Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 09:47 PM 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

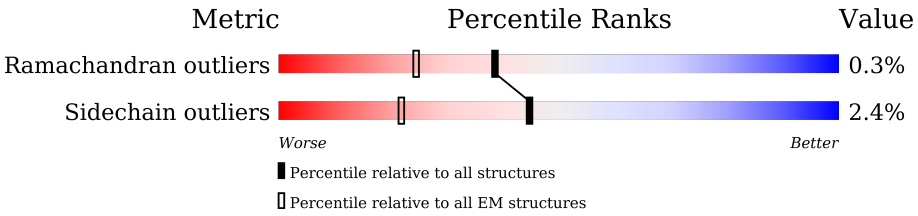
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 <=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	42% 97%
1	ZG	403	16% 95%
1	ZH	403	11% 97%
1	ZI	403	9% 97%
1	ZJ	403	11% 98%
1	ZK	403	17% 98%
1	ZL	403	15% 97%
1	ZM	403	12% 97%
1	ZN	403	13% 97%

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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	5% 96%
2	ZC	260	98%
2	ZD	260	98%
2	ZE	260	5% 99%
2	r	260	45% 95%
2	s	260	35% 95%
2	t	260	30% 94%
2	u	260	27% 93% 5%
2	v	260	27% 95%
2	w	260	15% 92% 7%
2	x	260	14% 92% 5%
2	y	260	12% 92% 5%
2	z	260	7% 93% 5%

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

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

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

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

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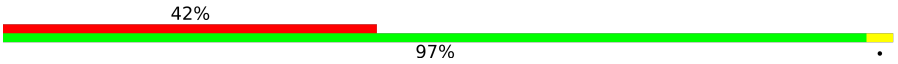
Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZA	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZB	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZC	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
2	ZD	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
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		

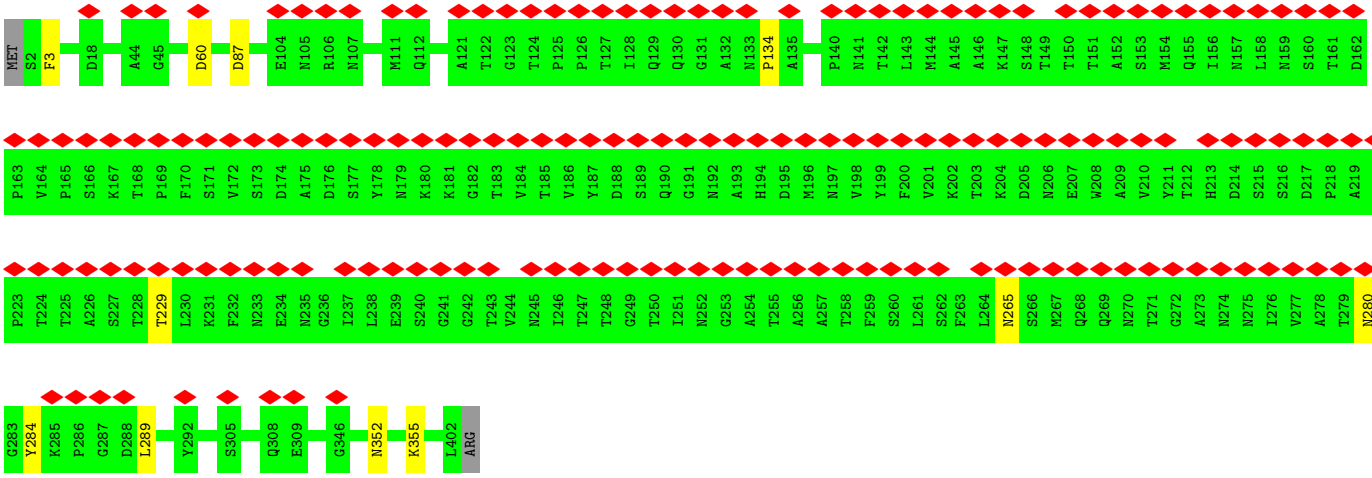
3 Residue-property plots (i)

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

• Molecule 1: Flagellar hook protein FlgE

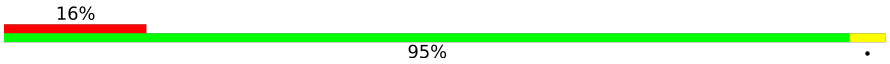
Chain ZF:

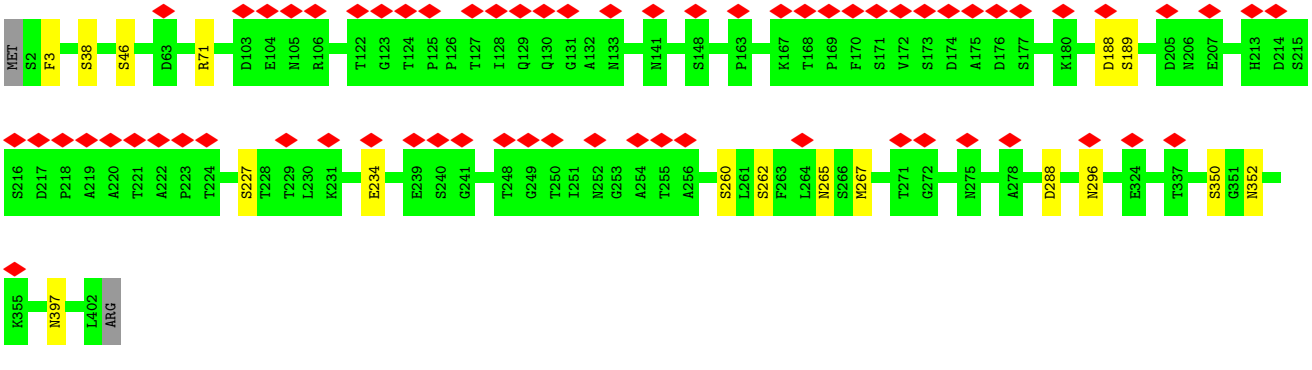




• Molecule 1: Flagellar hook protein FlgE

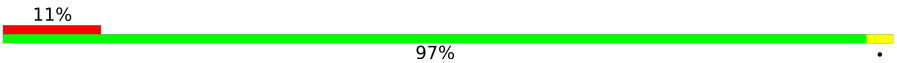
Chain ZG:

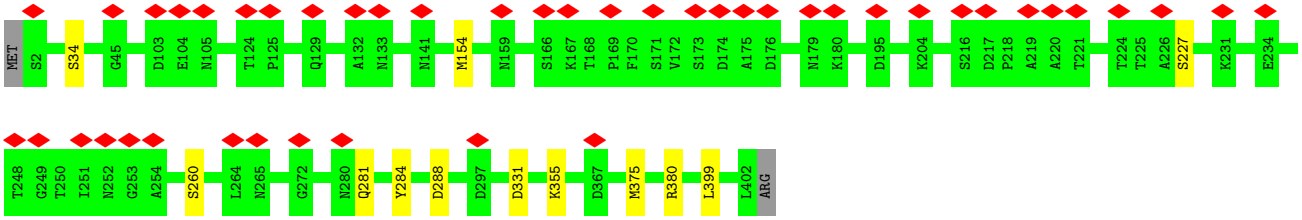




• Molecule 1: Flagellar hook protein FlgE

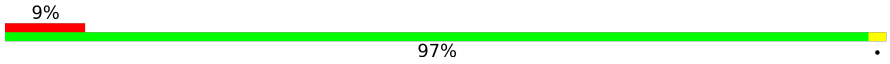
Chain ZH:





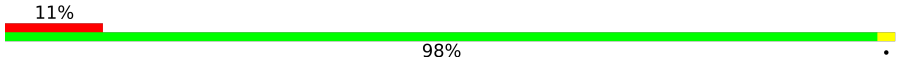
• Molecule 1: Flagellar hook protein FlgE

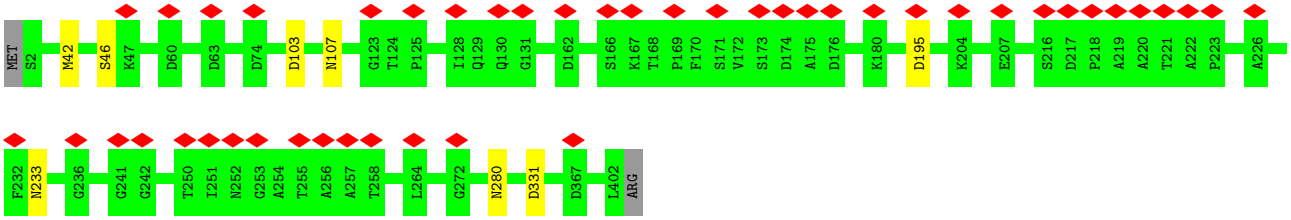
Chain ZI:



• Molecule 1: Flagellar hook protein FlgE

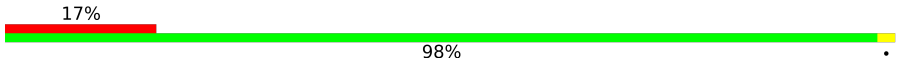
Chain ZJ:

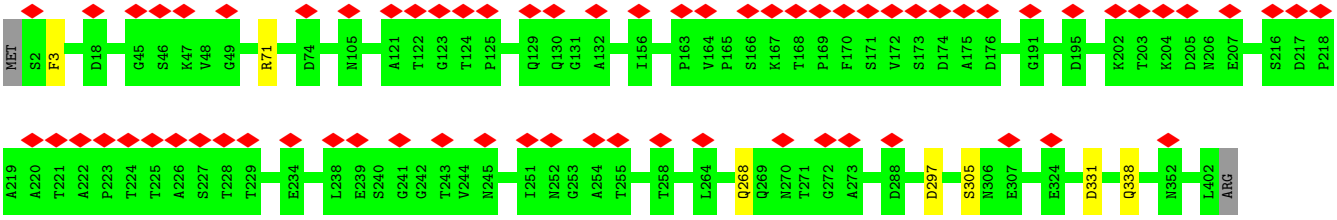




• Molecule 1: Flagellar hook protein FlgE

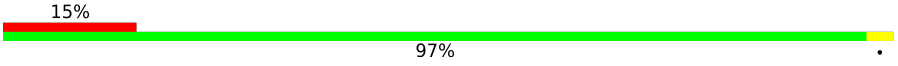
Chain ZK:

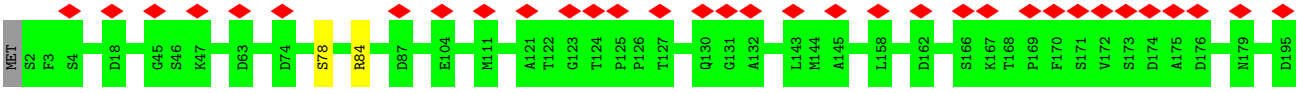


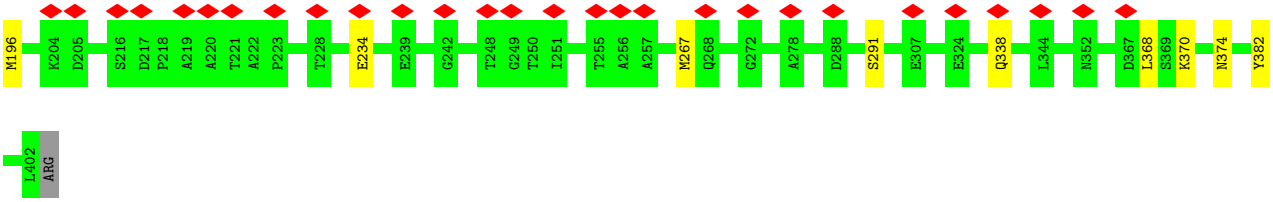


• Molecule 1: Flagellar hook protein FlgE

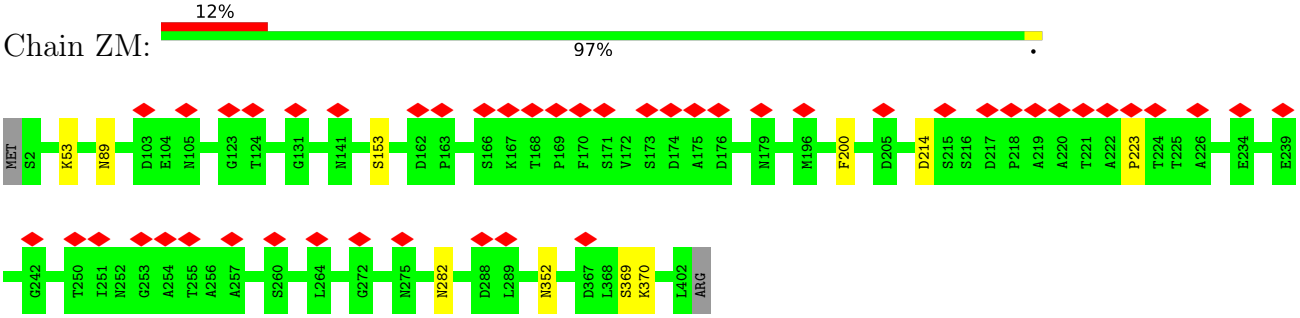
Chain ZL:



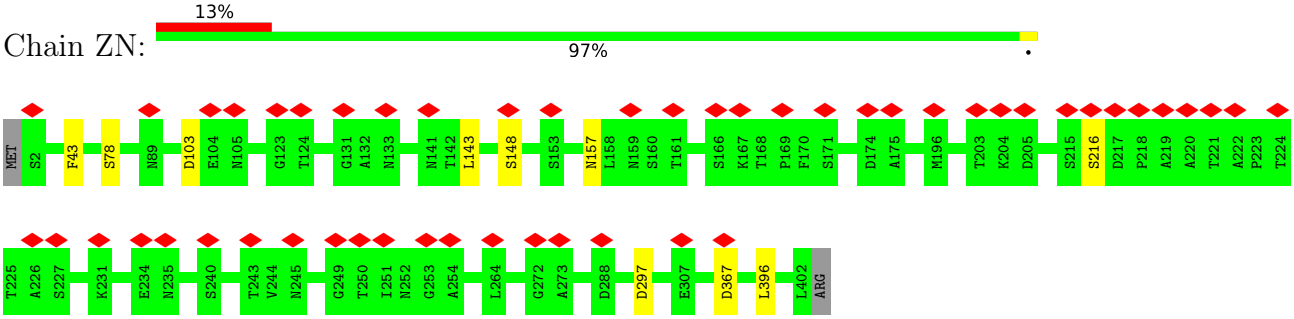




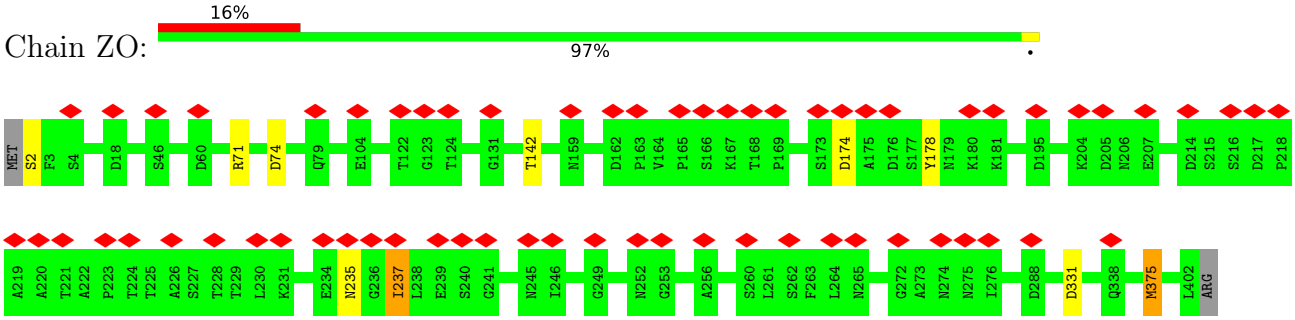
• Molecule 1: Flagellar hook protein FlgE



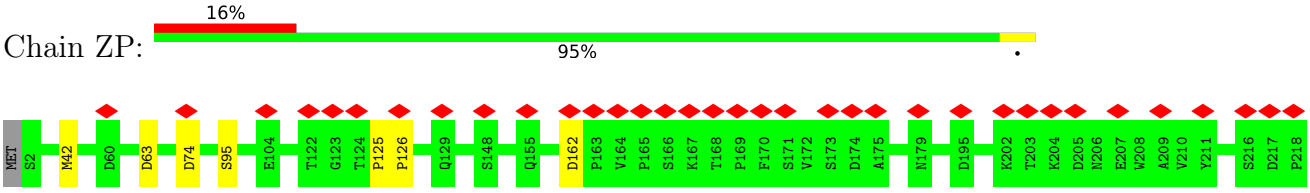
• Molecule 1: Flagellar hook protein FlgE

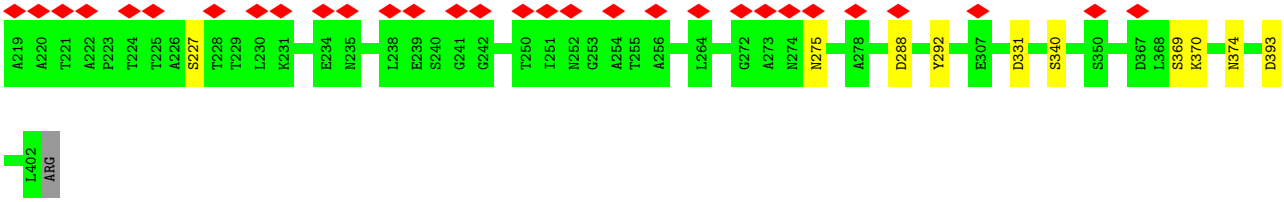


• Molecule 1: Flagellar hook protein FlgE



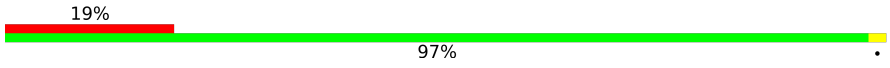
• Molecule 1: Flagellar hook protein FlgE

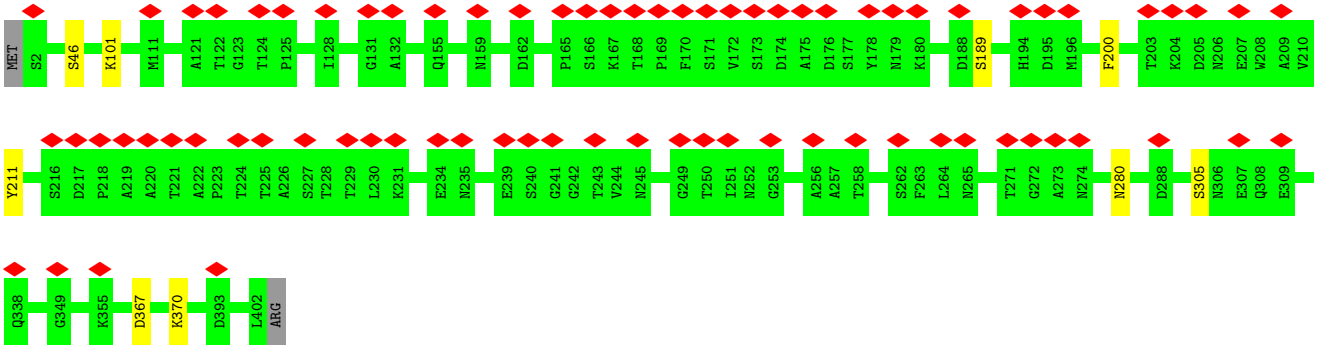




• Molecule 1: Flagellar hook protein FlgE

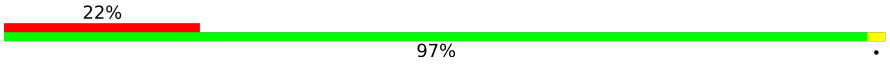
Chain ZQ:

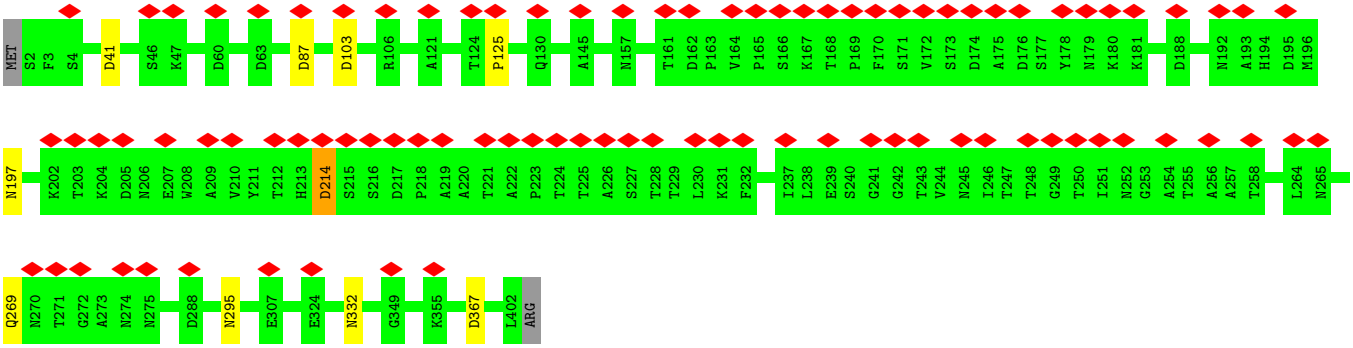




• Molecule 1: Flagellar hook protein FlgE

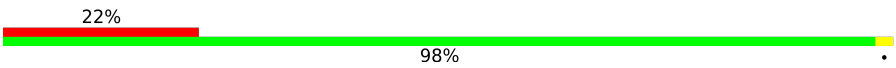
Chain ZR:

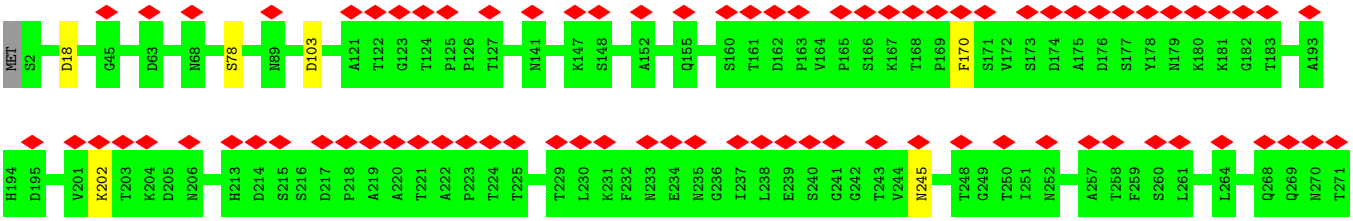


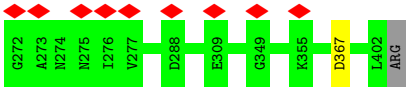


• Molecule 1: Flagellar hook protein FlgE

Chain ZS:

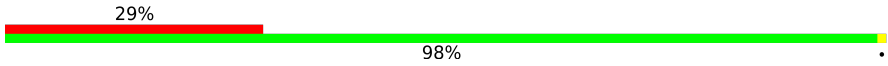


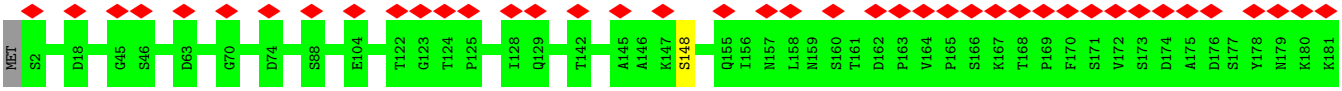


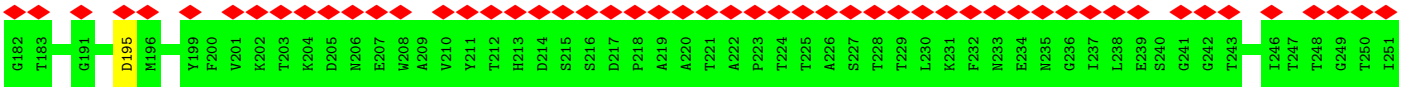


• Molecule 1: Flagellar hook protein FlgE

Chain ZT:

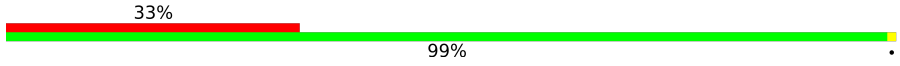


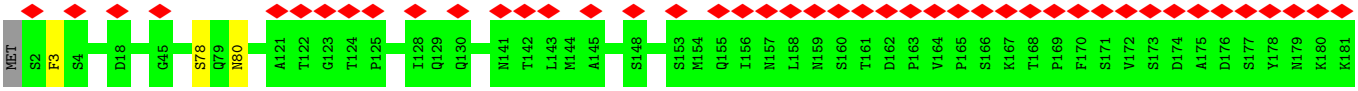


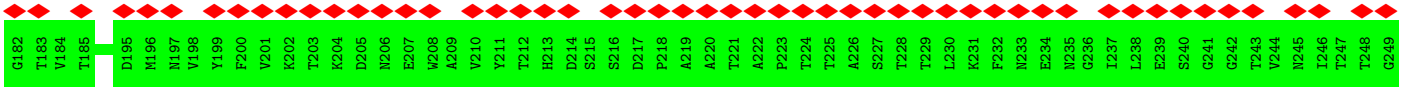


• Molecule 1: Flagellar hook protein FlgE

Chain ZU:

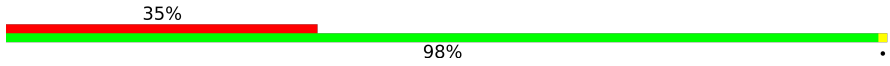


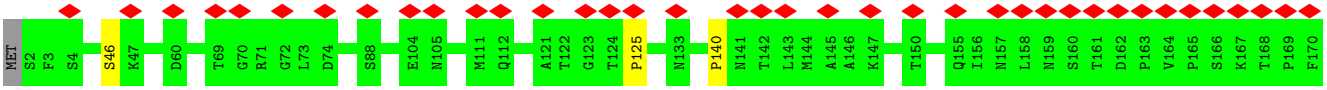


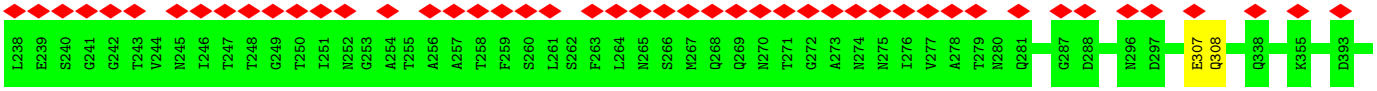


• Molecule 1: Flagellar hook protein FlgE

Chain ZV:

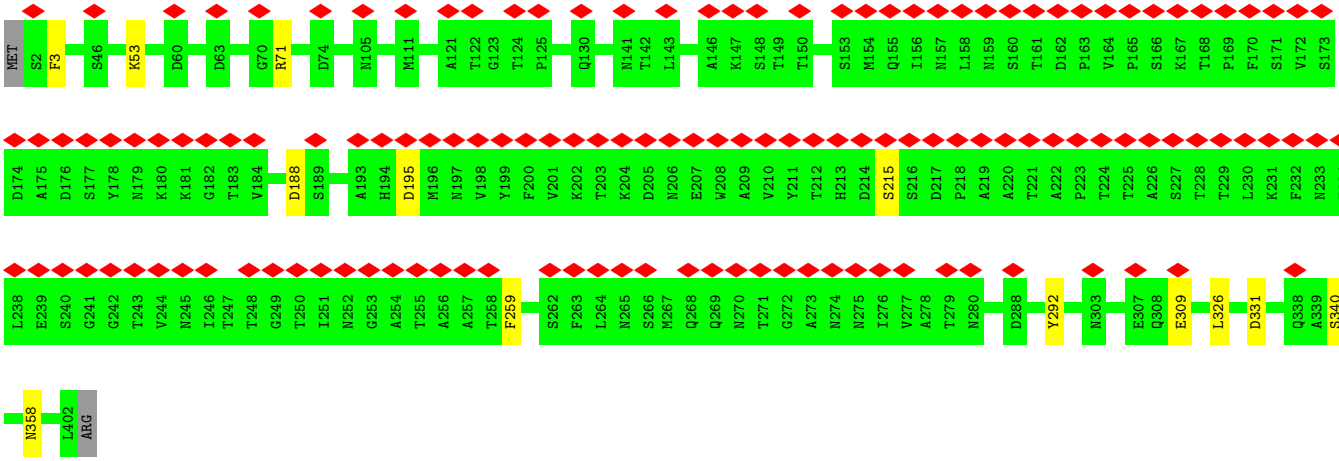






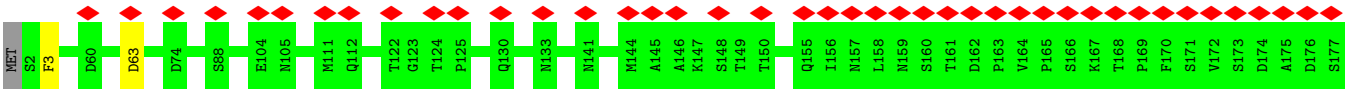
• Molecule 1: Flagellar hook protein FlgE

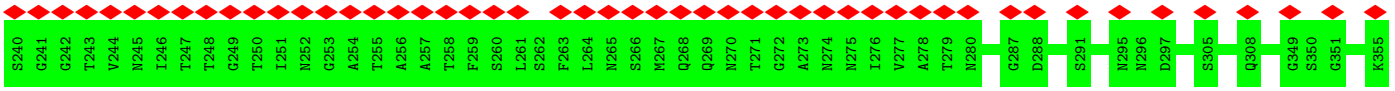
Chain ZW:



• Molecule 1: Flagellar hook protein FlgE

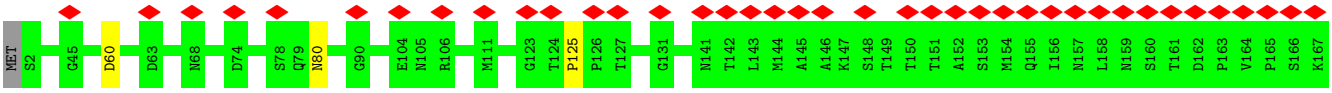
Chain ZX:

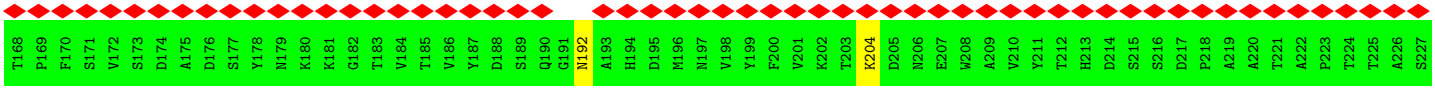


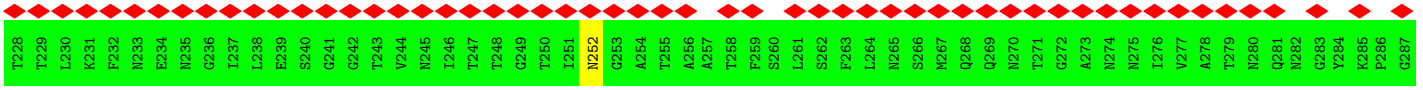


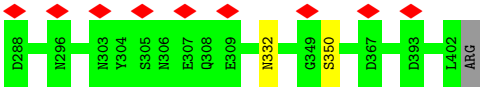
• Molecule 1: Flagellar hook protein FlgE

Chain ZY:



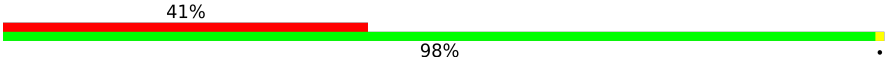


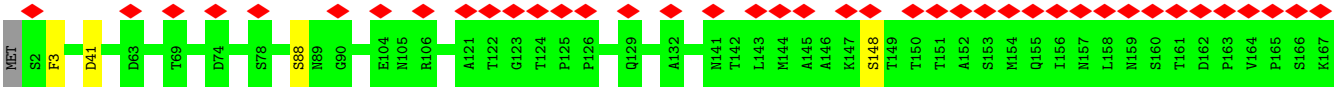


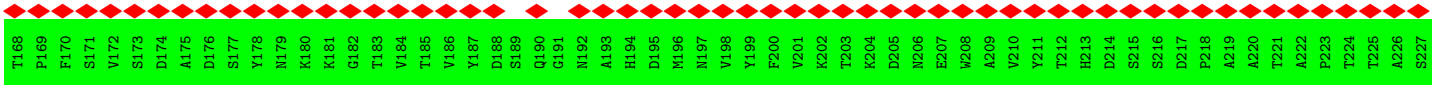


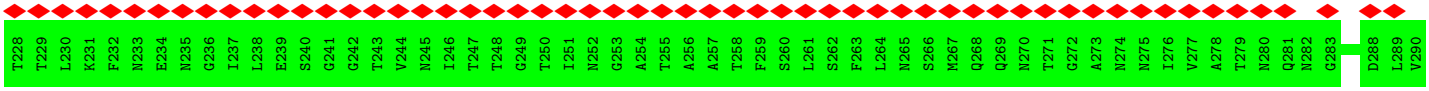
• Molecule 1: Flagellar hook protein FlgE

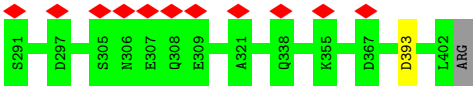
Chain ZZ:





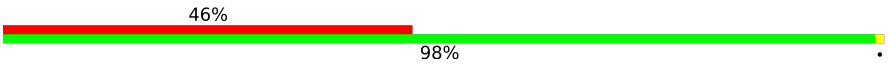


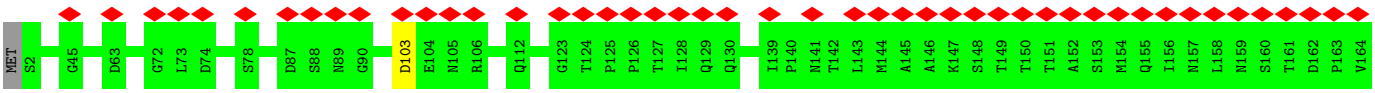


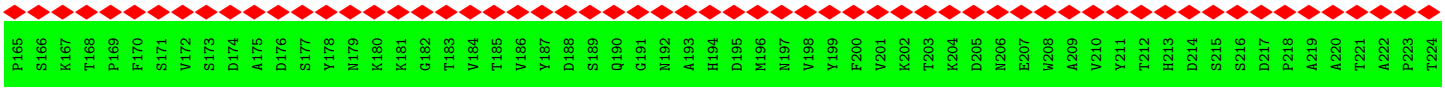


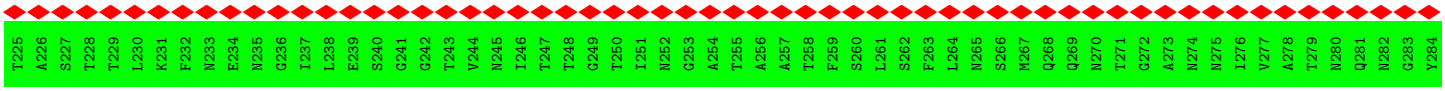
• Molecule 1: Flagellar hook protein FlgE

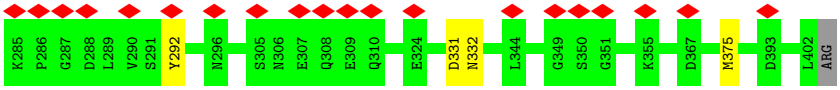
Chain Za:





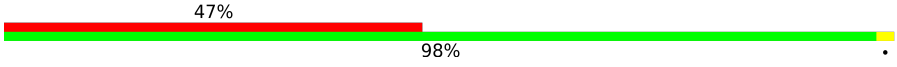


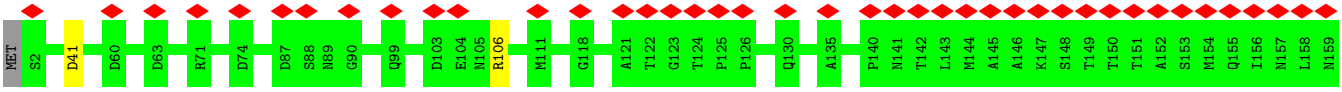


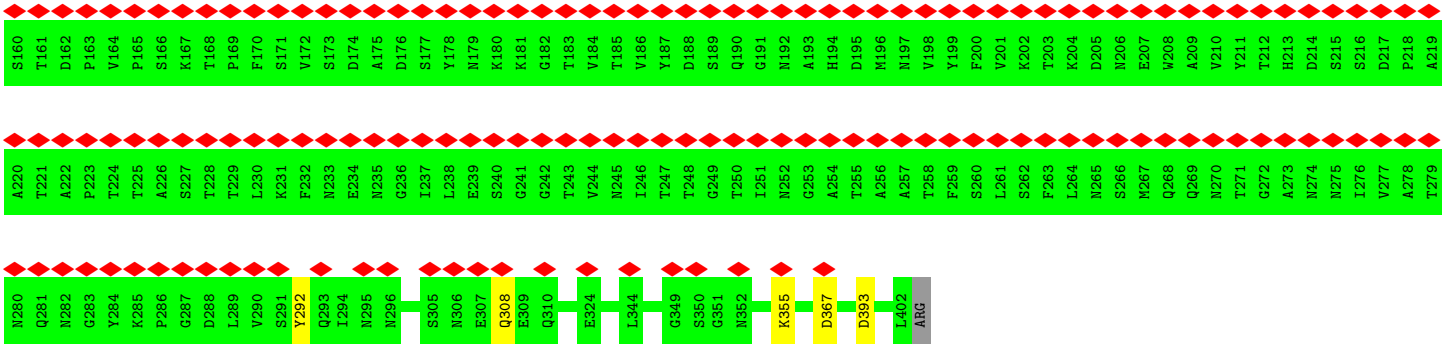


• Molecule 1: Flagellar hook protein FlgE

Chain Zb:

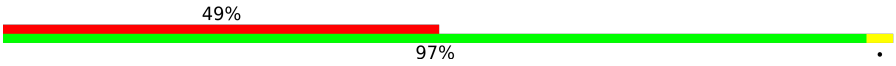


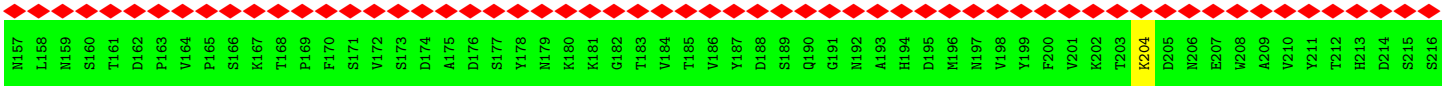


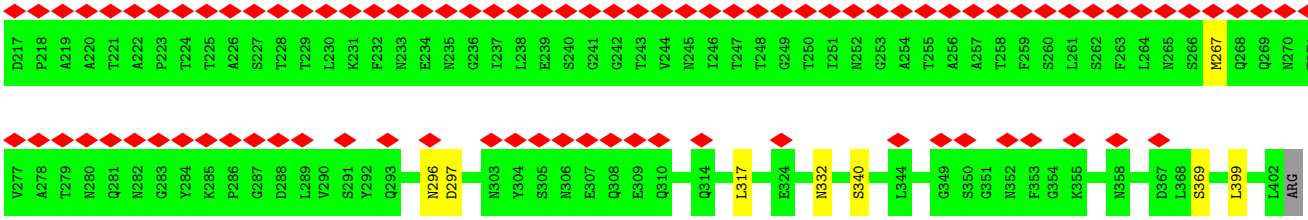


• Molecule 1: Flagellar hook protein FlgE

Chain Zc:

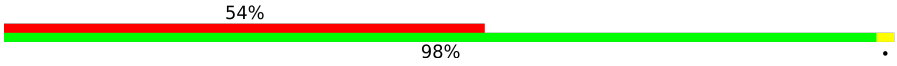


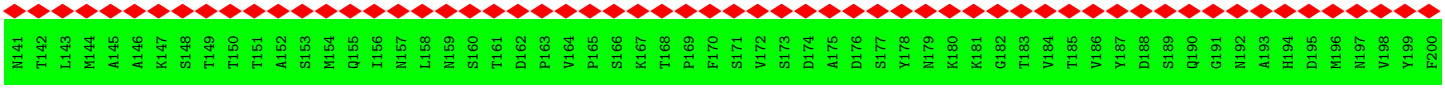


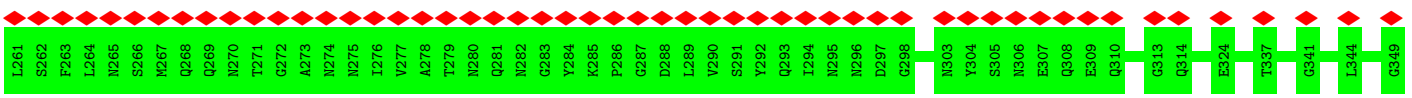


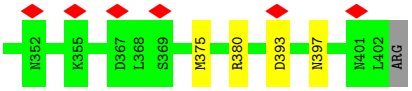
• Molecule 1: Flagellar hook protein FlgE

Chain Zd:



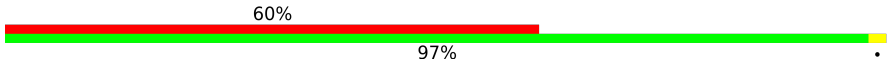


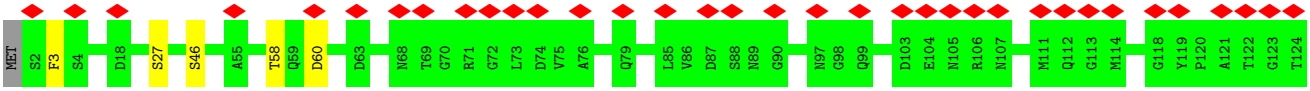


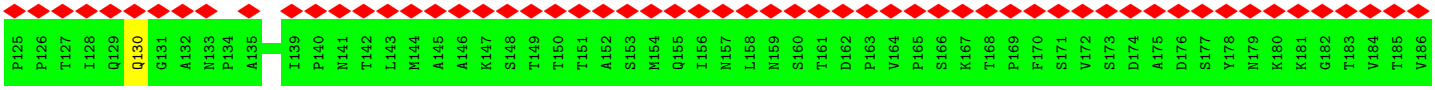


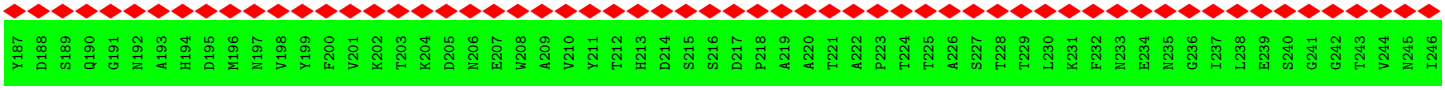
• Molecule 1: Flagellar hook protein FlgE

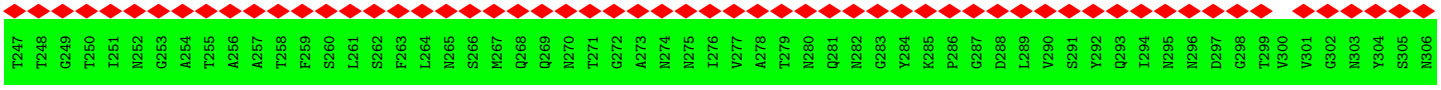
Chain Ze:

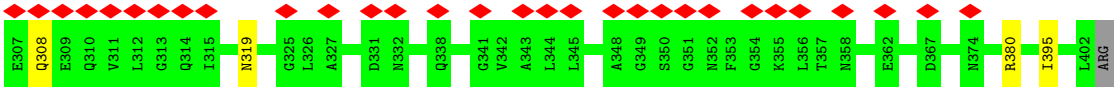






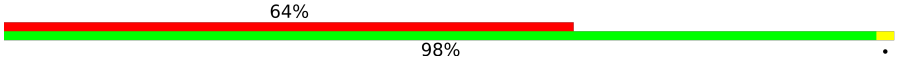


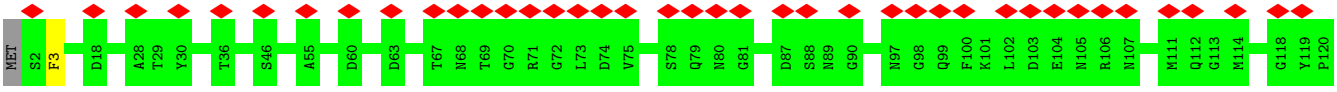


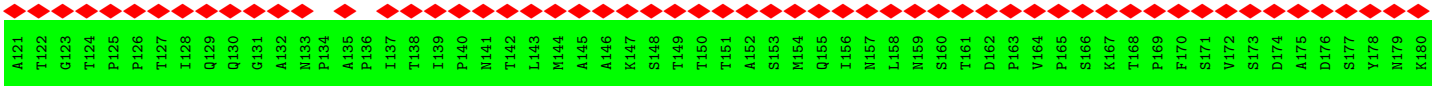


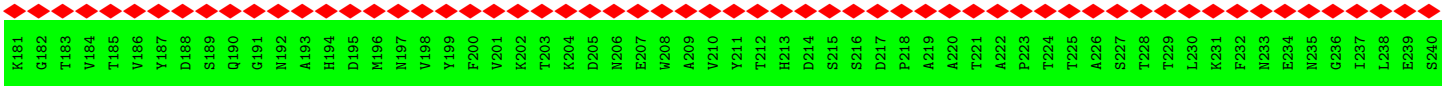
• Molecule 1: Flagellar hook protein FlgE

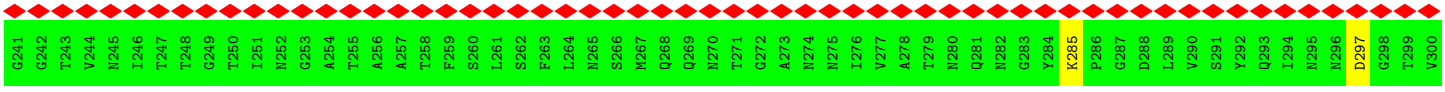
Chain Zf:

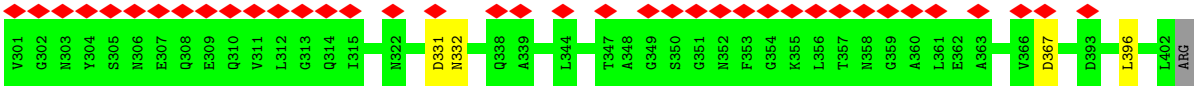






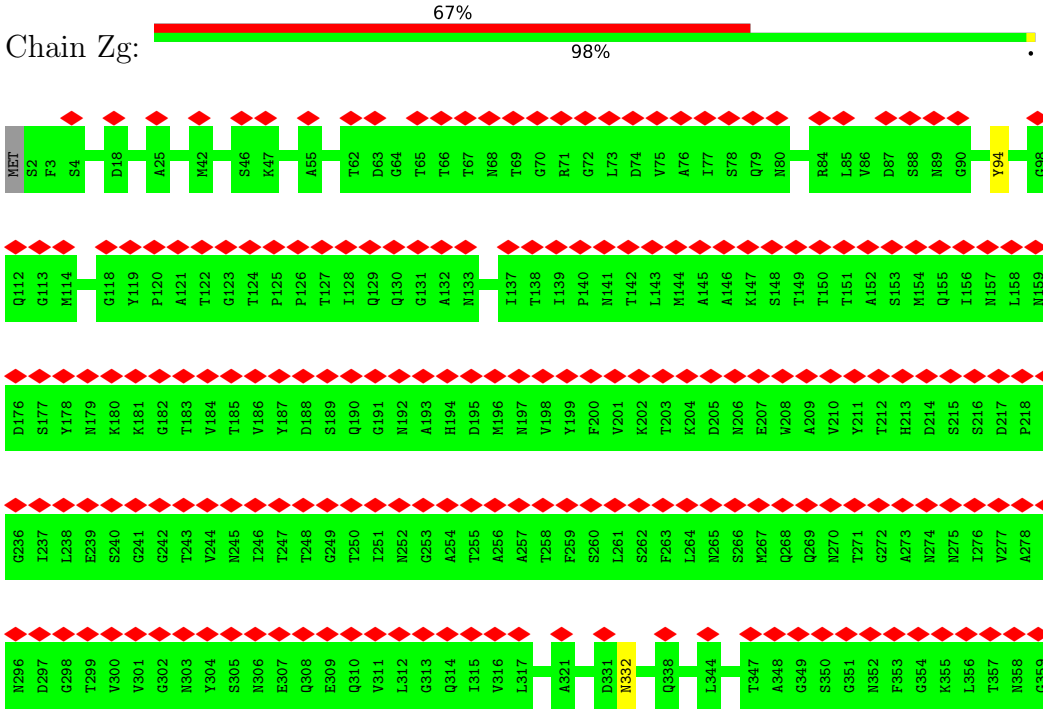






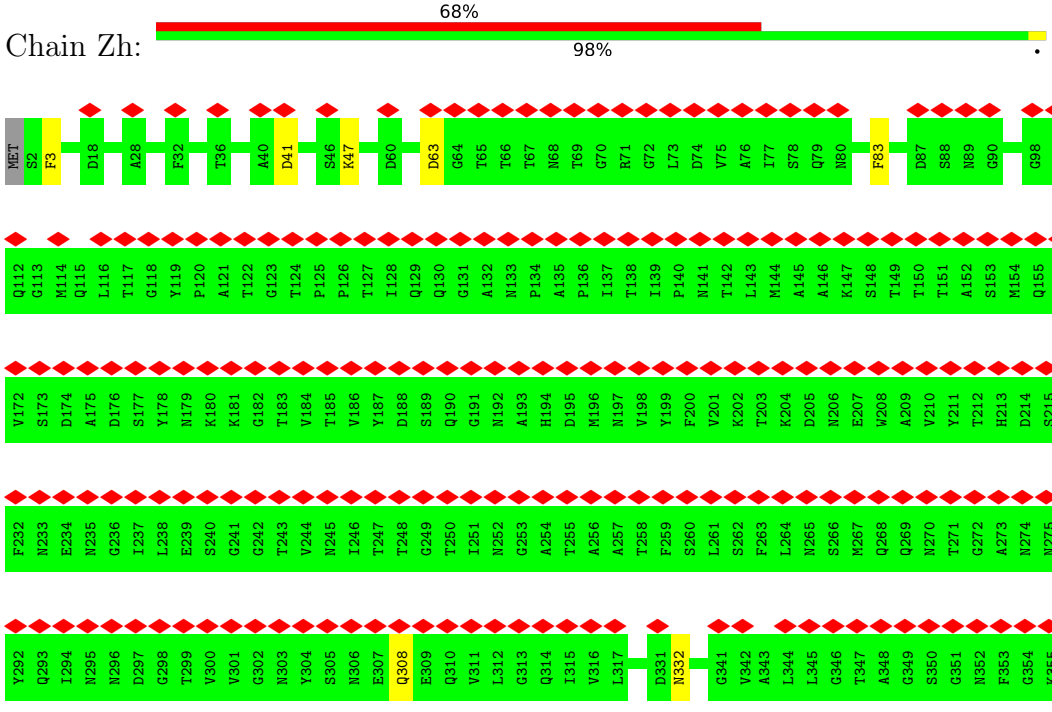
• Molecule 1: Flagellar hook protein FlgE

Chain Zg:



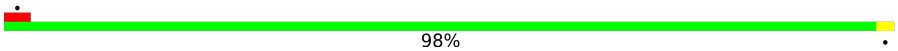
• Molecule 1: Flagellar hook protein FlgE

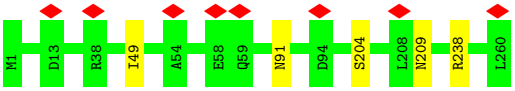
Chain Zh:



• Molecule 2: Flagellar basal-body rod protein FlgG

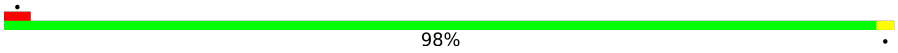
Chain 2:

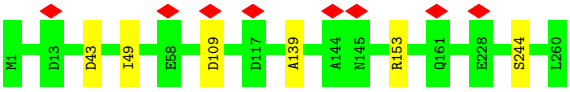




• Molecule 2: Flagellar basal-body rod protein FlgG

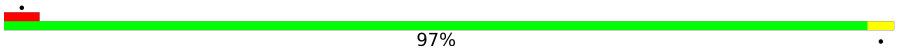
Chain 3:

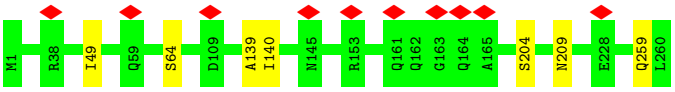




• Molecule 2: Flagellar basal-body rod protein FlgG

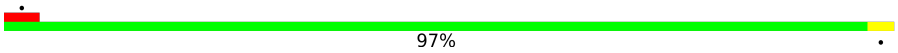
Chain 4:

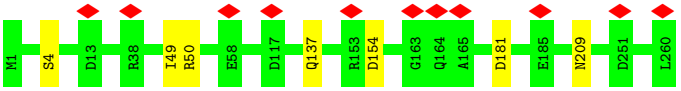




• Molecule 2: Flagellar basal-body rod protein FlgG

Chain 5:





• Molecule 2: Flagellar basal-body rod protein FlgG

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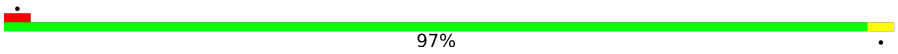
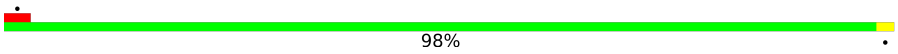
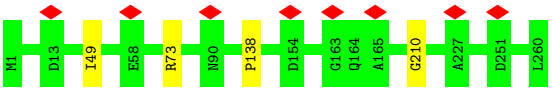


• Molecule 2: Flagellar basal-body rod protein FlgG

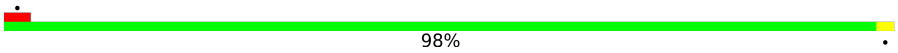
Chain 7:

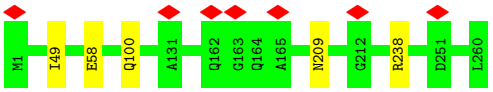




• Molecule 2: Flagellar basal-body rod protein FlgG

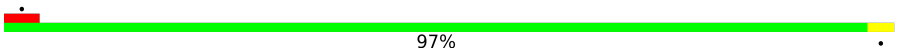
Chain 8:

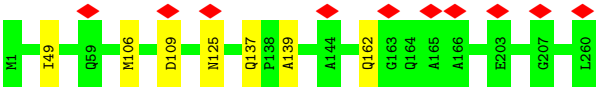




• Molecule 2: Flagellar basal-body rod protein FlgG

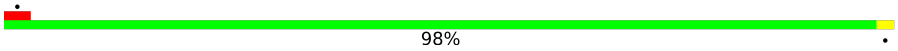
Chain 9:





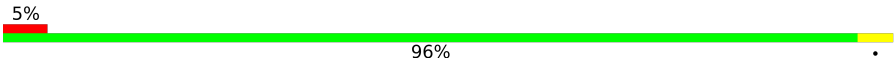
• Molecule 2: Flagellar basal-body rod protein FlgG

Chain ZA:



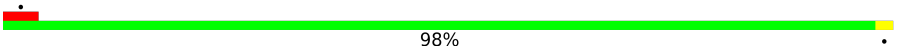
• Molecule 2: Flagellar basal-body rod protein FlgG

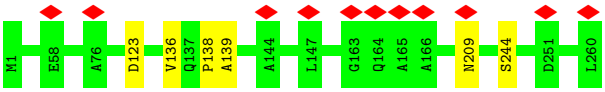
Chain ZB:



• Molecule 2: Flagellar basal-body rod protein FlgG

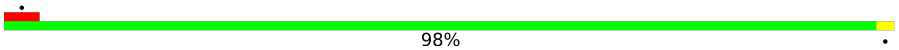
Chain ZC:

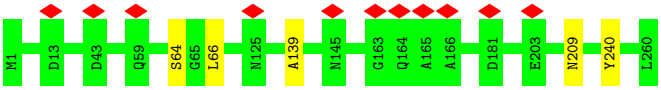




• Molecule 2: Flagellar basal-body rod protein FlgG

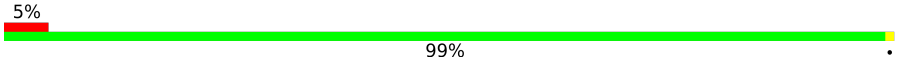
Chain ZD:

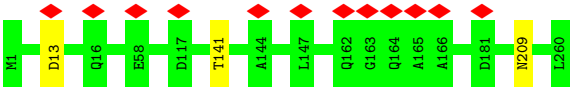




• Molecule 2: Flagellar basal-body rod protein FlgG

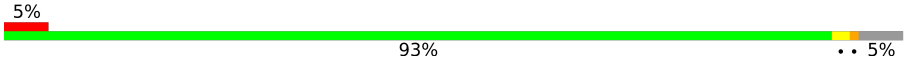
Chain ZE:

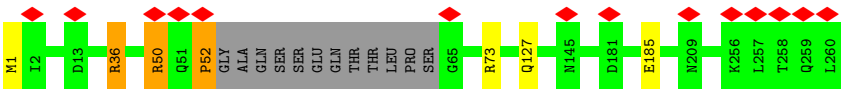




• Molecule 2: Flagellar basal-body rod protein FlgG

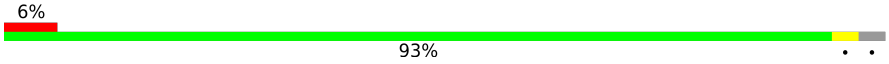
Chain 0:

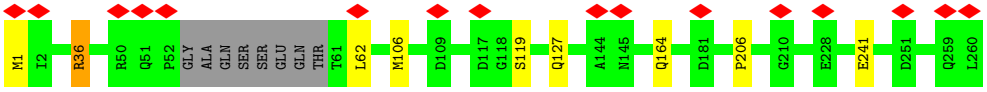




• Molecule 2: Flagellar basal-body rod protein FlgG

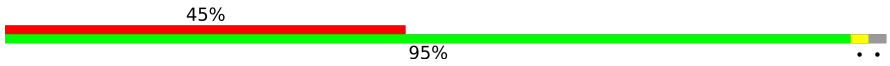
Chain 1:

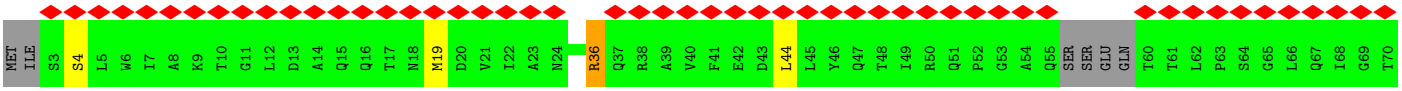


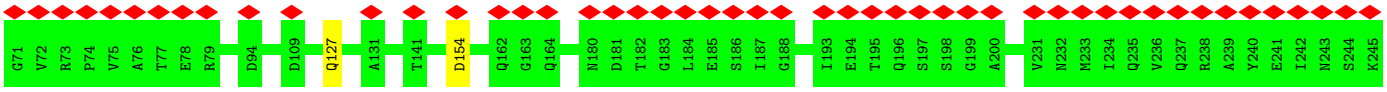


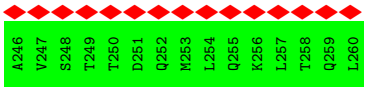
• Molecule 2: Flagellar basal-body rod protein FlgG

Chain r:



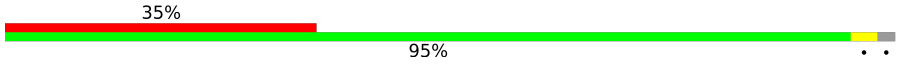


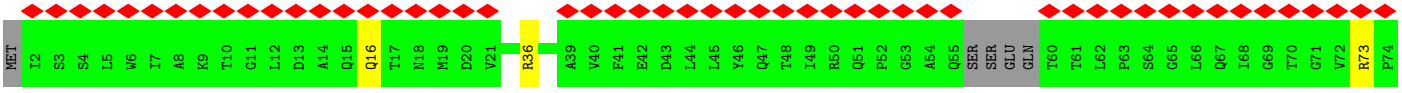


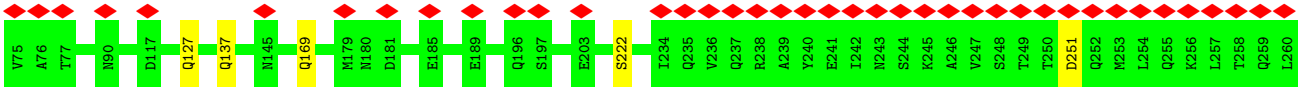


• Molecule 2: Flagellar basal-body rod protein FlgG

Chain s:







• Molecule 2: Flagellar basal-body rod protein FlgG

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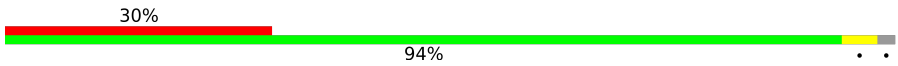

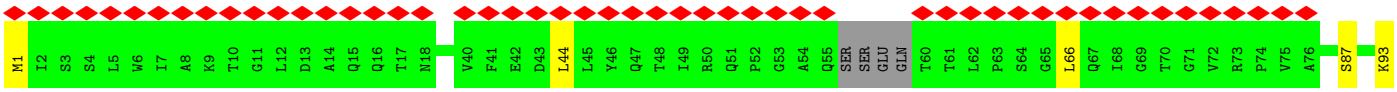

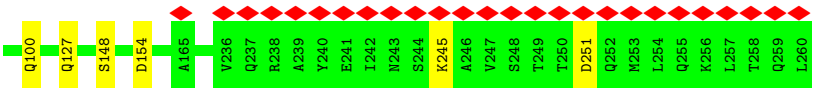

• Molecule 2: Flagellar basal-body rod protein FlgG

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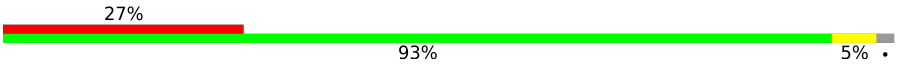
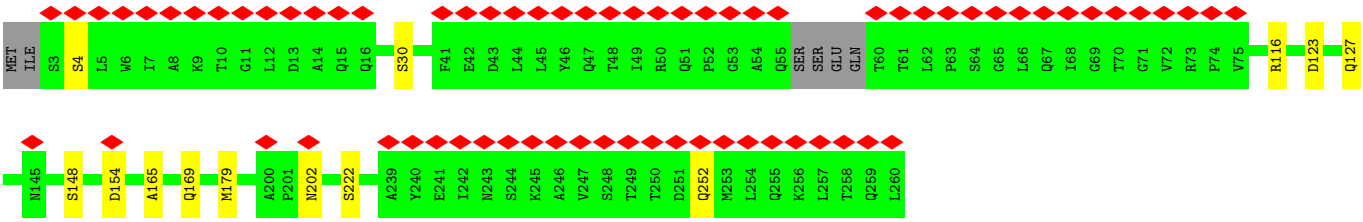
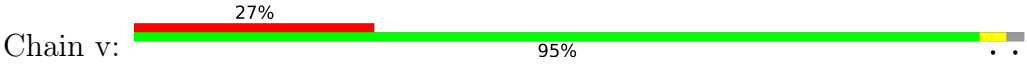
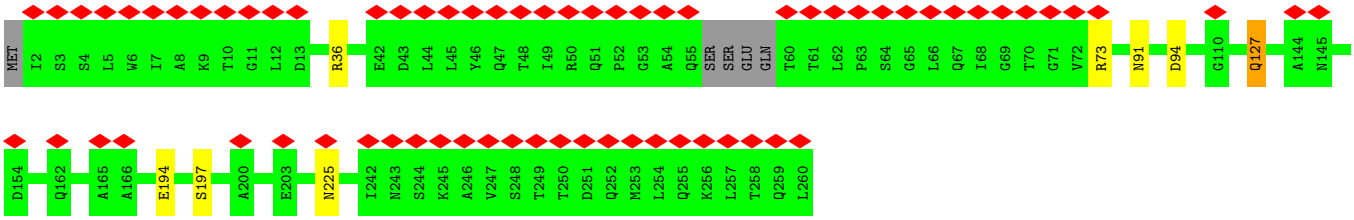


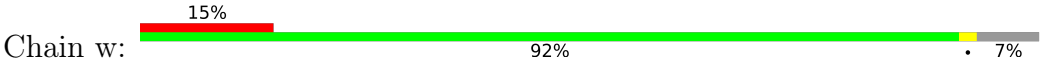


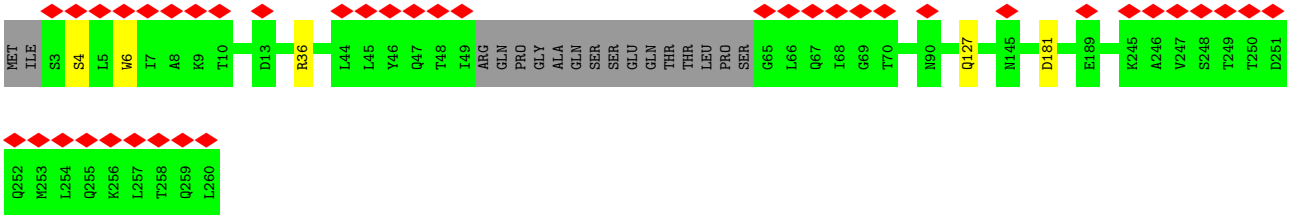
• Molecule 2: Flagellar basal-body rod protein FlgG



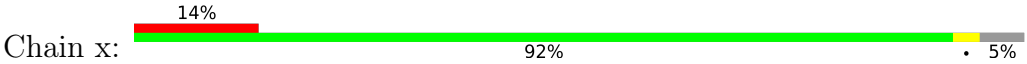


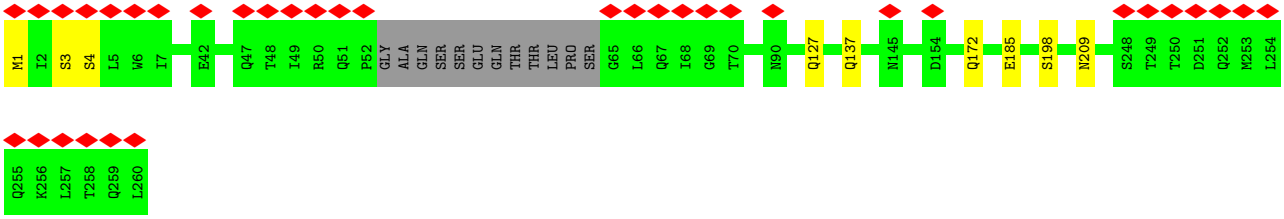
• Molecule 2: Flagellar basal-body rod protein FlgG



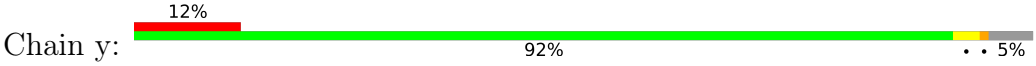


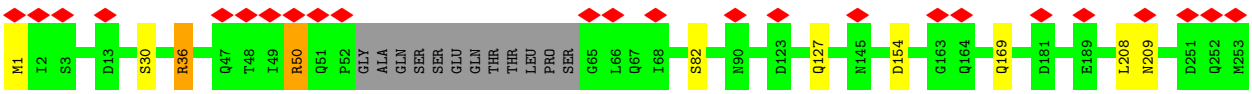
• Molecule 2: Flagellar basal-body rod protein FlgG

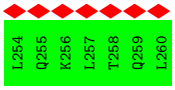




• Molecule 2: Flagellar basal-body rod protein FlgG

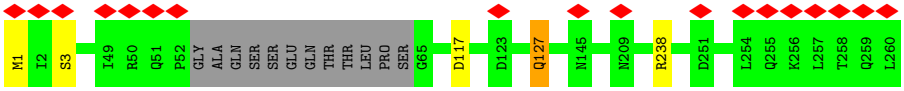






• Molecule 2: Flagellar basal-body rod protein FlgG

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.771	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

5.1 Standard geometry

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

All (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
1	ZR	125	PRO	CG-CD	-5.10	1.33	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	Zc	125	PRO	CA-N-CD	-11.21	95.80	111.50
1	ZV	140	PRO	CA-N-CD	-10.24	97.16	111.50
1	ZV	140	PRO	CA-CB-CG	-9.29	86.35	104.00
1	ZM	223	PRO	CA-N-CD	-8.43	99.70	111.50
1	ZR	125	PRO	N-CD-CG	-7.58	91.83	103.20
1	ZY	125	PRO	N-CD-CG	-7.47	92.00	103.20
2	u	154	ASP	CB-CG-OD2	6.25	123.93	118.30
1	ZR	214	ASP	CB-CG-OD1	6.02	123.72	118.30
1	Zc	125	PRO	N-CD-CG	-5.85	94.42	103.20
2	y	154	ASP	CB-CG-OD1	5.75	123.47	118.30
2	0	52	PRO	N-CA-CB	-5.72	96.31	102.60
1	ZS	18	ASP	CB-CG-OD1	5.67	123.40	118.30
1	ZV	125	PRO	CA-CB-CG	-5.66	93.25	104.00
1	ZP	125	PRO	CA-N-CD	-5.57	103.70	111.50
2	ZE	13	ASP	CB-CG-OD1	5.54	123.29	118.30
2	9	109	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0	36	ARG	Sidechain
2	0	50	ARG	Sidechain
2	1	36	ARG	Sidechain
2	5	50	ARG	Sidechain
2	6	153	ARG	Sidechain
2	8	238	ARG	Sidechain
2	ZA	79	ARG	Sidechain
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
1	Zb	106	ARG	Sidechain
1	Zd	380	ARG	Sidechain
1	Ze	380	ARG	Sidechain
2	r	36	ARG	Sidechain
2	u	116	ARG	Sidechain
2	y	36	ARG	Sidechain
2	y	50	ARG	Sidechain
2	z	238	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
2	ZB	164	GLN
2	ZC	139	ALA
1	ZI	375	MET
1	ZO	237	ILE
1	ZR	87	ASP
2	9	139	ALA
2	ZB	165	ALA
2	ZB	209	ASN

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Mol	Chain	Res	Type
2	ZC	209	ASN
2	ZD	209	ASN
2	ZE	209	ASN
2	u	165	ALA
2	x	4	SER
2	z	127	GLN
1	ZL	374	ASN
2	2	49	ILE
2	3	49	ILE
2	4	49	ILE
2	4	139	ALA
2	4	140	ILE
2	5	49	ILE
2	0	127	GLN
2	r	127	GLN
2	x	3	SER
2	y	127	GLN
1	ZO	142	THR
1	ZP	374	ASN
2	6	49	ILE
2	6	58	GLU
2	7	49	ILE
2	7	138	PRO
2	8	49	ILE
2	9	49	ILE
2	ZA	49	ILE
2	ZA	139	ALA
2	ZD	139	ALA
2	s	127	GLN
2	u	127	GLN
2	w	127	GLN
2	x	127	GLN
2	7	210	GLY
2	1	127	GLN
2	t	127	GLN
2	v	127	GLN
1	ZO	375	MET
2	3	139	ALA
1	ZI	325	GLY
2	ZC	138	PRO

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ZF	3	PHE

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Mol	Chain	Res	Type
1	ZF	60	ASP
1	ZF	87	ASP
1	ZF	134	PRO
1	ZF	229	THR
1	ZF	265	ASN
1	ZF	280	ASN
1	ZF	284	TYR
1	ZF	289	LEU
1	ZF	352	ASN
1	ZF	355	LYS
1	ZG	3	PHE
1	ZG	38	SER
1	ZG	188	ASP
1	ZG	189	SER
1	ZG	227	SER
1	ZG	234	GLU
1	ZG	260	SER
1	ZG	262	SER
1	ZG	265	ASN
1	ZG	267	MET
1	ZG	288	ASP
1	ZG	296	ASN
1	ZG	350	SER
1	ZG	352	ASN
1	ZG	397	ASN
1	ZH	34	SER
1	ZH	154	MET
1	ZH	227	SER
1	ZH	260	SER
1	ZH	281	GLN
1	ZH	284	TYR
1	ZH	288	ASP
1	ZH	331	ASP
1	ZH	355	LYS
1	ZH	375	MET
1	ZH	380	ARG
1	ZH	399	LEU
1	ZI	99	GLN
1	ZI	195	ASP
1	ZI	197	ASN
1	ZI	260	SER
1	ZI	352	ASN

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Mol	Chain	Res	Type
1	ZI	358	ASN
1	ZJ	42	MET
1	ZJ	46	SER
1	ZJ	103	ASP
1	ZJ	107	ASN
1	ZJ	195	ASP
1	ZJ	233	ASN
1	ZJ	280	ASN
1	ZJ	331	ASP
1	ZK	3	PHE
1	ZK	268	GLN
1	ZK	297	ASP
1	ZK	305	SER
1	ZK	331	ASP
1	ZK	338	GLN
1	ZL	78	SER
1	ZL	84	ARG
1	ZL	196	MET
1	ZL	234	GLU
1	ZL	267	MET
1	ZL	291	SER
1	ZL	338	GLN
1	ZL	368	LEU
1	ZL	370	LYS
1	ZL	382	TYR
1	ZM	53	LYS
1	ZM	89	ASN
1	ZM	153	SER
1	ZM	200	PHE
1	ZM	214	ASP
1	ZM	282	ASN
1	ZM	352	ASN
1	ZM	369	SER
1	ZM	370	LYS
1	ZN	43	PHE
1	ZN	78	SER
1	ZN	103	ASP
1	ZN	143	LEU
1	ZN	148	SER
1	ZN	157	ASN
1	ZN	216	SER
1	ZN	297	ASP

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Mol	Chain	Res	Type
1	ZN	367	ASP
1	ZN	396	LEU
1	ZO	2	SER
1	ZO	74	ASP
1	ZO	174	ASP
1	ZO	178	TYR
1	ZO	235	ASN
1	ZO	237	ILE
1	ZO	331	ASP
1	ZO	375	MET
1	ZP	42	MET
1	ZP	63	ASP
1	ZP	74	ASP
1	ZP	95	SER
1	ZP	126	PRO
1	ZP	162	ASP
1	ZP	227	SER
1	ZP	275	ASN
1	ZP	288	ASP
1	ZP	292	TYR
1	ZP	331	ASP
1	ZP	340	SER
1	ZP	369	SER
1	ZP	370	LYS
1	ZP	393	ASP
1	ZQ	46	SER
1	ZQ	101	LYS
1	ZQ	189	SER
1	ZQ	200	PHE
1	ZQ	211	TYR
1	ZQ	280	ASN
1	ZQ	305	SER
1	ZQ	367	ASP
1	ZQ	370	LYS
1	ZR	41	ASP
1	ZR	103	ASP
1	ZR	197	ASN
1	ZR	214	ASP
1	ZR	269	GLN
1	ZR	295	ASN
1	ZR	332	ASN
1	ZR	367	ASP

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Mol	Chain	Res	Type
1	ZS	78	SER
1	ZS	103	ASP
1	ZS	170	PHE
1	ZS	202	LYS
1	ZS	245	ASN
1	ZS	367	ASP
1	ZT	148	SER
1	ZT	195	ASP
1	ZT	262	SER
1	ZT	297	ASP
1	ZT	358	ASN
1	ZU	3	PHE
1	ZU	78	SER
1	ZU	80	ASN
1	ZU	340	SER
1	ZV	46	SER
1	ZV	232	PHE
1	ZV	307	GLU
1	ZV	308	GLN
1	ZW	3	PHE
1	ZW	53	LYS
1	ZW	188	ASP
1	ZW	195	ASP
1	ZW	215	SER
1	ZW	259	PHE
1	ZW	292	TYR
1	ZW	309	GLU
1	ZW	326	LEU
1	ZW	331	ASP
1	ZW	340	SER
1	ZW	358	ASN
1	ZX	3	PHE
1	ZX	63	ASP
1	ZX	195	ASP
1	ZY	60	ASP
1	ZY	80	ASN
1	ZY	192	ASN
1	ZY	204	LYS
1	ZY	252	ASN
1	ZY	332	ASN
1	ZY	350	SER
1	ZZ	3	PHE

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Mol	Chain	Res	Type
1	ZZ	41	ASP
1	ZZ	88	SER
1	ZZ	148	SER
1	ZZ	393	ASP
1	Za	103	ASP
1	Za	292	TYR
1	Za	331	ASP
1	Za	332	ASN
1	Za	375	MET
1	Zb	41	ASP
1	Zb	292	TYR
1	Zb	308	GLN
1	Zb	355	LYS
1	Zb	367	ASP
1	Zb	393	ASP
1	Zc	41	ASP
1	Zc	103	ASP
1	Zc	204	LYS
1	Zc	267	MET
1	Zc	296	ASN
1	Zc	297	ASP
1	Zc	317	LEU
1	Zc	332	ASN
1	Zc	340	SER
1	Zc	369	SER
1	Zc	399	LEU
1	Zd	41	ASP
1	Zd	114	MET
1	Zd	140	PRO
1	Zd	375	MET
1	Zd	393	ASP
1	Zd	397	ASN
1	Ze	3	PHE
1	Ze	27	SER
1	Ze	46	SER
1	Ze	58	THR
1	Ze	60	ASP
1	Ze	130	GLN
1	Ze	308	GLN
1	Ze	319	ASN
1	Ze	395	ILE
1	Zf	3	PHE

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Mol	Chain	Res	Type
1	Zf	285	LYS
1	Zf	297	ASP
1	Zf	331	ASP
1	Zf	332	ASN
1	Zf	367	ASP
1	Zf	396	LEU
1	Zg	94	TYR
1	Zg	103	ASP
1	Zg	292	TYR
1	Zg	332	ASN
1	Zg	367	ASP
1	Zg	370	LYS
1	Zh	3	PHE
1	Zh	41	ASP
1	Zh	47	LYS
1	Zh	63	ASP
1	Zh	83	PHE
1	Zh	162	ASP
1	Zh	308	GLN
1	Zh	332	ASN
2	2	91	ASN
2	2	204	SER
2	2	238	ARG
2	3	43	ASP
2	3	109	ASP
2	3	153	ARG
2	3	244	SER
2	4	64	SER
2	4	204	SER
2	4	209	ASN
2	4	259	GLN
2	5	4	SER
2	5	137	GLN
2	5	154	ASP
2	5	181	ASP
2	6	59	GLN
2	6	73	ARG
2	6	78	GLU
2	6	109	ASP
2	6	244	SER
2	7	73	ARG
2	8	58	GLU

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Mol	Chain	Res	Type
2	8	100	GLN
2	9	106	MET
2	9	125	ASN
2	9	137	GLN
2	9	162	GLN
2	ZA	136	VAL
2	ZA	248	SER
2	ZB	1	MET
2	ZB	4	SER
2	ZB	58	GLU
2	ZB	73	ARG
2	ZB	119	SER
2	ZB	137	GLN
2	ZB	143	PRO
2	ZB	244	SER
2	ZC	123	ASP
2	ZC	136	VAL
2	ZC	244	SER
2	ZD	64	SER
2	ZD	66	LEU
2	ZD	240	TYR
2	ZE	141	THR
2	0	1	MET
2	0	36	ARG
2	0	50	ARG
2	0	52	PRO
2	0	73	ARG
2	0	185	GLU
2	1	1	MET
2	1	36	ARG
2	1	62	LEU
2	1	106	MET
2	1	119	SER
2	1	164	GLN
2	1	206	PRO
2	1	241	GLU
2	r	4	SER
2	r	19	MET
2	r	36	ARG
2	r	44	LEU
2	r	154	ASP
2	s	16	GLN

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Mol	Chain	Res	Type
2	s	36	ARG
2	s	73	ARG
2	s	137	GLN
2	s	169	GLN
2	s	222	SER
2	s	251	ASP
2	t	1	MET
2	t	44	LEU
2	t	66	LEU
2	t	87	SER
2	t	93	LYS
2	t	100	GLN
2	t	148	SER
2	t	154	ASP
2	t	245	LYS
2	t	251	ASP
2	u	4	SER
2	u	30	SER
2	u	123	ASP
2	u	148	SER
2	u	169	GLN
2	u	179	MET
2	u	202	ASN
2	u	222	SER
2	u	252	GLN
2	v	36	ARG
2	v	73	ARG
2	v	91	ASN
2	v	94	ASP
2	v	127	GLN
2	v	194	GLU
2	v	197	SER
2	v	225	ASN
2	w	4	SER
2	w	6	TRP
2	w	36	ARG
2	w	181	ASP
2	x	1	MET
2	x	137	GLN
2	x	172	GLN
2	x	185	GLU
2	x	198	SER

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Mol	Chain	Res	Type
2	x	209	ASN
2	y	1	MET
2	y	30	SER
2	y	36	ARG
2	y	50	ARG
2	y	82	SER
2	y	169	GLN
2	y	208	LEU
2	y	209	ASN
2	z	1	MET
2	z	3	SER
2	z	117	ASP
2	z	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (370) such sidechains are listed below:

Mol	Chain	Res	Type
1	ZF	5	GLN
1	ZF	16	ASN
1	ZF	107	ASN
1	ZF	155	GLN
1	ZF	197	ASN
1	ZF	358	ASN
1	ZF	385	ASN
1	ZF	401	ASN
1	ZG	89	ASN
1	ZG	130	GLN
1	ZG	133	ASN
1	ZG	332	ASN
1	ZG	387	GLN
1	ZG	397	ASN
1	ZG	401	ASN
1	ZH	5	GLN
1	ZH	155	GLN
1	ZH	206	ASN
1	ZH	270	ASN
1	ZH	296	ASN
1	ZH	352	ASN
1	ZH	365	ASN
1	ZH	379	GLN
1	ZH	392	GLN
1	ZI	197	ASN

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Mol	Chain	Res	Type
1	ZI	269	GLN
1	ZI	323	ASN
1	ZI	385	ASN
1	ZI	387	GLN
1	ZI	392	GLN
1	ZI	394	GLN
1	ZI	401	ASN
1	ZJ	89	ASN
1	ZJ	107	ASN
1	ZJ	133	ASN
1	ZJ	159	ASN
1	ZJ	197	ASN
1	ZJ	265	ASN
1	ZJ	274	ASN
1	ZJ	282	ASN
1	ZJ	379	GLN
1	ZJ	392	GLN
1	ZJ	397	ASN
1	ZJ	401	ASN
1	ZK	107	ASN
1	ZK	197	ASN
1	ZK	252	ASN
1	ZK	303	ASN
1	ZK	319	ASN
1	ZK	392	GLN
1	ZK	401	ASN
1	ZL	5	GLN
1	ZL	79	GLN
1	ZL	89	ASN
1	ZL	179	ASN
1	ZL	190	GLN
1	ZL	197	ASN
1	ZL	269	GLN
1	ZL	282	ASN
1	ZL	310	GLN
1	ZL	338	GLN
1	ZL	401	ASN
1	ZM	5	GLN
1	ZM	59	GLN
1	ZM	89	ASN
1	ZM	197	ASN
1	ZM	213	HIS

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Mol	Chain	Res	Type
1	ZM	235	ASN
1	ZM	252	ASN
1	ZM	381	ASN
1	ZN	79	GLN
1	ZN	107	ASN
1	ZN	112	GLN
1	ZN	129	GLN
1	ZN	133	ASN
1	ZN	190	GLN
1	ZN	192	ASN
1	ZN	197	ASN
1	ZN	319	ASN
1	ZN	338	GLN
1	ZN	379	GLN
1	ZN	387	GLN
1	ZN	401	ASN
1	ZO	89	ASN
1	ZO	141	ASN
1	ZO	192	ASN
1	ZO	235	ASN
1	ZO	332	ASN
1	ZP	11	ASN
1	ZP	107	ASN
1	ZP	129	GLN
1	ZP	194	HIS
1	ZP	269	GLN
1	ZP	270	ASN
1	ZP	314	GLN
1	ZP	322	ASN
1	ZP	338	GLN
1	ZP	379	GLN
1	ZP	381	ASN
1	ZP	385	ASN
1	ZQ	89	ASN
1	ZQ	97	ASN
1	ZQ	133	ASN
1	ZQ	141	ASN
1	ZQ	155	GLN
1	ZQ	197	ASN
1	ZQ	233	ASN
1	ZQ	338	GLN
1	ZQ	387	GLN

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Mol	Chain	Res	Type
1	ZR	107	ASN
1	ZR	133	ASN
1	ZR	268	GLN
1	ZR	269	GLN
1	ZR	293	GLN
1	ZR	295	ASN
1	ZR	401	ASN
1	ZS	133	ASN
1	ZS	197	ASN
1	ZS	394	GLN
1	ZT	5	GLN
1	ZT	99	GLN
1	ZT	129	GLN
1	ZT	133	ASN
1	ZT	197	ASN
1	ZT	213	HIS
1	ZT	235	ASN
1	ZT	275	ASN
1	ZT	293	GLN
1	ZT	314	GLN
1	ZT	352	ASN
1	ZT	392	GLN
1	ZU	99	GLN
1	ZU	107	ASN
1	ZU	133	ASN
1	ZU	159	ASN
1	ZU	206	ASN
1	ZU	293	GLN
1	ZU	332	ASN
1	ZU	379	GLN
1	ZU	387	GLN
1	ZV	107	ASN
1	ZV	133	ASN
1	ZV	197	ASN
1	ZV	280	ASN
1	ZV	303	ASN
1	ZV	314	GLN
1	ZV	394	GLN
1	ZV	397	ASN
1	ZV	401	ASN
1	ZW	5	GLN
1	ZW	26	ASN

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Mol	Chain	Res	Type
1	ZW	107	ASN
1	ZW	129	GLN
1	ZW	133	ASN
1	ZW	155	GLN
1	ZW	197	ASN
1	ZW	252	ASN
1	ZW	310	GLN
1	ZW	314	GLN
1	ZW	332	ASN
1	ZX	80	ASN
1	ZX	133	ASN
1	ZX	159	ASN
1	ZX	314	GLN
1	ZX	352	ASN
1	ZY	5	GLN
1	ZY	115	GLN
1	ZY	159	ASN
1	ZY	197	ASN
1	ZY	268	GLN
1	ZY	392	GLN
1	ZZ	5	GLN
1	ZZ	99	GLN
1	ZZ	107	ASN
1	ZZ	133	ASN
1	ZZ	194	HIS
1	ZZ	197	ASN
1	ZZ	314	GLN
1	ZZ	332	ASN
1	ZZ	379	GLN
1	ZZ	394	GLN
1	ZZ	401	ASN
1	Za	115	GLN
1	Za	129	GLN
1	Za	133	ASN
1	Za	197	ASN
1	Za	387	GLN
1	Zb	5	GLN
1	Zb	79	GLN
1	Zb	107	ASN
1	Zb	129	GLN
1	Zb	133	ASN
1	Zb	197	ASN

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Mol	Chain	Res	Type
1	Zb	293	GLN
1	Zb	308	GLN
1	Zb	332	ASN
1	Zb	358	ASN
1	Zb	387	GLN
1	Zc	5	GLN
1	Zc	107	ASN
1	Zc	129	GLN
1	Zc	159	ASN
1	Zc	197	ASN
1	Zc	352	ASN
1	Zc	379	GLN
1	Zc	387	GLN
1	Zc	397	ASN
1	Zd	5	GLN
1	Zd	105	ASN
1	Zd	129	GLN
1	Zd	130	GLN
1	Zd	133	ASN
1	Zd	293	GLN
1	Zd	295	ASN
1	Zd	397	ASN
1	Ze	5	GLN
1	Ze	99	GLN
1	Ze	107	ASN
1	Ze	133	ASN
1	Ze	197	ASN
1	Ze	394	GLN
1	Zf	105	ASN
1	Zf	159	ASN
1	Zf	197	ASN
1	Zf	314	GLN
1	Zg	5	GLN
1	Zg	107	ASN
1	Zg	129	GLN
1	Zg	133	ASN
1	Zg	197	ASN
1	Zg	310	GLN
1	Zh	5	GLN
1	Zh	115	GLN
1	Zh	197	ASN
1	Zh	379	GLN

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Mol	Chain	Res	Type
1	Zh	392	GLN
2	2	164	GLN
2	2	180	ASN
2	2	255	GLN
2	3	24	ASN
2	3	67	GLN
2	3	161	GLN
2	3	190	ASN
2	3	255	GLN
2	4	37	GLN
2	4	47	GLN
2	4	125	ASN
2	4	127	GLN
2	4	174	ASN
2	4	216	GLN
2	4	235	GLN
2	4	243	ASN
2	4	259	GLN
2	5	55	GLN
2	5	85	ASN
2	5	100	GLN
2	5	121	GLN
2	5	237	GLN
2	5	252	GLN
2	6	16	GLN
2	6	59	GLN
2	6	91	ASN
2	6	121	GLN
2	6	127	GLN
2	6	135	GLN
2	6	209	ASN
2	6	237	GLN
2	7	24	ASN
2	7	55	GLN
2	7	164	GLN
2	7	235	GLN
2	8	83	GLN
2	8	91	ASN
2	8	196	GLN
2	9	37	GLN
2	9	55	GLN
2	9	85	ASN

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Mol	Chain	Res	Type
2	9	91	ASN
2	9	259	GLN
2	ZA	37	GLN
2	ZA	235	GLN
2	ZB	24	ASN
2	ZB	25	ASN
2	ZB	28	ASN
2	ZB	37	GLN
2	ZB	137	GLN
2	ZB	235	GLN
2	ZC	16	GLN
2	ZC	88	GLN
2	ZC	100	GLN
2	ZC	190	ASN
2	ZD	24	ASN
2	ZD	67	GLN
2	ZD	88	GLN
2	ZD	91	ASN
2	ZD	127	GLN
2	ZD	135	GLN
2	ZD	161	GLN
2	ZD	235	GLN
2	ZE	37	GLN
2	ZE	67	GLN
2	ZE	121	GLN
2	ZE	252	GLN
2	0	88	GLN
2	0	100	GLN
2	0	135	GLN
2	0	137	GLN
2	0	180	ASN
2	0	235	GLN
2	0	237	GLN
2	0	255	GLN
2	1	47	GLN
2	1	67	GLN
2	1	91	ASN
2	1	121	GLN
2	1	135	GLN
2	1	223	ASN
2	1	252	GLN
2	r	83	GLN

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Mol	Chain	Res	Type
2	r	85	ASN
2	r	121	GLN
2	r	135	GLN
2	r	172	GLN
2	r	174	ASN
2	r	223	ASN
2	s	16	GLN
2	s	28	ASN
2	s	169	GLN
2	s	223	ASN
2	s	259	GLN
2	t	85	ASN
2	t	104	GLN
2	t	127	GLN
2	t	162	GLN
2	t	259	GLN
2	u	16	GLN
2	u	32	ASN
2	u	196	GLN
2	v	90	ASN
2	v	161	GLN
2	v	164	GLN
2	v	169	GLN
2	v	172	GLN
2	v	223	ASN
2	v	232	ASN
2	w	28	ASN
2	w	121	GLN
2	w	135	GLN
2	w	196	GLN
2	w	223	ASN
2	w	235	GLN
2	x	32	ASN
2	x	104	GLN
2	x	121	GLN
2	x	127	GLN
2	x	145	ASN
2	x	209	ASN
2	y	25	ASN
2	y	37	GLN
2	y	51	GLN
2	y	67	GLN

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Mol	Chain	Res	Type
2	y	125	ASN
2	y	127	GLN
2	y	209	ASN
2	y	223	ASN
2	y	252	GLN
2	z	67	GLN
2	z	85	ASN
2	z	125	ASN
2	z	235	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.

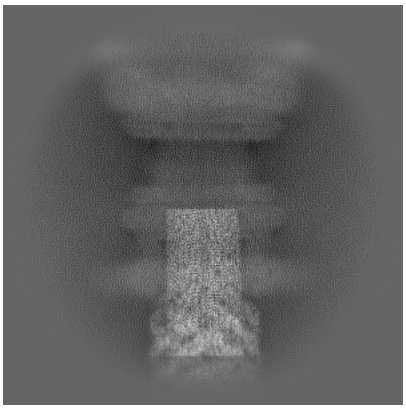
6 Map visualisation

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.

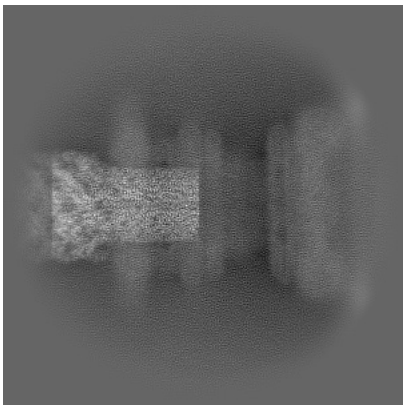
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

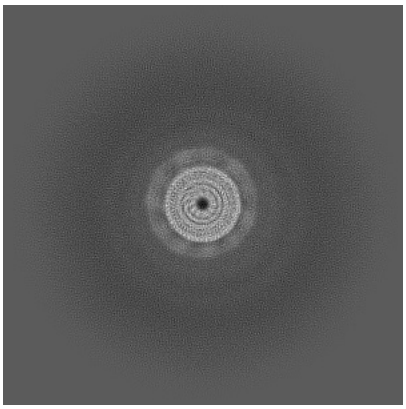
6.1.1 Primary map



X

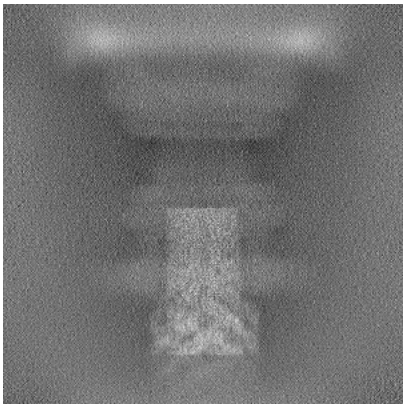


Y

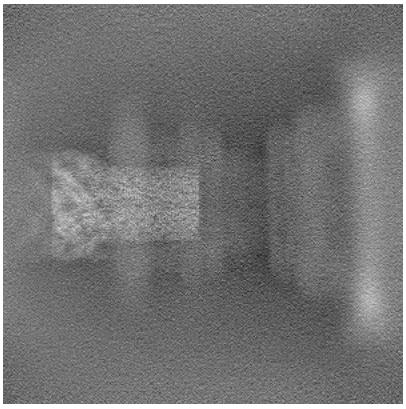


Z

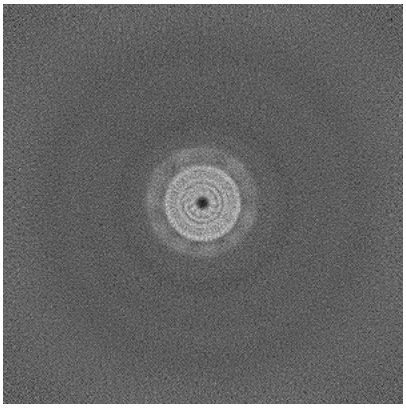
6.1.2 Raw map



X



Y

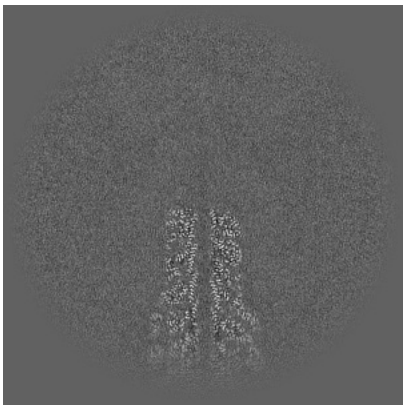


Z

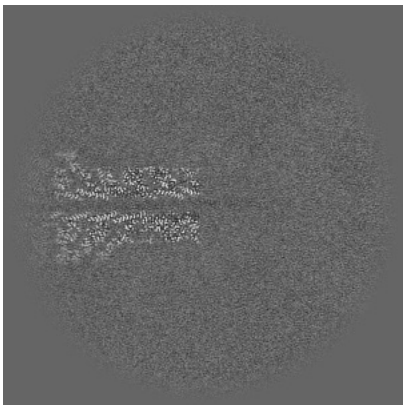
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

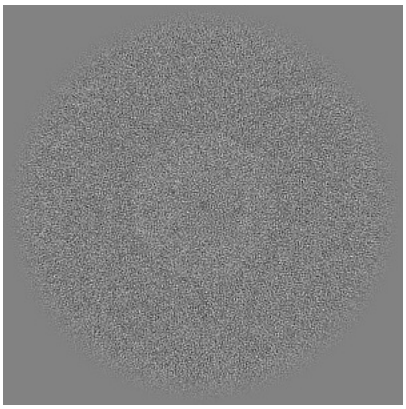
6.2.1 Primary map



X Index: 256

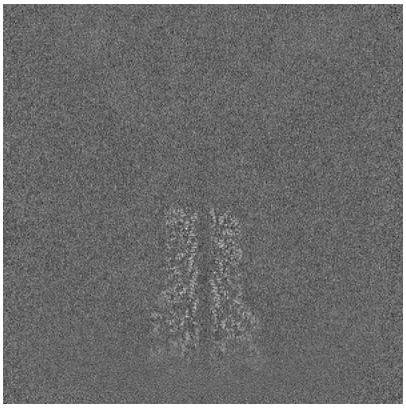


Y Index: 256

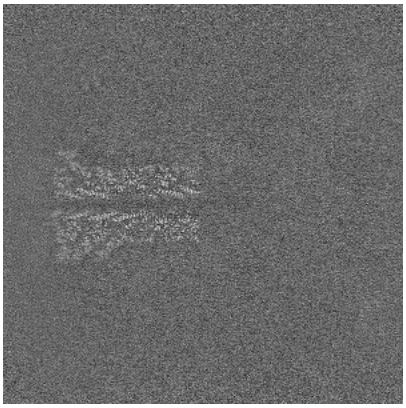


Z Index: 256

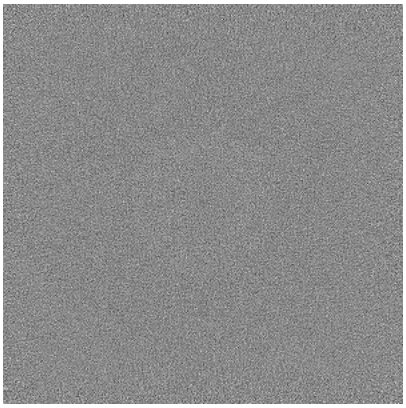
6.2.2 Raw map



X Index: 256



Y Index: 256

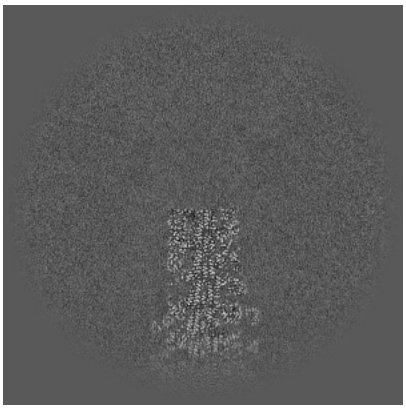


Z Index: 256

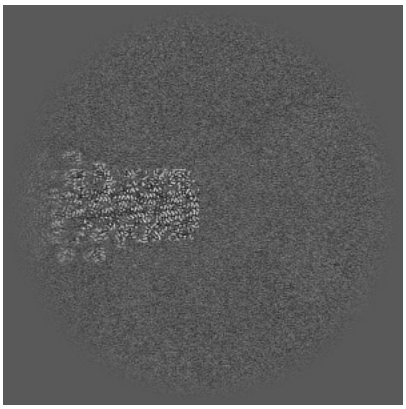
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

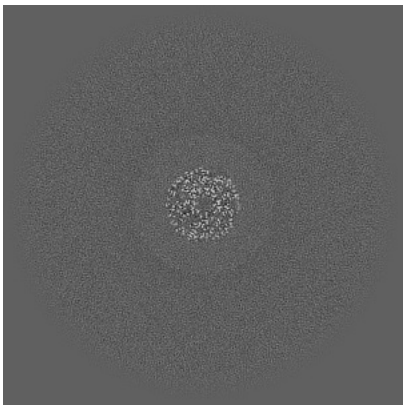
6.3.1 Primary map



X Index: 242

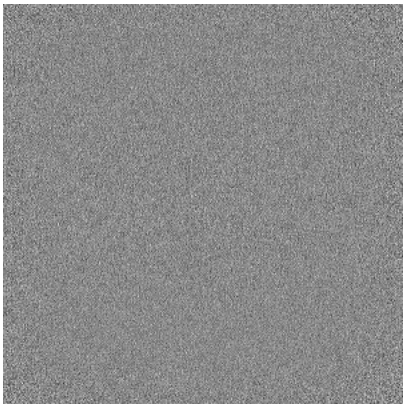


Y Index: 268

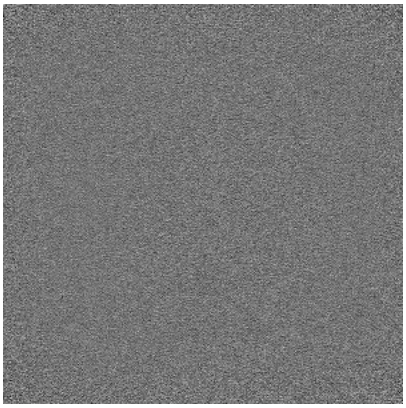


Z Index: 218

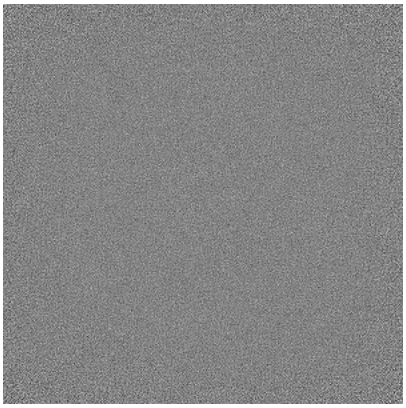
6.3.2 Raw map



X Index: 0



Y Index: 0

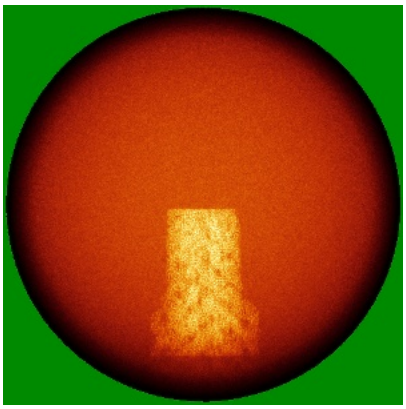


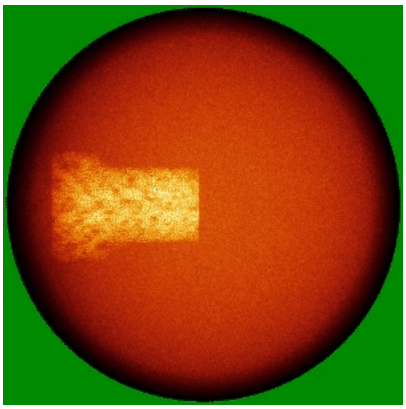
Z Index: 0

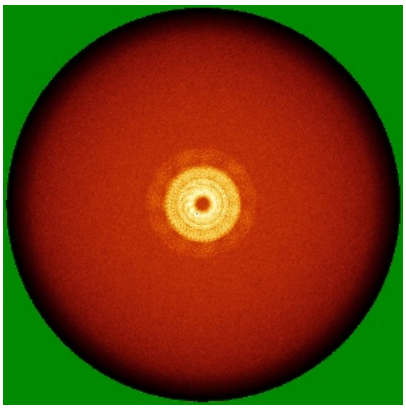
The images above show the largest variance slices of the map in three orthogonal directions.

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

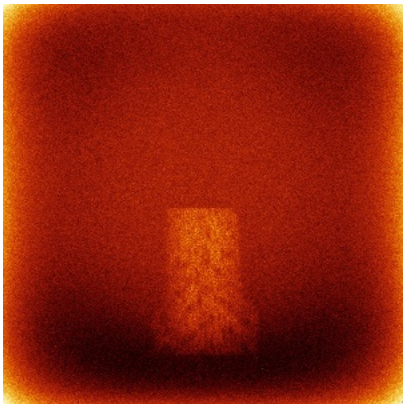
6.4.1 Primary map

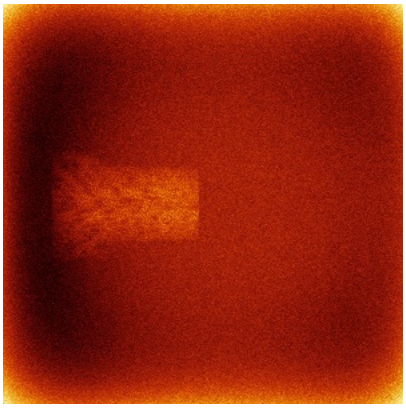

X

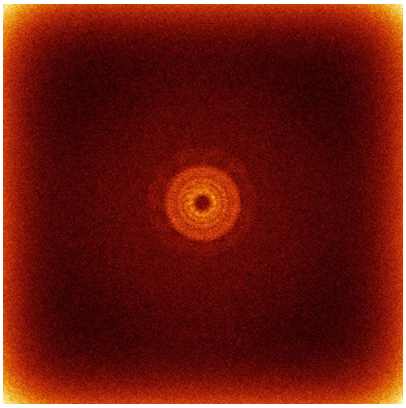

Y


Z

6.4.2 Raw map


X


Y


Z

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

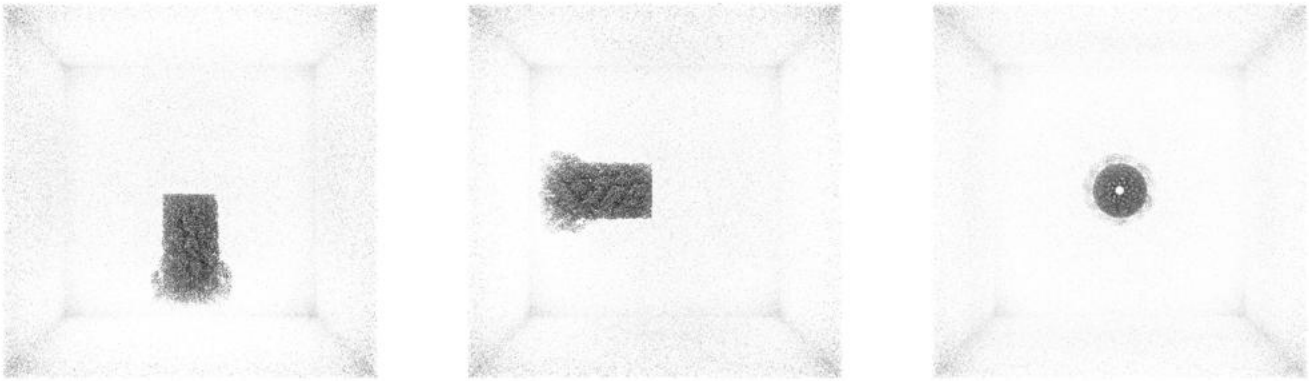
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map



X Y Z

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

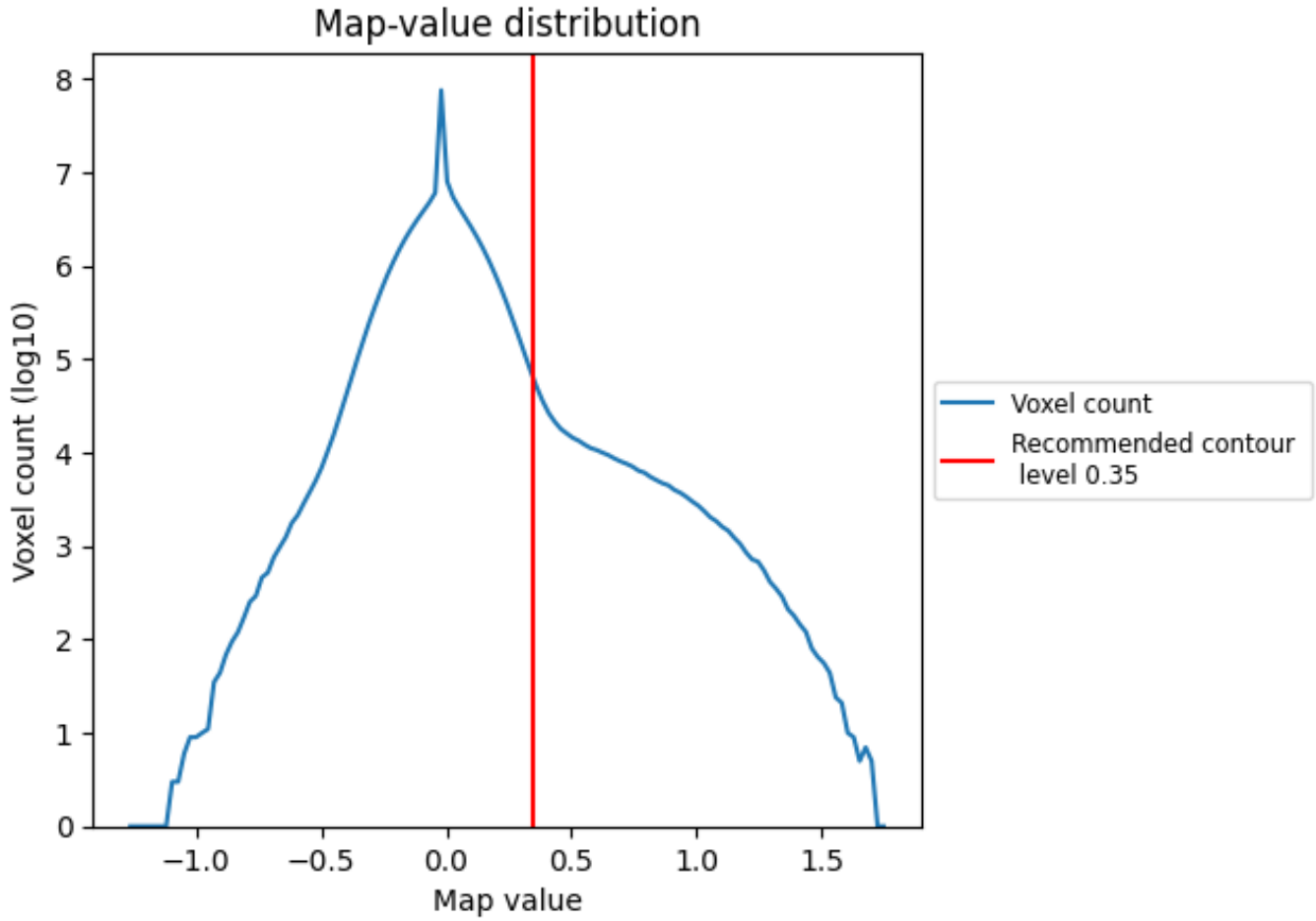
6.6 Mask visualisation (i)

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

7 Map analysis

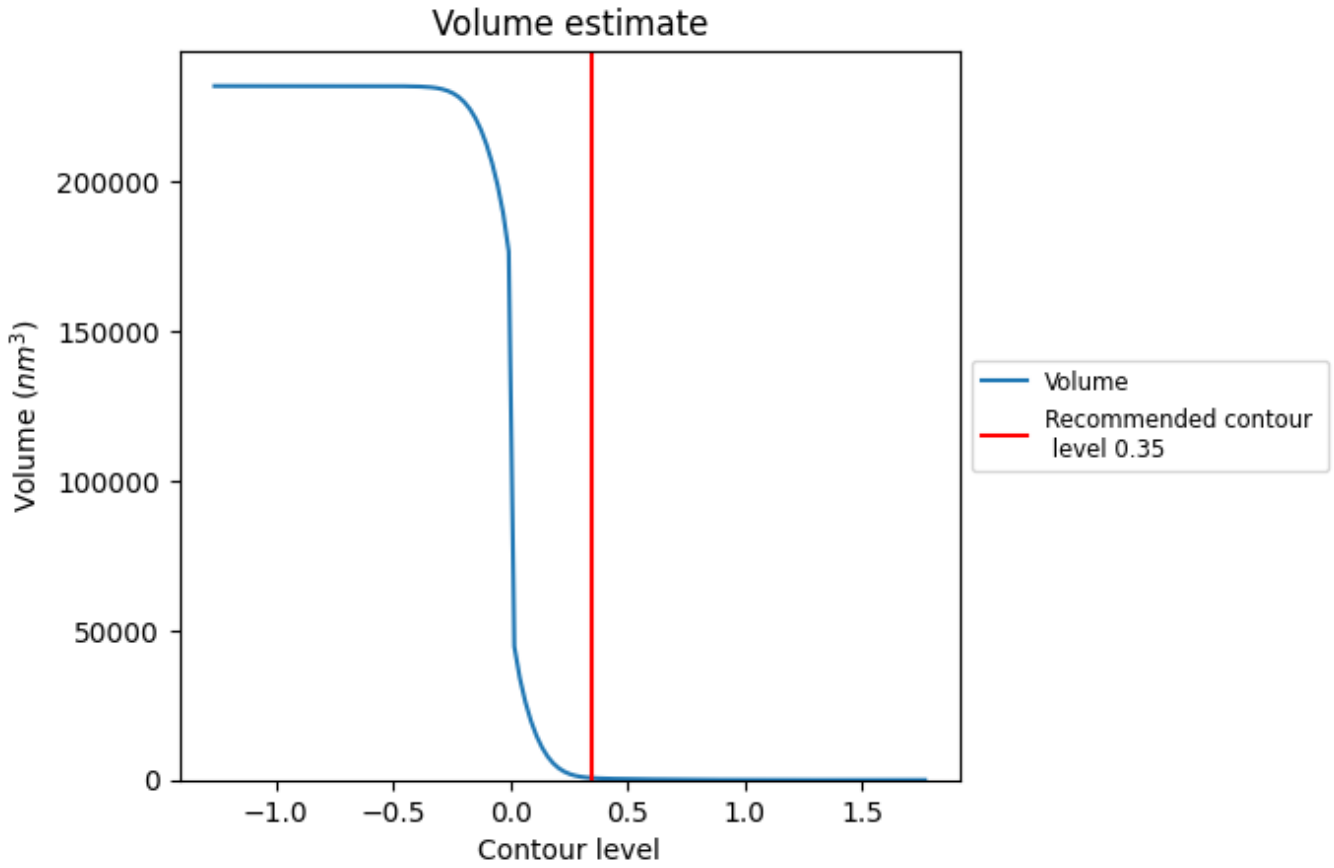
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

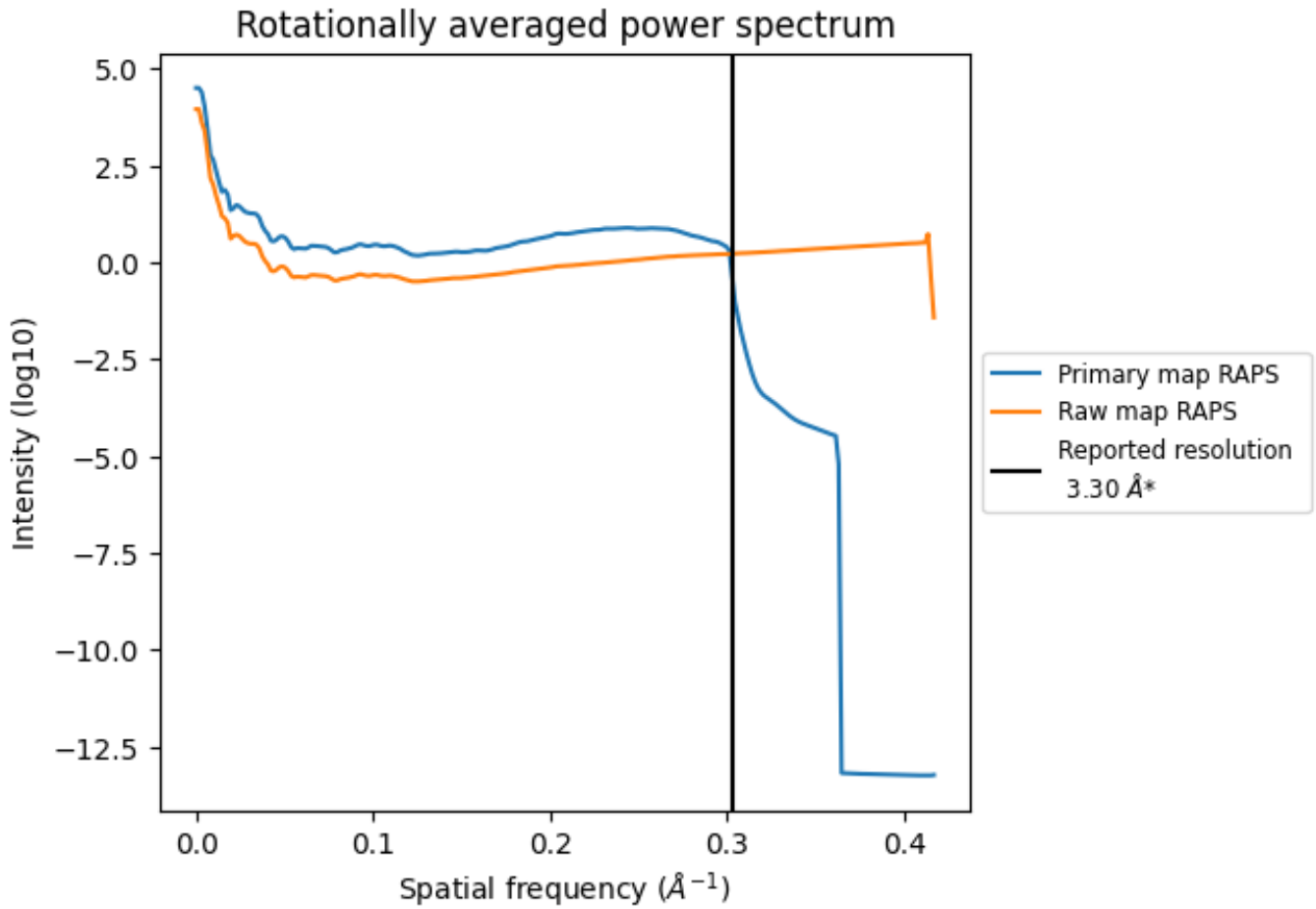
7.2 Volume estimate



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)

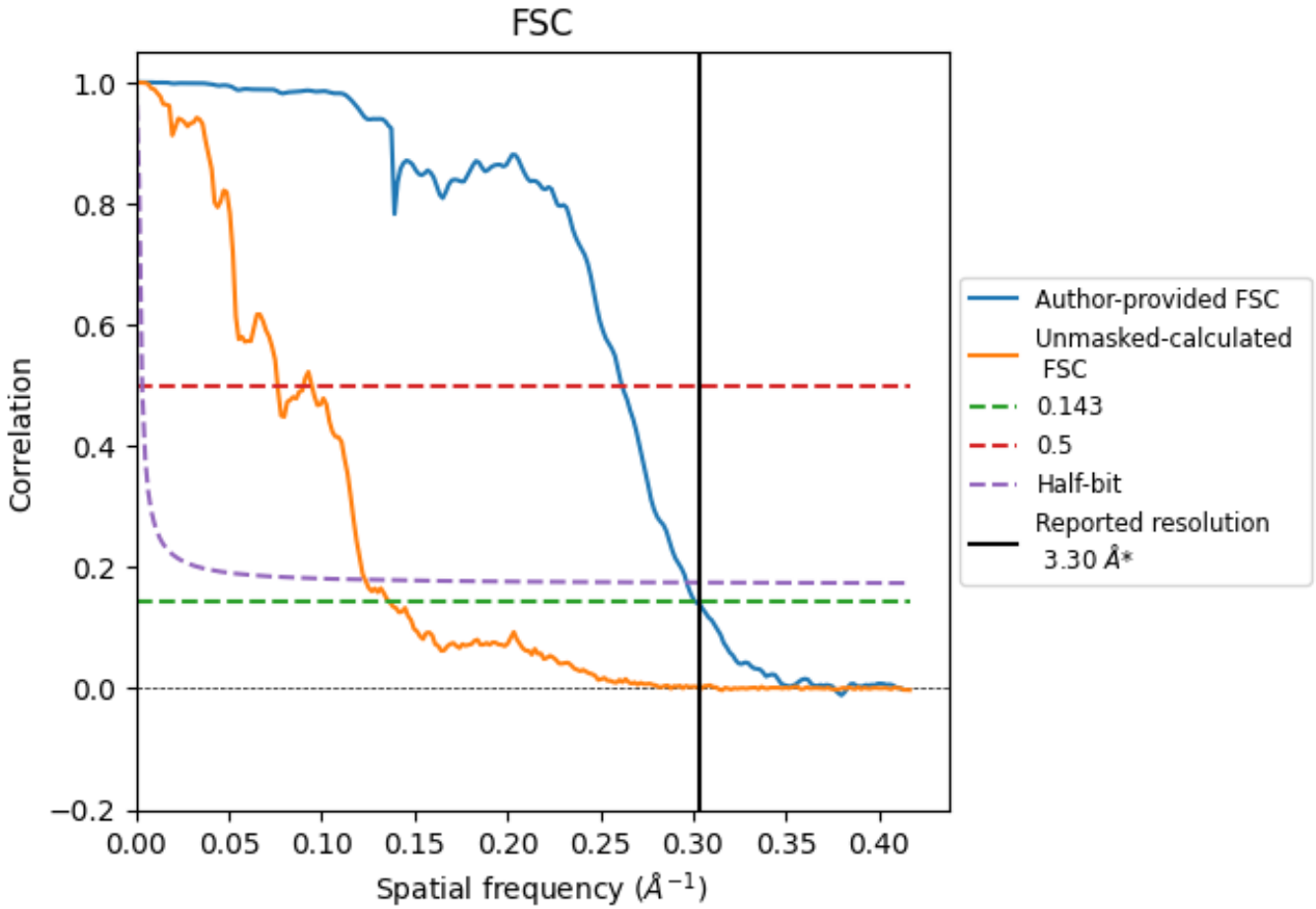


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

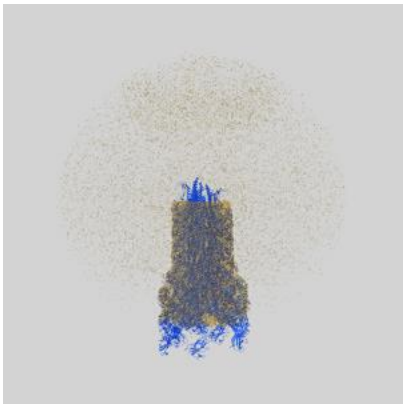
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.82	3.37
Unmasked-calculated*	7.32	13.12	8.10

*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 %

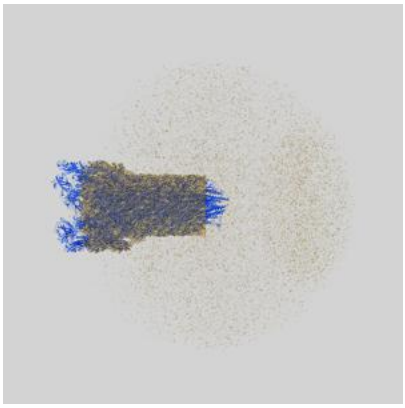
9 Map-model fit

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.

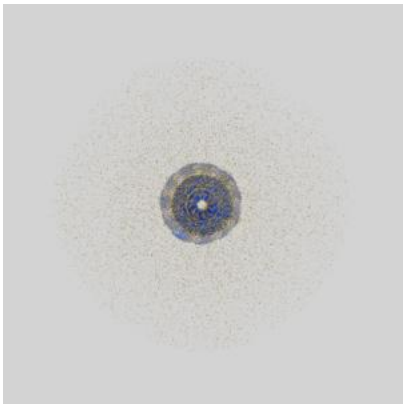
9.1 Map-model overlay



X



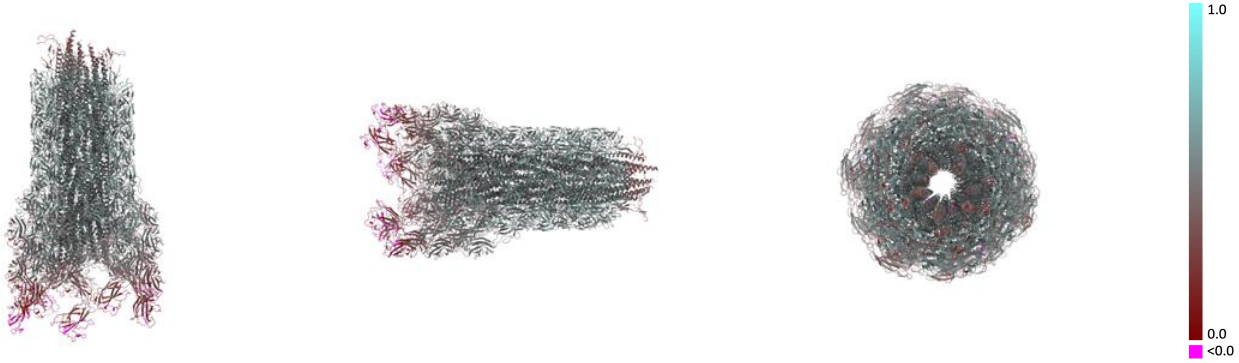
Y



Z

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

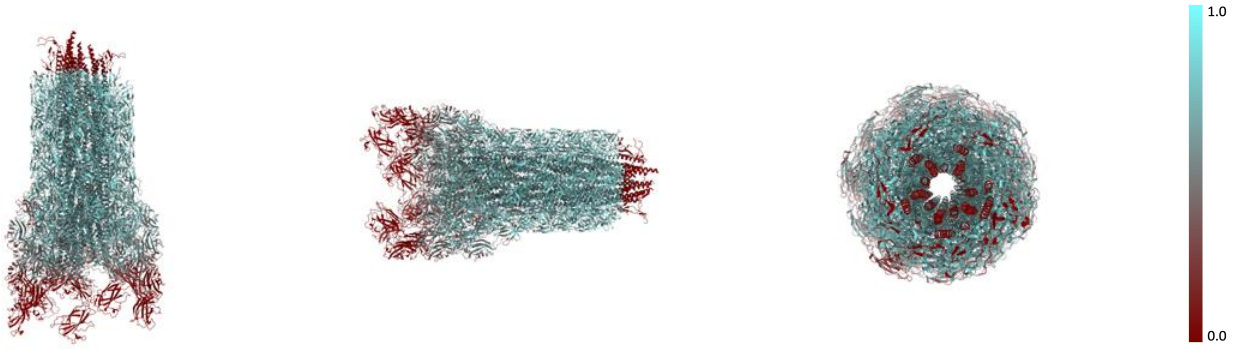
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

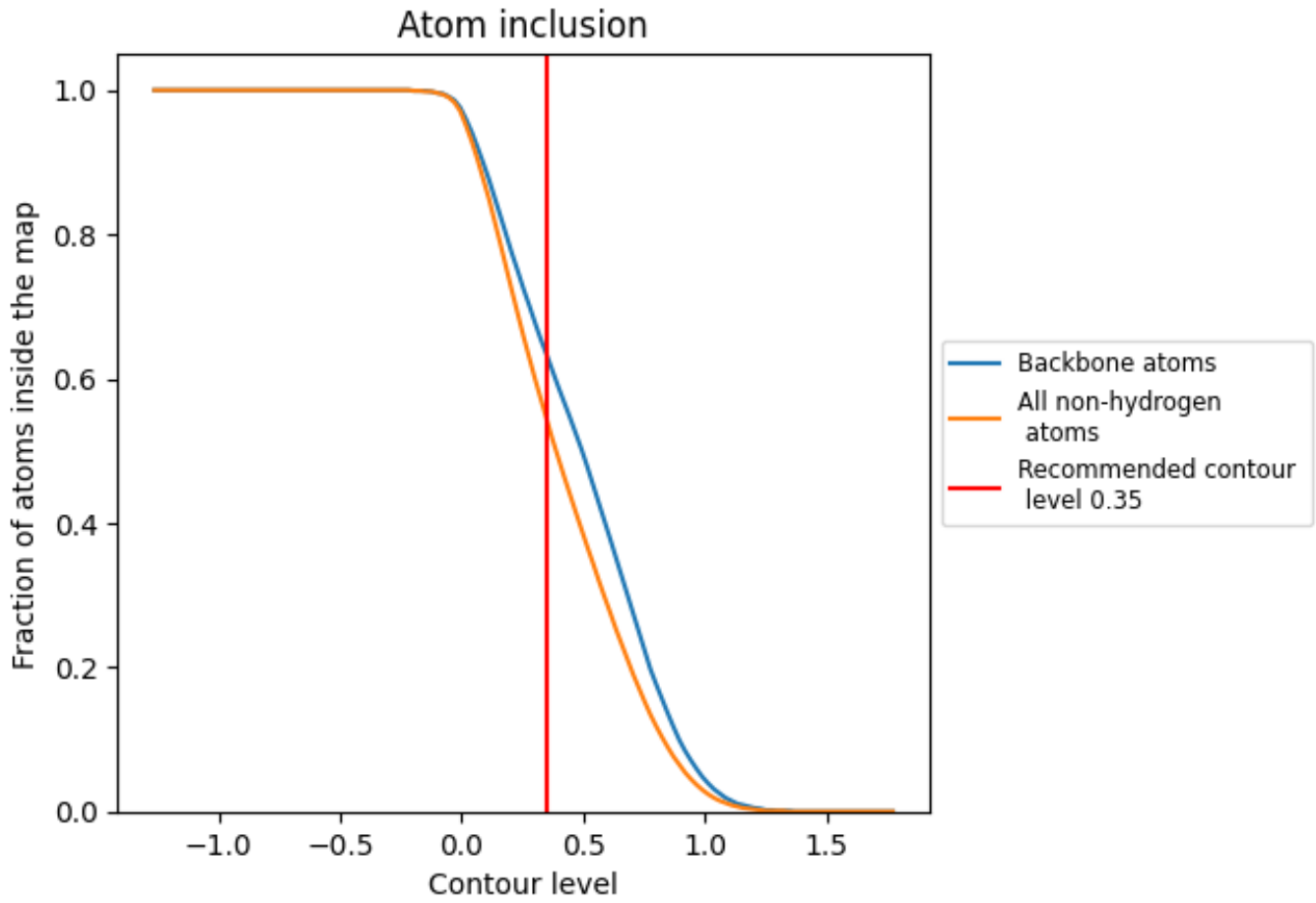
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 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