



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 06:39 PM UTC

PDB ID : 8WKK / pdb_00008wkk
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

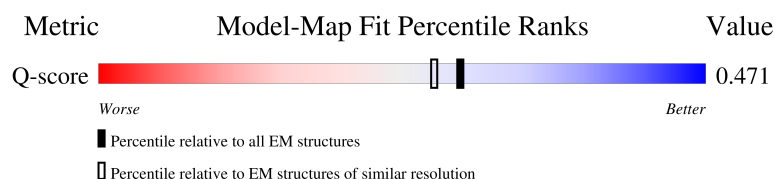
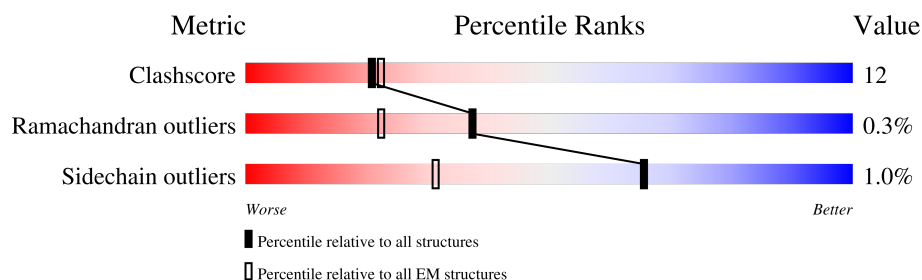
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	89% 79% 20% .
1	B	89	75% 67% 33%
1	C	89	71% 67% 33%
1	D	89	87% 64% 34% .

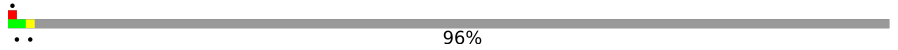
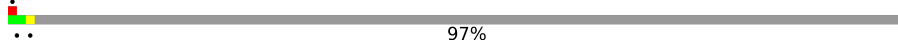
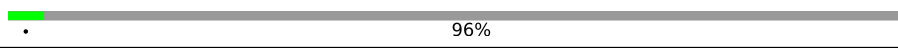
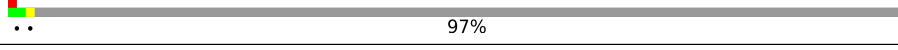
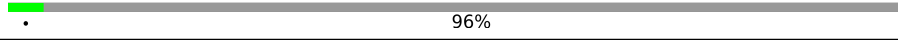
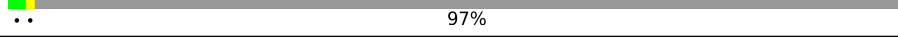
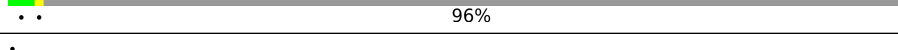
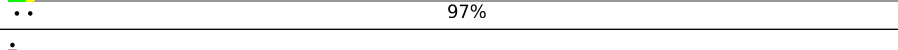
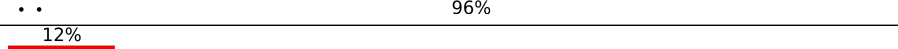
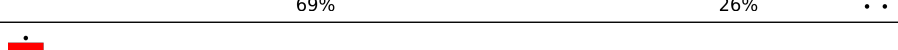
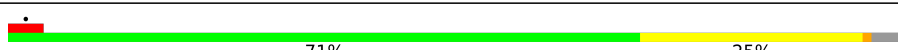
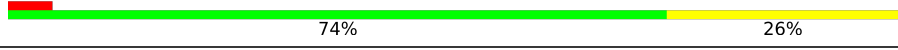
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Mol	Chain	Length	Quality of chain
2	E	264	
3	F	245	
3	G	245	
3	H	245	
3	I	245	
3	J	245	
4	K	104	
4	L	104	
4	M	104	
4	N	104	
4	O	104	
4	P	104	
5	Q	138	
5	R	138	
5	S	138	
5	T	138	
5	U	138	
6	V	134	
6	W	134	
6	X	134	
6	Y	134	
6	Z	134	
6	a	134	
7	b	560	
7	c	560	

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Mol	Chain	Length	Quality of chain
7	d	560	 96%
7	e	560	 97%
7	f	560	 96%
7	g	560	 97%
7	h	560	 96%
7	i	560	 97%
7	j	560	 96%
7	k	560	 97%
7	l	560	 96%
8	m	251	 12% 69% 26%
8	n	251	 66% 32%
8	o	251	 69% 29%
8	p	251	 68% 31%
8	q	251	 6% 70% 29%
9	0	260	 64% 30% 5%
9	1	260	 71% 25%
9	2	260	 76% 23%
9	3	260	 72% 27%
9	4	260	 69% 31%
9	5	260	 5% 69% 30%
9	6	260	 70% 29%
9	7	260	 5% 74% 26%
9	8	260	 71% 28%
9	9	260	 72% 27%
9	ZA	260	 73% 26%

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Mol	Chain	Length	Quality of chain
9	ZB	260	
9	ZC	260	
9	ZD	260	
9	ZE	260	
9	r	260	
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	

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Mol	Chain	Length	Quality of chain
10	ZR	403	
10	ZS	403	
10	ZT	403	
10	ZU	403	
10	ZV	403	
10	ZW	403	
10	ZX	403	
10	ZY	403	
10	ZZ	403	
10	Za	403	
10	Zb	403	
10	Zc	403	
10	Zd	403	
10	Ze	403	
10	Zf	403	
10	Zg	403	
10	Zh	403	

2 Entry composition

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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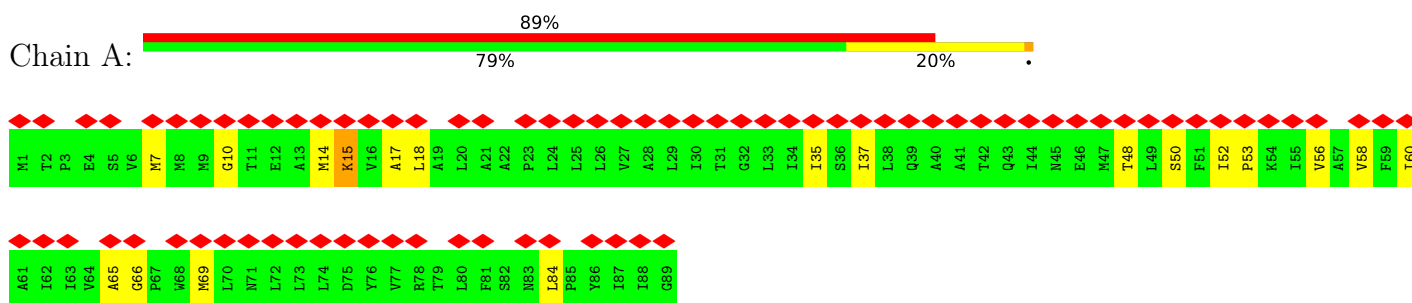
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Mol	Chain	Residues	Atoms					AltConf	Trace
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10	ZY	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	ZZ	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Za	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
10	Zb	401	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

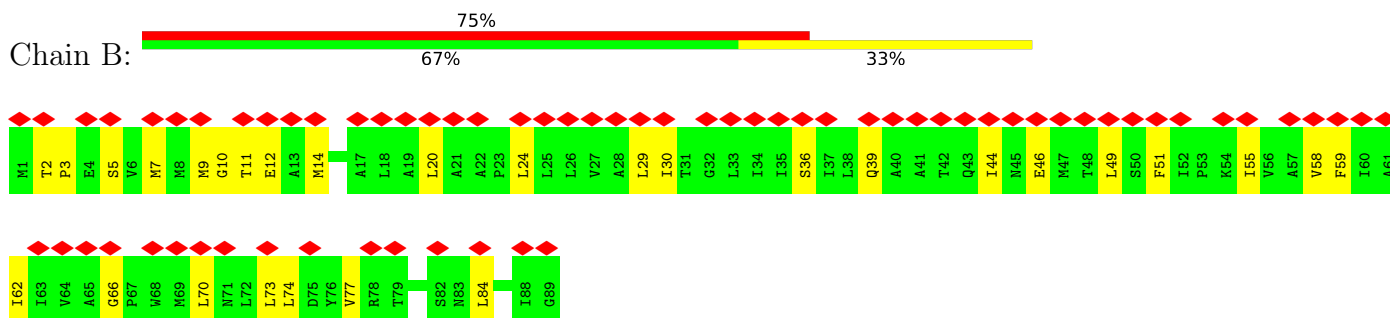
3 Residue-property plots

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.

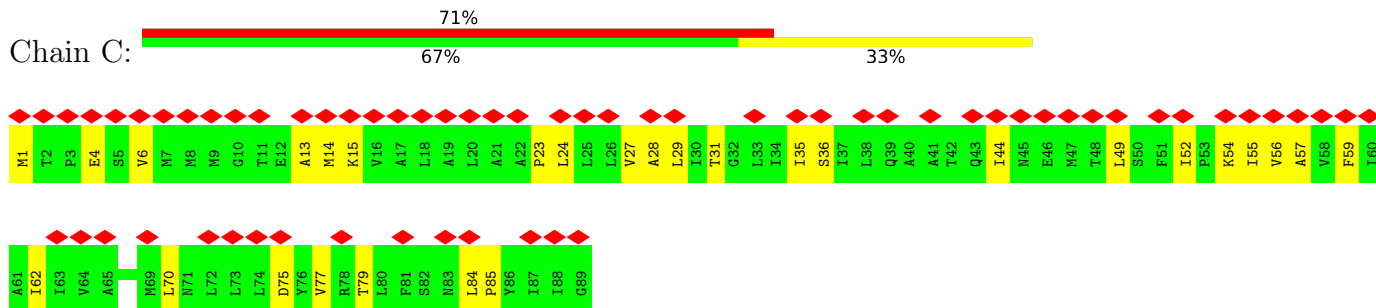
- Molecule 1: Flagellar biosynthetic protein FliQ



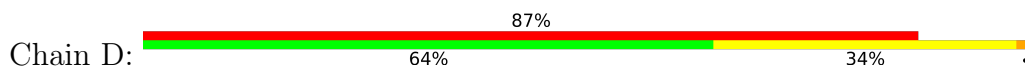
- Molecule 1: Flagellar biosynthetic protein FliQ

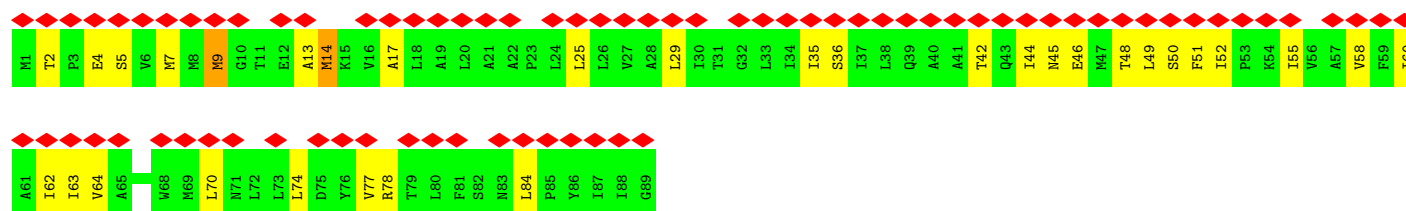


- Molecule 1: Flagellar biosynthetic protein FliQ

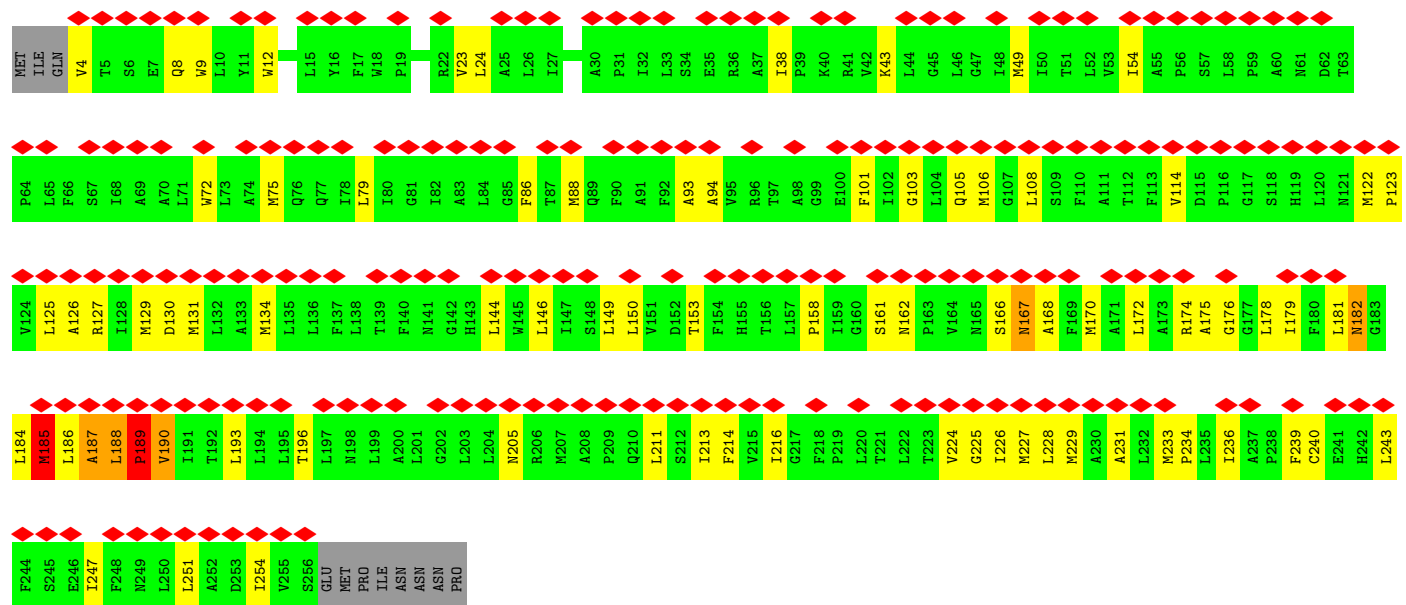
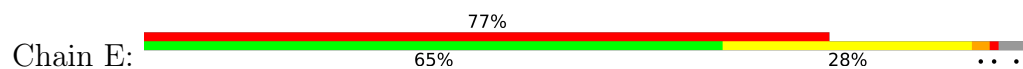


- Molecule 1: Flagellar biosynthetic protein FliQ

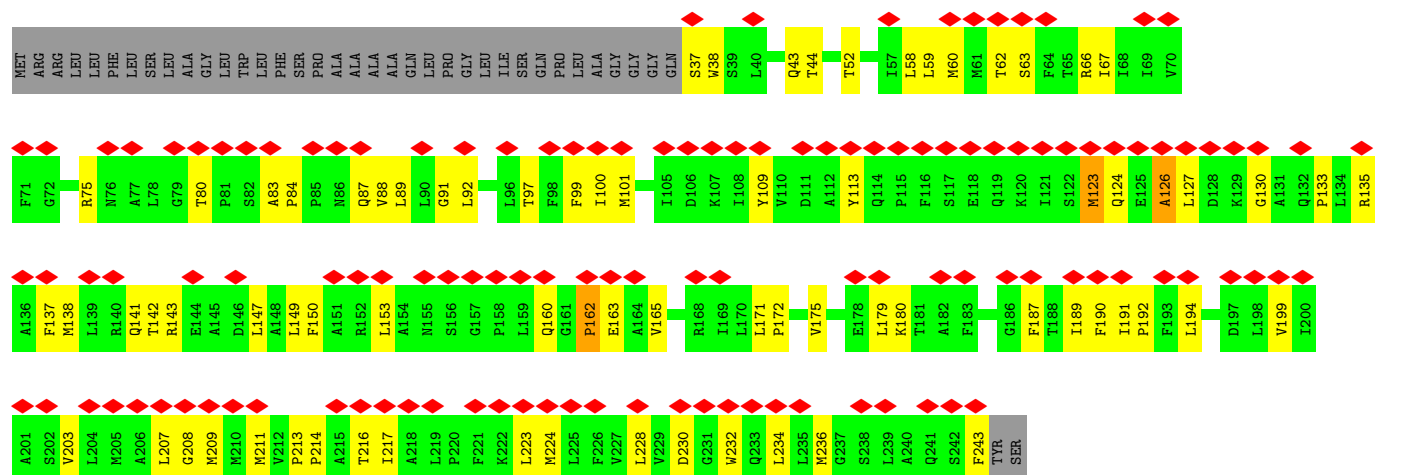




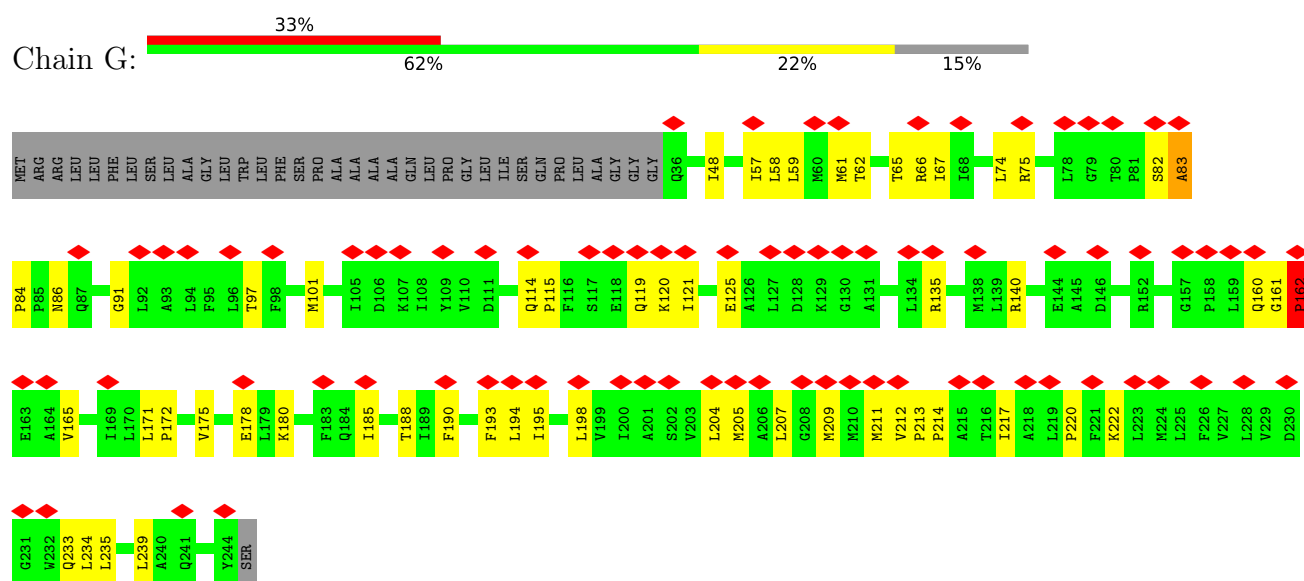
• Molecule 2: Flagellar biosynthetic protein FlIR



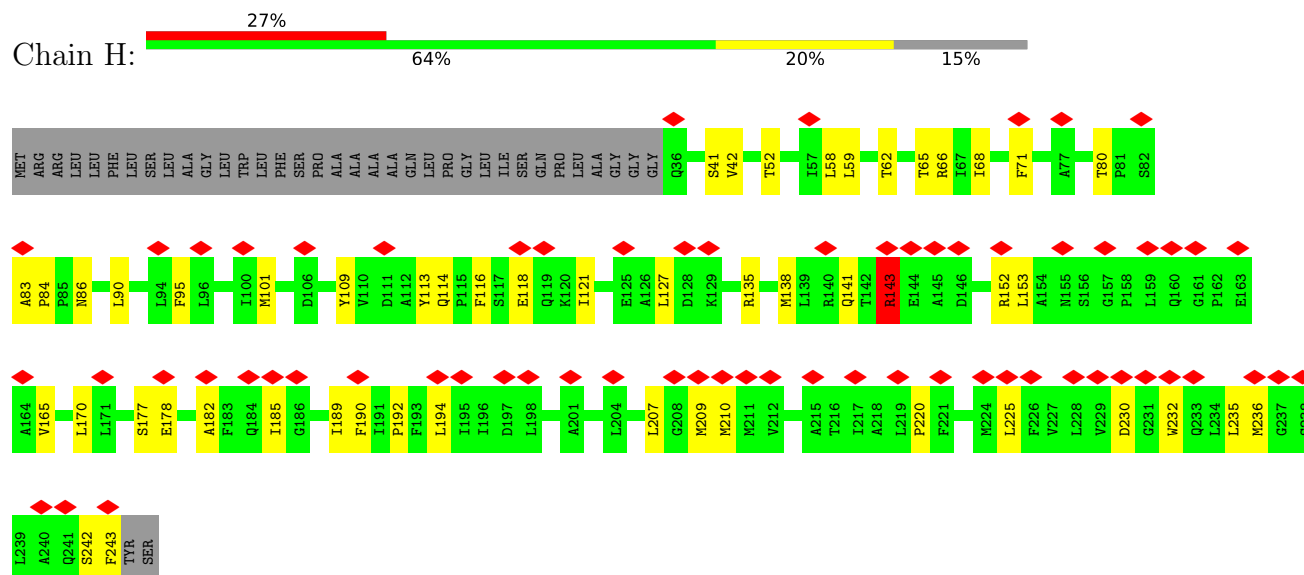
• Molecule 3: Flagellar biosynthetic protein FlIP



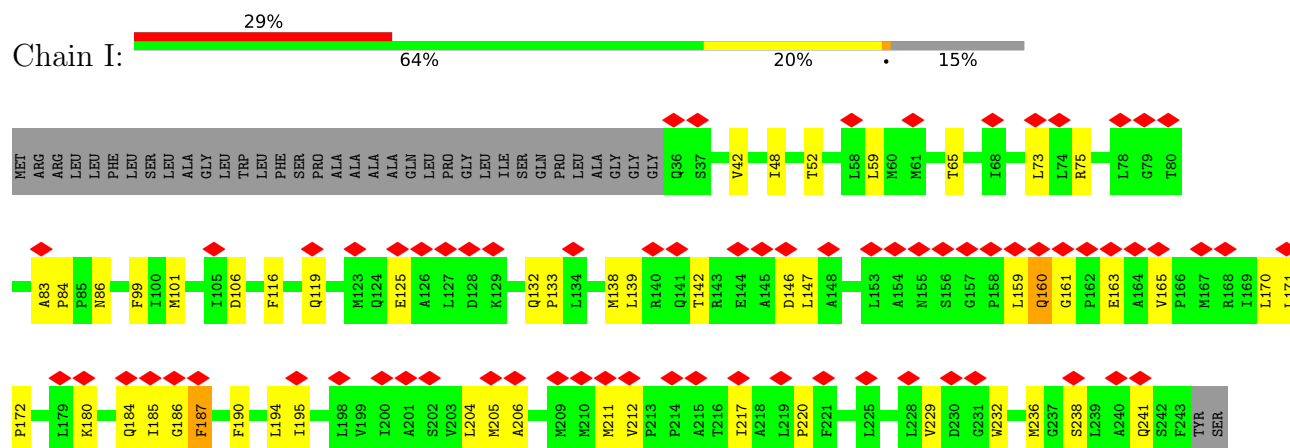
• Molecule 3: Flagellar biosynthetic protein FlIP



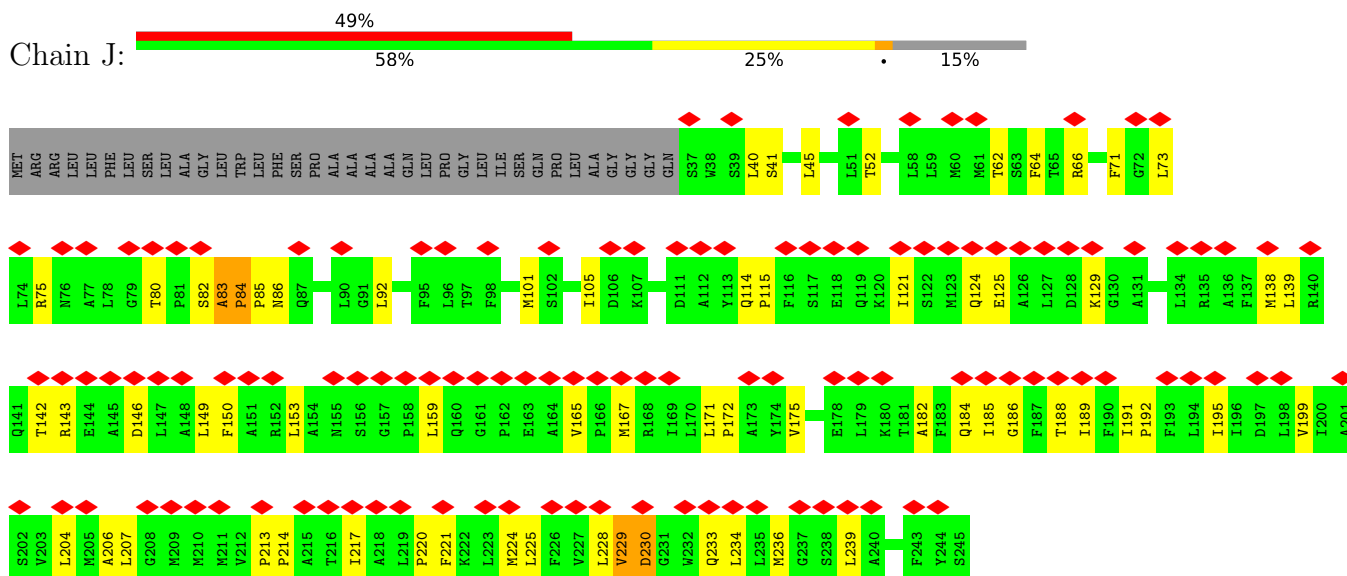
- Molecule 3: Flagellar biosynthetic protein FlpP



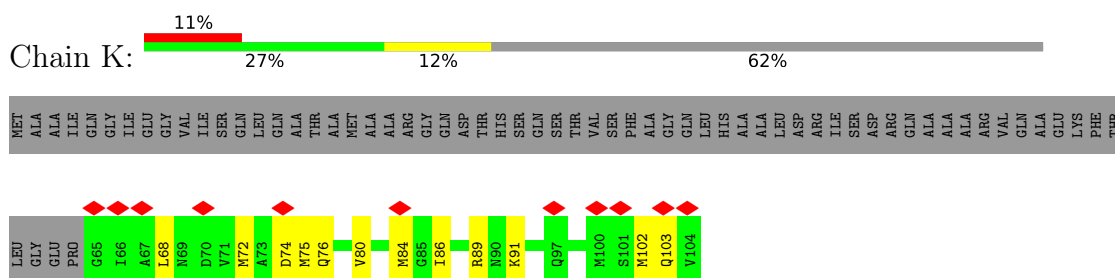
- Molecule 3: Flagellar biosynthetic protein FlhP



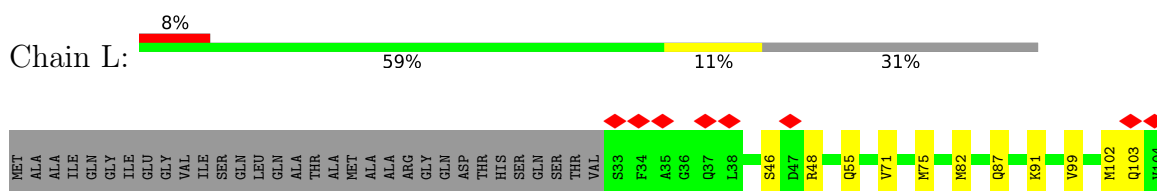
- Molecule 3: Flagellar biosynthetic protein FliP



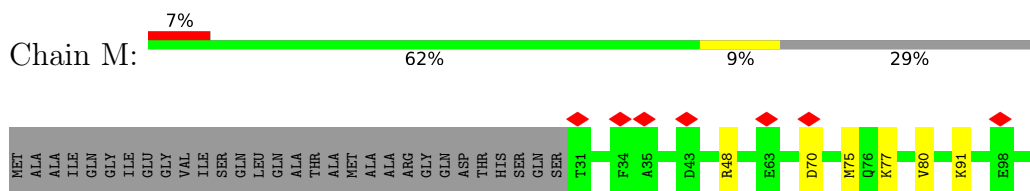
- Molecule 4: Flagellar hook-basal body complex protein FliE



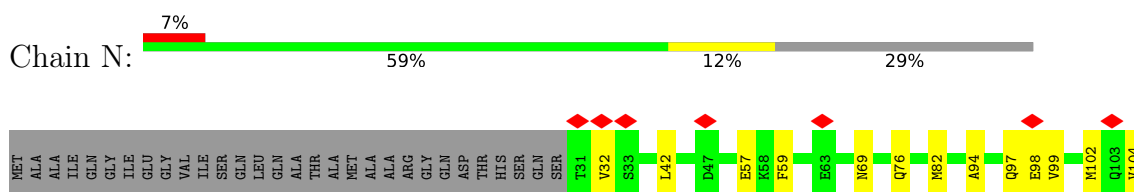
- Molecule 4: Flagellar hook-basal body complex protein FliE



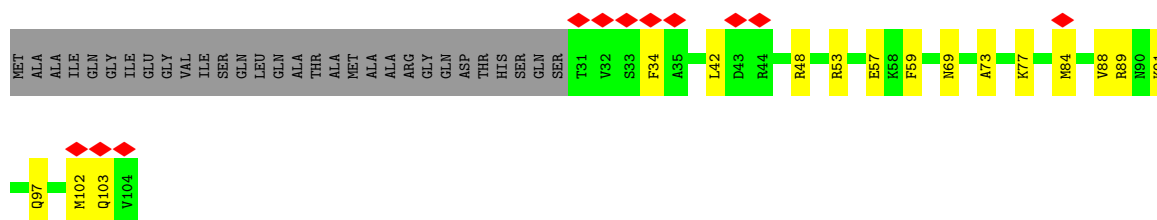
- Molecule 4: Flagellar hook-basal body complex protein FliE



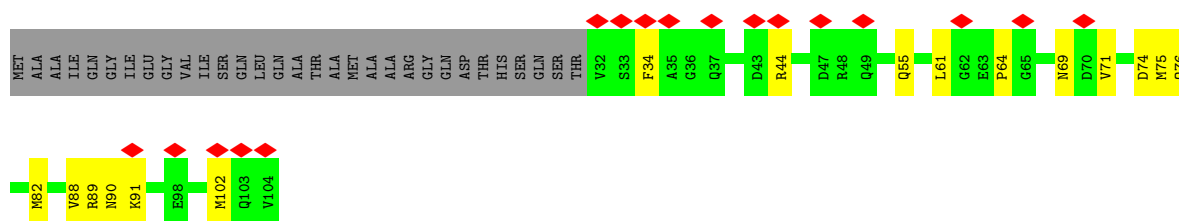
- Molecule 4: Flagellar hook-basal body complex protein FliE



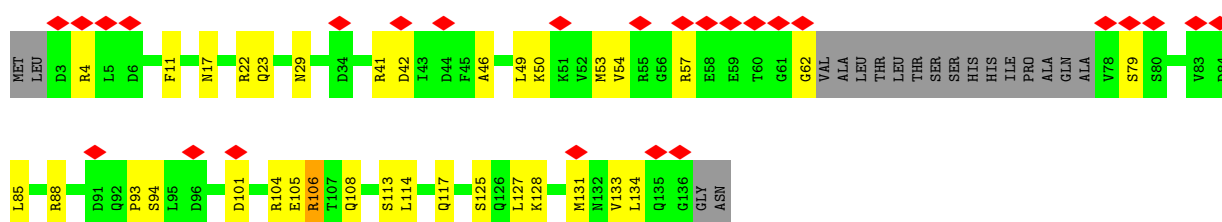
- Molecule 4: Flagellar hook-basal body complex protein FliE



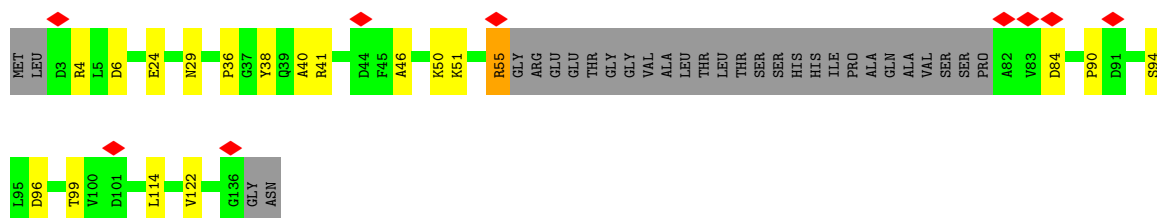
- Molecule 4: Flagellar hook-basal body complex protein FliE



- Molecule 5: Flagellar basal body rod protein FlgB



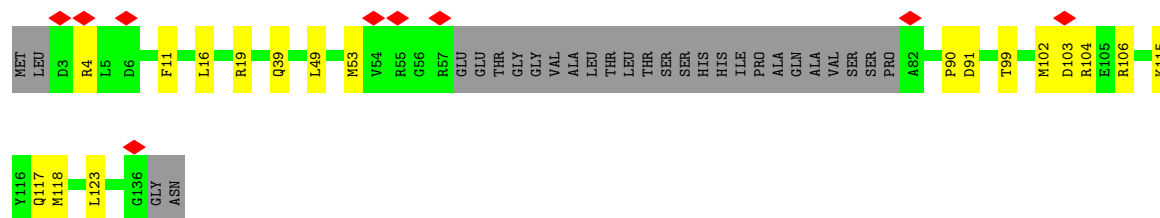
- Molecule 5: Flagellar basal body rod protein FlgB



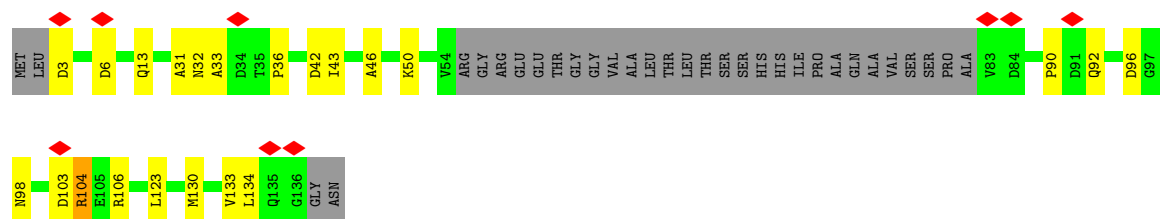
- Molecule 5: Flagellar basal body rod protein FlgB



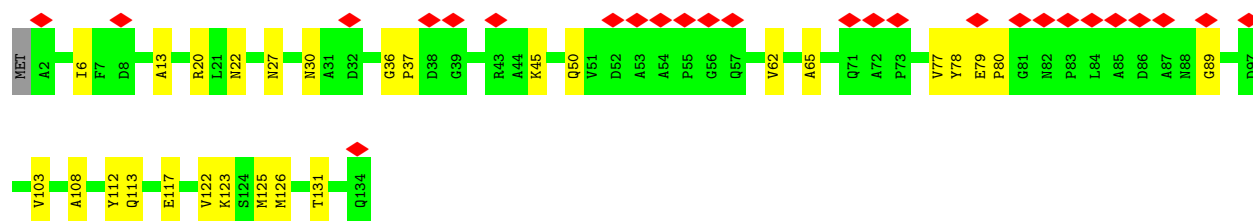
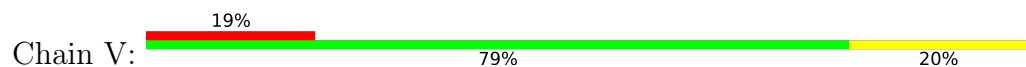
- Molecule 5: Flagellar basal body rod protein FlgB



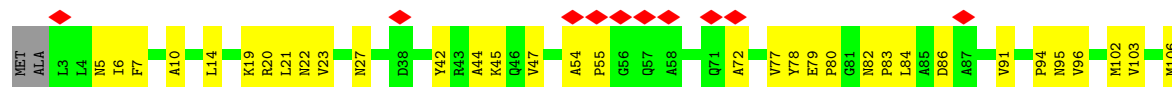
- Molecule 5: Flagellar basal body rod protein FlgB



- Molecule 6: Flagellar basal-body rod protein FlgC

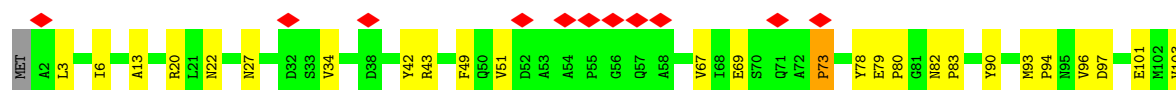
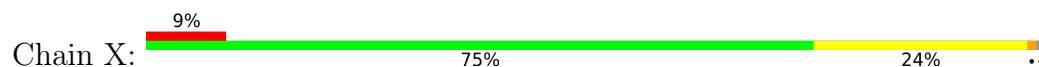


- Molecule 6: Flagellar basal-body rod protein FlgC

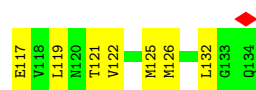
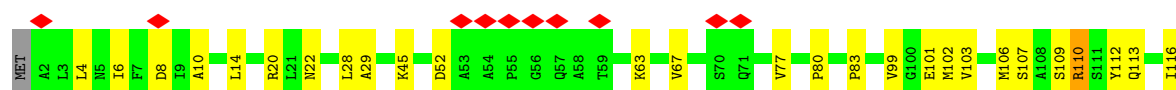
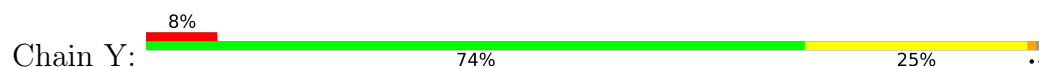




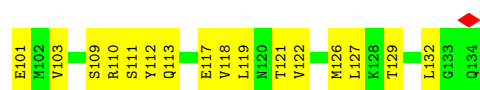
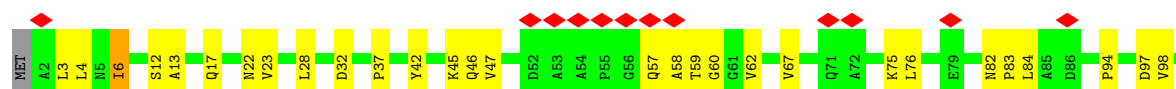
- Molecule 6: Flagellar basal-body rod protein FlgC



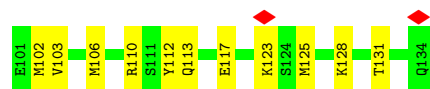
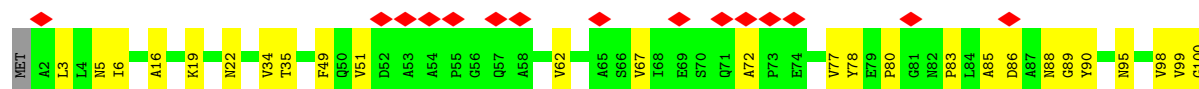
- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 6: Flagellar basal-body rod protein FlgC



- Molecule 7: Flagellar M-ring protein

98%

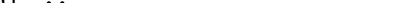
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97%

SER	GLU	GLN	VAL	GLY	ALA	GLY	TTR	P309	A315	P323	N324	GLU	GLU	PRO	PRO	ILE	ALA	THR	PRO	PRO	THR	THR	ASN	GLN	GLN	ASN	ALA	ALA	GLN	ASN	THR	THR	PRO	GLN	THR	THR	SER	SER	SER	THR	THR	THR	ASN	SER	ASN	ASN	SER	ALA	GLY	PRO	ARG	SER	THR	THR	GLN	ARG	ASN	GLU	THR	THR	SER	ASN	TTR	GLU	VAL	ASP	ASP
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[illegible]

- Molecule 7: Flagellar M-ring protein

Chain d:  96%

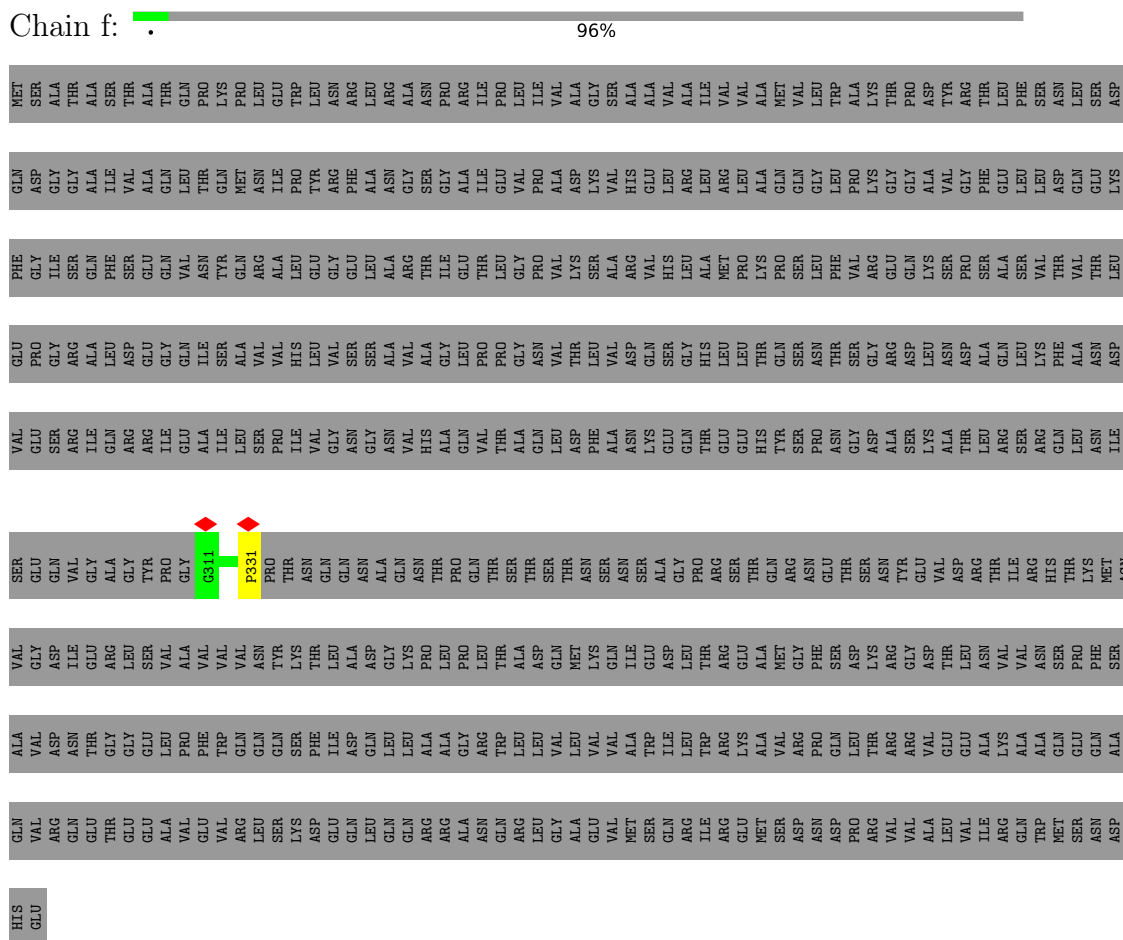
[illegible]

- Molecule 7: Flagellar M-ring protein

Chain e: 97%

[illegible]

- Molecule 7: Flagellar M-ring protein

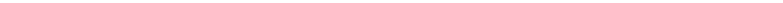


- Molecule 7: Flagellar M-ring protein



ASN	ASN	GLN
ASP	ALA	ALA
HIS	ARG	ARG
GLU	GLN	GLU
	THR	THR
	GLU	GLU
	GLU	GLU
	ALA	ALA
	VAL	VAL
	GLU	GLU
	VAL	VAL
	ARG	ARG
	ARG	LEU
	LEU	LEU
	LEU	LEU
	LYS	LYS
	ASP	ASP
	GLU	GLU
	GLN	GLN
	LEU	LEU
	GLN	GLN
	GLN	GLN
	ARG	ARG
	ARG	ARG
	ALA	ALA
	ASN	ASN
	GLN	GLN
	ARG	ARG
	LEU	LEU
	GLY	GLY
	ALA	ALA
	GLU	GLU
	VAL	VAL
	MET	MET
	SER	SER
	GLN	GLN
	ARG	ARG
	ILE	ILE
	GLU	GLU
	MET	MET
	SER	SER
	ASN	ASN
	ASP	ASP
	PRO	PRO
	ARG	ARG
	VAL	VAL
	VAL	VAL
	ALA	ALA
	LEU	LEU
	VAL	VAL
	ILE	ILE
	ARG	ARG
	GLN	GLN
	TRP	TRP
	MET	MET
	SER	SER

- Molecule 7: Flagellar M-ring protein

Chain i:  97%

NET	SER	ALA	THR	ALA	SER	THR	ALA	THR	GLN	PRO	PRO	LYS	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ARG	LEU	ARG	ALA	ALA	ASN	PRO	ARG	ILE	ILE	VAL	ALA	GLY	SER	ALA	ALA	ALA	VAL	VAL	ALA	ILE	VAL	VAL	VAL	VAL	MET	VAL	LEU	TRP	ALA	ALA	LYS	THR	PRO	ASP	SER	ASN	LEU	LEU	SER	ARG	THR	LEU	PHE	SER	ASN	LEU	LEU	SER	ARG
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Gln Asp Gln Gly Ala Ile Val Ala Gln Thr Met Asn Ile Pro Arg Phe Ala Ala Ser Gly Ala Ile Glu Val Val Pro Asp Lys Val His Glu Leu Leu Leu Gln Gln Gly Leu Leu Lys Gly Ala Val Val Phe Glu Leu Asp Gln Glu

PHE	GLY	ILE	GLN	GLN	PHE	SER	GLU	GLN	VAL	TYR	GLN	ARG	ALA	LEU	GLU	GLY	GLU	LEU	ALA	ARG	THR	ILE	GLU	THR	LEU	GLY	PRO	LYS	VAL	VAL	ARG	ALA	HIS	LEU	ALA	MET	PRO	PRO	LYS	PRO	SER	PRO	LEU	PHE	VAL	ARG	GLU	GLN	LYS	SER	SER	PRO	PRO	ALA	ALA	SER	VAL	THR	VAL	THR	LEU
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GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	ALA	VAL	HIS	LEU	VAL	SER	SER	ALA	ALA	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	THR	LEU	VAL	ASP	GLN	SER	GLY	HIS	LEU	LEU	ASN	ASP	ASP	GLN	LEU	PHE	LYS	ALA	ASN	ASP
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VAL	GLU	SER	ARG	ILE	GLN	ARG	ARG	ILE	GLU	ALA	ILE	LEU	SER	PRO	ILE	VAL	GLY	ASN	GLY	VAL	ASN	ASN	VAL	HIS	ALA	ALA	GLN	THR	THR	ALA	ALA	ALA	GLN	LEU	ASP	PHE	ASP	ASN	ASN	LYS	GLU	GLN	GLN	THR	GLU	GLU	GLY	HIS	TYR	SER	PRO	PRO	ASN	GLY	ASP	ALA	ALA	SER	LYS	ARG	GLN	ARG	ARG	LEU	LEU	ASN	ILE
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VAL	ASP	ARG	THR	ILE	ARG	HIS	THR	LYS	MET	ASN	VAL	VAL	GLY	ASP	ILE	GLU	ARG	LEU	SER	VAL	ALA	VAL	VAL	VAL	ASN	TYR	LYS	THR	LEU	LEU	ASP	GLY	LYS	PRO	PRO	LEU	LEU	THR	THR	LEU	ALA	ALA	ASP	GLN	MET	LYS	GLN	GLN	LEU	ILE	GLU	ASP	LEU	LEU	THR	THR	GLU	GLU	ARG	ALA	ALA	MET	GLY	PHE	SER	ASP	LYS	ARG	GLY
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ASP	THR	LEU	ASN	VAL	ASN	SER	PRO	PHE	SER	ALA	VAL	ASP	THR	GLY	GLY	GLU	LEU	PRO	PHE	TRP	GLN	GLN	SER	SER	PHE	ILE	ASP	ASP	GLN	LEU	LEU	ALA	ALA	ALA	GLY	ARG	TRP	TRP	LEU	LEU	VAL	VAL	LEU	VAL	VAL	ALA	ALA	TRP	ALA	TRP	ILE	LEU	LEU	TRP	ARG	LYS	ARG	THR	LEU	GLN	PRO	ARG	VAL	VAL	ALA	ALA	THR	LEU	THR	THR	ARG	ARG
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VAL	GLU	GLU	LYS	ALA	ALA	GLN	GLU	GLN	ALA	GLN	VAL	ARG	GLN	THR	GLU	GLU	ALA	VAL	GLU	VAL	ARG	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	GLN	ARG	ARG	ALA	ASN	GLN	ARG	ARG	MET	MET	SER	SER	GLN	ARG	TLE	ASP	ASN	ASP	PRO	ARG	VAL	VAL
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ALA
LEU
VAL
ILE
ARG
GLN
TRP
MET
SER
ASN
ASP
HIS
GLU

- Molecule 7: Flagellar M-ring protein

Chain j:  96%

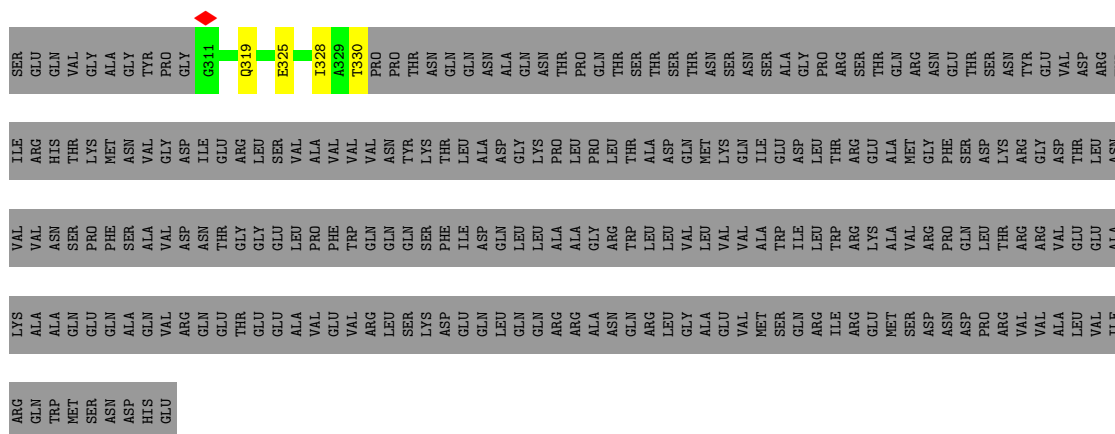
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Gln Asp Gly Gly Ala Ile Val Ala Ala Gln Leu Leu Thr Met Asn Ile Pro Arg Phe Ala Ala Gly Ser Gly Ala Ile Glu Val Val Pro Asp Lys Val Val His Hleu Leu Leu Arg Arg Arg Lys Gly Gly Ala Val Val Phe Glu Leu Leu Asp Asn Gln Gly

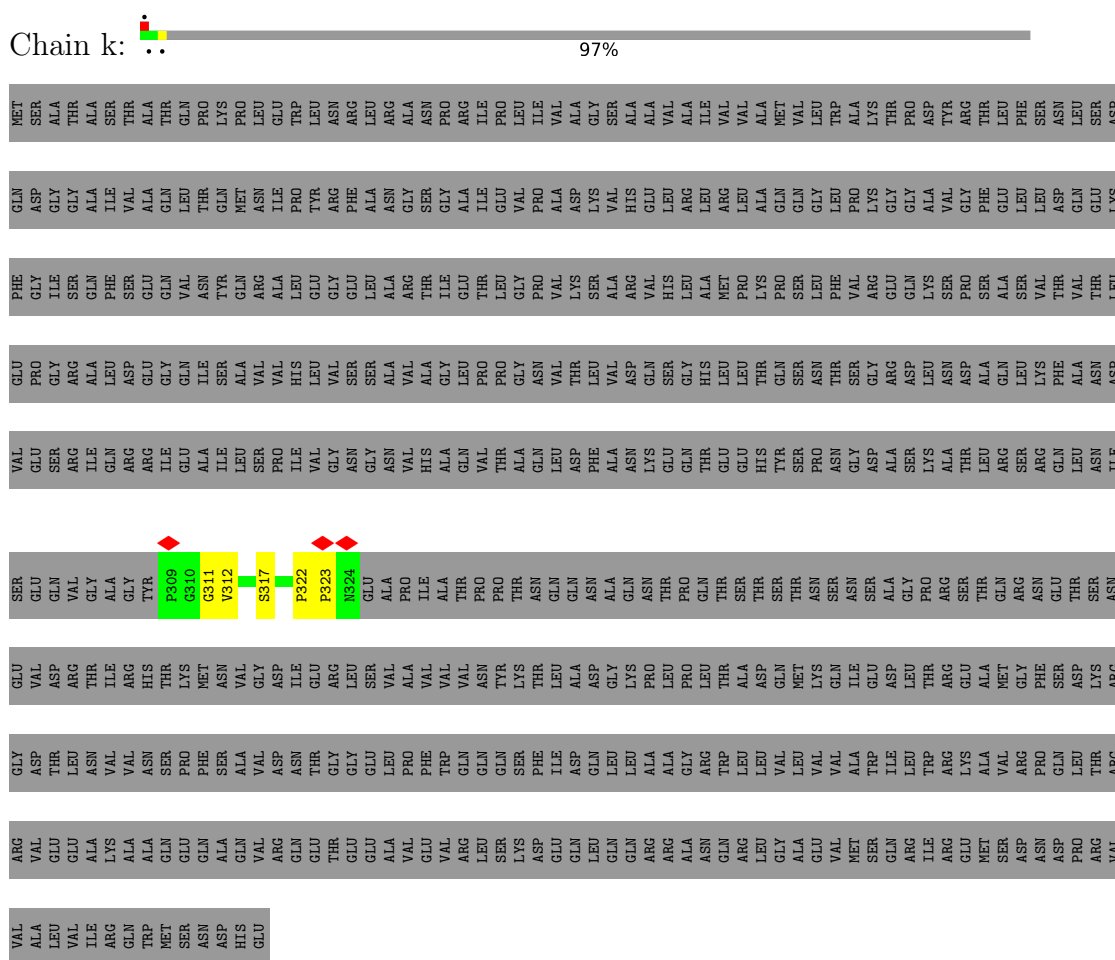
PHE
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VAL
THR
LEU

GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	HIS	VAL	SER	SER	ALA	VAL	ALA	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	THR	GLN	SER	ASN	THR	SER	GLY	ARG	ASP	ASP	ASN	ASN	ASP	ALA	GLN	LEU	LYS	PHE	LYS	ALA	ASN	ASP
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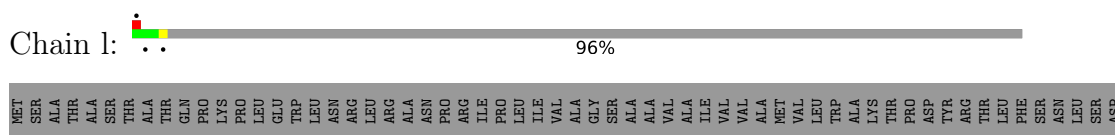
VAL	GLU	SER	ARG	ILE	GLN	ARG	ARG	ILE	GLU	ALA	ILE	LEU	SER	PRO	VAL	GLY	ASN	GLY	VAL	THR	ALA	ALA	GLN	LEU	ASP	PHE	ALA	ASN	LYS	GLN	GLN	THR	GLY	TYR	SER	PRO	ASN	GLY	ASP	ALA	SER	LYS	ALA	THR	LEU	ARG	SER	ARG	GLN	LEU	ASN	ILE
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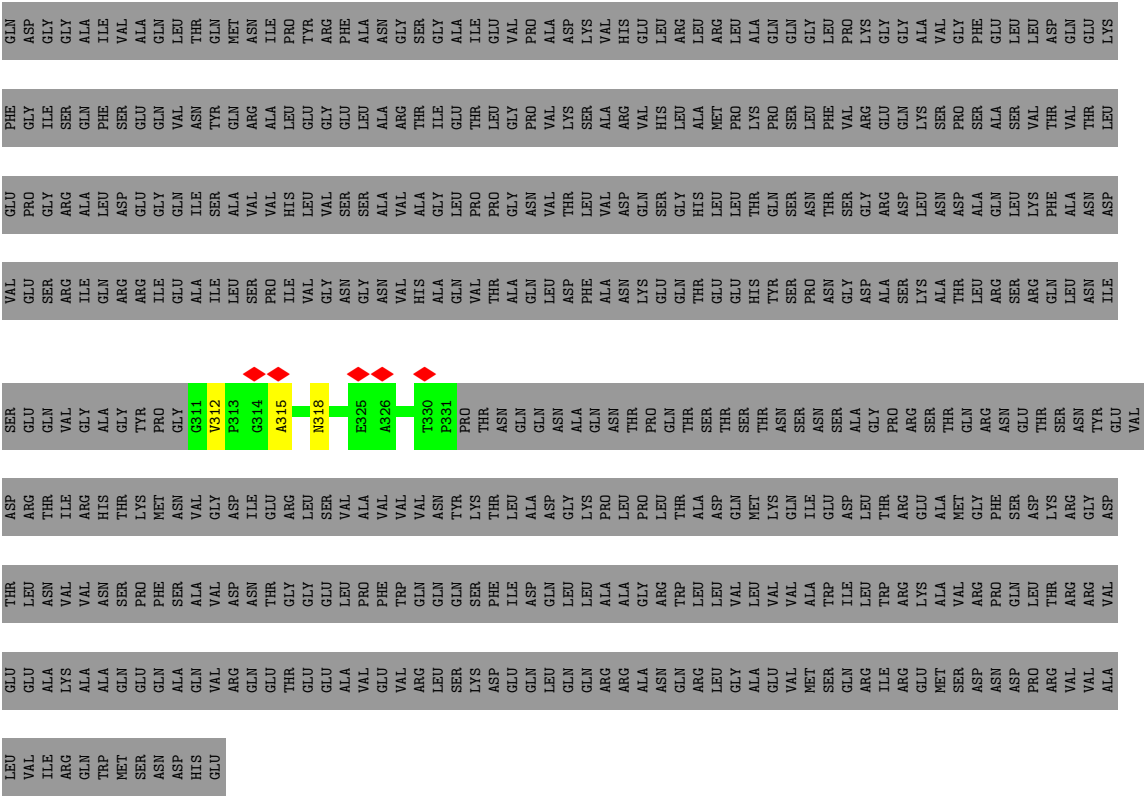


- Molecule 7: Flagellar M-ring protein

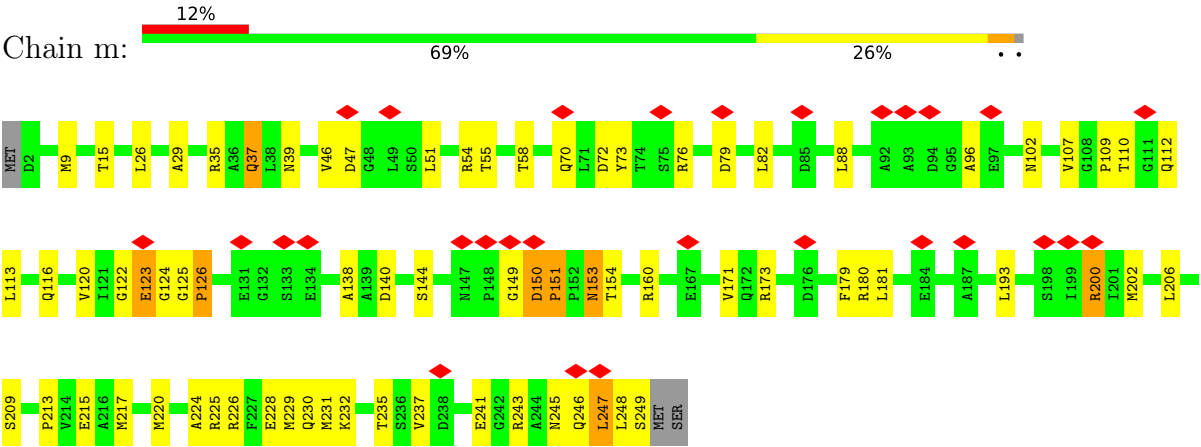


- Molecule 7: Flagellar M-ring protein

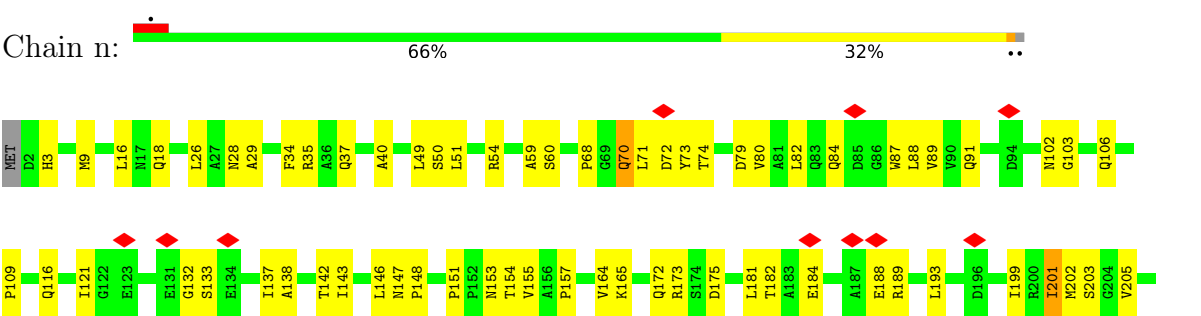




• Molecule 8: Flagellar basal-body rod protein FlgF

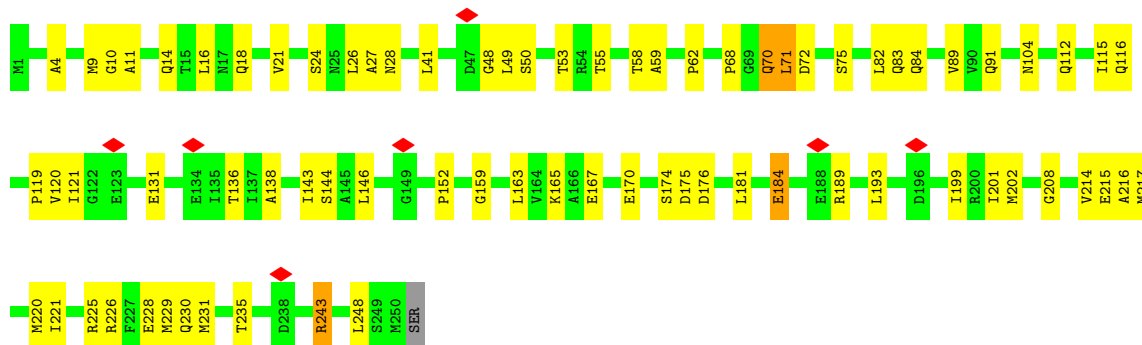


• Molecule 8: Flagellar basal-body rod protein FlgF

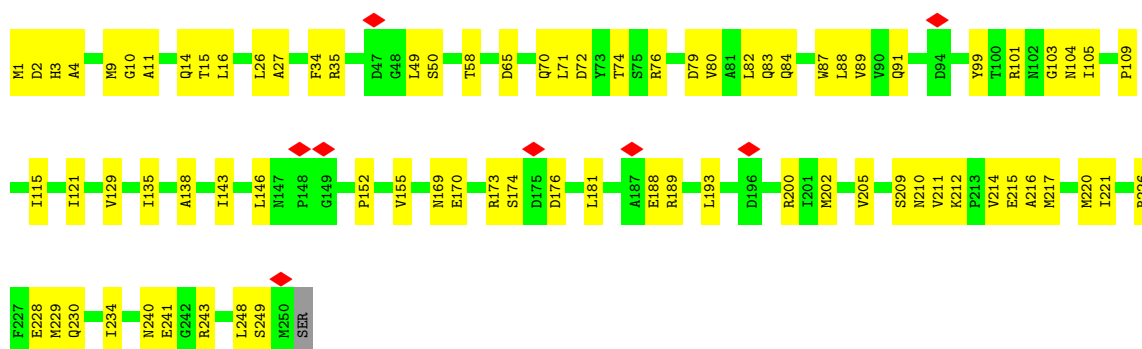




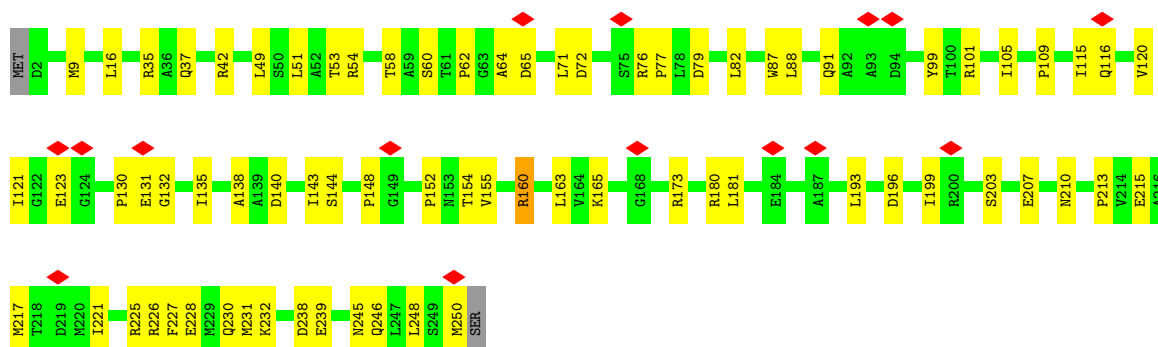
• Molecule 8: Flagellar basal-body rod protein FlgF



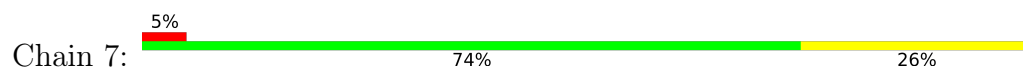
• Molecule 8: Flagellar basal-body rod protein FlgF

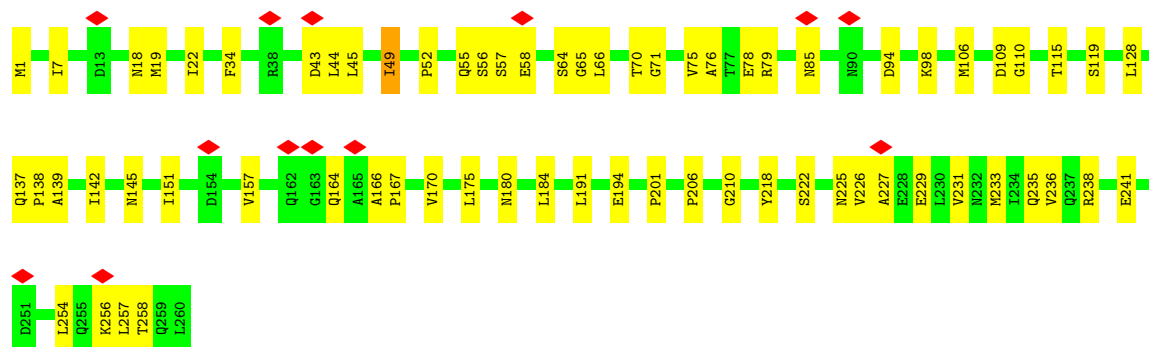


• Molecule 8: Flagellar basal-body rod protein FlgF



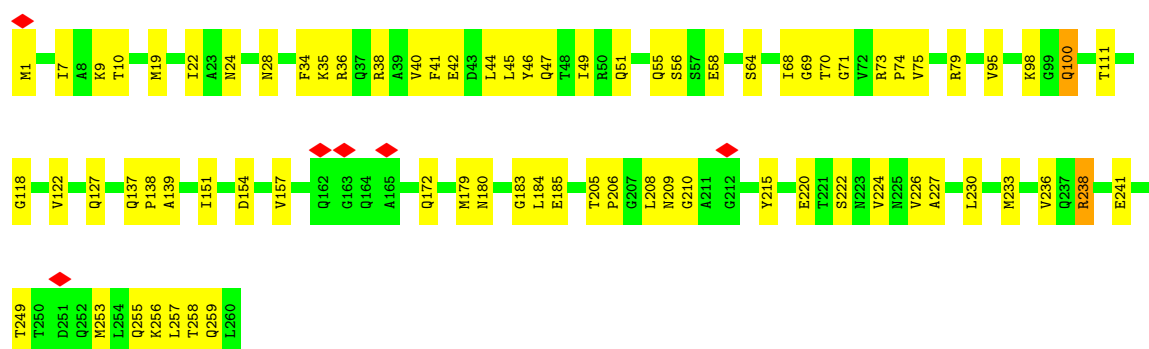
• Molecule 9: Flagellar basal-body rod protein FlgG





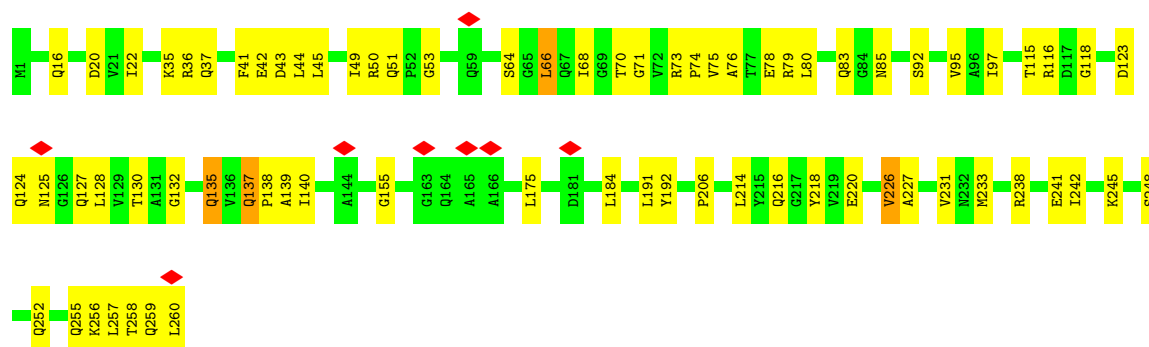
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain 8: 71% 28%



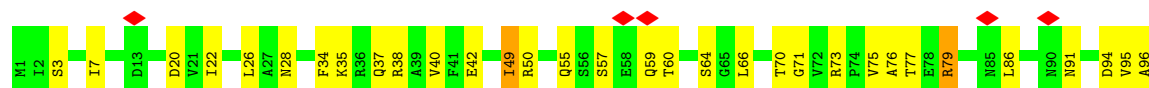
- Molecule 9: Flagellar basal-body rod protein FlgG

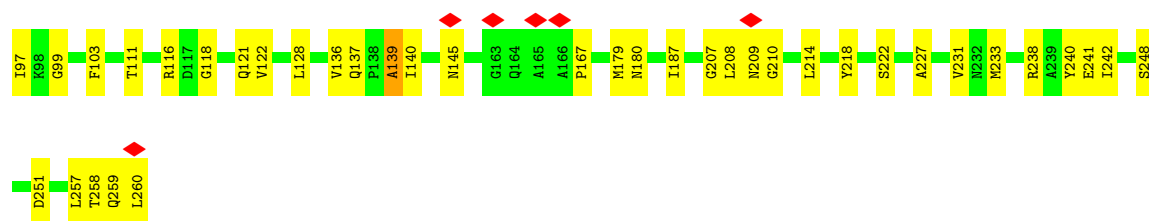
Chain 9: 72% 27%



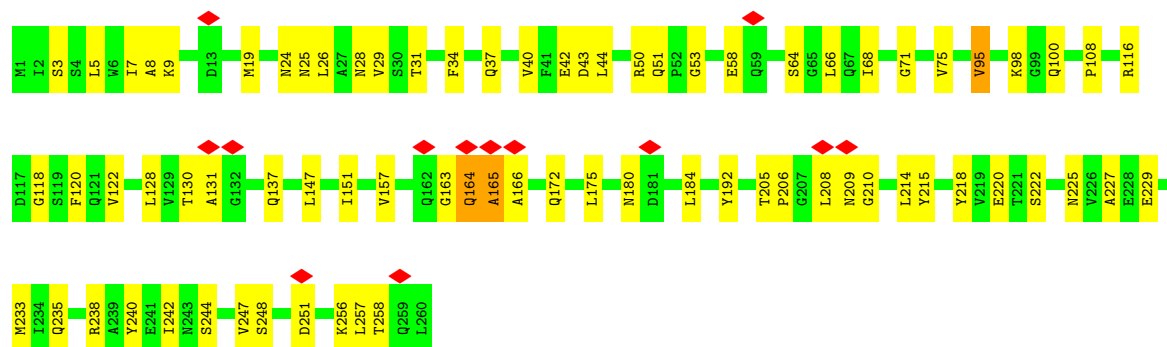
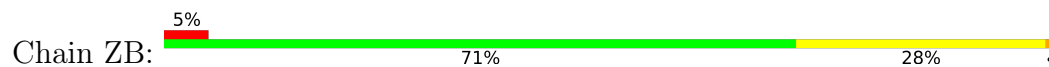
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain ZA: 73% 26%

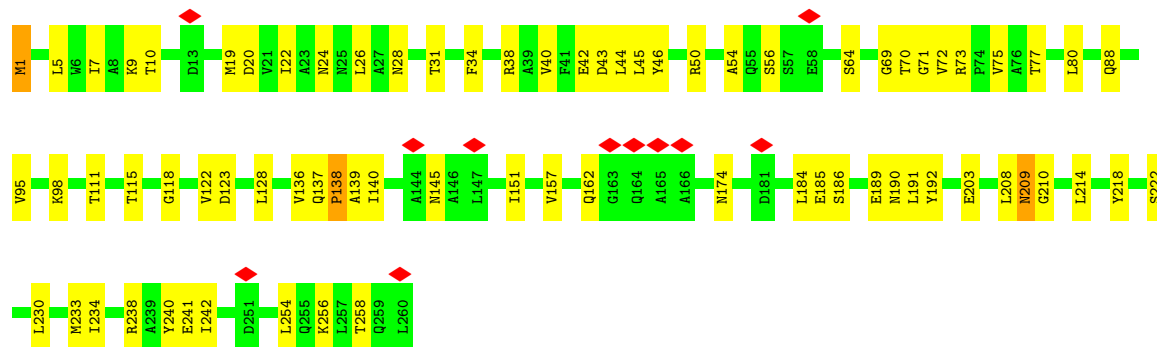




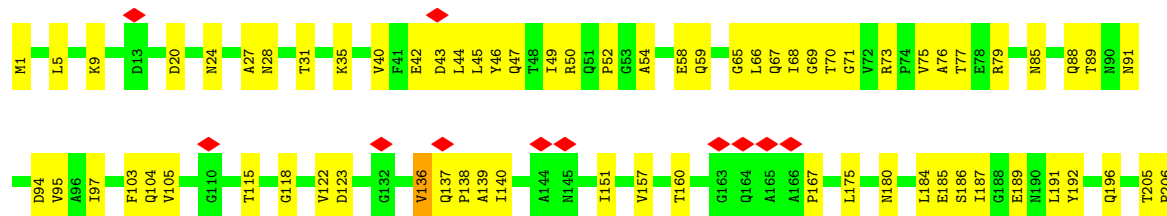
• Molecule 9: Flagellar basal-body rod protein FlgG



• Molecule 9: Flagellar basal-body rod protein FlgG

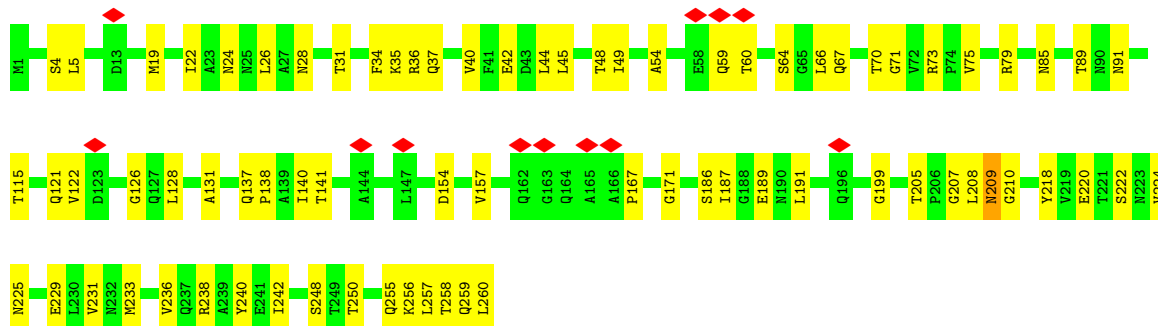
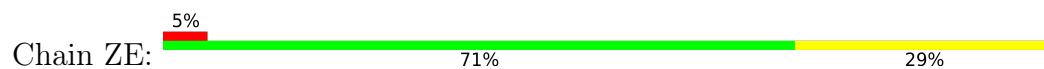


• Molecule 9: Flagellar basal-body rod protein FlgG

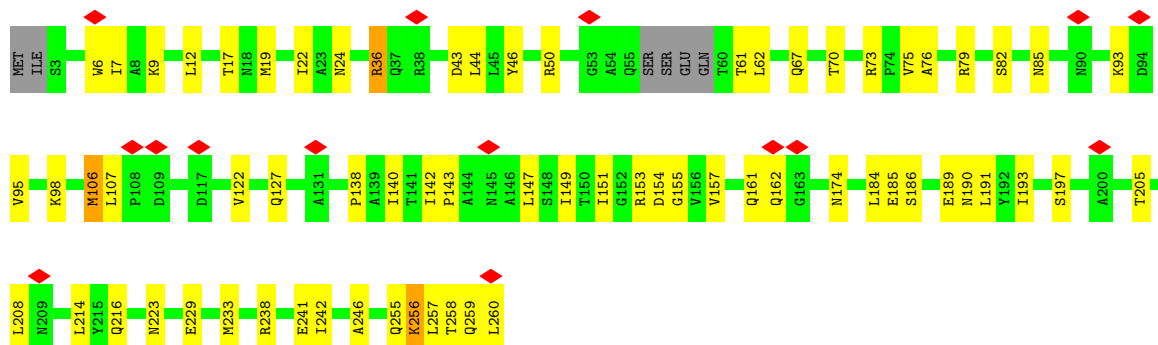




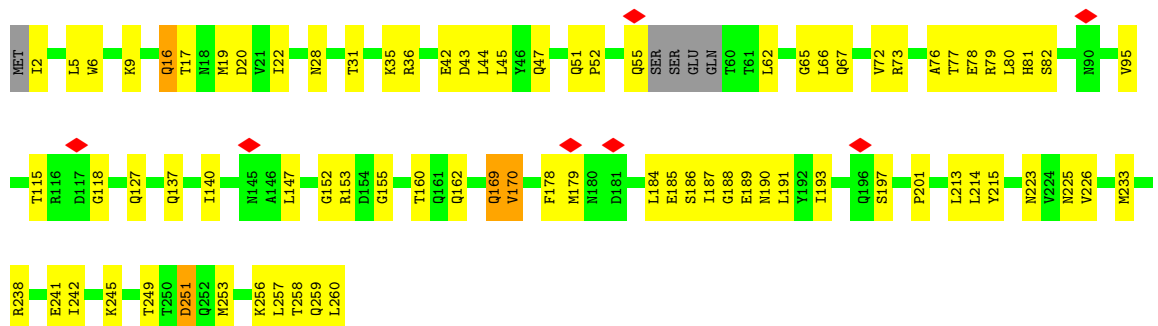
- Molecule 9: Flagellar basal-body rod protein FlgG



- Molecule 9: Flagellar basal-body rod protein FlgG

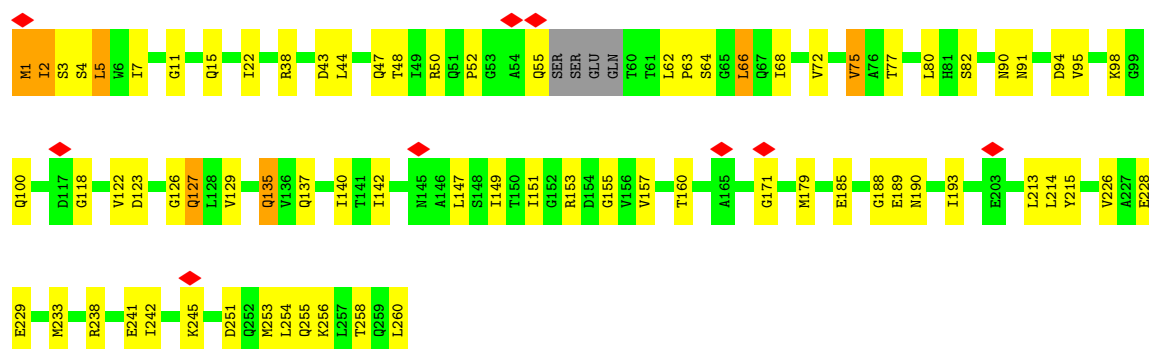


- Molecule 9: Flagellar basal-body rod protein FlgG

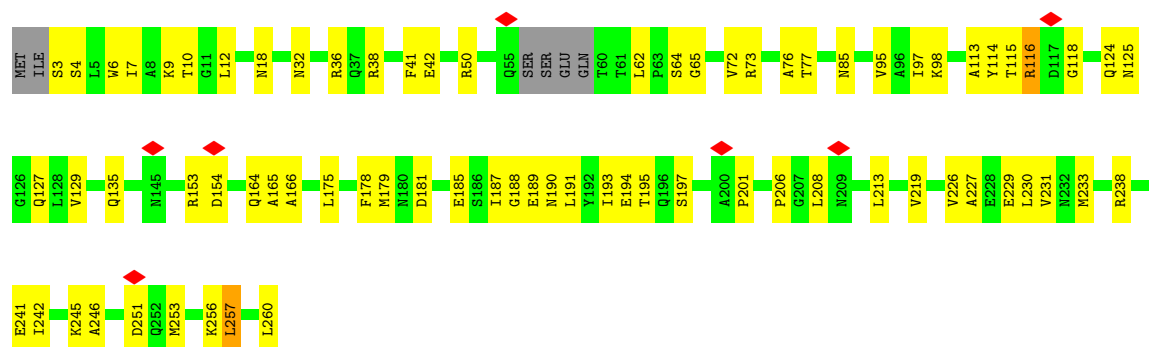


- Molecule 9: Flagellar basal-body rod protein FlgG

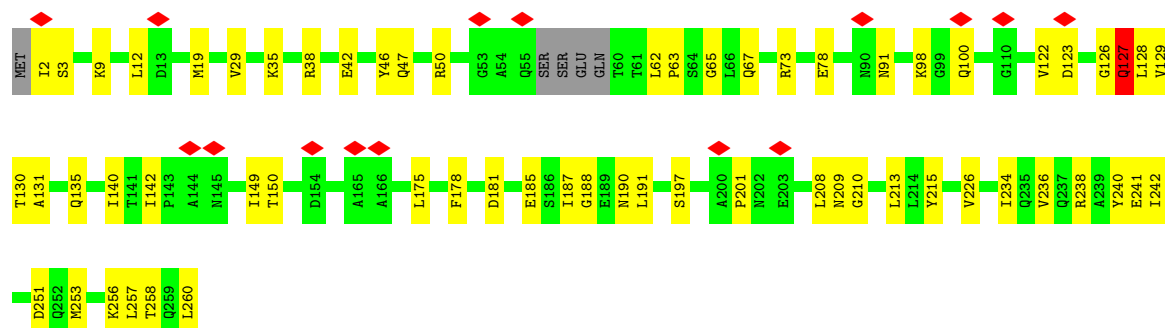
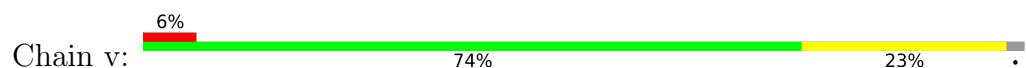




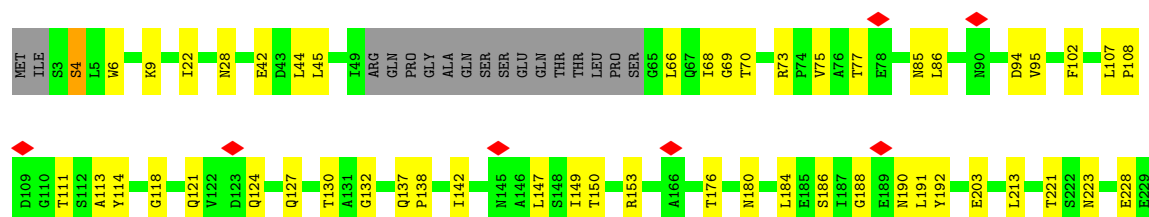
• Molecule 9: Flagellar basal-body rod protein FlgG



• Molecule 9: Flagellar basal-body rod protein FlgG



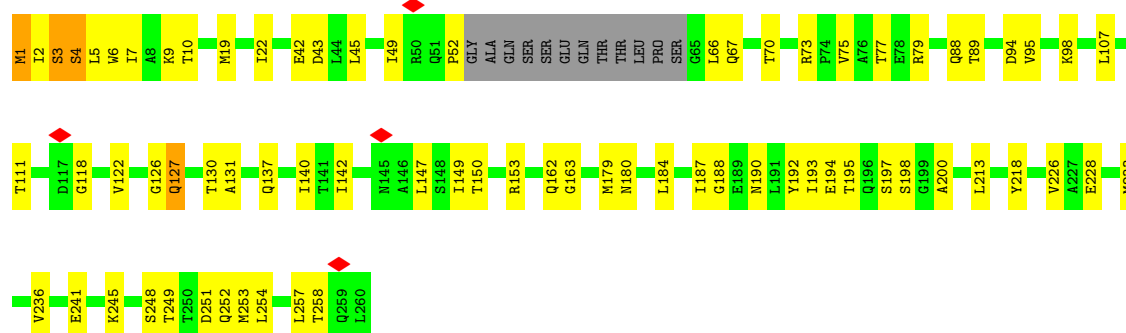
• Molecule 9: Flagellar basal-body rod protein FlgG





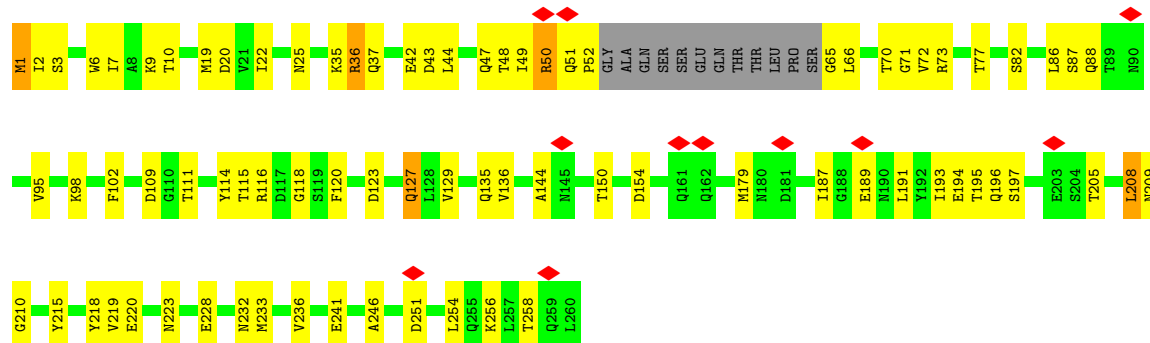
• Molecule 9: Flagellar basal-body rod protein FlgG

Chain x: 67% 27% 5%



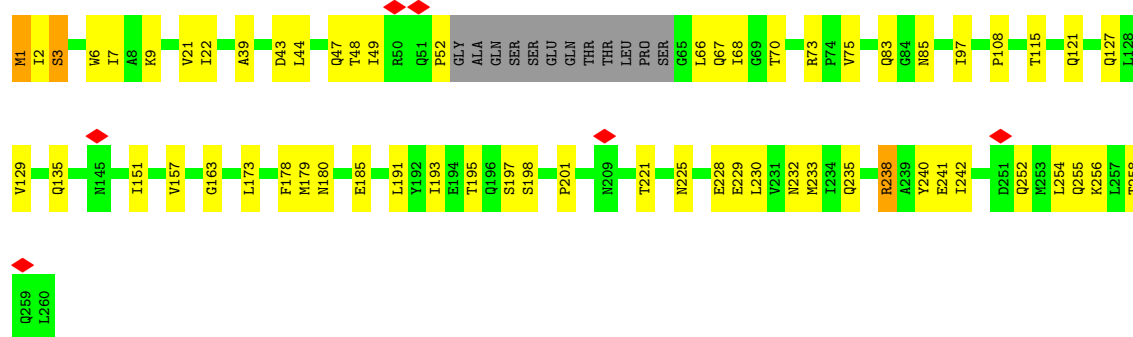
• Molecule 9: Flagellar basal-body rod protein FlgG

Chain y: 65% 29% 5%

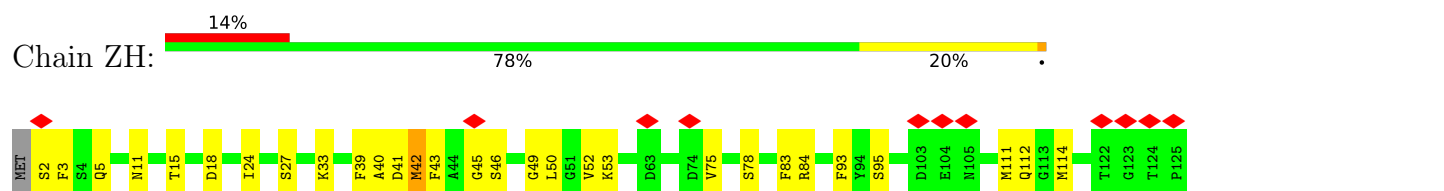


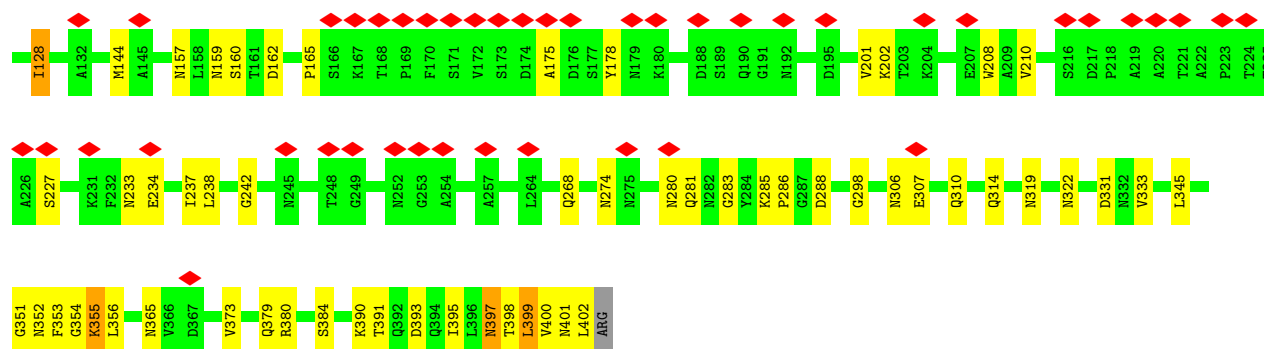
• Molecule 9: Flagellar basal-body rod protein FlgG

Chain z: 72% 22% 5%

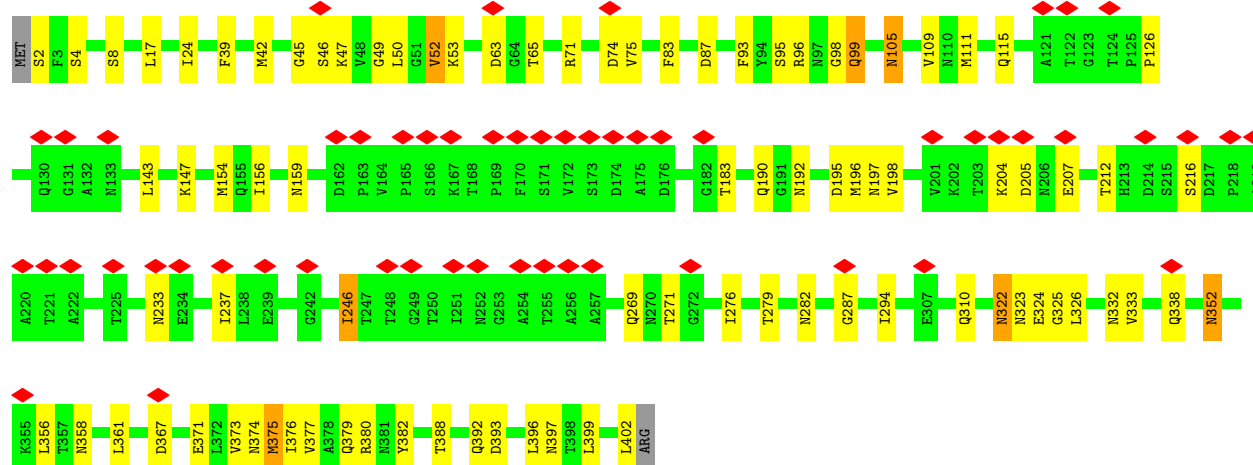
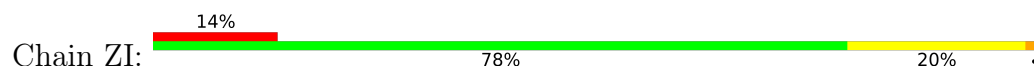


• Molecule 10: Flagellar hook protein FlgE

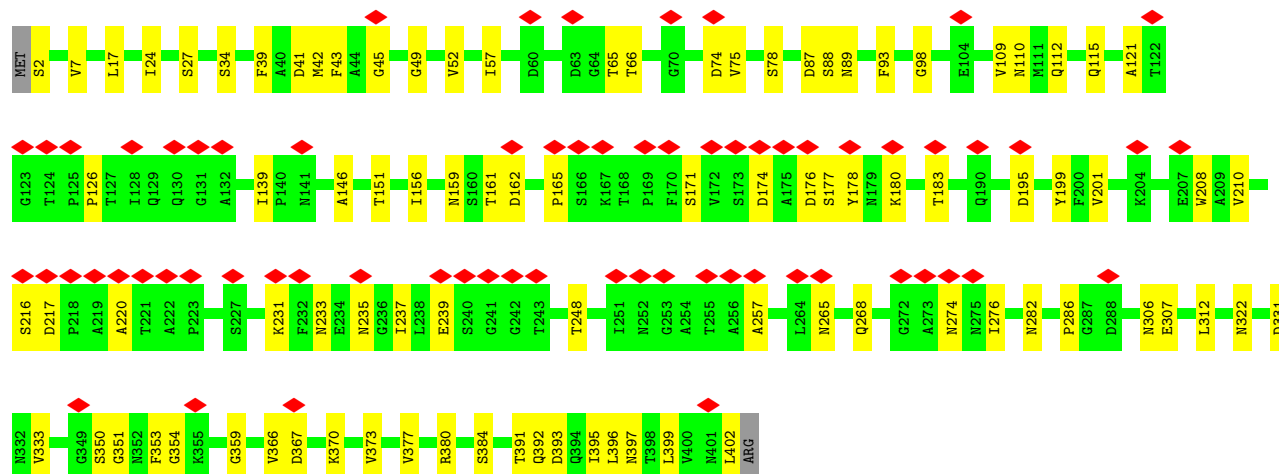
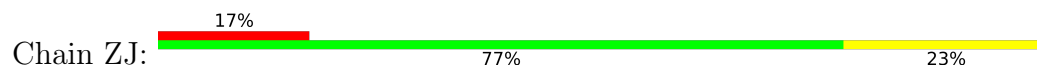




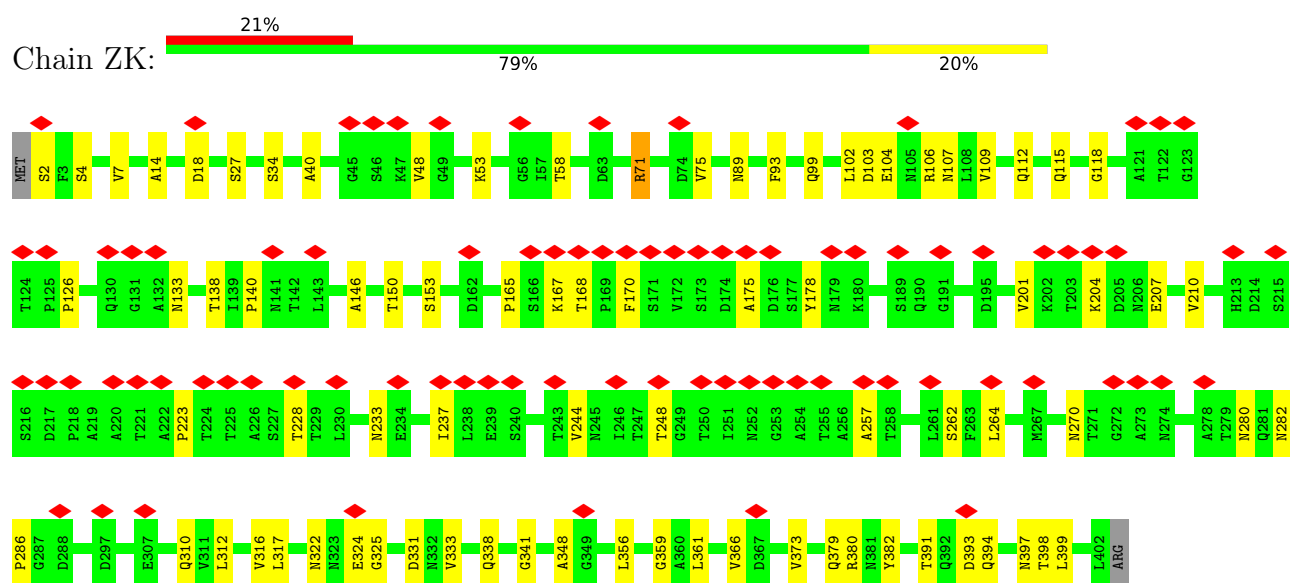
• Molecule 10: Flagellar hook protein FlgE



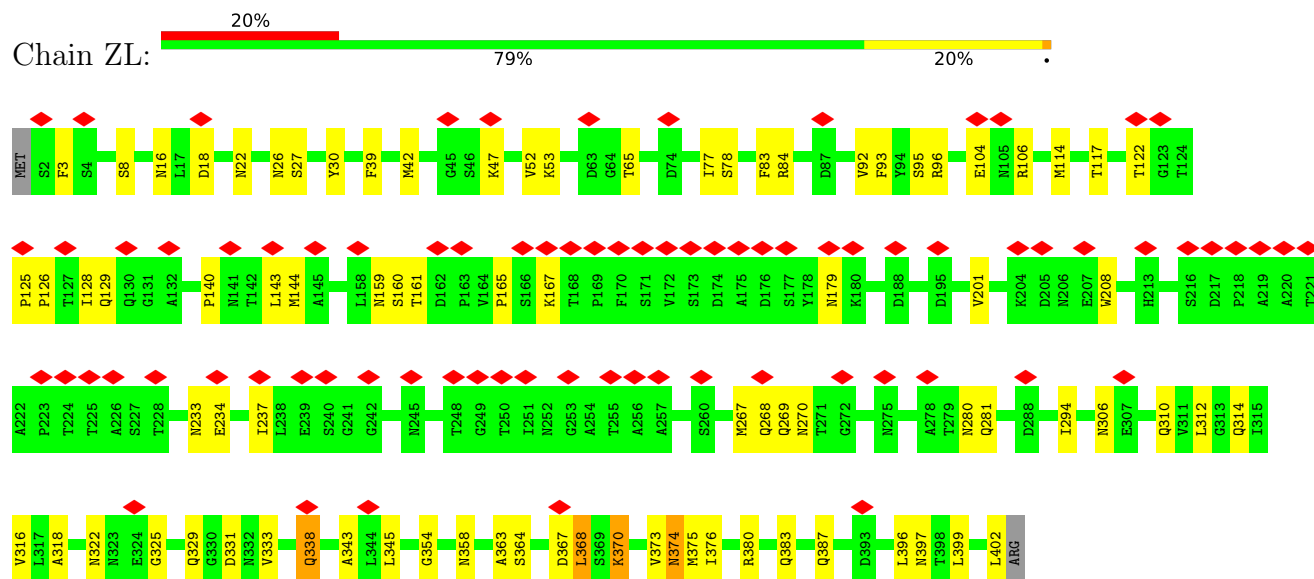
• Molecule 10: Flagellar hook protein FlgE



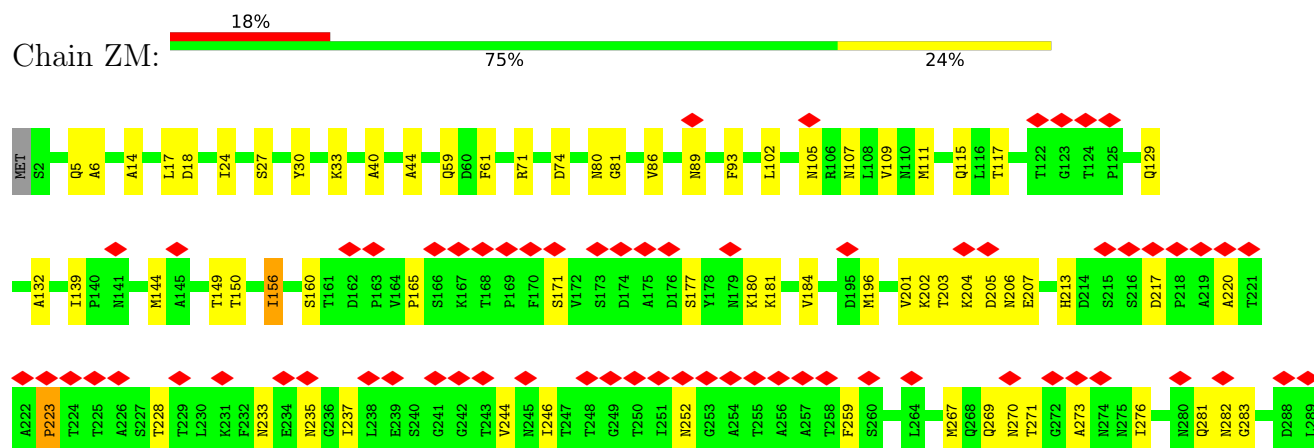
• Molecule 10: Flagellar hook protein FlgE

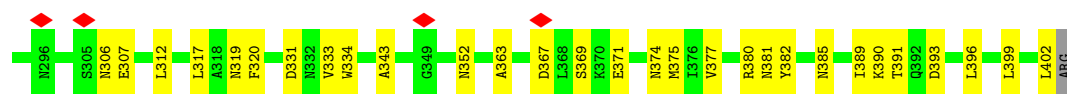


• Molecule 10: Flagellar hook protein FlgE

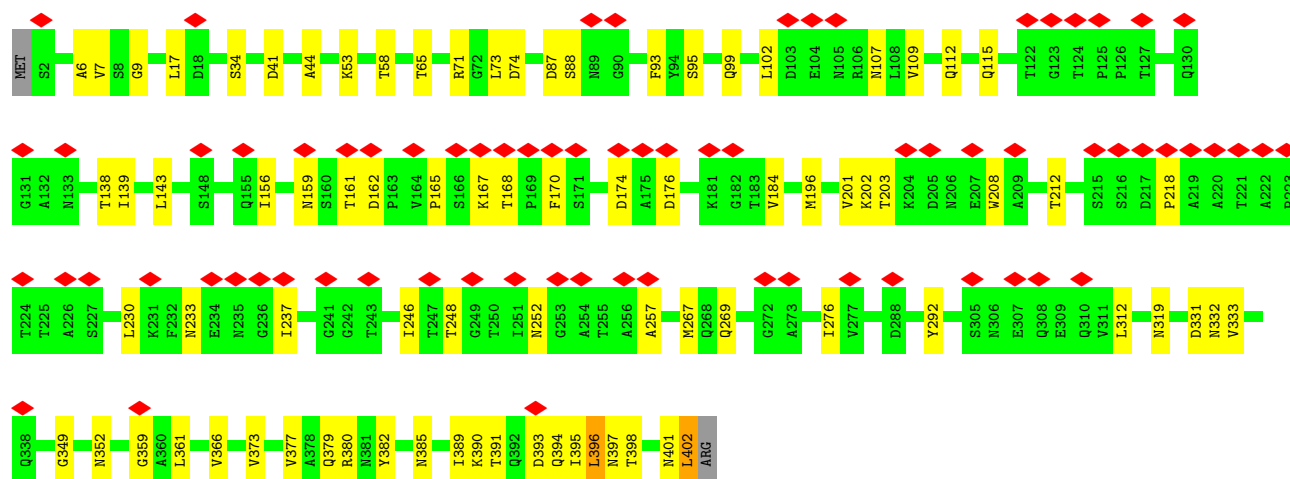
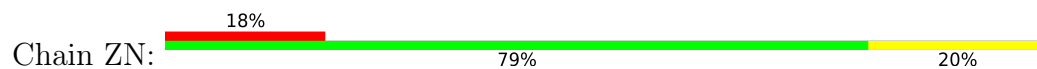


• Molecule 10: Flagellar hook protein FlgE

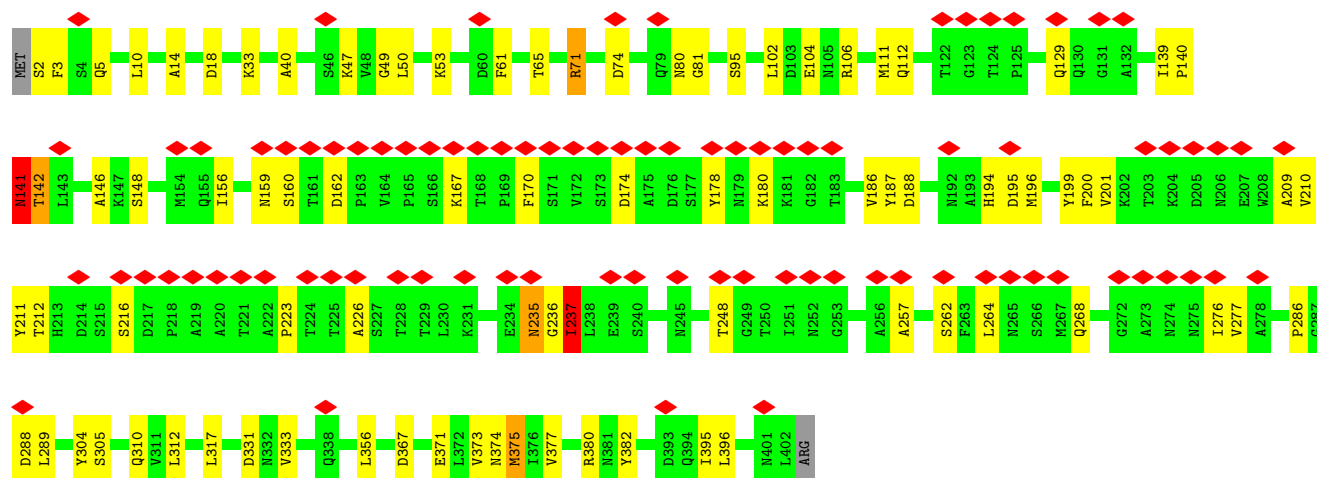
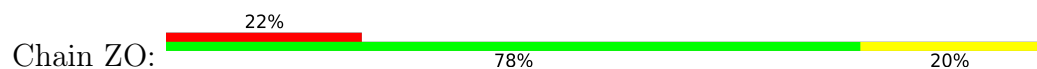




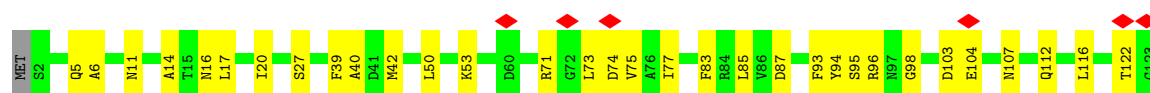
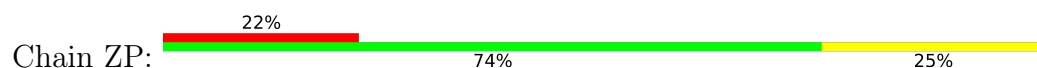
• Molecule 10: Flagellar hook protein FlgE

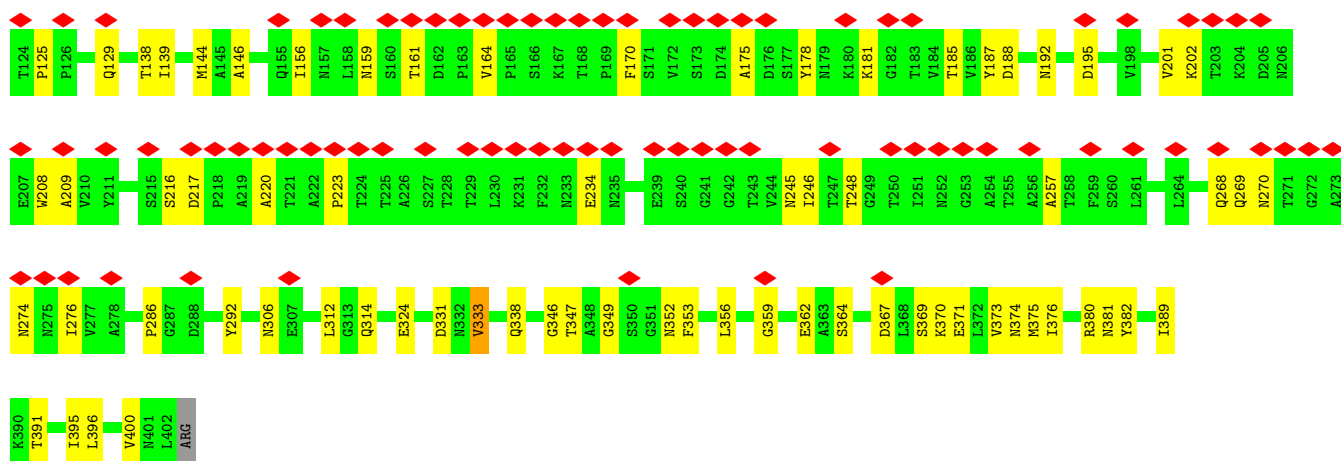


• Molecule 10: Flagellar hook protein FlgE

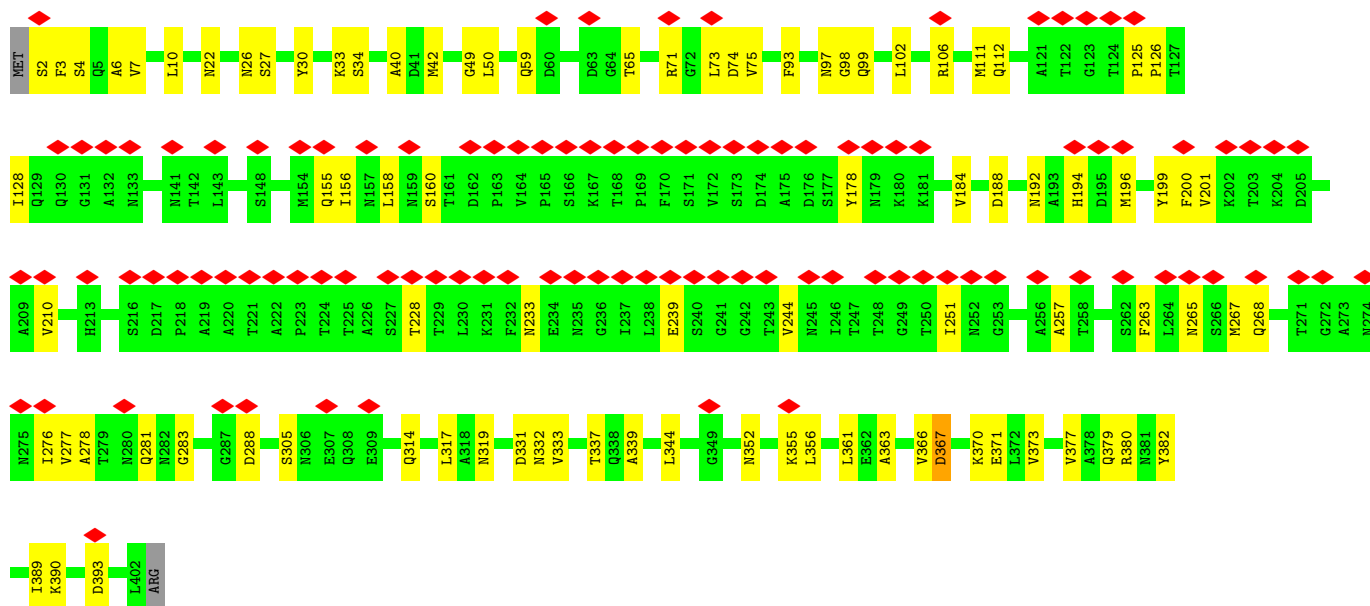
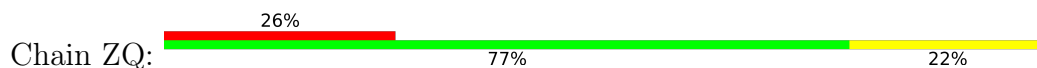


• Molecule 10: Flagellar hook protein FlgE

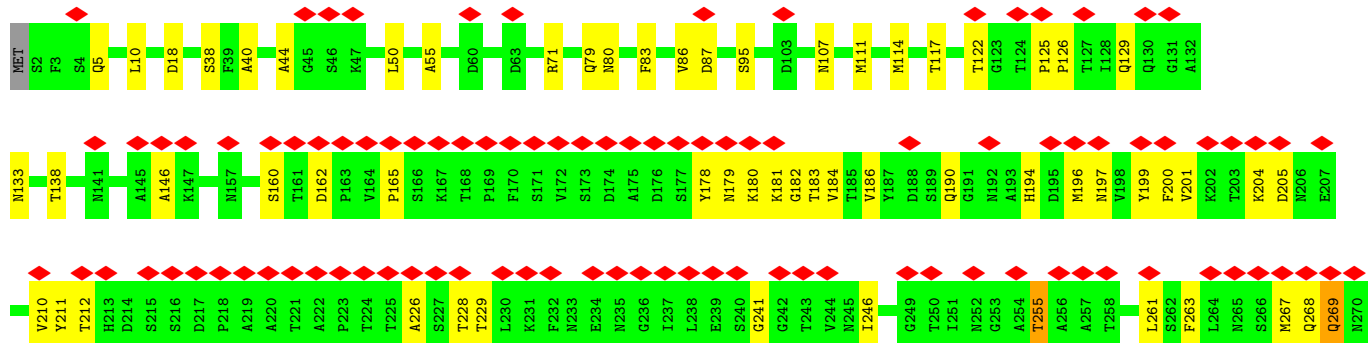
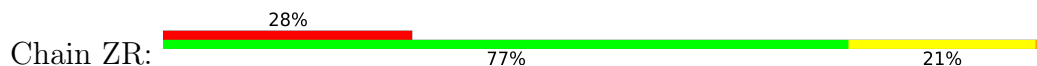




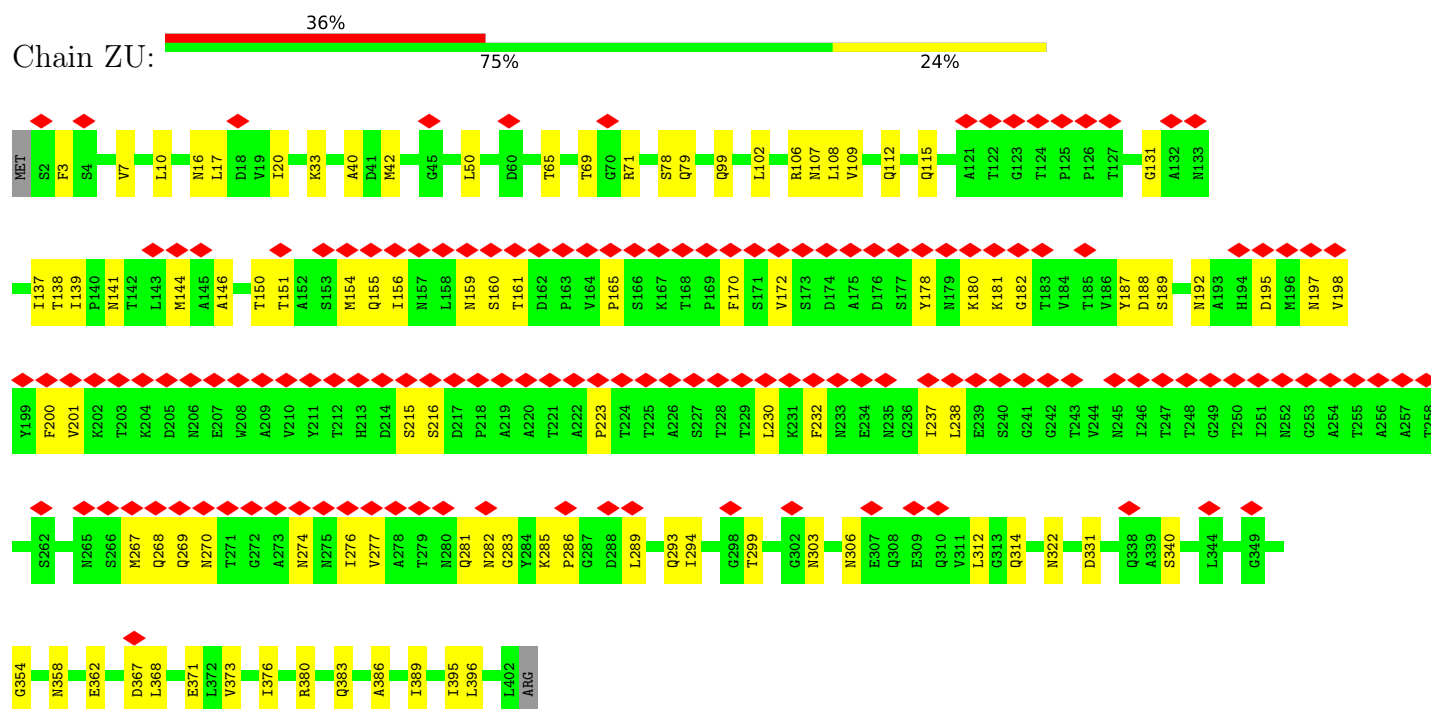
• Molecule 10: Flagellar hook protein FlgE



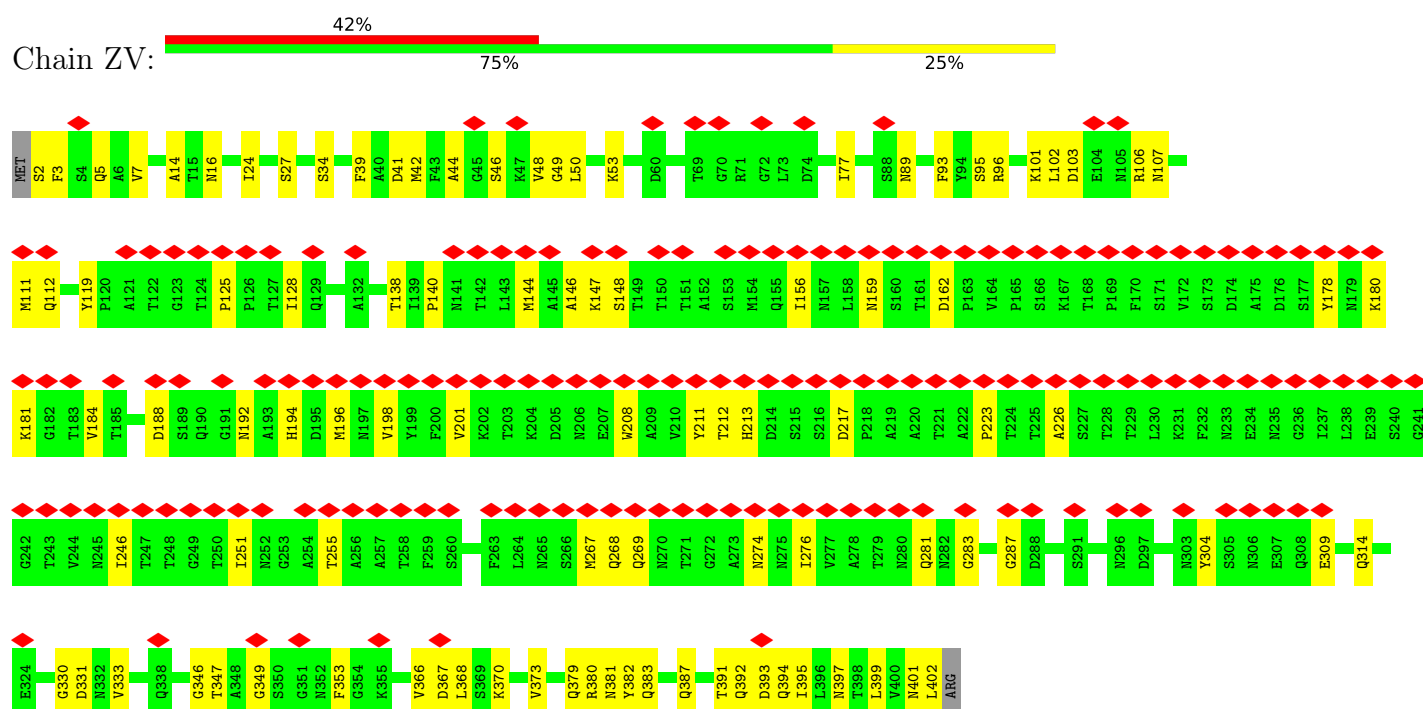
• Molecule 10: Flagellar hook protein FlgE



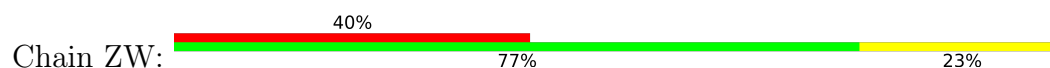
- Molecule 10: Flagellar hook protein FlgE

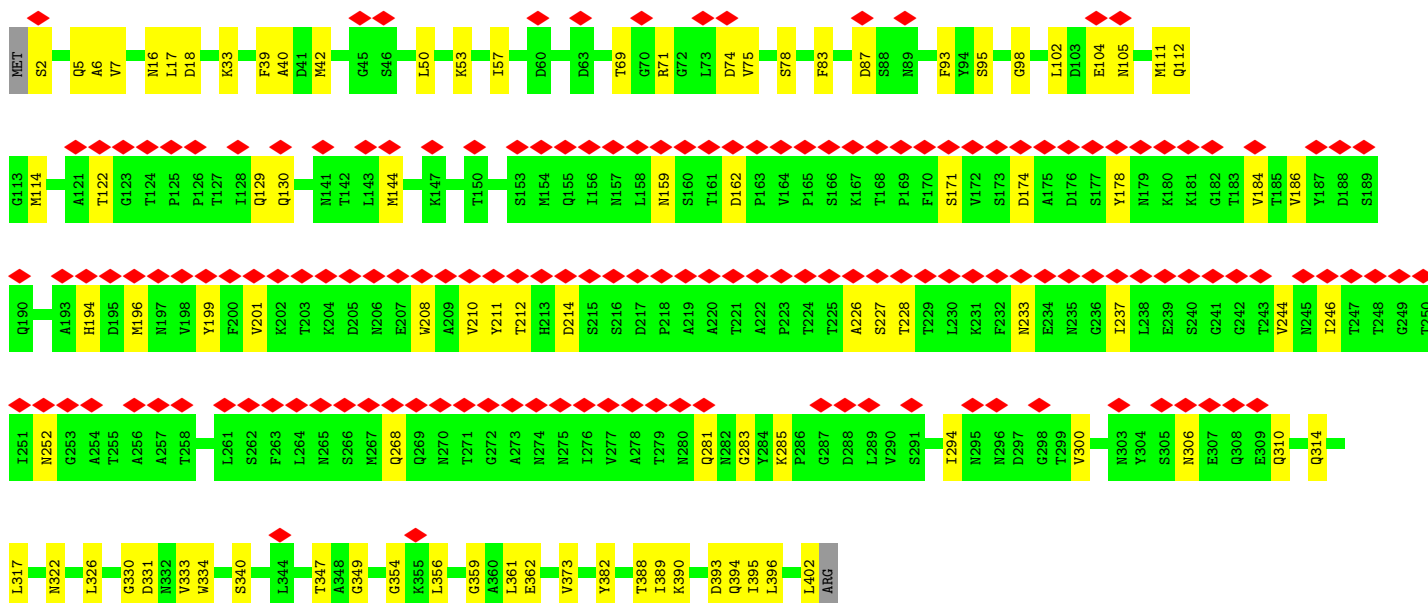


- Molecule 10: Flagellar hook protein FlgE

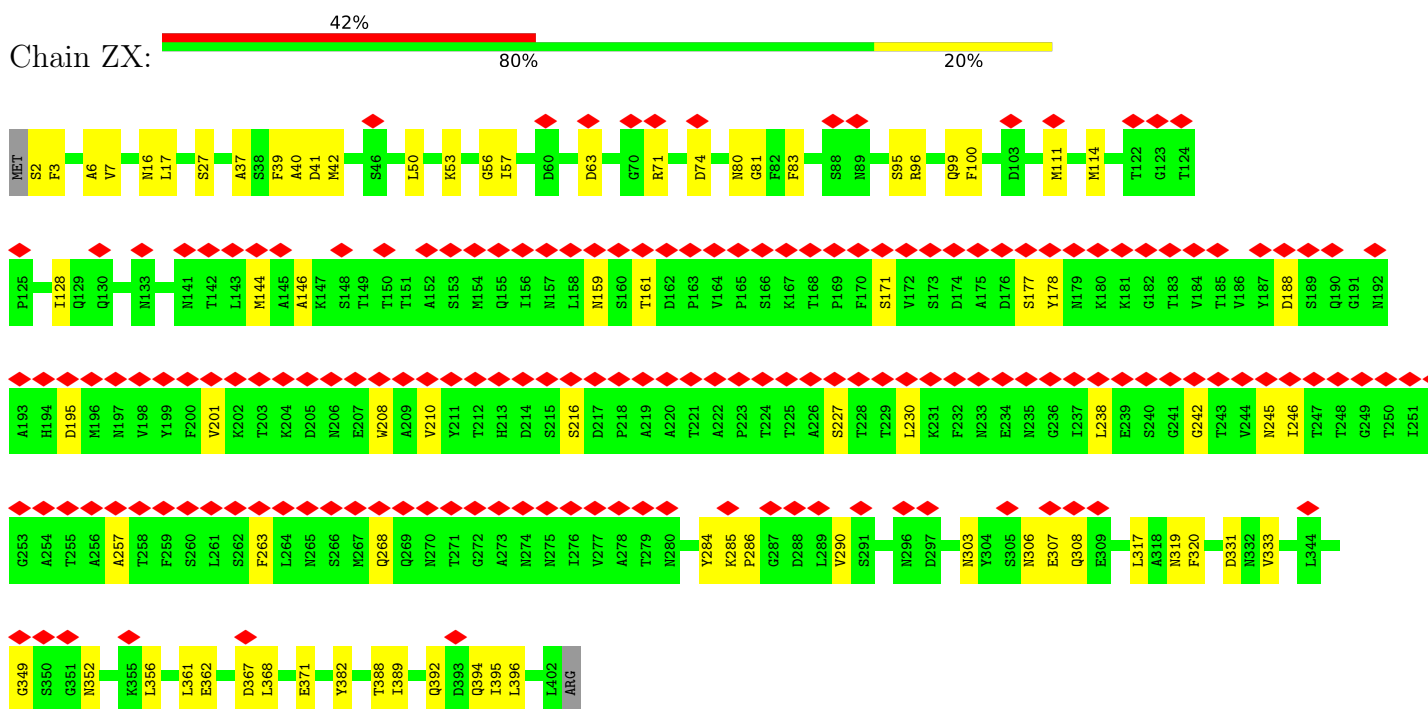


- Molecule 10: Flagellar hook protein FlgE

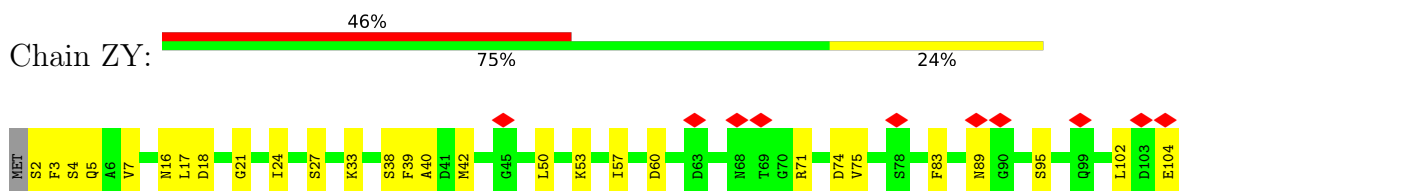


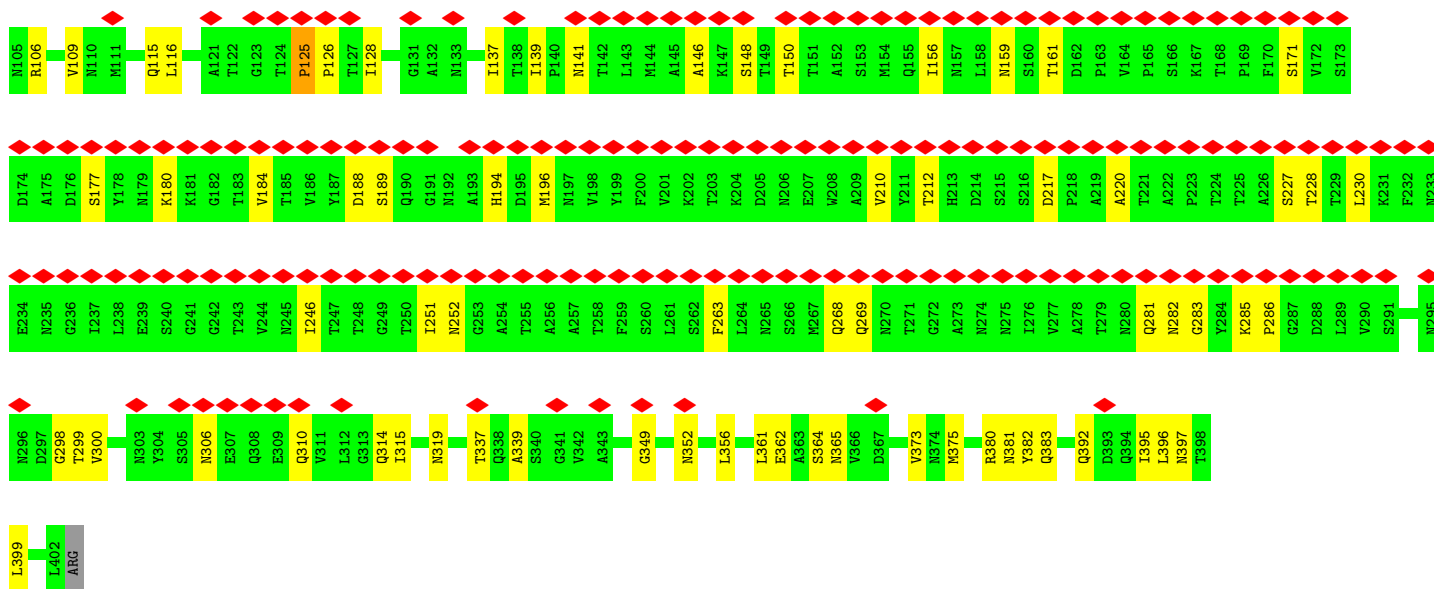


• Molecule 10: Flagellar hook protein FlgE

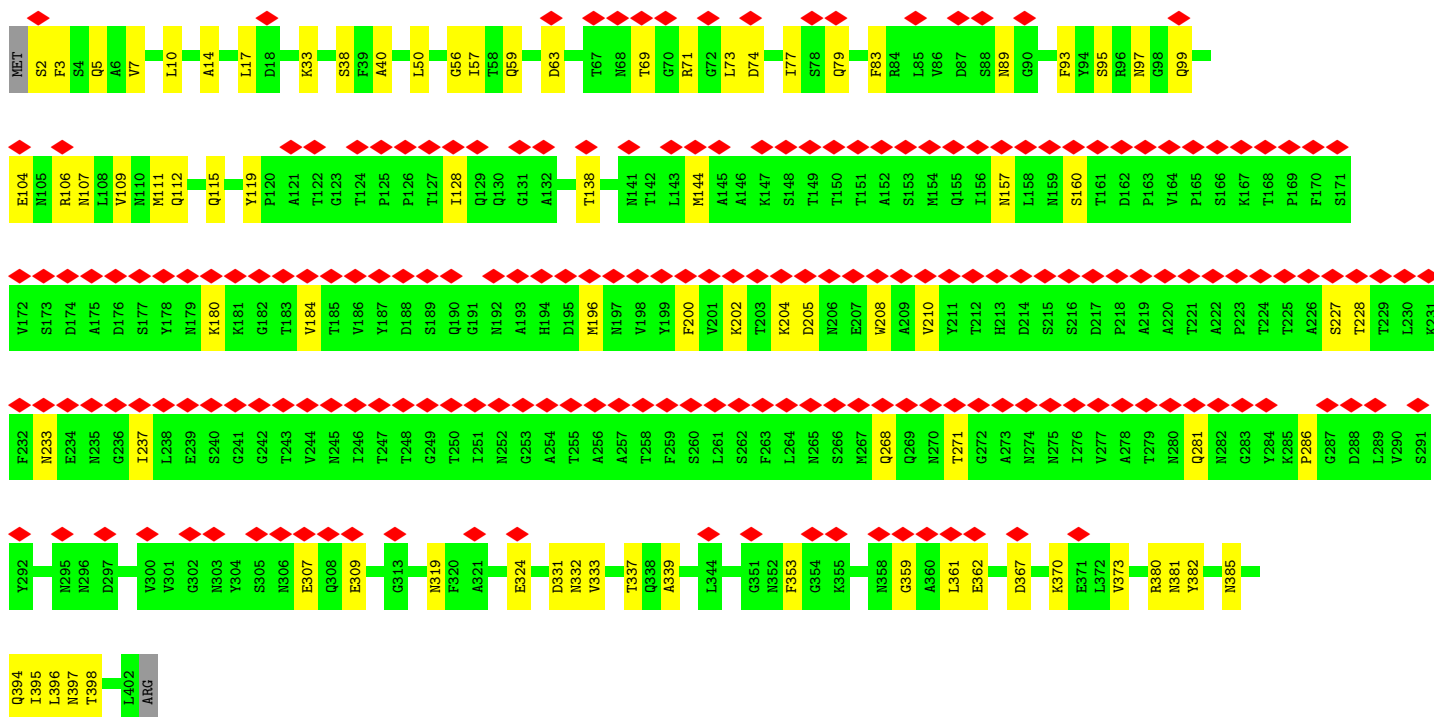
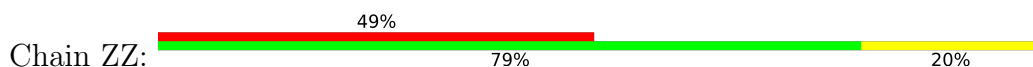


• Molecule 10: Flagellar hook protein FlgE

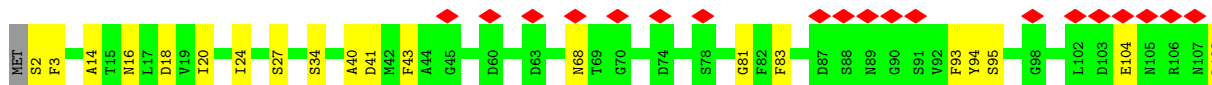
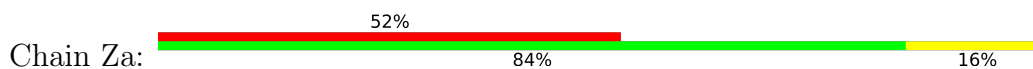


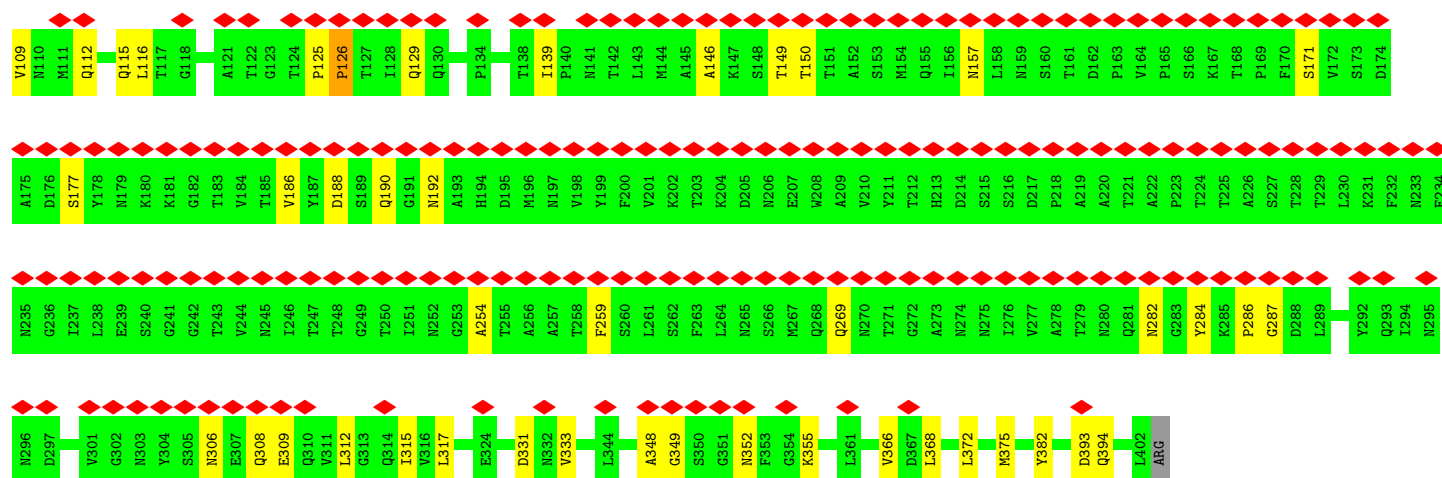


• Molecule 10: Flagellar hook protein FlgE

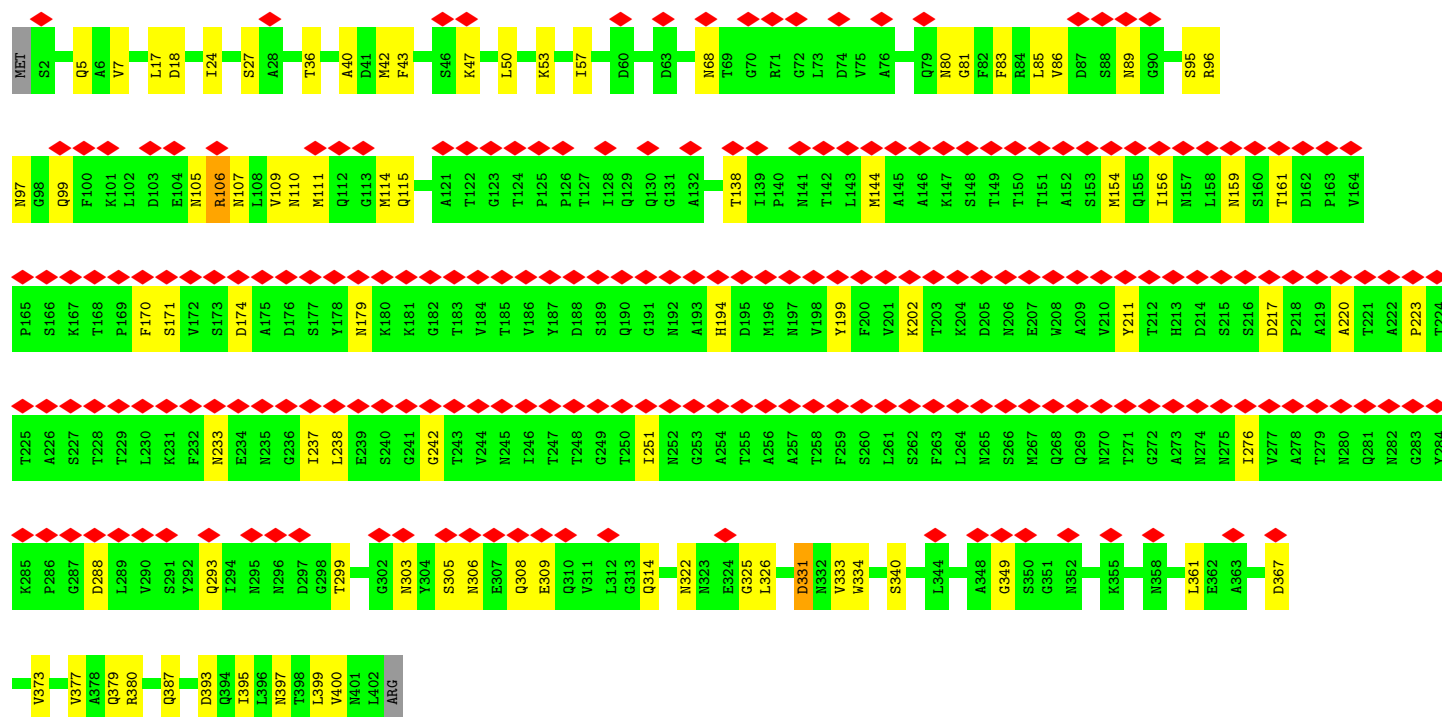
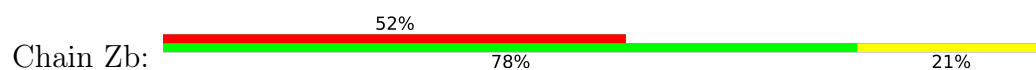


• Molecule 10: Flagellar hook protein FlgE

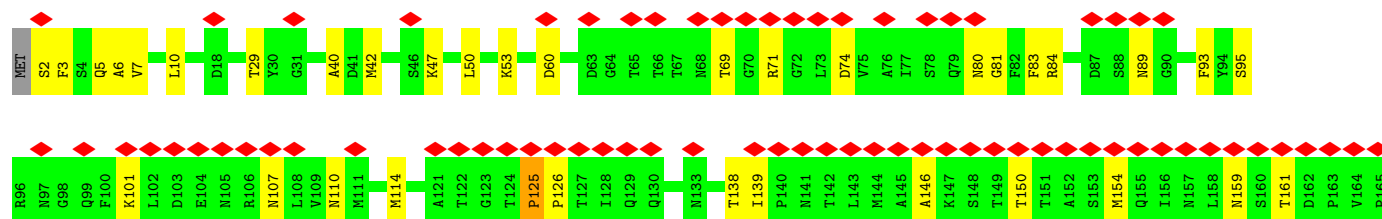
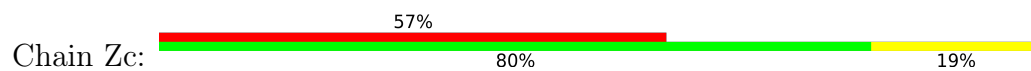


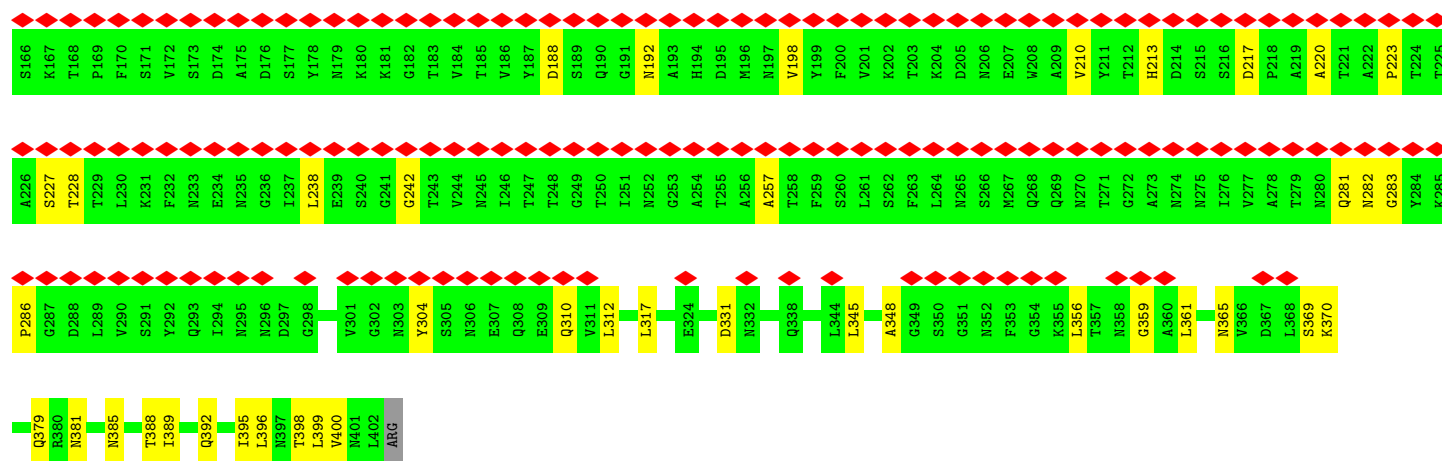


• Molecule 10: Flagellar hook protein FlgE

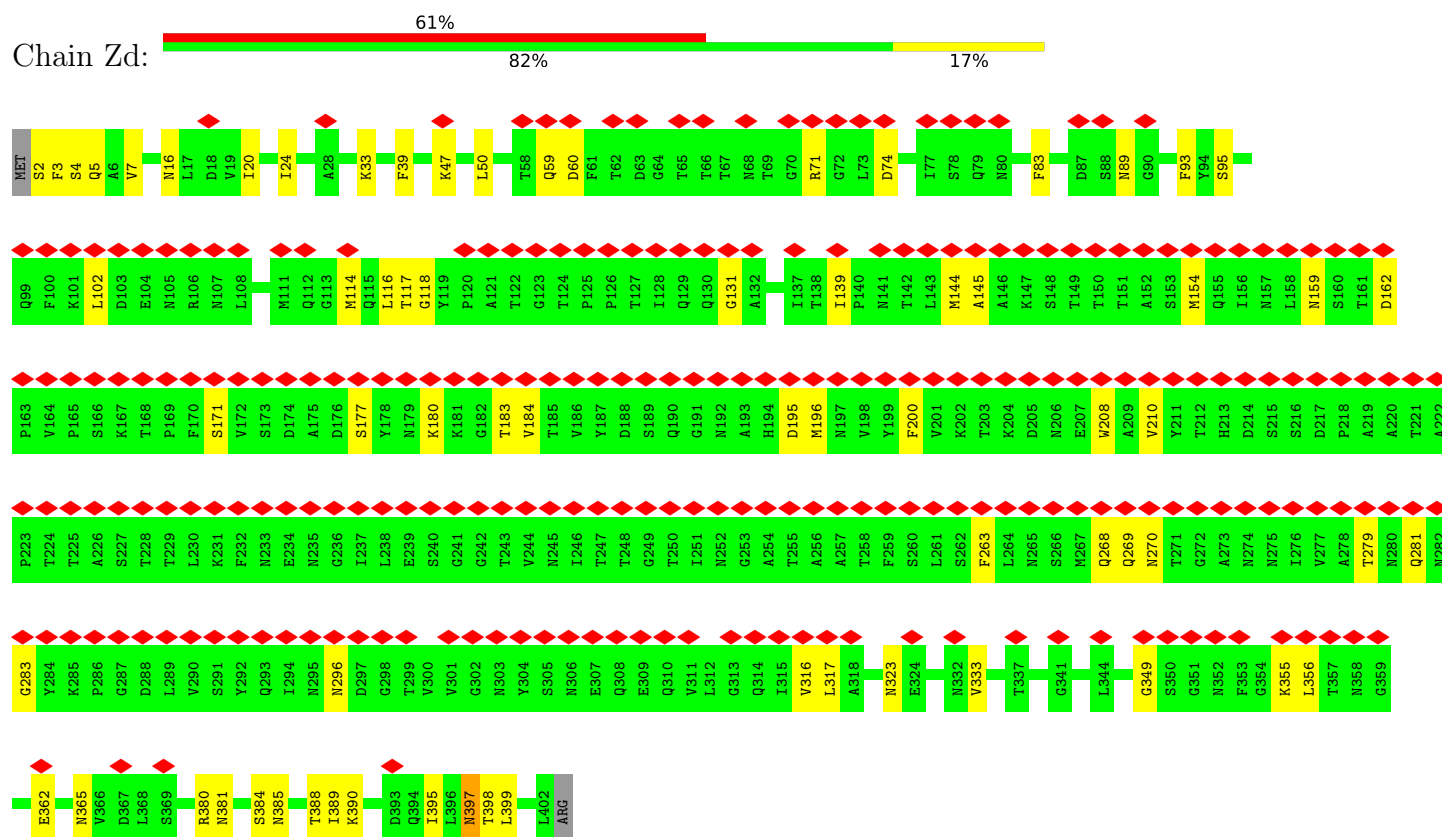


• Molecule 10: Flagellar hook protein FlgE

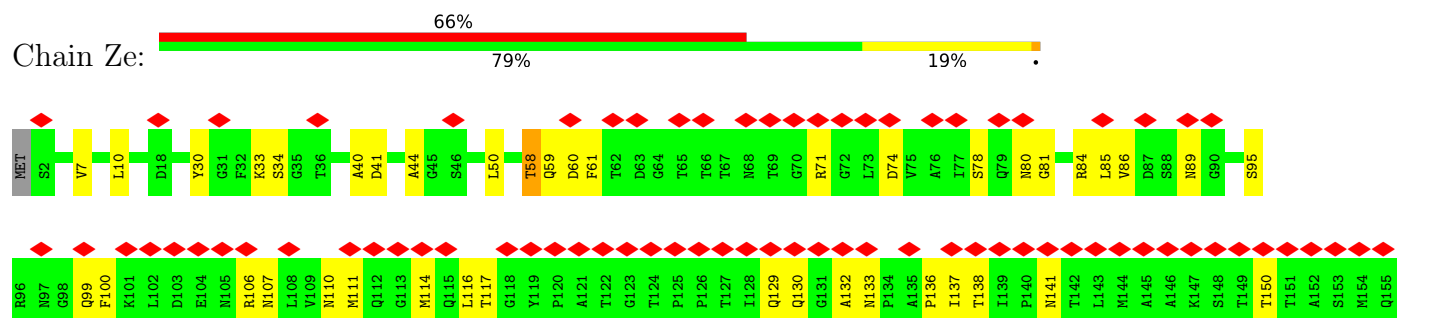


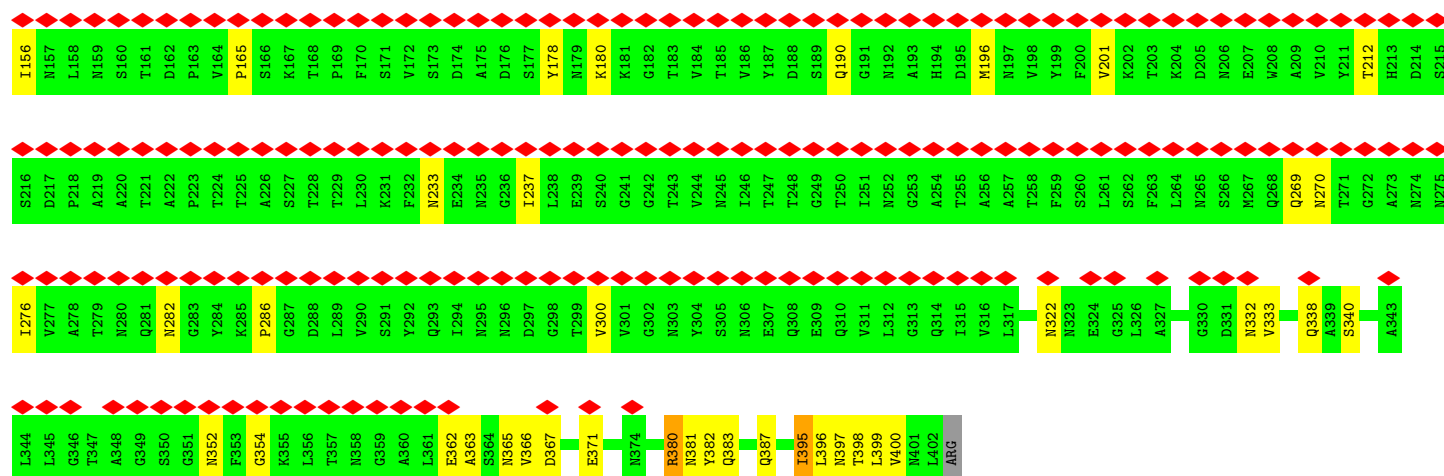


• Molecule 10: Flagellar hook protein FlgE

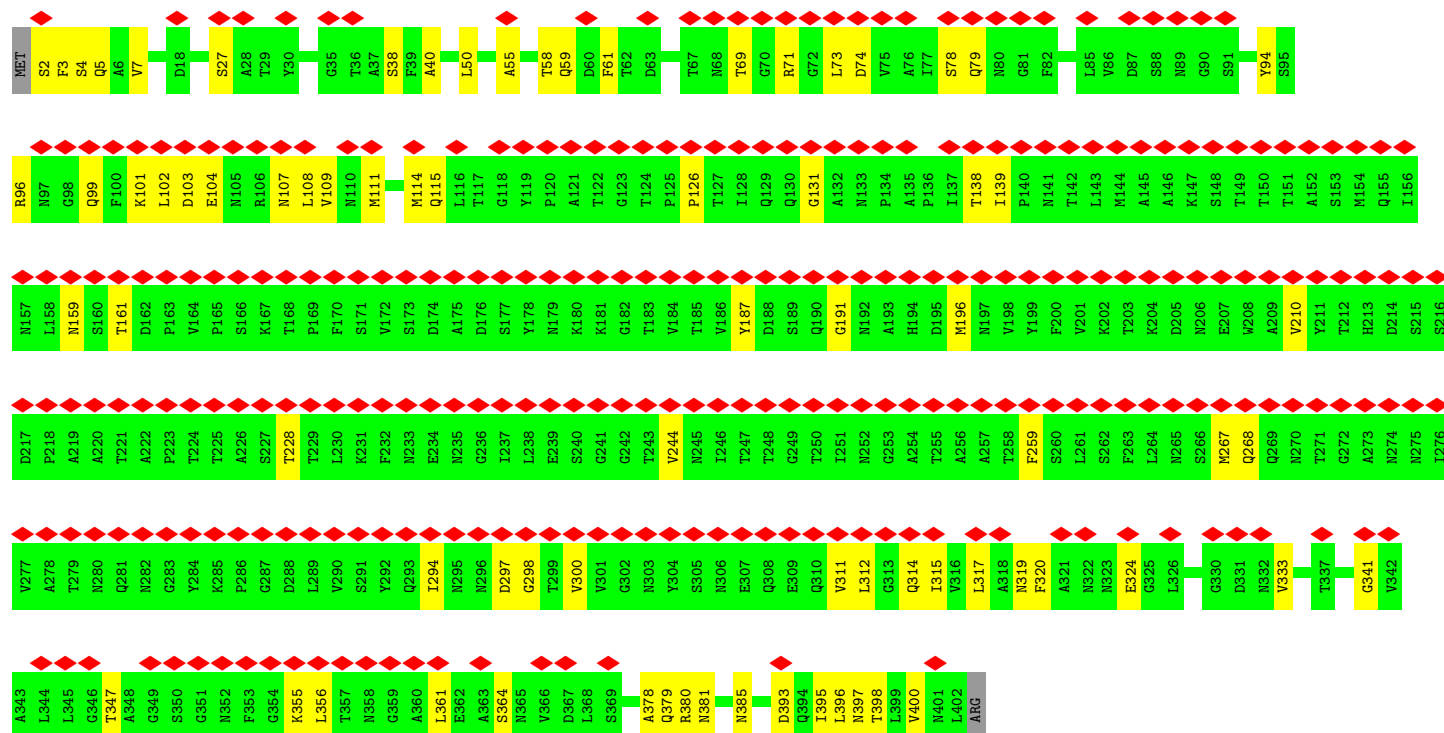
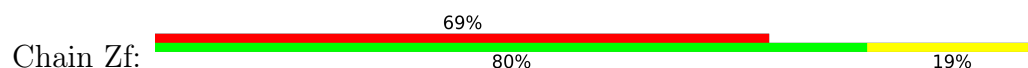


• Molecule 10: Flagellar hook protein FlgE

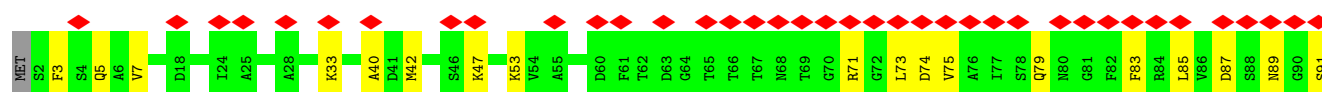
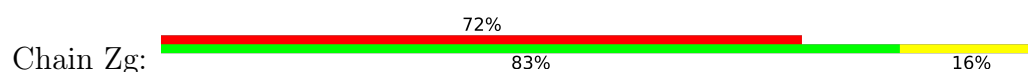


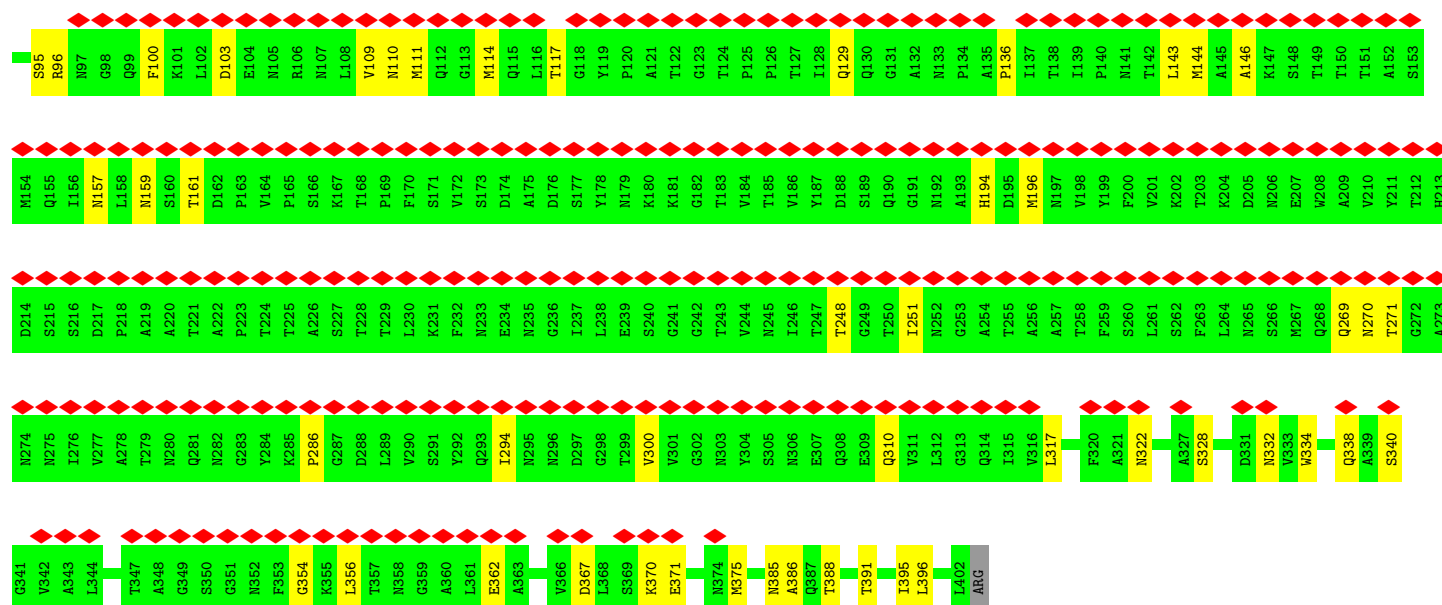


• Molecule 10: Flagellar hook protein FlgE

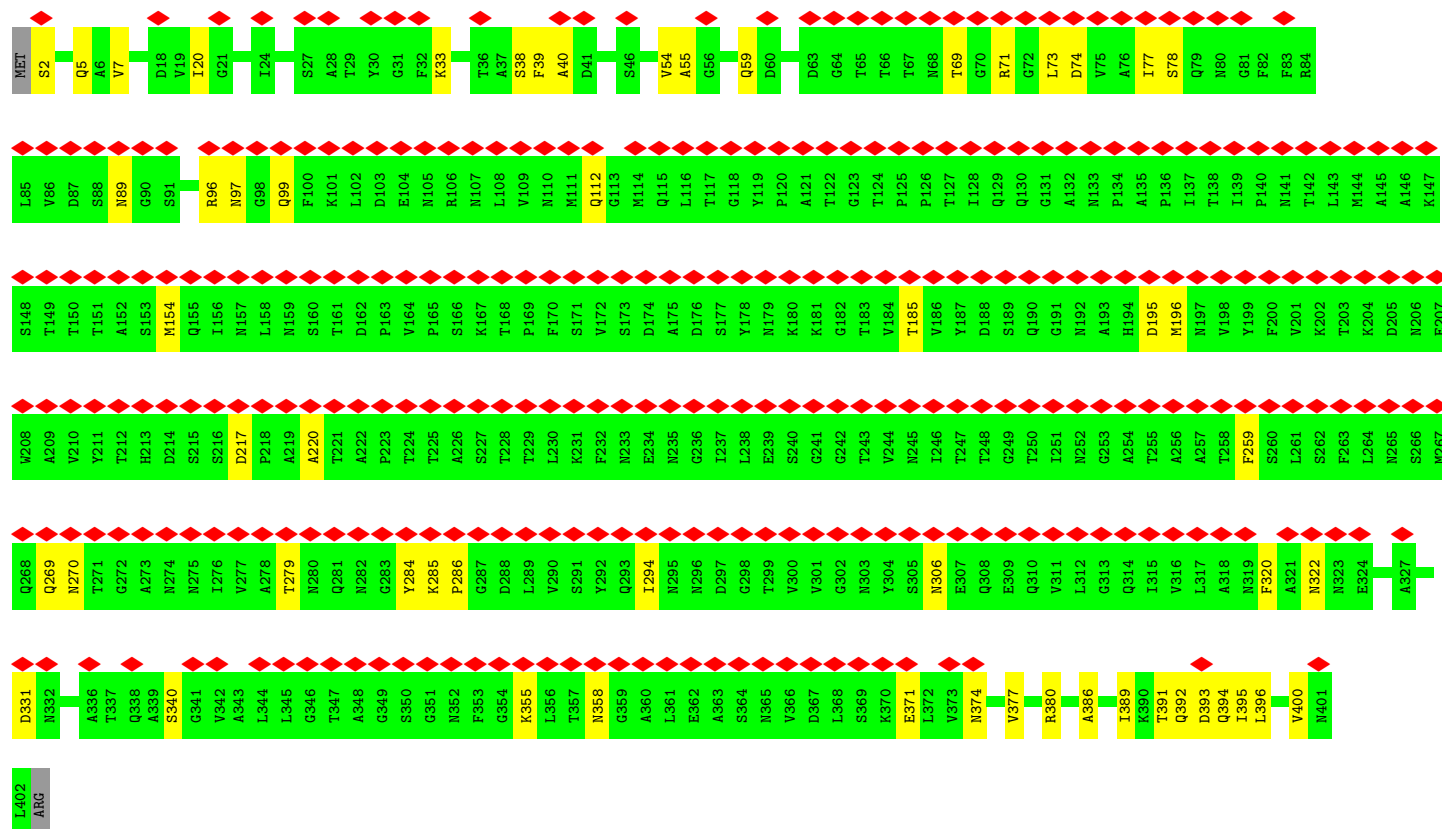
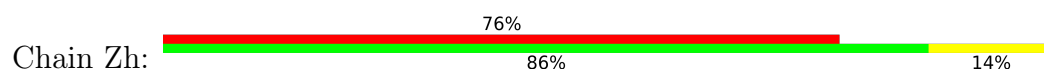


• Molecule 10: Flagellar hook protein FlgE





• 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 ($\text{\AA}$)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.26	0/681	0.49	0/930
1	B	0.16	0/681	0.42	0/930
1	C	0.23	0/681	0.44	0/930
1	D	0.26	0/681	0.55	0/930
2	E	0.45	3/1994 (0.2%)	0.61	3/2724 (0.1%)
3	F	0.33	0/1643	0.61	4/2237 (0.2%)
3	G	0.26	0/1665	0.46	2/2267 (0.1%)
3	H	0.22	0/1652	0.42	0/2249
3	I	0.22	0/1652	0.40	0/2249
3	J	0.30	0/1662	0.53	1/2263 (0.0%)
4	K	0.17	0/300	0.43	0/400
4	L	0.11	0/547	0.24	0/733
4	M	0.17	0/561	0.29	0/753
4	N	0.13	0/561	0.27	0/753
4	O	0.13	0/561	0.31	0/753
4	P	0.16	0/554	0.32	0/743
5	Q	0.21	0/930	0.46	0/1251
5	R	0.16	0/855	0.34	0/1150
5	S	0.18	0/855	0.39	0/1150
5	T	0.16	0/870	0.33	0/1169
5	U	0.18	0/839	0.35	0/1129
6	V	0.15	0/981	0.31	0/1334
6	W	0.13	0/976	0.32	0/1327
6	X	0.52	2/981 (0.2%)	0.98	3/1334 (0.2%)
6	Y	0.16	0/981	0.36	0/1334
6	Z	0.15	0/981	0.35	0/1334
6	a	0.19	0/981	0.36	0/1334
7	b	0.70	0/83	0.97	0/114
7	c	0.16	0/107	0.37	0/148
7	d	0.27	0/137	0.52	0/191
7	e	0.20	0/107	0.44	0/148
7	f	1.32	1/145 (0.7%)	1.50	3/203 (1.5%)
7	g	0.22	0/107	0.57	0/148
7	h	0.13	0/145	0.29	0/203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	i	0.14	0/107	0.41	0/148
7	j	0.25	0/137	0.66	0/191
7	k	0.16	0/107	0.30	0/148
7	l	0.26	0/145	0.44	0/203
8	m	0.36	0/1828	0.56	1/2492 (0.0%)
8	n	0.26	0/1836	0.47	0/2502
8	o	0.22	0/1844	0.44	0/2512
8	p	0.17	0/1844	0.37	0/2512
8	q	0.29	0/1836	0.49	1/2502 (0.0%)
9	0	0.28	0/1888	0.51	1/2564 (0.0%)
9	1	0.27	0/1917	0.52	0/2605
9	2	0.21	0/1973	0.46	0/2682
9	3	0.23	0/1973	0.47	0/2682
9	4	0.20	0/1973	0.46	0/2682
9	5	0.32	0/1973	0.58	0/2682
9	6	0.30	0/1973	0.57	0/2682
9	7	0.22	0/1973	0.45	0/2682
9	8	0.26	0/1973	0.52	0/2682
9	9	0.23	0/1973	0.54	2/2682 (0.1%)
9	ZA	0.27	0/1973	0.51	0/2682
9	ZB	0.26	0/1973	0.50	0/2682
9	ZC	0.23	0/1973	0.51	0/2682
9	ZD	0.25	0/1973	0.53	0/2682
9	ZE	0.23	0/1973	0.46	0/2682
9	r	0.35	0/1926	0.60	0/2618
9	s	0.40	0/1934	0.69	0/2629
9	t	0.35	0/1942	0.64	3/2639 (0.1%)
9	u	0.33	0/1926	0.60	2/2618 (0.1%)
9	v	0.31	0/1934	0.55	0/2629
9	w	0.32	0/1844	0.58	1/2505 (0.0%)
9	x	0.30	0/1888	0.53	0/2564
9	y	0.30	0/1888	0.57	0/2564
9	z	0.28	0/1888	0.50	0/2564
10	ZF	0.23	0/2991	0.48	2/4076 (0.0%)
10	ZG	0.29	1/2991 (0.0%)	0.53	4/4076 (0.1%)
10	ZH	0.24	0/2991	0.48	1/4076 (0.0%)
10	ZI	0.27	0/2991	0.50	1/4076 (0.0%)
10	ZJ	0.28	0/2991	0.51	0/4076
10	ZK	0.17	0/2991	0.39	0/4076
10	ZL	0.23	0/2991	0.44	0/4076
10	ZM	0.22	0/2991	0.49	1/4076 (0.0%)
10	ZN	0.21	0/2991	0.46	1/4076 (0.0%)
10	ZO	0.26	0/2991	0.49	1/4076 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	ZP	0.20	0/2991	0.43	1/4076 (0.0%)
10	ZQ	0.22	0/2991	0.48	0/4076
10	ZR	0.24	1/2991 (0.0%)	0.50	2/4076 (0.0%)
10	ZS	0.21	0/2991	0.44	0/4076
10	ZT	0.13	0/2991	0.35	0/4076
10	ZU	0.21	0/2991	0.43	0/4076
10	ZV	0.48	4/2991 (0.1%)	0.65	7/4076 (0.2%)
10	ZW	0.14	0/2991	0.37	0/4076
10	ZX	0.18	0/2991	0.41	0/4076
10	ZY	0.22	1/2991 (0.0%)	0.45	2/4076 (0.0%)
10	ZZ	0.13	0/2991	0.35	0/4076
10	Za	0.18	0/2991	0.41	1/4076 (0.0%)
10	Zb	0.25	0/2991	0.48	1/4076 (0.0%)
10	Zc	0.23	0/2991	0.49	3/4076 (0.1%)
10	Zd	0.25	0/2991	0.50	1/4076 (0.0%)
10	Ze	0.21	0/2991	0.48	0/4076
10	Zf	0.21	0/2991	0.45	0/4076
10	Zg	0.18	0/2991	0.42	0/4076
10	Zh	0.16	0/2991	0.38	0/4076
All	All	0.26	13/170184 (0.0%)	0.49	56/231624 (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

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	ZV	140	PRO	CG-CD	-15.65	0.97	1.50
7	f	331	PRO	CG-CD	-13.86	1.03	1.50
10	ZV	125	PRO	CG-CD	-12.77	1.17	1.51
6	X	73	PRO	CG-CD	-12.38	1.08	1.50
2	E	185	MET	C-O	9.78	1.35	1.24

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	73	PRO	CB-CG-CD	23.05	179.87	106.10
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
10	ZV	125	PRO	N-CD-CG	-14.54	86.35	103.80

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	143	ARG	Sidechain
5	Q	106	ARG	Sidechain
5	U	104	ARG	Sidechain
6	Y	110	ARG	Sidechain
6	a	110	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	670	0	739	15	0
1	B	670	0	739	28	0
1	C	670	0	739	28	0
1	D	670	0	739	40	0
2	E	1945	0	2063	81	0
3	F	1605	0	1701	63	0
3	G	1626	0	1718	48	0
3	H	1614	0	1709	40	0
3	I	1614	0	1709	43	0
3	J	1623	0	1715	65	0
4	K	300	0	311	15	0
4	L	543	0	550	10	0
4	M	557	0	566	10	0
4	N	557	0	566	13	0
4	O	557	0	566	18	0
4	P	550	0	559	18	0
5	Q	922	0	914	26	0
5	R	848	0	847	16	0
5	S	848	0	847	25	0
5	T	863	0	863	17	0
5	U	832	0	829	24	0
6	V	969	0	981	51	0
6	W	964	0	976	60	0
6	X	969	0	981	35	0
6	Y	969	0	981	37	0
6	Z	969	0	981	45	0
6	a	969	0	981	56	0
7	b	81	0	78	6	0
7	c	103	0	99	1	0
7	d	133	0	129	5	0
7	e	103	0	99	5	0
7	f	140	0	136	0	0
7	g	103	0	99	5	0
7	h	140	0	136	2	0
7	i	103	0	99	3	0
7	j	133	0	129	3	0
7	k	103	0	99	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	l	140	0	136	1	0
8	m	1804	0	1791	107	0
8	n	1812	0	1800	151	0
8	o	1820	0	1812	127	0
8	p	1820	0	1812	109	0
8	q	1812	0	1800	118	0
9	0	1866	0	1848	67	0
9	1	1894	0	1878	63	0
9	2	1949	0	1926	59	0
9	3	1949	0	1926	53	0
9	4	1949	0	1926	71	0
9	5	1949	0	1926	72	0
9	6	1949	0	1926	74	0
9	7	1949	0	1926	57	0
9	8	1949	0	1926	65	0
9	9	1949	0	1926	60	0
9	ZA	1949	0	1926	78	0
9	ZB	1949	0	1926	85	0
9	ZC	1949	0	1926	90	0
9	ZD	1949	0	1926	102	0
9	ZE	1949	0	1926	88	0
9	r	1903	0	1878	115	0
9	s	1911	0	1889	110	0
9	t	1919	0	1901	117	0
9	u	1903	0	1878	83	0
9	v	1911	0	1889	99	0
9	w	1823	0	1797	74	0
9	x	1866	0	1848	94	0
9	y	1866	0	1848	92	0
9	z	1866	0	1848	72	0
10	ZF	2947	0	2839	75	0
10	ZG	2947	0	2839	86	0
10	ZH	2947	0	2839	94	0
10	ZI	2947	0	2839	103	0
10	ZJ	2947	0	2839	87	0
10	ZK	2947	0	2839	68	0
10	ZL	2947	0	2839	64	0
10	ZM	2947	0	2839	70	0
10	ZN	2947	0	2839	71	0
10	ZO	2947	0	2839	72	0
10	ZP	2947	0	2839	79	0
10	ZQ	2947	0	2839	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	ZR	2947	0	2839	70	0
10	ZS	2947	0	2839	92	0
10	ZT	2947	0	2839	70	0
10	ZU	2947	0	2839	69	0
10	ZV	2947	0	2839	71	0
10	ZW	2947	0	2839	64	0
10	ZX	2947	0	2839	60	0
10	ZY	2947	0	2839	74	0
10	ZZ	2947	0	2839	61	0
10	Za	2947	0	2839	44	0
10	Zb	2947	0	2839	63	0
10	Zc	2947	0	2839	51	0
10	Zd	2947	0	2839	53	0
10	Ze	2947	0	2839	52	0
10	Zf	2947	0	2839	47	0
10	Zg	2947	0	2839	44	0
10	Zh	2947	0	2839	39	0
All	All	167771	0	164995	4002	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 4002 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:ZD:233:MET:CE	10:ZI:388:THR:HA	1.40	1.48
8:q:228:GLU:CB	9:w:258:THR:HG21	1.48	1.40
9:ZD:233:MET:HE1	10:ZI:388:THR:CA	1.55	1.36
6:V:77:VAL:HG13	9:r:6:TRP:NE1	1.41	1.32
9:ZE:122:VAL:O	10:ZJ:322:ASN:HB2	1.33	1.25

There are no symmetry-related clashes.

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%)	4	24
3	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
3	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	12	40
3	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
3	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	24	55
3	J	207/245 (84%)	200 (97%)	5 (2%)	2 (1%)	12	40
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	45
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	10	37
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	60
9	0	244/260 (94%)	236 (97%)	7 (3%)	1 (0%)	30	60
9	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	60
9	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	45
9	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	45
9	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	10	37
9	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	45
9	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	45
9	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	10	37
9	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	45
9	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	45
9	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	10	37
9	ZB	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	10	37
9	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	10	37
9	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	45
9	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	60
9	r	250/260 (96%)	237 (95%)	12 (5%)	1 (0%)	30	60
9	s	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	60
9	t	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	u	250/260 (96%)	242 (97%)	6 (2%)	2 (1%)	16	45
9	v	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	60
9	w	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	60
9	x	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	10	37
9	y	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	60
9	z	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	60
10	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	36	65
10	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
10	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	24	55
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%)	36	65
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	45
10	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	36	65
10	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
10	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	36	65
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	37	65

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	188	LEU
2	E	190	VAL
3	J	83	ALA
8	m	123	GLU
9	2	209	ASN

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%)	72 (97%)	2 (3%)	39	63
1	B	74/74 (100%)	74 (100%)	0	100	100
1	C	74/74 (100%)	74 (100%)	0	100	100
1	D	74/74 (100%)	72 (97%)	2 (3%)	39	63
2	E	210/221 (95%)	208 (99%)	2 (1%)	68	76
3	F	177/204 (87%)	174 (98%)	3 (2%)	53	71
3	G	179/204 (88%)	174 (97%)	5 (3%)	38	62
3	H	178/204 (87%)	176 (99%)	2 (1%)	65	76
3	I	178/204 (87%)	175 (98%)	3 (2%)	53	71
3	J	179/204 (88%)	178 (99%)	1 (1%)	78	81
4	K	33/79 (42%)	33 (100%)	0	100	100
4	L	56/79 (71%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M	58/79 (73%)	58 (100%)	0	100	100
4	N	58/79 (73%)	57 (98%)	1 (2%)	53	71
4	O	58/79 (73%)	58 (100%)	0	100	100
4	P	57/79 (72%)	56 (98%)	1 (2%)	51	70
5	Q	98/113 (87%)	96 (98%)	2 (2%)	48	68
5	R	90/113 (80%)	89 (99%)	1 (1%)	65	76
5	S	90/113 (80%)	90 (100%)	0	100	100
5	T	91/113 (80%)	91 (100%)	0	100	100
5	U	89/113 (79%)	88 (99%)	1 (1%)	65	76
6	V	104/105 (99%)	104 (100%)	0	100	100
6	W	104/105 (99%)	104 (100%)	0	100	100
6	X	104/105 (99%)	104 (100%)	0	100	100
6	Y	104/105 (99%)	103 (99%)	1 (1%)	68	76
6	Z	104/105 (99%)	102 (98%)	2 (2%)	50	68
6	a	104/105 (99%)	104 (100%)	0	100	100
7	b	8/467 (2%)	8 (100%)	0	100	100
7	c	11/467 (2%)	11 (100%)	0	100	100
7	d	14/467 (3%)	12 (86%)	2 (14%)	3	14
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%)	13	40
7	k	11/467 (2%)	11 (100%)	0	100	100
7	l	15/467 (3%)	14 (93%)	1 (7%)	15	42
8	m	190/193 (98%)	185 (97%)	5 (3%)	40	64
8	n	191/193 (99%)	189 (99%)	2 (1%)	68	76
8	o	192/193 (100%)	189 (98%)	3 (2%)	55	72
8	p	192/193 (100%)	192 (100%)	0	100	100
8	q	191/193 (99%)	190 (100%)	1 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	0	205/215 (95%)	200 (98%)	5 (2%)	43	65
9	1	209/215 (97%)	206 (99%)	3 (1%)	59	73
9	2	215/215 (100%)	214 (100%)	1 (0%)	81	83
9	3	215/215 (100%)	213 (99%)	2 (1%)	70	78
9	4	215/215 (100%)	214 (100%)	1 (0%)	81	83
9	5	215/215 (100%)	213 (99%)	2 (1%)	70	78
9	6	215/215 (100%)	212 (99%)	3 (1%)	59	73
9	7	215/215 (100%)	215 (100%)	0	100	100
9	8	215/215 (100%)	213 (99%)	2 (1%)	70	78
9	9	215/215 (100%)	212 (99%)	3 (1%)	59	73
9	ZA	215/215 (100%)	214 (100%)	1 (0%)	81	83
9	ZB	215/215 (100%)	211 (98%)	4 (2%)	50	68
9	ZC	215/215 (100%)	212 (99%)	3 (1%)	59	73
9	ZD	215/215 (100%)	213 (99%)	2 (1%)	70	78
9	ZE	215/215 (100%)	214 (100%)	1 (0%)	81	83
9	r	209/215 (97%)	206 (99%)	3 (1%)	59	73
9	s	210/215 (98%)	203 (97%)	7 (3%)	33	59
9	t	211/215 (98%)	206 (98%)	5 (2%)	43	65
9	u	209/215 (97%)	204 (98%)	5 (2%)	43	65
9	v	210/215 (98%)	207 (99%)	3 (1%)	59	73
9	w	200/215 (93%)	199 (100%)	1 (0%)	81	83
9	x	205/215 (95%)	203 (99%)	2 (1%)	68	76
9	y	205/215 (95%)	200 (98%)	5 (2%)	43	65
9	z	205/215 (95%)	201 (98%)	4 (2%)	48	68
10	ZF	321/323 (99%)	315 (98%)	6 (2%)	50	68
10	ZG	321/323 (99%)	316 (98%)	5 (2%)	55	72
10	ZH	321/323 (99%)	316 (98%)	5 (2%)	55	72
10	ZI	321/323 (99%)	316 (98%)	5 (2%)	55	72
10	ZJ	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	ZK	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	ZL	321/323 (99%)	318 (99%)	3 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	ZM	321/323 (99%)	318 (99%)	3 (1%)	70	78
10	ZN	321/323 (99%)	319 (99%)	2 (1%)	78	81
10	ZO	321/323 (99%)	318 (99%)	3 (1%)	70	78
10	ZP	321/323 (99%)	318 (99%)	3 (1%)	70	78
10	ZQ	321/323 (99%)	318 (99%)	3 (1%)	70	78
10	ZR	321/323 (99%)	318 (99%)	3 (1%)	70	78
10	ZS	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	ZT	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	ZU	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	ZV	321/323 (99%)	319 (99%)	2 (1%)	78	81
10	ZW	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	ZX	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	ZY	321/323 (99%)	321 (100%)	0	100	100
10	ZZ	321/323 (99%)	321 (100%)	0	100	100
10	Za	321/323 (99%)	321 (100%)	0	100	100
10	Zb	321/323 (99%)	318 (99%)	3 (1%)	70	78
10	Zc	321/323 (99%)	318 (99%)	3 (1%)	70	78
10	Zd	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	Ze	321/323 (99%)	319 (99%)	2 (1%)	78	81
10	Zf	321/323 (99%)	319 (99%)	2 (1%)	78	81
10	Zg	321/323 (99%)	320 (100%)	1 (0%)	86	86
10	Zh	321/323 (99%)	320 (100%)	1 (0%)	86	86
All	All	18273/23835 (77%)	18098 (99%)	175 (1%)	65	76

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	ZQ	367	ASP
9	s	16	GLN
10	ZR	331	ASP
10	Zc	369	SER
9	t	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 622 such sidechains are listed below:

Mol	Chain	Res	Type
10	ZZ	401	ASN
9	t	259	GLN
10	Zb	133	ASN
10	ZZ	394	GLN
10	Zf	107	ASN

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.

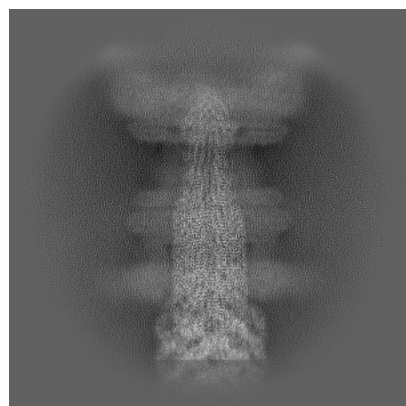
6 Map visualisation [i](#)

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.

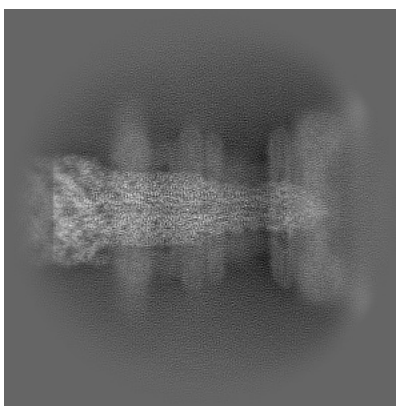
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

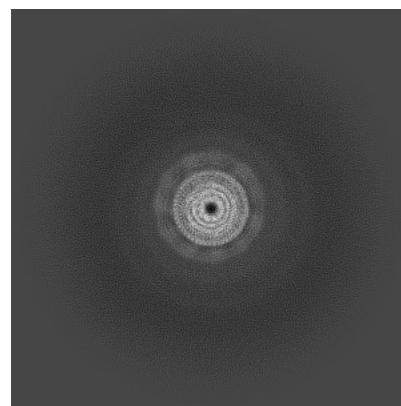
6.1.1 Primary map



X

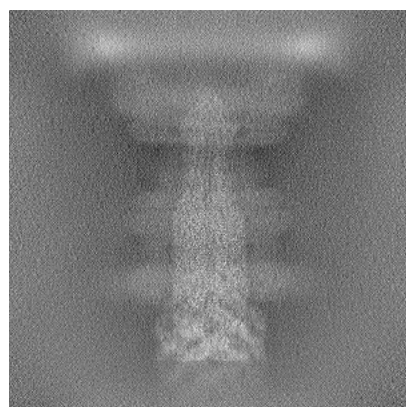


Y

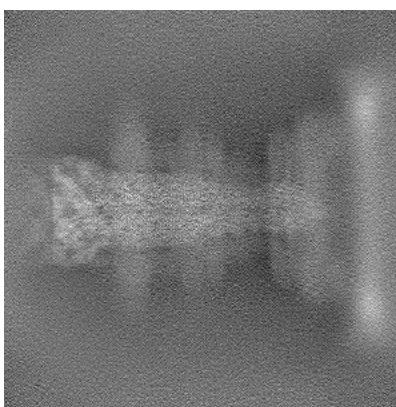


Z

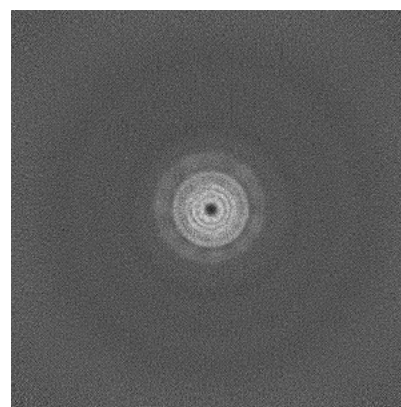
6.1.2 Raw map



X



Y

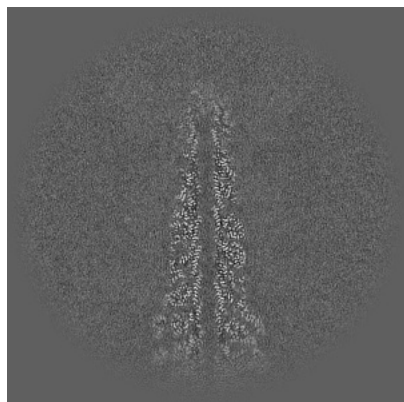


Z

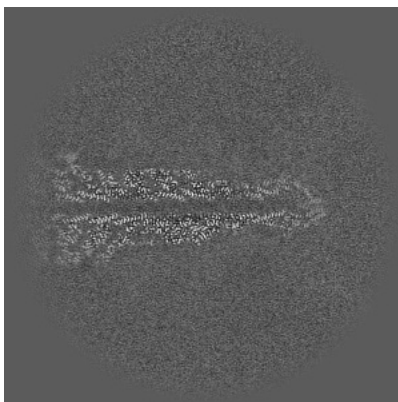
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

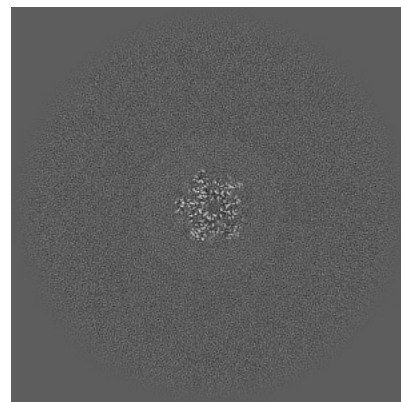
6.2.1 Primary map



X Index: 256

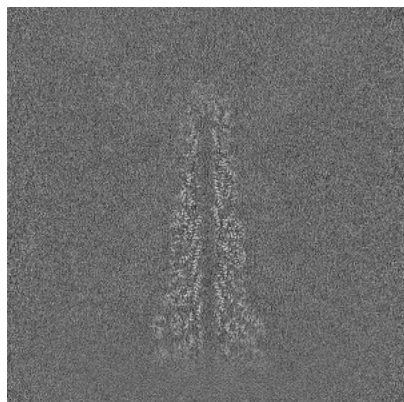


Y Index: 256

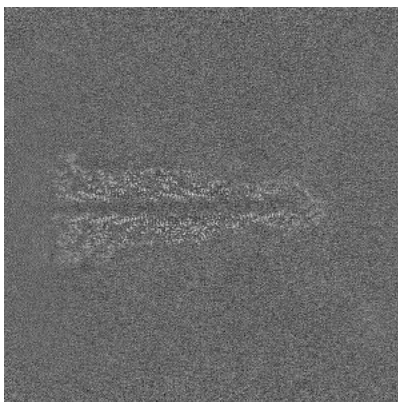


Z Index: 256

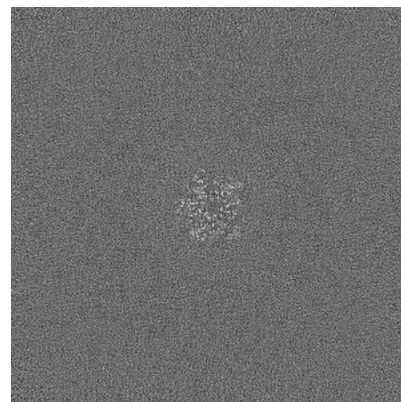
6.2.2 Raw map



X Index: 256



Y Index: 256

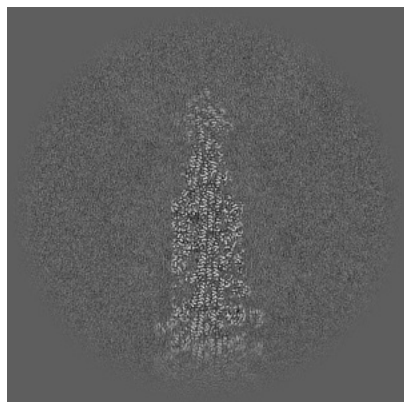


Z Index: 256

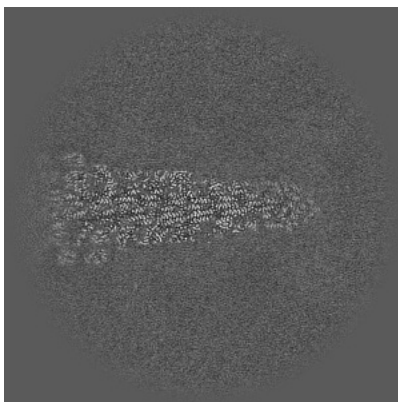
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

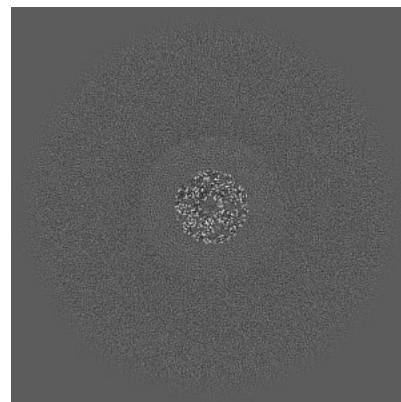
6.3.1 Primary map



X Index: 242

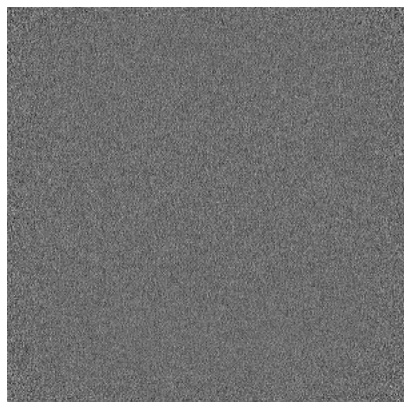


Y Index: 268

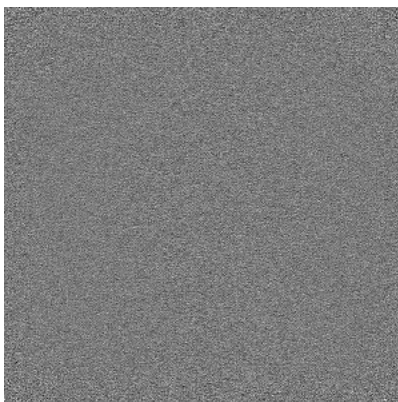


Z Index: 224

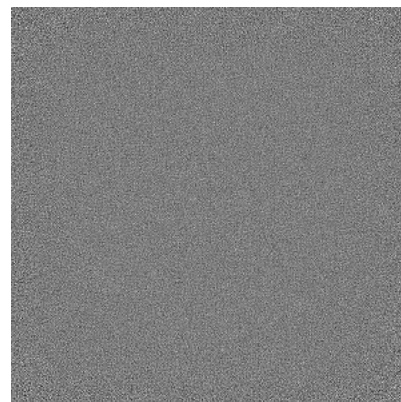
6.3.2 Raw map



X Index: 0



Y Index: 0

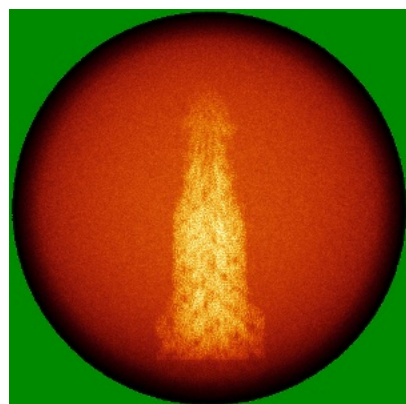


Z Index: 0

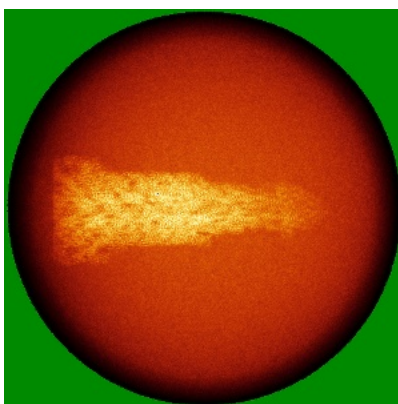
The images above show the largest variance slices of the map in three orthogonal directions.

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

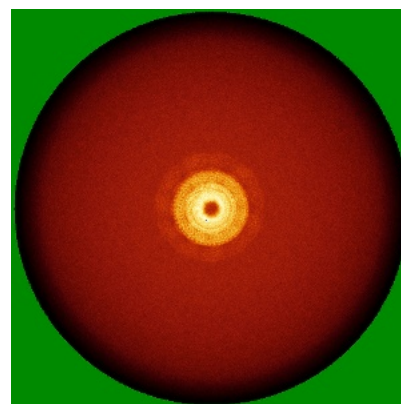
6.4.1 Primary map



X

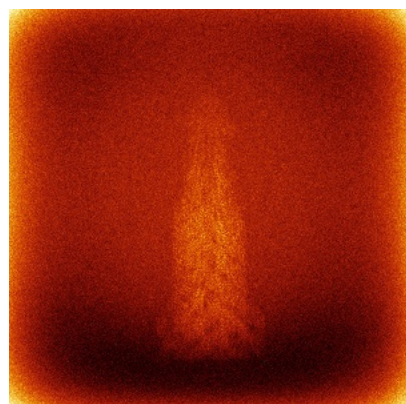


Y

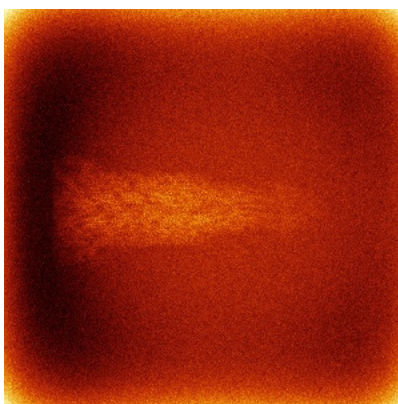


Z

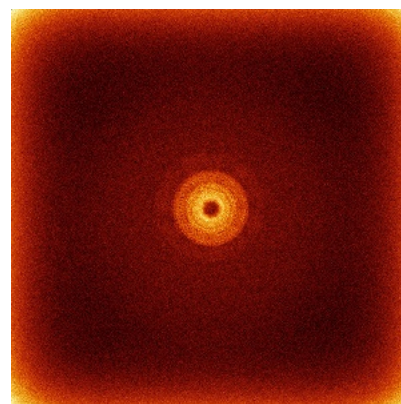
6.4.2 Raw map



X



Y

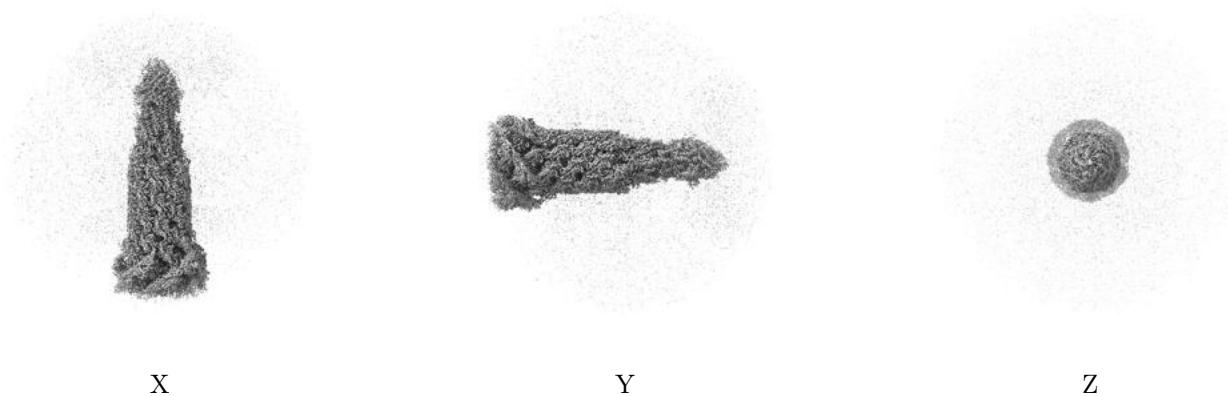


Z

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.

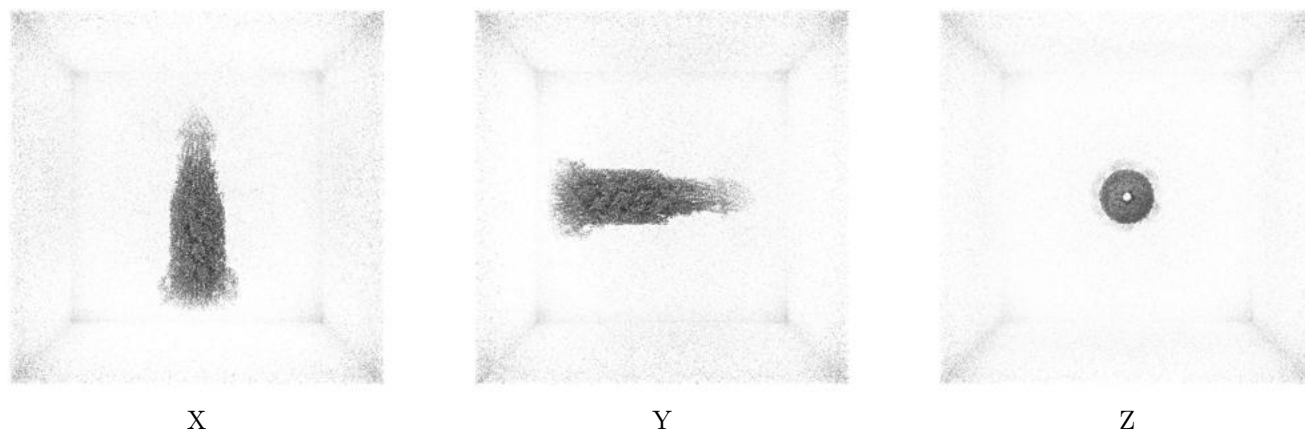
6.5 Orthogonal surface views [i](#)

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.

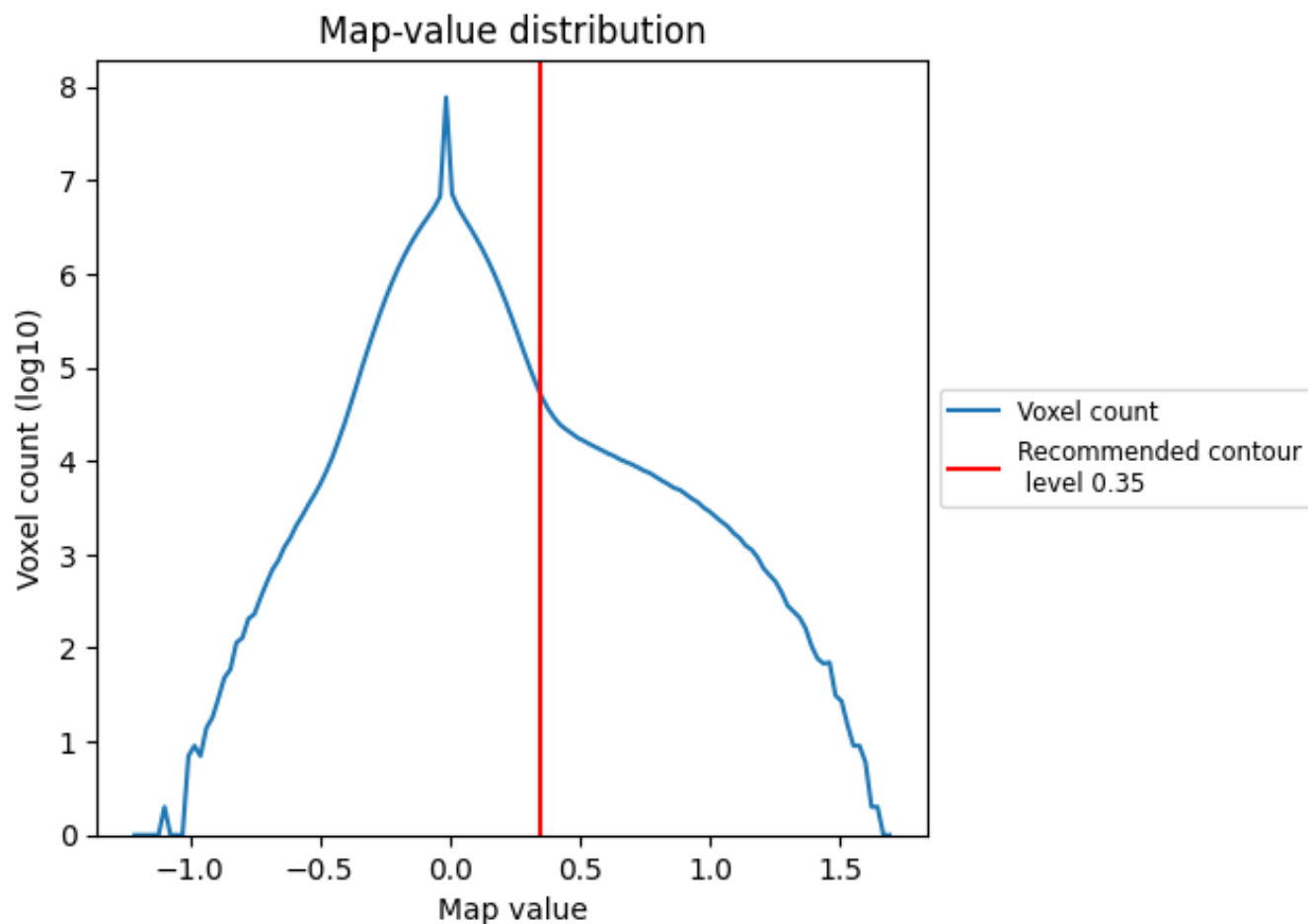
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

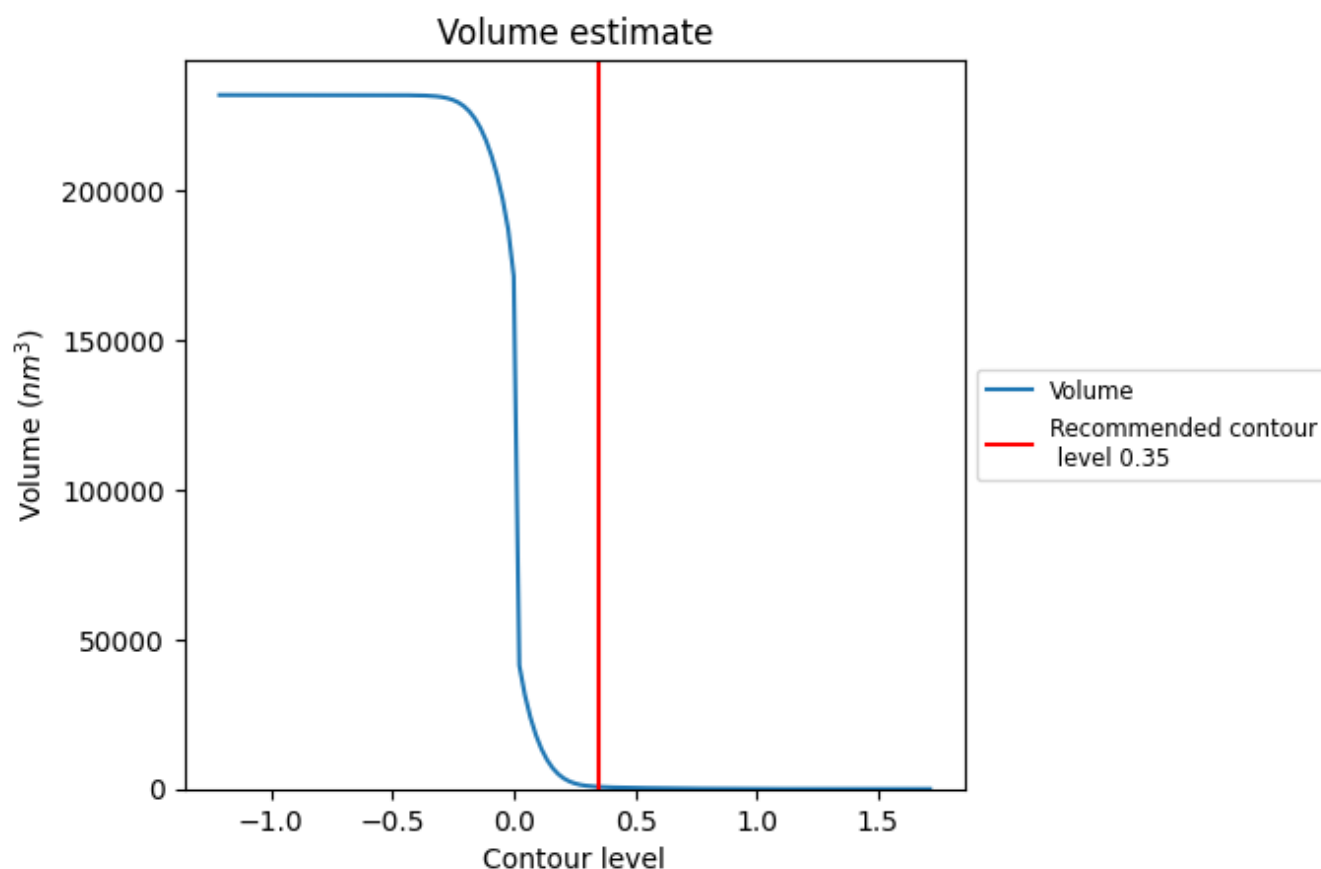
This section contains the results of statistical analysis of the map.

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.

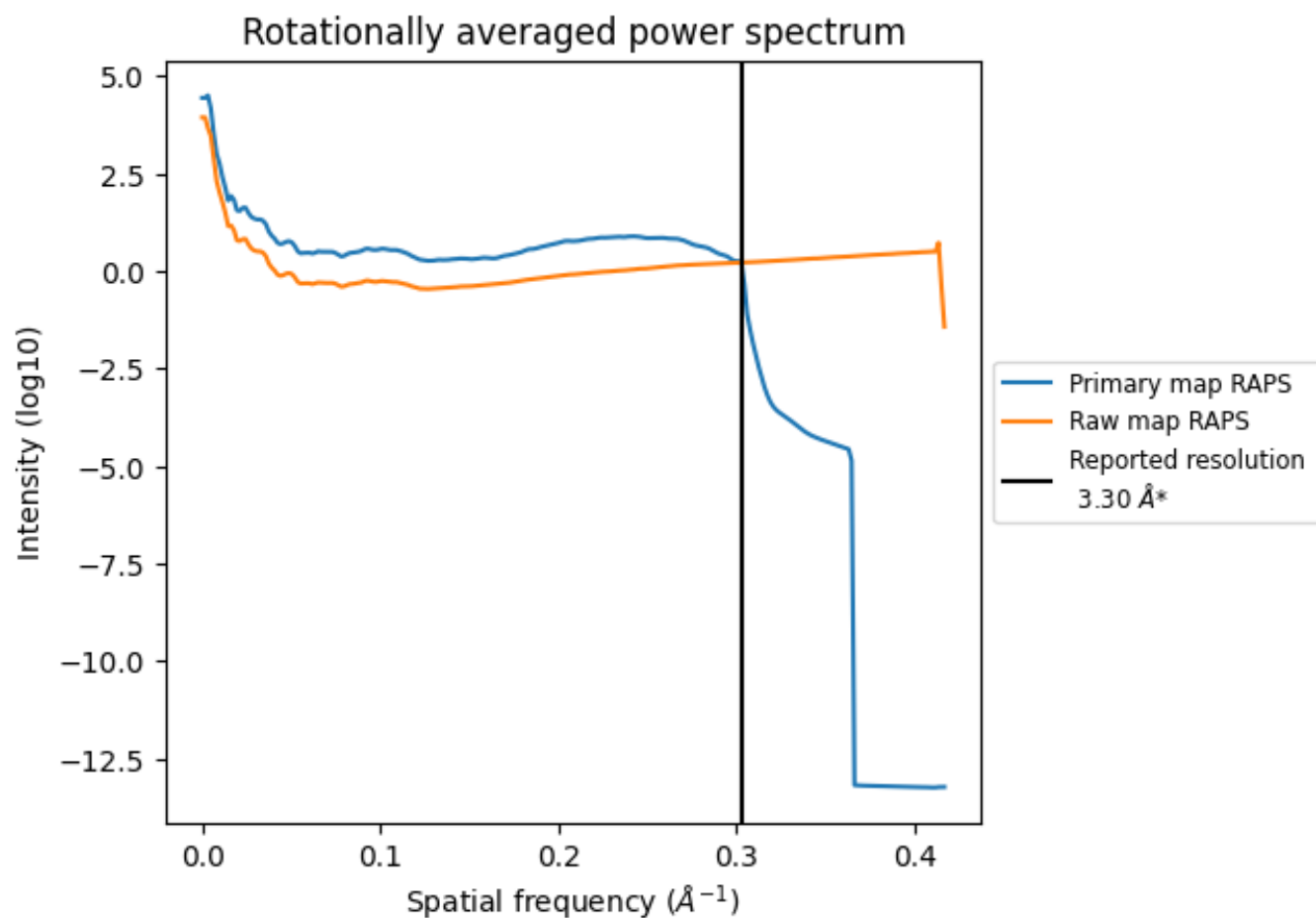
7.2 Volume estimate [i](#)



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 ⓘ

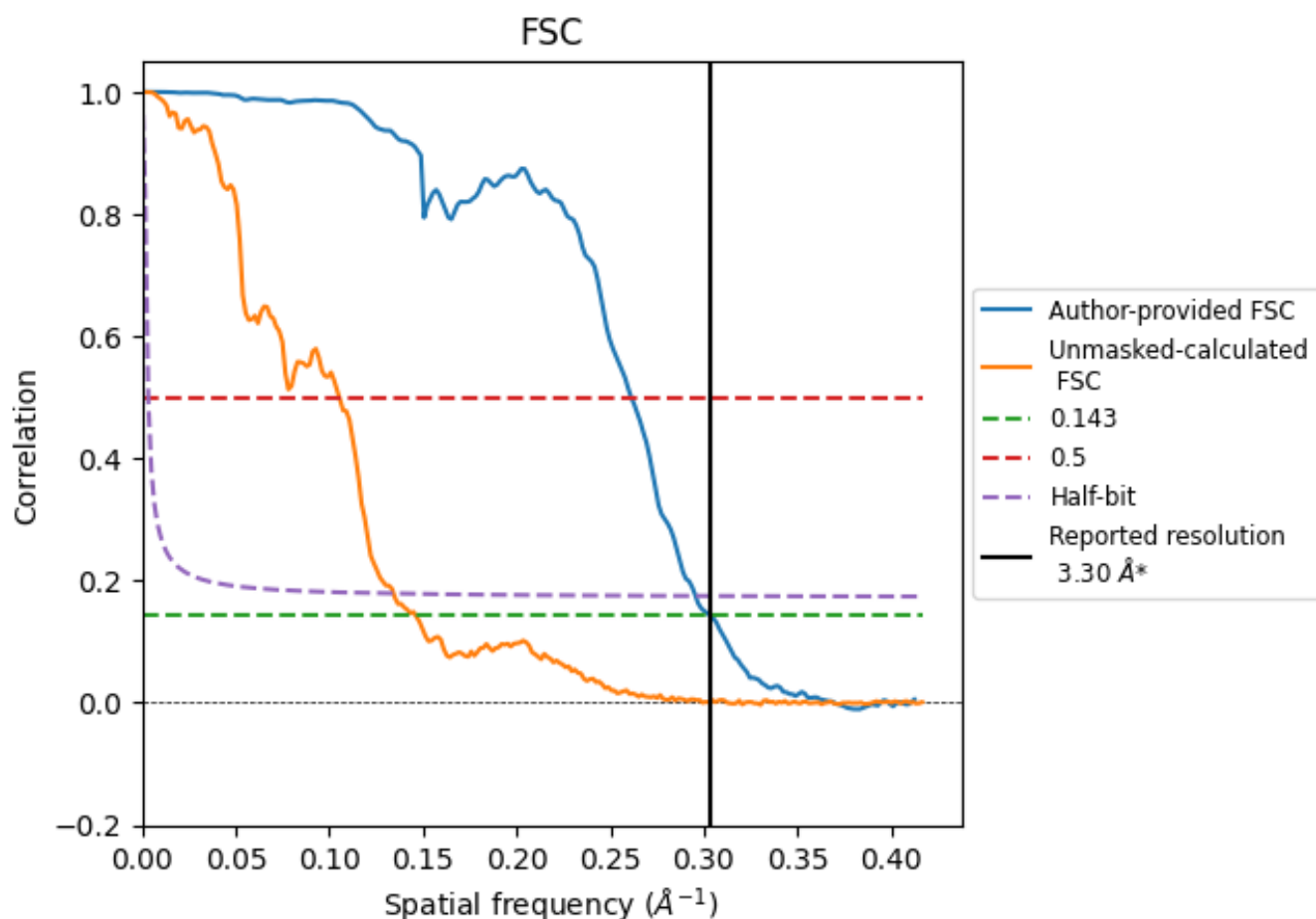


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

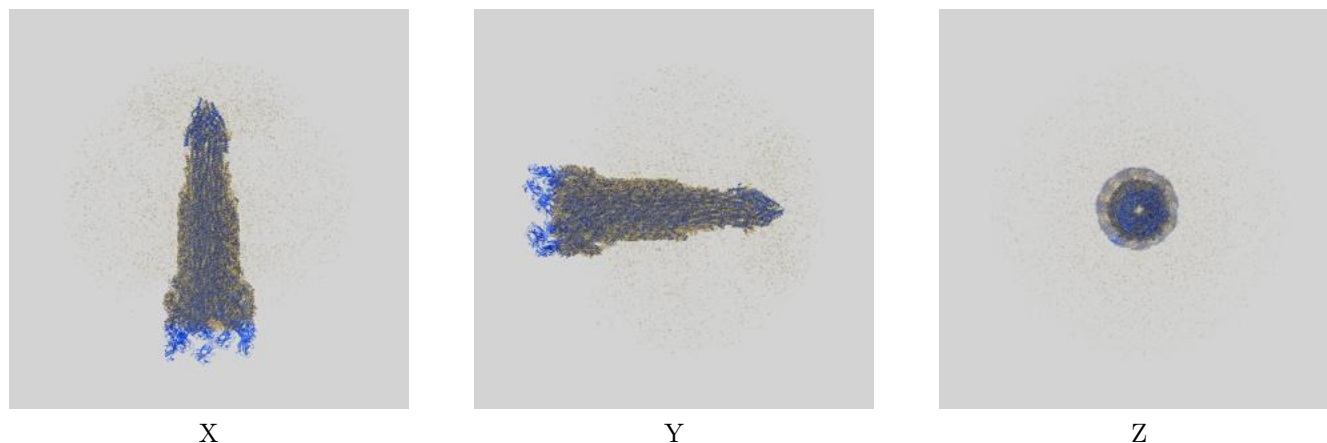
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.83	3.38
Unmasked-calculated*	6.85	9.51	7.45

*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](#)

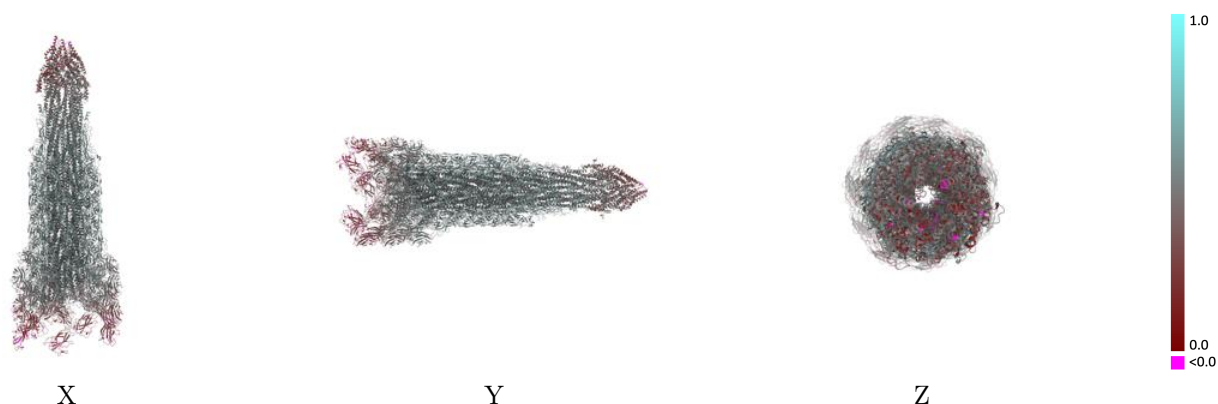
This section contains information regarding the fit between EMDB map EMD-37601 and PDB model 8WKK. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



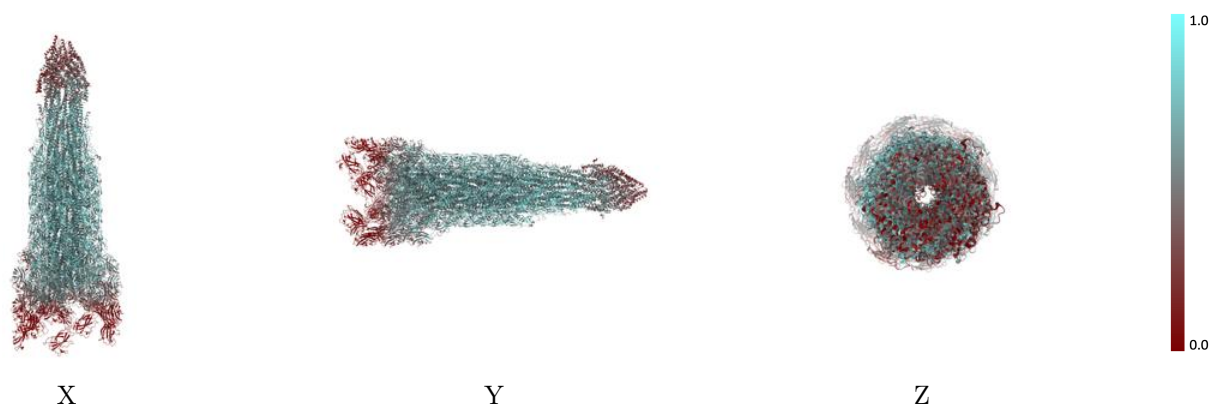
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



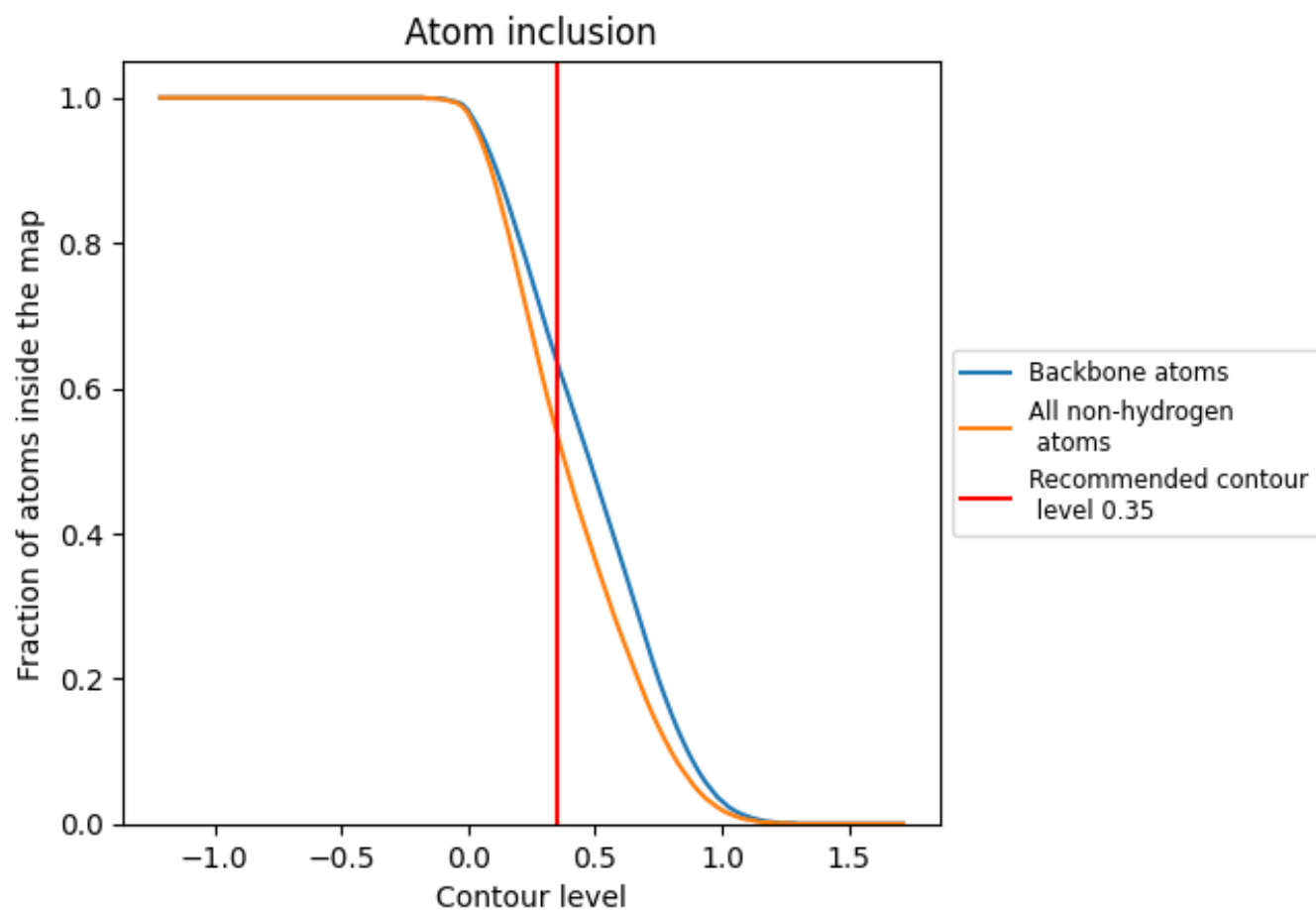
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 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	 0.5380	 0.4710
0	 0.7050	 0.5320
1	 0.6880	 0.5310
2	 0.6930	 0.5370
3	 0.6950	 0.5280
4	 0.6870	 0.5220
5	 0.6760	 0.5240
6	 0.6860	 0.5270
7	 0.6860	 0.5250
8	 0.6940	 0.5250
9	 0.6890	 0.5290
A	 0.1740	 0.2680
B	 0.3050	 0.3490
C	 0.3290	 0.3590
D	 0.2360	 0.3150
E	 0.2560	 0.3370
F	 0.3470	 0.3860
G	 0.4690	 0.4330
H	 0.5000	 0.4440
I	 0.4820	 0.4440
J	 0.3890	 0.4180
K	 0.4950	 0.4730
L	 0.5990	 0.4760
M	 0.6260	 0.4960
N	 0.6280	 0.5020
O	 0.5950	 0.4790
P	 0.5560	 0.4610
Q	 0.5750	 0.4810
R	 0.6770	 0.5040
S	 0.6950	 0.5210
T	 0.6770	 0.5130
U	 0.6510	 0.4950
V	 0.5880	 0.4940
W	 0.6810	 0.5180
X	 0.6760	 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