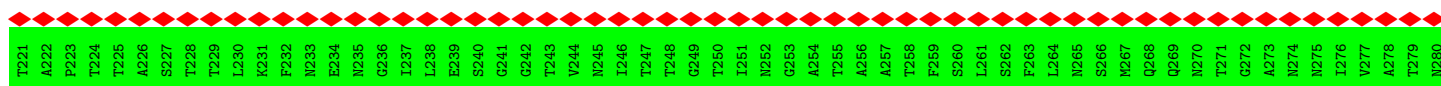
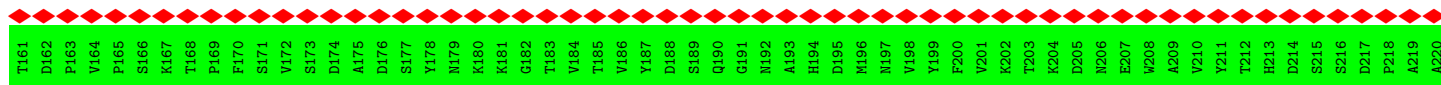


• Molecule 2: Flagellar hook protein FlgE

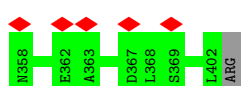
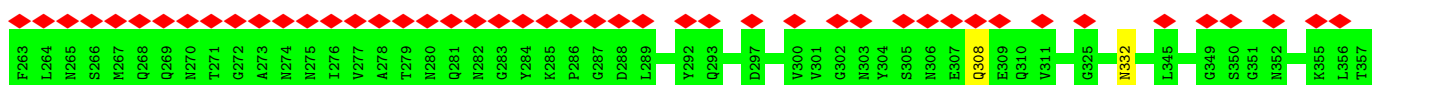
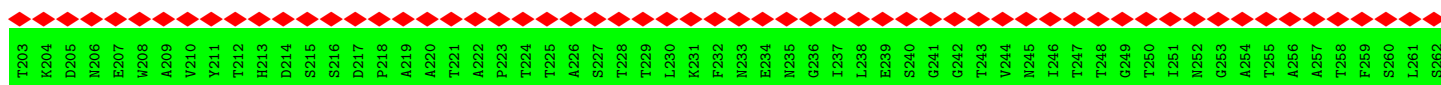
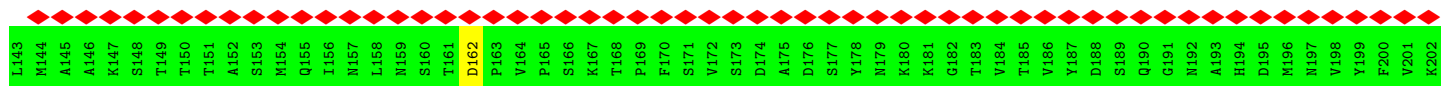




• Molecule 2: Flagellar hook protein FlgE



• Molecule 2: Flagellar hook protein FlgE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11858	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.810	Depositor
Minimum map value	-1.595	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	681.984, 681.984, 681.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332, 1.332, 1.332	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	0	0.33	0/1888	0.54	1/2564 (0.0%)
1	1	0.31	0/1917	0.51	0/2605
1	2	0.28	0/1973	0.51	0/2682
1	3	0.28	0/1973	0.52	0/2682
1	4	0.28	0/1973	0.51	0/2682
1	5	0.33	0/1973	0.52	0/2682
1	6	0.32	0/1973	0.54	0/2682
1	7	0.32	0/1973	0.53	0/2682
1	8	0.33	0/1973	0.56	0/2682
1	9	0.30	0/1973	0.53	1/2682 (0.0%)
1	ZA	0.31	0/1973	0.53	0/2682
1	ZB	0.29	0/1973	0.49	0/2682
1	ZC	0.34	0/1973	0.54	0/2682
1	ZD	0.31	0/1973	0.52	0/2682
1	ZE	0.30	0/1973	0.51	1/2682 (0.0%)
1	r	0.34	0/1926	0.53	0/2618
1	s	0.38	0/1934	0.59	0/2629
1	t	0.39	0/1942	0.56	0/2639
1	u	0.35	0/1926	0.58	1/2618 (0.0%)
1	v	0.34	0/1934	0.54	0/2629
1	w	0.34	0/1844	0.51	0/2505
1	x	0.33	0/1888	0.52	0/2564
1	y	0.33	0/1888	0.56	1/2564 (0.0%)
1	z	0.31	0/1888	0.51	0/2564
2	ZF	0.28	0/2991	0.49	0/4076
2	ZG	0.33	0/2991	0.52	1/4076 (0.0%)
2	ZH	0.29	0/2991	0.50	0/4076
2	ZI	0.30	0/2991	0.51	0/4076
2	ZJ	0.30	0/2991	0.49	0/4076
2	ZK	0.29	0/2991	0.50	0/4076
2	ZL	0.29	0/2991	0.49	0/4076
2	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
2	ZN	0.28	0/2991	0.51	0/4076
2	ZO	0.30	0/2991	0.50	0/4076

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
2	ZQ	0.29	0/2991	0.51	0/4076
2	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
2	ZS	0.29	0/2991	0.52	1/4076 (0.0%)
2	ZT	0.29	0/2991	0.48	0/4076
2	ZU	0.28	0/2991	0.50	0/4076
2	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
2	ZW	0.27	0/2991	0.49	0/4076
2	ZX	0.28	0/2991	0.48	0/4076
2	ZY	0.30	1/2991 (0.0%)	0.54	2/4076 (0.0%)
2	ZZ	0.26	0/2991	0.46	0/4076
2	Za	0.28	0/2991	0.49	0/4076
2	Zb	0.30	0/2991	0.49	0/4076
2	Zc	0.29	0/2991	0.52	2/4076 (0.0%)
2	Zd	0.29	0/2991	0.51	0/4076
2	Ze	0.28	0/2991	0.48	0/4076
2	Zf	0.27	0/2991	0.48	0/4076
2	Zg	0.28	0/2991	0.49	0/4076
2	Zh	0.28	0/2991	0.48	0/4076
All	All	0.31	6/133363 (0.0%)	0.52	22/181569 (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
1	0	0	2
1	1	0	1
1	5	0	2
1	7	0	1
1	8	0	2
1	ZA	0	2
1	ZD	0	1
1	ZE	0	3
1	r	0	1
1	u	0	1
1	w	0	1
1	x	0	1
1	y	0	2
1	z	0	3
2	ZI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	ZK	0	1
2	ZO	0	1
2	ZT	0	1
2	ZU	0	1
2	ZW	0	1
2	ZZ	0	1
2	Zd	0	1
2	Ze	0	1
All	All	0	32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	ZV	140	PRO	CG-CD	-16.12	0.97	1.50
2	ZV	125	PRO	CG-CD	-10.14	1.17	1.50
2	ZV	140	PRO	N-CD	8.33	1.59	1.47
2	ZV	125	PRO	N-CD	6.59	1.57	1.47
2	ZY	125	PRO	CG-CD	-5.44	1.32	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	ZV	140	PRO	N-CD-CG	-17.33	77.21	103.20
2	ZR	125	PRO	CA-N-CD	-13.96	91.96	111.50
2	ZY	125	PRO	CA-N-CD	-13.35	92.81	111.50
2	ZV	125	PRO	CA-N-CD	-13.25	92.95	111.50
2	ZV	125	PRO	N-CD-CG	-11.26	86.32	103.20

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	36	ARG	Sidechain
1	0	50	ARG	Sidechain
1	1	36	ARG	Sidechain
1	5	50	ARG	Sidechain
1	5	73	ARG	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	244/260 (94%)	236 (97%)	5 (2%)	3 (1%)	11	40
1	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	63
1	2	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	49
1	3	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	49
1	4	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	49
1	5	258/260 (99%)	240 (93%)	15 (6%)	3 (1%)	11	40
1	6	258/260 (99%)	244 (95%)	10 (4%)	4 (2%)	8	36
1	7	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	11	40
1	8	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	40
1	9	258/260 (99%)	244 (95%)	13 (5%)	1 (0%)	30	63
1	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	40
1	ZB	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	40
1	ZC	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	49
1	ZD	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	11	40
1	ZE	258/260 (99%)	242 (94%)	15 (6%)	1 (0%)	30	63
1	r	250/260 (96%)	238 (95%)	11 (4%)	1 (0%)	30	63
1	s	251/260 (96%)	234 (93%)	14 (6%)	3 (1%)	11	40
1	t	252/260 (97%)	234 (93%)	16 (6%)	2 (1%)	16	49
1	u	250/260 (96%)	239 (96%)	9 (4%)	2 (1%)	16	49
1	v	251/260 (96%)	235 (94%)	10 (4%)	6 (2%)	5	29
1	w	239/260 (92%)	231 (97%)	7 (3%)	1 (0%)	30	63
1	x	244/260 (94%)	229 (94%)	10 (4%)	5 (2%)	6	32
1	y	244/260 (94%)	234 (96%)	9 (4%)	1 (0%)	30	63
1	z	244/260 (94%)	239 (98%)	4 (2%)	1 (0%)	30	63
2	ZF	399/403 (99%)	387 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	ZG	399/403 (99%)	388 (97%)	10 (2%)	1 (0%)	37	69
2	ZH	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
2	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	58
2	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
2	ZK	399/403 (99%)	387 (97%)	11 (3%)	1 (0%)	37	69
2	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	69
2	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
2	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
2	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	49
2	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	69
2	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
2	ZR	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
2	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
2	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
2	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
2	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
2	ZW	399/403 (99%)	380 (95%)	18 (4%)	1 (0%)	37	69
2	ZX	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
2	ZY	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
2	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
2	Za	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
2	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
2	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
2	Zd	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
2	Ze	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	69
2	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
2	Zg	399/403 (99%)	383 (96%)	16 (4%)	0	100	100
2	Zh	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
All	All	17642/17927 (98%)	16971 (96%)	602 (3%)	69 (0%)	32	63

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	209	ASN
1	4	140	ILE
1	5	209	ASN
1	6	139	ALA
1	8	209	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	0	205/215 (95%)	198 (97%)	7 (3%)	32	55
1	1	209/215 (97%)	201 (96%)	8 (4%)	28	52
1	2	215/215 (100%)	213 (99%)	2 (1%)	75	82
1	3	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	4	215/215 (100%)	209 (97%)	6 (3%)	38	59
1	5	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	6	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	7	215/215 (100%)	214 (100%)	1 (0%)	86	90
1	8	215/215 (100%)	211 (98%)	4 (2%)	52	69
1	9	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	82
1	ZB	215/215 (100%)	208 (97%)	7 (3%)	33	56
1	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	ZD	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	ZE	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	r	209/215 (97%)	203 (97%)	6 (3%)	37	58
1	s	210/215 (98%)	201 (96%)	9 (4%)	25	49
1	t	211/215 (98%)	199 (94%)	12 (6%)	17	43
1	u	209/215 (97%)	198 (95%)	11 (5%)	19	44
1	v	210/215 (98%)	199 (95%)	11 (5%)	19	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	w	200/215 (93%)	195 (98%)	5 (2%)	42	62
1	x	205/215 (95%)	197 (96%)	8 (4%)	27	51
1	y	205/215 (95%)	197 (96%)	8 (4%)	27	51
1	z	205/215 (95%)	201 (98%)	4 (2%)	50	68
2	ZF	321/323 (99%)	309 (96%)	12 (4%)	29	53
2	ZG	321/323 (99%)	305 (95%)	16 (5%)	20	45
2	ZH	321/323 (99%)	308 (96%)	13 (4%)	27	50
2	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	62
2	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	56
2	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	59
2	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	56
2	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	62
2	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	46
2	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	59
2	ZR	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	ZT	321/323 (99%)	313 (98%)	8 (2%)	42	62
2	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	77
2	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	77
2	ZW	321/323 (99%)	307 (96%)	14 (4%)	24	48
2	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	82
2	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	73
2	Za	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	Zb	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	55
2	Zd	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Ze	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	Zh	321/323 (99%)	314 (98%)	7 (2%)	47	64
All	All	14382/14527 (99%)	14004 (97%)	378 (3%)	42	61

5 of 378 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	ZX	3	PHE
2	Zf	297	ASP
2	ZY	252	ASN
2	Zc	103	ASP
2	Zh	83	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 393 such sidechains are listed below:

Mol	Chain	Res	Type
2	ZU	269	GLN
2	Zb	5	GLN
2	ZV	280	ASN
2	ZX	352	ASN
2	Zc	5	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

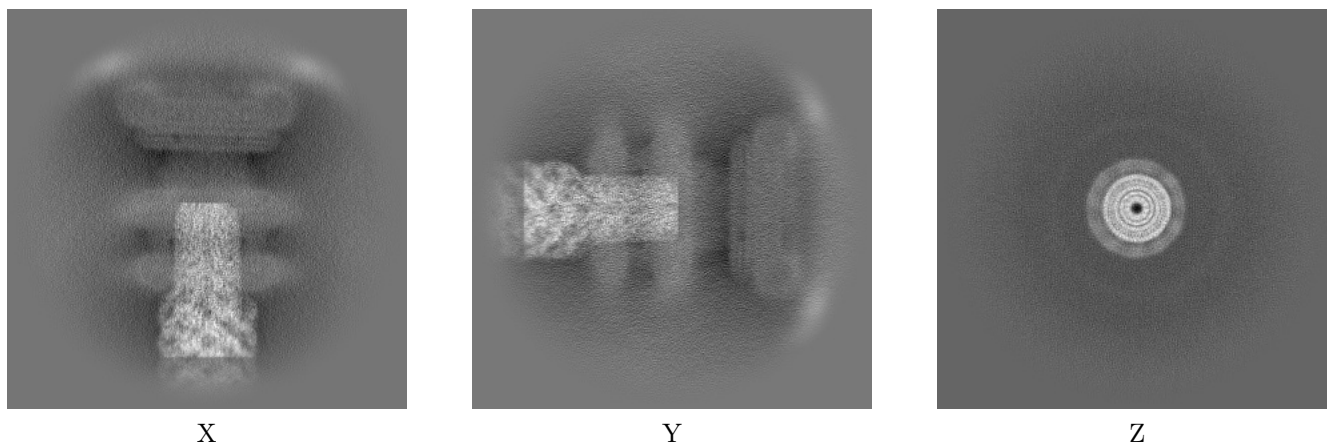
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37627. These allow visual inspection of the internal detail of the map and identification of artifacts.

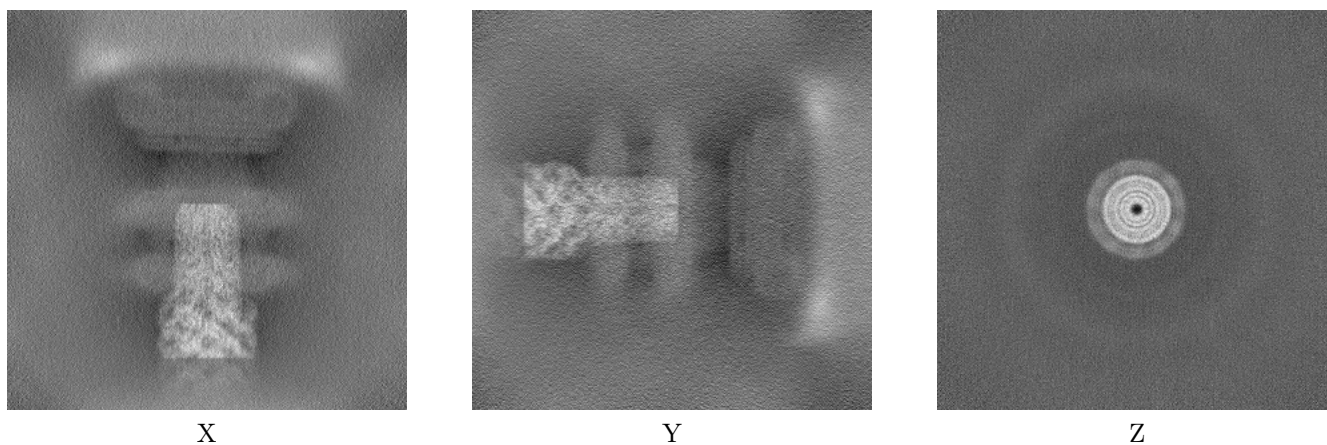
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



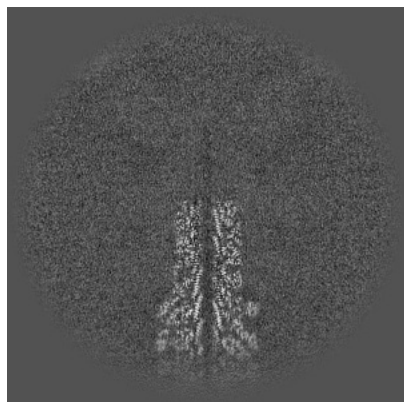
6.1.2 Raw map



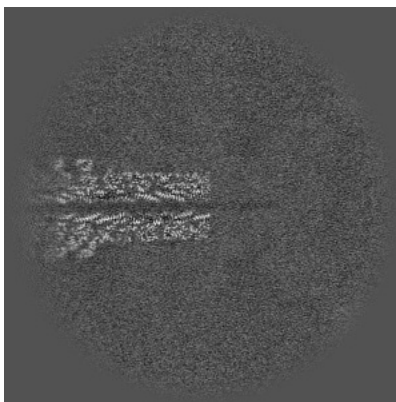
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

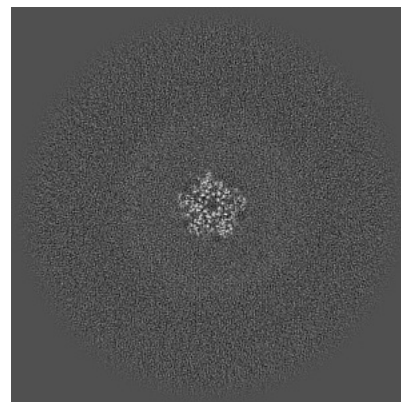
6.2.1 Primary map



X Index: 256

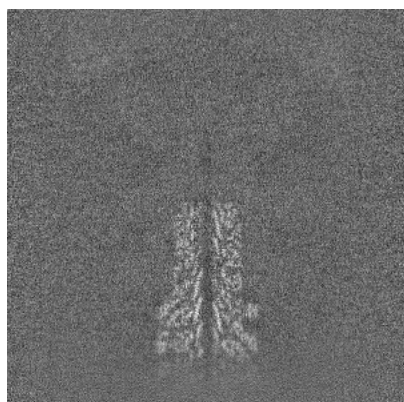


Y Index: 256

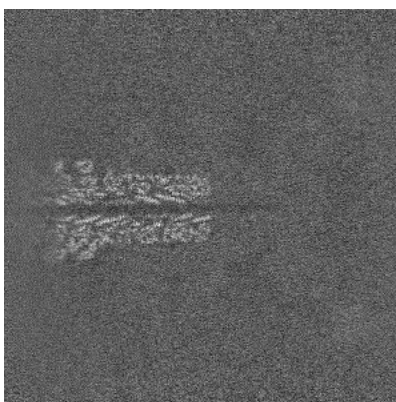


Z Index: 256

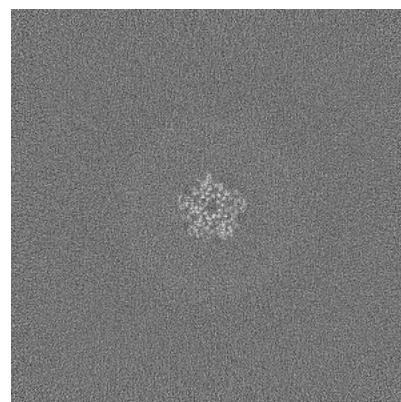
6.2.2 Raw map



X Index: 256



Y Index: 256

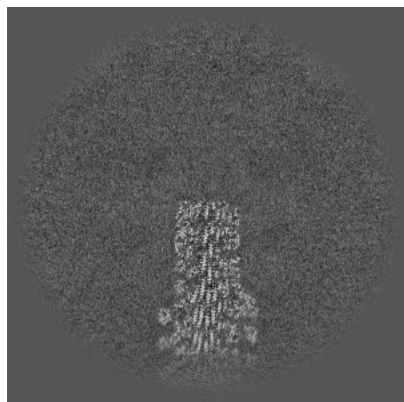


Z Index: 256

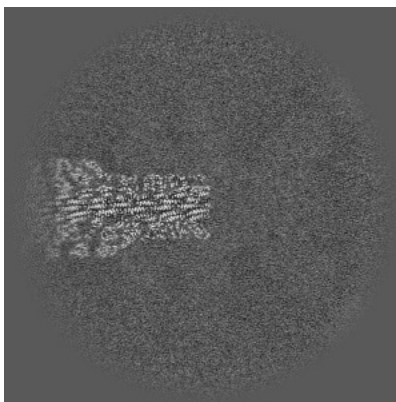
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

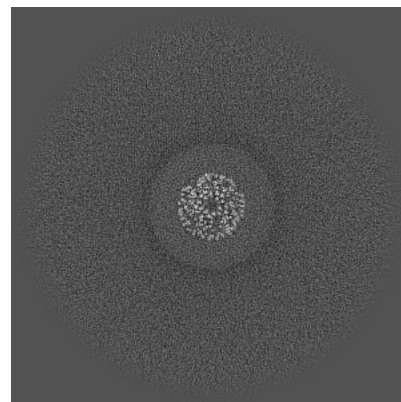
6.3.1 Primary map



X Index: 242

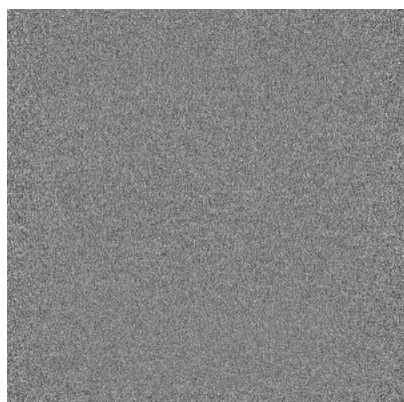


Y Index: 269

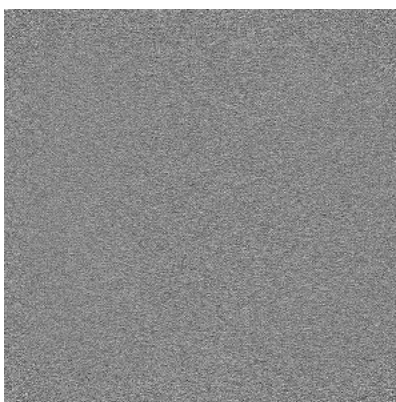


Z Index: 222

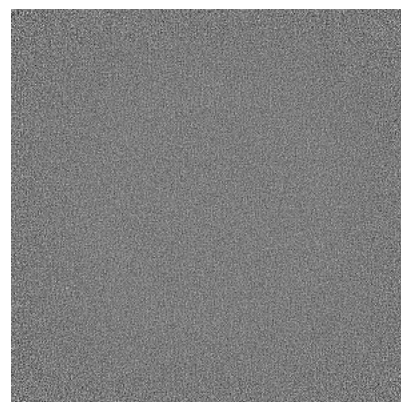
6.3.2 Raw map



X Index: 0



Y Index: 0

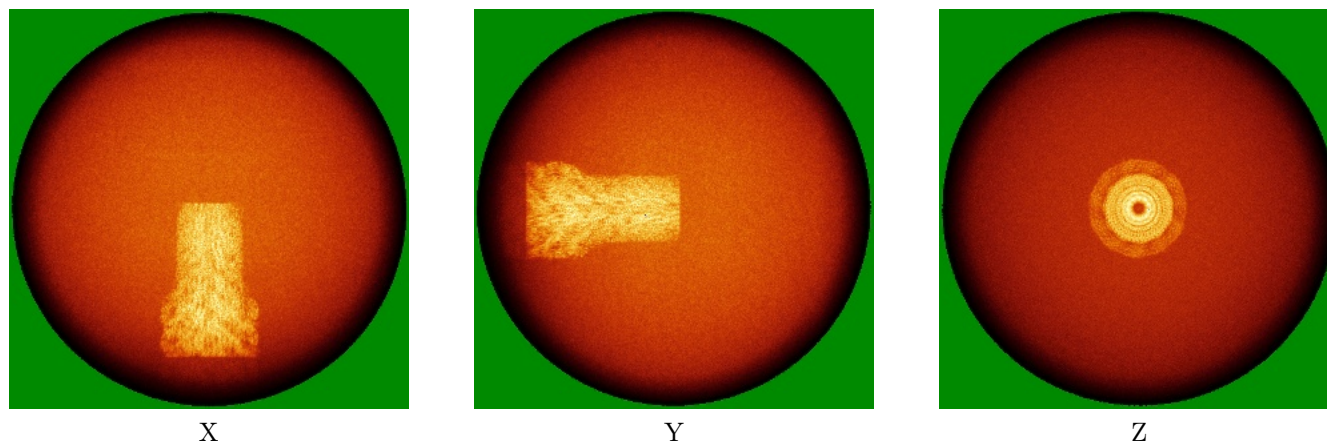


Z Index: 511

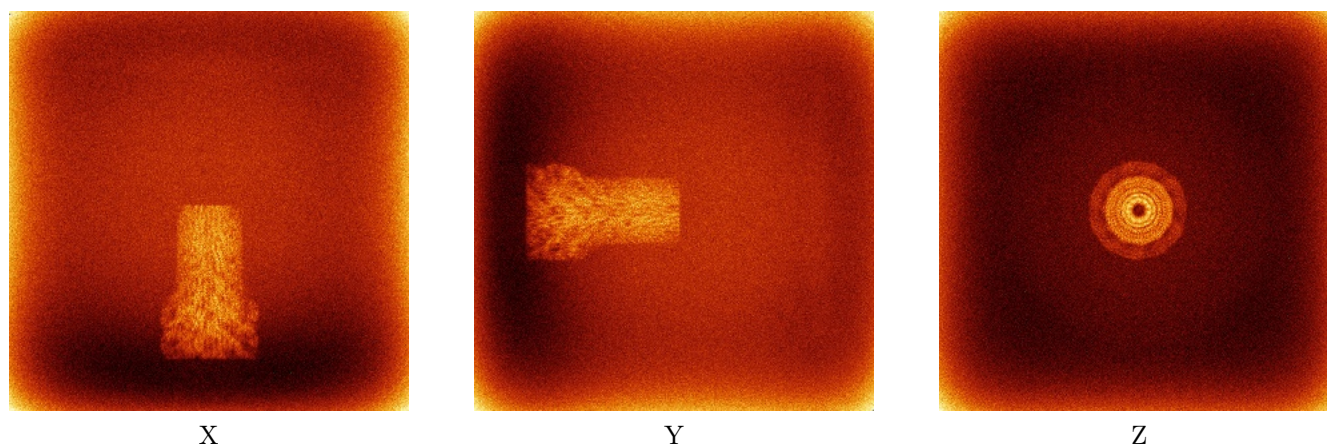
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



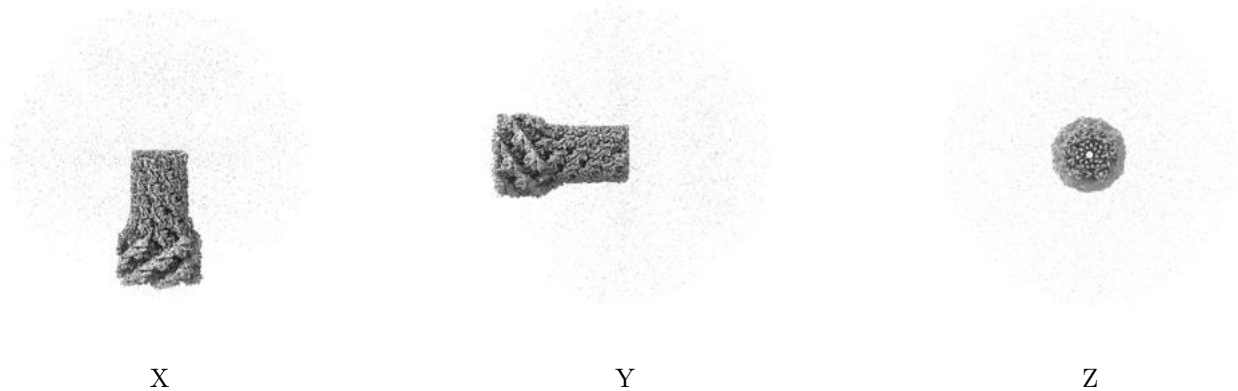
6.4.2 Raw map



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

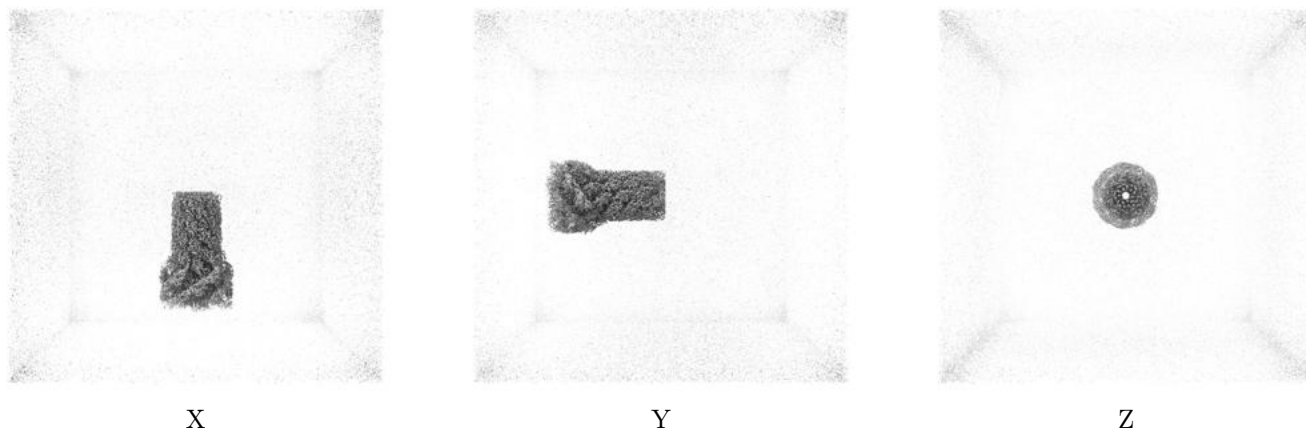
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

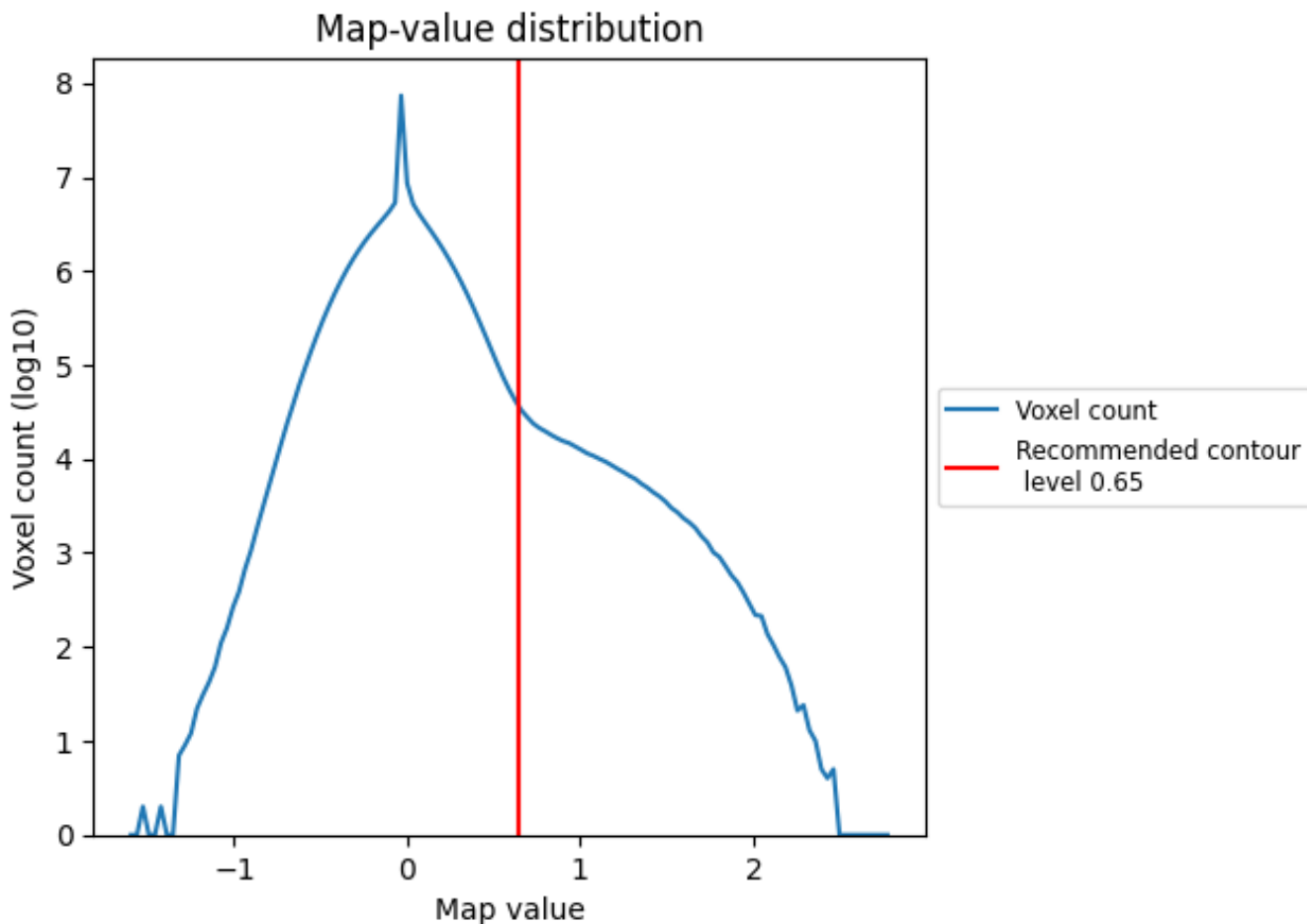
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

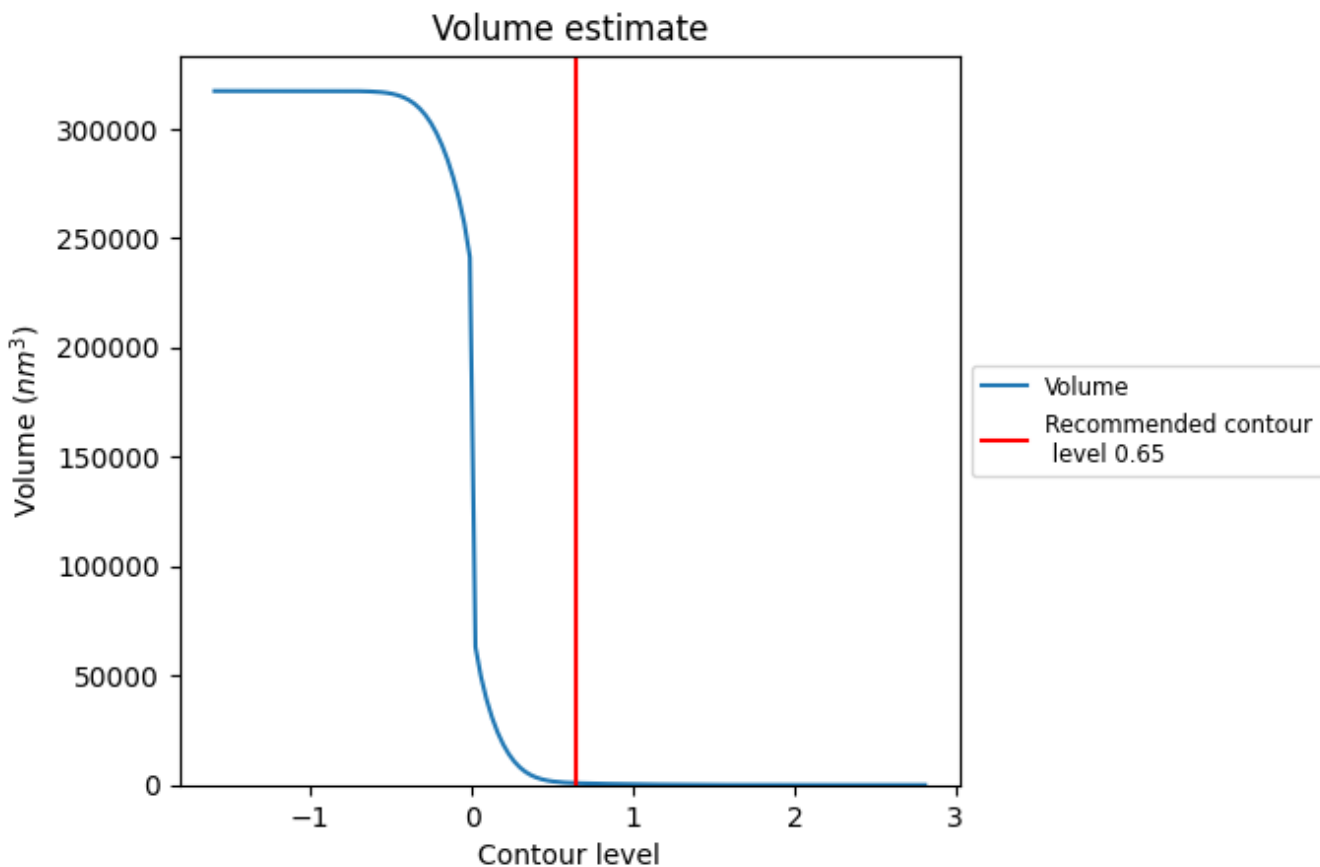
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

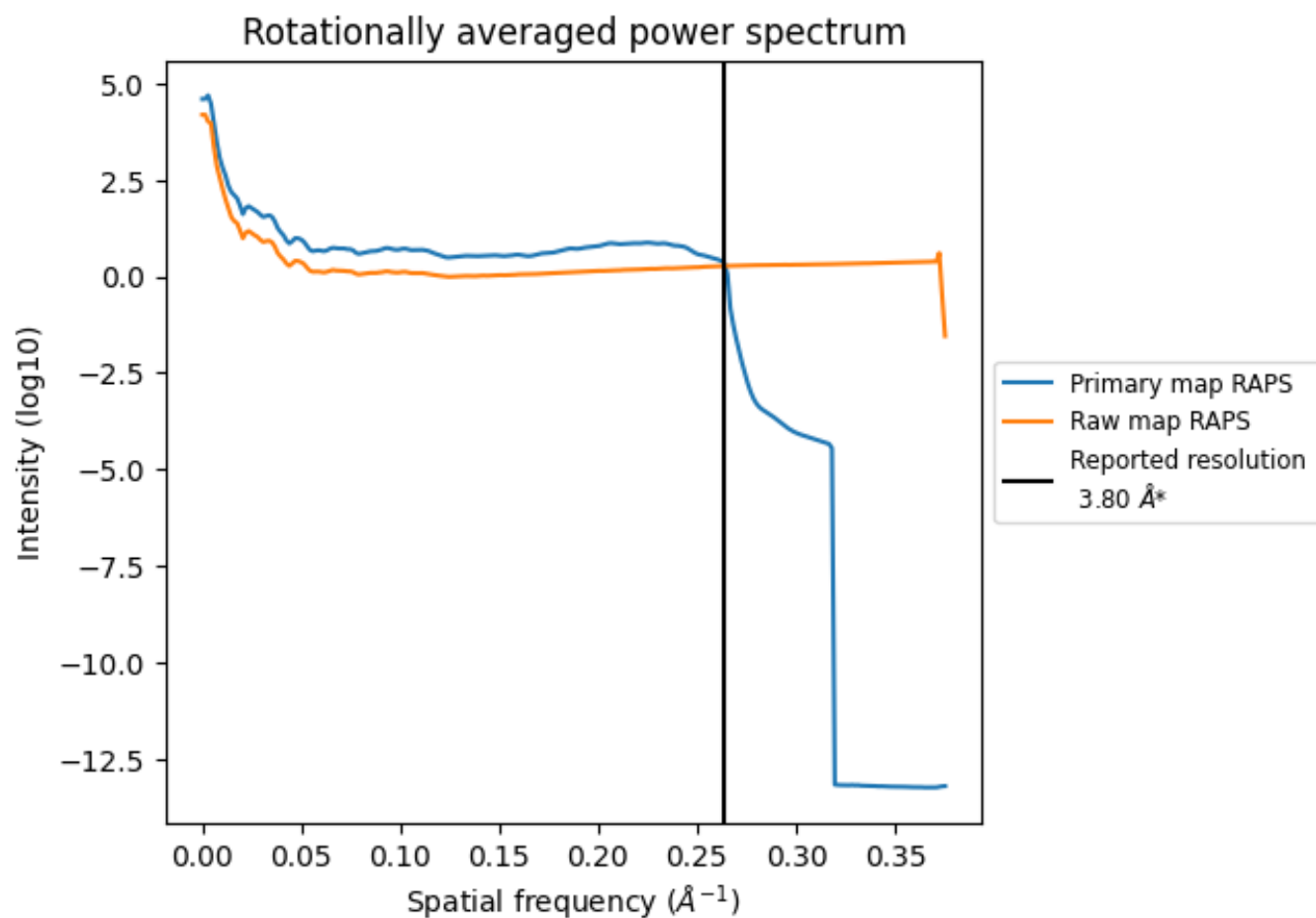
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 825 nm^3 ; this corresponds to an approximate mass of 745 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](#)

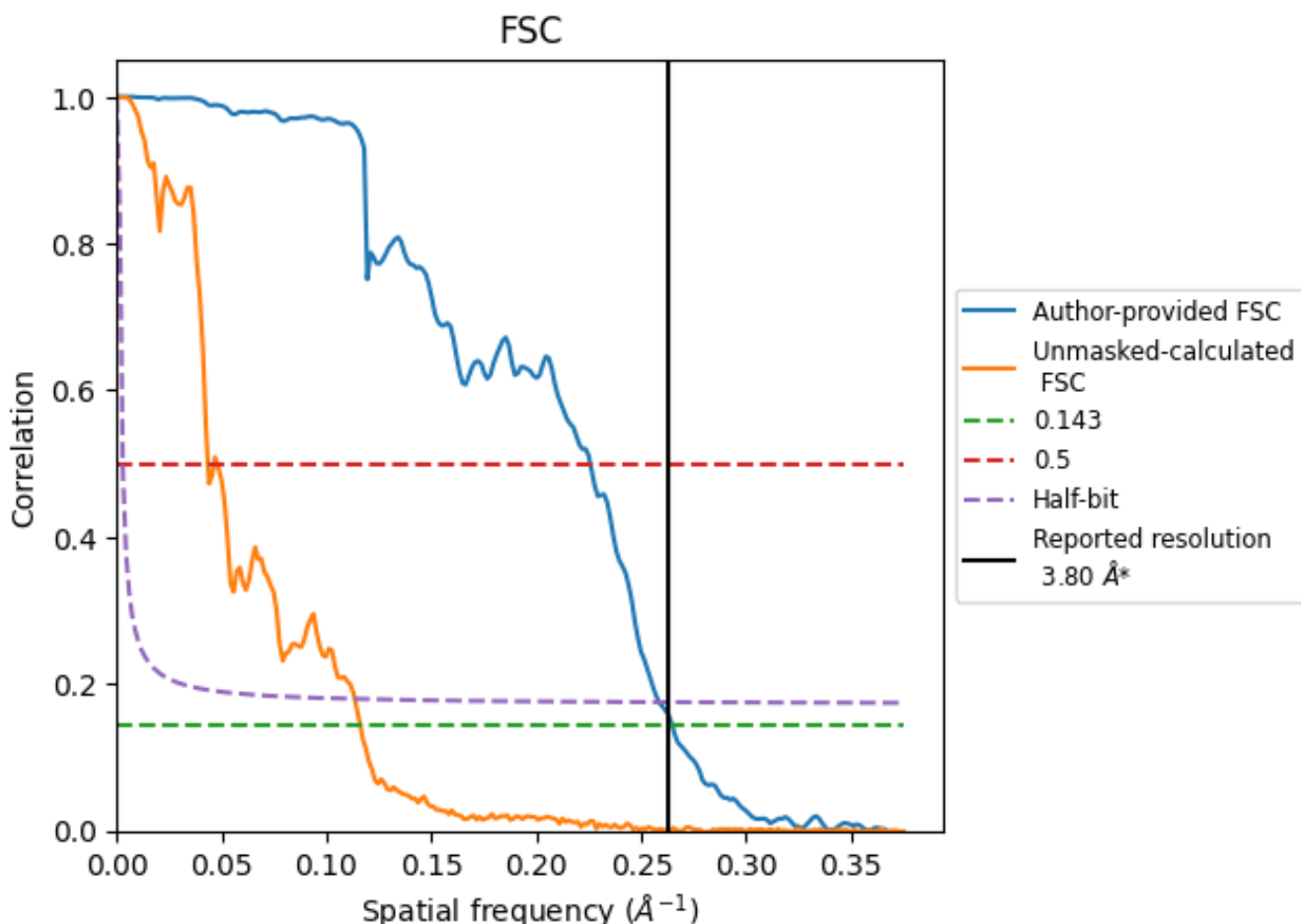


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

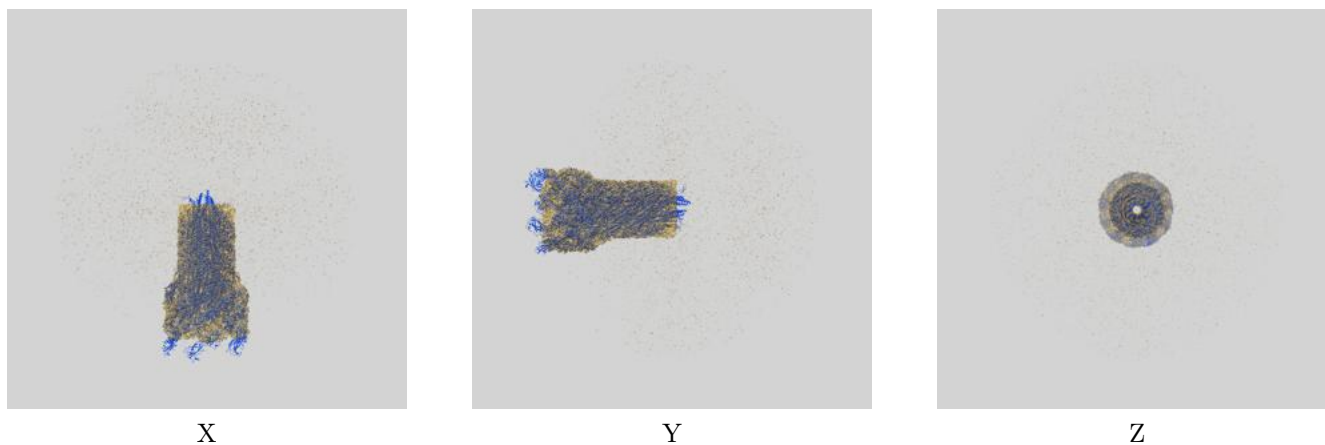
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.43	3.87
Unmasked-calculated*	8.61	22.99	8.81

*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 8.61 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

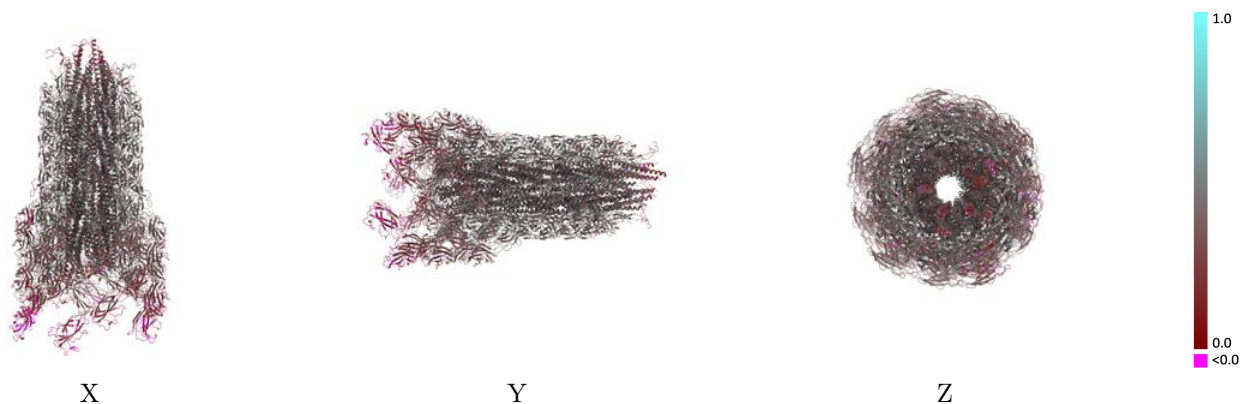
This section contains information regarding the fit between EMDB map EMD-37627 and PDB model 8WLP. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



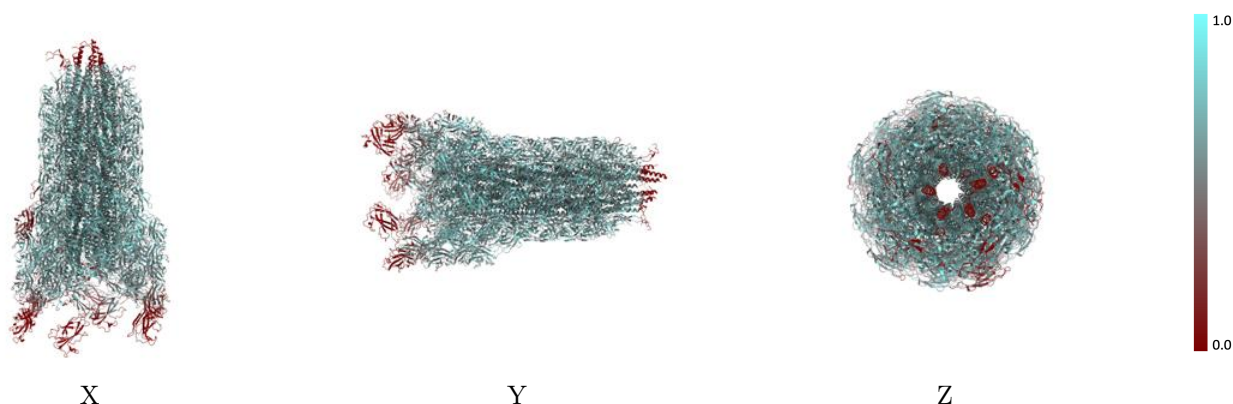
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



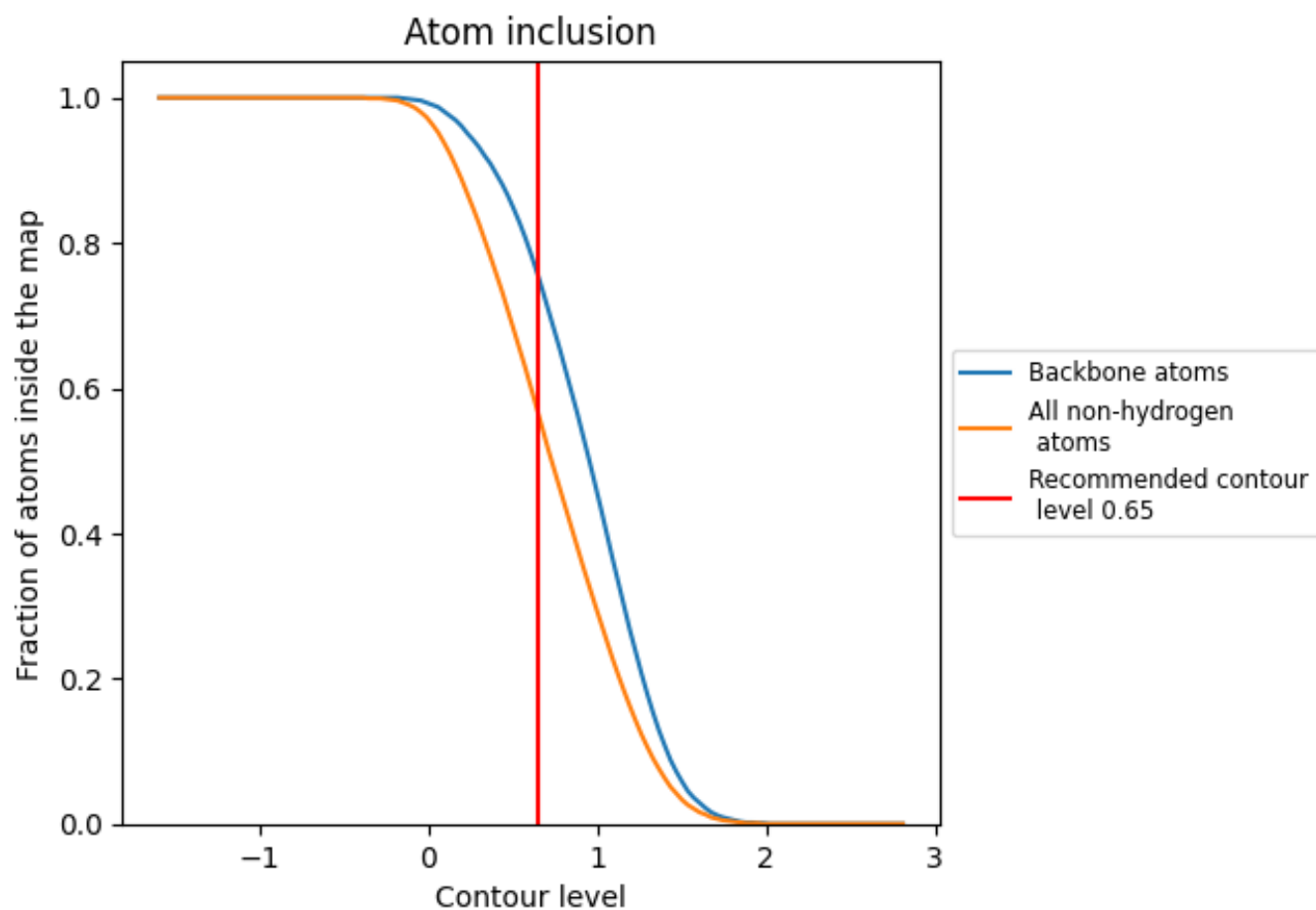
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 75% of all backbone atoms, 56% 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	 0.5650	 0.3590
0	 0.6200	 0.4090
1	 0.6050	 0.4030
2	 0.6140	 0.4080
3	 0.6160	 0.4020
4	 0.6230	 0.4010
5	 0.6080	 0.3990
6	 0.6250	 0.4080
7	 0.6330	 0.4170
8	 0.6260	 0.4080
9	 0.6080	 0.3990
ZA	 0.6240	 0.4060
ZB	 0.6260	 0.4040
ZC	 0.6400	 0.4230
ZD	 0.6210	 0.4140
ZE	 0.6030	 0.4010
ZF	 0.4190	 0.3260
ZG	 0.5800	 0.3720
ZH	 0.6210	 0.3780
ZI	 0.6340	 0.3840
ZJ	 0.6360	 0.3820
ZK	 0.6170	 0.3740
ZL	 0.6270	 0.3800
ZM	 0.6200	 0.3800
ZN	 0.6340	 0.3770
ZO	 0.6360	 0.3760
ZP	 0.6200	 0.3690
ZQ	 0.6250	 0.3680
ZR	 0.6150	 0.3610
ZS	 0.6160	 0.3620
ZT	 0.6080	 0.3590
ZU	 0.6080	 0.3510
ZV	 0.5990	 0.3450
ZW	 0.5910	 0.3450
ZX	 0.5820	 0.3390



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Chain	Atom inclusion	Q-score
ZY	 0.5560	 0.3320
ZZ	 0.5320	 0.3220
Za	 0.5120	 0.3250
Zb	 0.4700	 0.2900
Zc	 0.4540	 0.3000
Zd	 0.4340	 0.2930
Ze	 0.4000	 0.2790
Zf	 0.3830	 0.2600
Zg	 0.3550	 0.2490
Zh	 0.3370	 0.2420
r	 0.4350	 0.3310
s	 0.4860	 0.3630
t	 0.5090	 0.3710
u	 0.5370	 0.3820
v	 0.5680	 0.3940
w	 0.6050	 0.3940
x	 0.6020	 0.3960
y	 0.6140	 0.4040
z	 0.6090	 0.3950