



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2024 – 12:57 AM JST

PDB ID : 8WKI
EMDB ID : EMD-37600
Title : Cryo-EM structure of the distal rod-hook within the flagellar motor-hook complex in the CW state.
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-27
Resolution : 3.30 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

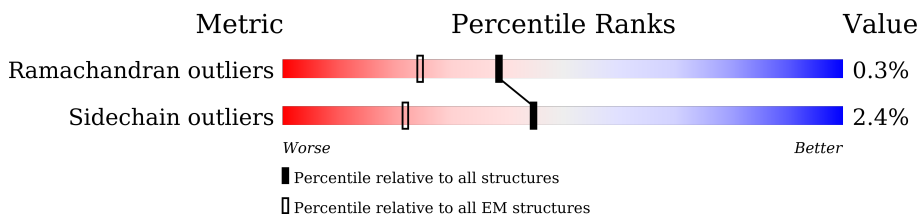
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	ZF	403	
1	ZG	403	
1	ZH	403	
1	ZI	403	
1	ZJ	403	
1	ZK	403	
1	ZL	403	
1	ZM	403	
1	ZN	403	

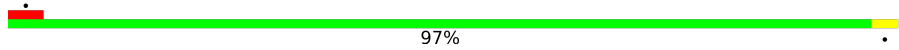
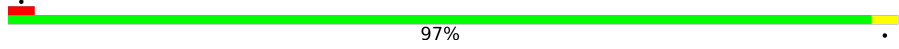
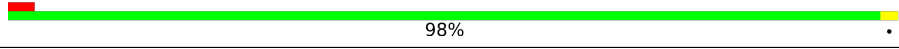
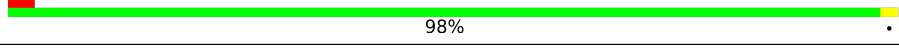
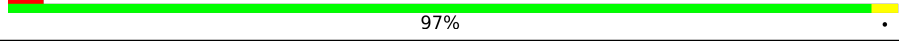
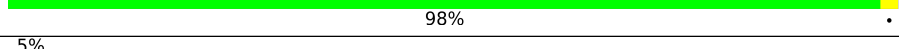
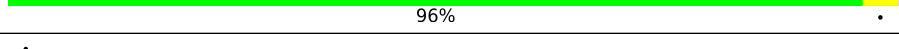
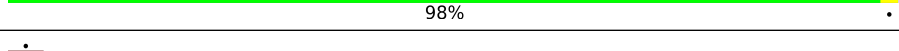
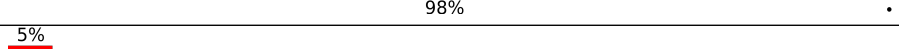
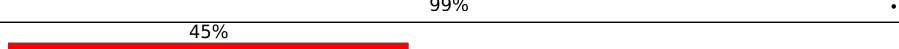
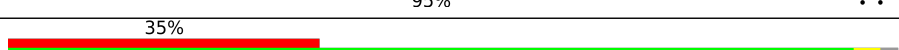
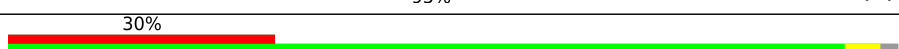

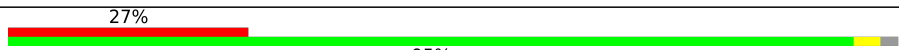
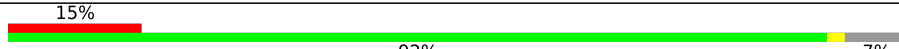
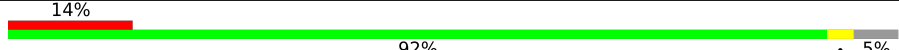

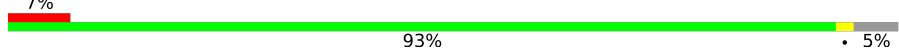

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Mol	Chain	Length	Quality of chain
1	ZO	403	16% 97%
1	ZP	403	16% 95%
1	ZQ	403	19% 97%
1	ZR	403	22% 97%
1	ZS	403	22% 98%
1	ZT	403	29% 98%
1	ZU	403	33% 99%
1	ZV	403	35% 98%
1	ZW	403	34% 96%
1	ZX	403	38% 99%
1	ZY	403	40% 98%
1	ZZ	403	41% 98%
1	Za	403	46% 98%
1	Zb	403	47% 98%
1	Zc	403	49% 97%
1	Zd	403	54% 98%
1	Ze	403	60% 97%
1	Zf	403	64% 98%
1	Zg	403	67% 98%
1	Zh	403	68% 98%
2	0	260	5% 93% 5%
2	1	260	6% 93%
2	2	260	98%
2	3	260	98%
2	4	260	97%

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Mol	Chain	Length	Quality of chain
2	5	260	 97%
2	6	260	 97%
2	7	260	 98%
2	8	260	 98%
2	9	260	 97%
2	ZA	260	 98%
2	ZB	260	 96%
2	ZC	260	 98%
2	ZD	260	 98%
2	ZE	260	 99%
2	r	260	 95%
2	s	260	 95%
2	t	260	 94%
2	u	260	 93%
2	v	260	 95%
2	w	260	 92%
2	x	260	 92%
2	y	260	 92%
2	z	260	 93%

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 hook protein FlgE.

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
2	3	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
2	4	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
2	5	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
2	6	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
2	7	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
2	8	260	Total 1949	C 1202	N 341	O 400	S 6	0	0

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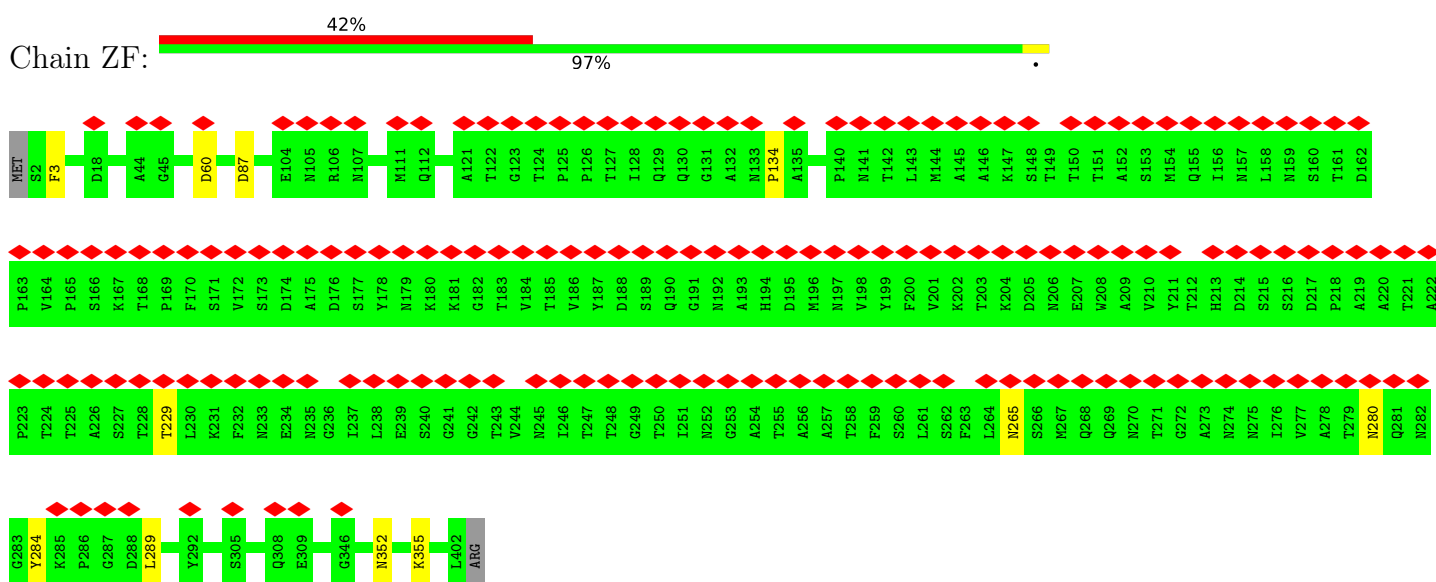
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZA	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZB	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZC	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZD	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZE	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	0	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
2	1	252	Total	C	N	O	S	0	0
			1894	1172	331	385	6		
2	r	254	Total	C	N	O	S	0	0
			1903	1175	334	389	5		
2	s	255	Total	C	N	O	S	0	0
			1911	1181	335	390	5		
2	t	256	Total	C	N	O	S	0	0
			1919	1186	336	391	6		
2	u	254	Total	C	N	O	S	0	0
			1903	1175	334	389	5		
2	v	255	Total	C	N	O	S	0	0
			1911	1181	335	390	5		
2	w	243	Total	C	N	O	S	0	0
			1823	1127	318	373	5		
2	x	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
2	y	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
2	z	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		

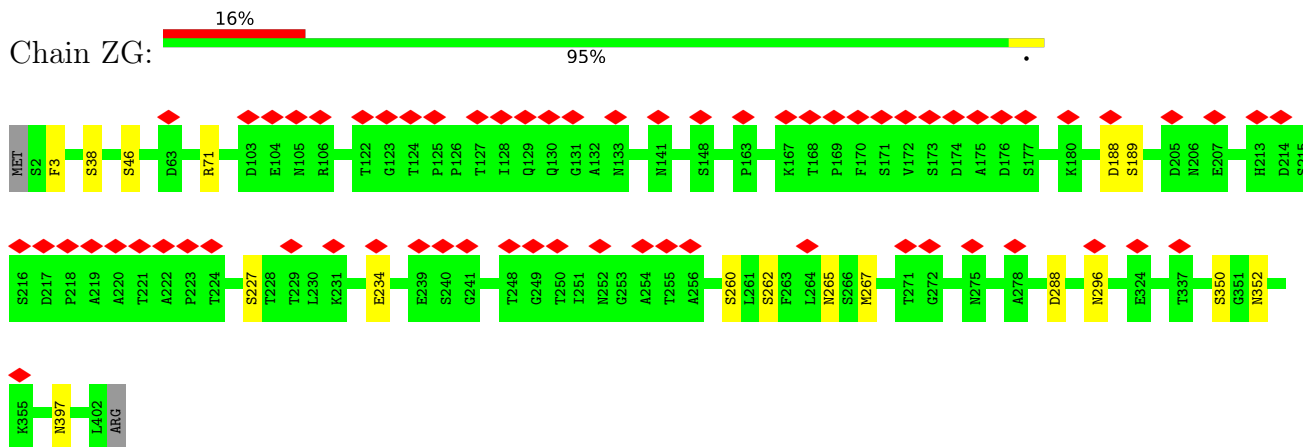
3 Residue-property plots

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

- Molecule 1: Flagellar hook protein FlgE

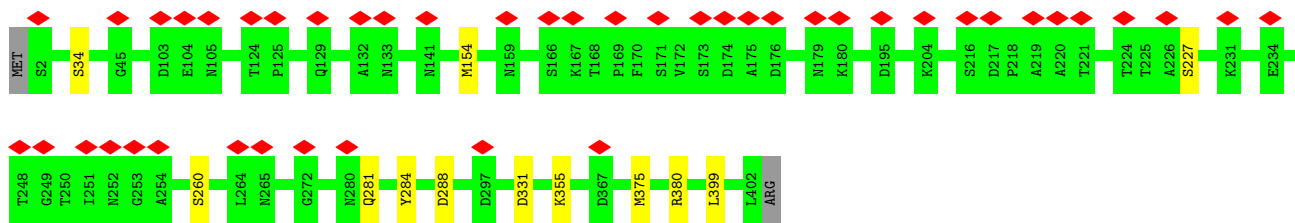


- Molecule 1: Flagellar hook protein FlgE

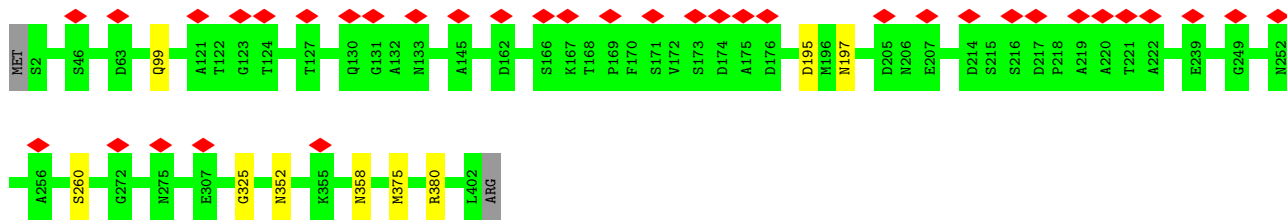


- Molecule 1: Flagellar hook protein FlgE

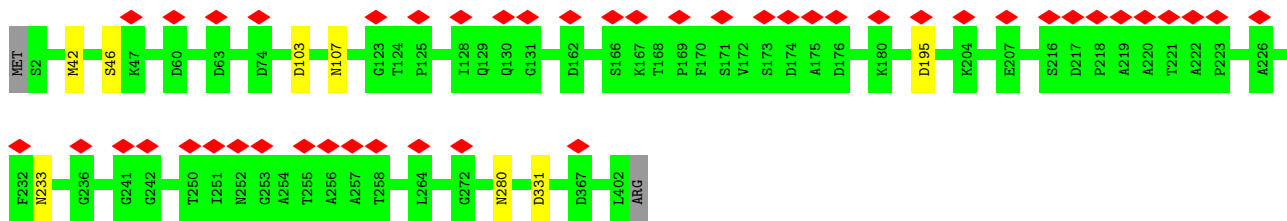




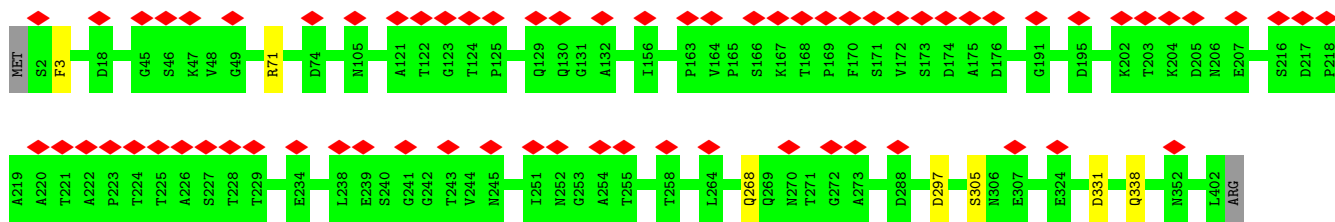
• Molecule 1: Flagellar hook protein FlgE



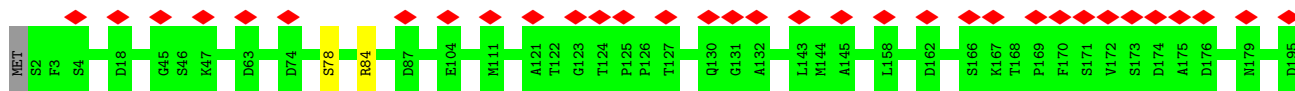
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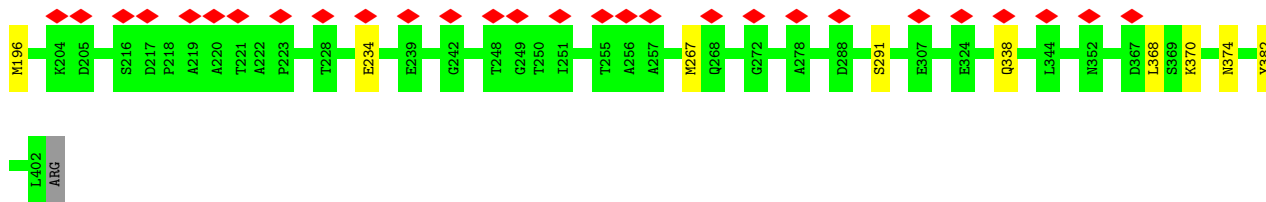


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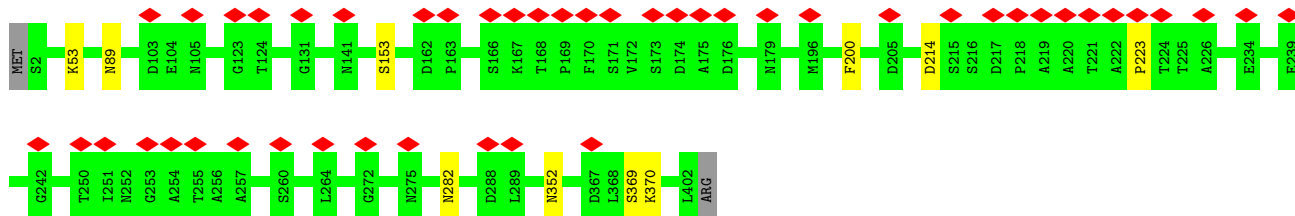


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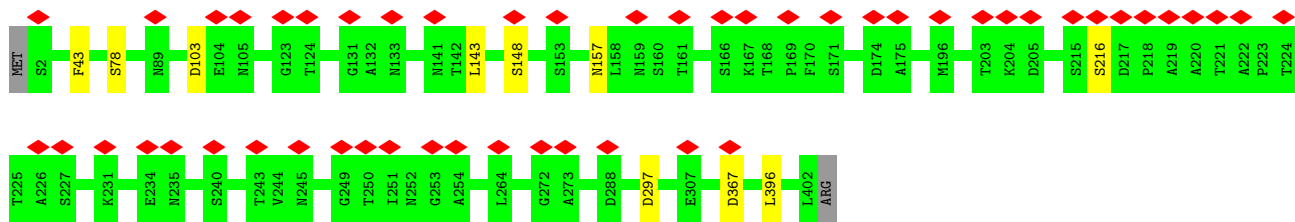




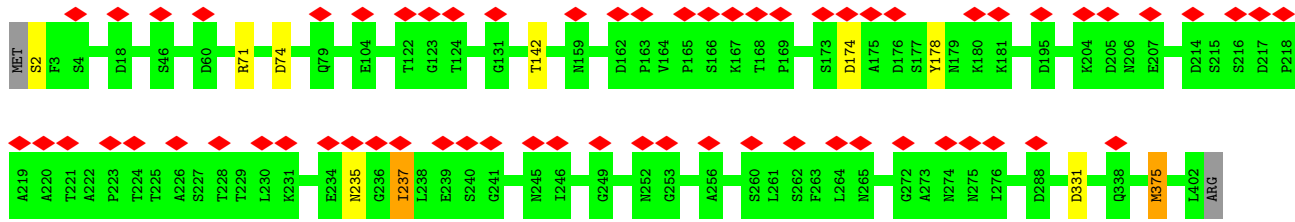
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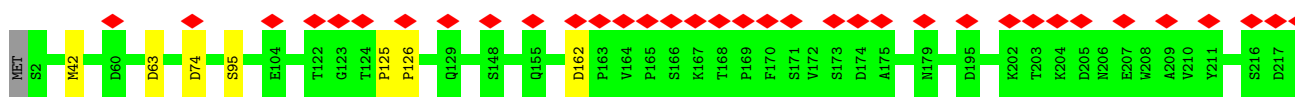
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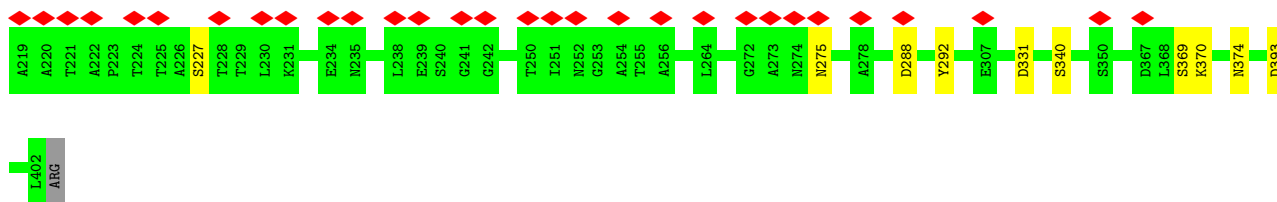


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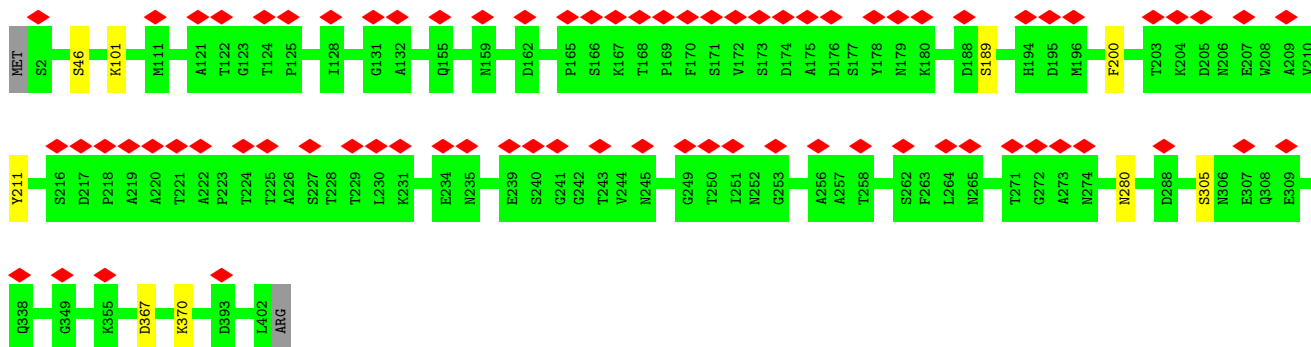


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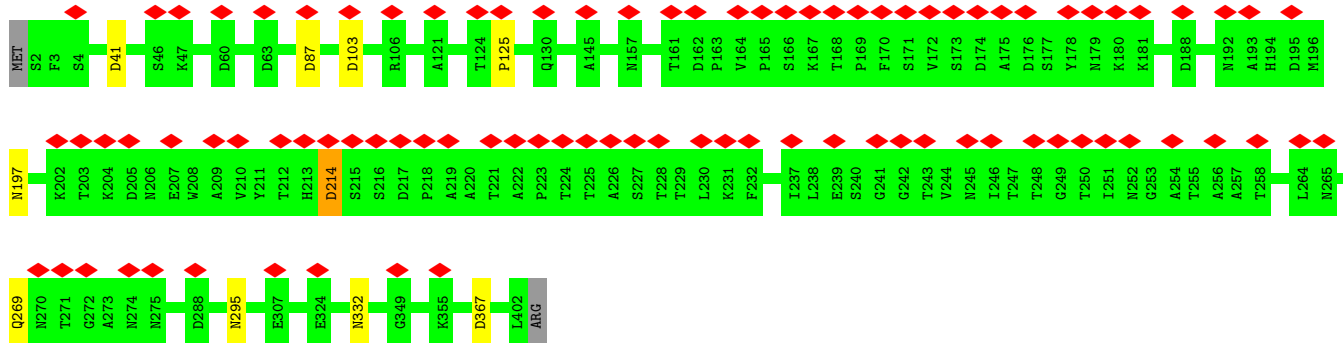




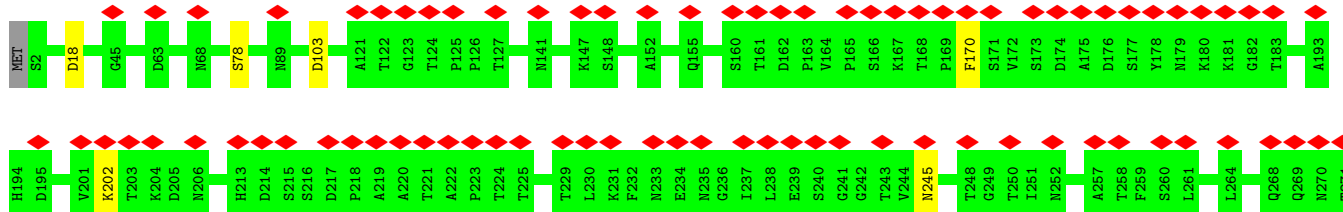
- Molecule 1: Flagellar hook protein FlgE

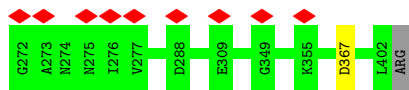


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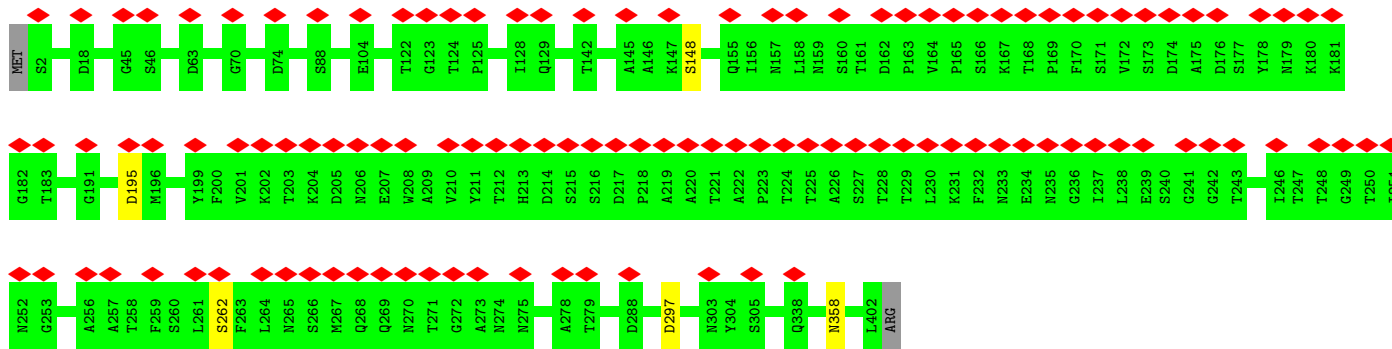


- Molecule 1: Flagellar hook protein FlgE

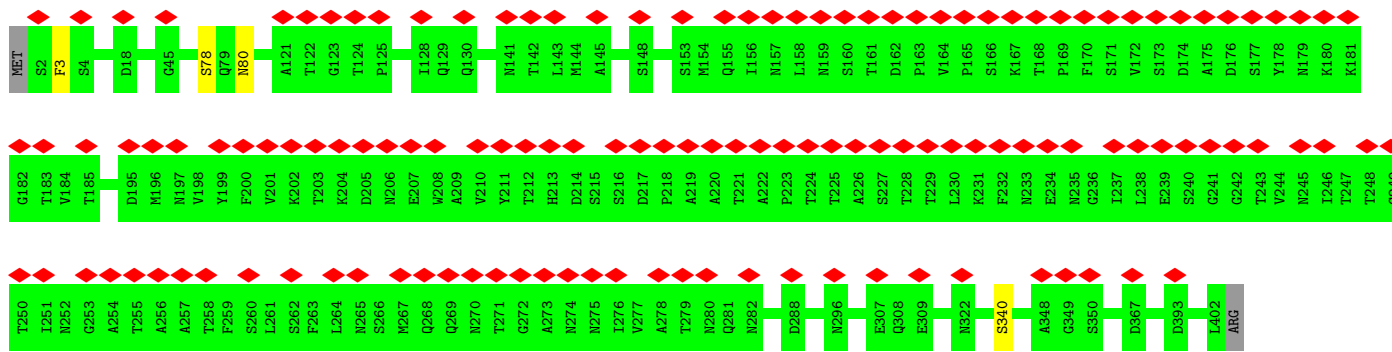




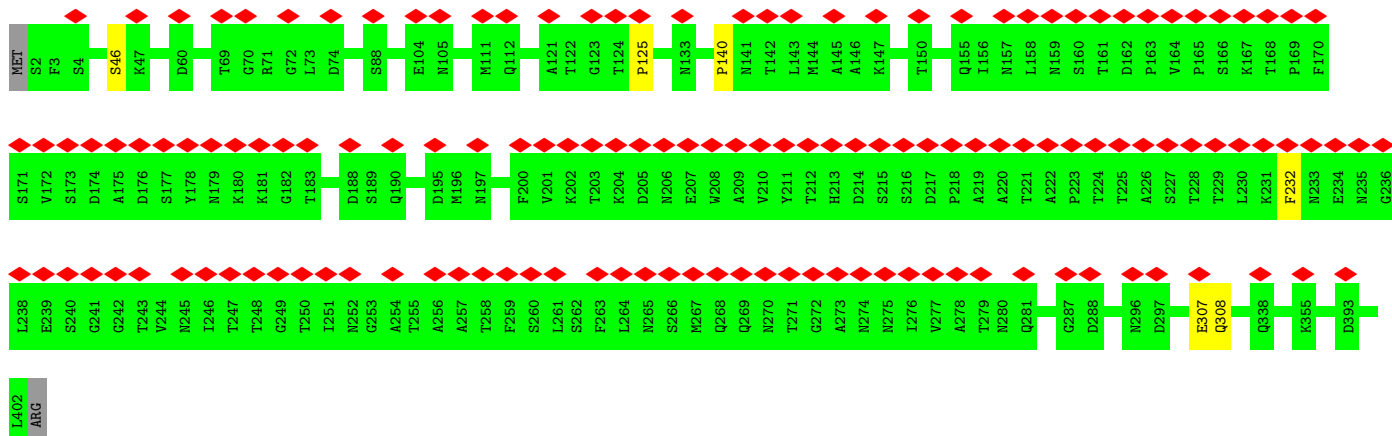
• Molecule 1: Flagellar hook protein FlgE



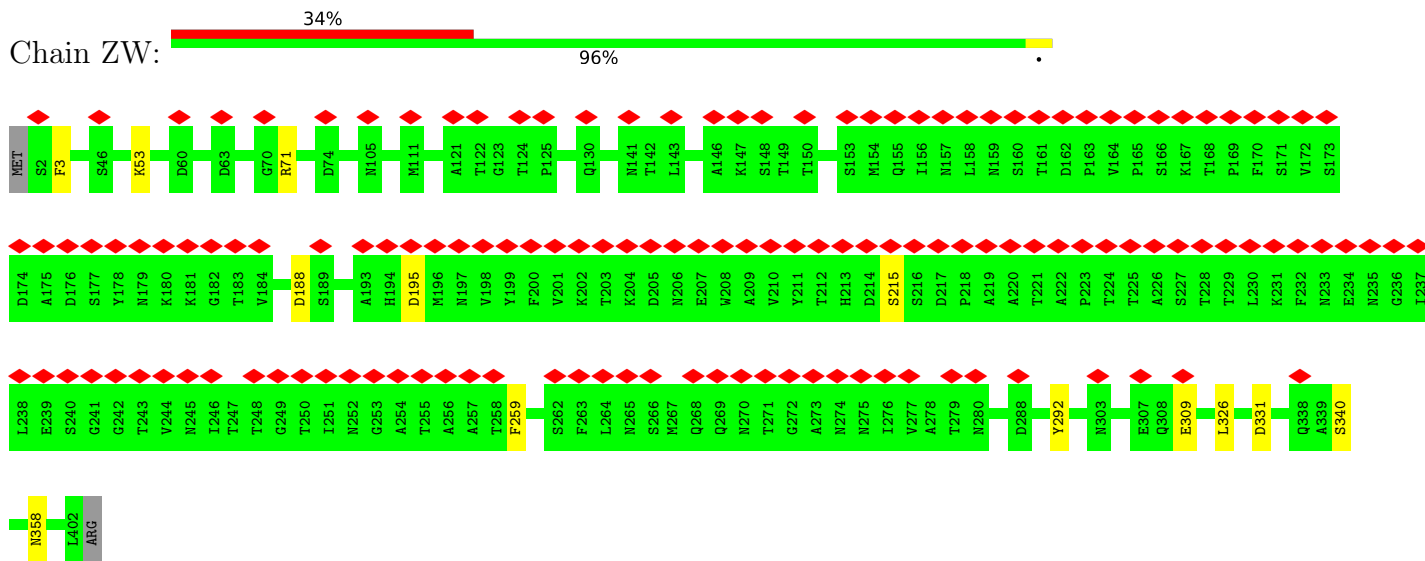
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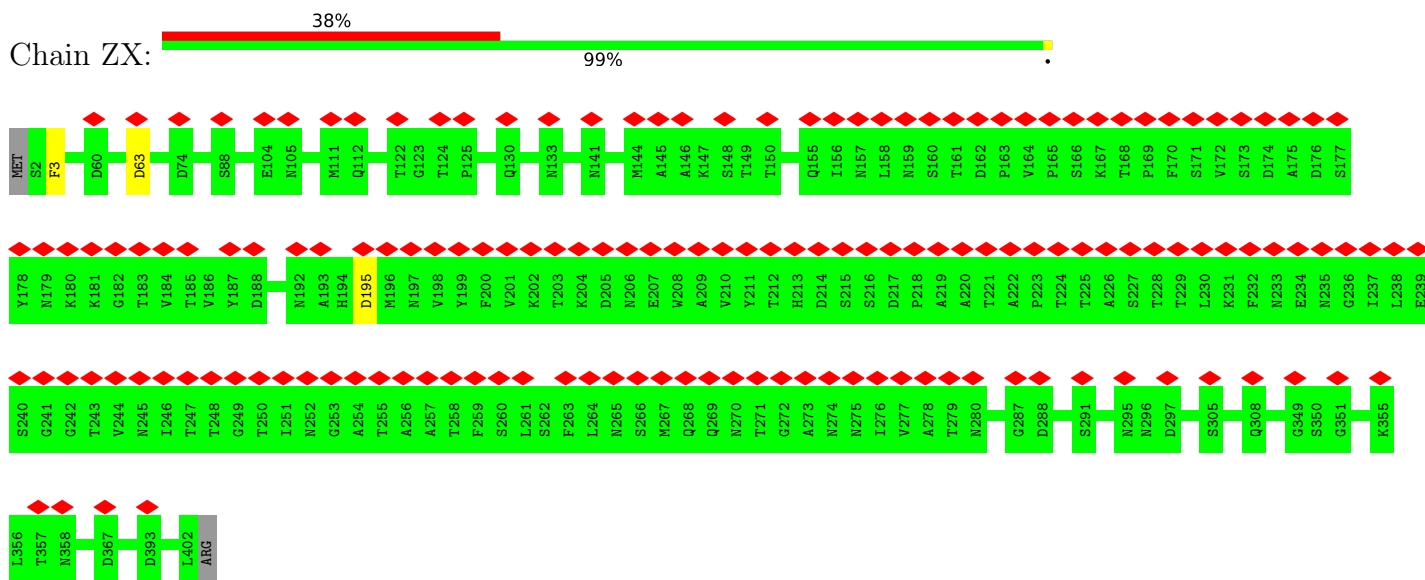
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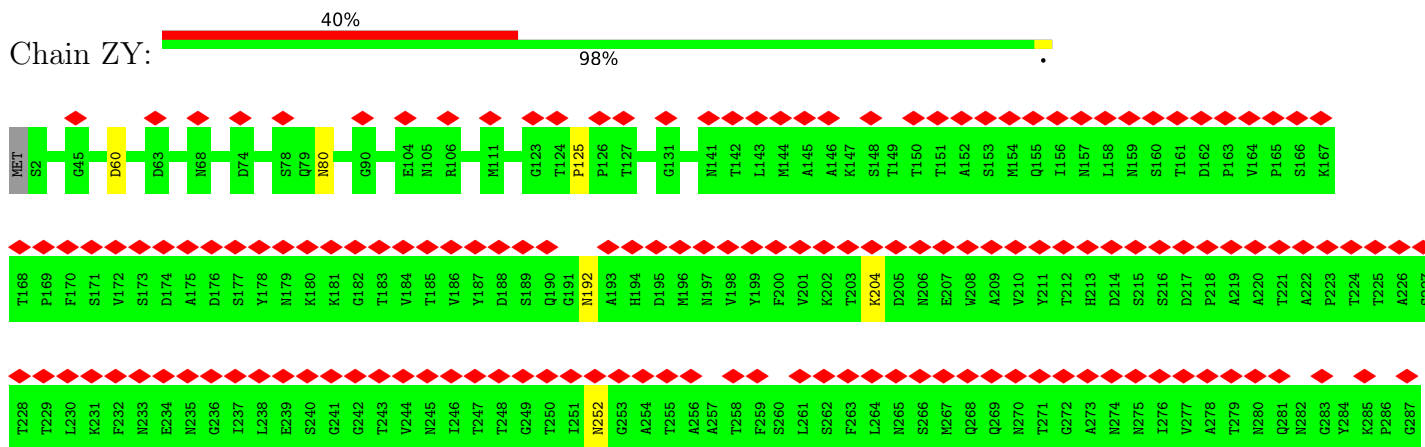
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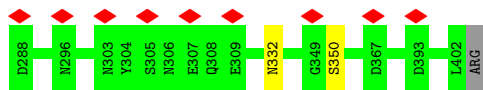


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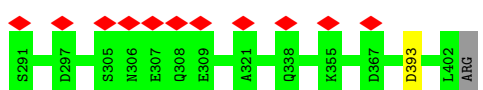
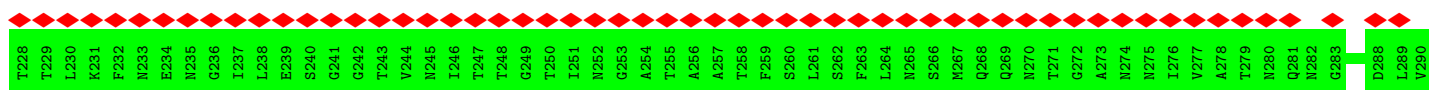
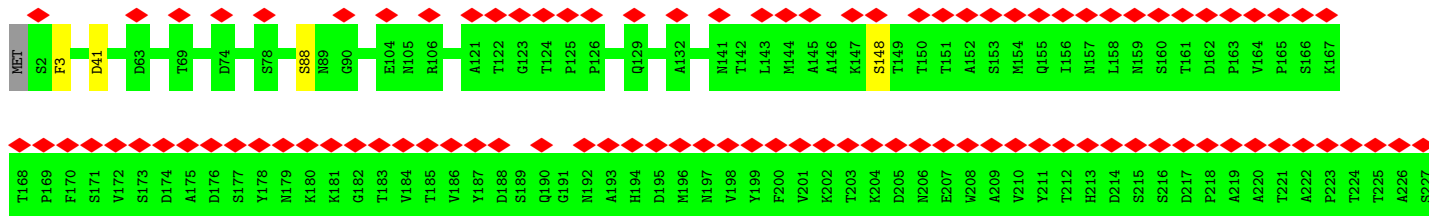
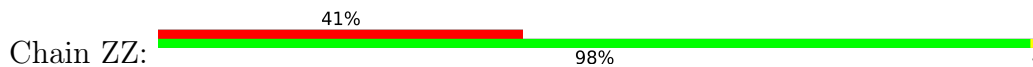


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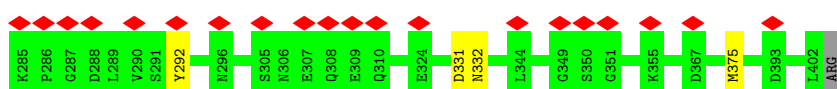
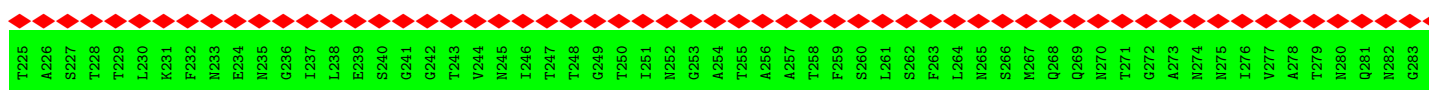
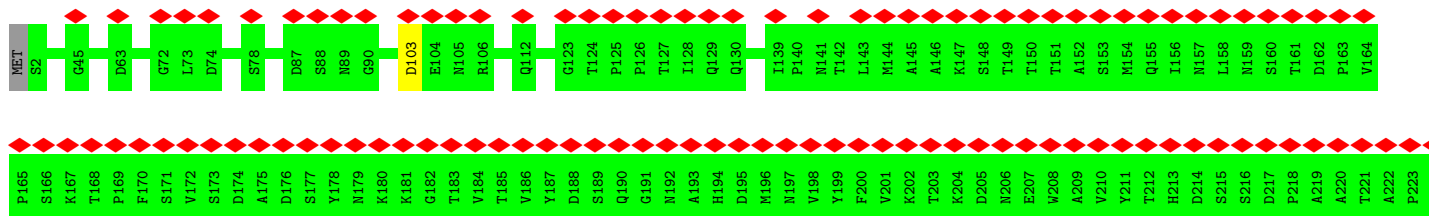




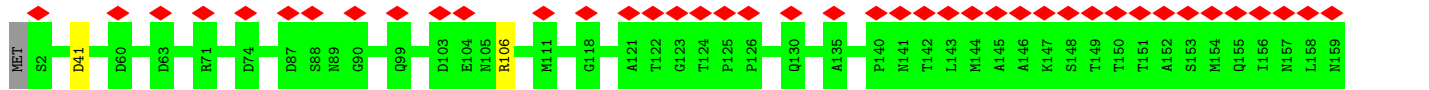
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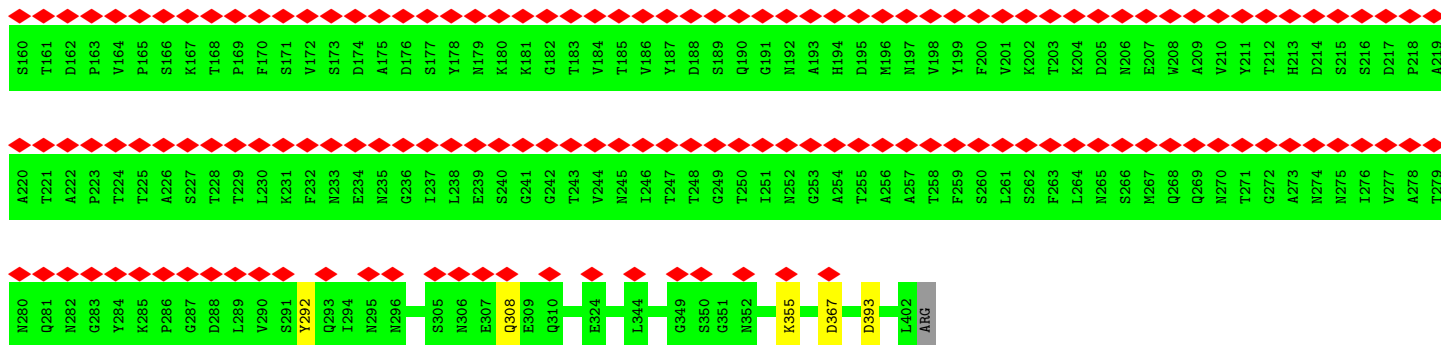


• Molecule 1: Flagellar hook protein FlgE

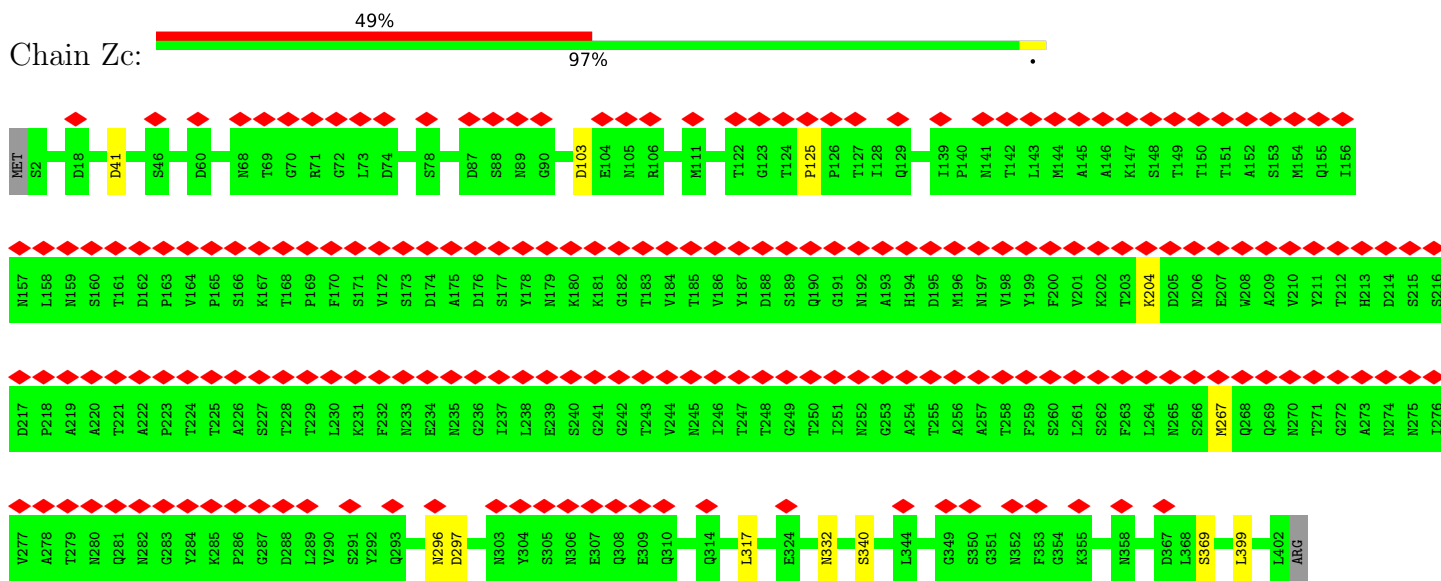


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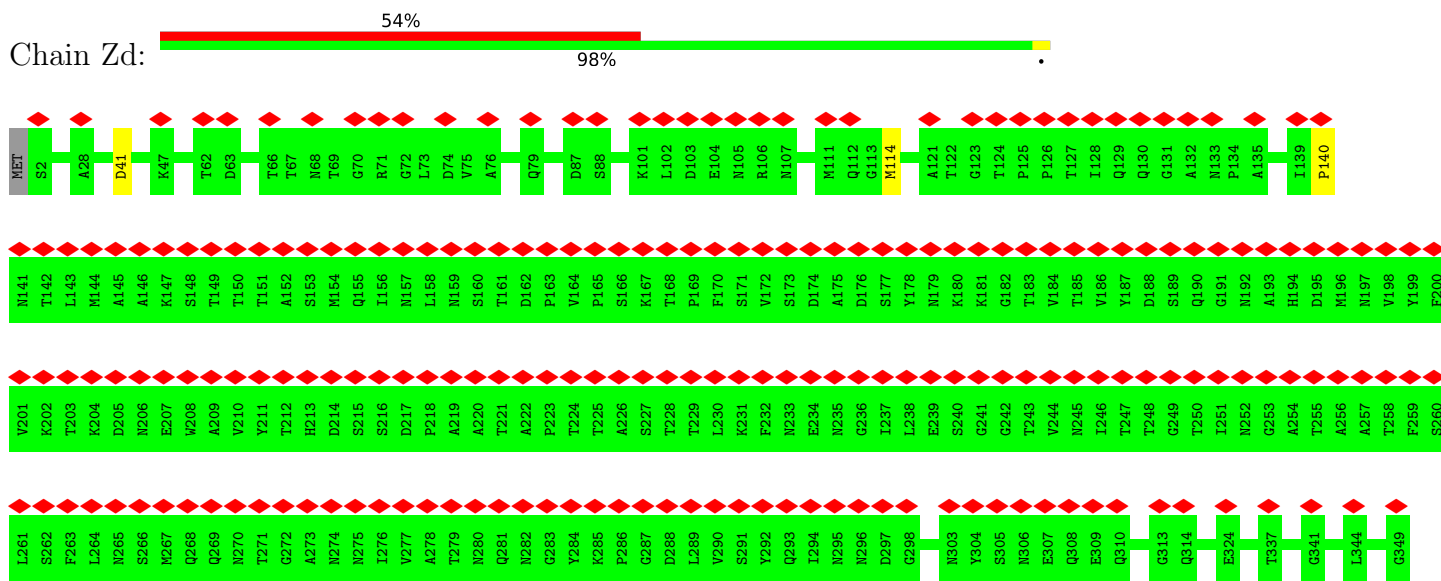




• Molecule 1: Flagellar hook protein FlgE

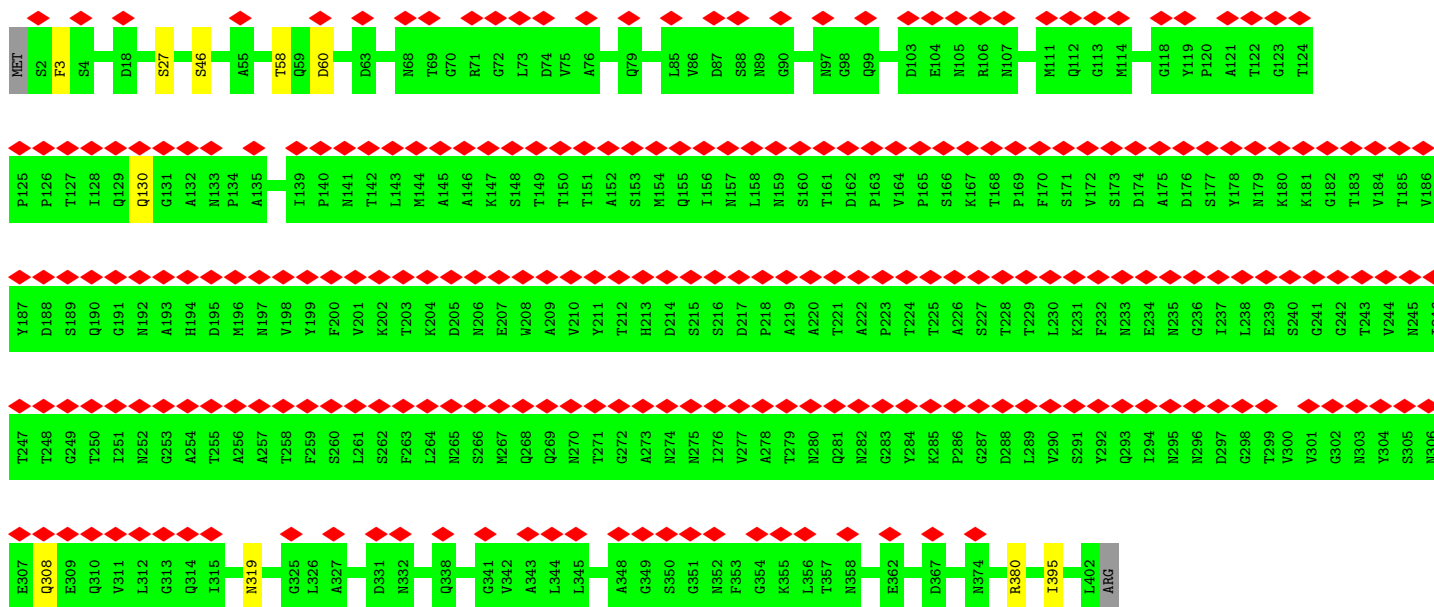


• Molecule 1: Flagellar hook protein FlgE

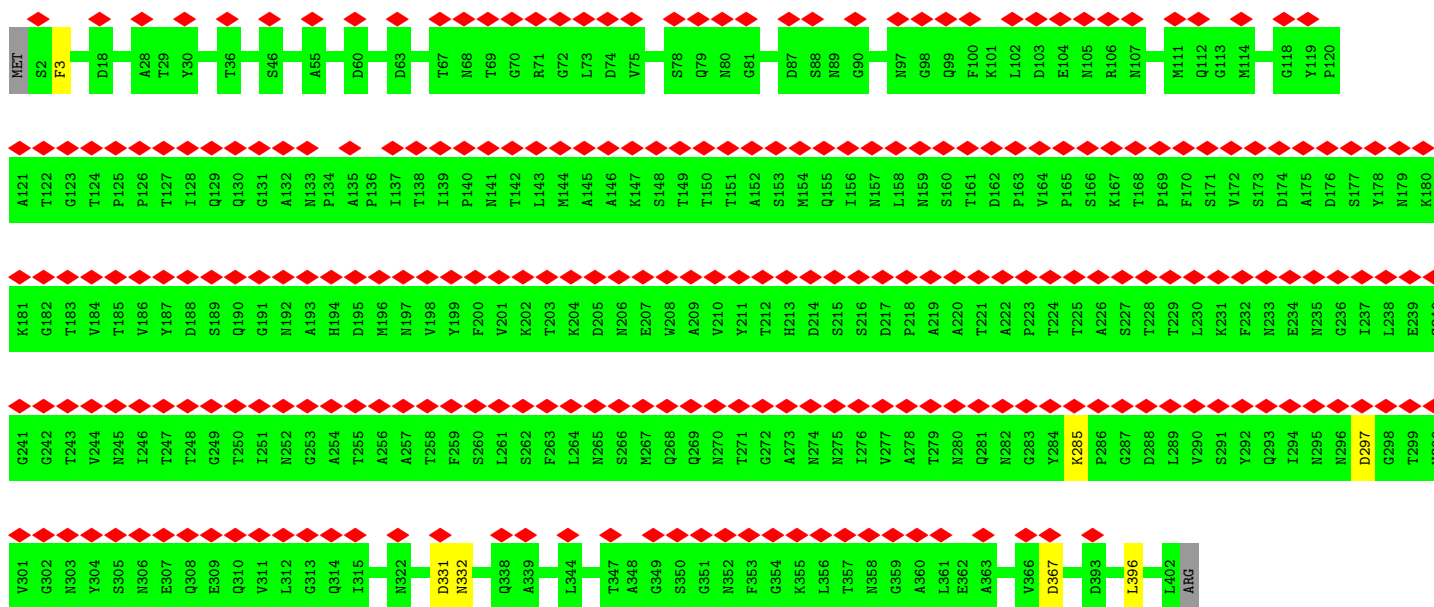




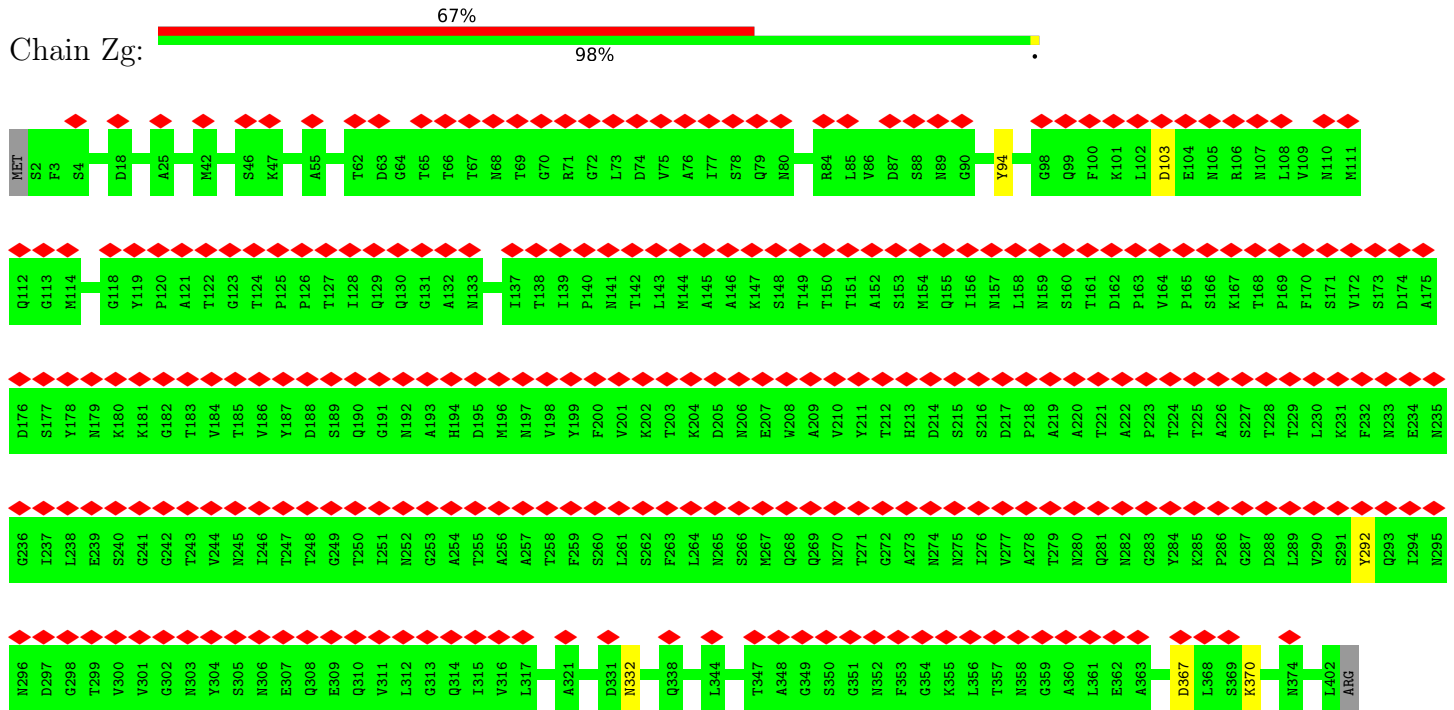
• Molecule 1: Flagellar hook protein FlgE



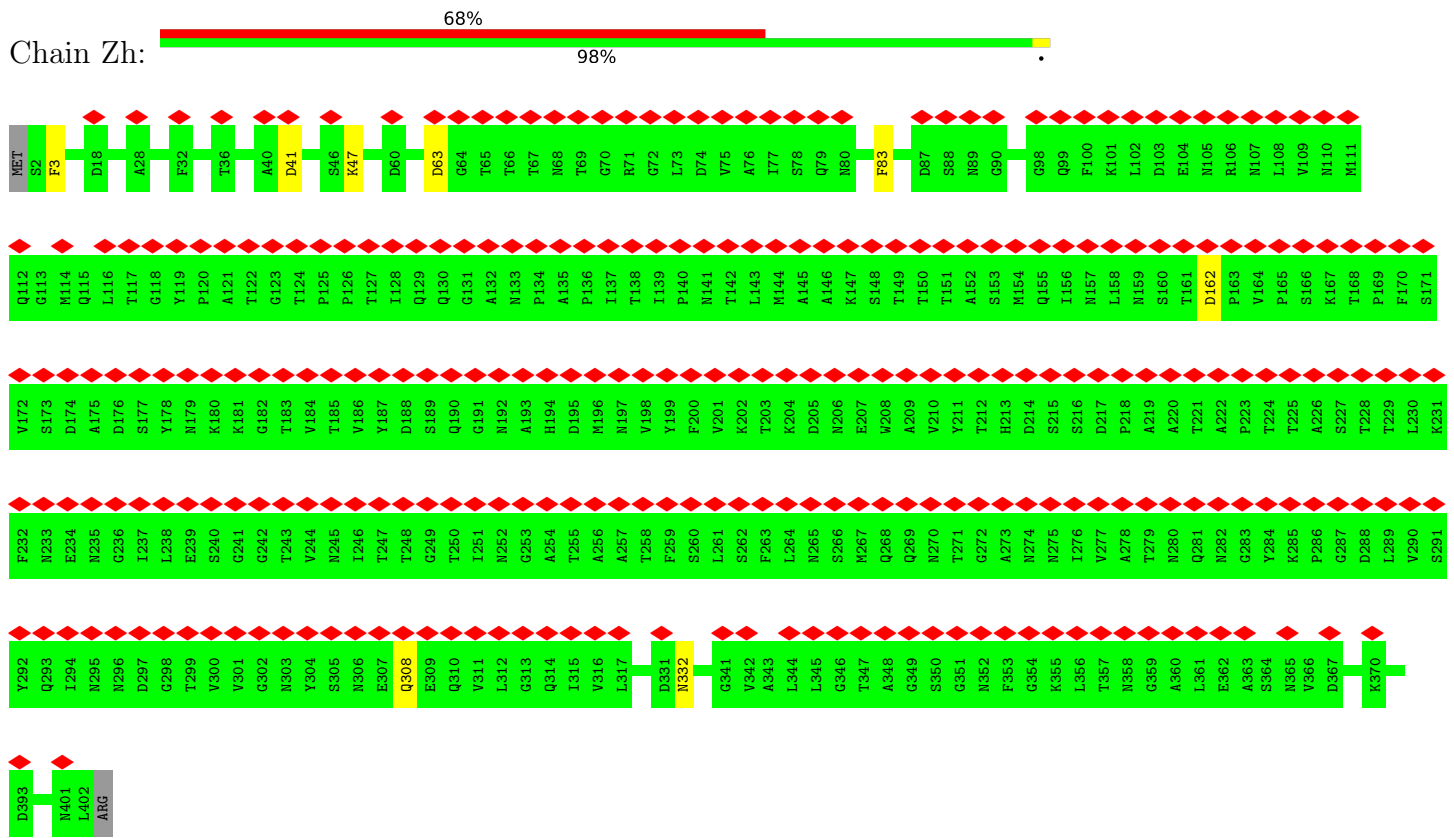
• Molecule 1: Flagellar hook protein FlgE



• Molecule 1: Flagellar hook protein FlgE

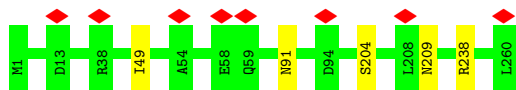


• Molecule 1: Flagellar hook protein FlgE

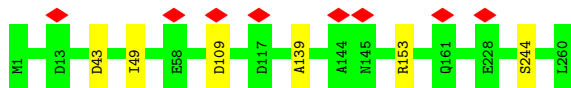


• Molecule 2: Flagellar basal-body rod protein FlgG





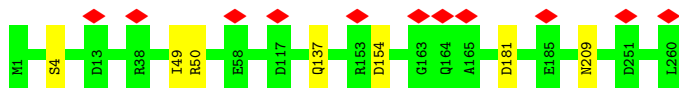
- Molecule 2: Flagellar basal-body rod protein FlgG



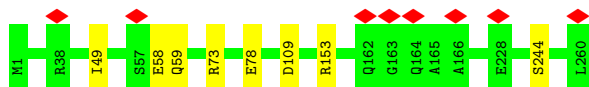
- Molecule 2: Flagellar basal-body rod protein FlgG



- Molecule 2: Flagellar basal-body rod protein FlgG



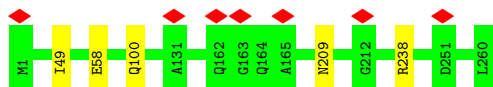
- Molecule 2: Flagellar basal-body rod protein FlgG



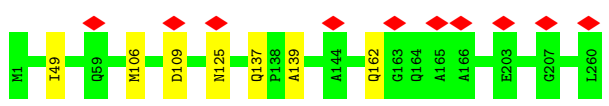
- Molecule 2: Flagellar basal-body rod protein FlgG



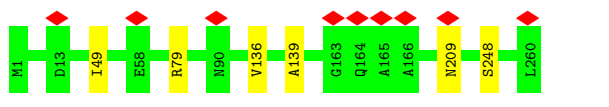
- Molecule 2: Flagellar basal-body rod protein FlgG



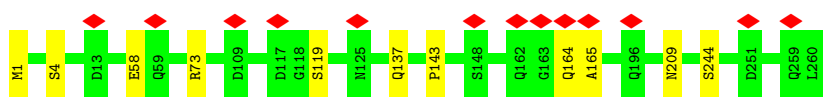
- Molecule 2: Flagellar basal-body rod protein FlgG



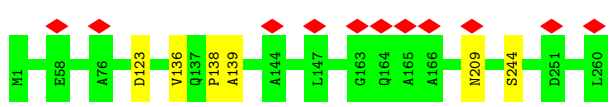
• Molecule 2: Flagellar basal-body rod protein FlgG



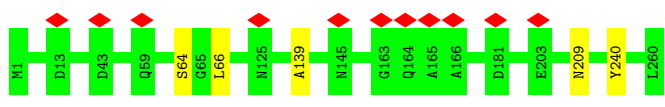
• Molecule 2: Flagellar basal-body rod protein FlgG



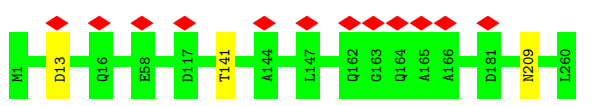
• Molecule 2: Flagellar basal-body rod protein FlgG



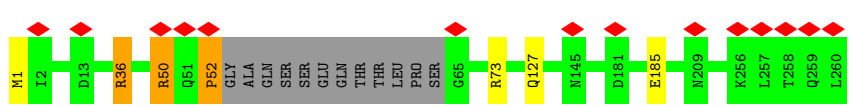
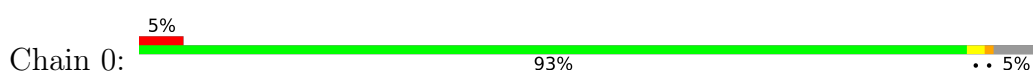
• Molecule 2: Flagellar basal-body rod protein FlgG



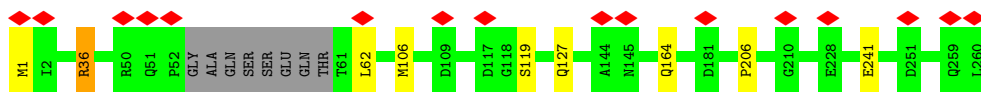
• Molecule 2: Flagellar basal-body rod protein FlgG



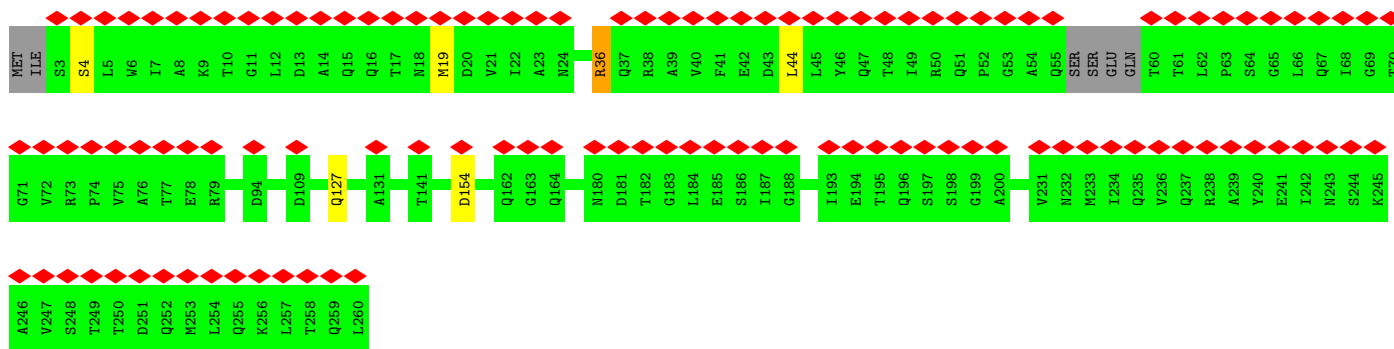
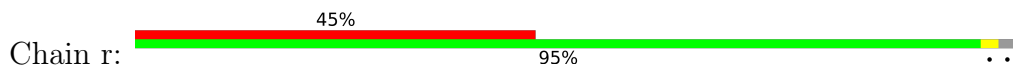
• Molecule 2: Flagellar basal-body rod protein FlgG



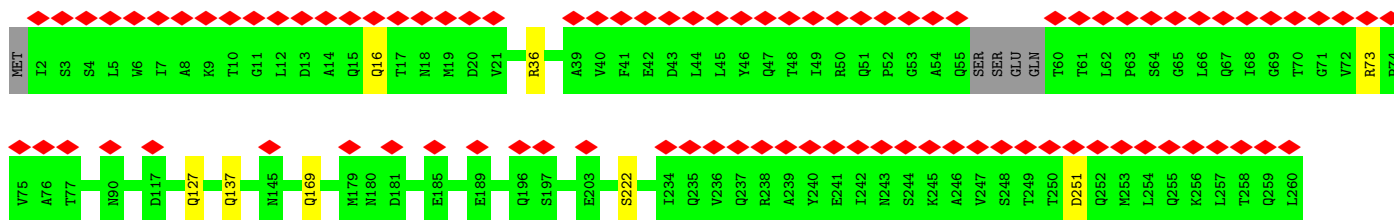
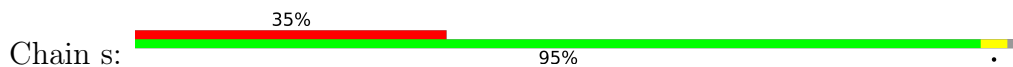
• Molecule 2: Flagellar basal-body rod protein FlgG



• Molecule 2: Flagellar basal-body rod protein FlgG



• Molecule 2: Flagellar basal-body rod protein FlgG

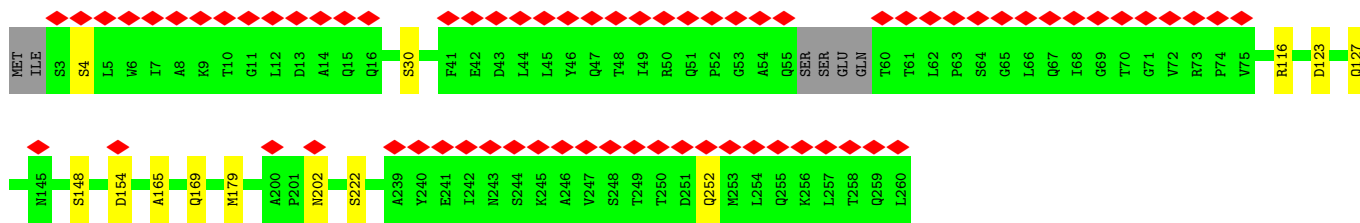


• Molecule 2: Flagellar basal-body rod protein FlgG

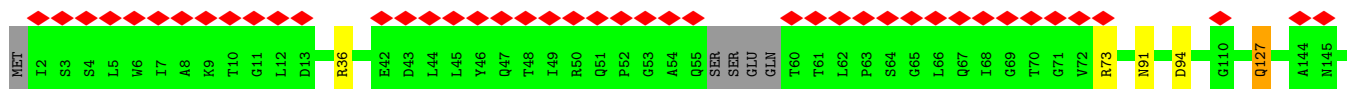


• Molecule 2: Flagellar basal-body rod protein FlgG

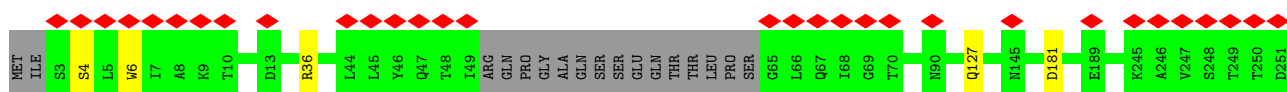
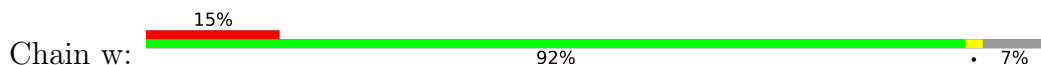




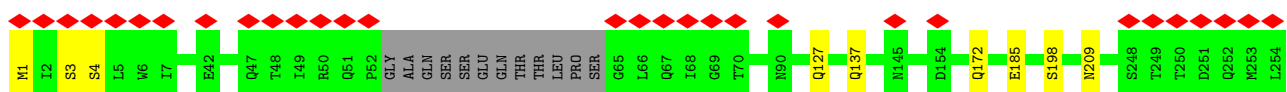
• Molecule 2: Flagellar basal-body rod protein FlgG



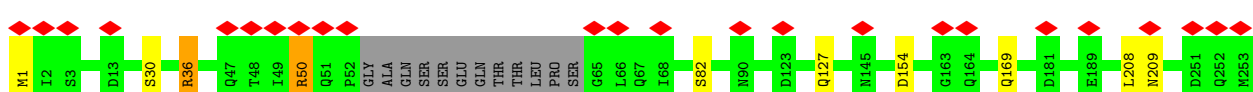
• Molecule 2: Flagellar basal-body rod protein FlgG

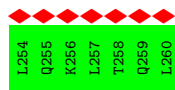


• Molecule 2: Flagellar basal-body rod protein FlgG

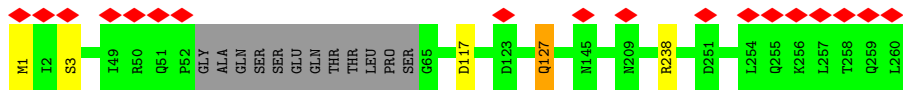
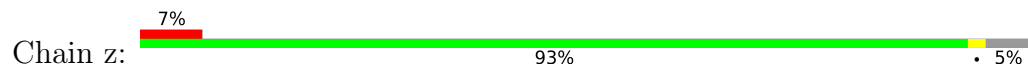


• Molecule 2: Flagellar basal-body rod protein FlgG





• Molecule 2: Flagellar basal-body rod protein FlgG



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.771	Depositor
Minimum map value	-1.263	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ZF	0.27	0/2991	0.49	0/4076
1	ZG	0.31	0/2991	0.50	0/4076
1	ZH	0.28	0/2991	0.50	0/4076
1	ZI	0.29	0/2991	0.51	0/4076
1	ZJ	0.31	0/2991	0.51	0/4076
1	ZK	0.26	0/2991	0.48	0/4076
1	ZL	0.28	0/2991	0.49	0/4076
1	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
1	ZN	0.28	0/2991	0.51	0/4076
1	ZO	0.30	0/2991	0.50	0/4076
1	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
1	ZQ	0.28	0/2991	0.51	0/4076
1	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
1	ZS	0.29	0/2991	0.52	1/4076 (0.0%)
1	ZT	0.26	0/2991	0.47	0/4076
1	ZU	0.27	0/2991	0.50	0/4076
1	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
1	ZW	0.25	0/2991	0.48	0/4076
1	ZX	0.28	0/2991	0.48	0/4076
1	ZY	0.29	1/2991 (0.0%)	0.54	2/4076 (0.0%)
1	ZZ	0.25	0/2991	0.46	0/4076
1	Za	0.27	0/2991	0.49	0/4076
1	Zb	0.28	0/2991	0.50	0/4076
1	Zc	0.29	0/2991	0.53	2/4076 (0.0%)
1	Zd	0.29	0/2991	0.50	0/4076
1	Ze	0.27	0/2991	0.48	0/4076
1	Zf	0.27	0/2991	0.48	0/4076
1	Zg	0.27	0/2991	0.49	0/4076
1	Zh	0.26	0/2991	0.48	0/4076
2	0	0.30	0/1888	0.52	1/2564 (0.0%)
2	1	0.31	0/1917	0.50	0/2605
2	2	0.27	0/1973	0.48	0/2682
2	3	0.28	0/1973	0.50	0/2682
2	4	0.28	0/1973	0.50	0/2682

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	5	0.32	0/1973	0.52	0/2682
2	6	0.30	0/1973	0.52	0/2682
2	7	0.28	0/1973	0.50	0/2682
2	8	0.30	0/1973	0.52	0/2682
2	9	0.29	0/1973	0.54	1/2682 (0.0%)
2	ZA	0.29	0/1973	0.52	0/2682
2	ZB	0.29	0/1973	0.49	0/2682
2	ZC	0.28	0/1973	0.51	0/2682
2	ZD	0.28	0/1973	0.51	0/2682
2	ZE	0.28	0/1973	0.50	1/2682 (0.0%)
2	r	0.33	0/1926	0.53	0/2618
2	s	0.36	0/1934	0.56	0/2629
2	t	0.33	0/1942	0.55	0/2639
2	u	0.32	0/1926	0.57	1/2618 (0.0%)
2	v	0.30	0/1934	0.51	0/2629
2	w	0.32	0/1844	0.51	0/2505
2	x	0.31	0/1888	0.51	0/2564
2	y	0.30	0/1888	0.54	1/2564 (0.0%)
2	z	0.30	0/1888	0.51	0/2564
All	All	0.29	6/133363 (0.0%)	0.51	21/181569 (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	ZG	0	1
1	ZI	0	1
1	ZK	0	1
1	ZO	0	1
1	ZW	0	1
1	Zb	0	1
1	Zd	0	1
1	Ze	0	1
2	0	0	2
2	1	0	1
2	5	0	1
2	6	0	1
2	8	0	1
2	ZA	0	1
2	r	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	u	0	1
2	y	0	2
2	z	0	1
All	All	0	20

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	ZV	140	PRO	CG-CD	-16.10	0.97	1.50
1	ZV	125	PRO	CG-CD	-10.15	1.17	1.50
1	ZV	140	PRO	N-CD	8.31	1.59	1.47
1	ZV	125	PRO	N-CD	6.64	1.57	1.47
1	ZY	125	PRO	CG-CD	-5.43	1.32	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ZV	140	PRO	N-CD-CG	-17.34	77.19	103.20
1	ZR	125	PRO	CA-N-CD	-13.96	91.96	111.50
1	ZY	125	PRO	CA-N-CD	-13.35	92.81	111.50
1	ZV	125	PRO	CA-N-CD	-13.26	92.94	111.50
1	ZV	125	PRO	N-CD-CG	-11.23	86.35	103.20

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	ZG	71	ARG	Sidechain
1	ZI	380	ARG	Sidechain
1	ZK	71	ARG	Sidechain
1	ZO	71	ARG	Sidechain
1	ZW	71	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

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	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
1	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	37	66
1	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
1	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	56
1	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
1	ZK	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
1	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	66
1	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
1	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
1	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	46
1	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	66
1	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
1	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	37	66
1	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
1	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
1	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
1	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
1	ZW	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
1	ZX	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
1	ZY	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
1	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
1	Za	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
1	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
1	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
1	Zd	399/403 (99%)	387 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ze	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
1	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
1	Zg	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
1	Zh	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
2	0	244/260 (94%)	236 (97%)	7 (3%)	1 (0%)	30	61
2	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	61
2	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	46
2	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	46
2	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	11	38
2	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	46
2	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	46
2	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	11	38
2	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	46
2	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	46
2	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	38
2	ZB	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	11	38
2	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	38
2	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	46
2	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	61
2	r	250/260 (96%)	237 (95%)	12 (5%)	1 (0%)	30	61
2	s	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	61
2	t	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	61
2	u	250/260 (96%)	242 (97%)	6 (2%)	2 (1%)	16	46
2	v	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	61
2	w	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	61
2	x	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	11	38
2	y	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	61
2	z	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	61
All	All	17642/17927 (98%)	17056 (97%)	533 (3%)	53 (0%)	38	66

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	ZG	46	SER
2	2	209	ASN
2	5	209	ASN
2	8	209	ASN
2	ZA	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	ZF	321/323 (99%)	310 (97%)	11 (3%)	32	59
1	ZG	321/323 (99%)	306 (95%)	15 (5%)	22	51
1	ZH	321/323 (99%)	309 (96%)	12 (4%)	29	56
1	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	72
1	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	67
1	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	72
1	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	61
1	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	64
1	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	61
1	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	67
1	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	51
1	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	64
1	ZR	321/323 (99%)	313 (98%)	8 (2%)	42	67
1	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	72
1	ZT	321/323 (99%)	316 (98%)	5 (2%)	58	76
1	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	80
1	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	80
1	ZW	321/323 (99%)	309 (96%)	12 (4%)	29	56
1	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	85
1	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	76
1	Za	321/323 (99%)	316 (98%)	5 (2%)	58	76
1	Zb	321/323 (99%)	315 (98%)	6 (2%)	52	72
1	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	59
1	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	72
1	Ze	321/323 (99%)	312 (97%)	9 (3%)	38	64
1	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	69
1	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	72
1	Zh	321/323 (99%)	313 (98%)	8 (2%)	42	67
2	0	205/215 (95%)	199 (97%)	6 (3%)	37	63
2	1	209/215 (97%)	201 (96%)	8 (4%)	28	56
2	2	215/215 (100%)	212 (99%)	3 (1%)	62	78
2	3	215/215 (100%)	211 (98%)	4 (2%)	52	72
2	4	215/215 (100%)	211 (98%)	4 (2%)	52	72
2	5	215/215 (100%)	211 (98%)	4 (2%)	52	72
2	6	215/215 (100%)	210 (98%)	5 (2%)	45	68
2	7	215/215 (100%)	214 (100%)	1 (0%)	86	91
2	8	215/215 (100%)	213 (99%)	2 (1%)	75	85
2	9	215/215 (100%)	211 (98%)	4 (2%)	52	72
2	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	85
2	ZB	215/215 (100%)	207 (96%)	8 (4%)	29	56
2	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	78
2	ZD	215/215 (100%)	212 (99%)	3 (1%)	62	78
2	ZE	215/215 (100%)	214 (100%)	1 (0%)	86	91
2	r	209/215 (97%)	204 (98%)	5 (2%)	44	68
2	s	210/215 (98%)	203 (97%)	7 (3%)	33	60
2	t	211/215 (98%)	201 (95%)	10 (5%)	22	51
2	u	209/215 (97%)	200 (96%)	9 (4%)	25	53
2	v	210/215 (98%)	202 (96%)	8 (4%)	28	56
2	w	200/215 (93%)	196 (98%)	4 (2%)	50	71
2	x	205/215 (95%)	199 (97%)	6 (3%)	37	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	y	205/215 (95%)	197 (96%)	8 (4%)	27	55
2	z	205/215 (95%)	201 (98%)	4 (2%)	50	71
All	All	14382/14527 (99%)	14032 (98%)	350 (2%)	45	68

5 of 350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	91	ASN
2	1	164	GLN
2	4	64	SER
2	ZB	1	MET
2	s	251	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 370 such sidechains are listed below:

Mol	Chain	Res	Type
1	Zh	5	GLN
2	ZB	235	GLN
2	2	255	GLN
2	6	59	GLN
2	ZE	67	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.

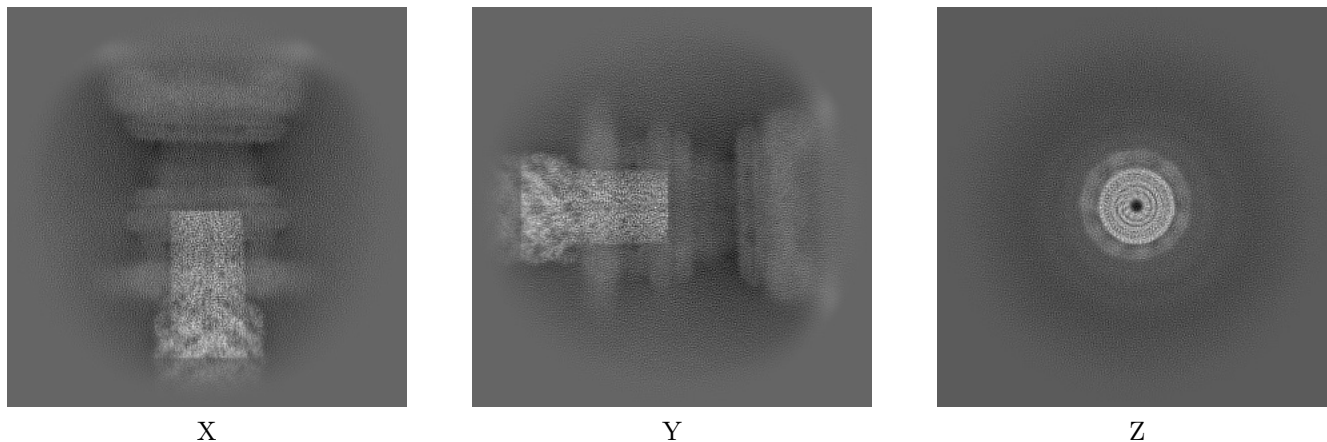
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37600. These allow visual inspection of the internal detail of the map and identification of artifacts.

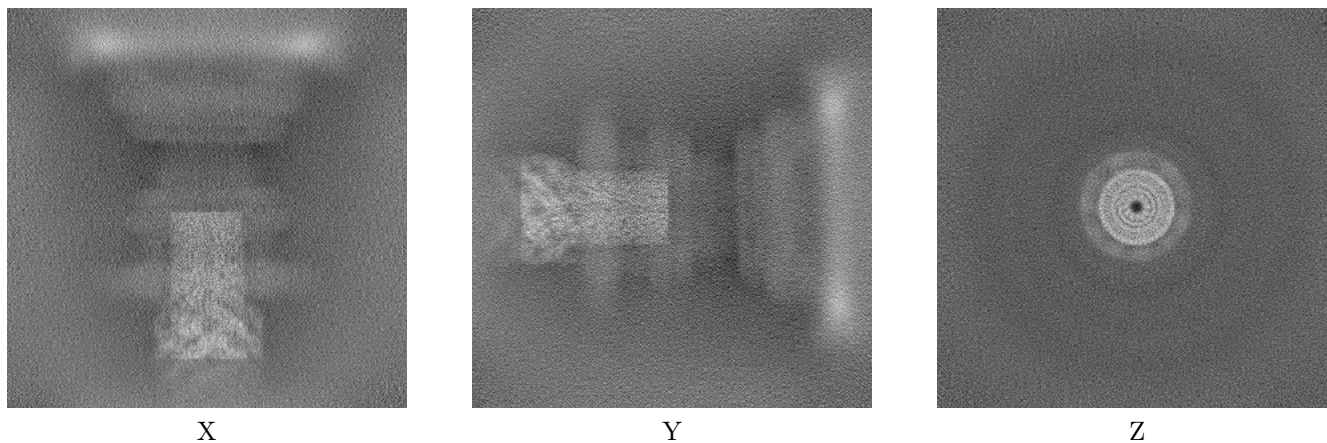
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



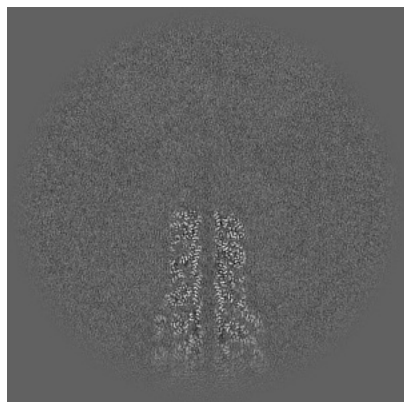
6.1.2 Raw map



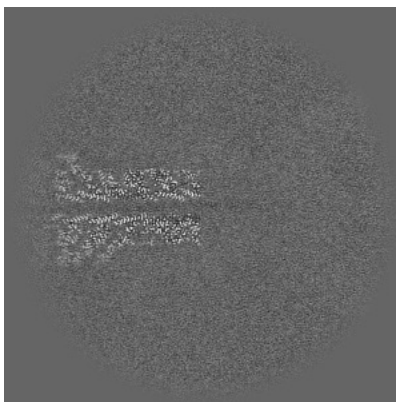
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

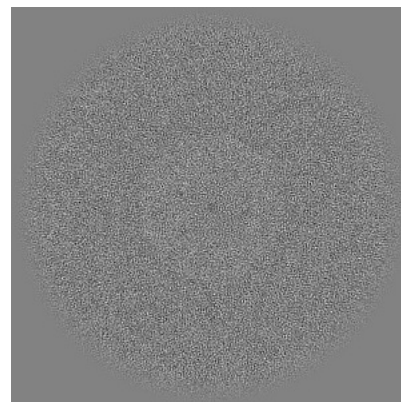
6.2.1 Primary map



X Index: 256

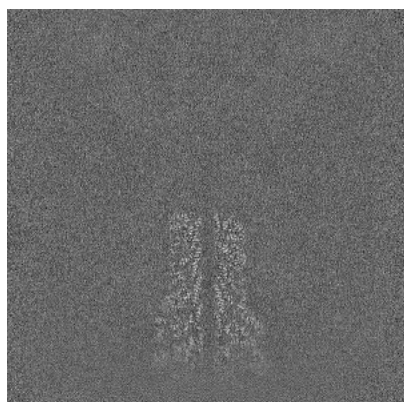


Y Index: 256

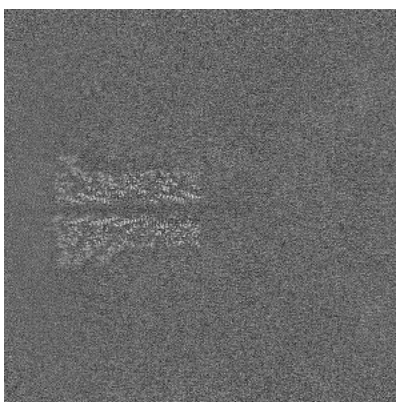


Z Index: 256

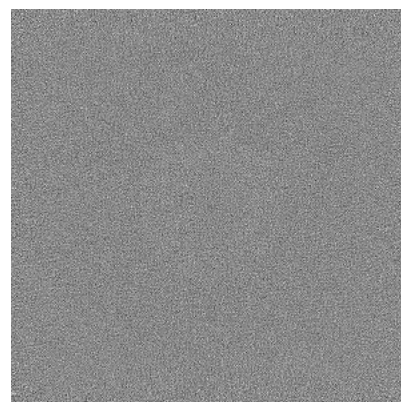
6.2.2 Raw map



X Index: 256



Y Index: 256

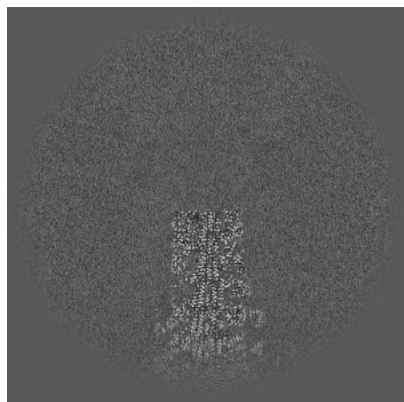


Z Index: 256

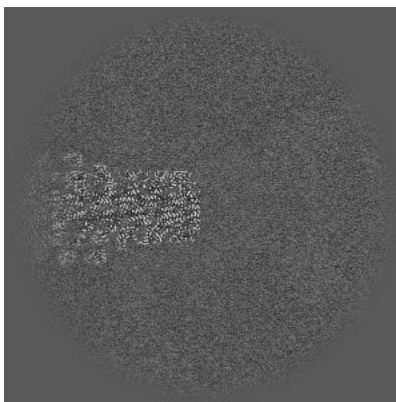
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

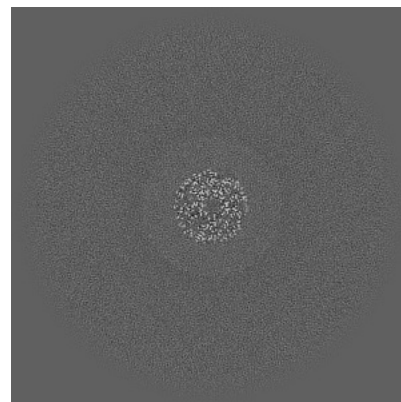
6.3.1 Primary map



X Index: 242

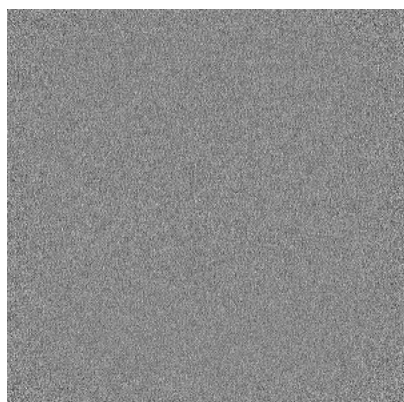


Y Index: 268

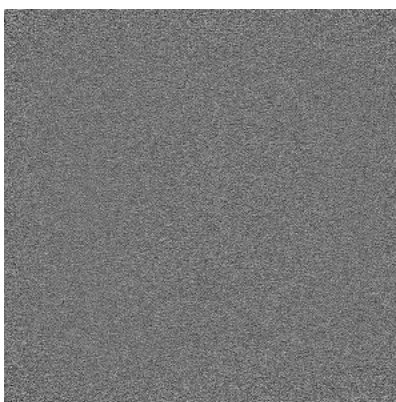


Z Index: 218

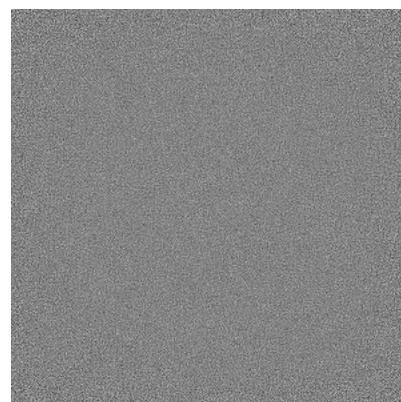
6.3.2 Raw map



X Index: 0



Y Index: 0

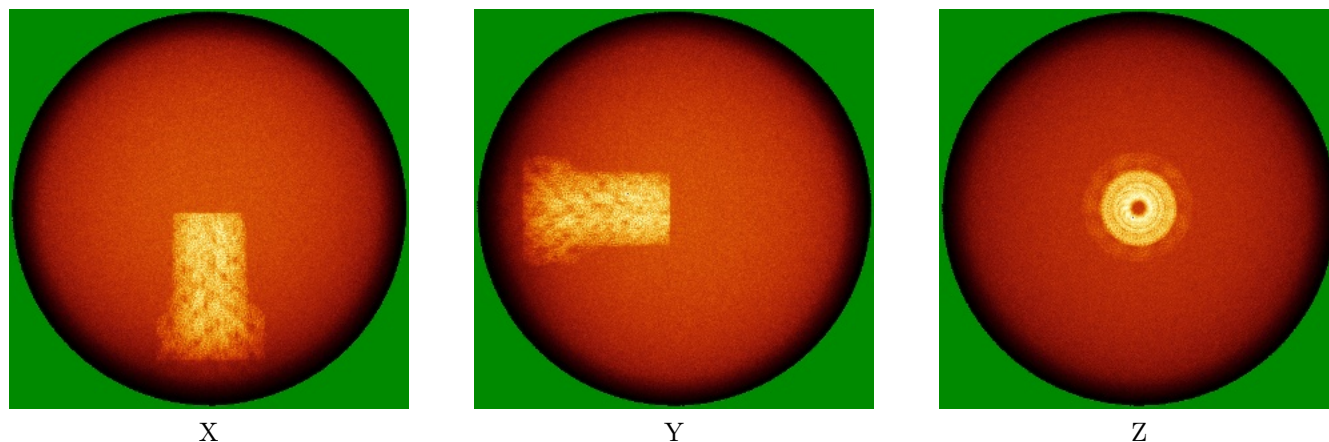


Z Index: 0

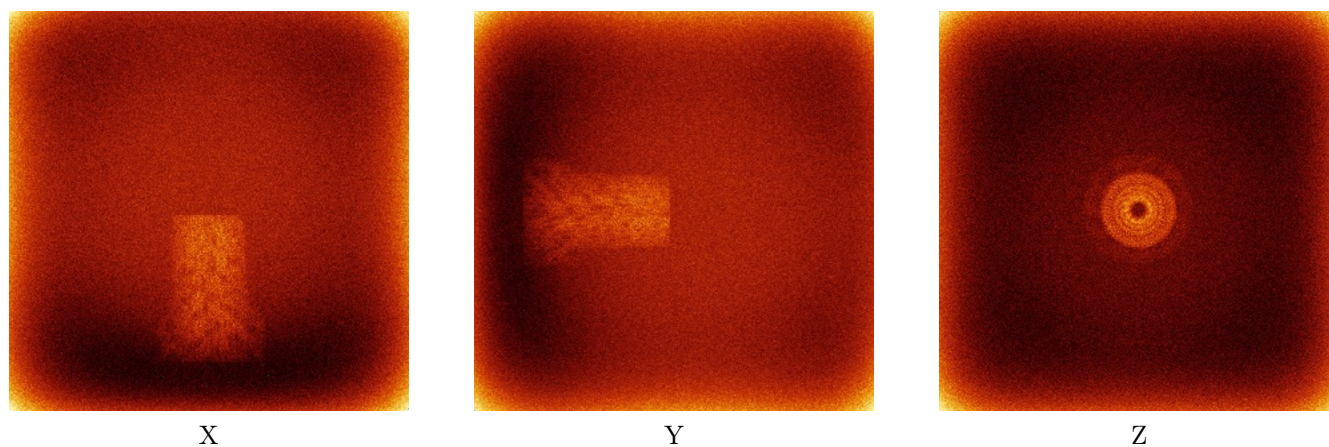
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



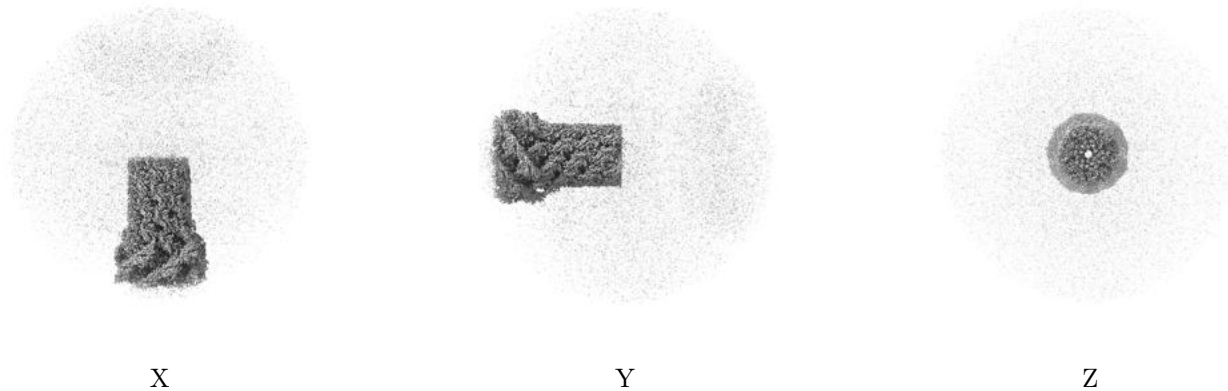
6.4.2 Raw map



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.

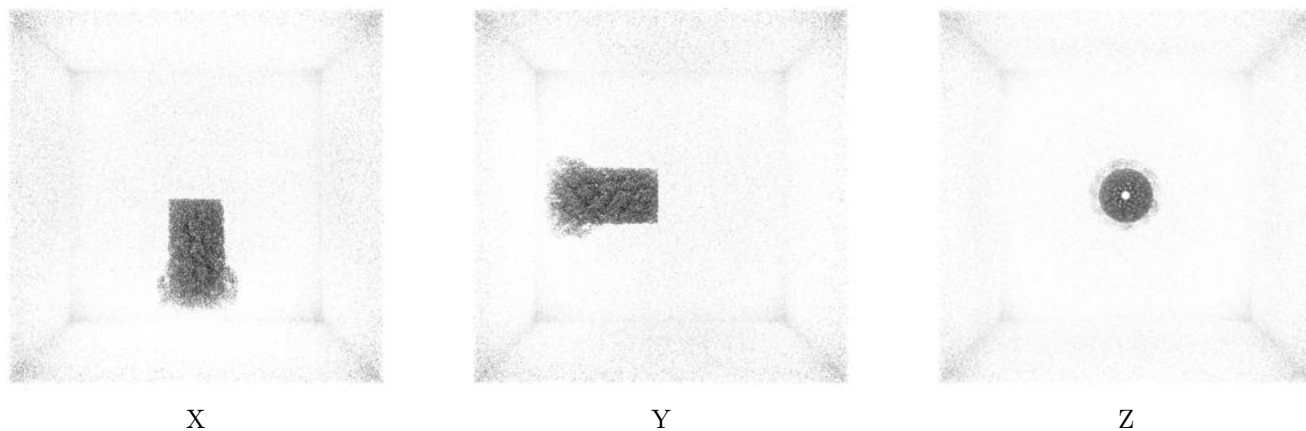
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

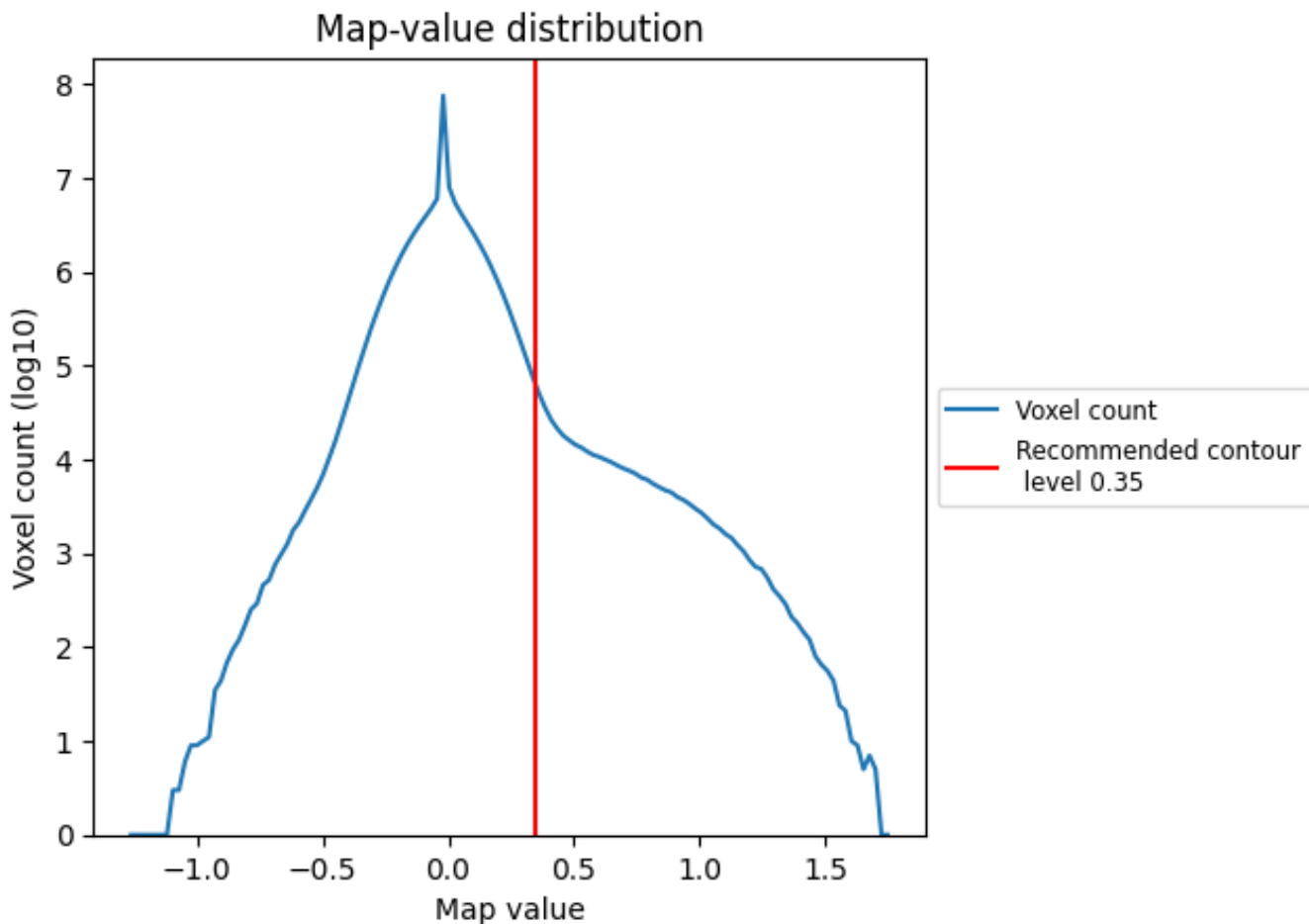
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

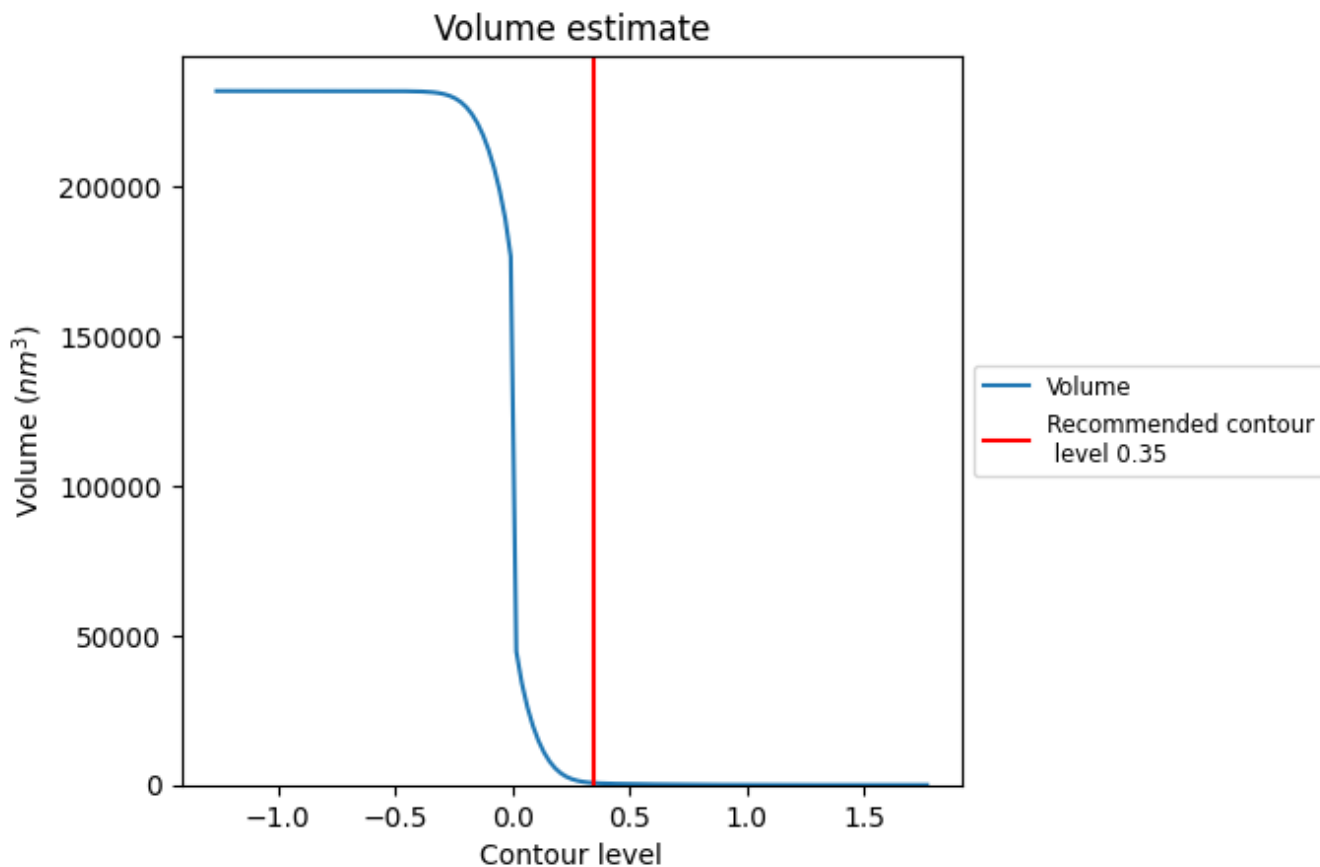
This section contains the results of statistical analysis of the map.

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.

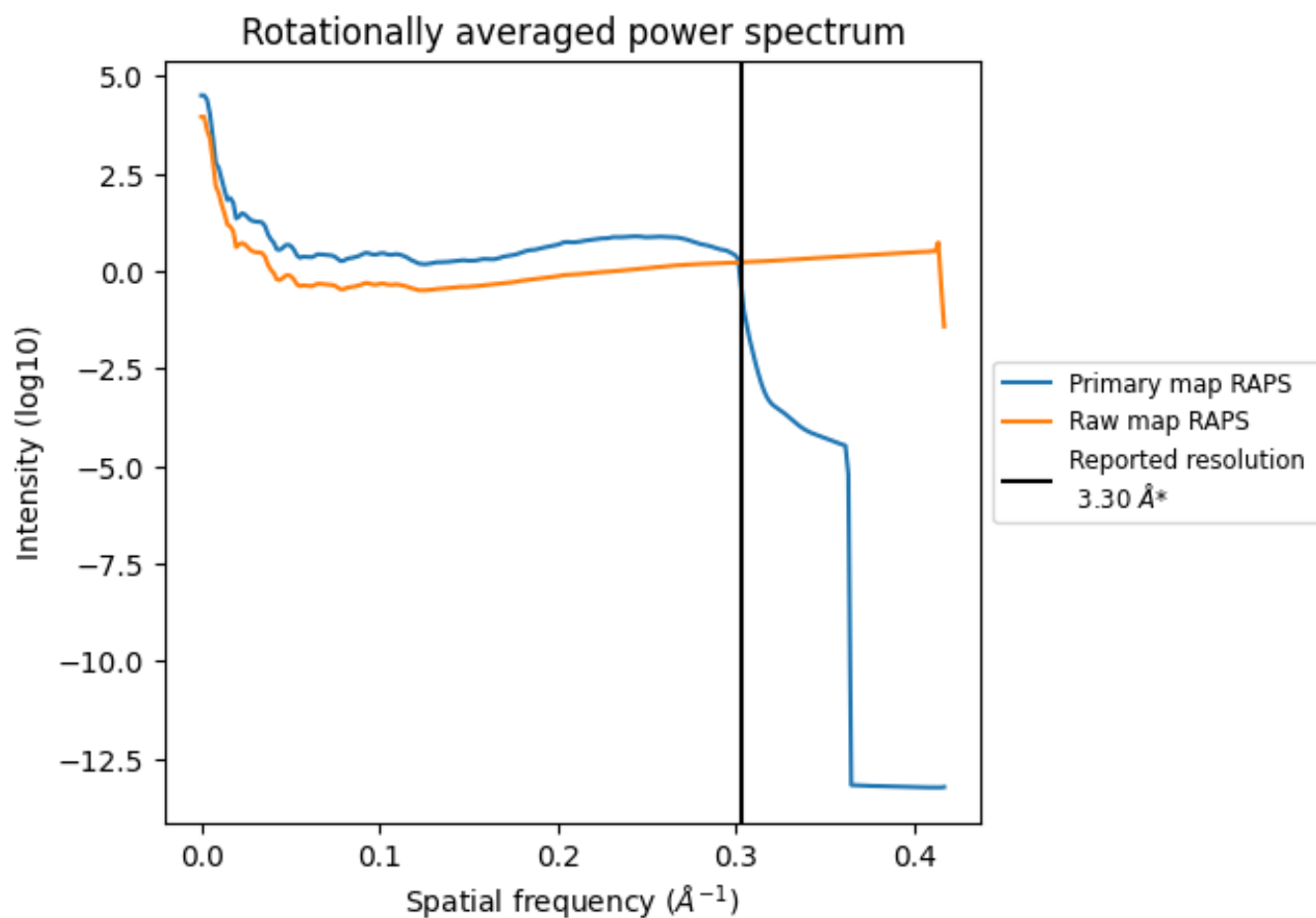
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 652 nm^3 ; this corresponds to an approximate mass of 589 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

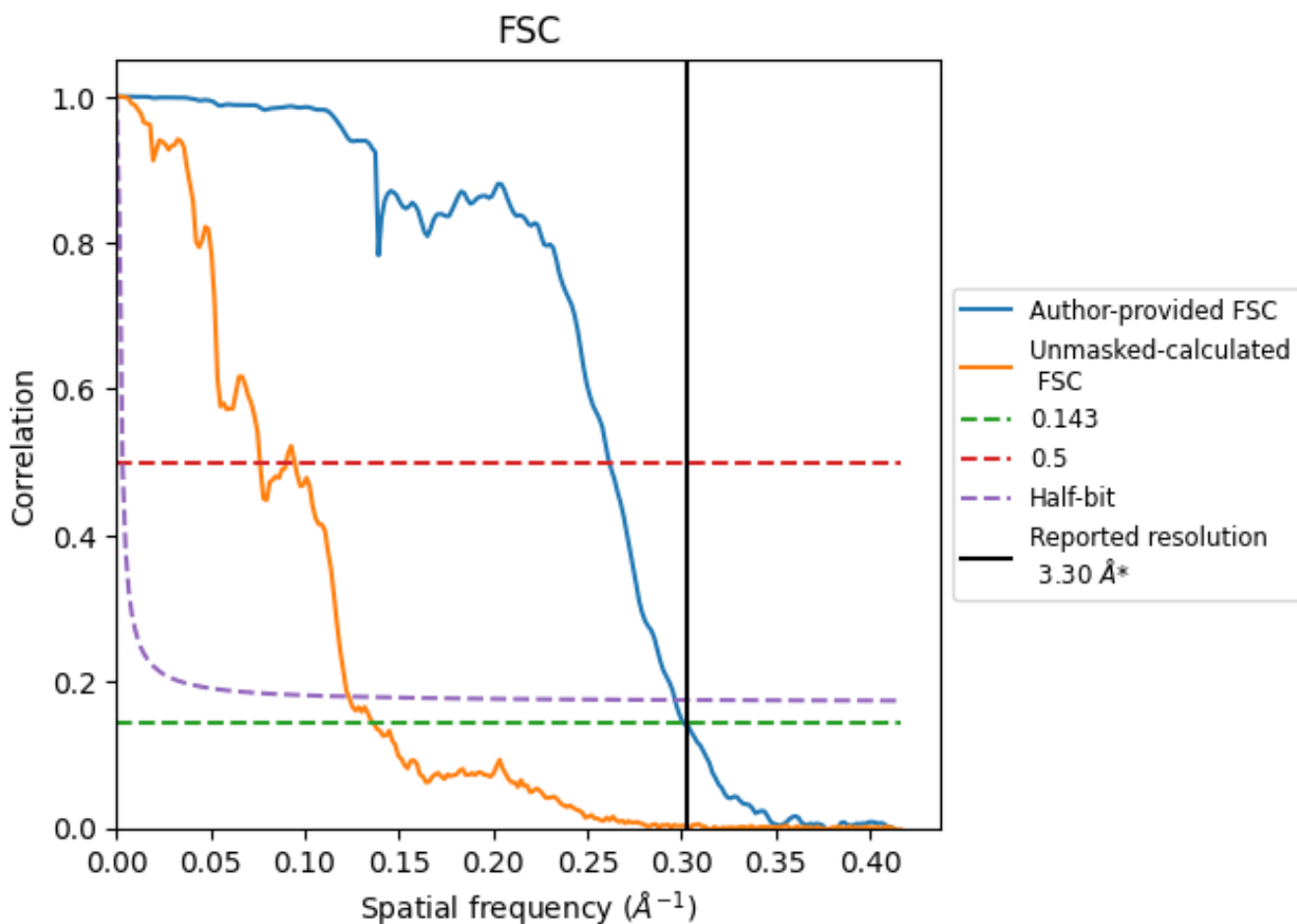


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates

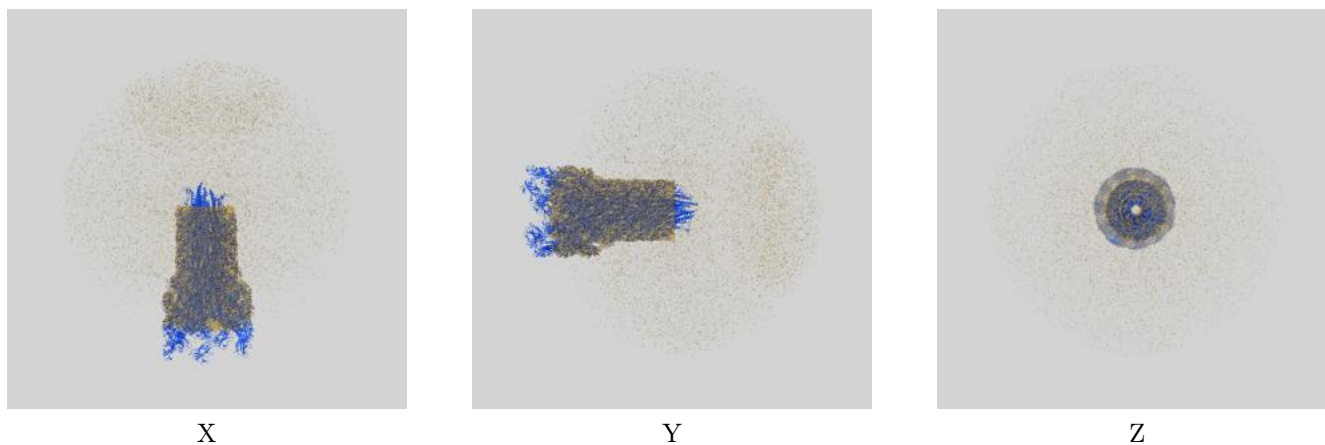
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.82	3.37
Unmasked-calculated*	7.32	13.12	8.10

*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 7.32 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

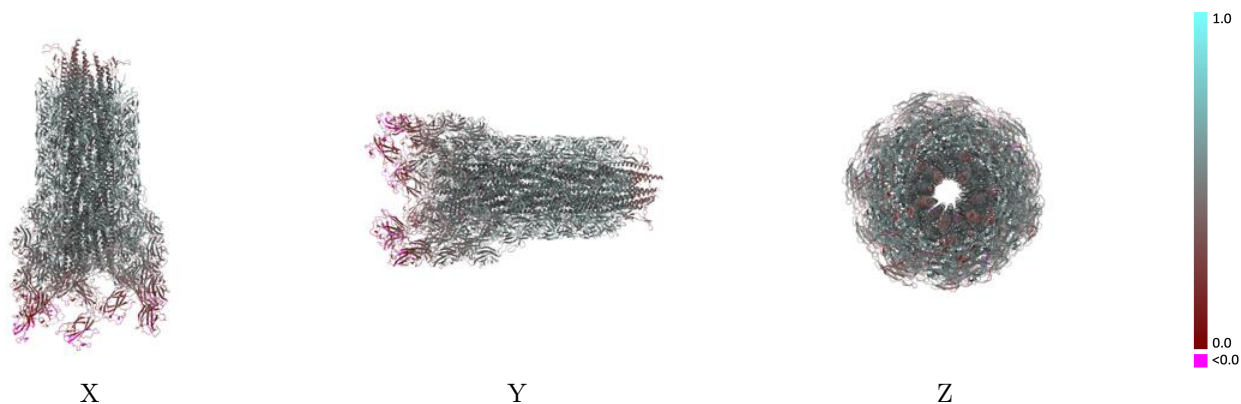
This section contains information regarding the fit between EMDB map EMD-37600 and PDB model 8WKI. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



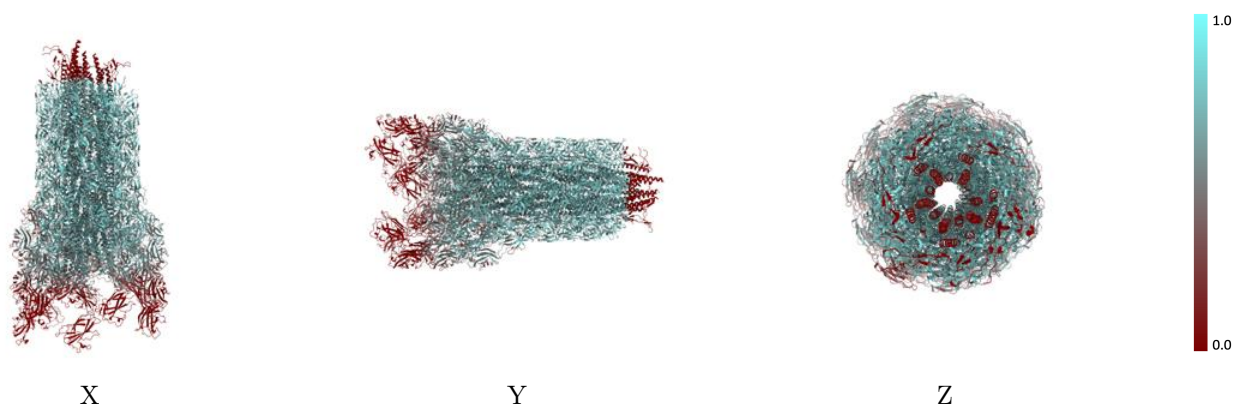
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



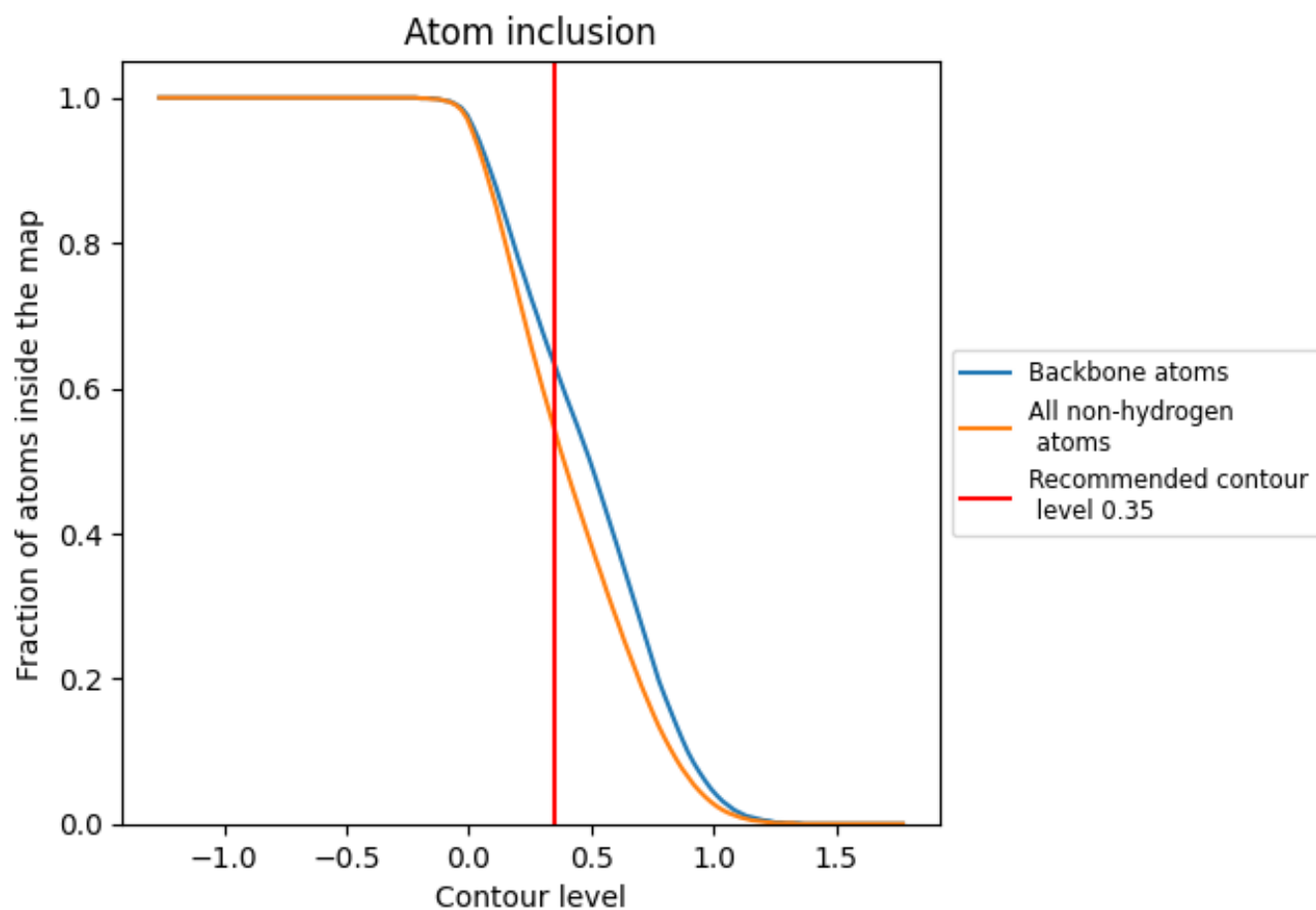
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5420	 0.4590
0	 0.6870	 0.5200
1	 0.6850	 0.5230
2	 0.7000	 0.5280
3	 0.7040	 0.5250
4	 0.6980	 0.5180
5	 0.6900	 0.5190
6	 0.6990	 0.5230
7	 0.7000	 0.5200
8	 0.7000	 0.5210
9	 0.6990	 0.5260
ZA	 0.6910	 0.5180
ZB	 0.7000	 0.5220
ZC	 0.6940	 0.5190
ZD	 0.6860	 0.5150
ZE	 0.6730	 0.5130
ZF	 0.4460	 0.4510
ZG	 0.6020	 0.4950
ZH	 0.6340	 0.4920
ZI	 0.6440	 0.4980
ZJ	 0.6340	 0.4890
ZK	 0.6060	 0.4800
ZL	 0.6200	 0.4840
ZM	 0.6340	 0.4920
ZN	 0.6290	 0.4840
ZO	 0.6130	 0.4850
ZP	 0.6100	 0.4790
ZQ	 0.5790	 0.4750
ZR	 0.5760	 0.4670
ZS	 0.5690	 0.4650
ZT	 0.5340	 0.4550
ZU	 0.5080	 0.4460
ZV	 0.4910	 0.4370
ZW	 0.4800	 0.4340
ZX	 0.4570	 0.4240



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Chain	Atom inclusion	Q-score
ZY	█ 0.4400	█ 0.4130
ZZ	█ 0.4130	█ 0.4010
Za	█ 0.3880	█ 0.3920
Zb	█ 0.3760	█ 0.3860
Zc	█ 0.3630	█ 0.3800
Zd	█ 0.3300	█ 0.3560
Ze	█ 0.2970	█ 0.3500
Zf	█ 0.2660	█ 0.3330
Zg	█ 0.2440	█ 0.3040
Zh	█ 0.2240	█ 0.3140
r	█ 0.3760	█ 0.4510
s	█ 0.4570	█ 0.4630
t	█ 0.4930	█ 0.4710
u	█ 0.5110	█ 0.4850
v	█ 0.5410	█ 0.4830
w	█ 0.6050	█ 0.5060
x	█ 0.6110	█ 0.4960
y	█ 0.6250	█ 0.5030
z	█ 0.6700	█ 0.5150