



Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 10:48 PM JST

PDB ID : 8WKK
EMDB ID : EMD-37601
Title : Cryo-EM structure of the whole rod with export apparatus and hook within the flagellar motor-hook complex in the CW state.
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-28
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:

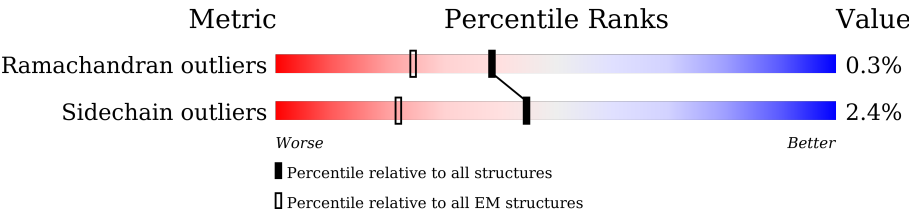
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	89	<div> <div>89%</div> <div>99%</div> </div>
1	B	89	<div> <div>75%</div> <div>99%</div> </div>
1	C	89	<div> <div>71%</div> <div>100%</div> </div>
1	D	89	<div> <div>87%</div> <div>99%</div> </div>
2	E	264	<div> <div>77%</div> <div>91%</div> </div>
3	F	245	<div> <div>51%</div> <div>81%</div> <div>16%</div> </div>
3	G	245	<div> <div>33%</div> <div>82%</div> <div>15%</div> </div>
3	H	245	<div> <div>27%</div> <div>83%</div> <div>15%</div> </div>
3	I	245	<div> <div>29%</div> <div>82%</div> <div>15%</div> </div>

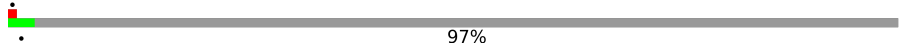
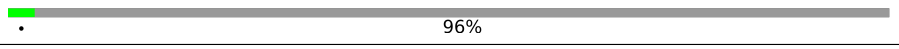
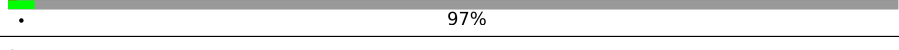
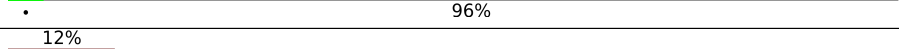
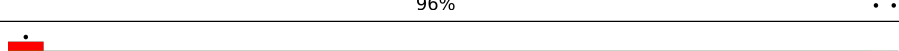
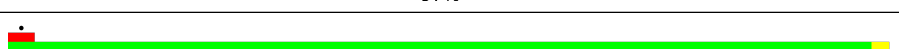
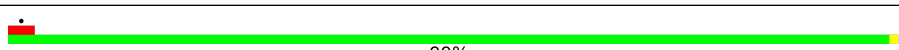

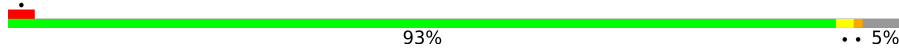
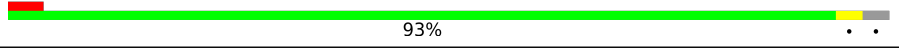
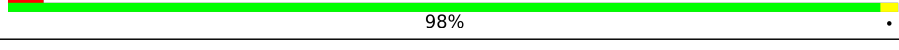
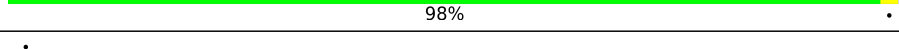
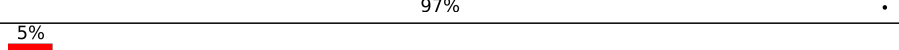
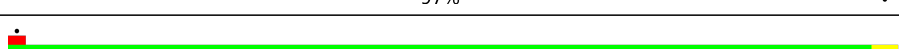
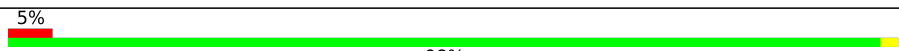
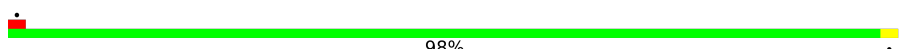
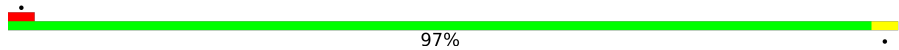
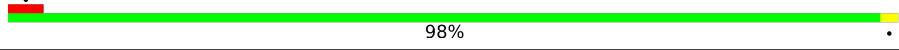
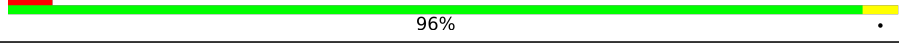
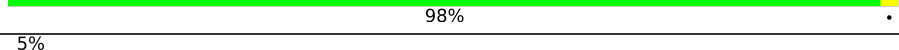
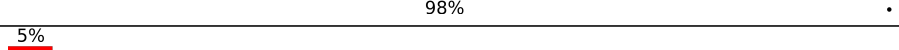
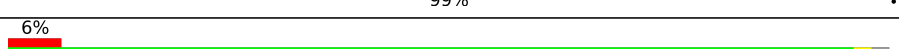



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Mol	Chain	Length	Quality of chain
3	J	245	
4	K	104	
4	L	104	
4	M	104	
4	N	104	
4	O	104	
4	P	104	
5	Q	138	
5	R	138	
5	S	138	
5	T	138	
5	U	138	
6	V	134	
6	W	134	
6	X	134	
6	Y	134	
6	Z	134	
6	a	134	
7	b	560	
7	c	560	
7	d	560	
7	e	560	
7	f	560	
7	g	560	
7	h	560	

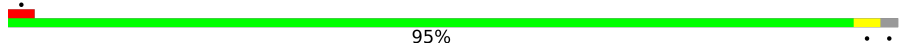
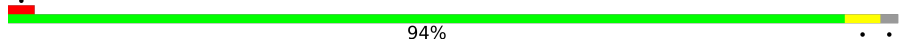
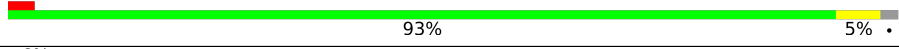
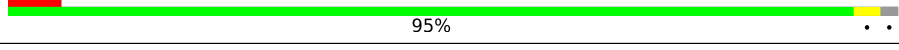
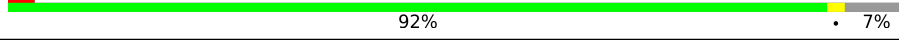
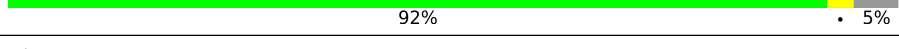
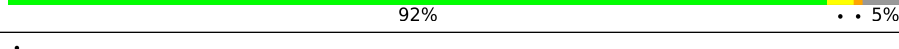
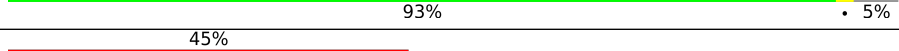
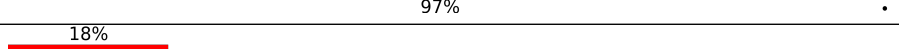
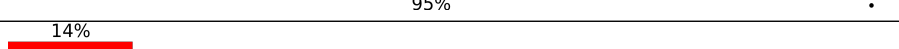
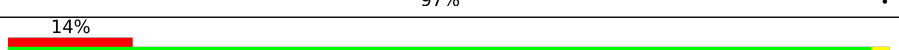
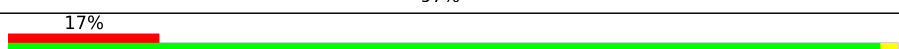
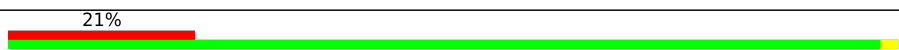
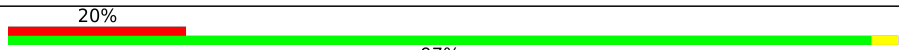
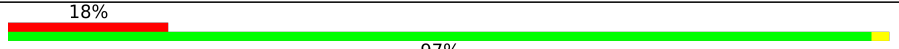


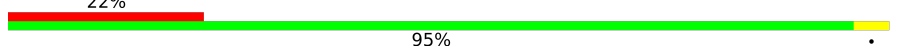
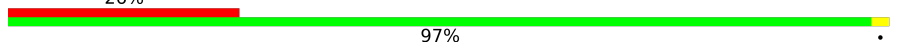
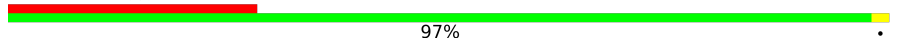
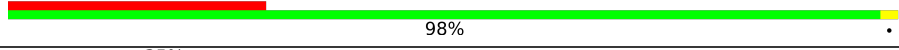
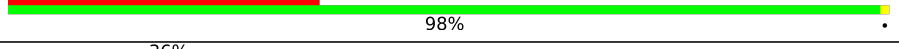
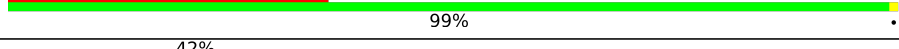
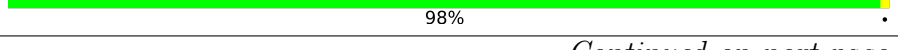

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Mol	Chain	Length	Quality of chain
7	i	560	 97%
7	j	560	 96%
7	k	560	 97%
7	l	560	 96%
8	m	251	 12% 96%
8	n	251	 97%
8	o	251	 97%
8	p	251	 99%
8	q	251	 6% 98%
9	0	260	 93% 5%
9	1	260	 93%
9	2	260	 98%
9	3	260	 98%
9	4	260	 97%
9	5	260	 5% 97%
9	6	260	 97%
9	7	260	 5% 98%
9	8	260	 98%
9	9	260	 97%
9	ZA	260	 98%
9	ZB	260	 5% 96%
9	ZC	260	 98%
9	ZD	260	 5% 98%
9	ZE	260	 5% 99%
9	r	260	 6% 95%

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Mol	Chain	Length	Quality of chain
9	s	260	
9	t	260	
9	u	260	
9	v	260	
9	w	260	
9	x	260	
9	y	260	
9	z	260	
10	ZF	403	
10	ZG	403	
10	ZH	403	
10	ZI	403	
10	ZJ	403	
10	ZK	403	
10	ZL	403	
10	ZM	403	
10	ZN	403	
10	ZO	403	
10	ZP	403	
10	ZQ	403	
10	ZR	403	
10	ZS	403	
10	ZT	403	
10	ZU	403	
10	ZV	403	

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Mol	Chain	Length	Quality of chain
10	ZW	403	<div> <div>40%</div> <div>96%</div> <div>.</div> </div>
10	ZX	403	<div> <div>42%</div> <div>99%</div> <div>.</div> </div>
10	ZY	403	<div> <div>46%</div> <div>98%</div> <div>.</div> </div>
10	ZZ	403	<div> <div>49%</div> <div>98%</div> <div>.</div> </div>
10	Za	403	<div> <div>52%</div> <div>98%</div> <div>.</div> </div>
10	Zb	403	<div> <div>52%</div> <div>98%</div> <div>.</div> </div>
10	Zc	403	<div> <div>57%</div> <div>97%</div> <div>.</div> </div>
10	Zd	403	<div> <div>61%</div> <div>98%</div> <div>.</div> </div>
10	Ze	403	<div> <div>66%</div> <div>97%</div> <div>.</div> </div>
10	Zf	403	<div> <div>69%</div> <div>98%</div> <div>.</div> </div>
10	Zg	403	<div> <div>72%</div> <div>98%</div> <div>.</div> </div>
10	Zh	403	<div> <div>76%</div> <div>98%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 167771 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 biosynthetic protein FliQ.

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

- Molecule 2 is a protein called Flagellar biosynthetic protein FliR.

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

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

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

- Molecule 4 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	40	Total	C	N	O	S	0	0
			300	185	52	57	6		
4	L	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
4	M	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
4	N	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
4	O	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
4	P	73	Total	C	N	O	S	0	0
			550	340	100	104	6		

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

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

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

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

- Molecule 7 is a protein called Flagellar M-ring protein.

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

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

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

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
9	1	252	Total	C	N	O	S	0	0
			1894	1172	331	385	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	3	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	4	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	5	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	6	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	7	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	8	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	9	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZA	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZB	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZC	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZD	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	ZE	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
9	r	254	Total 1903	C 1175	N 334	O 389	S 5	0	0
9	s	255	Total 1911	C 1181	N 335	O 390	S 5	0	0
9	t	256	Total 1919	C 1186	N 336	O 391	S 6	0	0
9	u	254	Total 1903	C 1175	N 334	O 389	S 5	0	0
9	v	255	Total 1911	C 1181	N 335	O 390	S 5	0	0
9	w	243	Total 1823	C 1127	N 318	O 373	S 5	0	0
9	x	248	Total 1866	C 1154	N 327	O 379	S 6	0	0
9	y	248	Total 1866	C 1154	N 327	O 379	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	z	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		

- Molecule 10 is a protein called Flagellar hook protein FlgE.

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

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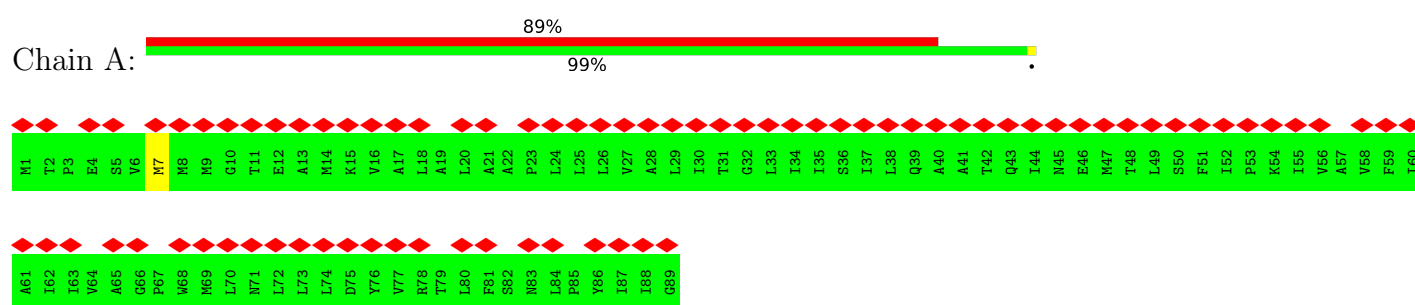
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Mol	Chain	Residues	Atoms					AltConf	Trace
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10	ZY	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	ZZ	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Za	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zb	401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

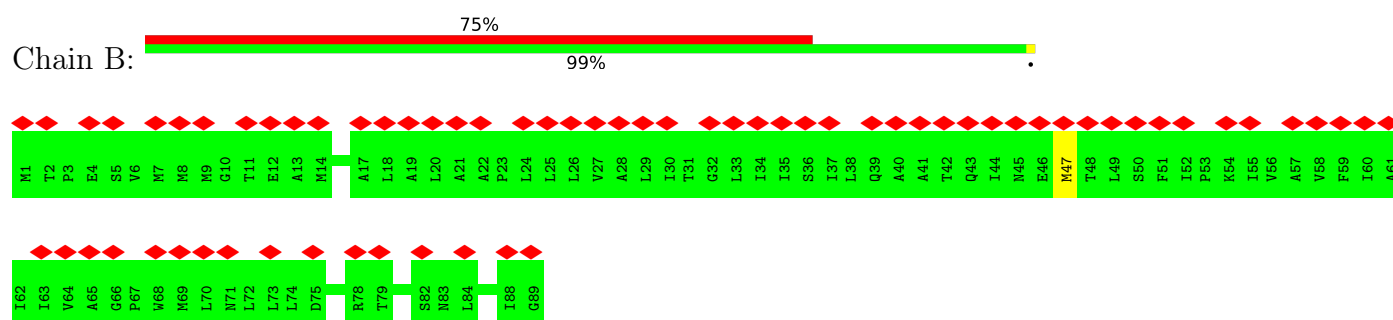
3 Residue-property plots

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.

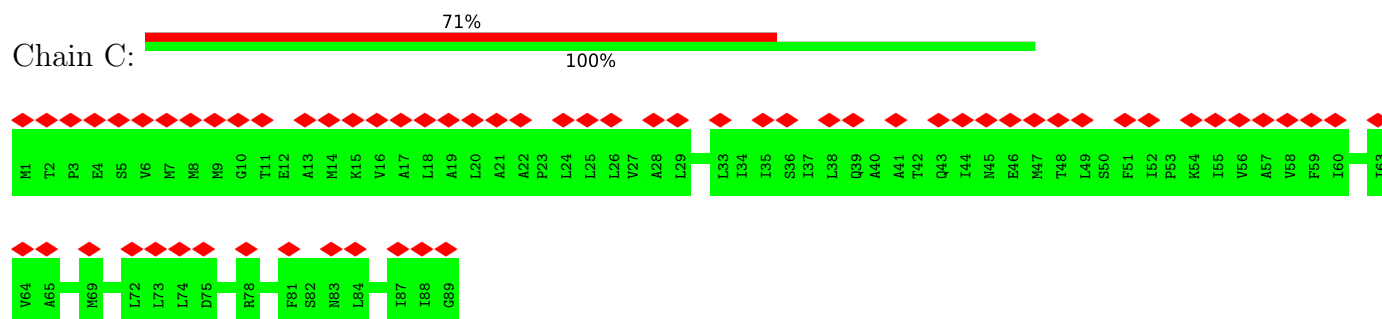
• Molecule 1: Flagellar biosynthetic protein FliQ



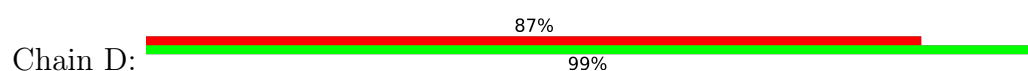
• Molecule 1: Flagellar biosynthetic protein FliQ

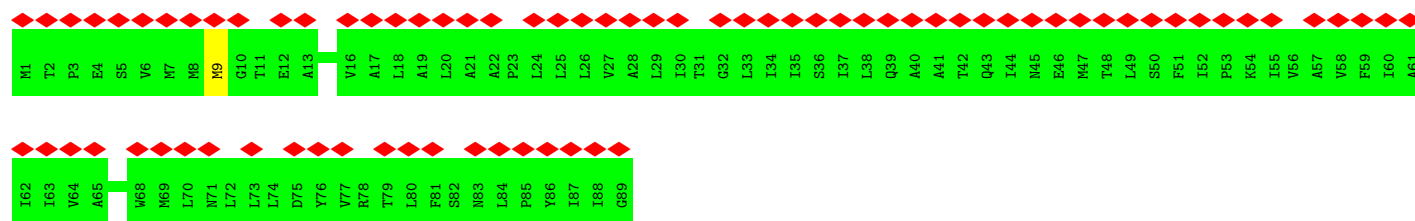


• Molecule 1: Flagellar biosynthetic protein FliQ

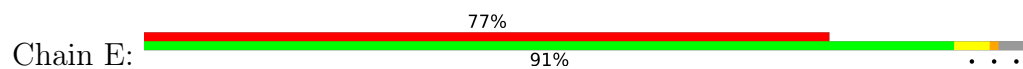


• Molecule 1: Flagellar biosynthetic protein FliQ

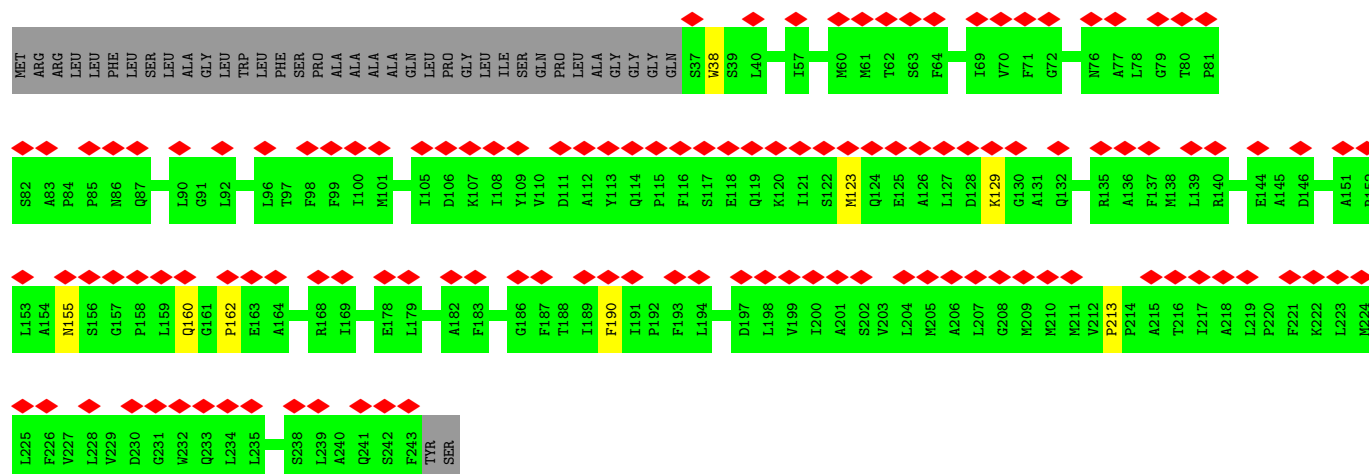
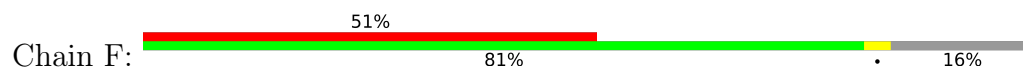




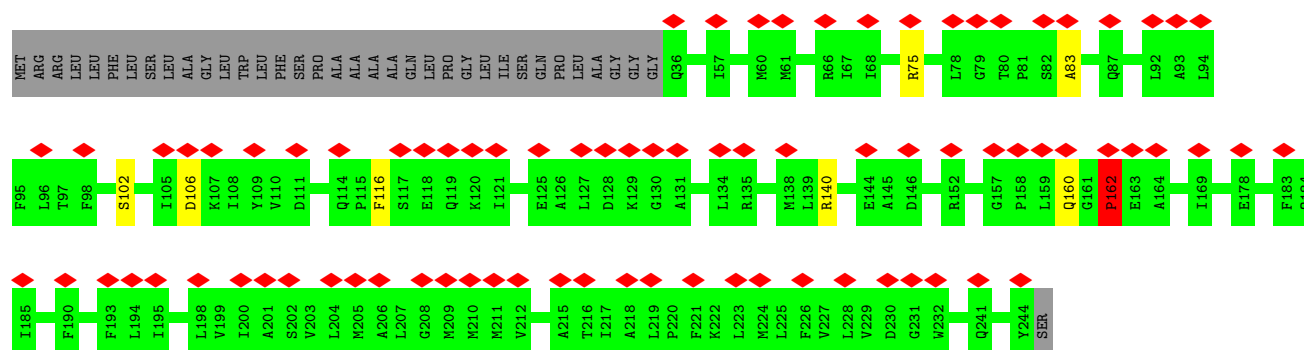
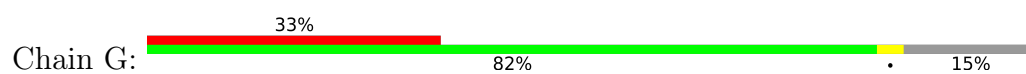
• Molecule 2: Flagellar biosynthetic protein FliR



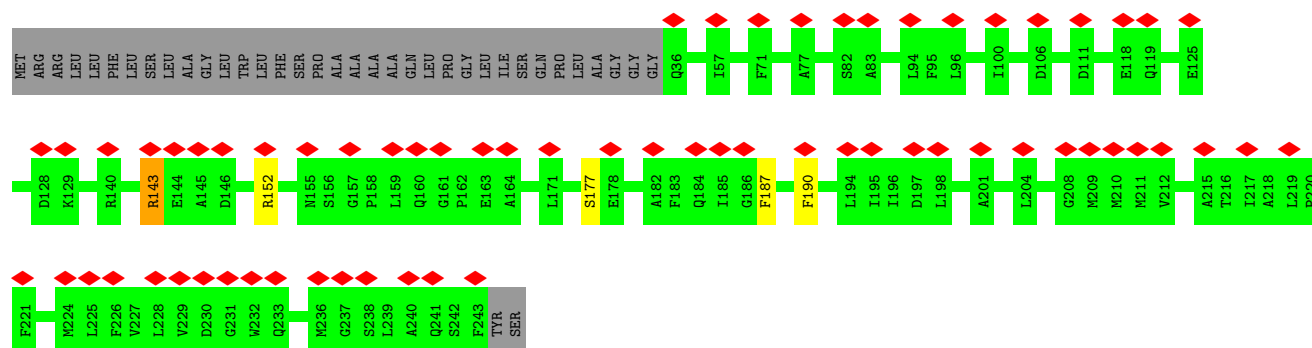
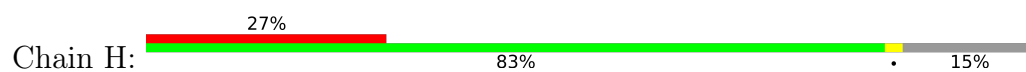
• Molecule 3: Flagellar biosynthetic protein FliP



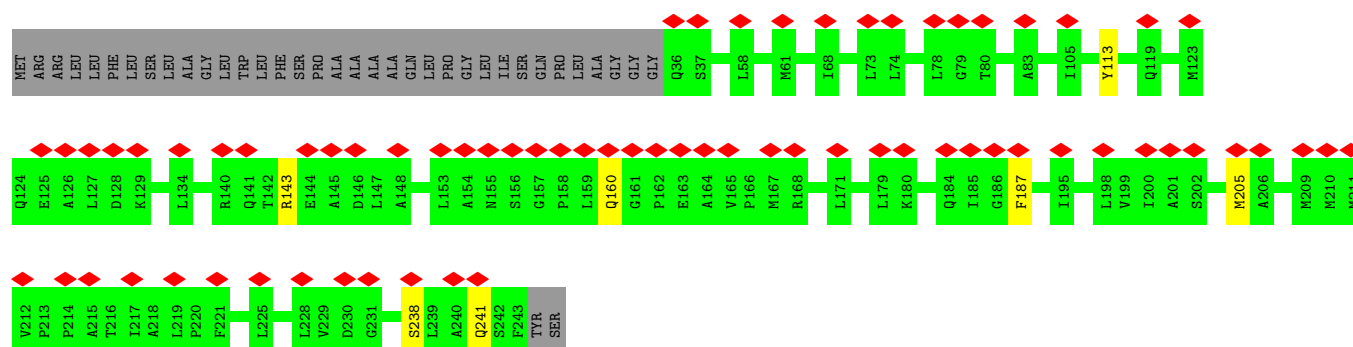
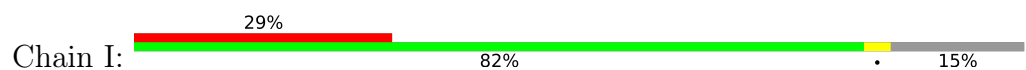
• Molecule 3: Flagellar biosynthetic protein FliP



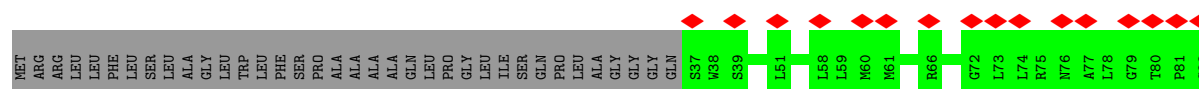
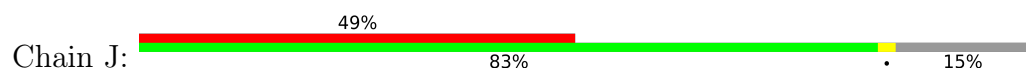
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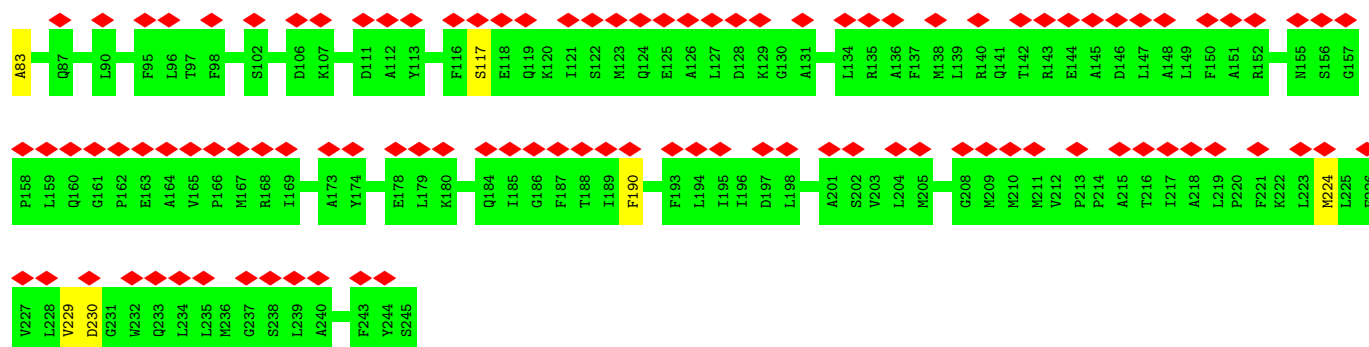


• Molecule 3: Flagellar biosynthetic protein FliP

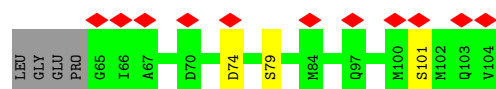
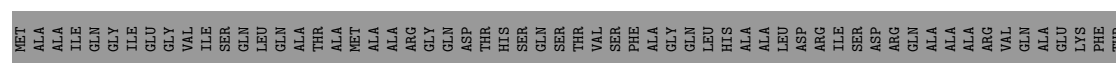


• Molecule 3: Flagellar biosynthetic protein FliP

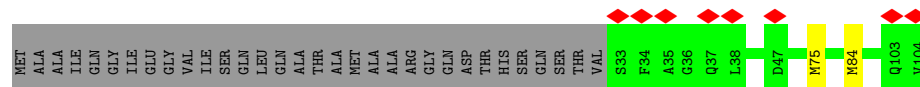




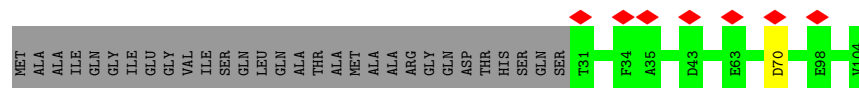
- Molecule 4: Flagellar hook-basal body complex protein FliE



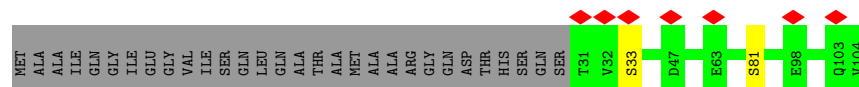
- Molecule 4: Flagellar hook-basal body complex protein FliE



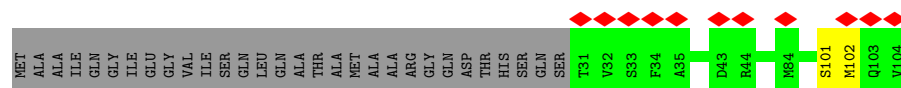
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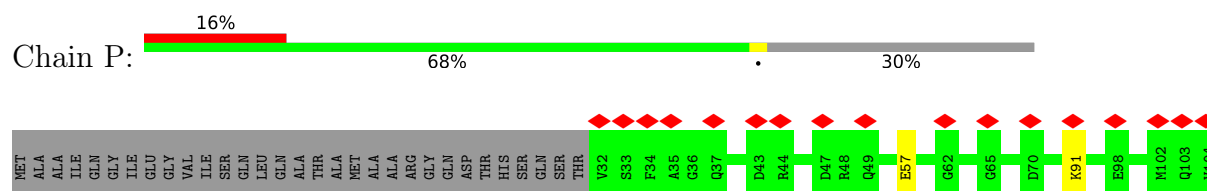
- Molecule 4: Flagellar hook-basal body complex protein FliE



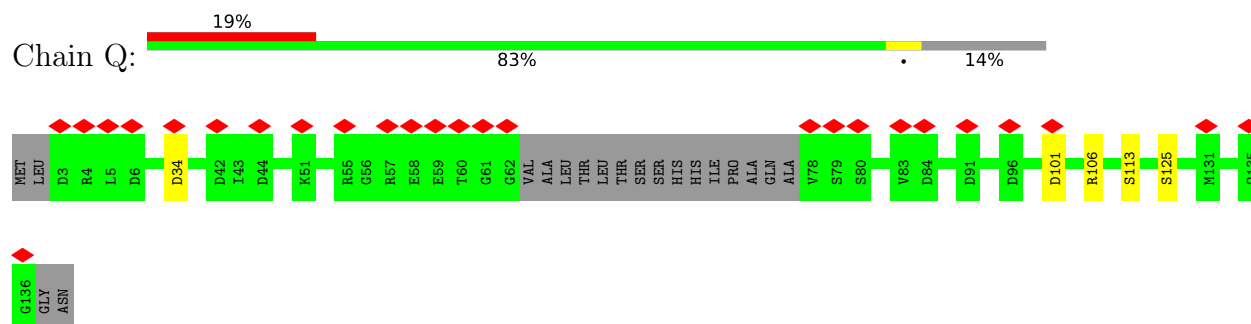
- Molecule 4: Flagellar hook-basal body complex protein FliE



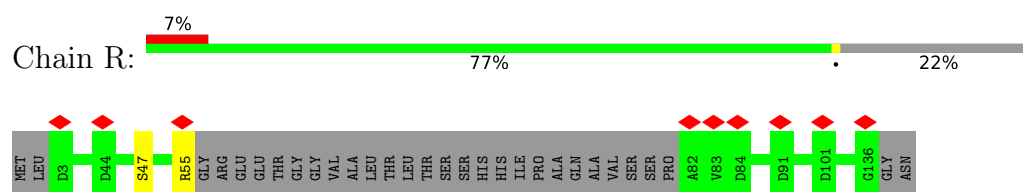
- Molecule 4: Flagellar hook-basal body complex protein FliE



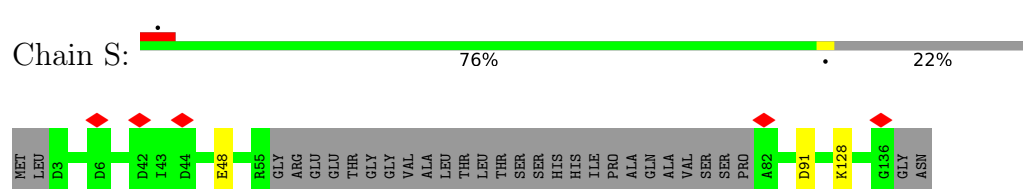
- Molecule 5: Flagellar basal body rod protein FlgB



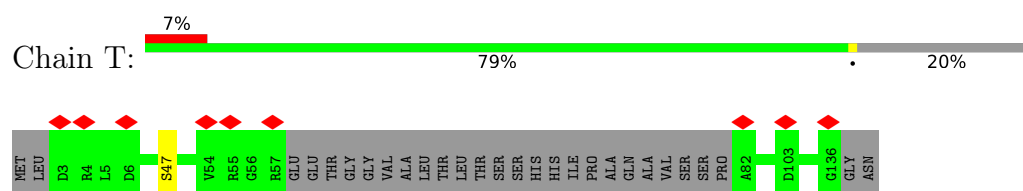
- Molecule 5: Flagellar basal body rod protein FlgB



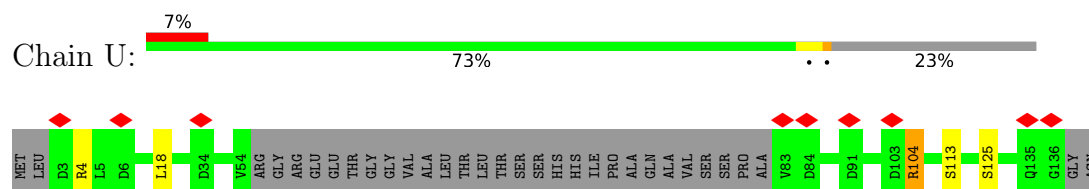
- Molecule 5: Flagellar basal body rod protein FlgB



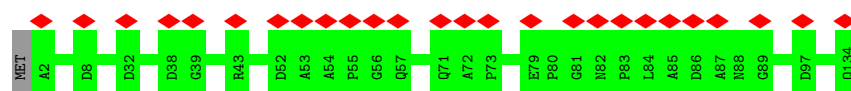
- Molecule 5: Flagellar basal body rod protein FlgB



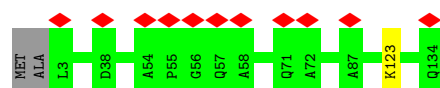
- Molecule 5: Flagellar basal body rod protein FlgB



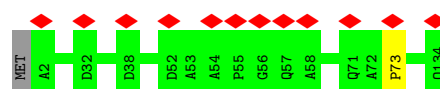
- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 6: Flagellar basal-body rod protein FlgC



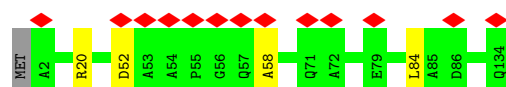
- Molecule 6: Flagellar basal-body rod protein FlgC



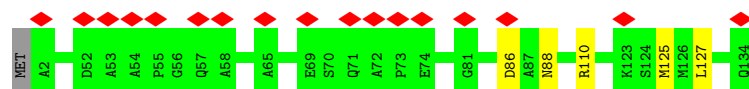
- Molecule 6: Flagellar basal-body rod protein FlgC



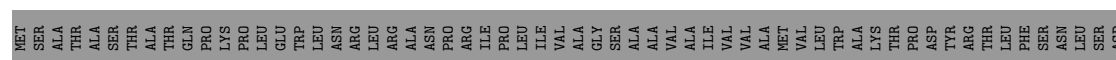
- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 7: Flagellar M-ring protein



[illegible]

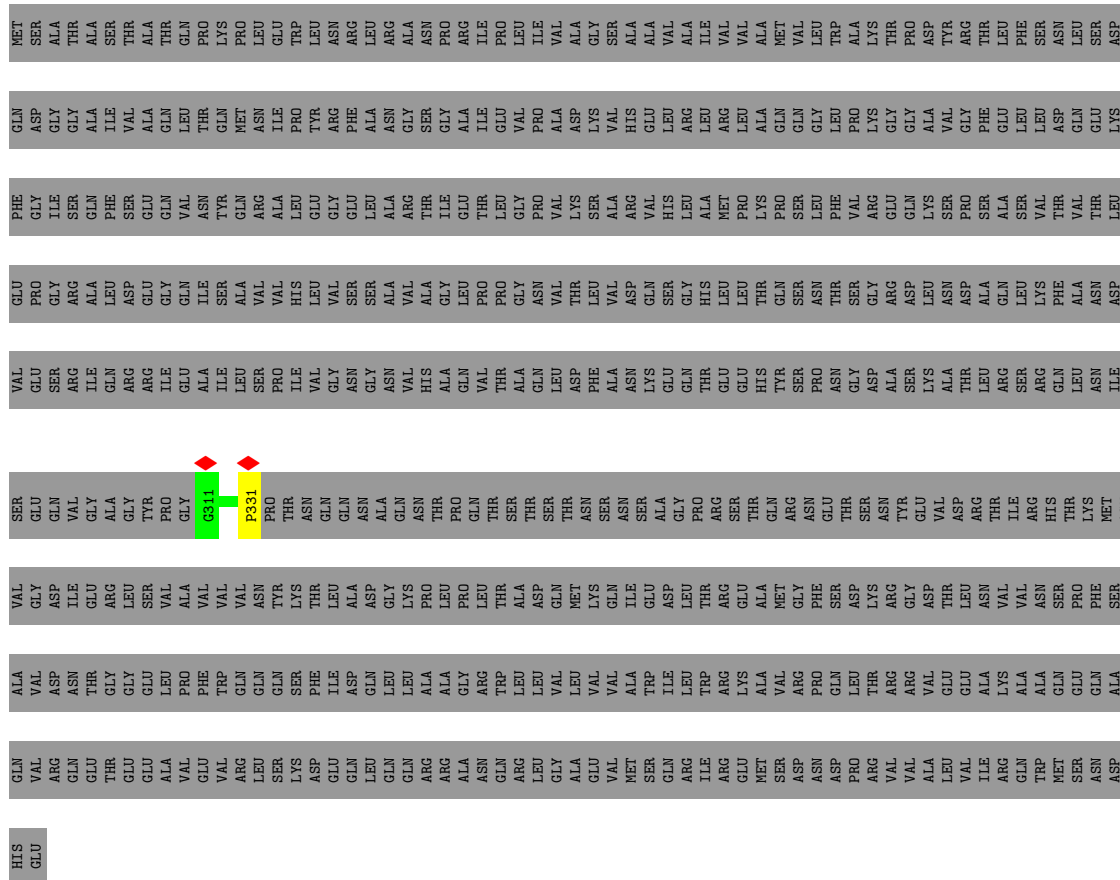
- Molecule 7: Flagellar M-ring protein

[illegible]



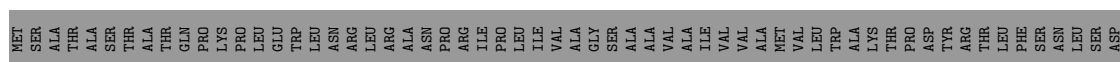
- Molecule 7: Flagellar M-ring protein

Chain f: 



- Molecule 7: Flagellar M-ring protein

Chain g:  97%



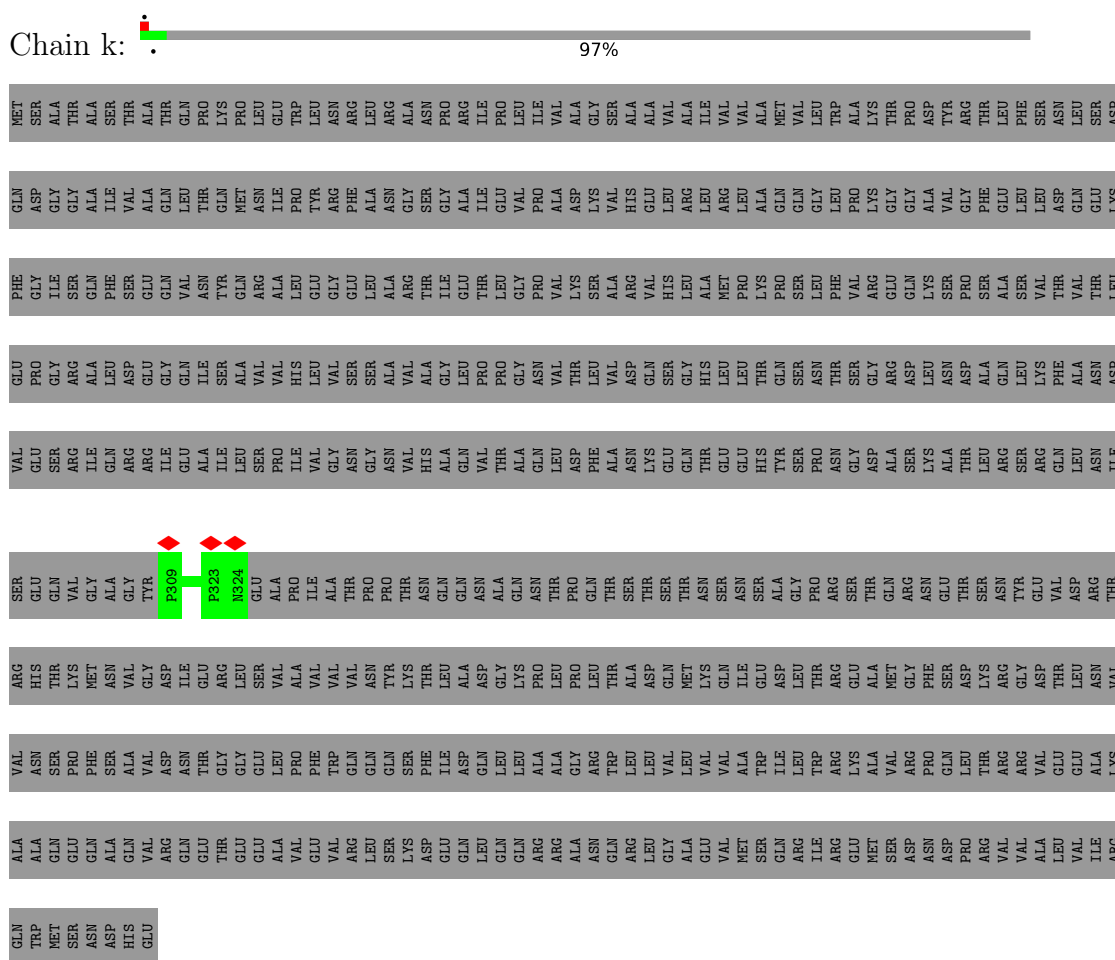
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- Molecule 7: Flagellar M-ring protein

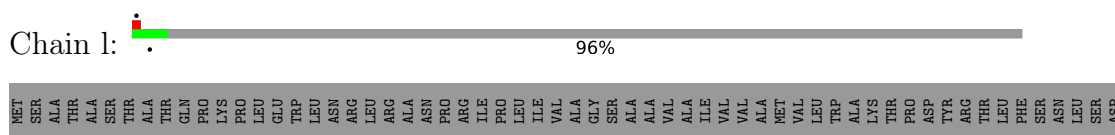
Chain h:  96%

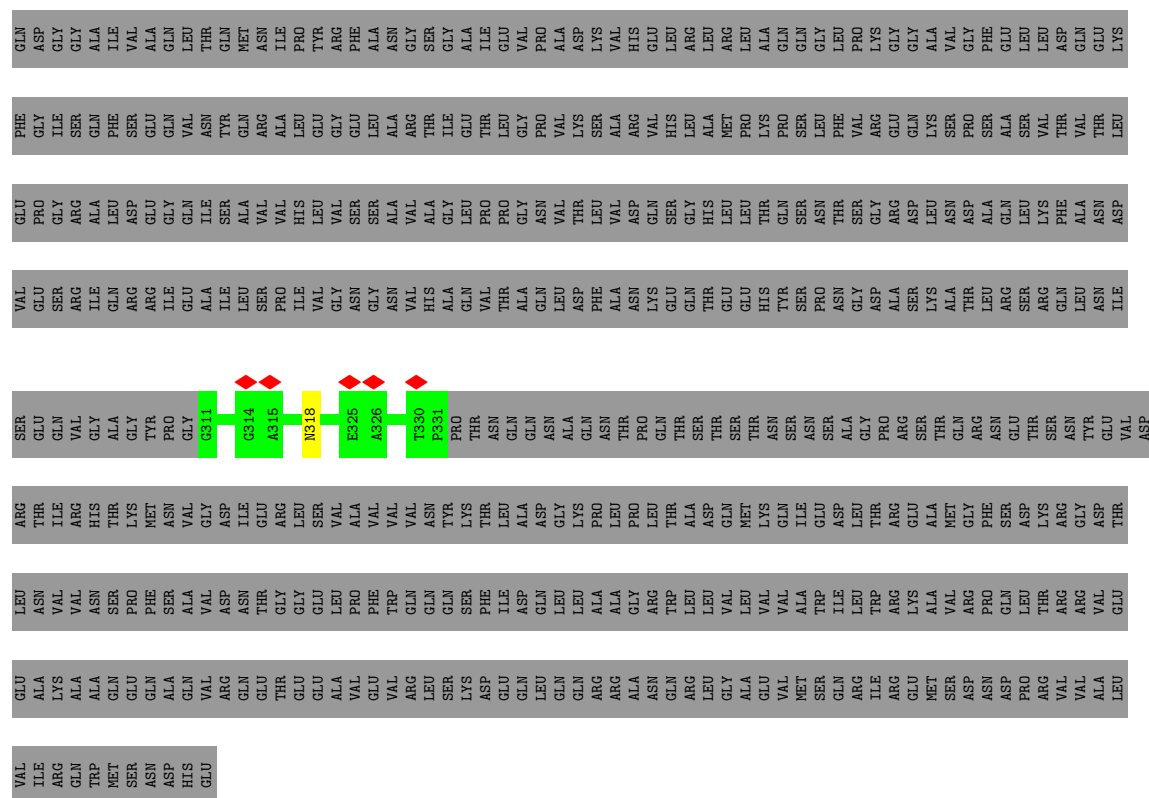
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- Molecule 7: Flagellar M-ring protein

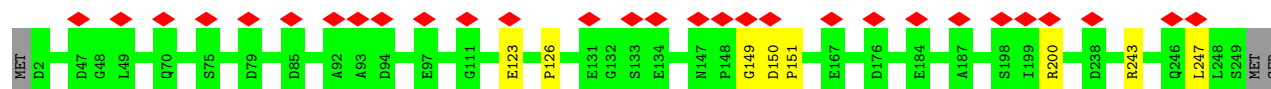


- Molecule 7: Flagellar M-ring protein

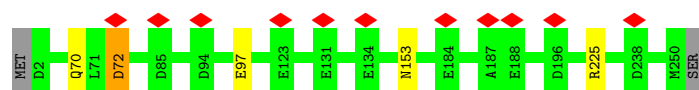




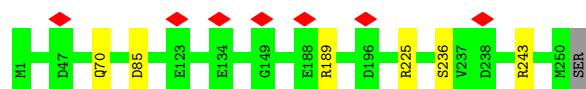
• Molecule 8: Flagellar basal-body rod protein FlgF



• Molecule 8: Flagellar basal-body rod protein FlgF

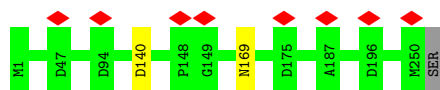


• Molecule 8: Flagellar basal-body rod protein FlgF



• Molecule 8: Flagellar basal-body rod protein FlgF





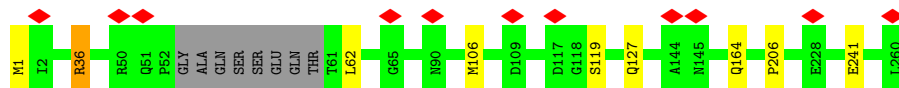
- Molecule 8: Flagellar basal-body rod protein FlgF



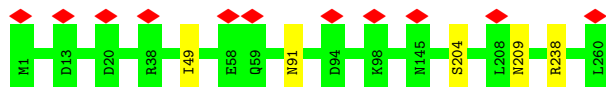
- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG



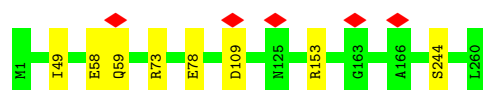
- Molecule 9: Flagellar basal-body rod protein FlgG



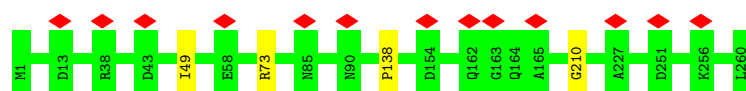
- Molecule 9: Flagellar basal-body rod protein FlgG



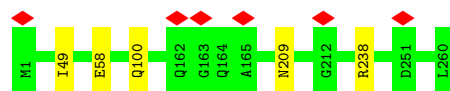
- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG



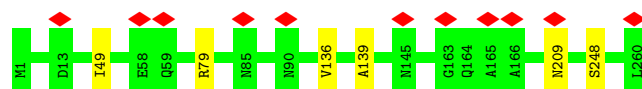
- Molecule 9: Flagellar basal-body rod protein FlgG



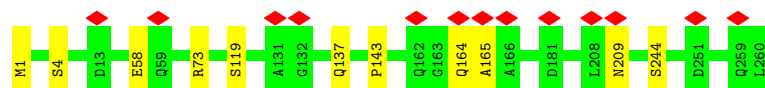
- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG

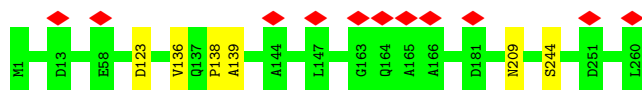


- Molecule 9: Flagellar basal-body rod protein FlgG



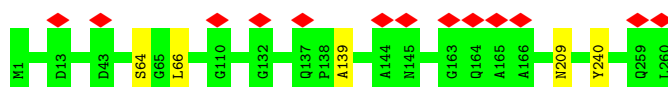
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain ZC:  98%



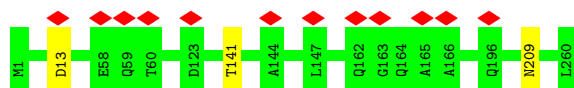
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain ZD:  98%



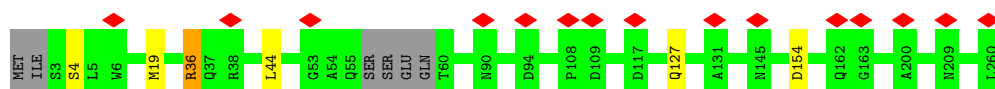
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain ZE:  99%



- Molecule 9: Flagellar basal-body rod protein FlgG

Chain r:  95%



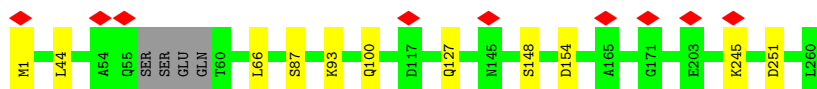
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain s:  95%



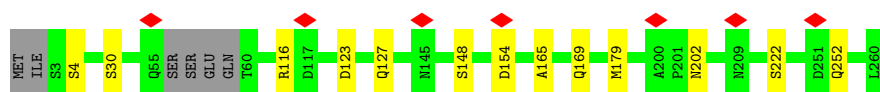
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain t:  94%

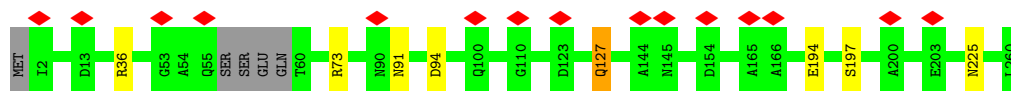


- Molecule 9: Flagellar basal-body rod protein FlgG

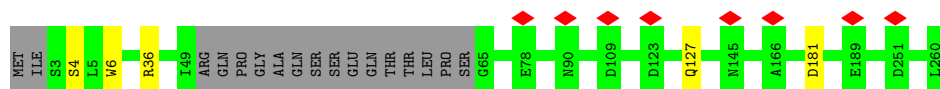
Chain u:  93%



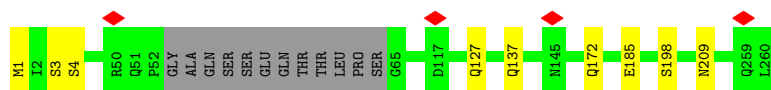
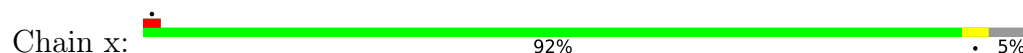
- Molecule 9: Flagellar basal-body rod protein FlgG



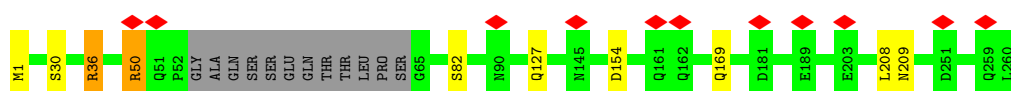
- Molecule 9: Flagellar basal-body rod protein FlgG



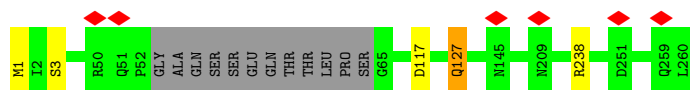
- Molecule 9: Flagellar basal-body rod protein FlgG



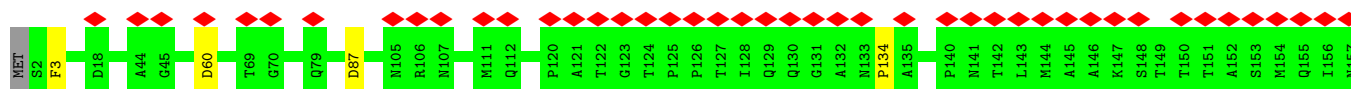
- Molecule 9: Flagellar basal-body rod protein FlgG

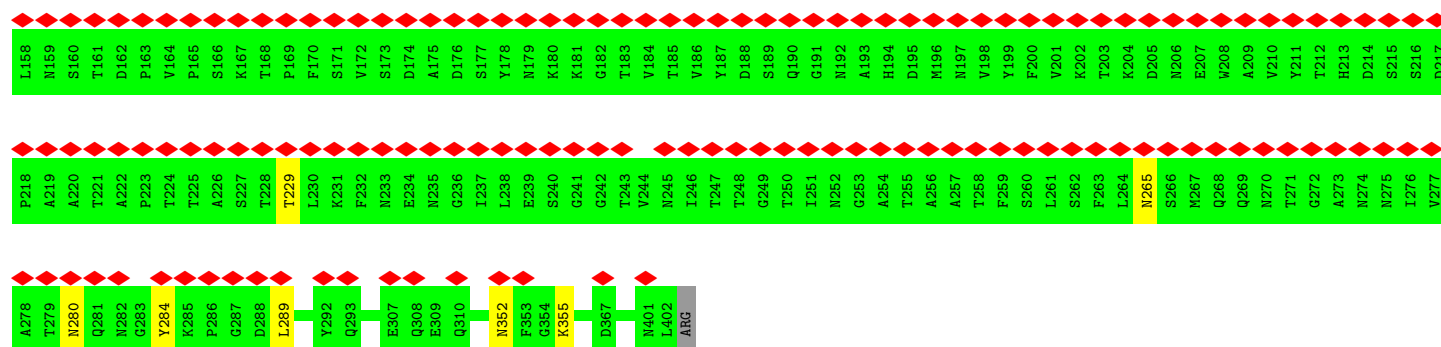


- Molecule 9: Flagellar basal-body rod protein FlgG

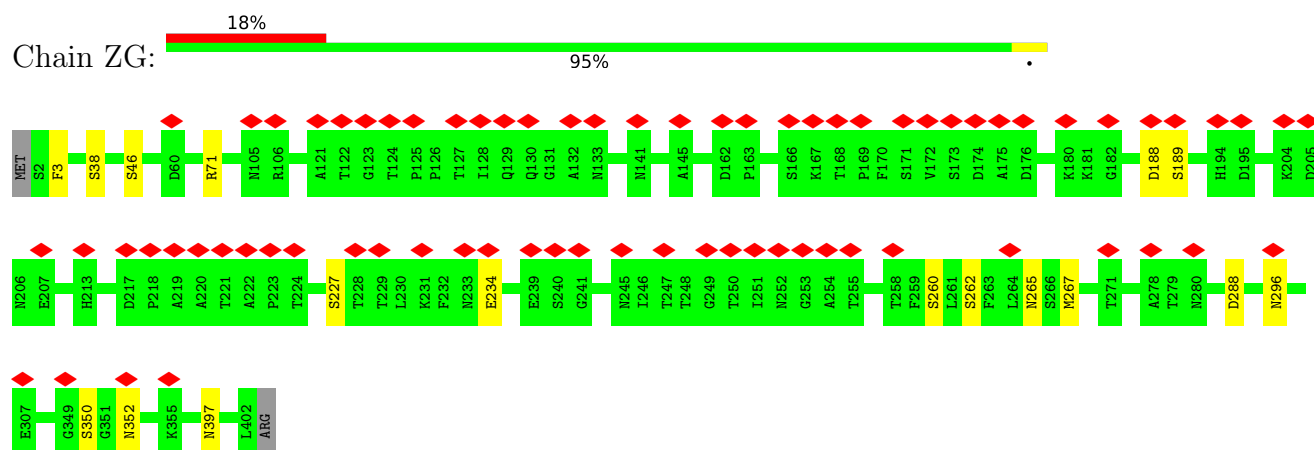


- Molecule 10: Flagellar hook protein FlgE

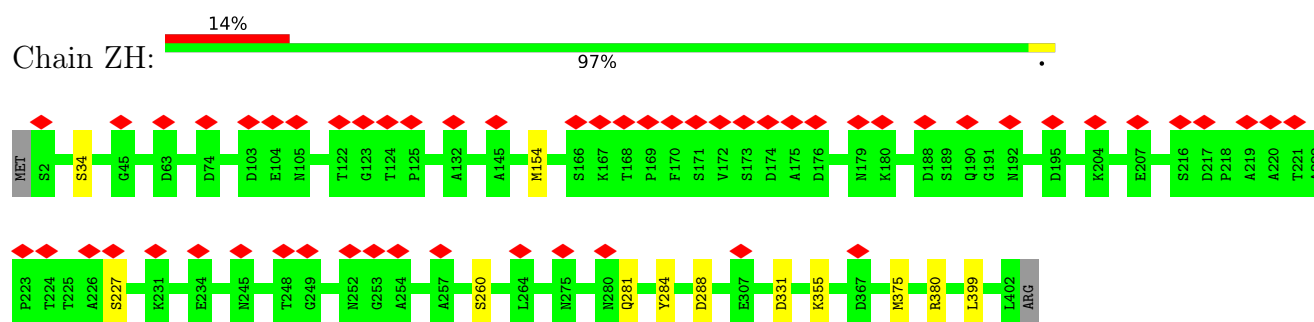




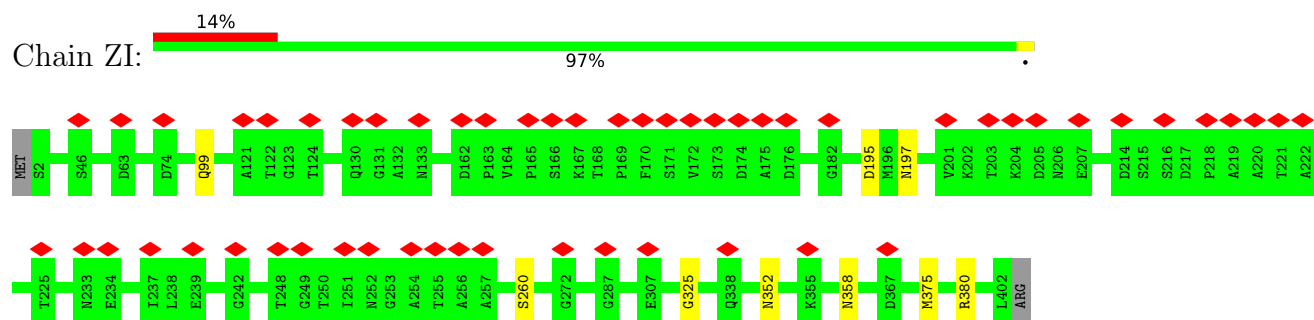
• Molecule 10: Flagellar hook protein FlgE



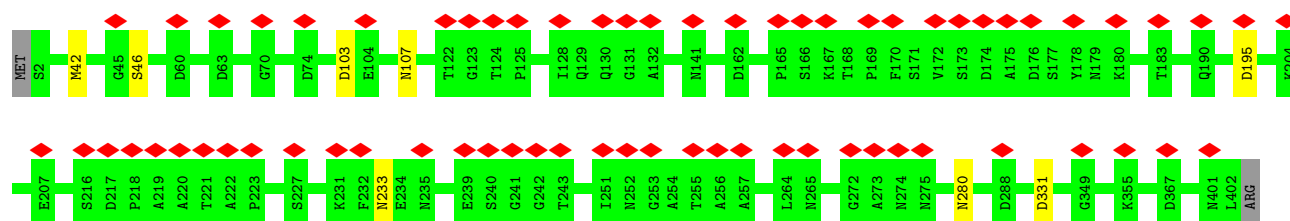
• Molecule 10: Flagellar hook protein FlgE



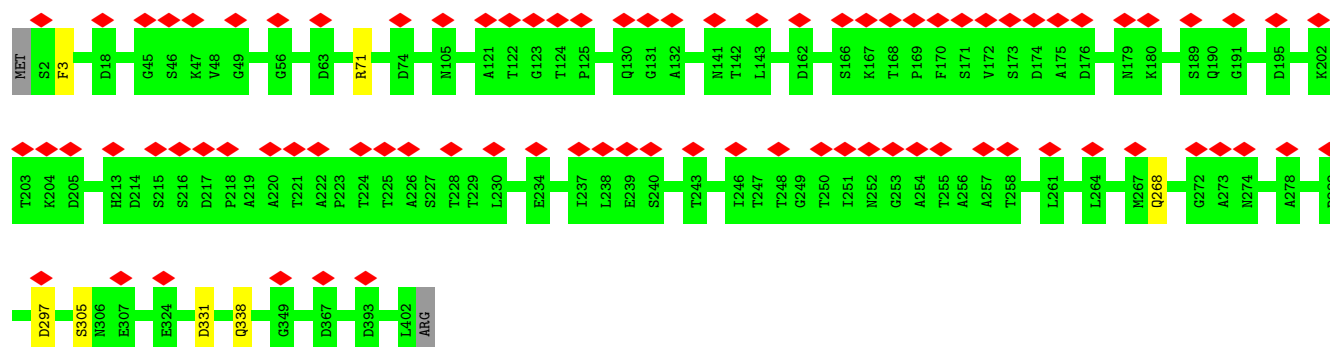
• Molecule 10: Flagellar hook protein FlgE



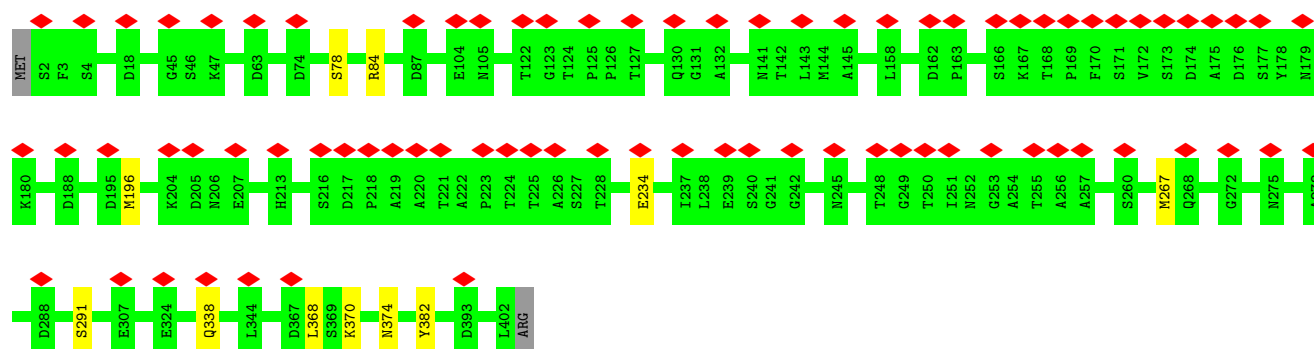
• Molecule 10: Flagellar hook protein FlgE



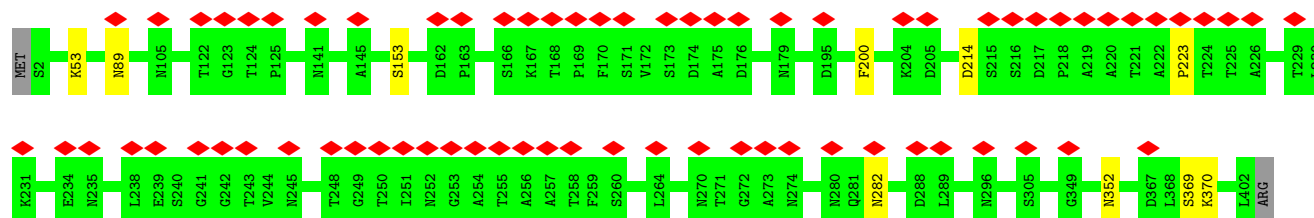
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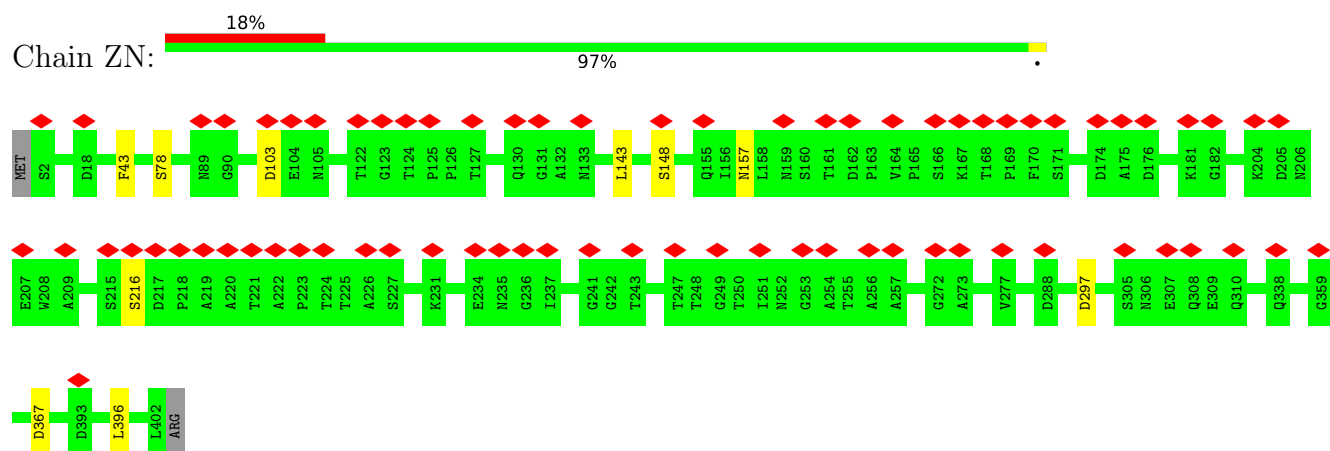
• Molecule 10: Flagellar hook protein FlgE



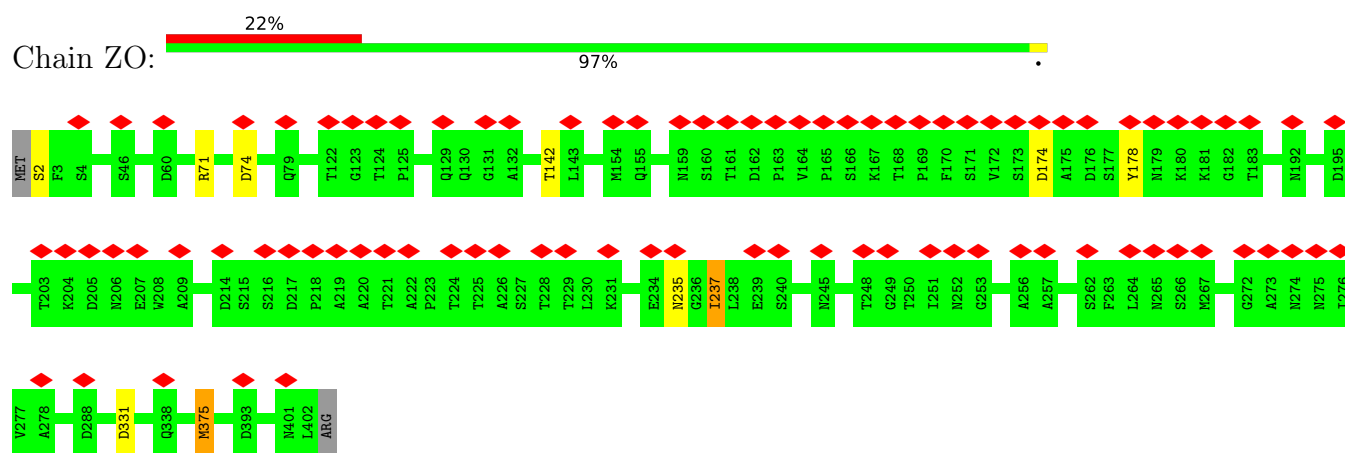
• Molecule 10: Flagellar hook protein FlgE



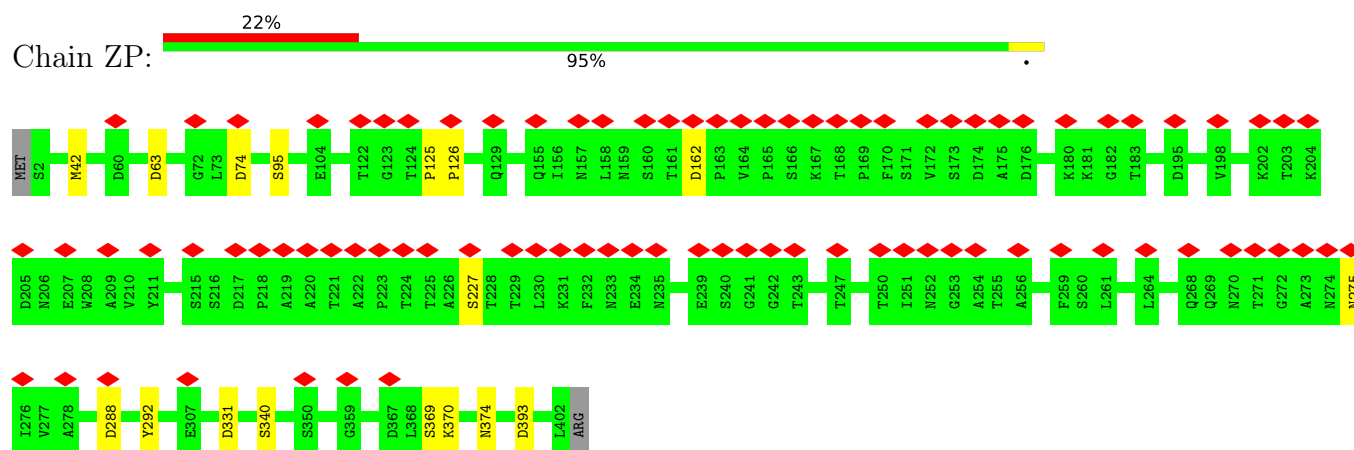
- Molecule 10: Flagellar hook protein FlgE



- Molecule 10: Flagellar hook protein FlgE

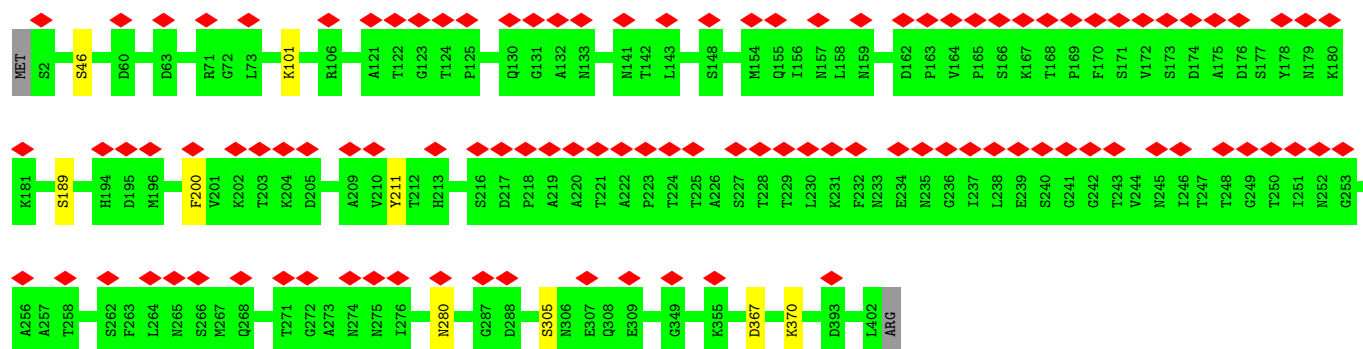


- Molecule 10: Flagellar hook protein FlgE

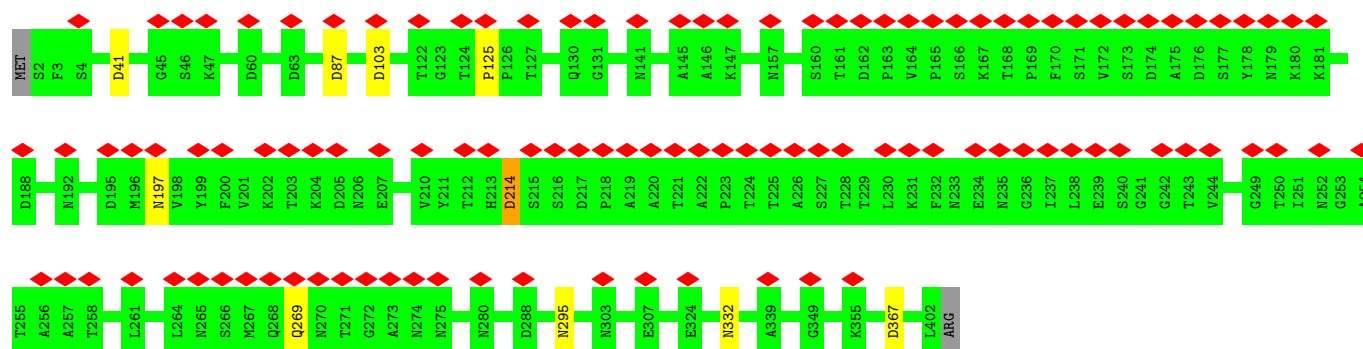


- Molecule 10: Flagellar hook protein FlgE

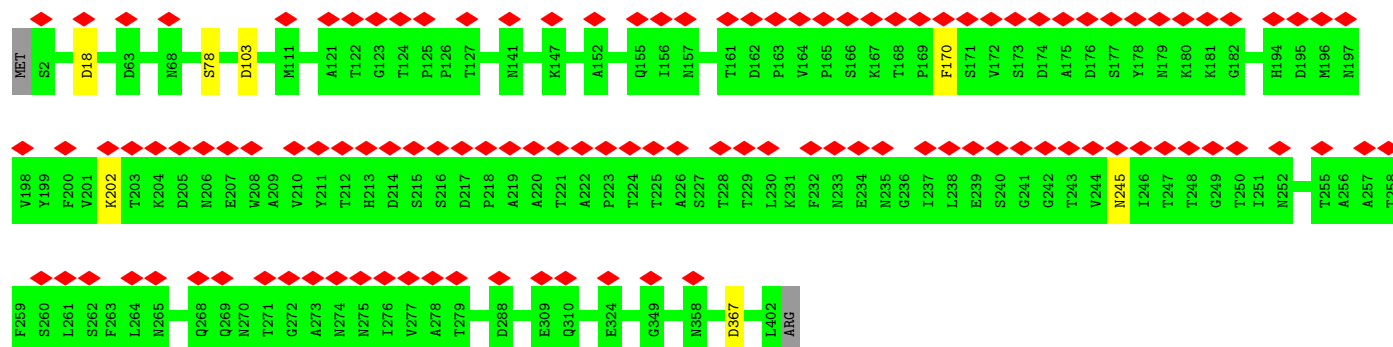




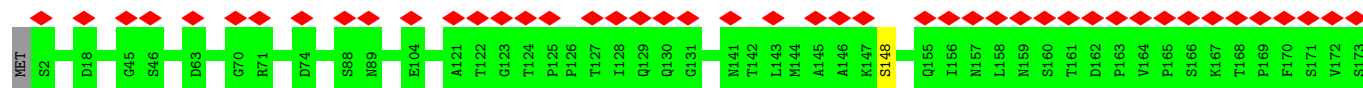
• Molecule 10: Flagellar hook protein FlgE

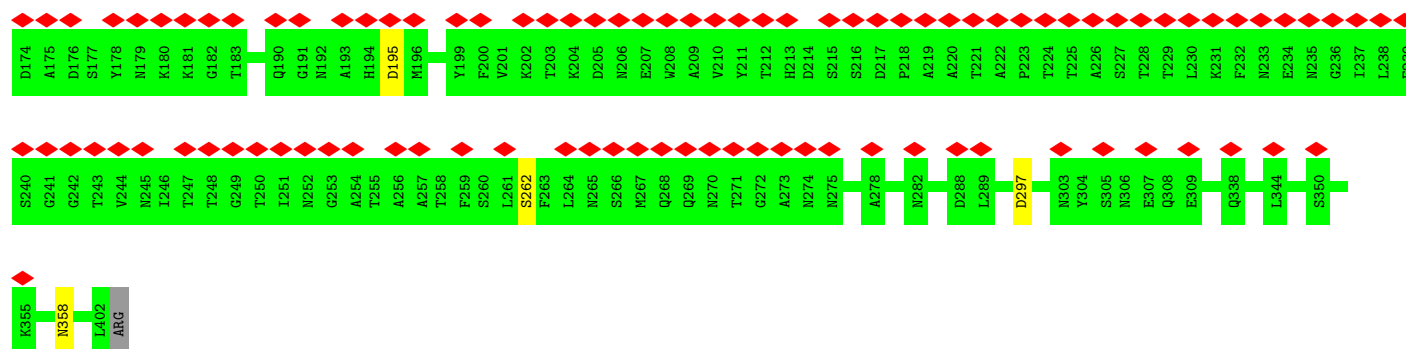


• Molecule 10: Flagellar hook protein FlgE

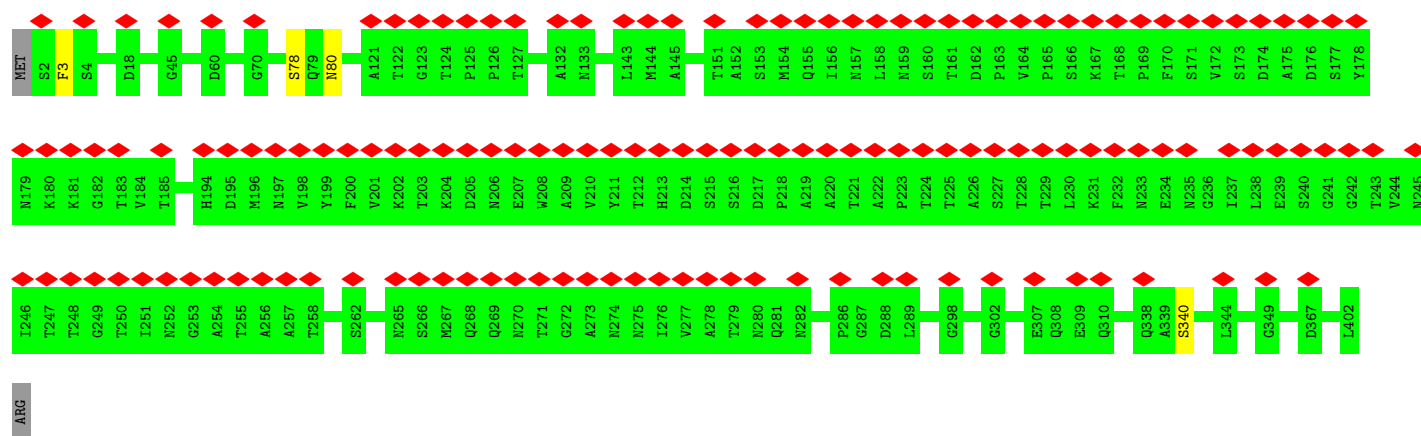


• Molecule 10: Flagellar hook protein FlgE

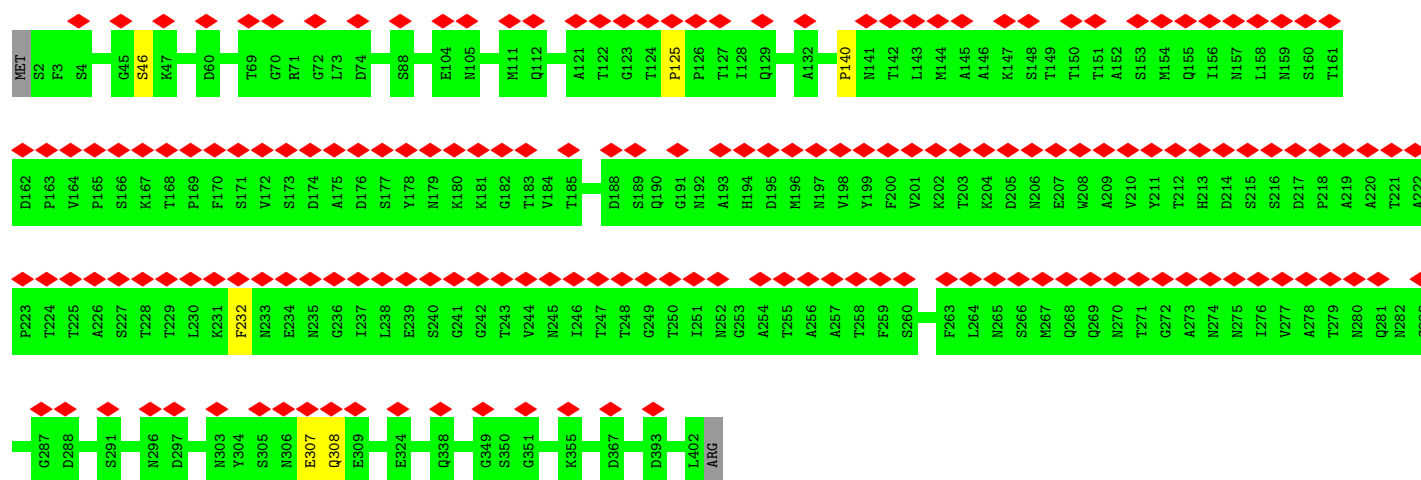




• Molecule 10: Flagellar hook protein FlgE

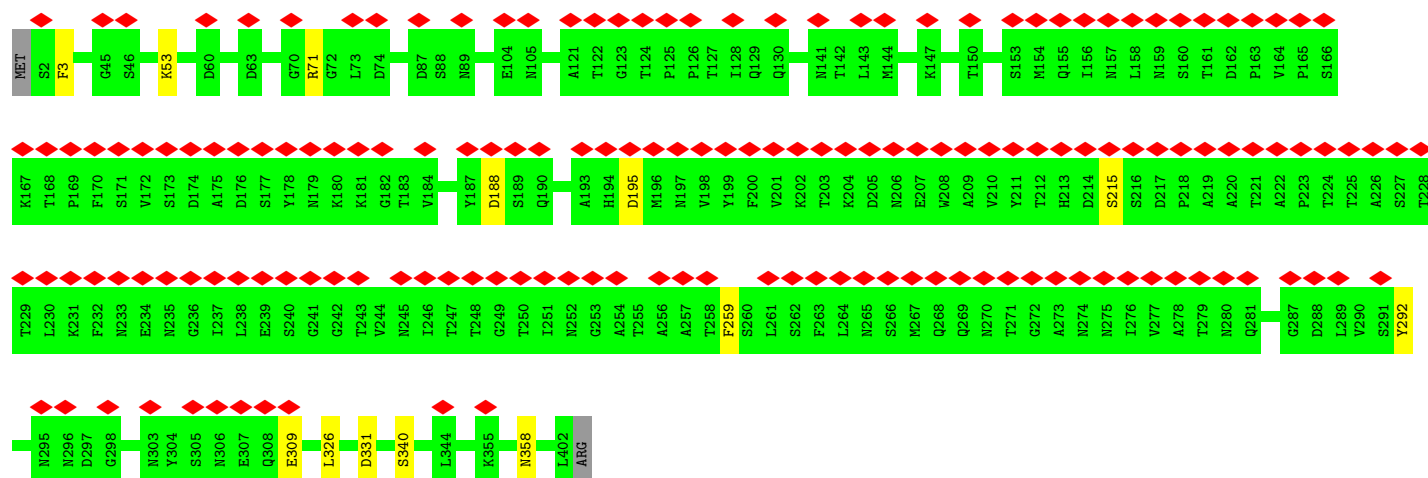


• Molecule 10: Flagellar hook protein FlgE

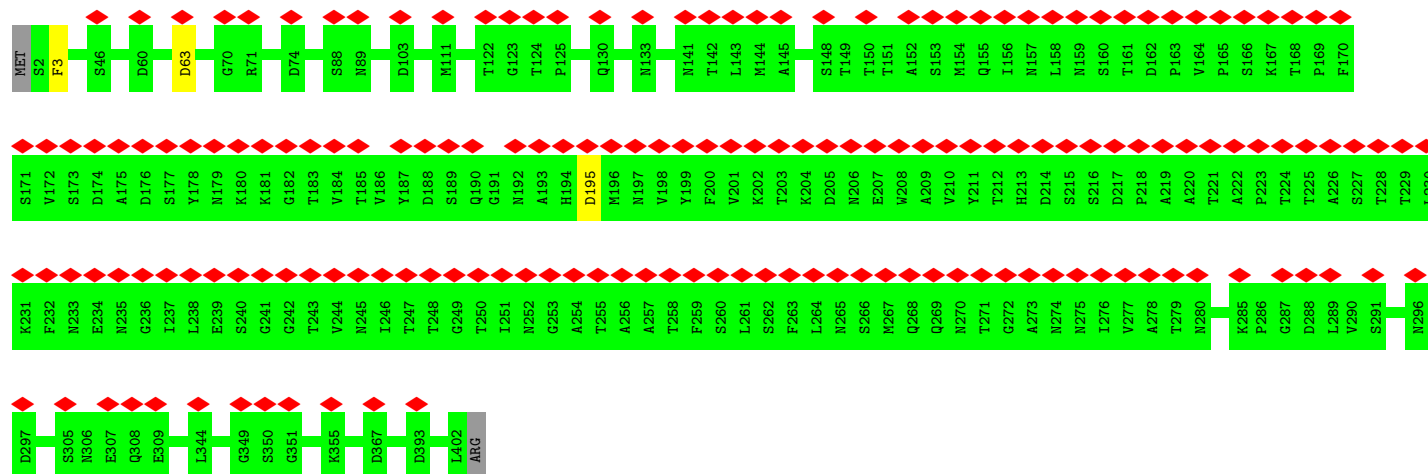
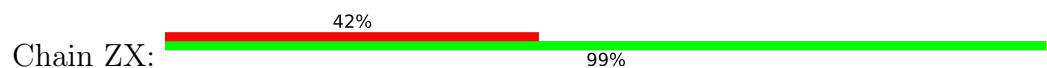


• Molecule 10: Flagellar hook protein FlgE

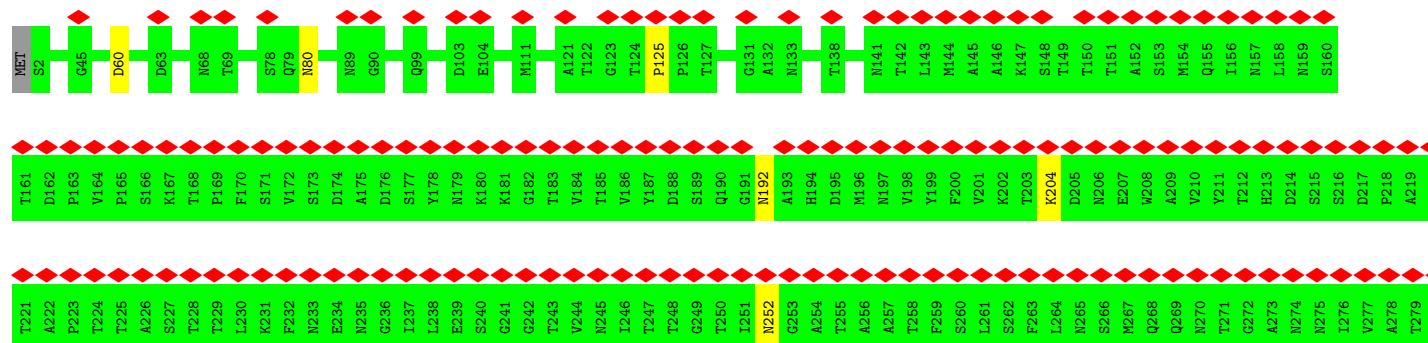


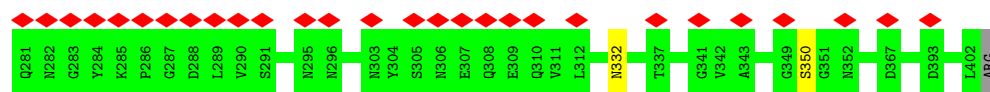


• Molecule 10: Flagellar hook protein FlgE

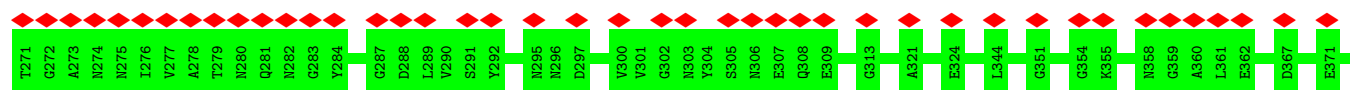
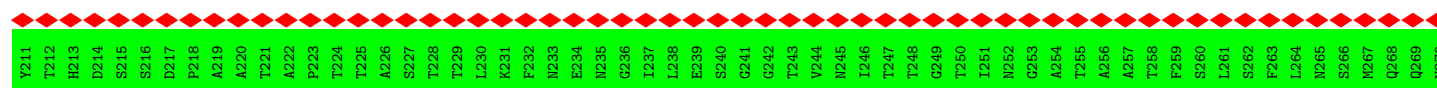
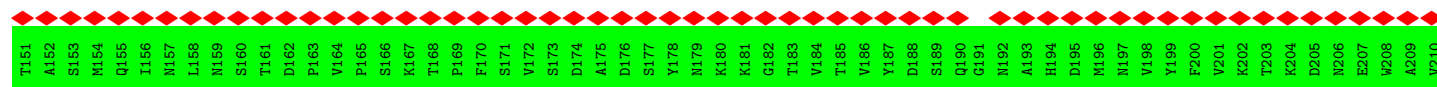
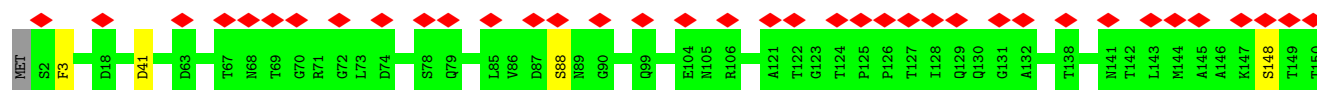


• Molecule 10: Flagellar hook protein FlgE

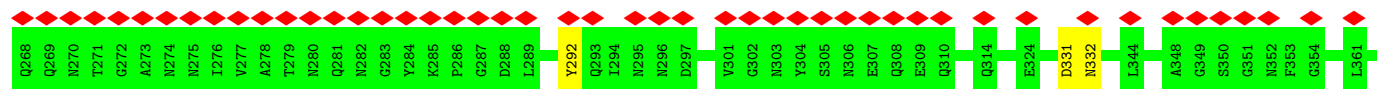
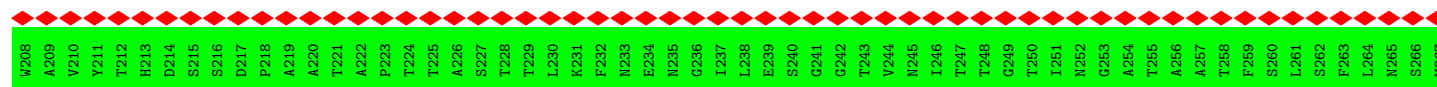
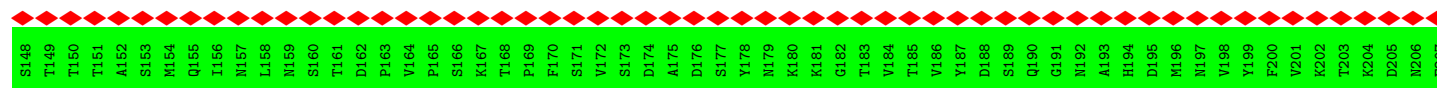
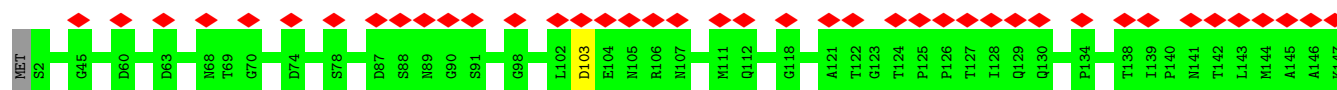




• Molecule 10: Flagellar hook protein FlgE

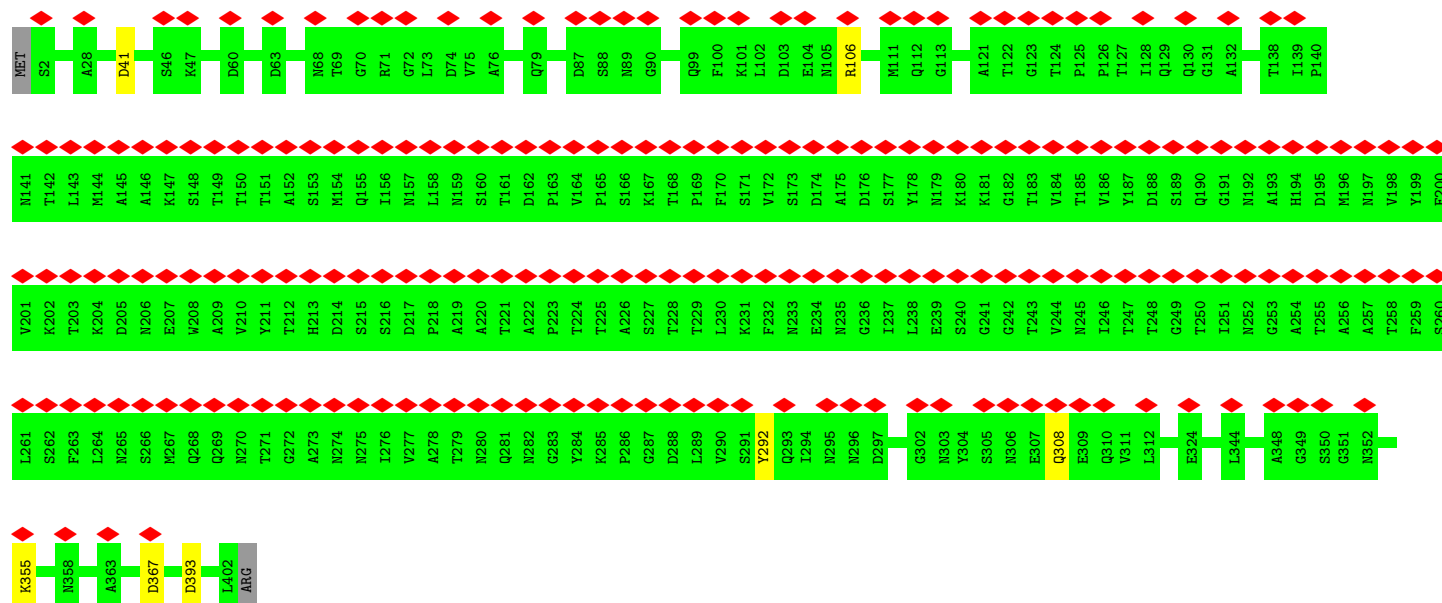


• Molecule 10: Flagellar hook protein FlgE

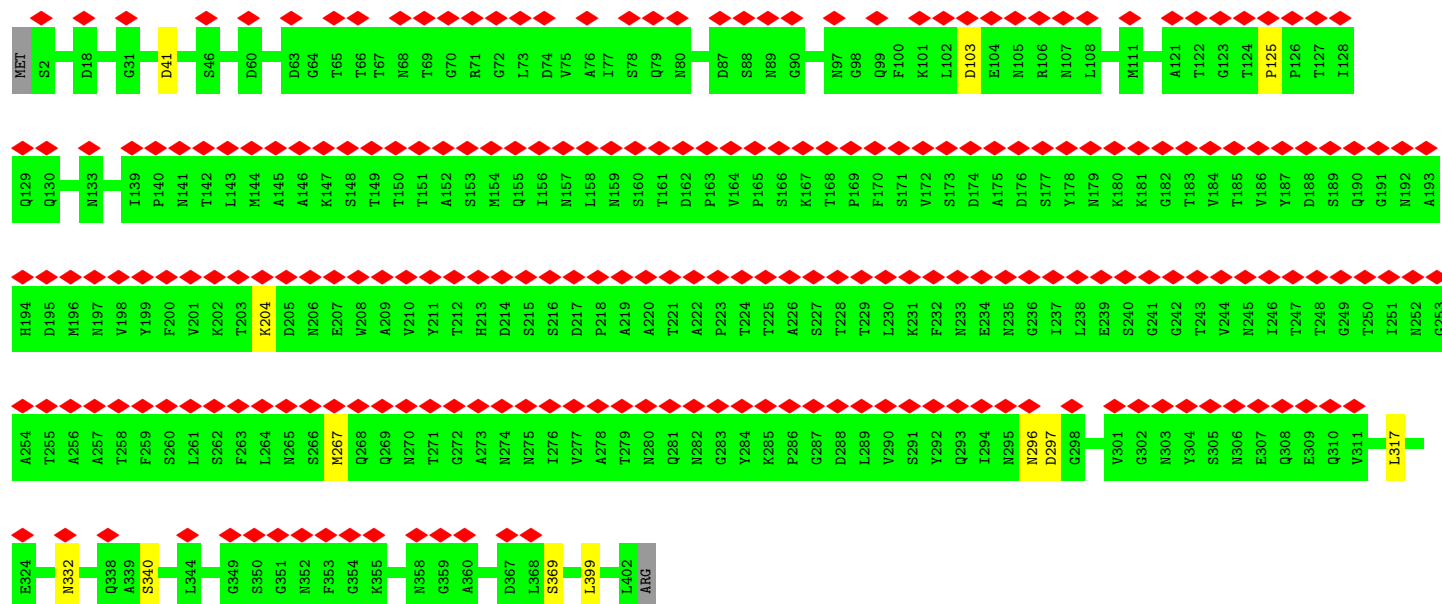


• Molecule 10: Flagellar hook protein FlgE

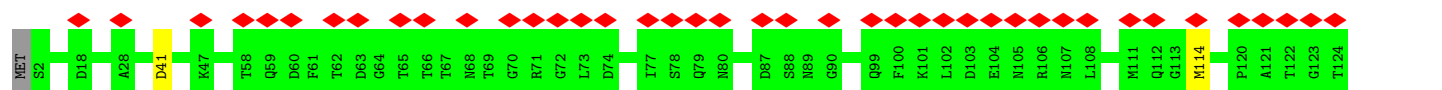


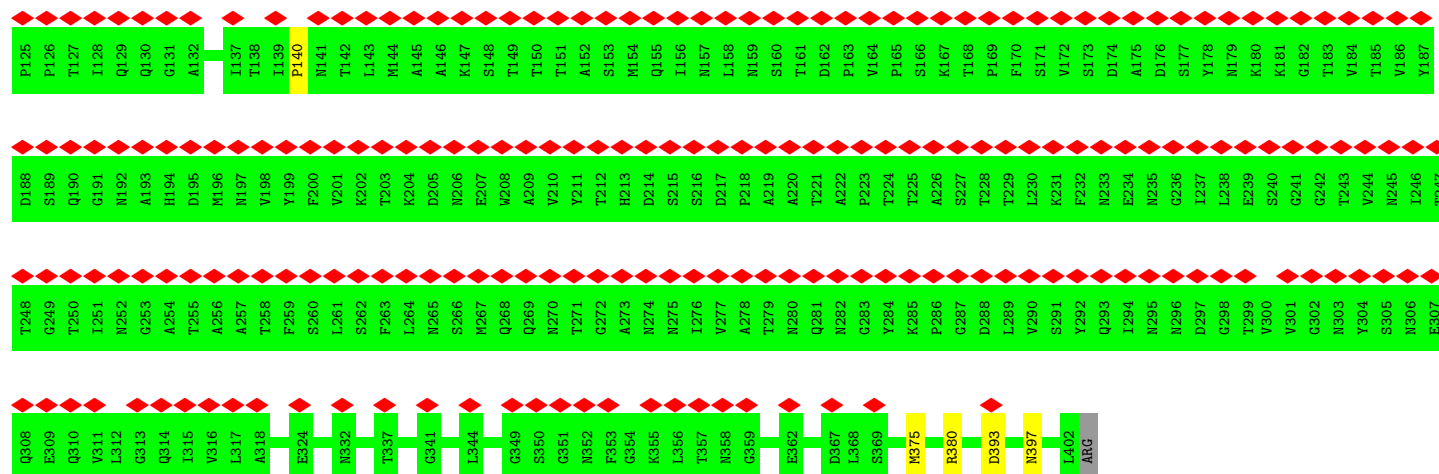


• Molecule 10: Flagellar hook protein FlgE



• Molecule 10: Flagellar hook protein FlgE

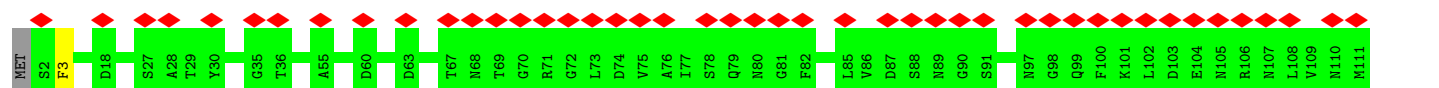




• Molecule 10: Flagellar hook protein FlgE

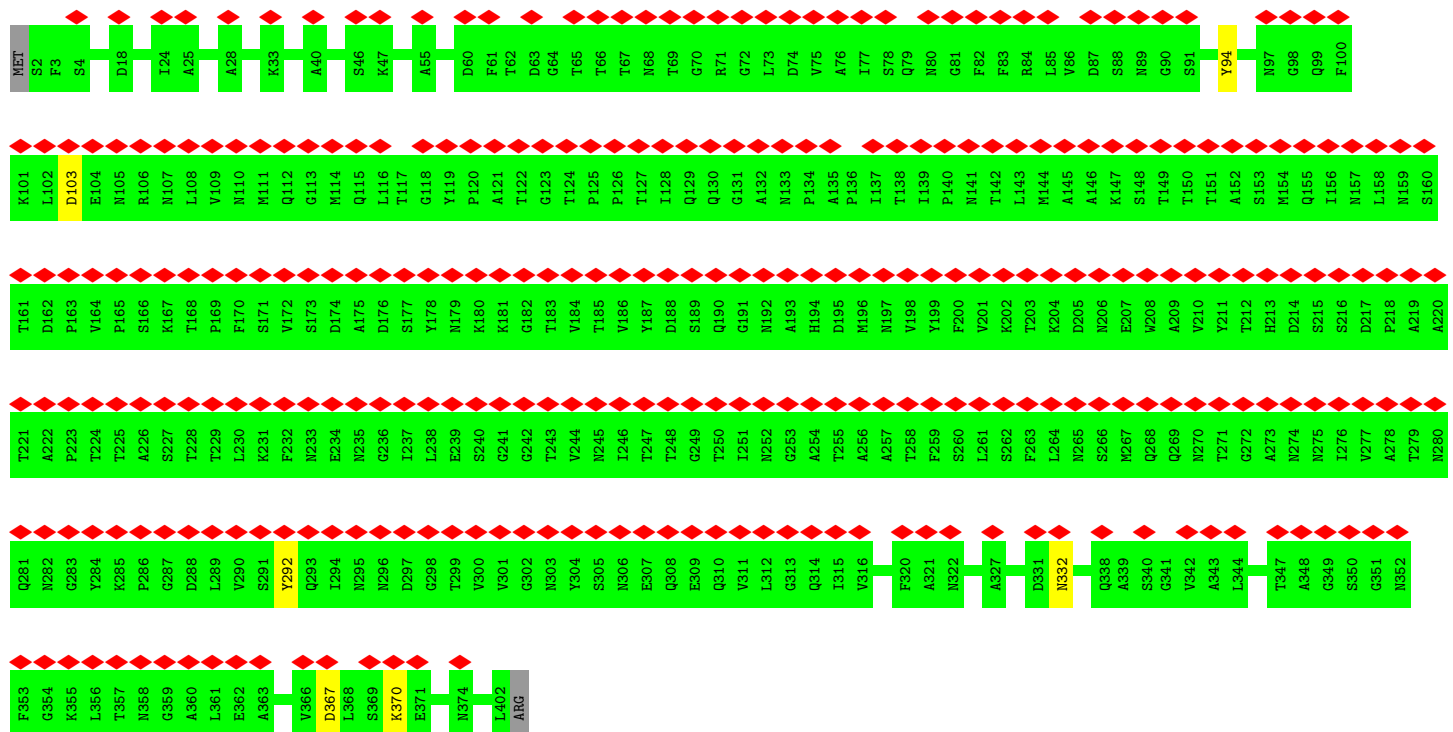
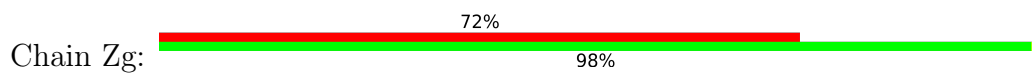


• Molecule 10: Flagellar hook protein FlgE

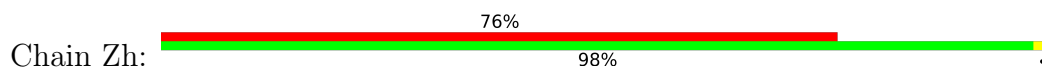


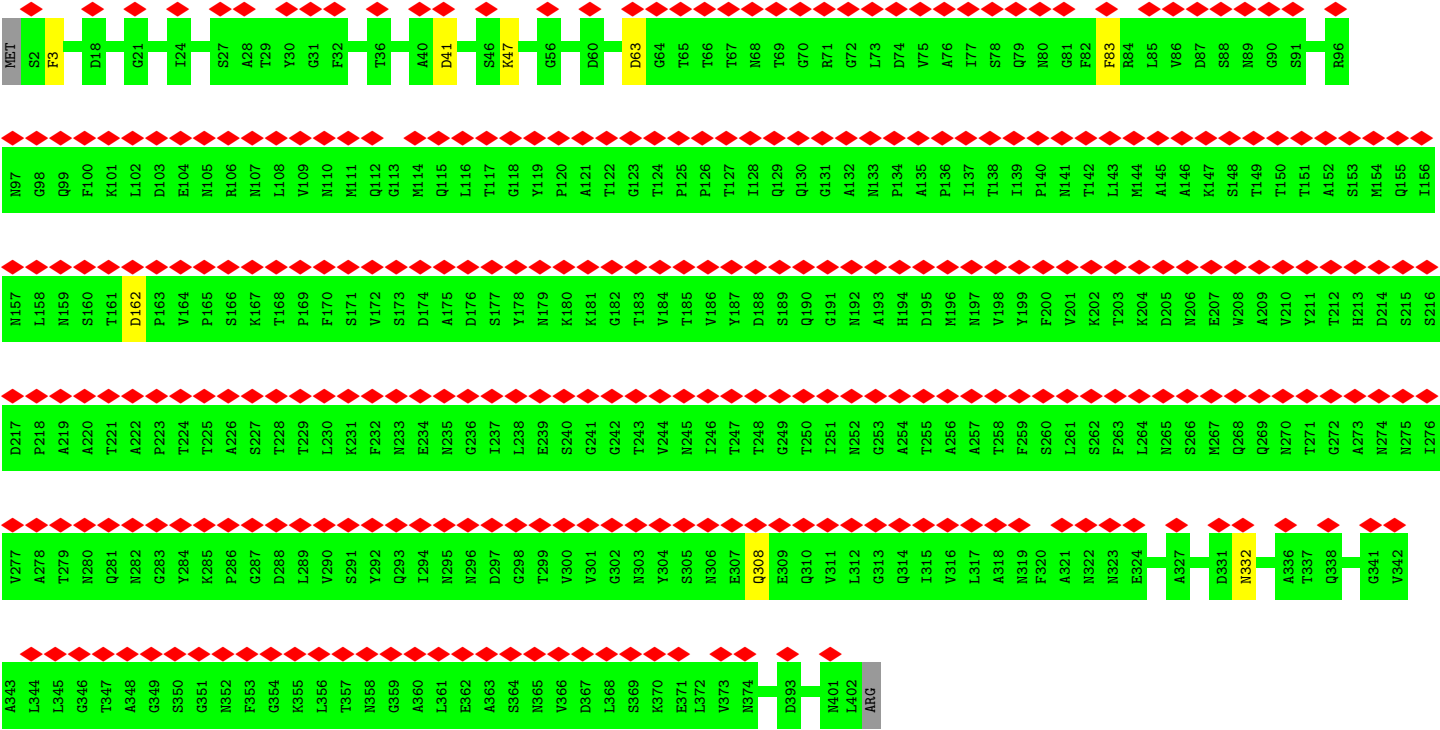


• Molecule 10: Flagellar hook protein FlgE



• Molecule 10: Flagellar hook protein FlgE





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	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	1.715	Depositor
Minimum map value	-1.213	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.080	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	A	0.29	0/681	0.47	0/930
1	B	0.26	0/681	0.49	0/930
1	C	0.28	0/681	0.48	0/930
1	D	0.28	0/681	0.49	0/930
2	E	0.38	1/1994 (0.1%)	0.56	1/2724 (0.0%)
3	F	0.36	0/1643	0.62	2/2237 (0.1%)
3	G	0.29	0/1665	0.49	1/2267 (0.0%)
3	H	0.29	0/1652	0.48	0/2249
3	I	0.28	0/1652	0.46	0/2249
3	J	0.30	0/1662	0.49	0/2263
4	K	0.26	0/300	0.47	0/400
4	L	0.25	0/547	0.44	0/733
4	M	0.26	0/561	0.44	0/753
4	N	0.25	0/561	0.46	0/753
4	O	0.26	0/561	0.49	0/753
4	P	0.27	0/554	0.46	0/743
5	Q	0.28	0/930	0.54	0/1251
5	R	0.26	0/855	0.48	0/1150
5	S	0.27	0/855	0.54	0/1150
5	T	0.25	0/870	0.49	0/1169
5	U	0.26	0/839	0.47	0/1129
6	V	0.28	0/981	0.44	0/1334
6	W	0.26	0/976	0.46	0/1327
6	X	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
6	Y	0.28	0/981	0.52	0/1334
6	Z	0.26	0/981	0.47	0/1334
6	a	0.28	0/981	0.47	0/1334
7	b	0.52	0/83	0.63	0/114
7	c	0.26	0/107	0.38	0/148
7	d	0.30	0/137	0.49	0/191
7	e	0.28	0/107	0.56	0/148
7	f	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
7	g	0.32	0/107	0.51	0/148
7	h	0.26	0/145	0.43	0/203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	i	0.30	0/107	0.38	0/148
7	j	0.30	0/137	0.57	0/191
7	k	0.30	0/107	0.37	0/148
7	l	0.29	0/145	0.45	0/203
8	m	0.33	0/1828	0.56	0/2492
8	n	0.28	0/1836	0.54	1/2502 (0.0%)
8	o	0.28	0/1844	0.54	0/2512
8	p	0.27	0/1844	0.53	0/2512
8	q	0.31	0/1836	0.55	0/2502
9	0	0.30	0/1888	0.52	1/2564 (0.0%)
9	1	0.31	0/1917	0.50	0/2605
9	2	0.27	0/1973	0.48	0/2682
9	3	0.28	0/1973	0.50	0/2682
9	4	0.28	0/1973	0.50	0/2682
9	5	0.32	0/1973	0.52	0/2682
9	6	0.30	0/1973	0.52	0/2682
9	7	0.28	0/1973	0.50	0/2682
9	8	0.30	0/1973	0.52	0/2682
9	9	0.29	0/1973	0.54	1/2682 (0.0%)
9	ZA	0.29	0/1973	0.52	0/2682
9	ZB	0.29	0/1973	0.49	0/2682
9	ZC	0.28	0/1973	0.51	0/2682
9	ZD	0.28	0/1973	0.51	0/2682
9	ZE	0.28	0/1973	0.50	1/2682 (0.0%)
9	r	0.33	0/1926	0.53	0/2618
9	s	0.36	0/1934	0.56	0/2629
9	t	0.33	0/1942	0.55	0/2639
9	u	0.32	0/1926	0.57	1/2618 (0.0%)
9	v	0.30	0/1934	0.51	0/2629
9	w	0.32	0/1844	0.51	0/2505
9	x	0.31	0/1888	0.51	0/2564
9	y	0.30	0/1888	0.54	1/2564 (0.0%)
9	z	0.30	0/1888	0.51	0/2564
10	ZF	0.27	0/2991	0.49	0/4076
10	ZG	0.31	0/2991	0.50	0/4076
10	ZH	0.28	0/2991	0.50	0/4076
10	ZI	0.29	0/2991	0.51	0/4076
10	ZJ	0.31	0/2991	0.51	0/4076
10	ZK	0.26	0/2991	0.48	0/4076
10	ZL	0.28	0/2991	0.49	0/4076
10	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
10	ZN	0.28	0/2991	0.51	0/4076
10	ZO	0.30	0/2991	0.50	0/4076

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
10	ZQ	0.28	0/2991	0.51	0/4076
10	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
10	ZS	0.29	0/2991	0.52	1/4076 (0.0%)
10	ZT	0.26	0/2991	0.47	0/4076
10	ZU	0.27	0/2991	0.50	0/4076
10	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
10	ZW	0.25	0/2991	0.48	0/4076
10	ZX	0.28	0/2991	0.48	0/4076
10	ZY	0.29	1/2991 (0.0%)	0.54	2/4076 (0.0%)
10	ZZ	0.25	0/2991	0.46	0/4076
10	Za	0.27	0/2991	0.49	0/4076
10	Zb	0.28	0/2991	0.50	0/4076
10	Zc	0.29	0/2991	0.53	2/4076 (0.0%)
10	Zd	0.29	0/2991	0.50	0/4076
10	Ze	0.27	0/2991	0.48	0/4076
10	Zf	0.27	0/2991	0.48	0/4076
10	Zg	0.27	0/2991	0.49	0/4076
10	Zh	0.26	0/2991	0.48	0/4076
All	All	0.30	10/170184 (0.0%)	0.52	32/231624 (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
3	H	0	1
5	Q	0	1
5	U	0	1
6	Y	0	1
6	a	0	1
8	m	0	2
8	n	0	1
8	o	0	1
8	q	0	1
9	0	0	2
9	1	0	1
9	5	0	1
9	6	0	1
9	8	0	1
9	ZA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	r	0	1
9	u	0	1
9	y	0	2
9	z	0	1
10	ZG	0	1
10	ZI	0	1
10	ZK	0	1
10	ZO	0	1
10	ZW	0	1
10	Zb	0	1
10	Zd	0	1
10	Ze	0	1
All	All	0	30

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	ZV	140	PRO	CG-CD	-16.10	0.97	1.50
7	f	331	PRO	CG-CD	-14.24	1.03	1.50
6	X	73	PRO	CG-CD	-12.72	1.08	1.50
10	ZV	125	PRO	CG-CD	-10.15	1.17	1.50
10	ZV	140	PRO	N-CD	8.31	1.59	1.47
6	X	73	PRO	CB-CG	-7.64	1.11	1.50
10	ZV	125	PRO	N-CD	6.64	1.57	1.47
2	E	185	MET	C-O	6.30	1.35	1.23
10	ZY	125	PRO	CG-CD	-5.43	1.32	1.50
10	ZR	125	PRO	CG-CD	-5.10	1.33	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	73	PRO	CB-CG-CD	18.81	179.87	106.50
6	X	73	PRO	N-CD-CG	-18.79	75.01	103.20
10	ZV	140	PRO	N-CD-CG	-17.34	77.19	103.20
7	f	331	PRO	N-CD-CG	-16.10	79.05	103.20
6	X	73	PRO	CA-CB-CG	-13.99	77.42	104.00
10	ZR	125	PRO	CA-N-CD	-13.96	91.96	111.50
10	ZY	125	PRO	CA-N-CD	-13.35	92.81	111.50
10	ZV	125	PRO	CA-N-CD	-13.26	92.94	111.50
3	F	162	PRO	CA-N-CD	-12.03	94.66	111.50
10	ZV	125	PRO	N-CD-CG	-11.23	86.35	103.20
10	Zc	125	PRO	CA-N-CD	-11.21	95.80	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	ZV	140	PRO	CA-N-CD	-10.24	97.16	111.50
10	ZV	140	PRO	CA-CB-CG	-9.29	86.35	104.00
7	f	331	PRO	CA-CB-CG	-9.01	86.89	104.00
10	ZM	223	PRO	CA-N-CD	-8.43	99.70	111.50
10	ZR	125	PRO	N-CD-CG	-7.58	91.83	103.20
10	ZY	125	PRO	N-CD-CG	-7.47	92.00	103.20
7	f	331	PRO	N-CA-CB	-7.05	94.84	103.30
3	F	162	PRO	N-CD-CG	-6.55	93.37	103.20
9	u	154	ASP	CB-CG-OD2	6.25	123.93	118.30
10	ZR	214	ASP	CB-CG-OD1	6.02	123.72	118.30
10	Zc	125	PRO	N-CD-CG	-5.85	94.42	103.20
9	y	154	ASP	CB-CG-OD1	5.75	123.47	118.30
9	0	52	PRO	N-CA-CB	-5.72	96.31	102.60
10	ZS	18	ASP	CB-CG-OD1	5.67	123.40	118.30
10	ZV	125	PRO	CA-CB-CG	-5.66	93.25	104.00
10	ZP	125	PRO	CA-N-CD	-5.57	103.70	111.50
9	ZE	13	ASP	CB-CG-OD1	5.54	123.29	118.30
2	E	189	PRO	CA-N-CD	-5.49	103.81	111.50
3	G	162	PRO	N-CA-CB	-5.32	96.75	102.60
8	n	72	ASP	CB-CG-OD1	5.25	123.03	118.30
9	9	109	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	0	36	ARG	Sidechain
9	0	50	ARG	Sidechain
9	1	36	ARG	Sidechain
9	5	50	ARG	Sidechain
9	6	153	ARG	Sidechain
9	8	238	ARG	Sidechain
3	H	143	ARG	Sidechain
5	Q	106	ARG	Sidechain
5	U	104	ARG	Sidechain
6	Y	110	ARG	Sidechain
9	ZA	79	ARG	Sidechain
10	ZG	71	ARG	Sidechain
10	ZI	380	ARG	Sidechain
10	ZK	71	ARG	Sidechain
10	ZO	71	ARG	Sidechain
10	ZW	71	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	Zb	106	ARG	Sidechain
10	Zd	380	ARG	Sidechain
10	Ze	380	ARG	Sidechain
6	a	110	ARG	Sidechain
8	m	200	ARG	Sidechain
8	m	243	ARG	Sidechain
8	n	225	ARG	Sidechain
8	o	243	ARG	Sidechain
8	q	160	ARG	Sidechain
9	r	36	ARG	Sidechain
9	u	116	ARG	Sidechain
9	y	36	ARG	Sidechain
9	y	50	ARG	Sidechain
9	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	A	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
1	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
1	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
1	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
2	E	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	5	25
3	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
3	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	42
3	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	56
3	J	207/245 (84%)	200 (97%)	5 (2%)	2 (1%)	13	42
4	K	38/104 (36%)	36 (95%)	2 (5%)	0	100	100
4	L	70/104 (67%)	70 (100%)	0	0	100	100
4	M	72/104 (69%)	70 (97%)	2 (3%)	0	100	100
4	N	72/104 (69%)	72 (100%)	0	0	100	100
4	O	72/104 (69%)	72 (100%)	0	0	100	100
4	P	71/104 (68%)	71 (100%)	0	0	100	100
5	Q	115/138 (83%)	115 (100%)	0	0	100	100
5	R	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
5	S	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
5	T	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
5	U	102/138 (74%)	101 (99%)	1 (1%)	0	100	100
6	V	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
6	W	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
6	X	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
6	Y	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
6	Z	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	46
6	a	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
7	b	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
7	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
7	d	18/560 (3%)	18 (100%)	0	0	100	100
7	e	14/560 (2%)	14 (100%)	0	0	100	100
7	f	19/560 (3%)	19 (100%)	0	0	100	100
7	g	14/560 (2%)	13 (93%)	1 (7%)	0	100	100
7	h	19/560 (3%)	19 (100%)	0	0	100	100
7	i	14/560 (2%)	14 (100%)	0	0	100	100
7	j	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
7	k	14/560 (2%)	14 (100%)	0	0	100	100
7	l	19/560 (3%)	19 (100%)	0	0	100	100
8	m	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	n	247/251 (98%)	241 (98%)	6 (2%)	0	100	100
8	o	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
8	p	248/251 (99%)	240 (97%)	8 (3%)	0	100	100
8	q	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	61
9	0	244/260 (94%)	236 (97%)	7 (3%)	1 (0%)	30	61
9	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	61
9	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	46
9	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	46
9	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	11	38
9	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	46
9	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	46
9	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	11	38
9	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	46
9	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	46
9	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	38
9	ZB	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	11	38
9	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	38
9	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	46
9	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	61
9	r	250/260 (96%)	237 (95%)	12 (5%)	1 (0%)	30	61
9	s	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	61
9	t	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	61
9	u	250/260 (96%)	242 (97%)	6 (2%)	2 (1%)	16	46
9	v	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	61
9	w	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	61
9	x	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	11	38
9	y	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	61
9	z	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	61
10	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	37	66
10	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	56
10	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
10	ZK	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	66
10	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	46
10	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	66
10	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	37	66
10	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
10	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	ZW	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
10	ZX	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	ZY	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
10	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	Za	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
10	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
10	Zd	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
10	Ze	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
10	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
10	Zg	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
10	Zh	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
All	All	22393/29305 (76%)	21644 (97%)	680 (3%)	69 (0%)	38	66

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	188	LEU
2	E	190	VAL

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Mol	Chain	Res	Type
3	J	83	ALA
8	m	123	GLU
9	2	209	ASN
9	5	209	ASN
9	8	209	ASN
9	ZA	209	ASN
9	ZB	164	GLN
9	ZC	139	ALA
10	ZG	46	SER
2	E	167	ASN
2	E	213	ILE
3	G	83	ALA
3	I	160	GLN
9	9	139	ALA
9	ZB	165	ALA
9	ZB	209	ASN
9	ZC	209	ASN
9	ZD	209	ASN
9	ZE	209	ASN
10	ZI	375	MET
10	ZO	237	ILE
10	ZR	87	ASP
9	u	165	ALA
9	x	4	SER
9	z	127	GLN
2	E	189	PRO
8	m	151	PRO
9	0	127	GLN
9	2	49	ILE
9	3	49	ILE
9	4	49	ILE
9	4	139	ALA
9	4	140	ILE
9	5	49	ILE
10	ZL	374	ASN
9	r	127	GLN
9	x	3	SER
9	y	127	GLN
9	6	49	ILE
9	6	58	GLU
9	7	49	ILE
9	7	138	PRO

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Mol	Chain	Res	Type
9	8	49	ILE
9	9	49	ILE
9	ZA	49	ILE
9	ZA	139	ALA
9	ZD	139	ALA
10	ZO	142	THR
10	ZP	374	ASN
9	s	127	GLN
9	u	127	GLN
9	w	127	GLN
9	x	127	GLN
3	G	162	PRO
9	1	127	GLN
9	7	210	GLY
9	t	127	GLN
9	v	127	GLN
2	E	187	ALA
6	Z	58	ALA
9	3	139	ALA
10	ZO	375	MET
8	m	149	GLY
8	q	132	GLY
10	ZI	325	GLY
3	J	229	VAL
9	ZC	138	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	74/74 (100%)	73 (99%)	1 (1%)	62	78
1	B	74/74 (100%)	73 (99%)	1 (1%)	62	78
1	C	74/74 (100%)	74 (100%)	0	100	100
1	D	74/74 (100%)	73 (99%)	1 (1%)	62	78
2	E	210/221 (95%)	204 (97%)	6 (3%)	37	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	177/204 (87%)	170 (96%)	7 (4%)	27	55
3	G	179/204 (88%)	172 (96%)	7 (4%)	27	55
3	H	178/204 (87%)	173 (97%)	5 (3%)	38	64
3	I	178/204 (87%)	172 (97%)	6 (3%)	32	59
3	J	179/204 (88%)	175 (98%)	4 (2%)	47	69
4	K	33/79 (42%)	30 (91%)	3 (9%)	7	27
4	L	56/79 (71%)	54 (96%)	2 (4%)	30	57
4	M	58/79 (73%)	57 (98%)	1 (2%)	56	74
4	N	58/79 (73%)	56 (97%)	2 (3%)	32	59
4	O	58/79 (73%)	56 (97%)	2 (3%)	32	59
4	P	57/79 (72%)	55 (96%)	2 (4%)	31	58
5	Q	98/113 (87%)	94 (96%)	4 (4%)	26	54
5	R	90/113 (80%)	88 (98%)	2 (2%)	47	69
5	S	90/113 (80%)	87 (97%)	3 (3%)	33	60
5	T	91/113 (80%)	90 (99%)	1 (1%)	70	82
5	U	89/113 (79%)	84 (94%)	5 (6%)	17	45
6	V	104/105 (99%)	104 (100%)	0	100	100
6	W	104/105 (99%)	103 (99%)	1 (1%)	73	84
6	X	104/105 (99%)	104 (100%)	0	100	100
6	Y	104/105 (99%)	102 (98%)	2 (2%)	52	72
6	Z	104/105 (99%)	101 (97%)	3 (3%)	37	63
6	a	104/105 (99%)	100 (96%)	4 (4%)	28	56
7	b	8/467 (2%)	8 (100%)	0	100	100
7	c	11/467 (2%)	10 (91%)	1 (9%)	7	27
7	d	14/467 (3%)	12 (86%)	2 (14%)	2	12
7	e	11/467 (2%)	11 (100%)	0	100	100
7	f	15/467 (3%)	15 (100%)	0	100	100
7	g	11/467 (2%)	11 (100%)	0	100	100
7	h	15/467 (3%)	15 (100%)	0	100	100
7	i	11/467 (2%)	11 (100%)	0	100	100
7	j	14/467 (3%)	13 (93%)	1 (7%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	k	11/467 (2%)	11 (100%)	0	100	100
7	l	15/467 (3%)	14 (93%)	1 (7%)	13	39
8	m	190/193 (98%)	187 (98%)	3 (2%)	58	76
8	n	191/193 (99%)	187 (98%)	4 (2%)	48	70
8	o	192/193 (100%)	187 (97%)	5 (3%)	41	66
8	p	192/193 (100%)	190 (99%)	2 (1%)	73	84
8	q	191/193 (99%)	190 (100%)	1 (0%)	86	91
9	0	205/215 (95%)	199 (97%)	6 (3%)	37	63
9	1	209/215 (97%)	201 (96%)	8 (4%)	28	56
9	2	215/215 (100%)	212 (99%)	3 (1%)	62	78
9	3	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	4	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	5	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	6	215/215 (100%)	210 (98%)	5 (2%)	45	68
9	7	215/215 (100%)	214 (100%)	1 (0%)	86	91
9	8	215/215 (100%)	213 (99%)	2 (1%)	75	85
9	9	215/215 (100%)	211 (98%)	4 (2%)	52	72
9	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	85
9	ZB	215/215 (100%)	207 (96%)	8 (4%)	29	56
9	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	78
9	ZD	215/215 (100%)	212 (99%)	3 (1%)	62	78
9	ZE	215/215 (100%)	214 (100%)	1 (0%)	86	91
9	r	209/215 (97%)	204 (98%)	5 (2%)	44	68
9	s	210/215 (98%)	203 (97%)	7 (3%)	33	60
9	t	211/215 (98%)	201 (95%)	10 (5%)	22	51
9	u	209/215 (97%)	200 (96%)	9 (4%)	25	53
9	v	210/215 (98%)	202 (96%)	8 (4%)	28	56
9	w	200/215 (93%)	196 (98%)	4 (2%)	50	71
9	x	205/215 (95%)	199 (97%)	6 (3%)	37	63
9	y	205/215 (95%)	197 (96%)	8 (4%)	27	55
9	z	205/215 (95%)	201 (98%)	4 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	ZF	321/323 (99%)	310 (97%)	11 (3%)	32	59
10	ZG	321/323 (99%)	306 (95%)	15 (5%)	22	51
10	ZH	321/323 (99%)	309 (96%)	12 (4%)	29	56
10	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	67
10	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	61
10	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	64
10	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	61
10	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	67
10	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	51
10	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	64
10	ZR	321/323 (99%)	313 (98%)	8 (2%)	42	67
10	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	ZT	321/323 (99%)	316 (98%)	5 (2%)	58	76
10	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	80
10	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	80
10	ZW	321/323 (99%)	309 (96%)	12 (4%)	29	56
10	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	85
10	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	69
10	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	76
10	Za	321/323 (99%)	316 (98%)	5 (2%)	58	76
10	Zb	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	59
10	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	Ze	321/323 (99%)	312 (97%)	9 (3%)	38	64
10	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	69
10	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	72
10	Zh	321/323 (99%)	313 (98%)	8 (2%)	42	67
All	All	18273/23835 (77%)	17828 (98%)	445 (2%)	45	68

All (445) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	B	47	MET
1	D	9	MET
2	E	36	ARG
2	E	86	PHE
2	E	185	MET
2	E	214	PHE
2	E	227	MET
2	E	229	MET
3	F	38	TRP
3	F	123	MET
3	F	129	LYS
3	F	155	ASN
3	F	160	GLN
3	F	190	PHE
3	F	213	PRO
3	G	75	ARG
3	G	102	SER
3	G	106	ASP
3	G	116	PHE
3	G	140	ARG
3	G	160	GLN
3	G	162	PRO
3	H	143	ARG
3	H	152	ARG
3	H	177	SER
3	H	187	PHE
3	H	190	PHE
3	I	113	TYR
3	I	143	ARG
3	I	187	PHE
3	I	205	MET
3	I	238	SER
3	I	241	GLN
3	J	117	SER
3	J	190	PHE
3	J	224	MET
3	J	230	ASP
4	K	74	ASP
4	K	79	SER
4	K	101	SER
4	L	75	MET
4	L	84	MET

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Mol	Chain	Res	Type
4	M	70	ASP
4	N	33	SER
4	N	81	SER
4	O	101	SER
4	O	102	MET
4	P	57	GLU
4	P	91	LYS
5	Q	34	ASP
5	Q	101	ASP
5	Q	113	SER
5	Q	125	SER
5	R	47	SER
5	R	55	ARG
5	S	48	GLU
5	S	91	ASP
5	S	128	LYS
5	T	47	SER
5	U	4	ARG
5	U	18	LEU
5	U	104	ARG
5	U	113	SER
5	U	125	SER
6	W	123	LYS
6	Y	30	ASN
6	Y	120	ASN
6	Z	20	ARG
6	Z	52	ASP
6	Z	84	LEU
6	a	86	ASP
6	a	88	ASN
6	a	125	MET
6	a	127	LEU
7	c	324	ASN
7	d	318	ASN
7	d	319	GLN
7	j	319	GLN
7	l	318	ASN
8	m	126	PRO
8	m	150	ASP
8	m	247	LEU
8	n	70	GLN
8	n	72	ASP

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Mol	Chain	Res	Type
8	n	97	GLU
8	n	153	ASN
8	o	70	GLN
8	o	85	ASP
8	o	189	ARG
8	o	225	ARG
8	o	236	SER
8	p	140	ASP
8	p	169	ASN
8	q	175	ASP
9	0	1	MET
9	0	36	ARG
9	0	50	ARG
9	0	52	PRO
9	0	73	ARG
9	0	185	GLU
9	1	1	MET
9	1	36	ARG
9	1	62	LEU
9	1	106	MET
9	1	119	SER
9	1	164	GLN
9	1	206	PRO
9	1	241	GLU
9	2	91	ASN
9	2	204	SER
9	2	238	ARG
9	3	43	ASP
9	3	109	ASP
9	3	153	ARG
9	3	244	SER
9	4	64	SER
9	4	204	SER
9	4	209	ASN
9	4	259	GLN
9	5	4	SER
9	5	137	GLN
9	5	154	ASP
9	5	181	ASP
9	6	59	GLN
9	6	73	ARG
9	6	78	GLU

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Mol	Chain	Res	Type
9	6	109	ASP
9	6	244	SER
9	7	73	ARG
9	8	58	GLU
9	8	100	GLN
9	9	106	MET
9	9	125	ASN
9	9	137	GLN
9	9	162	GLN
9	ZA	136	VAL
9	ZA	248	SER
9	ZB	1	MET
9	ZB	4	SER
9	ZB	58	GLU
9	ZB	73	ARG
9	ZB	119	SER
9	ZB	137	GLN
9	ZB	143	PRO
9	ZB	244	SER
9	ZC	123	ASP
9	ZC	136	VAL
9	ZC	244	SER
9	ZD	64	SER
9	ZD	66	LEU
9	ZD	240	TYR
9	ZE	141	THR
10	ZF	3	PHE
10	ZF	60	ASP
10	ZF	87	ASP
10	ZF	134	PRO
10	ZF	229	THR
10	ZF	265	ASN
10	ZF	280	ASN
10	ZF	284	TYR
10	ZF	289	LEU
10	ZF	352	ASN
10	ZF	355	LYS
10	ZG	3	PHE
10	ZG	38	SER
10	ZG	188	ASP
10	ZG	189	SER
10	ZG	227	SER

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Mol	Chain	Res	Type
10	ZG	234	GLU
10	ZG	260	SER
10	ZG	262	SER
10	ZG	265	ASN
10	ZG	267	MET
10	ZG	288	ASP
10	ZG	296	ASN
10	ZG	350	SER
10	ZG	352	ASN
10	ZG	397	ASN
10	ZH	34	SER
10	ZH	154	MET
10	ZH	227	SER
10	ZH	260	SER
10	ZH	281	GLN
10	ZH	284	TYR
10	ZH	288	ASP
10	ZH	331	ASP
10	ZH	355	LYS
10	ZH	375	MET
10	ZH	380	ARG
10	ZH	399	LEU
10	ZI	99	GLN
10	ZI	195	ASP
10	ZI	197	ASN
10	ZI	260	SER
10	ZI	352	ASN
10	ZI	358	ASN
10	ZJ	42	MET
10	ZJ	46	SER
10	ZJ	103	ASP
10	ZJ	107	ASN
10	ZJ	195	ASP
10	ZJ	233	ASN
10	ZJ	280	ASN
10	ZJ	331	ASP
10	ZK	3	PHE
10	ZK	268	GLN
10	ZK	297	ASP
10	ZK	305	SER
10	ZK	331	ASP
10	ZK	338	GLN

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Mol	Chain	Res	Type
10	ZL	78	SER
10	ZL	84	ARG
10	ZL	196	MET
10	ZL	234	GLU
10	ZL	267	MET
10	ZL	291	SER
10	ZL	338	GLN
10	ZL	368	LEU
10	ZL	370	LYS
10	ZL	382	TYR
10	ZM	53	LYS
10	ZM	89	ASN
10	ZM	153	SER
10	ZM	200	PHE
10	ZM	214	ASP
10	ZM	282	ASN
10	ZM	352	ASN
10	ZM	369	SER
10	ZM	370	LYS
10	ZN	43	PHE
10	ZN	78	SER
10	ZN	103	ASP
10	ZN	143	LEU
10	ZN	148	SER
10	ZN	157	ASN
10	ZN	216	SER
10	ZN	297	ASP
10	ZN	367	ASP
10	ZN	396	LEU
10	ZO	2	SER
10	ZO	74	ASP
10	ZO	174	ASP
10	ZO	178	TYR
10	ZO	235	ASN
10	ZO	237	ILE
10	ZO	331	ASP
10	ZO	375	MET
10	ZP	42	MET
10	ZP	63	ASP
10	ZP	74	ASP
10	ZP	95	SER
10	ZP	126	PRO

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Mol	Chain	Res	Type
10	ZP	162	ASP
10	ZP	227	SER
10	ZP	275	ASN
10	ZP	288	ASP
10	ZP	292	TYR
10	ZP	331	ASP
10	ZP	340	SER
10	ZP	369	SER
10	ZP	370	LYS
10	ZP	393	ASP
10	ZQ	46	SER
10	ZQ	101	LYS
10	ZQ	189	SER
10	ZQ	200	PHE
10	ZQ	211	TYR
10	ZQ	280	ASN
10	ZQ	305	SER
10	ZQ	367	ASP
10	ZQ	370	LYS
10	ZR	41	ASP
10	ZR	103	ASP
10	ZR	197	ASN
10	ZR	214	ASP
10	ZR	269	GLN
10	ZR	295	ASN
10	ZR	332	ASN
10	ZR	367	ASP
10	ZS	78	SER
10	ZS	103	ASP
10	ZS	170	PHE
10	ZS	202	LYS
10	ZS	245	ASN
10	ZS	367	ASP
10	ZT	148	SER
10	ZT	195	ASP
10	ZT	262	SER
10	ZT	297	ASP
10	ZT	358	ASN
10	ZU	3	PHE
10	ZU	78	SER
10	ZU	80	ASN
10	ZU	340	SER

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Mol	Chain	Res	Type
10	ZV	46	SER
10	ZV	232	PHE
10	ZV	307	GLU
10	ZV	308	GLN
10	ZW	3	PHE
10	ZW	53	LYS
10	ZW	188	ASP
10	ZW	195	ASP
10	ZW	215	SER
10	ZW	259	PHE
10	ZW	292	TYR
10	ZW	309	GLU
10	ZW	326	LEU
10	ZW	331	ASP
10	ZW	340	SER
10	ZW	358	ASN
10	ZX	3	PHE
10	ZX	63	ASP
10	ZX	195	ASP
10	ZY	60	ASP
10	ZY	80	ASN
10	ZY	192	ASN
10	ZY	204	LYS
10	ZY	252	ASN
10	ZY	332	ASN
10	ZY	350	SER
10	ZZ	3	PHE
10	ZZ	41	ASP
10	ZZ	88	SER
10	ZZ	148	SER
10	ZZ	393	ASP
10	Za	103	ASP
10	Za	292	TYR
10	Za	331	ASP
10	Za	332	ASN
10	Za	375	MET
10	Zb	41	ASP
10	Zb	292	TYR
10	Zb	308	GLN
10	Zb	355	LYS
10	Zb	367	ASP
10	Zb	393	ASP

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Mol	Chain	Res	Type
10	Zc	41	ASP
10	Zc	103	ASP
10	Zc	204	LYS
10	Zc	267	MET
10	Zc	296	ASN
10	Zc	297	ASP
10	Zc	317	LEU
10	Zc	332	ASN
10	Zc	340	SER
10	Zc	369	SER
10	Zc	399	LEU
10	Zd	41	ASP
10	Zd	114	MET
10	Zd	140	PRO
10	Zd	375	MET
10	Zd	393	ASP
10	Zd	397	ASN
10	Ze	3	PHE
10	Ze	27	SER
10	Ze	46	SER
10	Ze	58	THR
10	Ze	60	ASP
10	Ze	130	GLN
10	Ze	308	GLN
10	Ze	319	ASN
10	Ze	395	ILE
10	Zf	3	PHE
10	Zf	285	LYS
10	Zf	297	ASP
10	Zf	331	ASP
10	Zf	332	ASN
10	Zf	367	ASP
10	Zf	396	LEU
10	Zg	94	TYR
10	Zg	103	ASP
10	Zg	292	TYR
10	Zg	332	ASN
10	Zg	367	ASP
10	Zg	370	LYS
10	Zh	3	PHE
10	Zh	41	ASP
10	Zh	47	LYS

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Mol	Chain	Res	Type
10	Zh	63	ASP
10	Zh	83	PHE
10	Zh	162	ASP
10	Zh	308	GLN
10	Zh	332	ASN
9	r	4	SER
9	r	19	MET
9	r	36	ARG
9	r	44	LEU
9	r	154	ASP
9	s	16	GLN
9	s	36	ARG
9	s	73	ARG
9	s	137	GLN
9	s	169	GLN
9	s	222	SER
9	s	251	ASP
9	t	1	MET
9	t	44	LEU
9	t	66	LEU
9	t	87	SER
9	t	93	LYS
9	t	100	GLN
9	t	148	SER
9	t	154	ASP
9	t	245	LYS
9	t	251	ASP
9	u	4	SER
9	u	30	SER
9	u	123	ASP
9	u	148	SER
9	u	169	GLN
9	u	179	MET
9	u	202	ASN
9	u	222	SER
9	u	252	GLN
9	v	36	ARG
9	v	73	ARG
9	v	91	ASN
9	v	94	ASP
9	v	127	GLN
9	v	194	GLU

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Mol	Chain	Res	Type
9	v	197	SER
9	v	225	ASN
9	w	4	SER
9	w	6	TRP
9	w	36	ARG
9	w	181	ASP
9	x	1	MET
9	x	137	GLN
9	x	172	GLN
9	x	185	GLU
9	x	198	SER
9	x	209	ASN
9	y	1	MET
9	y	30	SER
9	y	36	ARG
9	y	50	ARG
9	y	82	SER
9	y	169	GLN
9	y	208	LEU
9	y	209	ASN
9	z	1	MET
9	z	3	SER
9	z	117	ASP
9	z	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (449) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	39	GLN
2	E	162	ASN
2	E	182	ASN
2	E	205	ASN
3	F	119	GLN
3	F	141	GLN
3	H	36	GLN
3	H	233	GLN
3	I	160	GLN
3	I	184	GLN
3	J	114	GLN
3	J	155	ASN
4	K	103	GLN
4	L	90	ASN

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Mol	Chain	Res	Type
4	M	83	GLN
4	M	103	GLN
4	N	87	GLN
4	O	39	HIS
4	O	55	GLN
4	O	97	GLN
4	P	76	GLN
5	Q	17	ASN
5	Q	23	GLN
5	R	23	GLN
5	R	29	ASN
5	R	92	GLN
5	R	117	GLN
5	S	32	ASN
5	S	92	GLN
5	S	135	GLN
5	T	17	ASN
5	T	21	GLN
5	T	32	ASN
5	T	117	GLN
5	U	13	GLN
5	U	112	ASN
6	V	30	ASN
6	W	22	ASN
6	W	120	ASN
6	X	22	ASN
6	X	50	GLN
6	X	57	GLN
6	X	134	GLN
6	Z	17	GLN
6	a	5	ASN
6	a	57	GLN
6	a	115	ASN
7	b	319	GLN
7	h	324	ASN
7	l	318	ASN
7	l	324	ASN
8	m	102	ASN
8	n	18	GLN
8	n	172	GLN
8	n	210	ASN
8	n	223	ASN

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Mol	Chain	Res	Type
8	n	240	ASN
8	o	18	GLN
8	o	28	ASN
8	o	70	GLN
8	o	104	ASN
8	o	106	GLN
8	o	186	GLN
8	p	17	ASN
8	p	28	ASN
8	p	104	ASN
8	p	106	GLN
8	p	153	ASN
8	p	210	ASN
8	p	240	ASN
8	q	18	GLN
8	q	37	GLN
8	q	112	GLN
8	q	116	GLN
9	0	88	GLN
9	0	100	GLN
9	0	135	GLN
9	0	137	GLN
9	0	180	ASN
9	0	235	GLN
9	0	237	GLN
9	0	255	GLN
9	1	47	GLN
9	1	67	GLN
9	1	91	ASN
9	1	121	GLN
9	1	135	GLN
9	1	223	ASN
9	1	252	GLN
9	2	164	GLN
9	2	180	ASN
9	2	255	GLN
9	3	24	ASN
9	3	67	GLN
9	3	161	GLN
9	3	190	ASN
9	3	255	GLN
9	4	37	GLN

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Mol	Chain	Res	Type
9	4	47	GLN
9	4	51	GLN
9	4	125	ASN
9	4	127	GLN
9	4	174	ASN
9	4	216	GLN
9	4	235	GLN
9	4	243	ASN
9	4	259	GLN
9	5	51	GLN
9	5	55	GLN
9	5	85	ASN
9	5	100	GLN
9	5	121	GLN
9	5	237	GLN
9	5	252	GLN
9	6	16	GLN
9	6	59	GLN
9	6	91	ASN
9	6	121	GLN
9	6	127	GLN
9	6	135	GLN
9	6	209	ASN
9	6	237	GLN
9	7	24	ASN
9	7	55	GLN
9	7	164	GLN
9	7	235	GLN
9	8	83	GLN
9	8	91	ASN
9	8	196	GLN
9	9	37	GLN
9	9	55	GLN
9	9	85	ASN
9	9	91	ASN
9	9	259	GLN
9	ZA	37	GLN
9	ZA	235	GLN
9	ZB	24	ASN
9	ZB	25	ASN
9	ZB	28	ASN
9	ZB	37	GLN

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Mol	Chain	Res	Type
9	ZB	137	GLN
9	ZB	235	GLN
9	ZC	16	GLN
9	ZC	88	GLN
9	ZC	100	GLN
9	ZC	190	ASN
9	ZD	24	ASN
9	ZD	67	GLN
9	ZD	88	GLN
9	ZD	91	ASN
9	ZD	127	GLN
9	ZD	135	GLN
9	ZD	161	GLN
9	ZD	235	GLN
9	ZE	37	GLN
9	ZE	67	GLN
9	ZE	121	GLN
9	ZE	252	GLN
10	ZF	5	GLN
10	ZF	16	ASN
10	ZF	107	ASN
10	ZF	155	GLN
10	ZF	197	ASN
10	ZF	358	ASN
10	ZF	385	ASN
10	ZF	401	ASN
10	ZG	89	ASN
10	ZG	130	GLN
10	ZG	133	ASN
10	ZG	332	ASN
10	ZG	387	GLN
10	ZG	397	ASN
10	ZG	401	ASN
10	ZH	5	GLN
10	ZH	155	GLN
10	ZH	206	ASN
10	ZH	270	ASN
10	ZH	296	ASN
10	ZH	352	ASN
10	ZH	365	ASN
10	ZH	379	GLN
10	ZH	392	GLN

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

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Mol	Chain	Res	Type
10	ZM	213	HIS
10	ZM	235	ASN
10	ZM	252	ASN
10	ZM	381	ASN
10	ZN	79	GLN
10	ZN	107	ASN
10	ZN	112	GLN
10	ZN	129	GLN
10	ZN	133	ASN
10	ZN	190	GLN
10	ZN	192	ASN
10	ZN	197	ASN
10	ZN	319	ASN
10	ZN	338	GLN
10	ZN	379	GLN
10	ZN	387	GLN
10	ZN	401	ASN
10	ZO	89	ASN
10	ZO	141	ASN
10	ZO	192	ASN
10	ZO	235	ASN
10	ZO	332	ASN
10	ZP	11	ASN
10	ZP	107	ASN
10	ZP	129	GLN
10	ZP	194	HIS
10	ZP	269	GLN
10	ZP	270	ASN
10	ZP	314	GLN
10	ZP	322	ASN
10	ZP	338	GLN
10	ZP	379	GLN
10	ZP	381	ASN
10	ZP	385	ASN
10	ZQ	89	ASN
10	ZQ	97	ASN
10	ZQ	133	ASN
10	ZQ	141	ASN
10	ZQ	155	GLN
10	ZQ	197	ASN
10	ZQ	233	ASN
10	ZQ	338	GLN

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

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Mol	Chain	Res	Type
10	ZW	26	ASN
10	ZW	107	ASN
10	ZW	129	GLN
10	ZW	133	ASN
10	ZW	155	GLN
10	ZW	197	ASN
10	ZW	252	ASN
10	ZW	310	GLN
10	ZW	314	GLN
10	ZW	332	ASN
10	ZX	80	ASN
10	ZX	133	ASN
10	ZX	159	ASN
10	ZX	314	GLN
10	ZX	352	ASN
10	ZY	5	GLN
10	ZY	115	GLN
10	ZY	159	ASN
10	ZY	197	ASN
10	ZY	268	GLN
10	ZY	392	GLN
10	ZZ	5	GLN
10	ZZ	99	GLN
10	ZZ	107	ASN
10	ZZ	133	ASN
10	ZZ	194	HIS
10	ZZ	197	ASN
10	ZZ	314	GLN
10	ZZ	332	ASN
10	ZZ	379	GLN
10	ZZ	394	GLN
10	ZZ	401	ASN
10	Za	115	GLN
10	Za	129	GLN
10	Za	133	ASN
10	Za	197	ASN
10	Za	387	GLN
10	Zb	5	GLN
10	Zb	79	GLN
10	Zb	107	ASN
10	Zb	129	GLN
10	Zb	133	ASN

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

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Mol	Chain	Res	Type
10	Zh	379	GLN
10	Zh	392	GLN
9	r	47	GLN
9	r	83	GLN
9	r	85	ASN
9	r	121	GLN
9	r	135	GLN
9	r	172	GLN
9	r	174	ASN
9	r	223	ASN
9	s	16	GLN
9	s	28	ASN
9	s	169	GLN
9	s	223	ASN
9	s	259	GLN
9	t	47	GLN
9	t	85	ASN
9	t	104	GLN
9	t	127	GLN
9	t	162	GLN
9	t	259	GLN
9	u	16	GLN
9	u	32	ASN
9	u	196	GLN
9	v	47	GLN
9	v	90	ASN
9	v	161	GLN
9	v	164	GLN
9	v	169	GLN
9	v	172	GLN
9	v	223	ASN
9	v	232	ASN
9	w	28	ASN
9	w	121	GLN
9	w	135	GLN
9	w	196	GLN
9	w	223	ASN
9	w	235	GLN
9	x	32	ASN
9	x	104	GLN
9	x	121	GLN
9	x	127	GLN

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Mol	Chain	Res	Type
9	x	145	ASN
9	x	209	ASN
9	y	25	ASN
9	y	37	GLN
9	y	51	GLN
9	y	67	GLN
9	y	125	ASN
9	y	127	GLN
9	y	209	ASN
9	y	223	ASN
9	y	252	GLN
9	z	67	GLN
9	z	85	ASN
9	z	125	ASN
9	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.

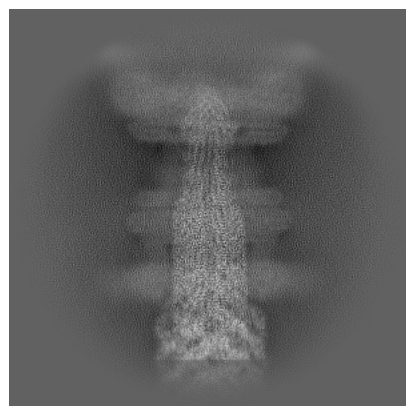
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37601. These allow visual inspection of the internal detail of the map and identification of artifacts.

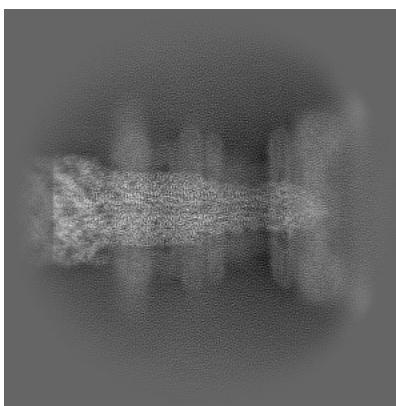
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

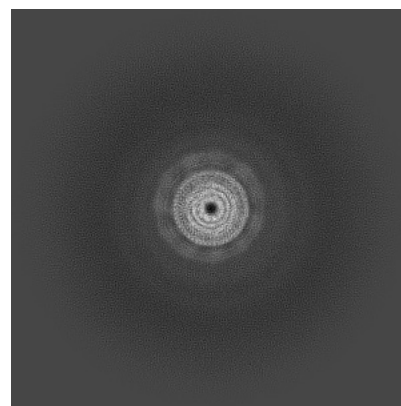
6.1.1 Primary map



X

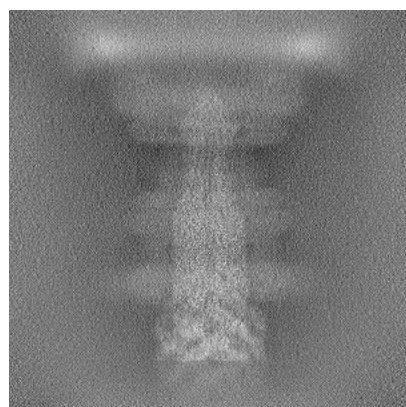


Y

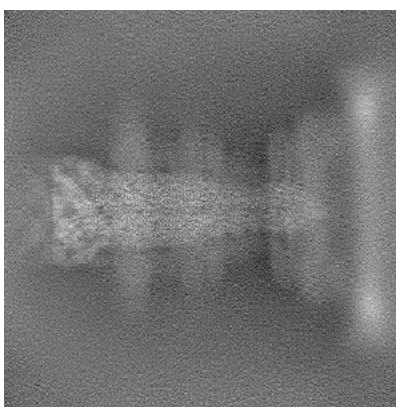


Z

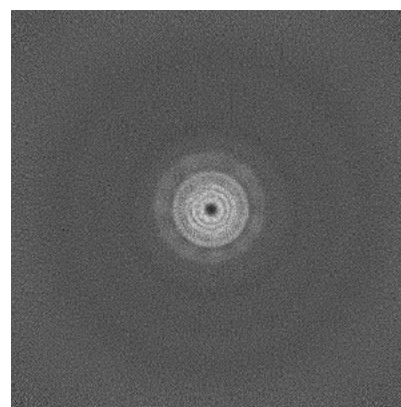
6.1.2 Raw map



X



Y

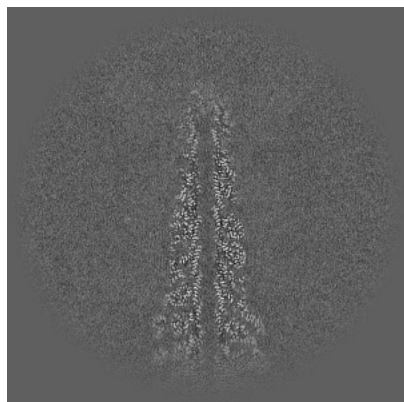


Z

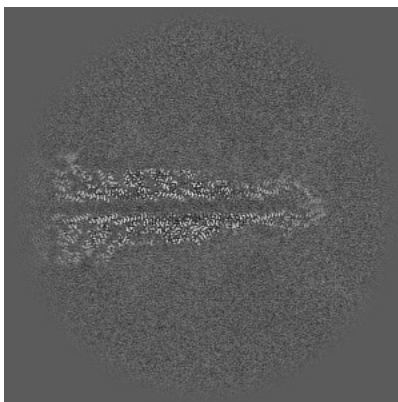
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

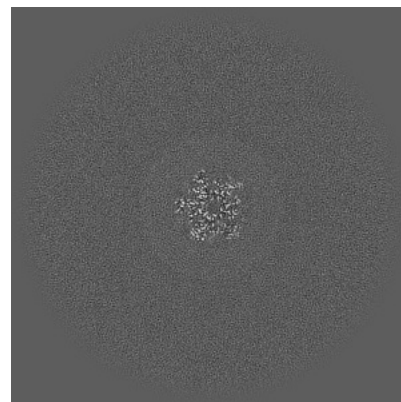
6.2.1 Primary map



X Index: 256

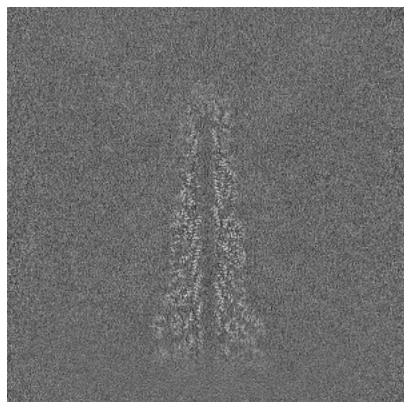


Y Index: 256

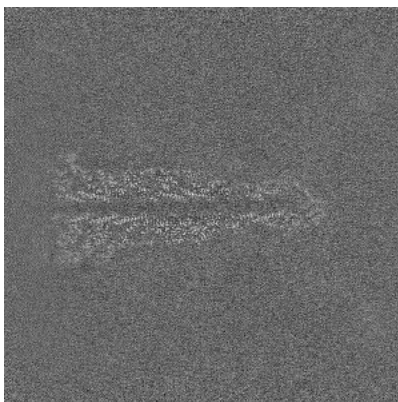


Z Index: 256

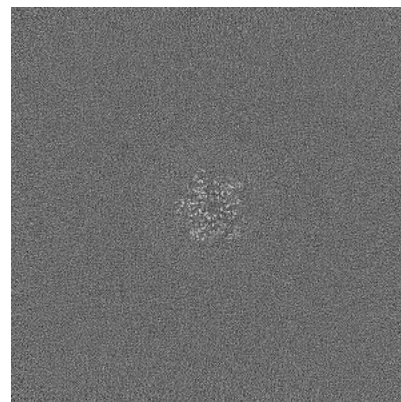
6.2.2 Raw map



X Index: 256



Y Index: 256

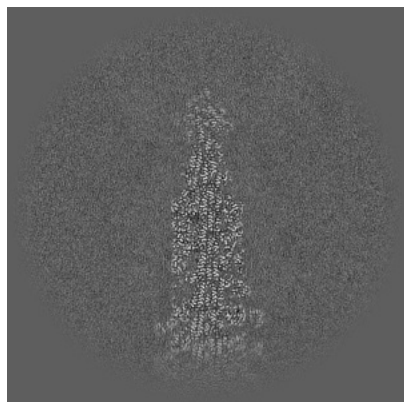


Z Index: 256

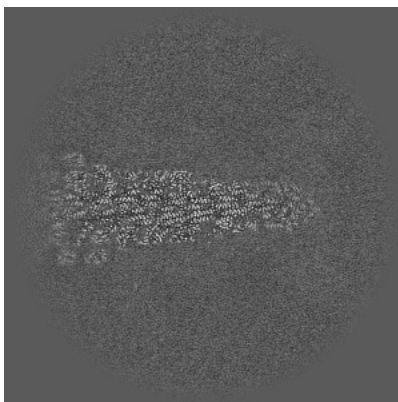
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

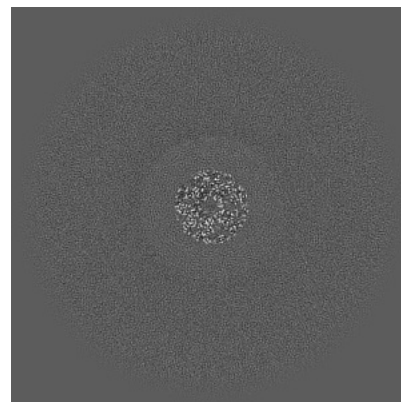
6.3.1 Primary map



X Index: 242

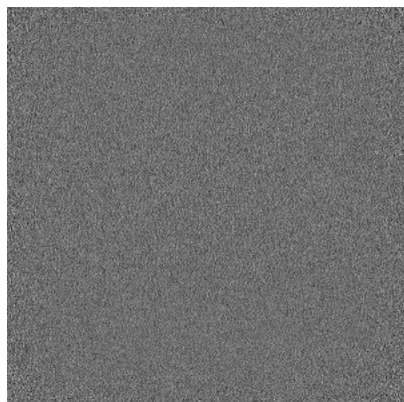


Y Index: 268

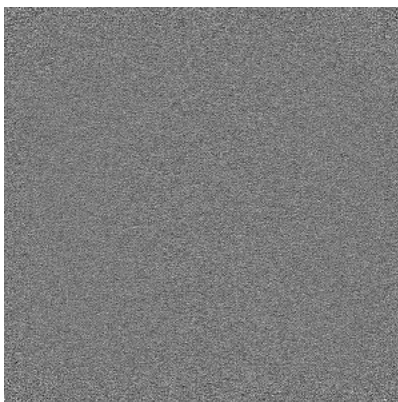


Z Index: 224

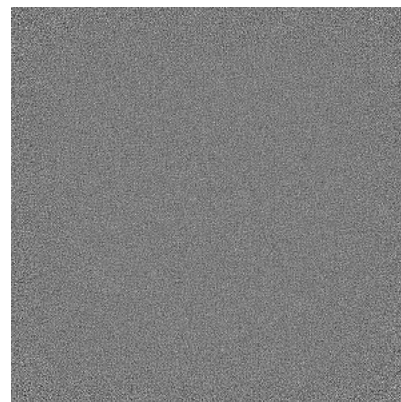
6.3.2 Raw map



X Index: 0



Y Index: 0

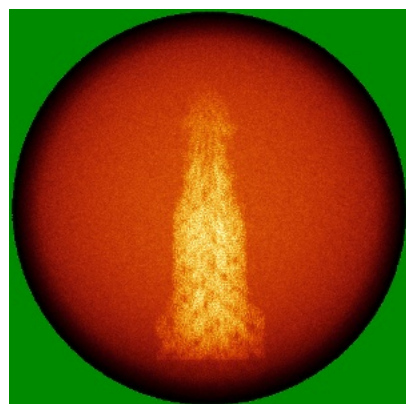


Z Index: 0

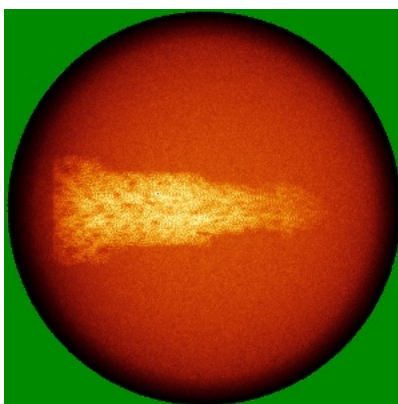
The images above show the largest variance slices of the map in three orthogonal directions.

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

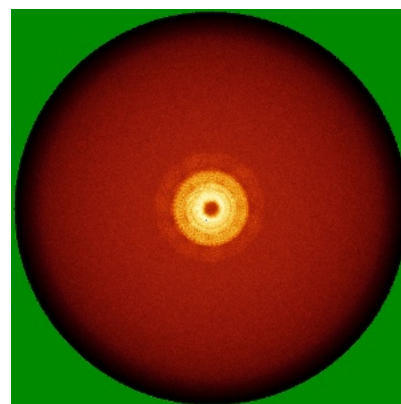
6.4.1 Primary map



X

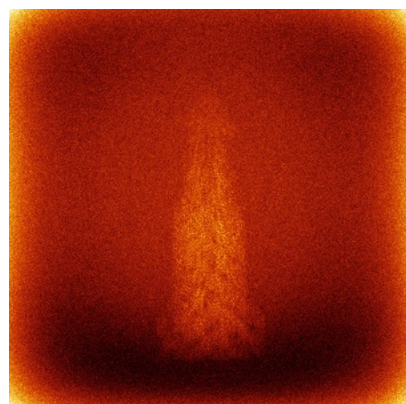


Y

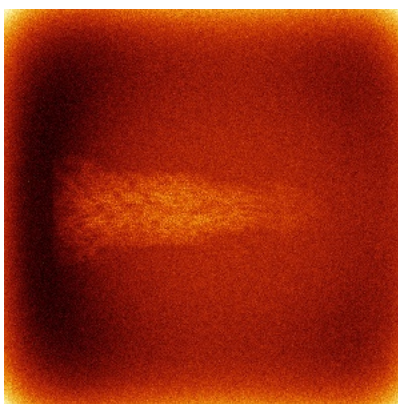


Z

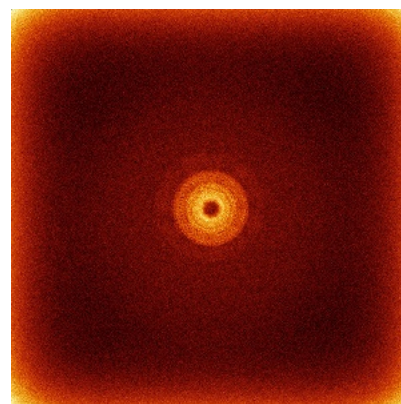
6.4.2 Raw map



X



Y

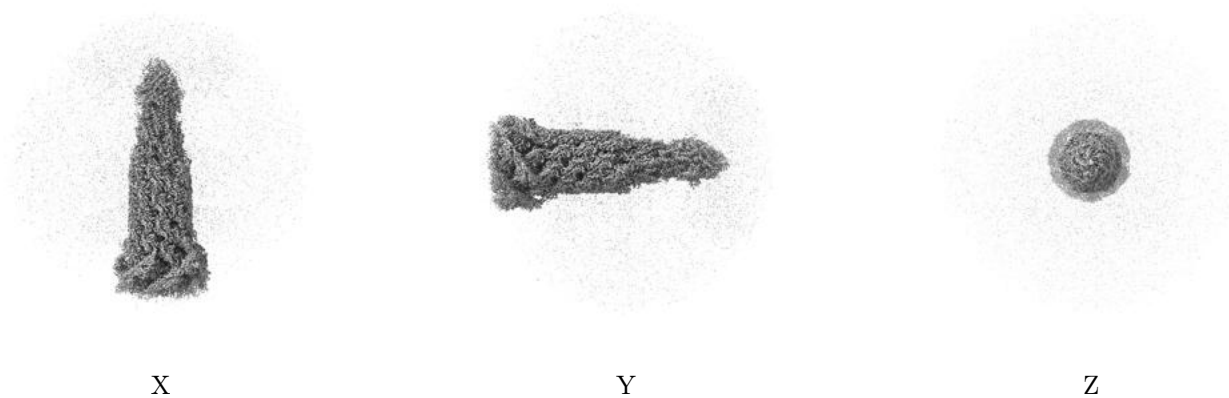


Z

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.

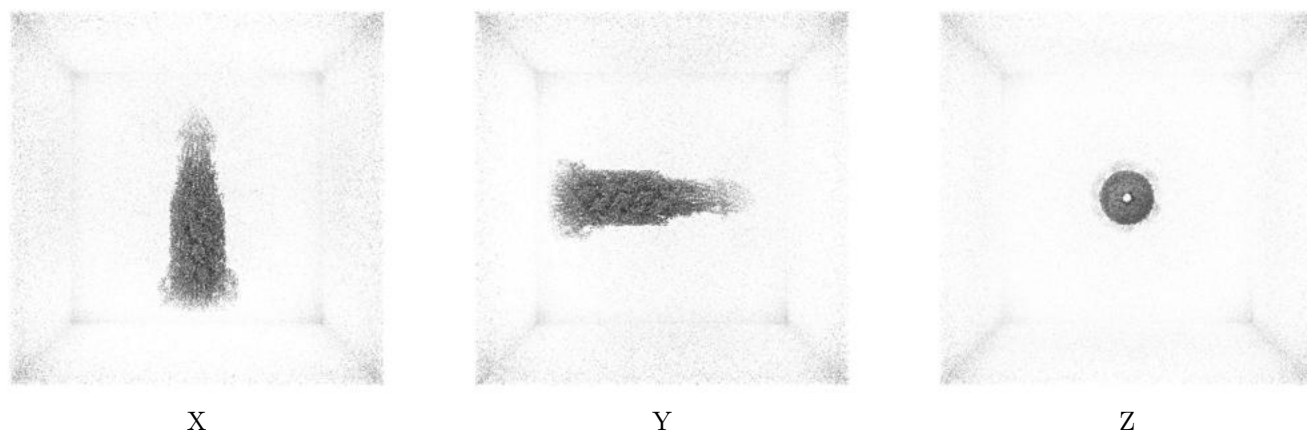
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

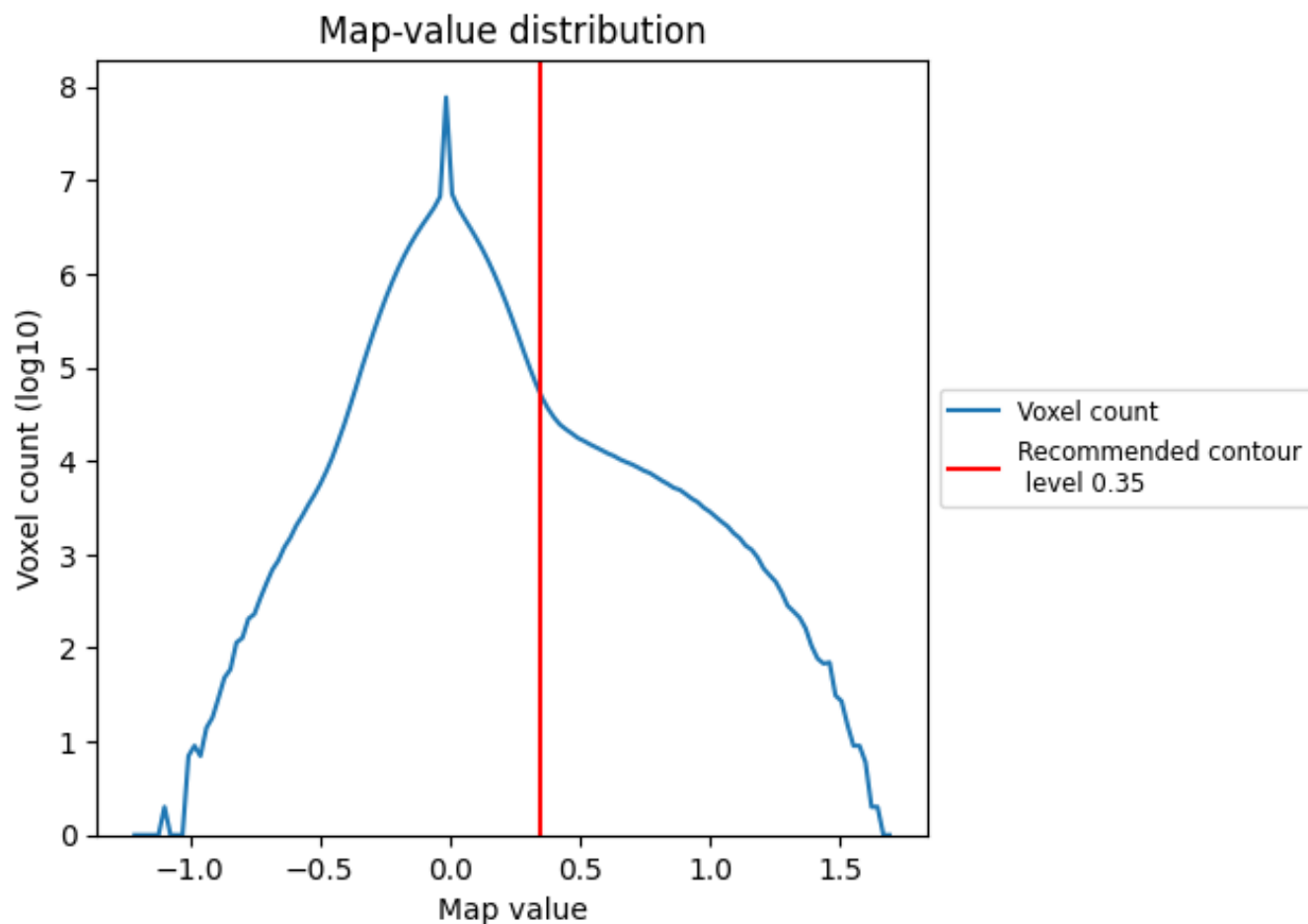
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

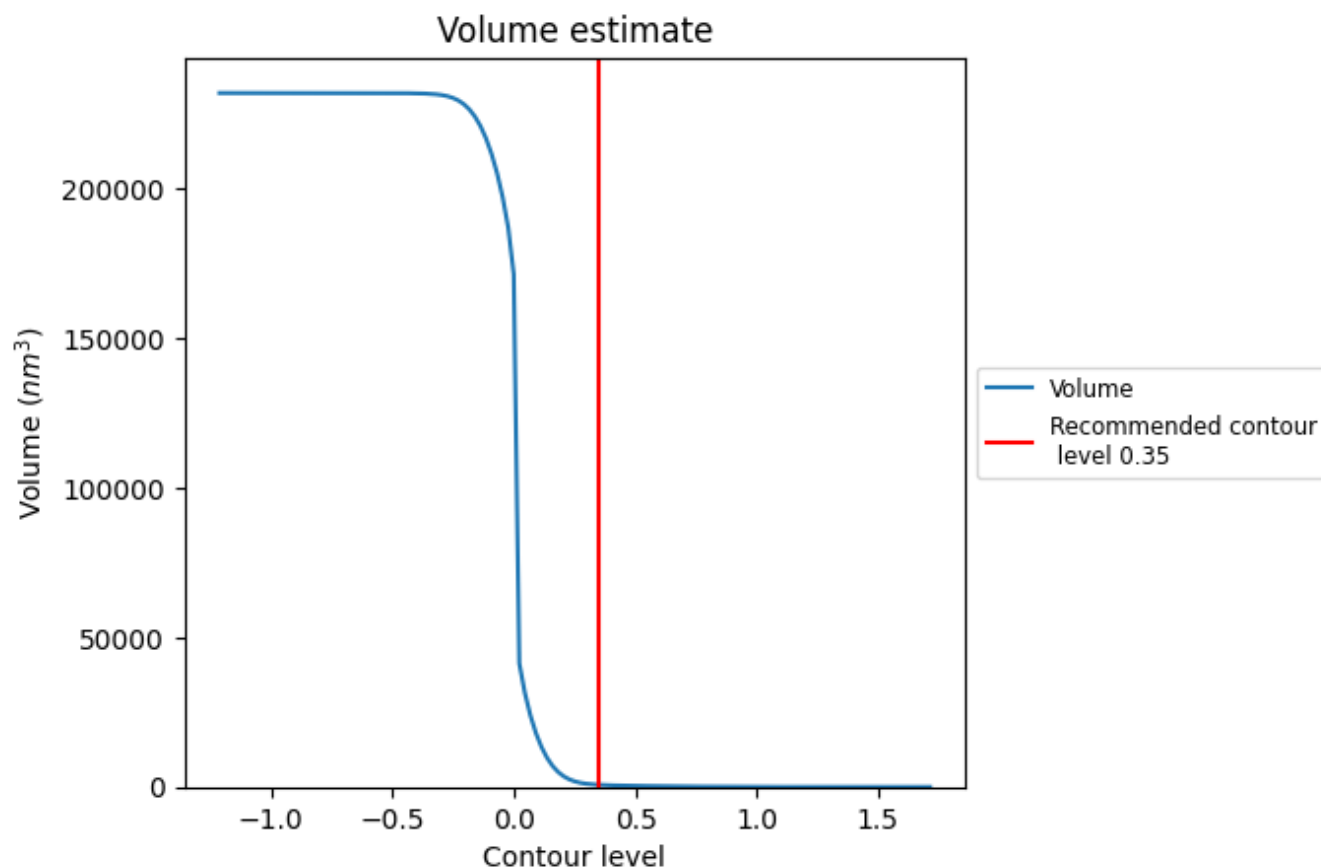
This section contains the results of statistical analysis of the map.

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.

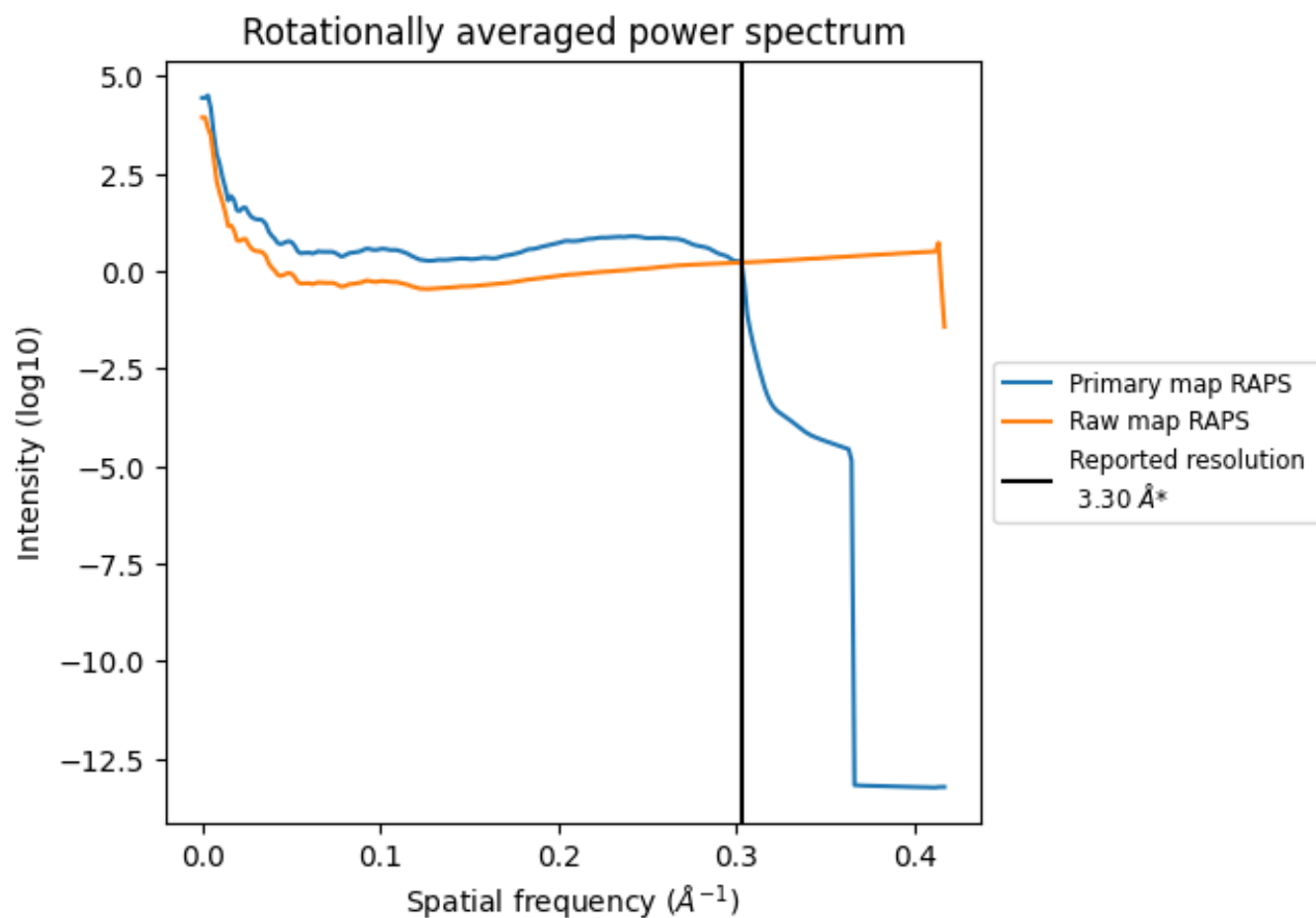
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 705 nm³; this corresponds to an approximate mass of 637 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

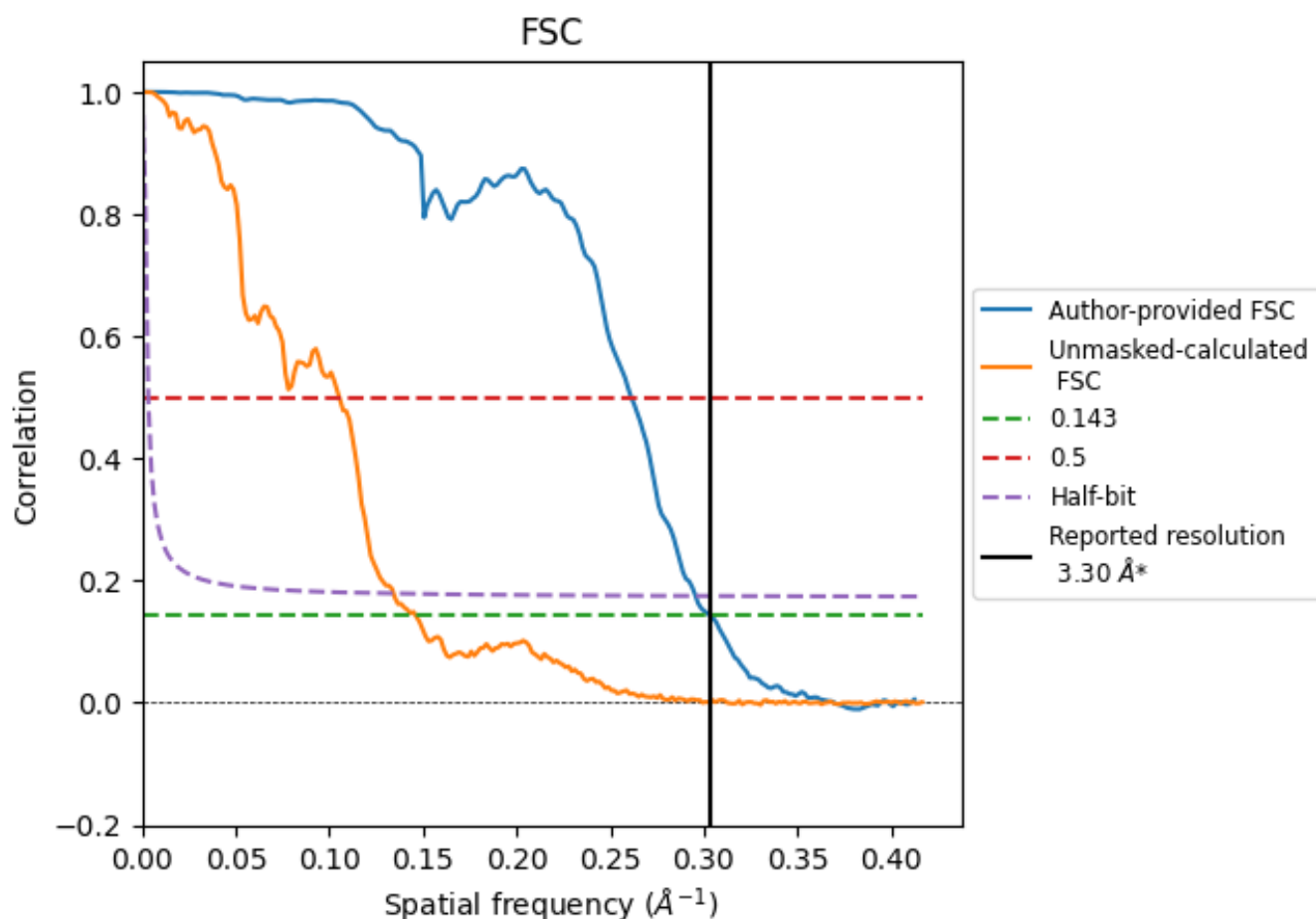


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [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 \AA^{-1}

8.2 Resolution estimates [i](#)

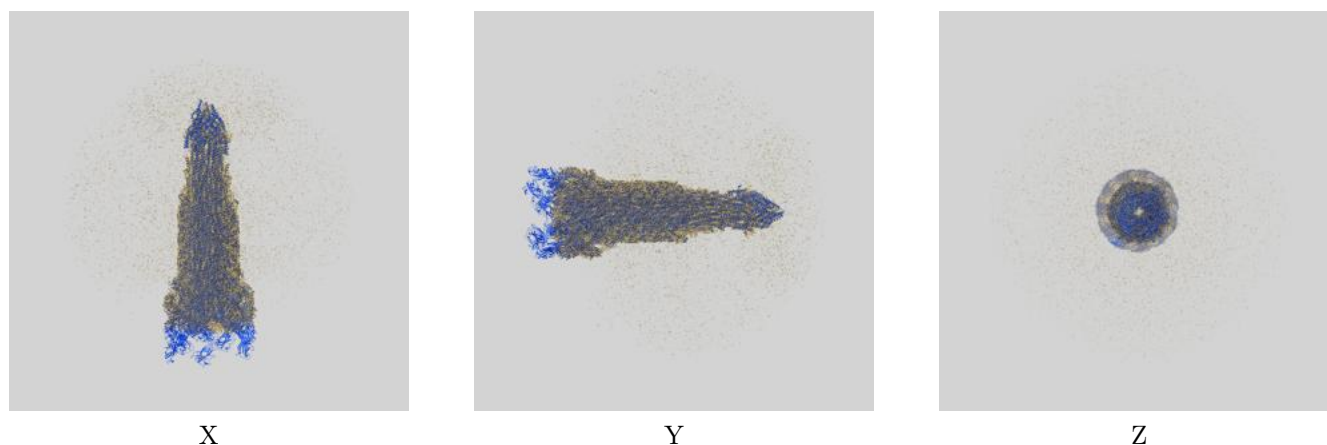
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.83	3.38
Unmasked-calculated*	6.85	9.51	7.45

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

9 Map-model fit [i](#)

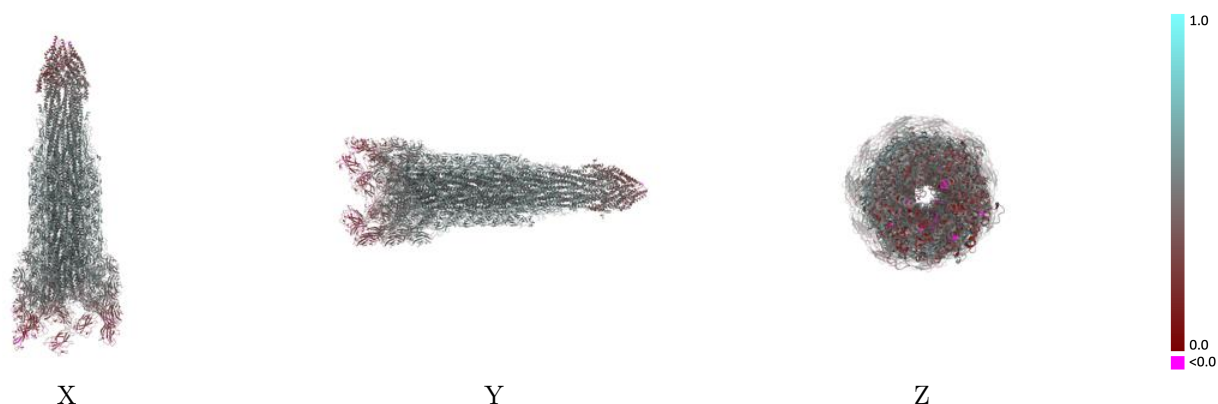
This section contains information regarding the fit between EMDB map EMD-37601 and PDB model 8WKK. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



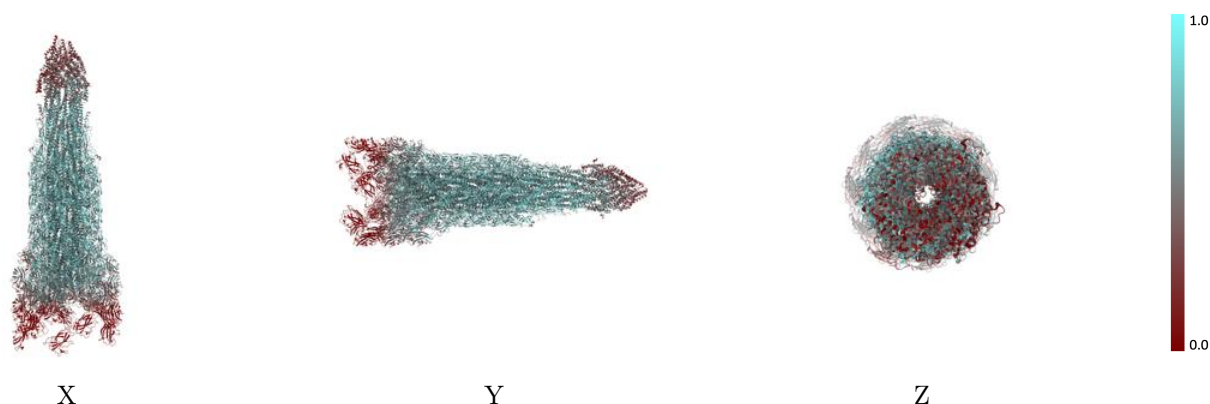
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



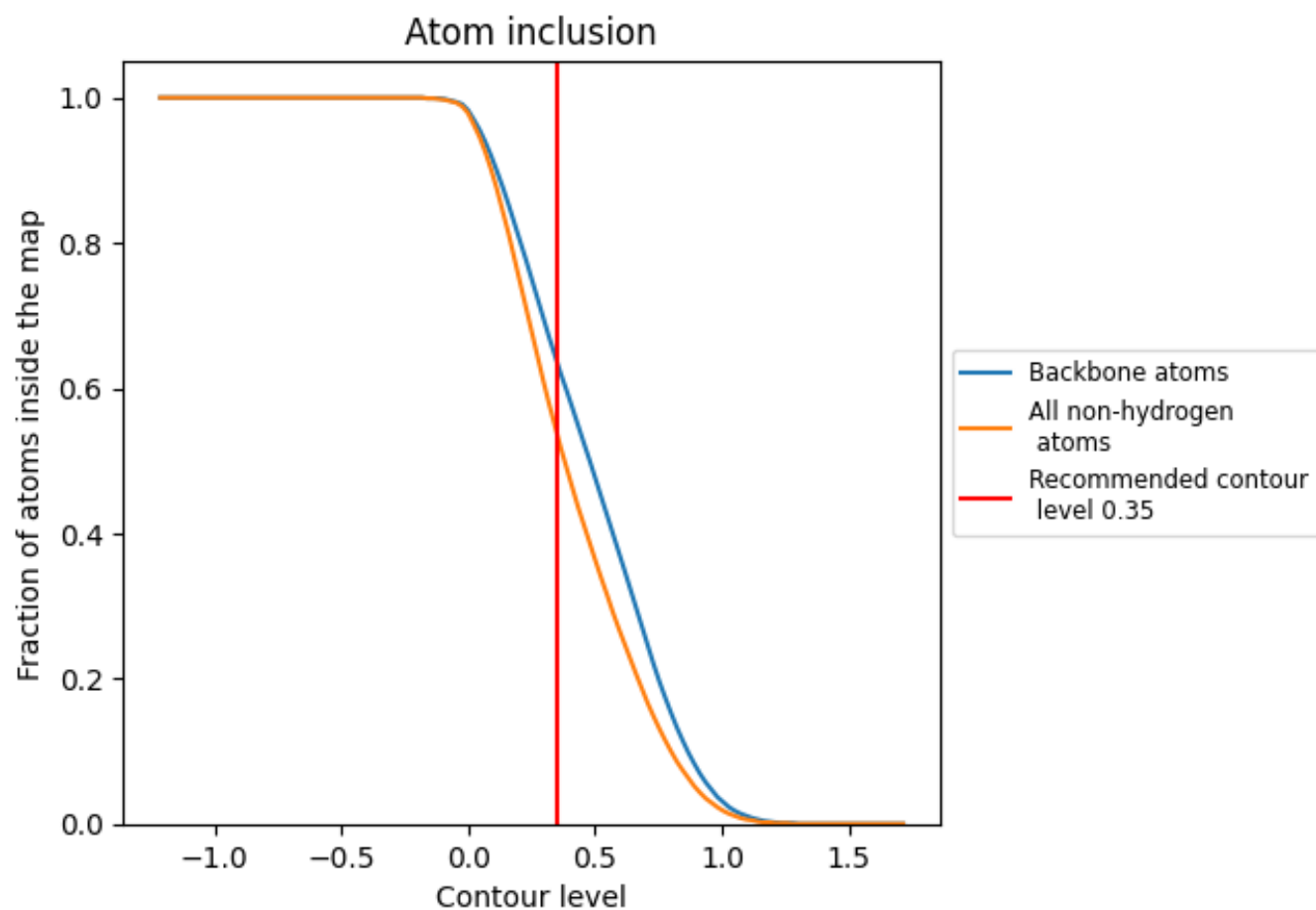
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 64% 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	<div></div> 0.5380	<div></div> 0.4710
0	<div></div> 0.7050	<div></div> 0.5320
1	<div></div> 0.6880	<div></div> 0.5310
2	<div></div> 0.6930	<div></div> 0.5370
3	<div></div> 0.6950	<div></div> 0.5280
4	<div></div> 0.6870	<div></div> 0.5220
5	<div></div> 0.6760	<div></div> 0.5240
6	<div></div> 0.6860	<div></div> 0.5270
7	<div></div> 0.6860	<div></div> 0.5250
8	<div></div> 0.6940	<div></div> 0.5250
9	<div></div> 0.6890	<div></div> 0.5290
A	<div></div> 0.1740	<div></div> 0.2680
B	<div></div> 0.3050	<div></div> 0.3490
C	<div></div> 0.3290	<div></div> 0.3590
D	<div></div> 0.2360	<div></div> 0.3150
E	<div></div> 0.2560	<div></div> 0.3370
F	<div></div> 0.3470	<div></div> 0.3860
G	<div></div> 0.4690	<div></div> 0.4330
H	<div></div> 0.5000	<div></div> 0.4440
I	<div></div> 0.4820	<div></div> 0.4440
J	<div></div> 0.3890	<div></div> 0.4180
K	<div></div> 0.4950	<div></div> 0.4730
L	<div></div> 0.5990	<div></div> 0.4760
M	<div></div> 0.6260	<div></div> 0.4960
N	<div></div> 0.6280	<div></div> 0.5020
O	<div></div> 0.5950	<div></div> 0.4790
P	<div></div> 0.5560	<div></div> 0.4610
Q	<div></div> 0.5750	<div></div> 0.4810
R	<div></div> 0.6770	<div></div> 0.5040
S	<div></div> 0.6950	<div></div> 0.5210
T	<div></div> 0.6770	<div></div> 0.5130
U	<div></div> 0.6510	<div></div> 0.4950
V	<div></div> 0.5880	<div></div> 0.4940
W	<div></div> 0.6810	<div></div> 0.5180
X	<div></div> 0.6760	<div></div> 0.5290











































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Chain	Atom inclusion	Q-score
Y	 0.6770	 0.5160
Z	 0.6570	 0.5150
ZA	 0.6710	 0.5200
ZB	 0.6810	 0.5250
ZC	 0.6810	 0.5230
ZD	 0.6720	 0.5170
ZE	 0.6580	 0.5170
ZF	 0.4120	 0.4580
ZG	 0.5850	 0.5040
ZH	 0.6120	 0.5040
ZI	 0.6150	 0.5040
ZJ	 0.6050	 0.4980
ZK	 0.5810	 0.4940
ZL	 0.5860	 0.4880
ZM	 0.5930	 0.4940
ZN	 0.5990	 0.4910
ZO	 0.5750	 0.4910
ZP	 0.5670	 0.4840
ZQ	 0.5360	 0.4750
ZR	 0.5370	 0.4690
ZS	 0.5260	 0.4690
ZT	 0.4920	 0.4610
ZU	 0.4740	 0.4570
ZV	 0.4360	 0.4420
ZW	 0.4360	 0.4430
ZX	 0.4120	 0.4300
ZY	 0.3940	 0.4240
ZZ	 0.3630	 0.4160
Za	 0.3520	 0.4020
Zb	 0.3390	 0.4000
Zc	 0.3060	 0.3940
Zd	 0.2840	 0.3690
Ze	 0.2500	 0.3670
Zf	 0.2250	 0.3470
Zg	 0.2030	 0.3190
Zh	 0.1840	 0.3290
a	 0.6240	 0.5050
b	 0.3700	 0.4480
c	 0.5630	 0.4860
d	 0.5040	 0.4980
e	 0.5730	 0.5260
f	 0.6430	 0.5100

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Chain	Atom inclusion	Q-score
g	 0.5920	 0.4950
h	 0.6570	 0.5050
i	 0.5340	 0.4690
j	 0.6470	 0.4990
k	 0.5630	 0.4830
l	 0.5430	 0.5030
m	 0.6420	 0.5150
n	 0.7010	 0.5350
o	 0.7130	 0.5350
p	 0.7130	 0.5320
q	 0.6710	 0.5170
r	 0.6570	 0.5270
s	 0.6960	 0.5350
t	 0.6940	 0.5340
u	 0.6980	 0.5390
v	 0.6900	 0.5310
w	 0.7100	 0.5340
x	 0.6920	 0.5290
y	 0.6920	 0.5300
z	 0.7000	 0.5370