



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 05:11 am GMT

PDB ID : 7BIN
EMDB ID : EMD-12192
Title : Salmonella export gate and rod refined in focussed C1 map
Authors : Johnson, S.; Furlong, E.; Lea, S.M.
Deposited on : 2021-01-12
Resolution : 3.20 Å (reported)

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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Mol	Chain	Length	Quality of chain
3	J	89	100% 98%
4	K	104	35% 37% 62%
4	L	104	61% 72% 28%
4	M	104	57% 72% 28%
4	N	104	55% 72% 28%
4	O	104	56% 72% 28%
4	P	104	64% 72% 28%
5	Q	138	88% 96%
5	R	138	59% 87% 13%
5	S	138	56% 88% 12%
5	T	138	48% 76% 23%
5	U	138	64% 84% 14%
6	V	134	76% 98%
6	W	134	60% 99%
6	X	134	57% 98%
6	Y	134	54% 99%
6	Z	134	55% 98%
6	a	134	75% 99%
7	b	251	79% 98%
7	c	251	65% 98%
7	d	251	62% 99%
7	e	251	59% 98%
7	f	251	66% 98%
8	1	260	80% 100%
8	2	260	82% 100%

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Mol	Chain	Length	Quality of chain
8	3	260	88% 100%
8	4	260	99% 99%
8	g	260	71% 100%
8	h	260	55% 100%
8	i	260	58% 100%
8	j	260	55% 100%
8	k	260	58% 100%
8	l	260	52% 96%
8	m	260	52% 96%
8	n	260	49% 95%
8	o	260	52% 96%
8	p	260	53% 96%
8	q	260	55% 96%
8	r	260	56% 100%
8	s	260	60% 100%
8	t	260	60% 99%
8	u	260	61% 100%
8	v	260	63% 100%
8	w	260	59% 100%
8	x	260	71% 100%
8	y	260	79% 100%
8	z	260	85% 99%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 81721 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 FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	209	Total 1623	C 1084	N 251	O 276	S 12	0	0
1	B	209	Total 1623	C 1084	N 251	O 276	S 12	0	0
1	C	209	Total 1623	C 1084	N 251	O 276	S 12	0	0
1	D	209	Total 1623	C 1084	N 251	O 276	S 12	0	0
1	E	209	Total 1623	C 1084	N 251	O 276	S 12	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	MET	VAL	conflict	UNP Q8Z5R3
B	236	MET	VAL	conflict	UNP Q8Z5R3
C	236	MET	VAL	conflict	UNP Q8Z5R3
D	236	MET	VAL	conflict	UNP Q8Z5R3
E	236	MET	VAL	conflict	UNP Q8Z5R3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	258	Total 1986	C 1329	N 314	O 327	S 16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	89	Total 670	C 449	N 100	O 114	S 7	0	0
3	H	89	Total 670	C 449	N 100	O 114	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
3	J	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	39	Total	C	N	O	S	0	0
			296	183	51	56	6		
4	L	75	Total	C	N	O	S	0	0
			563	347	102	108	6		
4	M	75	Total	C	N	O	S	0	0
			563	347	102	108	6		
4	N	75	Total	C	N	O	S	0	0
			563	347	102	108	6		
4	O	75	Total	C	N	O	S	0	0
			563	347	102	108	6		
4	P	75	Total	C	N	O	S	0	0
			563	347	102	108	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	133	Total	C	N	O	S	0	0
			1023	630	188	200	5		
5	R	120	Total	C	N	O	S	0	0
			932	578	169	180	5		
5	S	122	Total	C	N	O	S	0	0
			942	583	173	181	5		
5	T	106	Total	C	N	O	S	0	0
			835	516	153	161	5		
5	U	119	Total	C	N	O	S	0	0
			925	573	168	179	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
6	Y	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
6	Z	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
6	a	132	Total	C	N	O	S	0	0
			964	601	166	192	5		

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
7	c	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
7	d	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
7	e	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
7	f	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	h	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	i	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	j	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	k	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	l	249	Total	C	N	O	S	0	0
			1871	1157	328	381	5		
8	m	249	Total	C	N	O	S	0	0
			1871	1157	328	381	5		
8	n	249	Total	C	N	O	S	0	0
			1871	1157	328	381	5		

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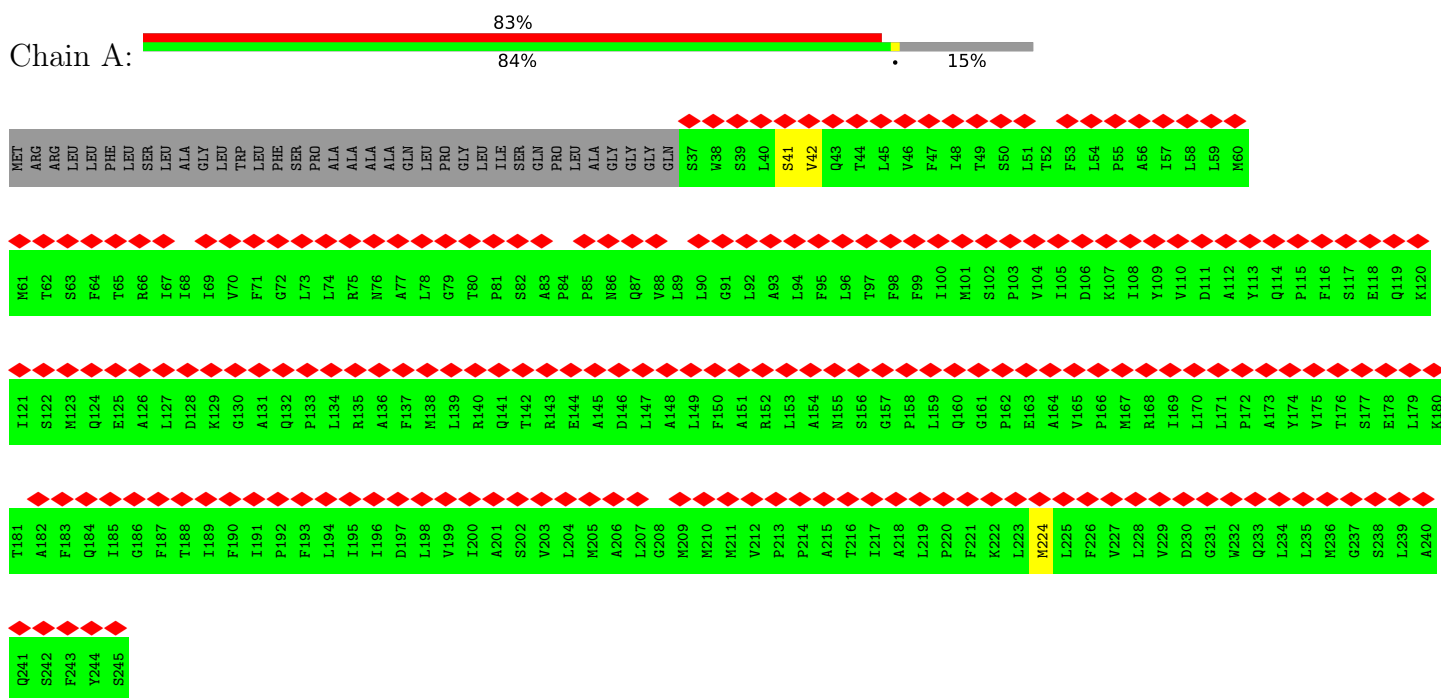
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Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	249	Total	C	N	O	S	0	0
			1871	1157	328	381	5		
8	p	249	Total	C	N	O	S	0	0
			1871	1157	328	381	5		
8	q	251	Total	C	N	O	S	0	0
			1886	1167	330	384	5		
8	r	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	s	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	t	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	u	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	v	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	w	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	x	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	y	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	z	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	1	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	2	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	3	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	4	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		

3 Residue-property plots [i](#)

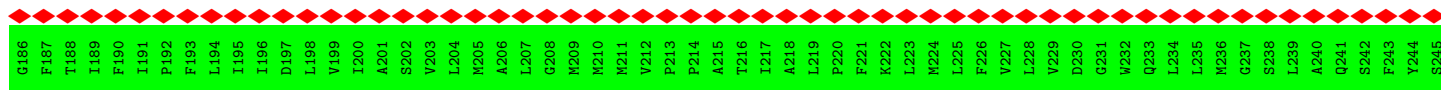
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Flagellar biosynthetic protein Flp

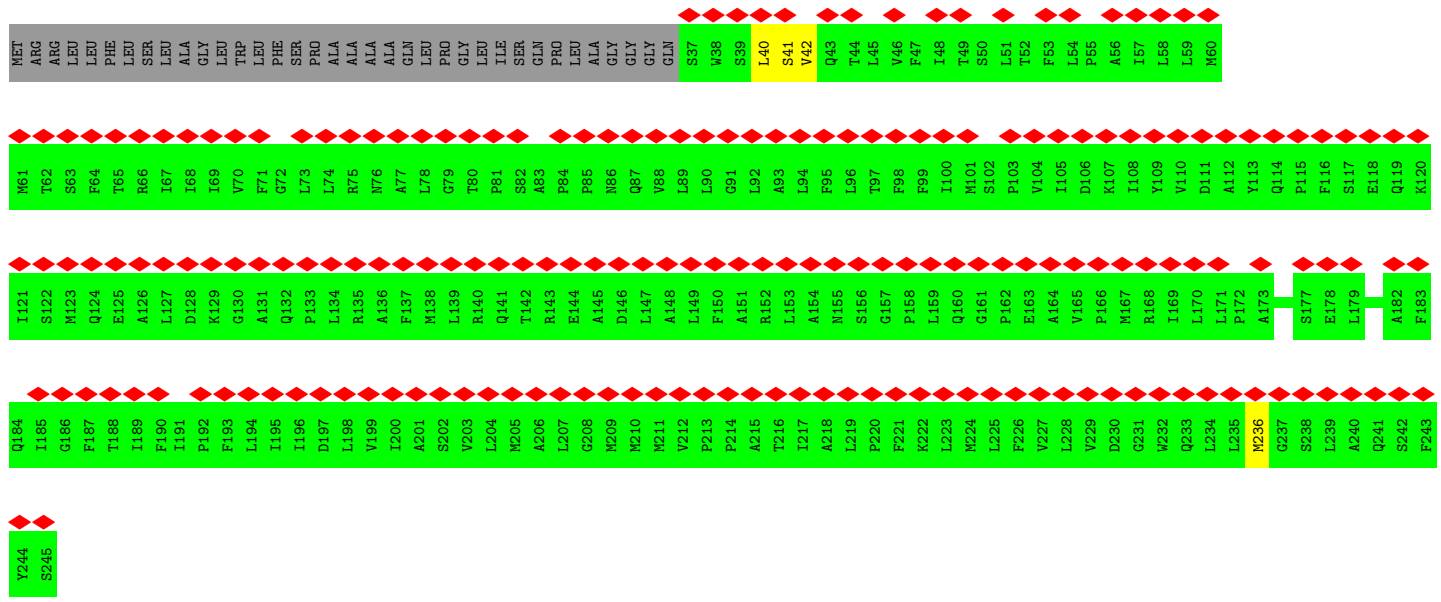
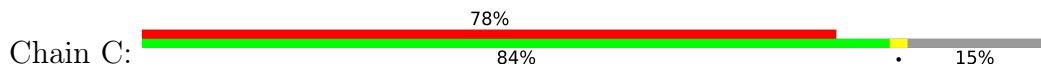


• Molecule 1: Flagellar biosynthetic protein Flp

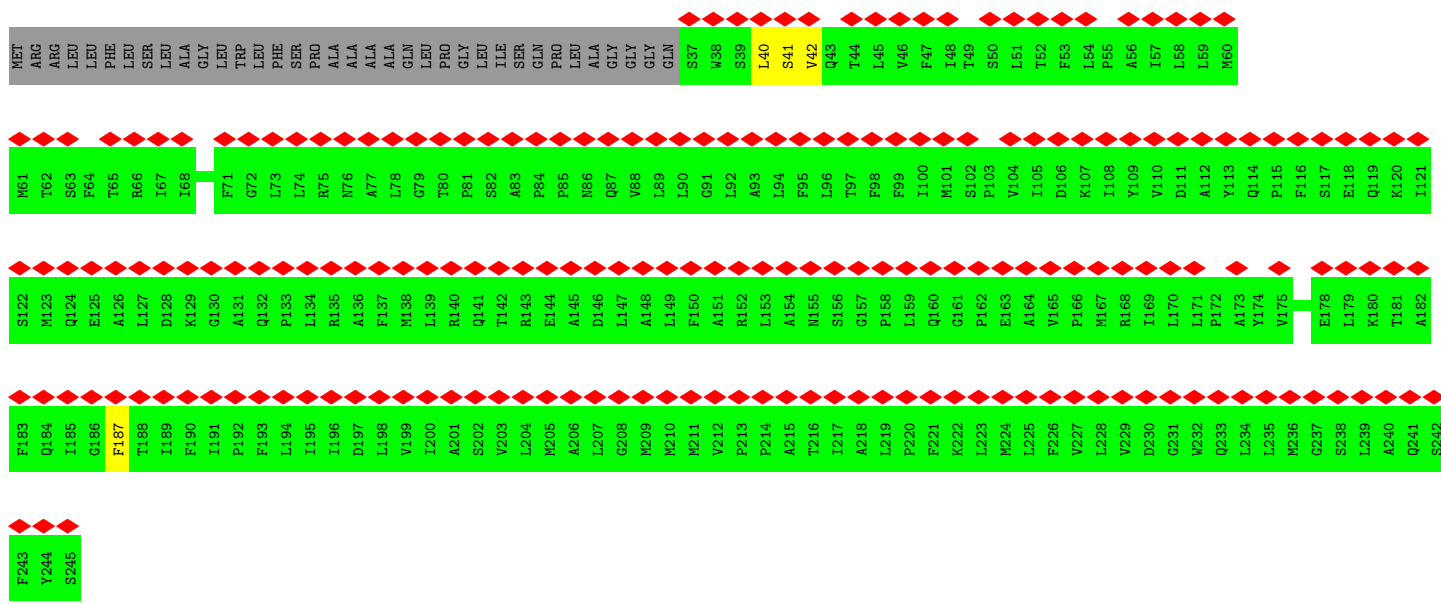
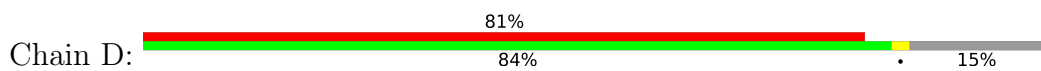




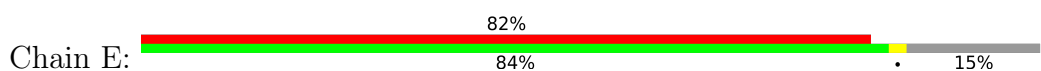
• Molecule 1: Flagellar biosynthetic protein FliP

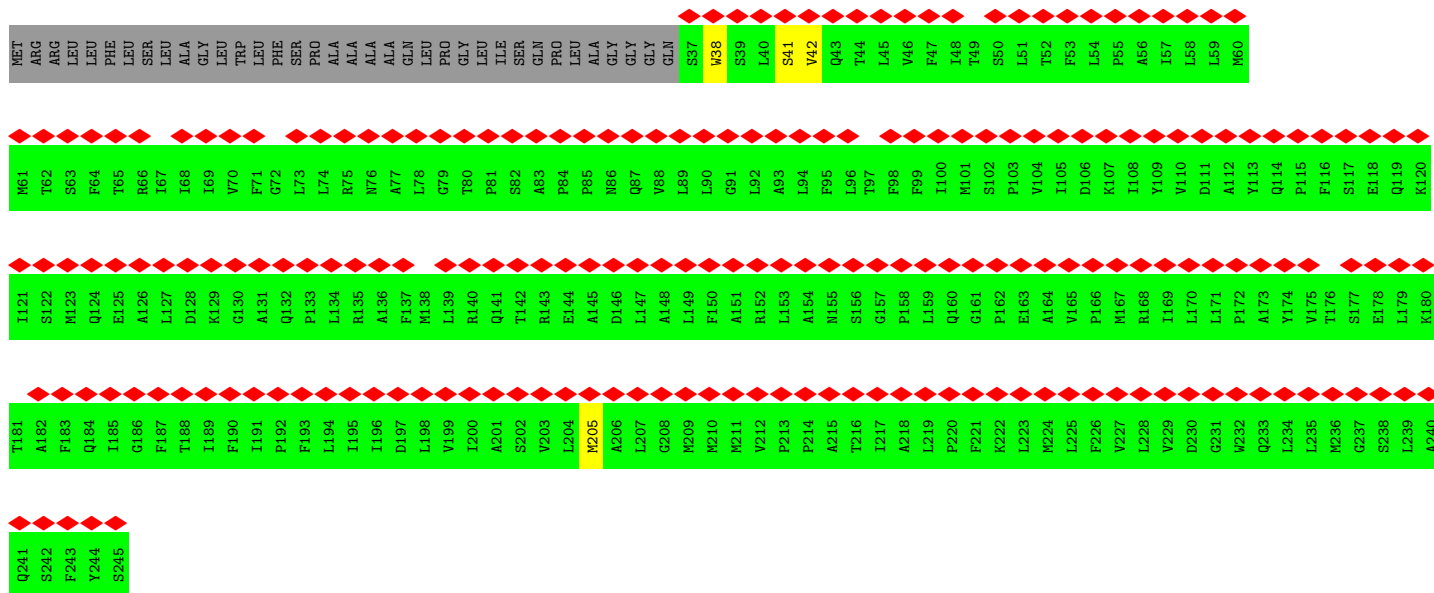


• Molecule 1: Flagellar biosynthetic protein FliP

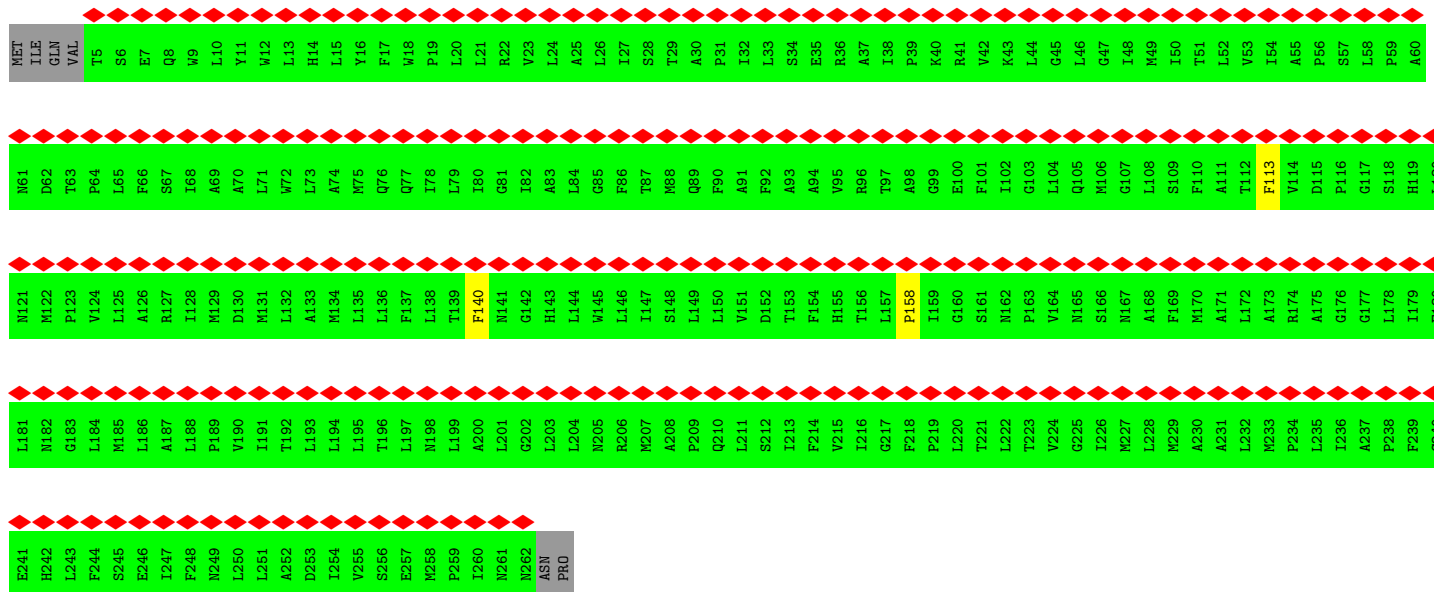


• Molecule 1: Flagellar biosynthetic protein FliP

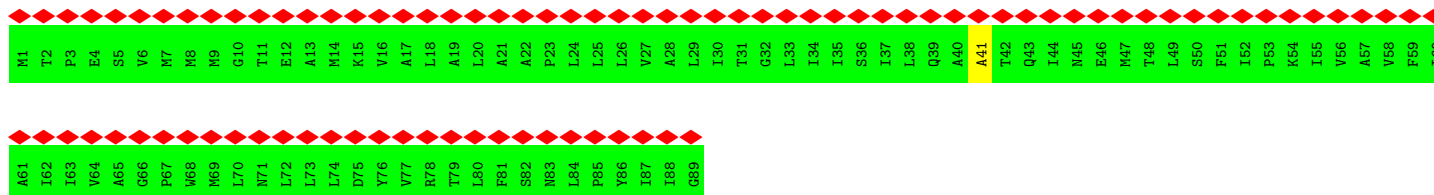




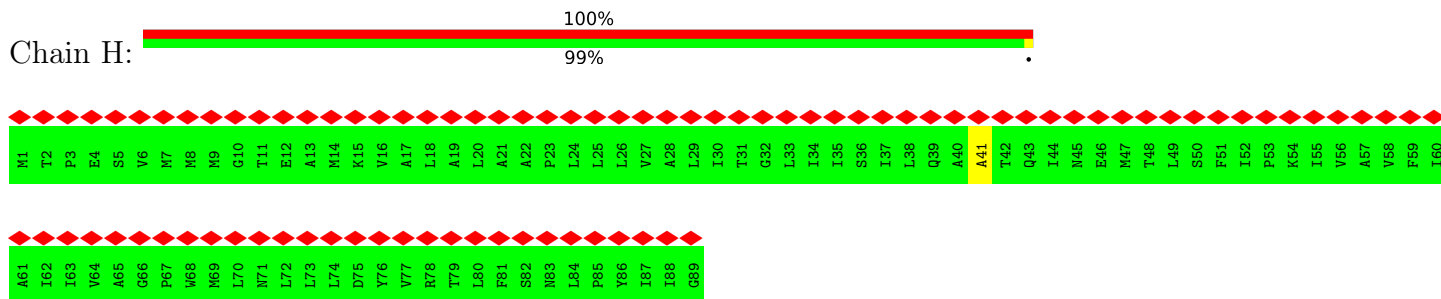
• Molecule 2: Flagellar biosynthetic protein FliR



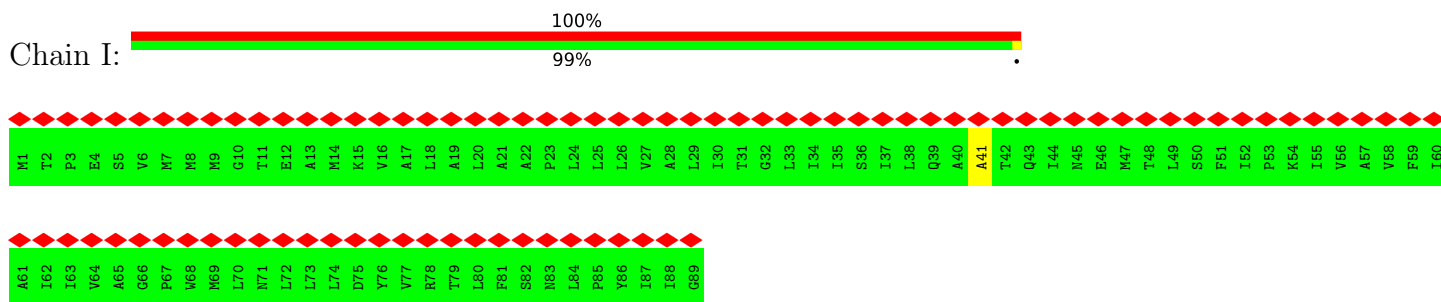
• Molecule 3: Flagellar biosynthetic protein FliQ



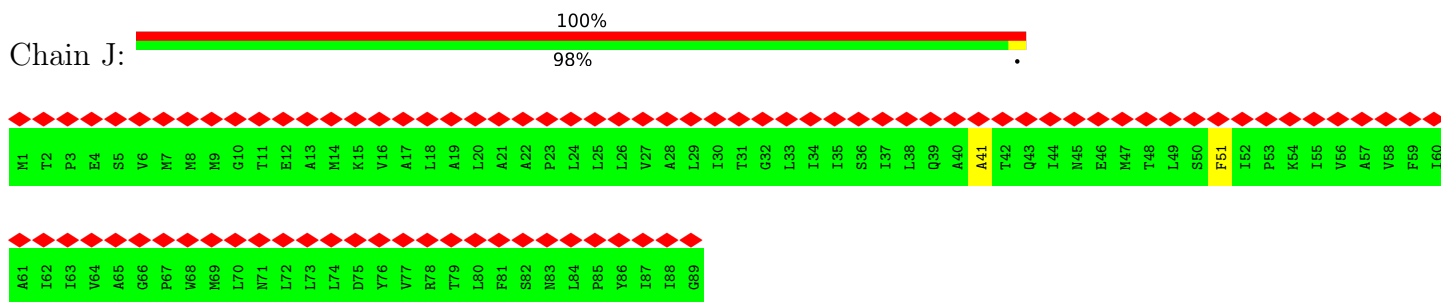
• Molecule 3: Flagellar biosynthetic protein FliQ



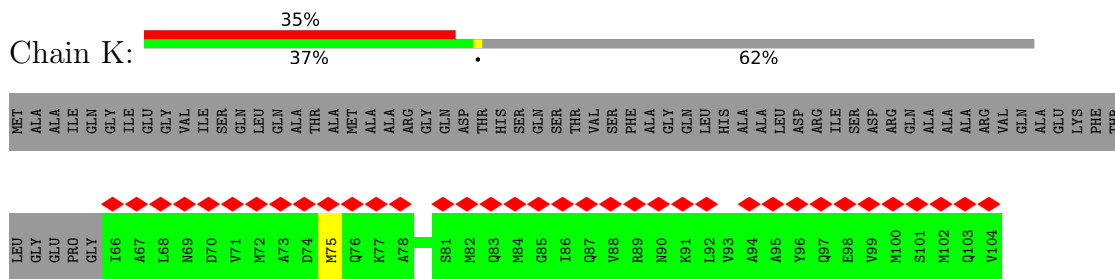
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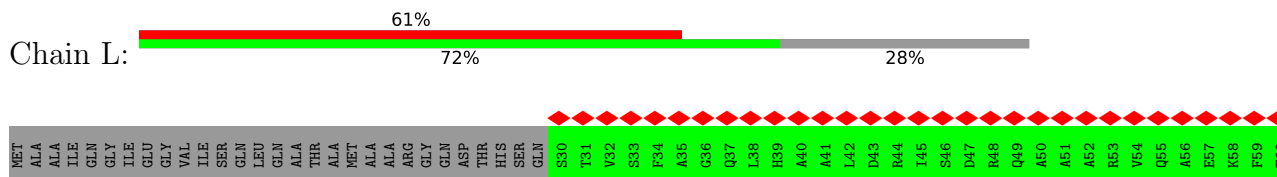
• Molecule 3: Flagellar biosynthetic protein FliQ

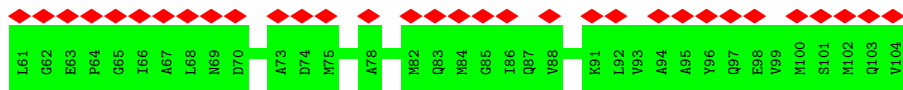


• Molecule 4: Flagellar hook-basal body complex protein FliE

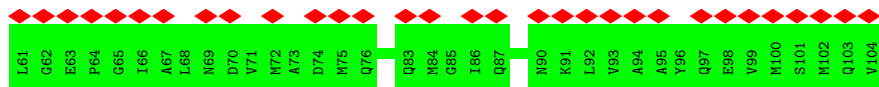
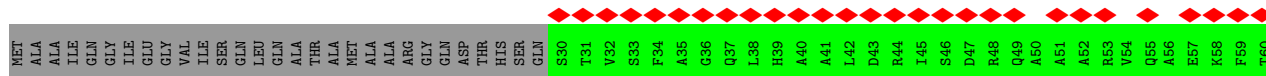
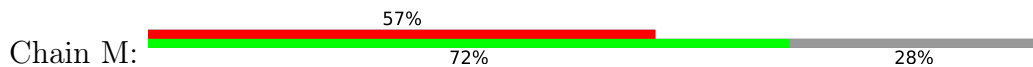


• Molecule 4: Flagellar hook-basal body complex protein FliE

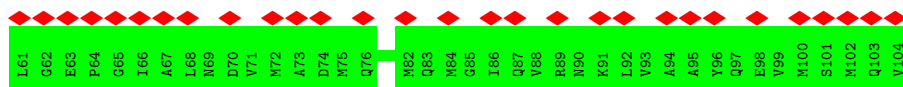
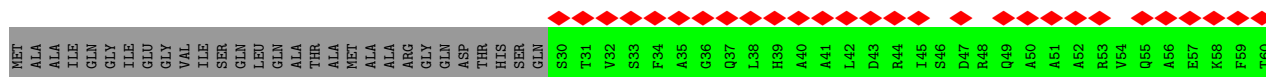




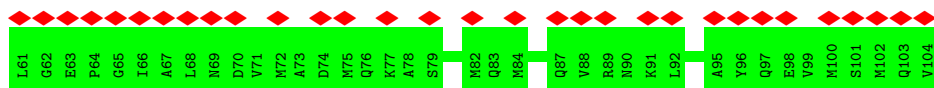
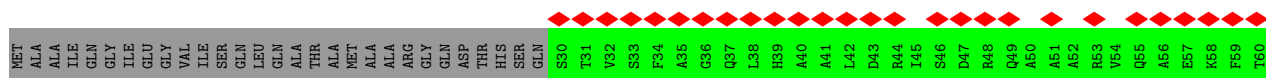
• Molecule 4: Flagellar hook-basal body complex protein FliE



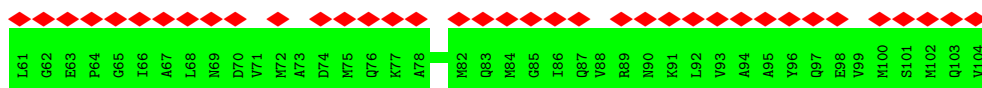
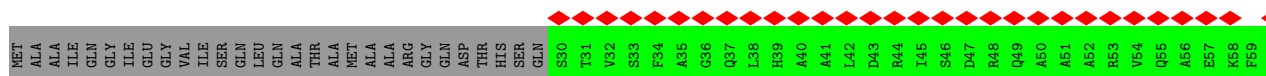
• Molecule 4: Flagellar hook-basal body complex protein FliE



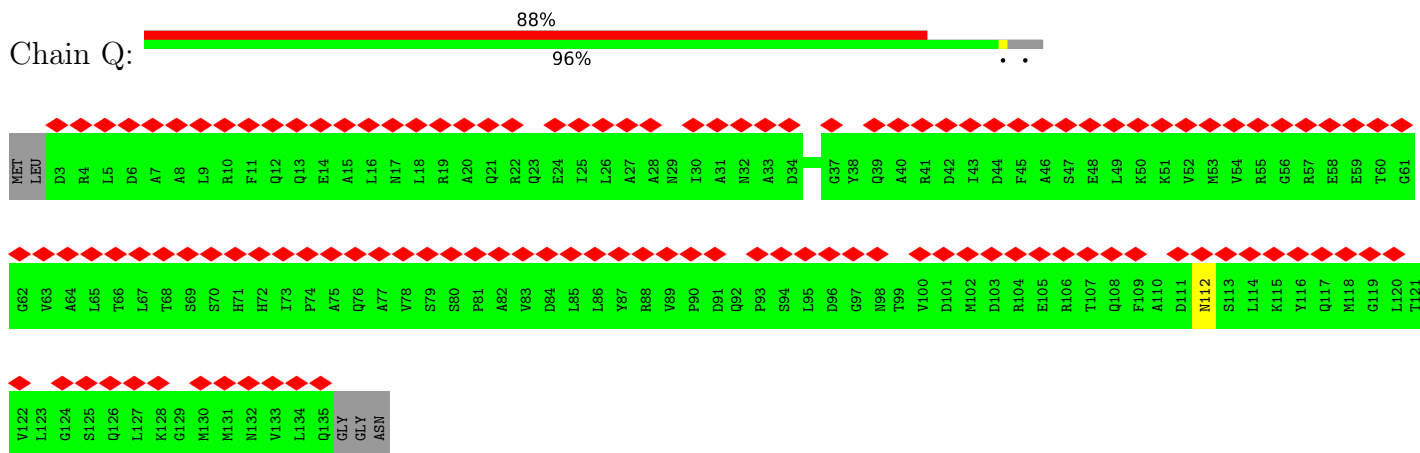
• Molecule 4: Flagellar hook-basal body complex protein FliE



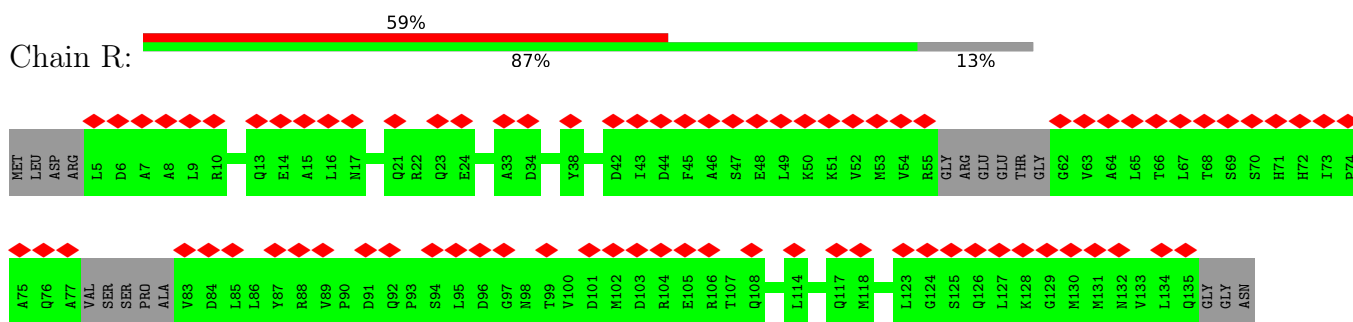
• Molecule 4: Flagellar hook-basal body complex protein FliE



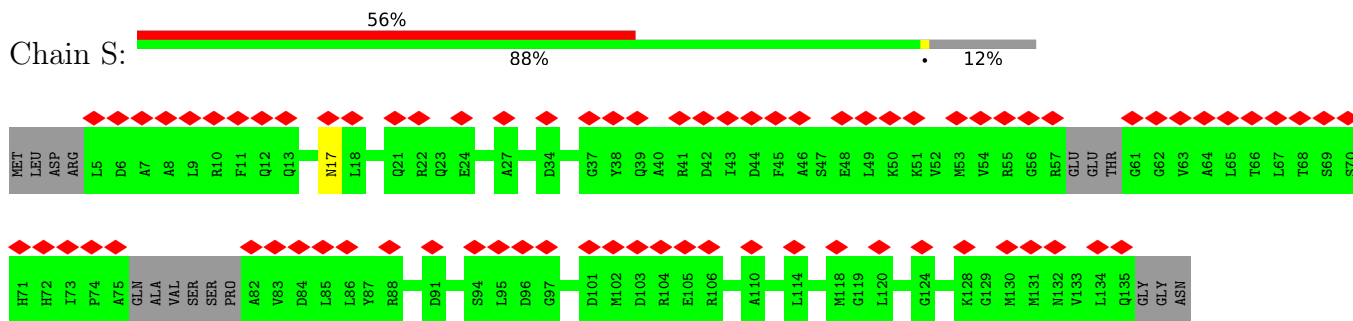
• Molecule 5: Flagellar basal body rod protein FlgB



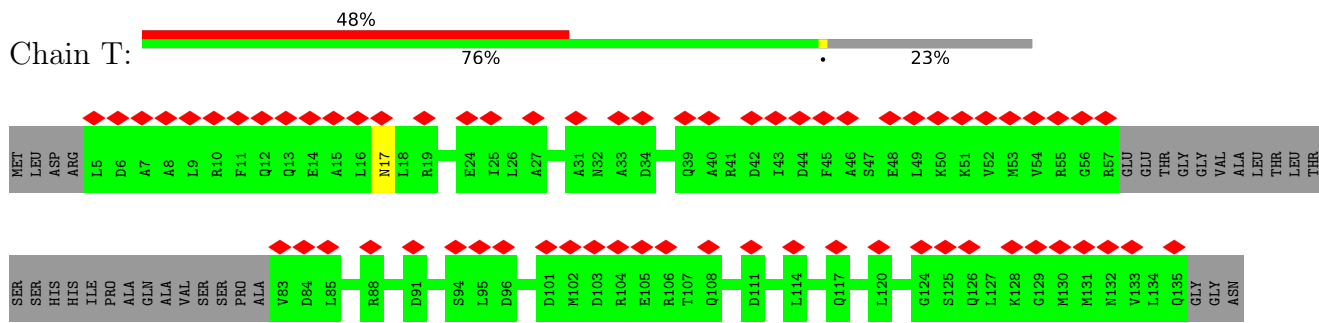
• Molecule 5: Flagellar basal body rod protein FlgB



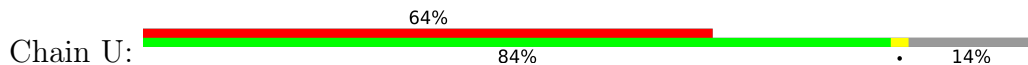
• Molecule 5: Flagellar basal body rod protein FlgB

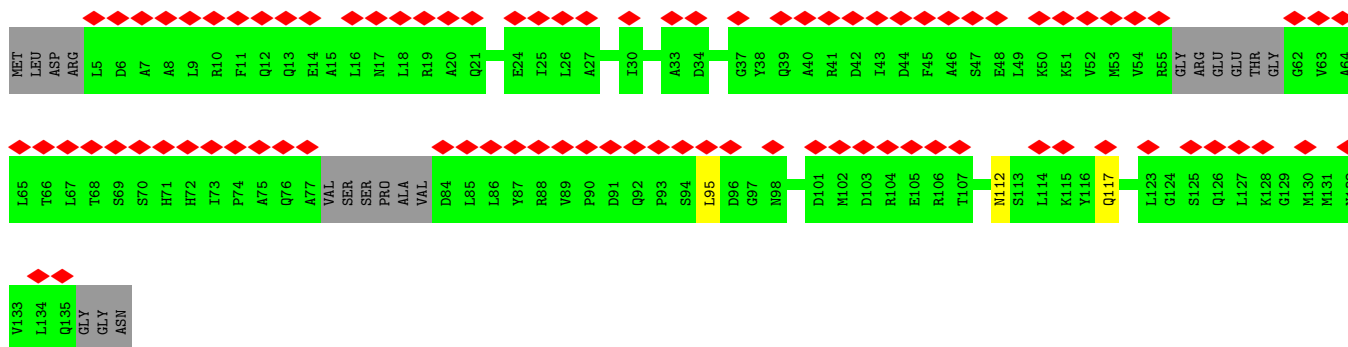


• Molecule 5: Flagellar basal body rod protein FlgB

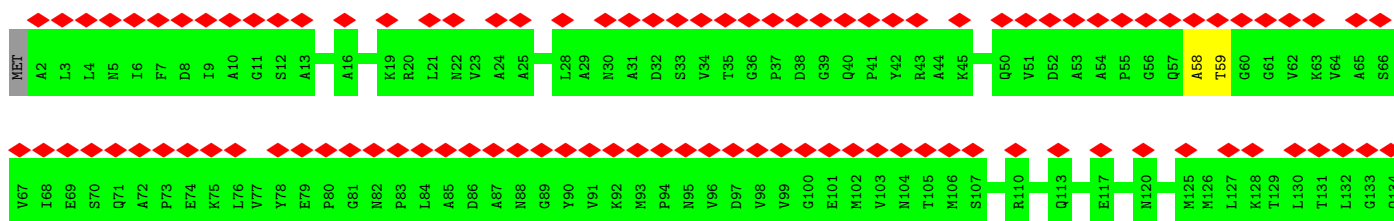
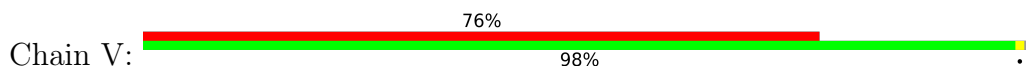


• Molecule 5: Flagellar basal body rod protein FlgB

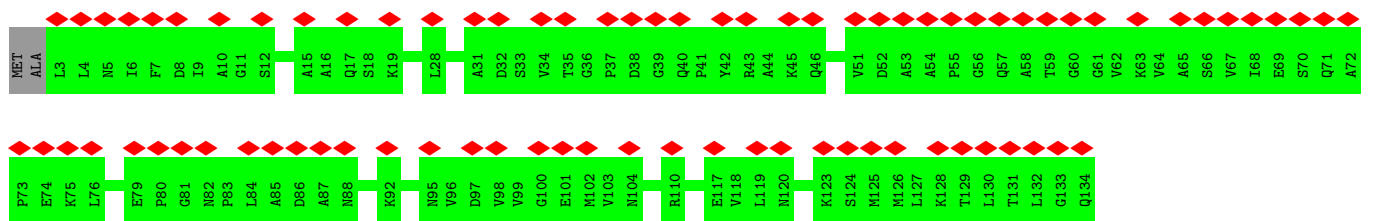




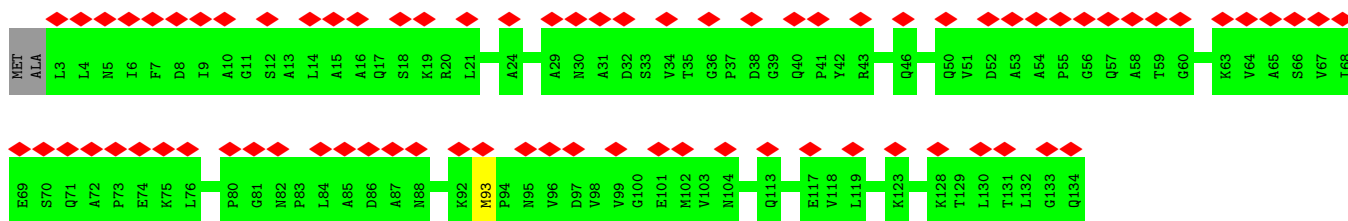
• Molecule 6: Flagellar basal-body rod protein FlgC



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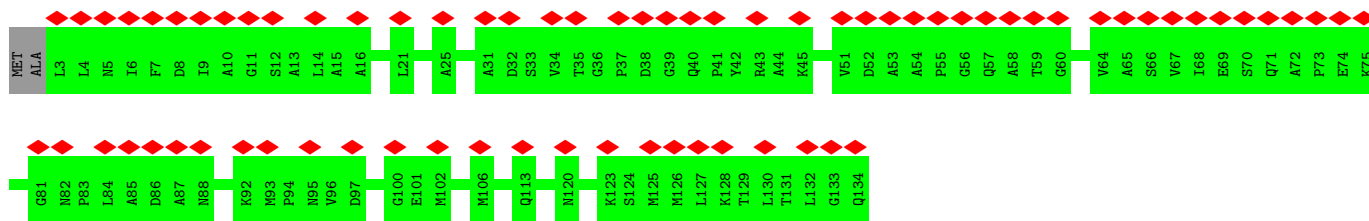


• Molecule 6: Flagellar basal-body rod protein FlgC

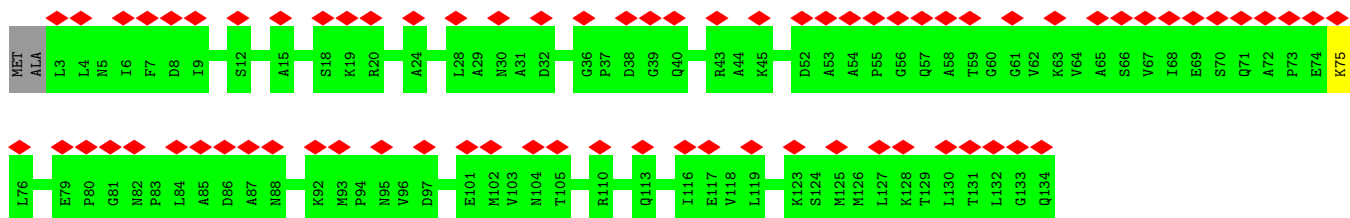


• Molecule 6: Flagellar basal-body rod protein FlgC

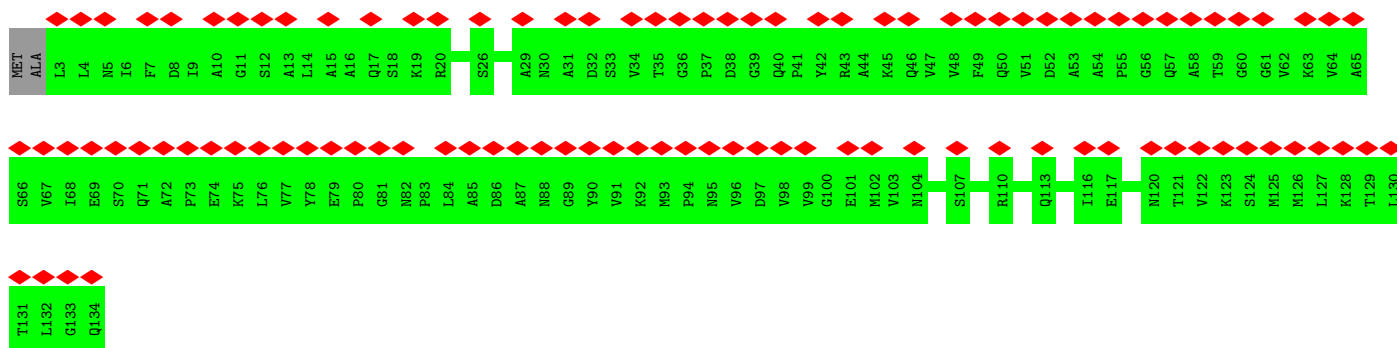
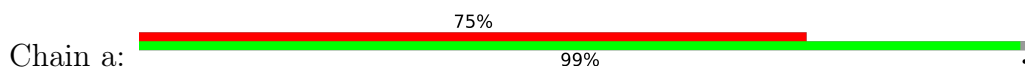




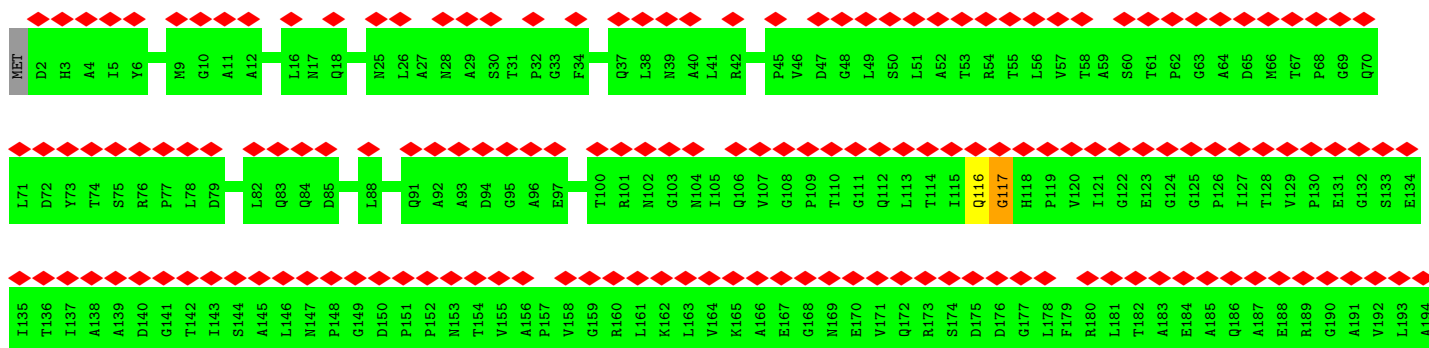
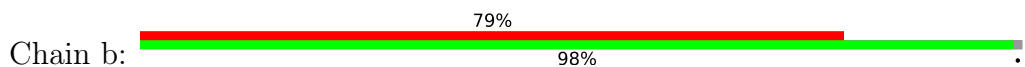
• Molecule 6: Flagellar basal-body rod protein FlgC

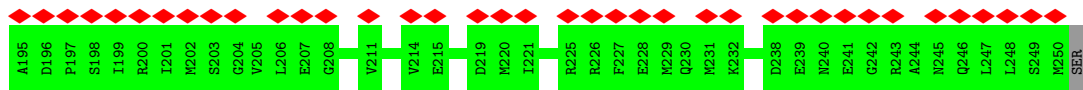


• Molecule 6: Flagellar basal-body rod protein FlgC

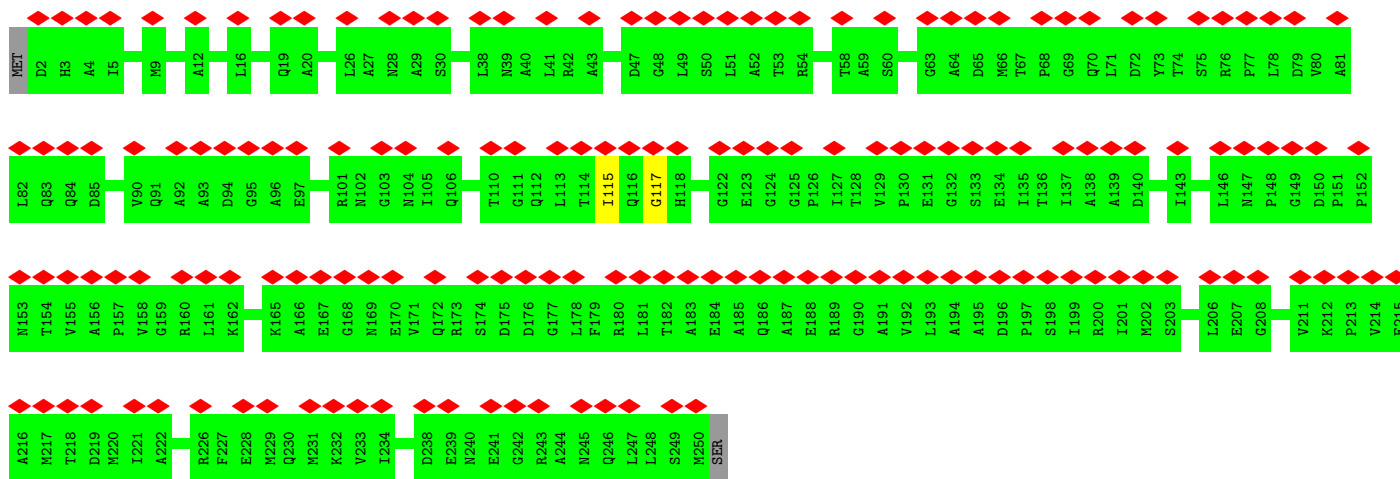


• Molecule 7: Flagellar basal-body rod protein FlgF

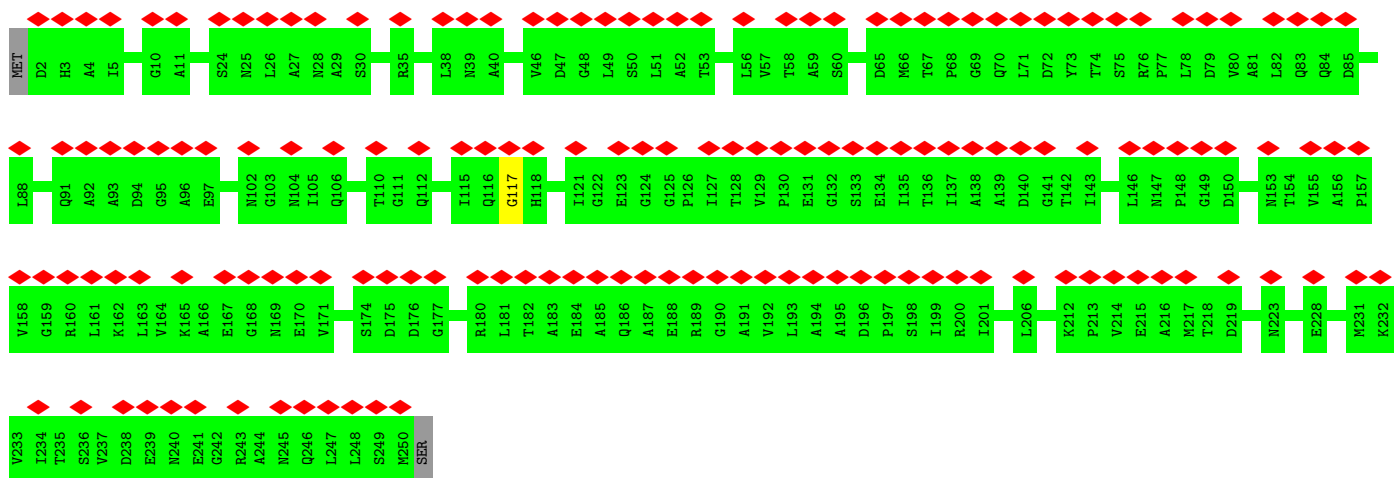




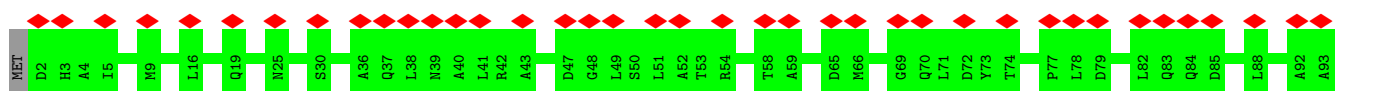
• Molecule 7: Flagellar basal-body rod protein FlgF

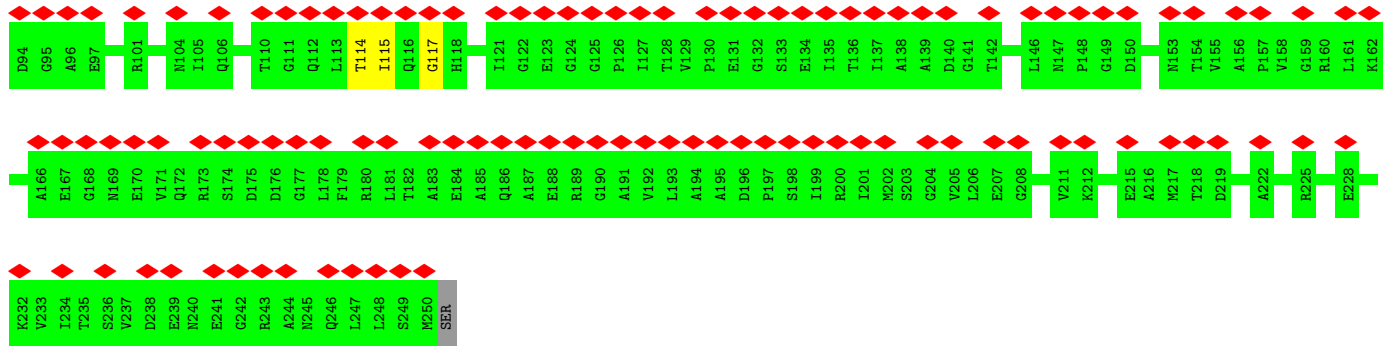


• Molecule 7: Flagellar basal-body rod protein FlgF

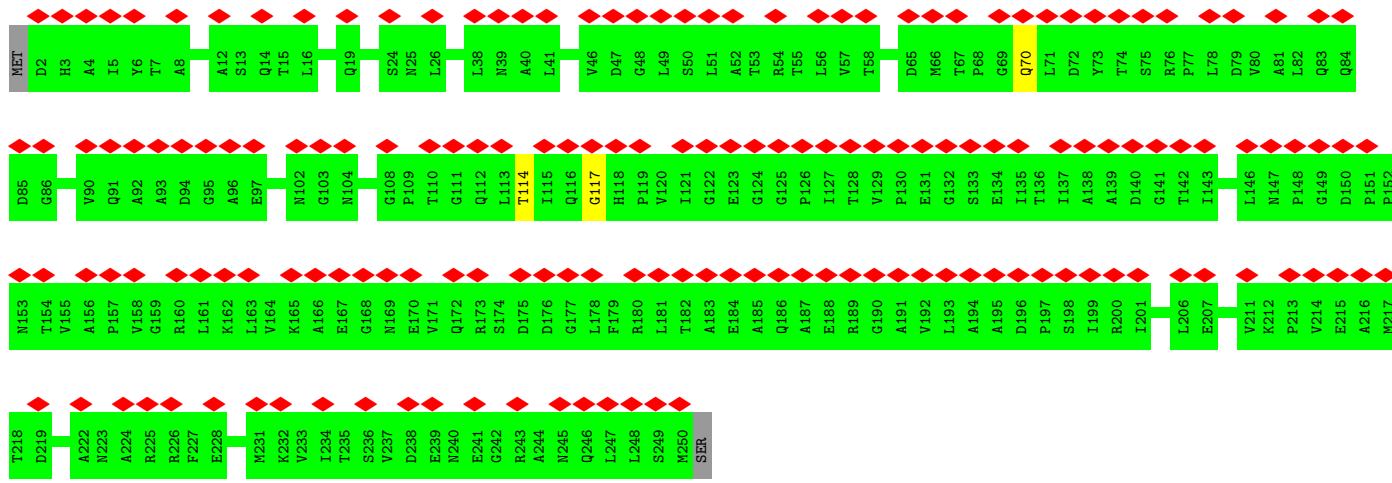


• Molecule 7: Flagellar basal-body rod protein FlgF

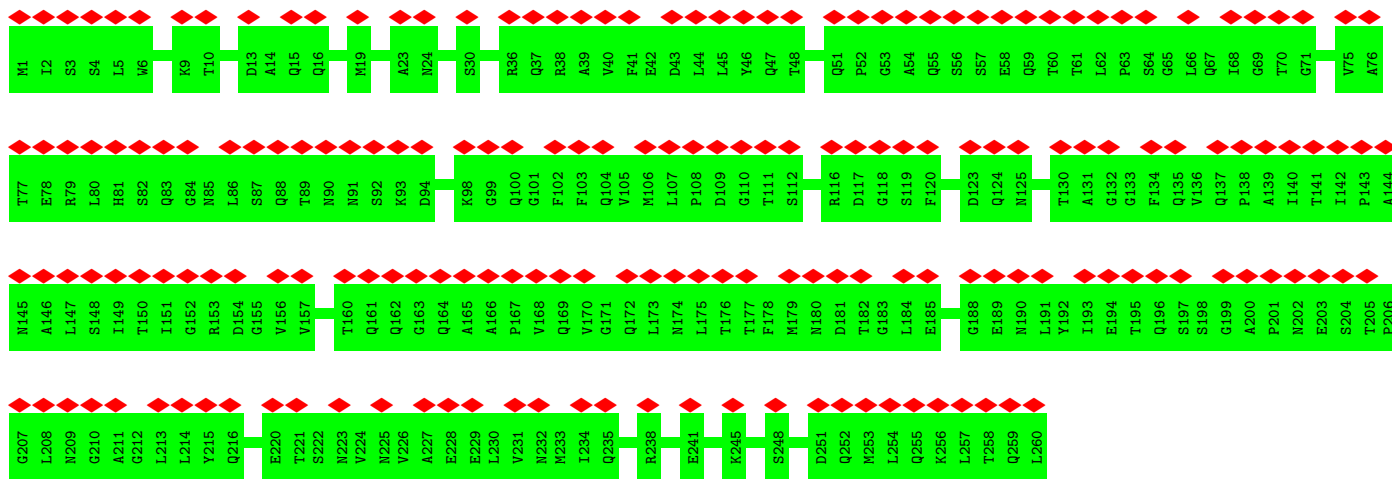




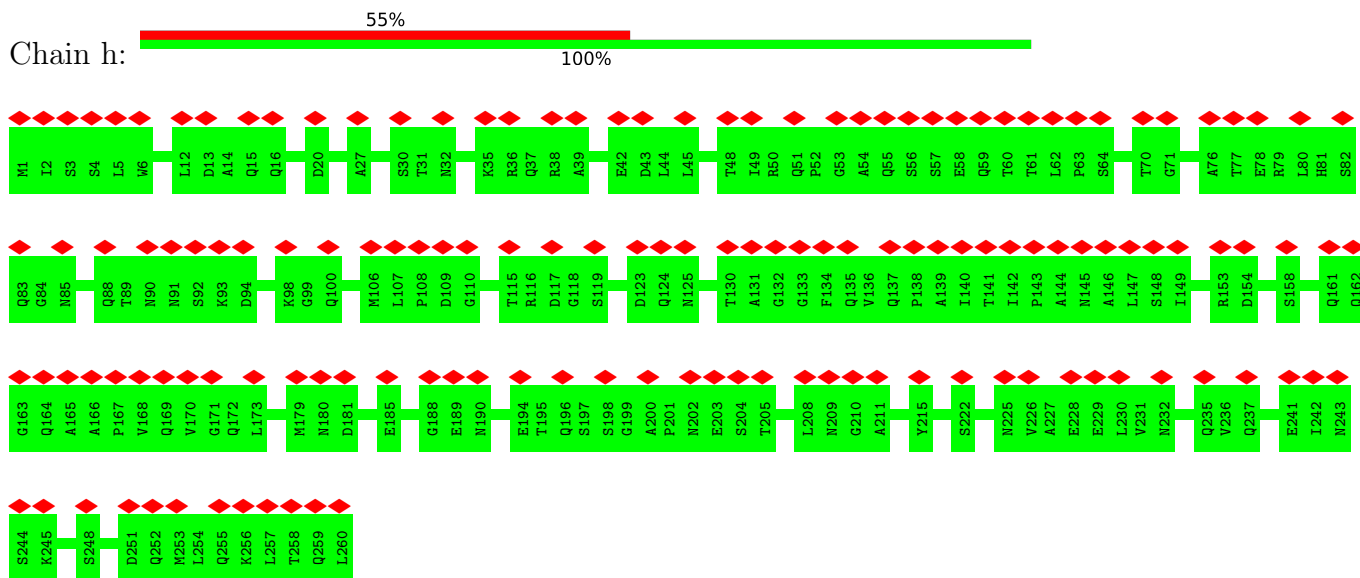
• Molecule 7: Flagellar basal-body rod protein FlgF



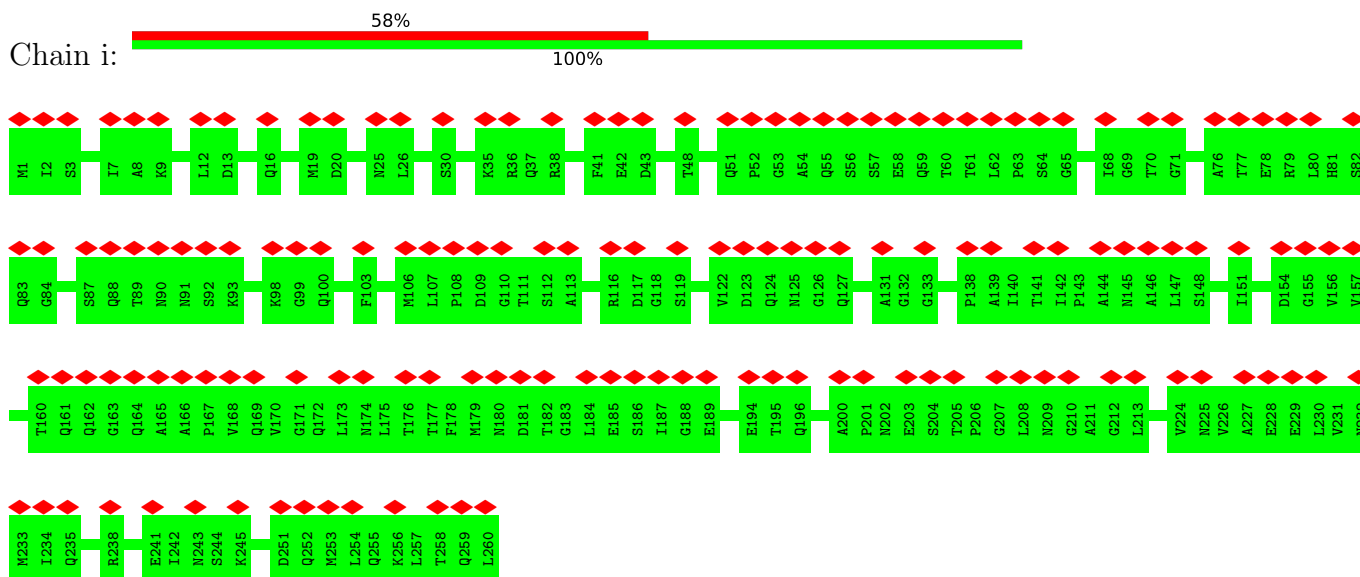
• Molecule 8: Flagellar basal-body rod protein FlgG



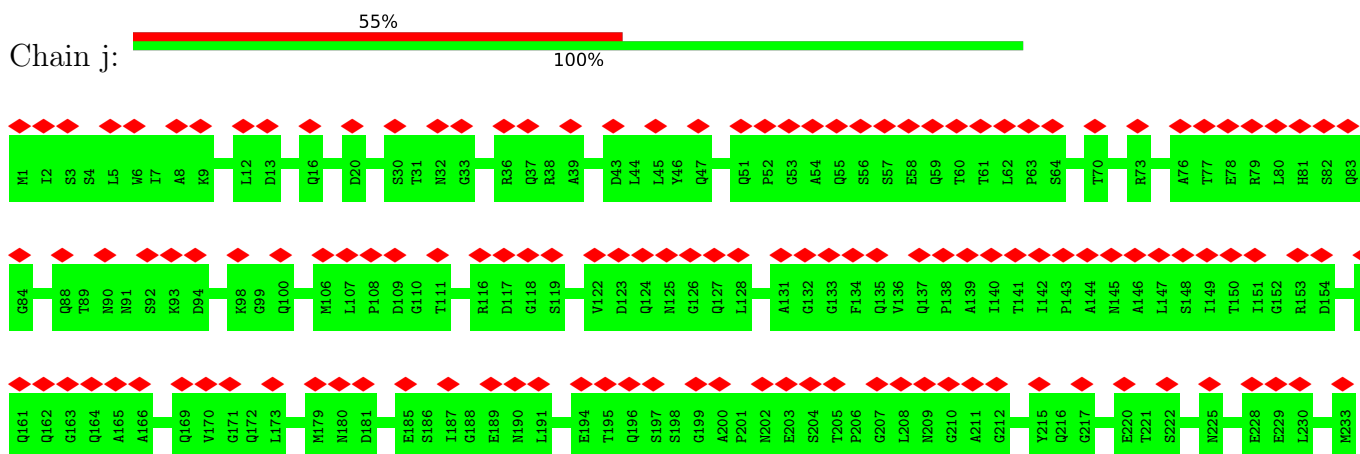
• Molecule 8: Flagellar basal-body rod protein FlgG

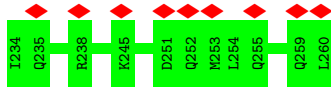


• Molecule 8: Flagellar basal-body rod protein FlgG

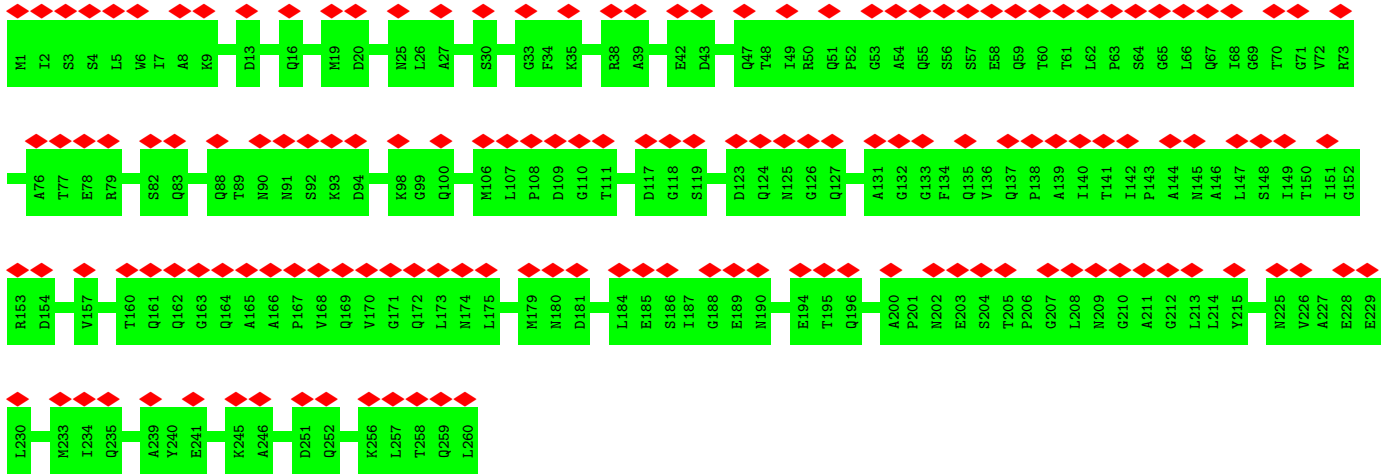


• Molecule 8: Flagellar basal-body rod protein FlgG

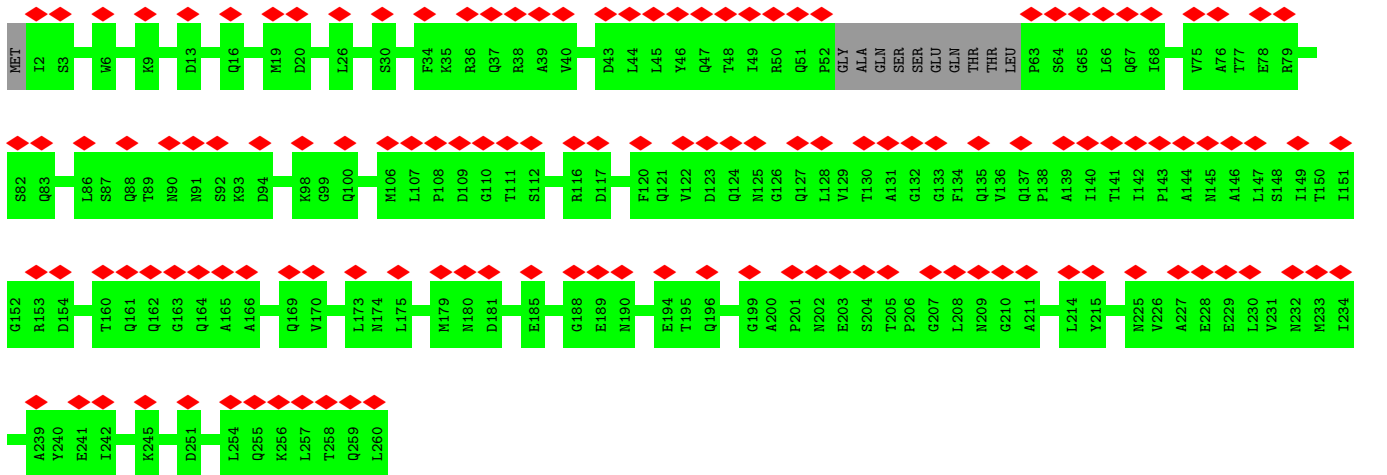
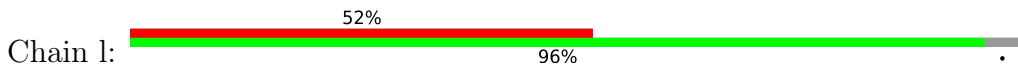




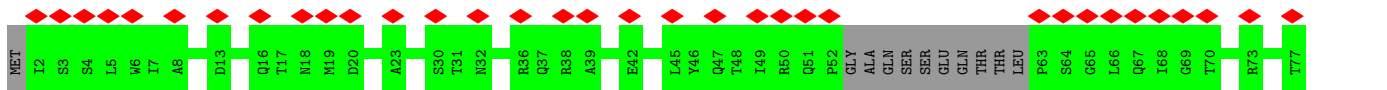
• Molecule 8: Flagellar basal-body rod protein FlgG

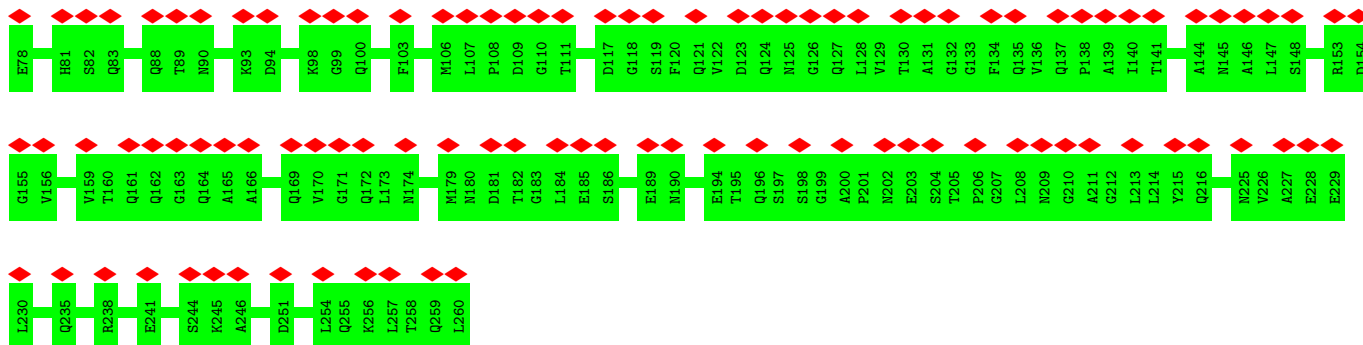


• Molecule 8: Flagellar basal-body rod protein FlgG



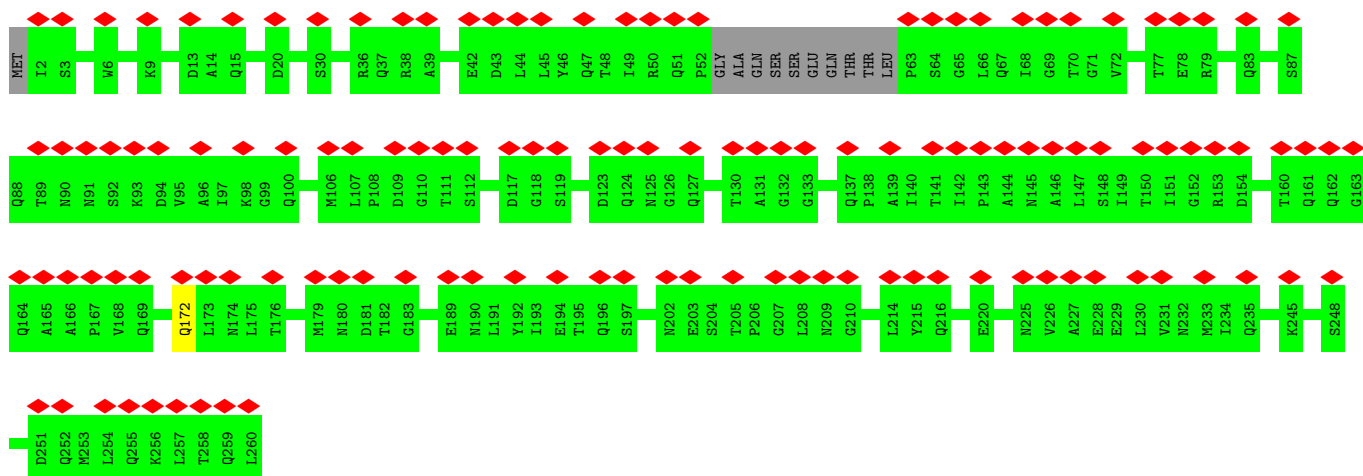
• Molecule 8: Flagellar basal-body rod protein FlgG





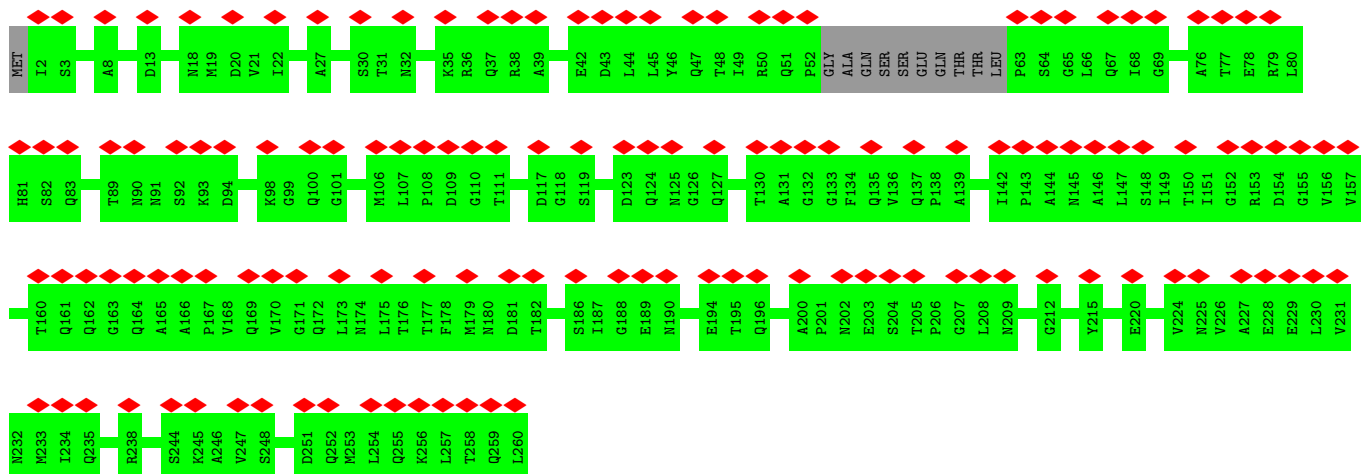
- Molecule 8: Flagellar basal-body rod protein FlgG

Chain n: 49% 95%

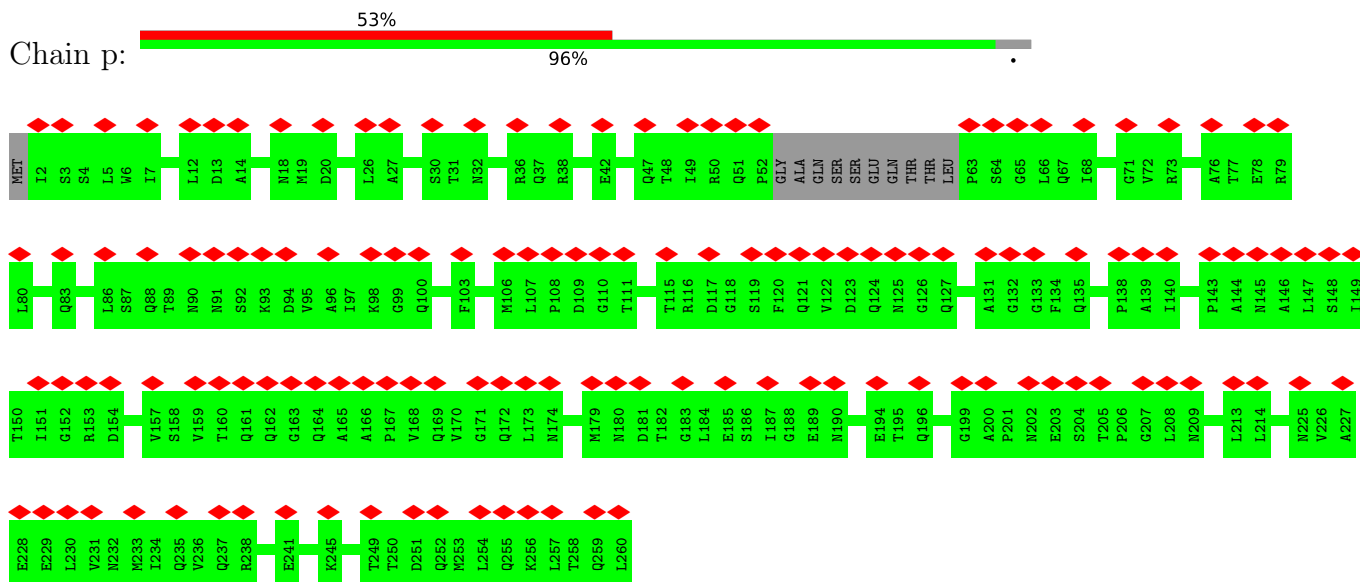


- Molecule 8: Flagellar basal-body rod protein FlgG

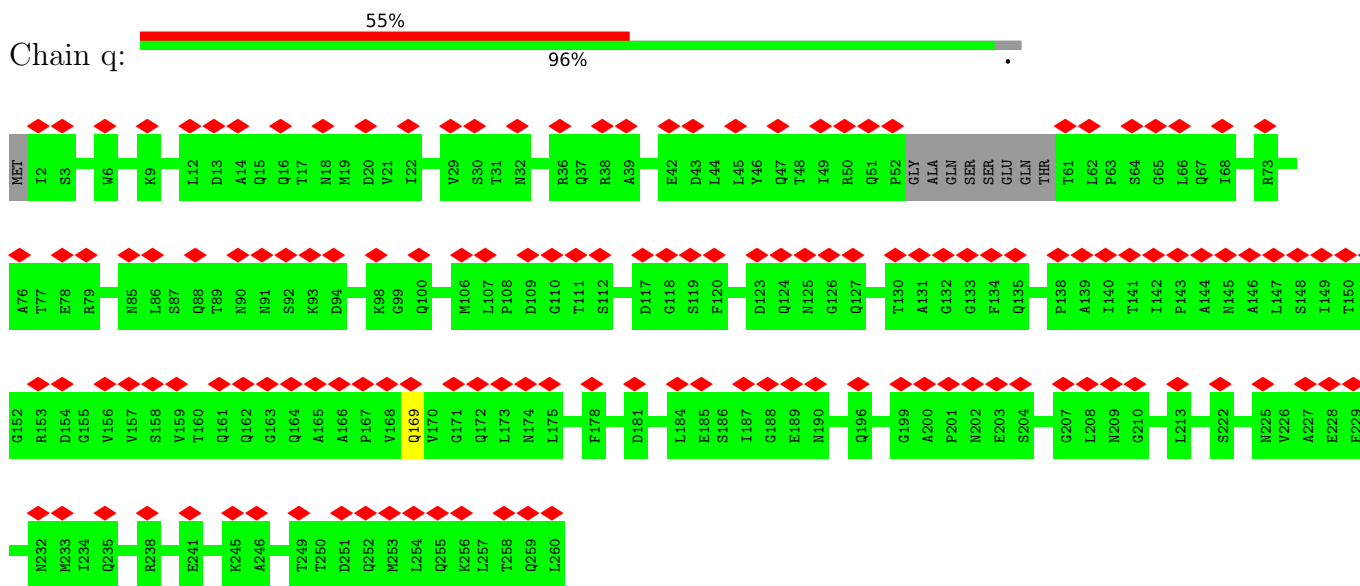
Chain o: 52% 96%



- Molecule 8: Flagellar basal-body rod protein FlgG

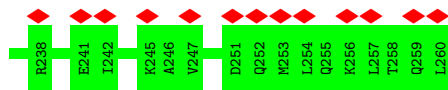


• Molecule 8: Flagellar basal-body rod protein FlgG

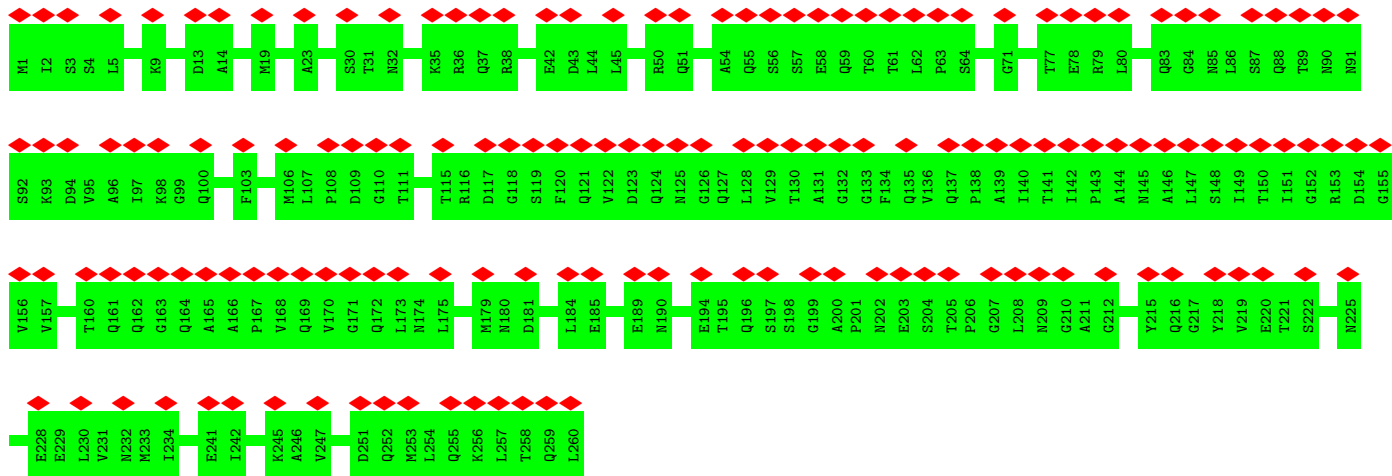


• Molecule 8: Flagellar basal-body rod protein FlgG

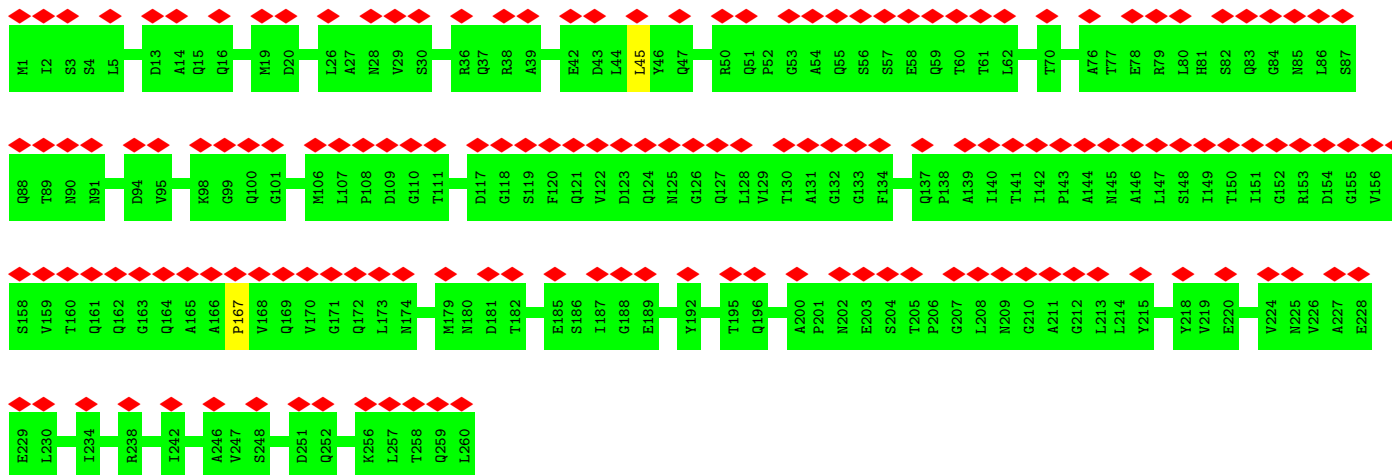




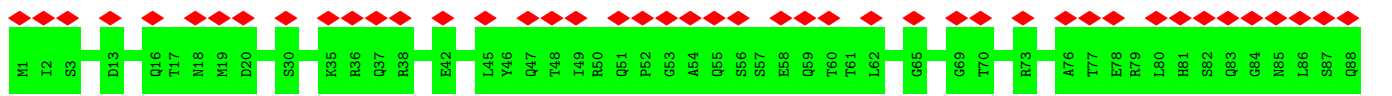
• Molecule 8: Flagellar basal-body rod protein FlgG

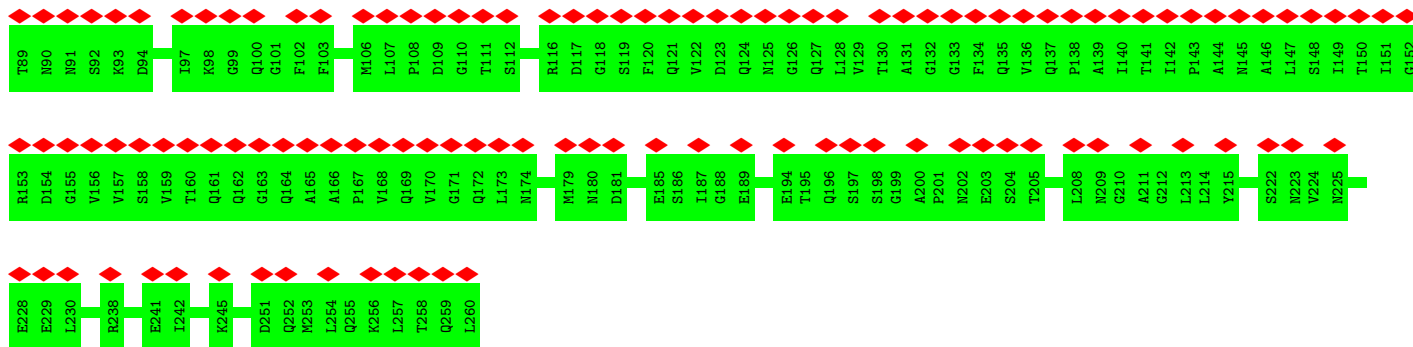


• Molecule 8: Flagellar basal-body rod protein FlgG

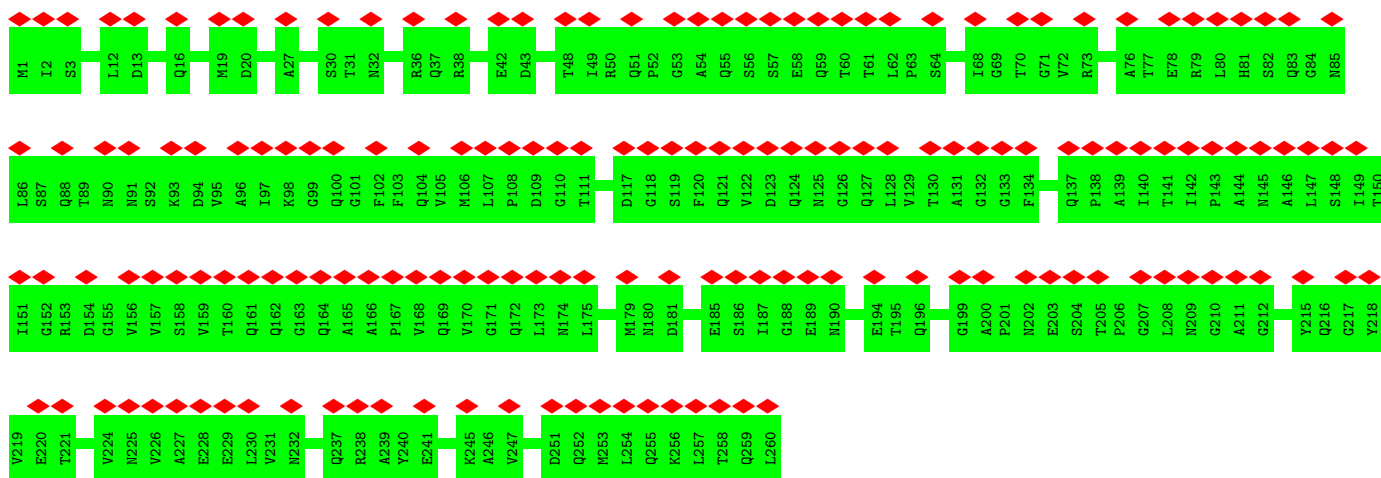


• Molecule 8: Flagellar basal-body rod protein FlgG

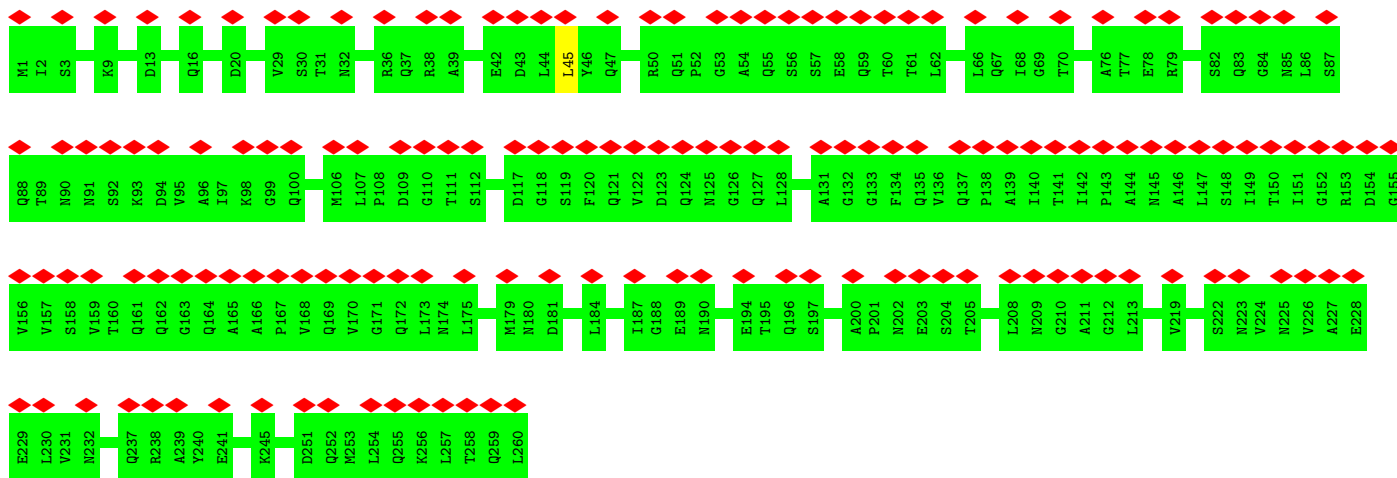




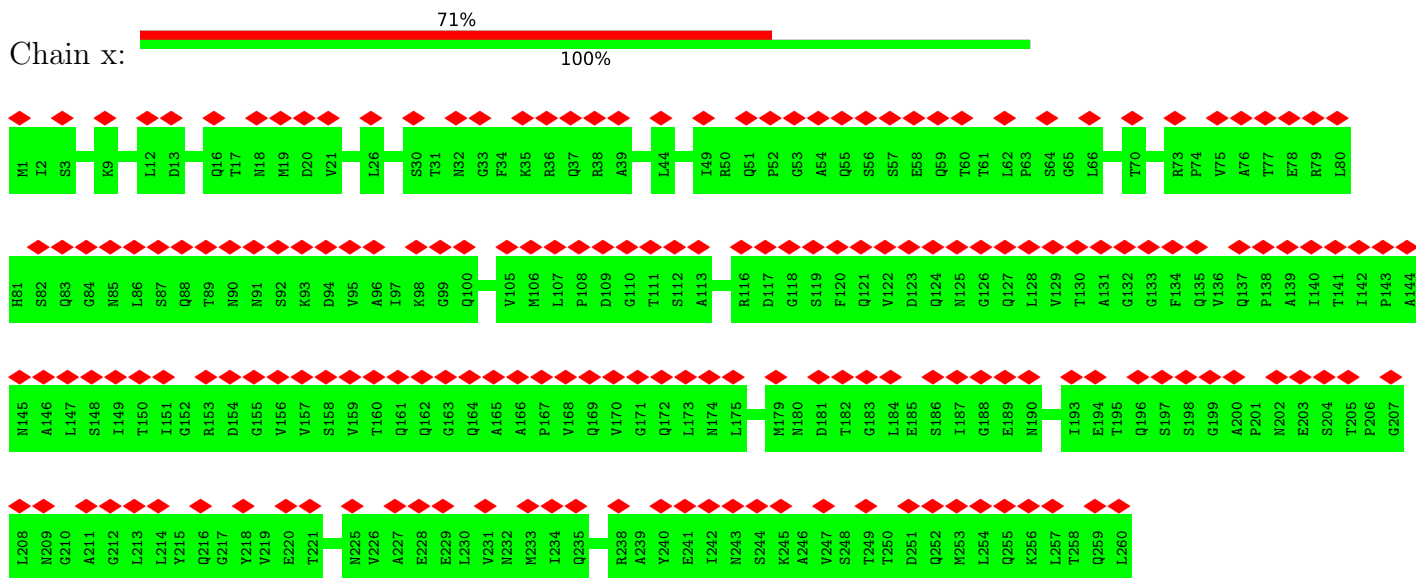
• Molecule 8: Flagellar basal-body rod protein FlgG



• Molecule 8: Flagellar basal-body rod protein FlgG



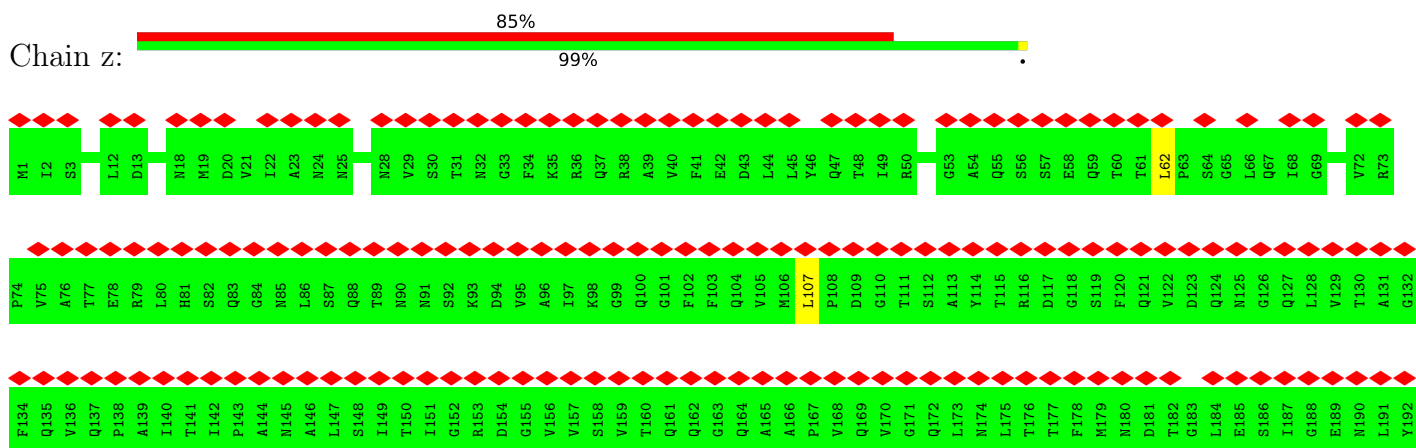
• Molecule 8: Flagellar basal-body rod protein FlgG

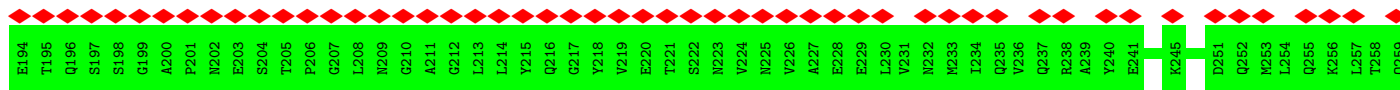


• Molecule 8: Flagellar basal-body rod protein FlgG



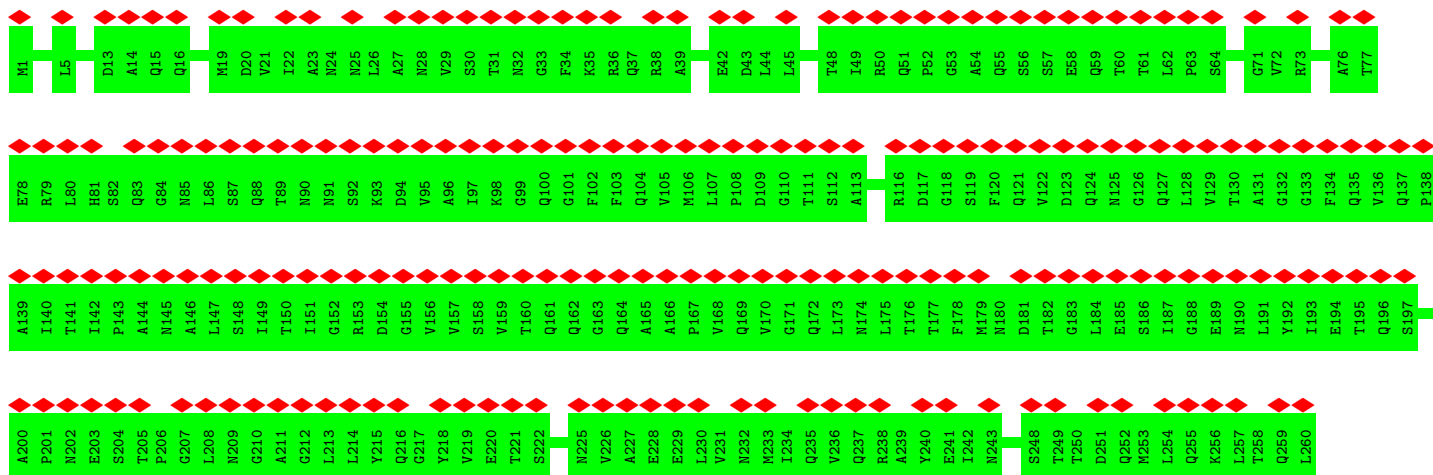
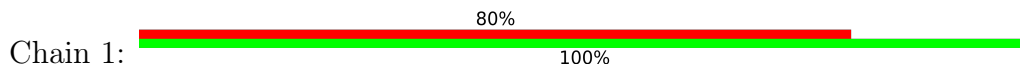
• Molecule 8: Flagellar basal-body rod protein FlgG



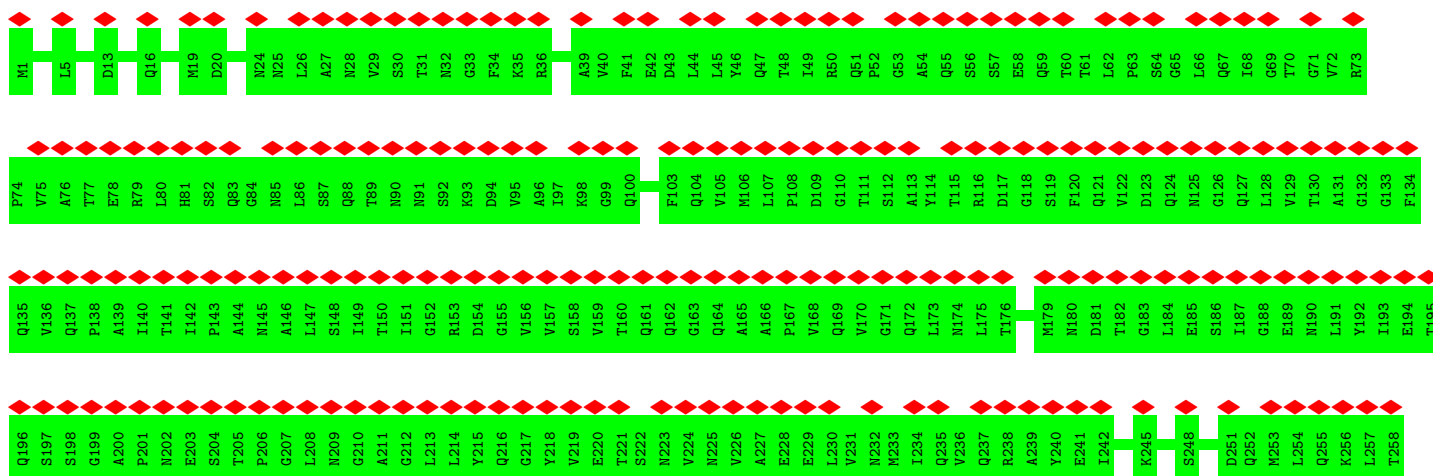
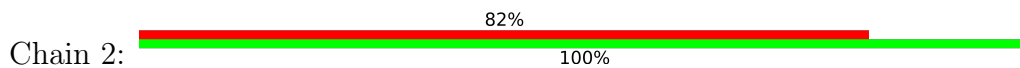


L260

• Molecule 8: Flagellar basal-body rod protein FlgG



• Molecule 8: Flagellar basal-body rod protein FlgG



Q259
L260

• Molecule 8: Flagellar basal-body rod protein FlgG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60497	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 ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	638.976, 638.976, 638.976	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	0.39	0/1662	0.62	1/2263 (0.0%)
1	B	0.41	0/1662	0.61	0/2263
1	C	0.40	0/1662	0.61	0/2263
1	D	0.43	1/1662 (0.1%)	0.58	0/2263
1	E	0.61	1/1662 (0.1%)	0.71	1/2263 (0.0%)
2	F	0.35	0/2035	0.58	0/2777
3	G	0.34	0/681	0.61	0/930
3	H	0.34	0/681	0.55	0/930
3	I	0.37	0/681	0.53	0/930
3	J	2.82	6/681 (0.9%)	0.65	0/930
4	K	0.35	0/296	0.60	1/395 (0.3%)
4	L	0.33	0/567	0.44	0/761
4	M	0.36	0/567	0.45	0/761
4	N	0.36	0/567	0.46	0/761
4	O	0.34	0/567	0.47	0/761
4	P	0.36	0/567	0.47	0/761
5	Q	0.39	0/1035	0.52	0/1399
5	R	0.37	0/941	0.53	0/1269
5	S	0.40	0/951	0.51	0/1281
5	T	0.40	0/842	0.53	0/1132
5	U	0.37	0/934	0.50	0/1259
6	V	0.44	0/981	0.65	0/1334
6	W	0.44	0/976	0.57	0/1327
6	X	0.48	0/976	0.56	0/1327
6	Y	0.46	0/976	0.56	0/1327
6	Z	0.46	0/976	0.55	0/1327
6	a	0.42	0/976	0.57	0/1327
7	b	0.39	0/1836	0.59	0/2502
7	c	0.42	0/1836	0.59	0/2502
7	d	0.44	0/1836	0.58	0/2502
7	e	0.43	0/1836	0.56	0/2502
7	f	0.40	0/1836	0.56	0/2502
8	1	0.38	0/1973	0.55	0/2682
8	2	0.37	0/1973	0.54	0/2682

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	3	0.36	0/1973	0.55	1/2682 (0.0%)
8	4	0.31	0/1973	0.56	1/2682 (0.0%)
8	g	0.41	0/1973	0.52	0/2682
8	h	0.43	0/1973	0.51	0/2682
8	i	0.43	0/1973	0.53	0/2682
8	j	0.44	0/1973	0.52	0/2682
8	k	0.43	0/1973	0.54	0/2682
8	l	0.43	0/1894	0.51	0/2573
8	m	0.46	0/1894	0.54	0/2573
8	n	0.43	0/1894	0.51	0/2573
8	o	0.44	0/1894	0.53	0/2573
8	p	0.44	0/1894	0.52	0/2573
8	q	0.43	0/1909	0.52	0/2595
8	r	0.42	0/1973	0.56	0/2682
8	s	0.43	0/1973	0.56	0/2682
8	t	0.42	0/1973	0.58	2/2682 (0.1%)
8	u	0.42	0/1973	0.56	0/2682
8	v	0.43	0/1973	0.54	0/2682
8	w	0.42	0/1973	0.57	1/2682 (0.0%)
8	x	0.39	0/1973	0.54	0/2682
8	y	0.36	0/1973	0.53	0/2682
8	z	0.35	0/1973	0.54	2/2682 (0.1%)
All	All	0.48	8/82837 (0.0%)	0.55	10/112567 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
2	F	0	2
3	G	0	1
3	H	0	1
3	I	0	1
3	J	0	1
5	U	0	1
7	b	0	2
7	c	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	d	0	1
7	e	0	3
7	f	0	3
All	All	0	25

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	51	PHE	CE2-CZ	34.87	2.03	1.37
3	J	51	PHE	CE1-CZ	33.72	2.01	1.37
3	J	51	PHE	CD1-CE1	32.60	2.04	1.39
3	J	51	PHE	CD2-CE2	31.33	2.02	1.39
3	J	51	PHE	CG-CD1	21.84	1.71	1.38
3	J	51	PHE	CG-CD2	21.32	1.70	1.38
1	E	205	MET	SD-CE	19.73	2.88	1.77
1	D	187	PHE	CB-CG	-5.18	1.42	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	205	MET	CG-SD-CE	20.16	132.46	100.20
8	t	167	PRO	CA-N-CD	-8.46	99.66	111.50
1	A	224	MET	CB-CG-SD	-6.22	93.75	112.40
8	t	45	LEU	CB-CG-CD2	-6.03	100.74	111.00
8	3	45	LEU	CA-CB-CG	5.80	128.63	115.30
8	4	253	MET	CG-SD-CE	-5.73	91.03	100.20
4	K	75	MET	CA-CB-CG	5.60	122.82	113.30
8	w	45	LEU	CB-CG-CD2	-5.23	102.11	111.00
8	z	107	LEU	CA-CB-CG	5.12	127.07	115.30
8	z	62	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	LEU	Peptide
1	B	41	SER	Peptide
1	C	40	LEU	Peptide
1	C	41	SER	Peptide
1	D	40	LEU	Peptide
1	D	41	SER	Peptide

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Mol	Chain	Res	Type	Group
1	E	38	TRP	Peptide
2	F	113	PHE	Peptide
2	F	140	PHE	Peptide
3	G	41	ALA	Peptide
3	H	41	ALA	Peptide
3	I	41	ALA	Peptide
3	J	41	ALA	Peptide
5	U	95	LEU	Peptide
7	b	116	GLN	Peptide
7	b	117	GLY	Peptide
7	c	115	ILE	Peptide
7	c	117	GLY	Peptide
7	d	117	GLY	Peptide
7	e	114	THR	Peptide
7	e	115	ILE	Peptide
7	e	117	GLY	Peptide
7	f	114	THR	Peptide
7	f	117	GLY	Peptide
7	f	70	GLN	Peptide

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	207/245 (84%)	182 (88%)	23 (11%)	2 (1%)	15	54
1	B	207/245 (84%)	183 (88%)	22 (11%)	2 (1%)	15	54
1	C	207/245 (84%)	177 (86%)	29 (14%)	1 (0%)	29	67
1	D	207/245 (84%)	181 (87%)	25 (12%)	1 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	207/245 (84%)	183 (88%)	22 (11%)	2 (1%)	15	54
2	F	254/264 (96%)	223 (88%)	30 (12%)	1 (0%)	34	69
3	G	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
3	H	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
3	I	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
3	J	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
4	K	37/104 (36%)	37 (100%)	0	0	100	100
4	L	73/104 (70%)	68 (93%)	5 (7%)	0	100	100
4	M	73/104 (70%)	68 (93%)	5 (7%)	0	100	100
4	N	73/104 (70%)	69 (94%)	4 (6%)	0	100	100
4	O	73/104 (70%)	69 (94%)	4 (6%)	0	100	100
4	P	73/104 (70%)	68 (93%)	5 (7%)	0	100	100
5	Q	131/138 (95%)	115 (88%)	16 (12%)	0	100	100
5	R	114/138 (83%)	98 (86%)	16 (14%)	0	100	100
5	S	116/138 (84%)	104 (90%)	12 (10%)	0	100	100
5	T	102/138 (74%)	95 (93%)	7 (7%)	0	100	100
5	U	113/138 (82%)	102 (90%)	11 (10%)	0	100	100
6	V	131/134 (98%)	112 (86%)	18 (14%)	1 (1%)	19	58
6	W	130/134 (97%)	108 (83%)	22 (17%)	0	100	100
6	X	130/134 (97%)	107 (82%)	22 (17%)	1 (1%)	19	58
6	Y	130/134 (97%)	109 (84%)	21 (16%)	0	100	100
6	Z	130/134 (97%)	113 (87%)	17 (13%)	0	100	100
6	a	130/134 (97%)	109 (84%)	21 (16%)	0	100	100
7	b	247/251 (98%)	217 (88%)	29 (12%)	1 (0%)	34	69
7	c	247/251 (98%)	212 (86%)	35 (14%)	0	100	100
7	d	247/251 (98%)	215 (87%)	32 (13%)	0	100	100
7	e	247/251 (98%)	212 (86%)	35 (14%)	0	100	100
7	f	247/251 (98%)	210 (85%)	37 (15%)	0	100	100
8	1	258/260 (99%)	231 (90%)	27 (10%)	0	100	100
8	2	258/260 (99%)	231 (90%)	27 (10%)	0	100	100
8	3	258/260 (99%)	232 (90%)	26 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	4	258/260 (99%)	239 (93%)	19 (7%)	0	100	100
8	g	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
8	h	258/260 (99%)	239 (93%)	19 (7%)	0	100	100
8	i	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
8	j	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
8	k	258/260 (99%)	242 (94%)	16 (6%)	0	100	100
8	l	245/260 (94%)	229 (94%)	16 (6%)	0	100	100
8	m	245/260 (94%)	230 (94%)	15 (6%)	0	100	100
8	n	245/260 (94%)	232 (95%)	13 (5%)	0	100	100
8	o	245/260 (94%)	230 (94%)	15 (6%)	0	100	100
8	p	245/260 (94%)	232 (95%)	13 (5%)	0	100	100
8	q	247/260 (95%)	233 (94%)	14 (6%)	0	100	100
8	r	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
8	s	258/260 (99%)	230 (89%)	28 (11%)	0	100	100
8	t	258/260 (99%)	236 (92%)	22 (8%)	0	100	100
8	u	258/260 (99%)	234 (91%)	24 (9%)	0	100	100
8	v	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
8	w	258/260 (99%)	232 (90%)	26 (10%)	0	100	100
8	x	258/260 (99%)	236 (92%)	22 (8%)	0	100	100
8	y	258/260 (99%)	238 (92%)	20 (8%)	0	100	100
8	z	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
All	All	10747/11458 (94%)	9685 (90%)	1050 (10%)	12 (0%)	54	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	VAL
1	C	42	VAL
1	D	42	VAL
1	A	42	VAL
1	E	42	VAL
1	E	41	SER
1	A	41	SER
1	B	41	SER
6	V	58	ALA

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Mol	Chain	Res	Type
2	F	158	PRO
7	b	117	GLY
6	X	93	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/204 (88%)	179 (100%)	0	100	100
1	B	179/204 (88%)	179 (100%)	0	100	100
1	C	179/204 (88%)	178 (99%)	1 (1%)	86	94
1	D	179/204 (88%)	179 (100%)	0	100	100
1	E	179/204 (88%)	179 (100%)	0	100	100
2	F	215/221 (97%)	215 (100%)	0	100	100
3	G	74/74 (100%)	74 (100%)	0	100	100
3	H	74/74 (100%)	74 (100%)	0	100	100
3	I	74/74 (100%)	74 (100%)	0	100	100
3	J	74/74 (100%)	74 (100%)	0	100	100
4	K	33/79 (42%)	33 (100%)	0	100	100
4	L	59/79 (75%)	59 (100%)	0	100	100
4	M	59/79 (75%)	59 (100%)	0	100	100
4	N	59/79 (75%)	59 (100%)	0	100	100
4	O	59/79 (75%)	59 (100%)	0	100	100
4	P	59/79 (75%)	59 (100%)	0	100	100
5	Q	109/113 (96%)	108 (99%)	1 (1%)	78	91
5	R	100/113 (88%)	100 (100%)	0	100	100
5	S	100/113 (88%)	99 (99%)	1 (1%)	76	90
5	T	89/113 (79%)	88 (99%)	1 (1%)	73	88
5	U	99/113 (88%)	97 (98%)	2 (2%)	55	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	V	104/105 (99%)	103 (99%)	1 (1%)	76	90
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%)	104 (100%)	0	100	100
6	Z	104/105 (99%)	103 (99%)	1 (1%)	76	90
6	a	104/105 (99%)	104 (100%)	0	100	100
7	b	191/193 (99%)	191 (100%)	0	100	100
7	c	191/193 (99%)	191 (100%)	0	100	100
7	d	191/193 (99%)	191 (100%)	0	100	100
7	e	191/193 (99%)	191 (100%)	0	100	100
7	f	191/193 (99%)	191 (100%)	0	100	100
8	1	215/215 (100%)	215 (100%)	0	100	100
8	2	215/215 (100%)	215 (100%)	0	100	100
8	3	215/215 (100%)	215 (100%)	0	100	100
8	4	215/215 (100%)	214 (100%)	1 (0%)	88	95
8	g	215/215 (100%)	215 (100%)	0	100	100
8	h	215/215 (100%)	215 (100%)	0	100	100
8	i	215/215 (100%)	215 (100%)	0	100	100
8	j	215/215 (100%)	215 (100%)	0	100	100
8	k	215/215 (100%)	215 (100%)	0	100	100
8	l	206/215 (96%)	206 (100%)	0	100	100
8	m	206/215 (96%)	206 (100%)	0	100	100
8	n	206/215 (96%)	205 (100%)	1 (0%)	88	95
8	o	206/215 (96%)	206 (100%)	0	100	100
8	p	206/215 (96%)	206 (100%)	0	100	100
8	q	208/215 (97%)	207 (100%)	1 (0%)	88	95
8	r	215/215 (100%)	214 (100%)	1 (0%)	88	95
8	s	215/215 (100%)	215 (100%)	0	100	100
8	t	215/215 (100%)	215 (100%)	0	100	100
8	u	215/215 (100%)	215 (100%)	0	100	100
8	v	215/215 (100%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	w	215/215 (100%)	215 (100%)	0	100	100
8	x	215/215 (100%)	215 (100%)	0	100	100
8	y	215/215 (100%)	214 (100%)	1 (0%)	88	95
8	z	215/215 (100%)	215 (100%)	0	100	100
All	All	8918/9331 (96%)	8905 (100%)	13 (0%)	93	98

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	236	MET
5	Q	112	ASN
5	S	17	ASN
5	T	17	ASN
5	U	112	ASN
5	U	117	GLN
6	V	59	THR
6	Z	75	LYS
8	n	172	GLN
8	q	169	GLN
8	r	135	GLN
8	y	196	GLN
8	4	243	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	C	119	GLN
2	F	105	GLN
5	Q	13	GLN
5	Q	92	GLN
5	Q	112	ASN
5	S	92	GLN
5	T	92	GLN
6	V	134	GLN
6	W	22	ASN
6	X	22	ASN
7	b	37	GLN
7	c	230	GLN
7	e	83	GLN

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Mol	Chain	Res	Type
7	e	106	GLN
8	g	67	GLN
8	h	24	ASN
8	h	47	GLN
8	h	67	GLN
8	i	121	GLN
8	j	169	GLN
8	k	135	GLN
8	m	67	GLN
8	m	135	GLN
8	o	67	GLN
8	o	127	GLN
8	o	169	GLN
8	o	235	GLN
8	p	85	ASN
8	p	88	GLN
8	p	145	ASN
8	r	180	ASN
8	t	67	GLN
8	t	127	GLN
8	t	137	GLN
8	u	55	GLN
8	v	88	GLN
8	w	83	GLN
8	y	16	GLN
8	y	91	ASN
8	3	255	GLN
8	4	47	GLN
8	4	55	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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	115:ASP	C	116:PRO	N	5.09

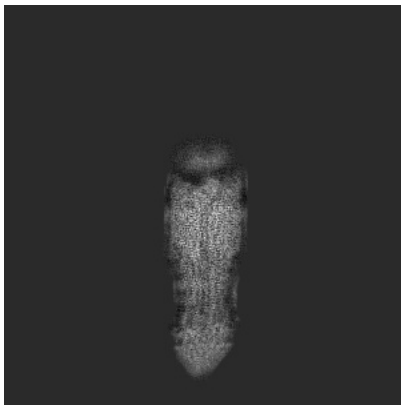
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12192. These allow visual inspection of the internal detail of the map and identification of artifacts.

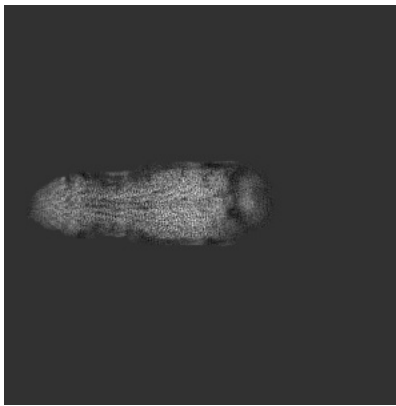
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

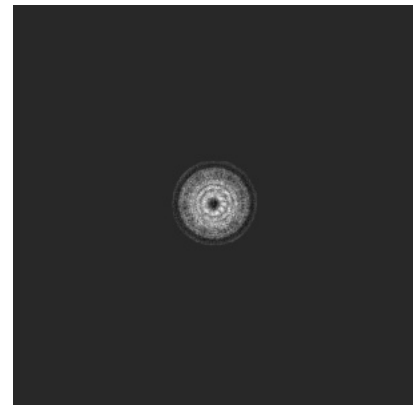
6.1.1 Primary map



X

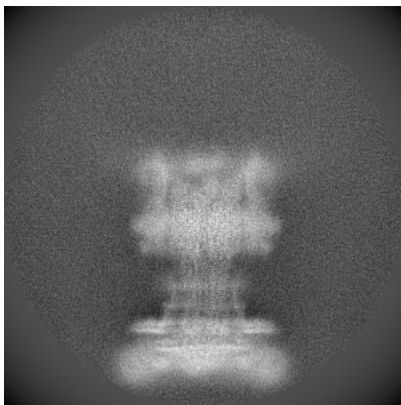


Y

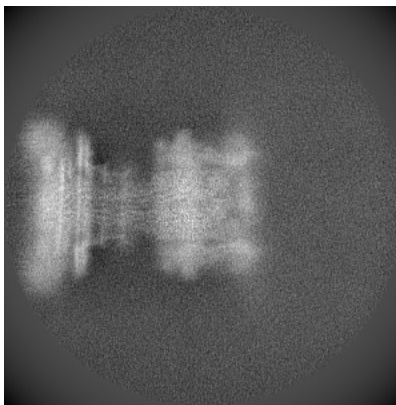


Z

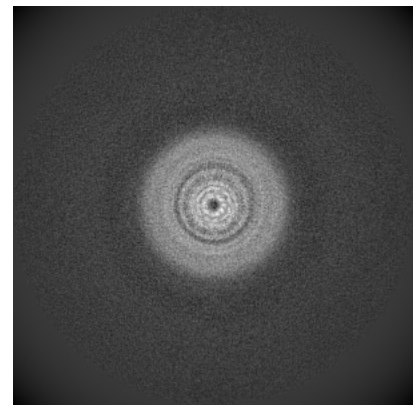
6.1.2 Raw map



X



Y

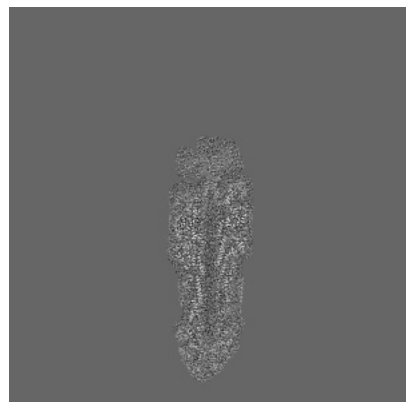


Z

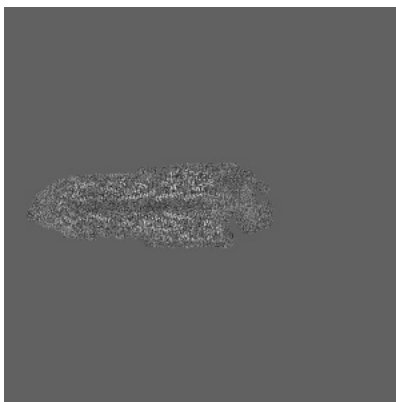
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

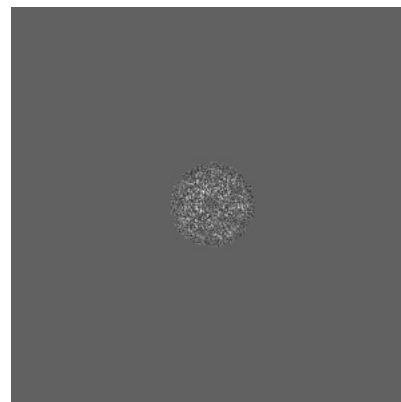
6.2.1 Primary map



X Index: 384

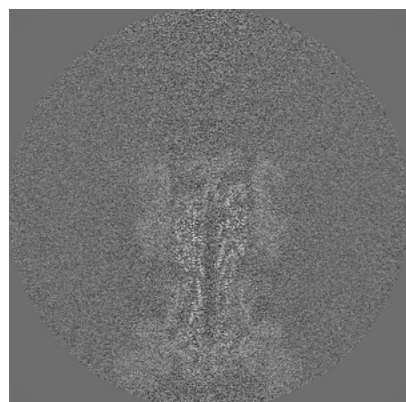


Y Index: 384

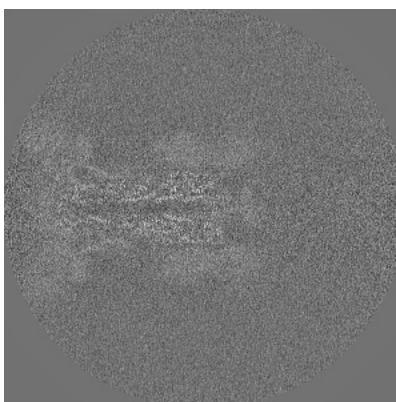


Z Index: 384

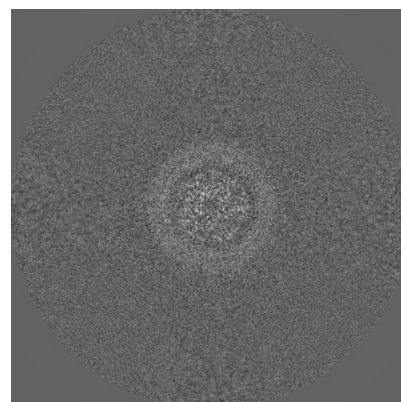
6.2.2 Raw map



X Index: 384



Y Index: 384

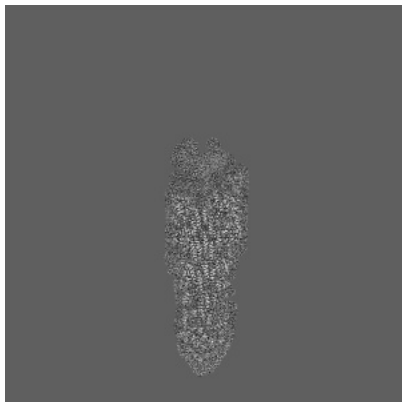


Z Index: 384

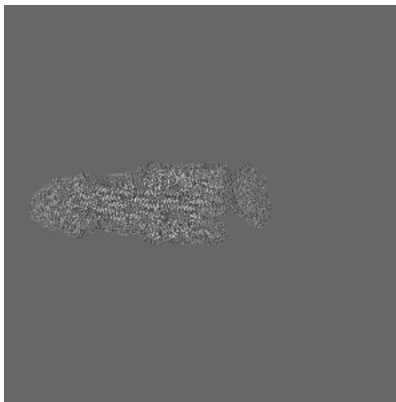
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

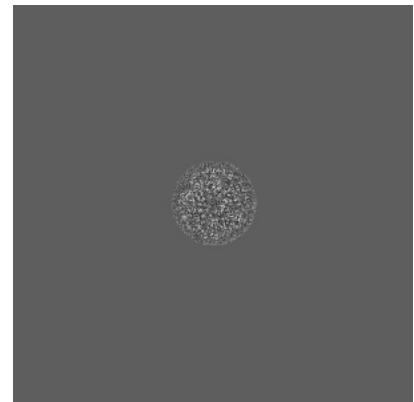
6.3.1 Primary map



X Index: 404

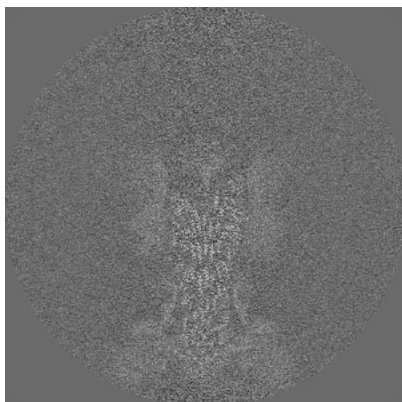


Y Index: 366

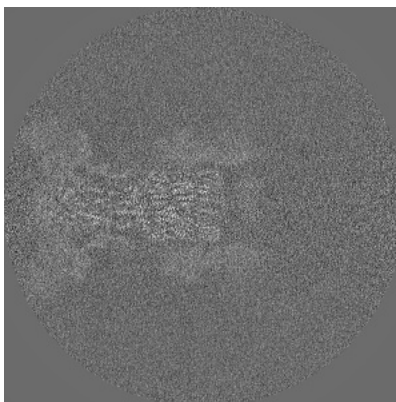


Z Index: 355

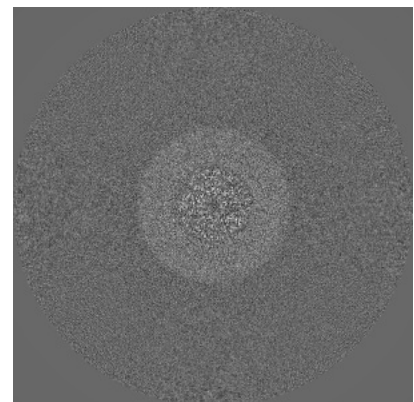
6.3.2 Raw map



X Index: 403



Y Index: 371



Z Index: 354

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

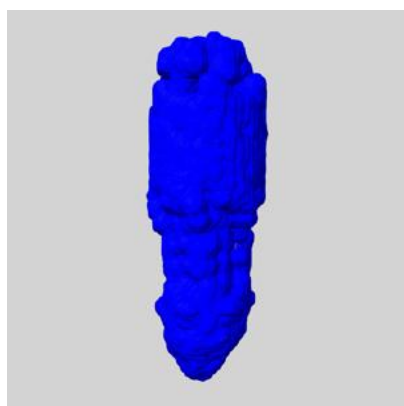
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

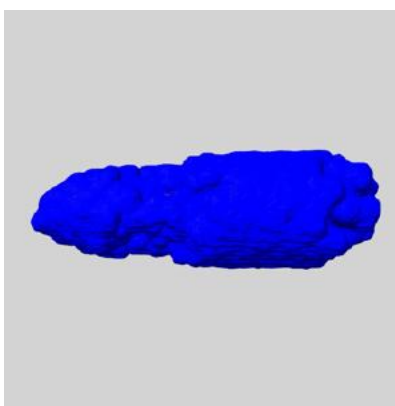
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

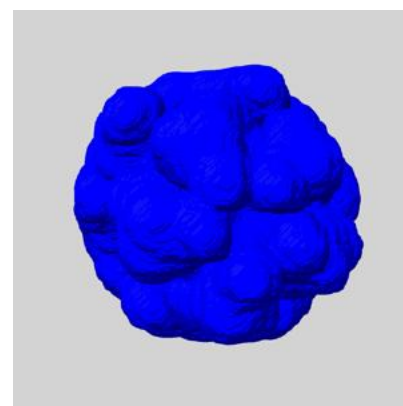
6.5.1 emd_12192_msk_1.map [i](#)



X



Y

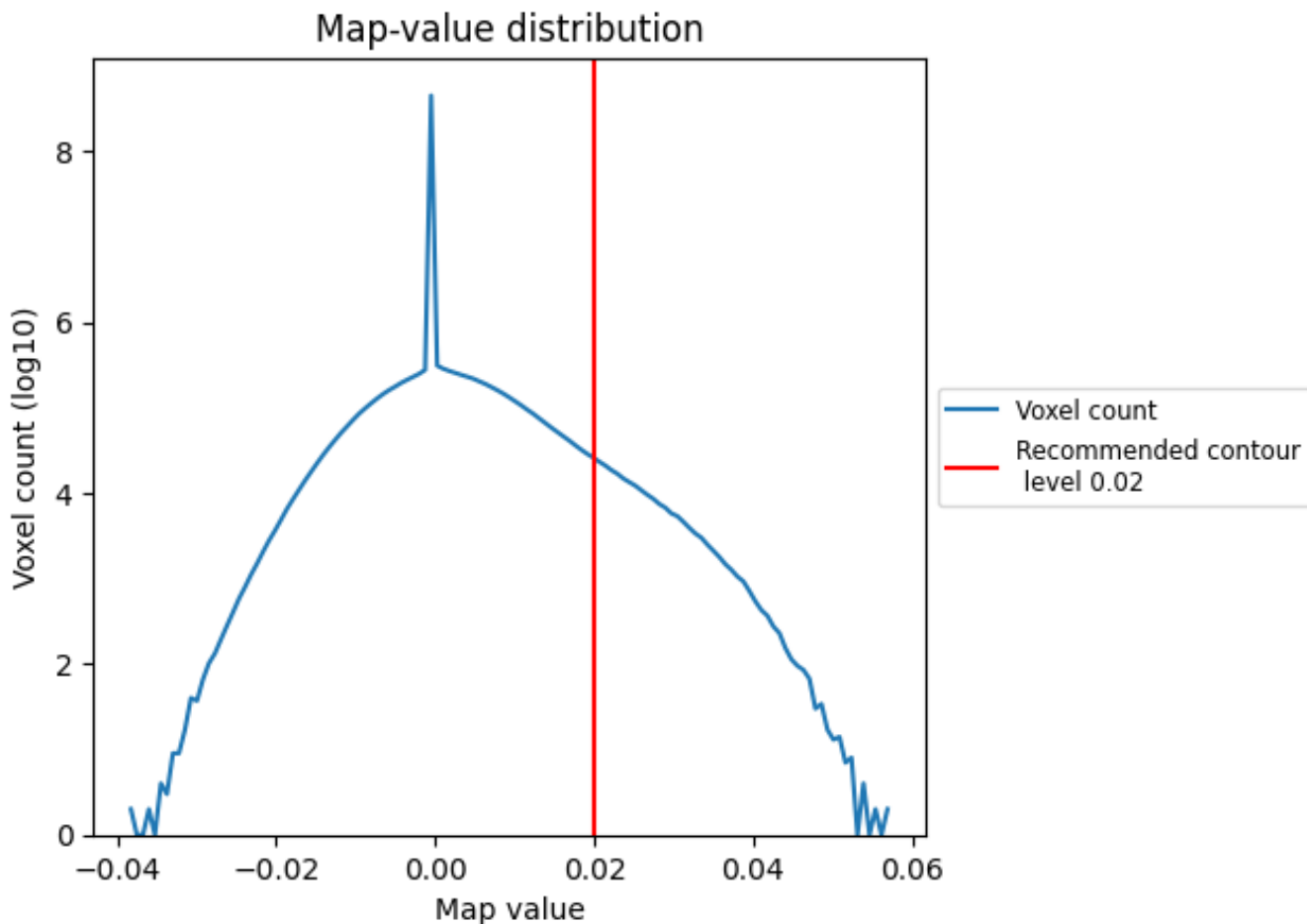


Z

7 Map analysis [i](#)

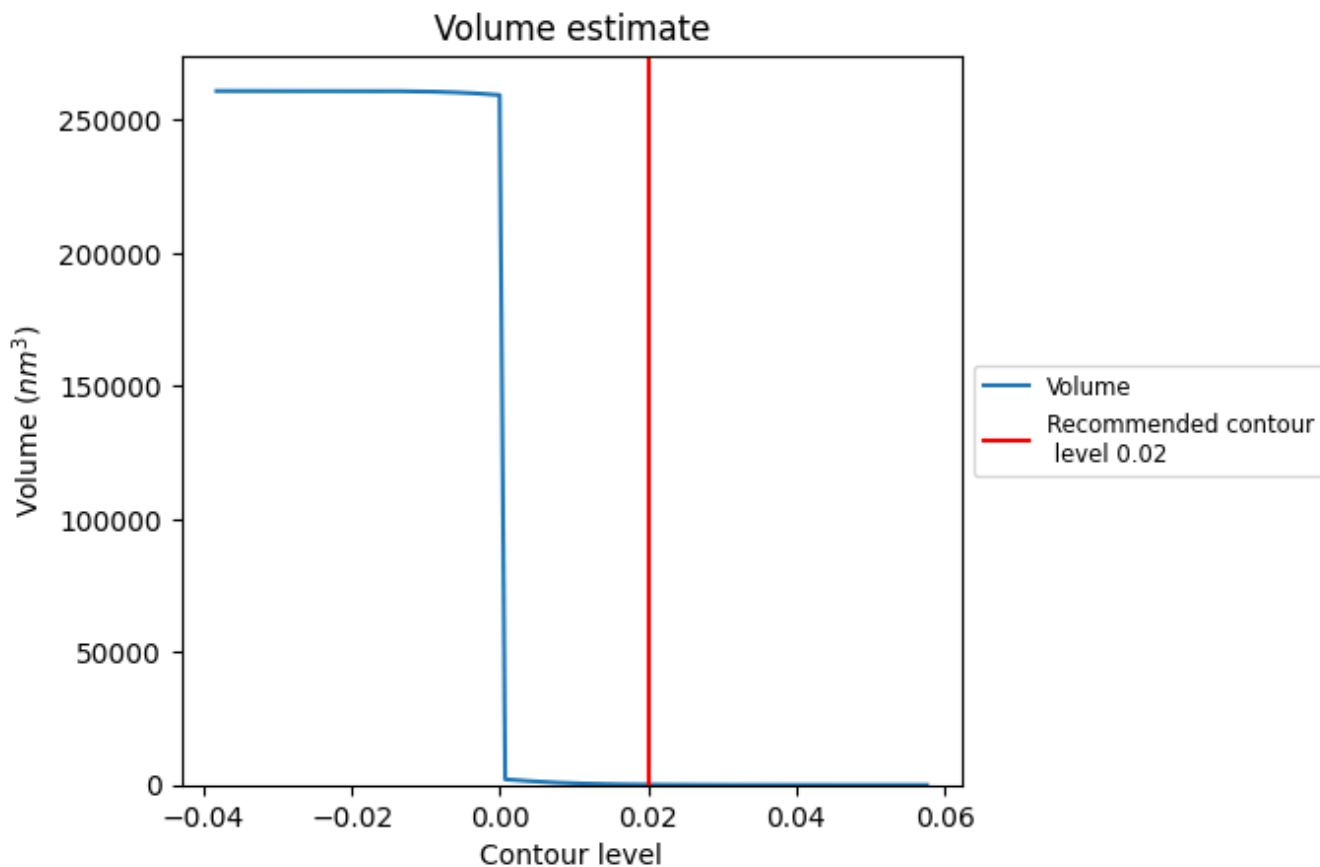
This section contains the results of statistical analysis of the map.

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.

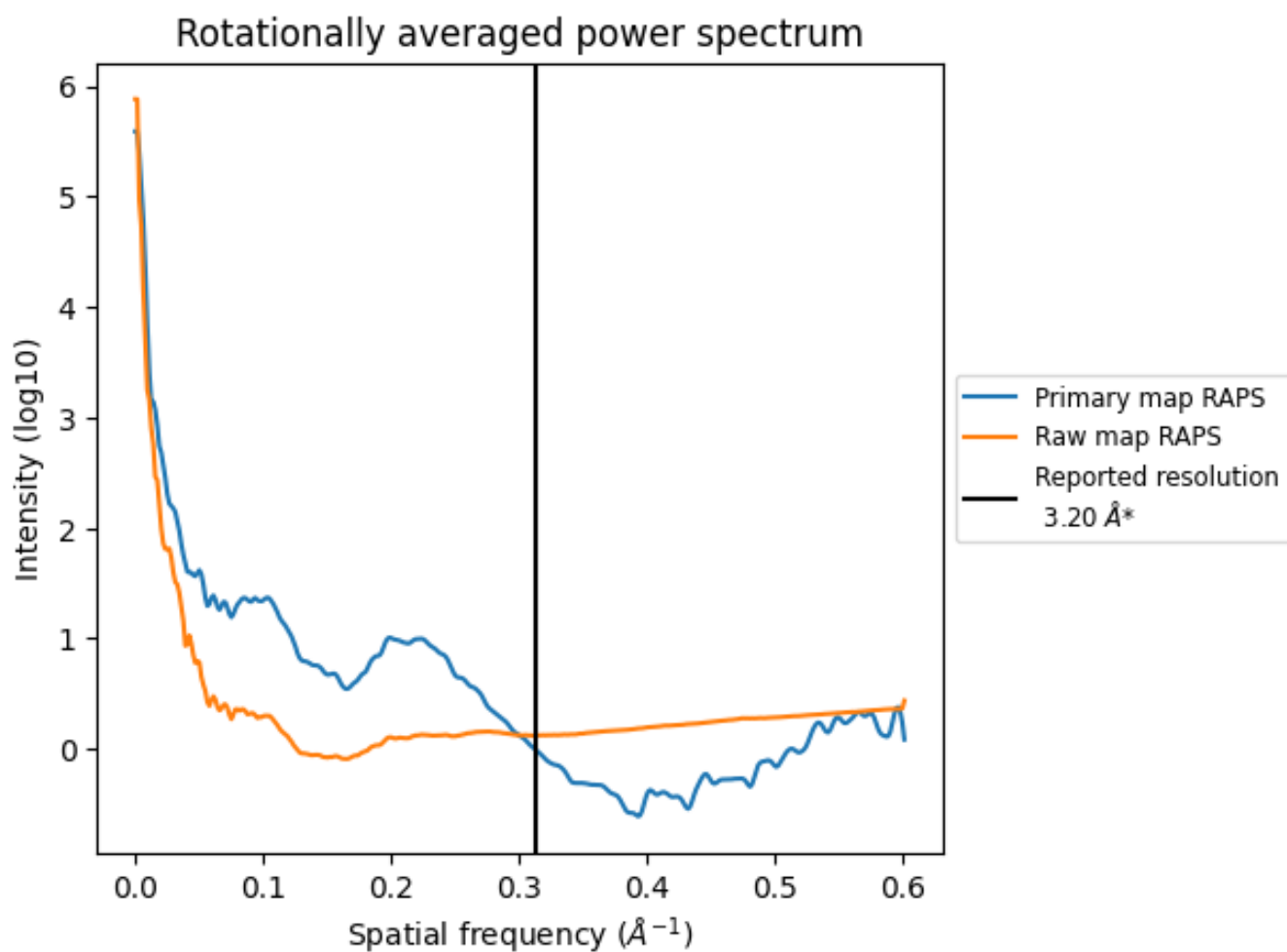
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 117 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

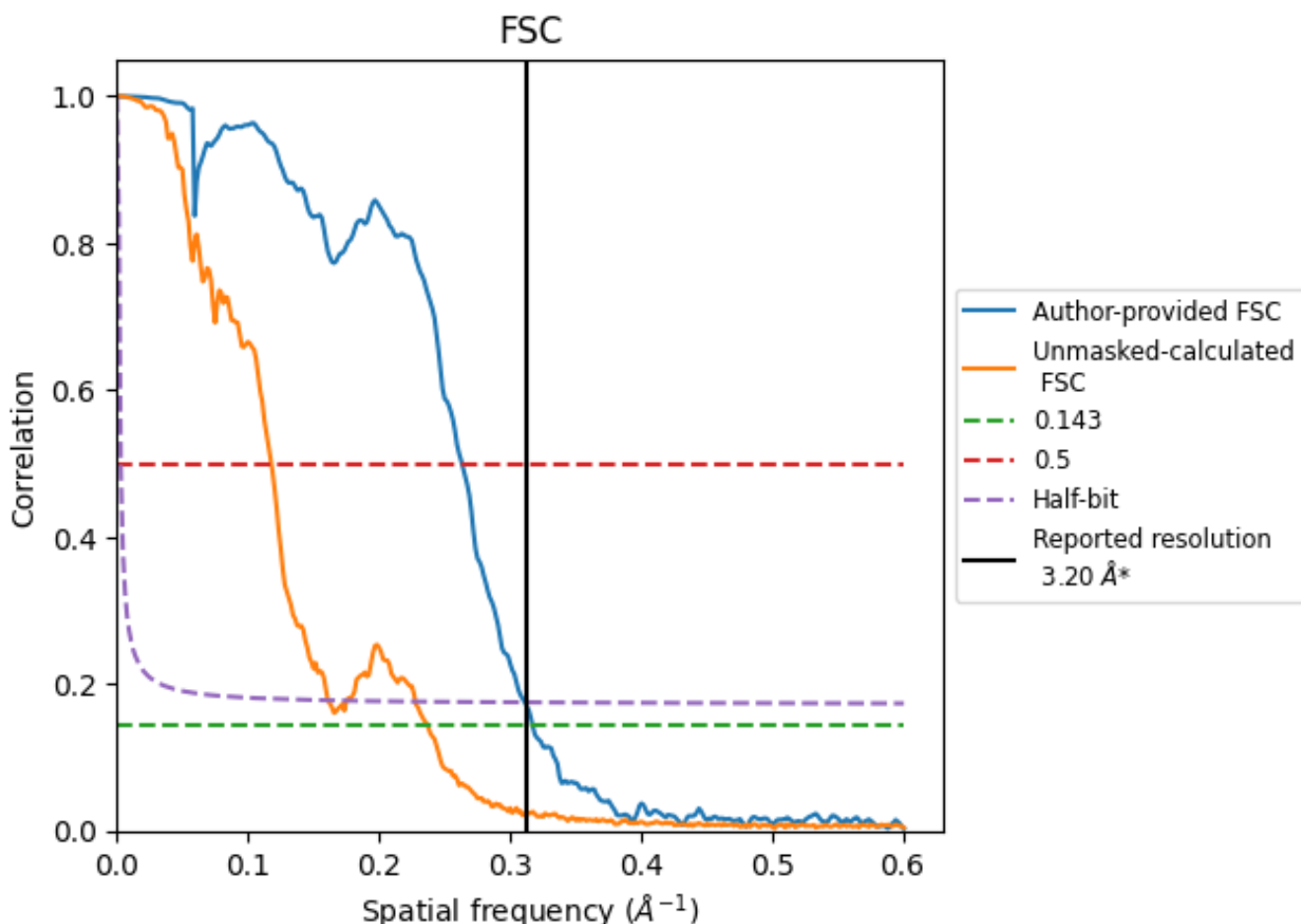


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

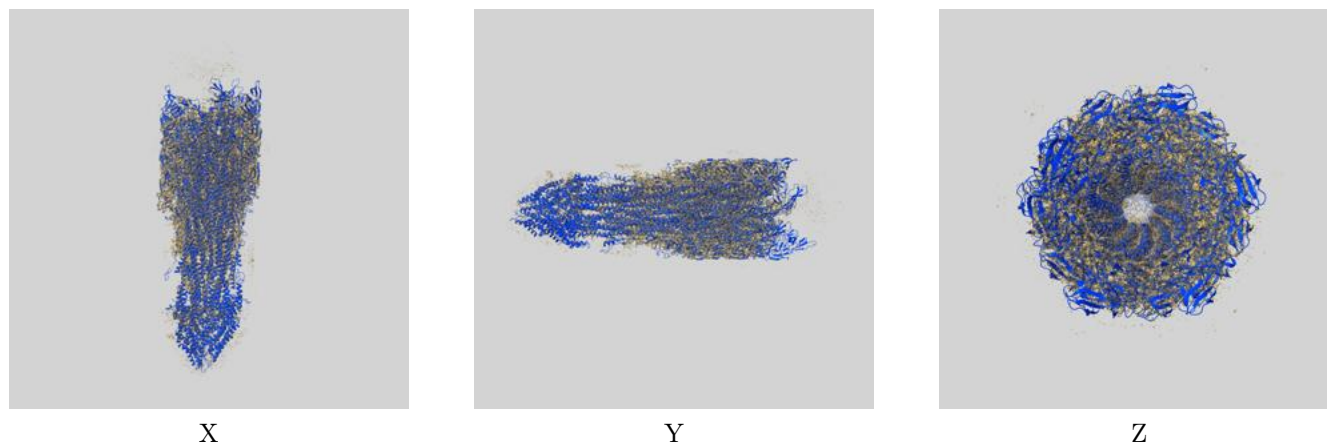
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.80	3.21
Unmasked-calculated*	4.22	8.47	6.20

*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 4.22 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

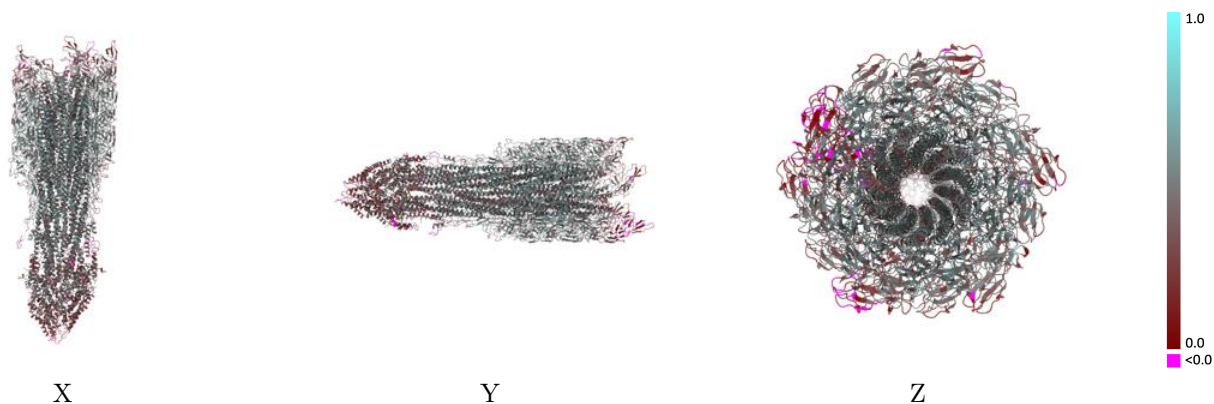
This section contains information regarding the fit between EMDB map EMD-12192 and PDB model 7BIN. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



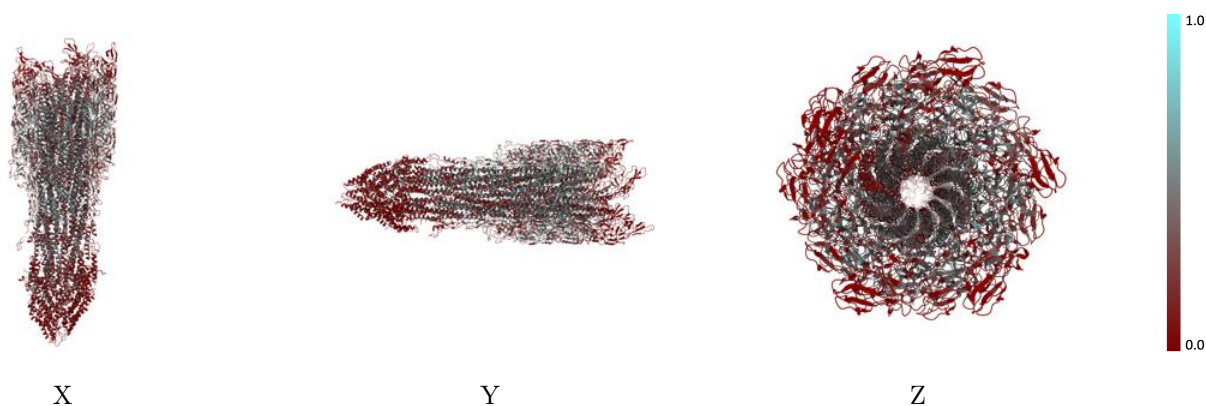
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



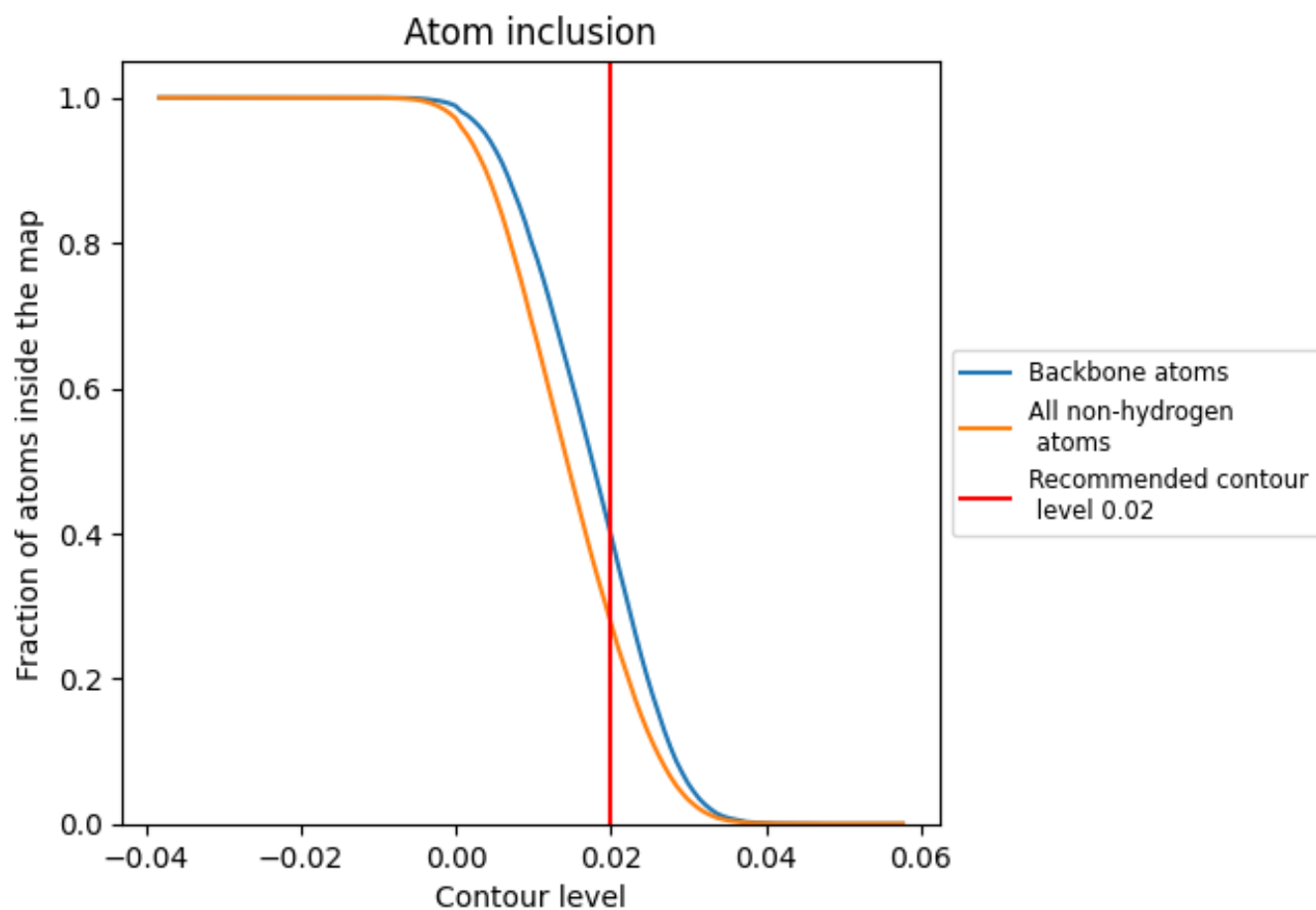
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 28% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2760	 0.4340
1	 0.2160	 0.4090
2	 0.2227	 0.4130
3	 0.1750	 0.4010
4	 0.0457	 0.2250
A	 0.1004	 0.3440
B	 0.1454	 0.3610
C	 0.1659	 0.3820
D	 0.1478	 0.3630
E	 0.0811	 0.3210
F	 0.0448	 0.2890
G	 0.0436	 0.2750
H	 0.0662	 0.2870
I	 0.0511	 0.2790
J	 0.0226	 0.2350
K	 0.1843	 0.3990
L	 0.2310	 0.4310
M	 0.2780	 0.4570
N	 0.2870	 0.4400
O	 0.2635	 0.4330
P	 0.2166	 0.4120
Q	 0.2010	 0.4150
R	 0.3034	 0.4100
S	 0.3214	 0.4200
T	 0.3538	 0.4770
U	 0.2759	 0.3970
V	 0.2294	 0.3980
W	 0.3197	 0.4540
X	 0.3532	 0.4680
Y	 0.3711	 0.4790
Z	 0.3543	 0.4610
a	 0.2652	 0.4250
b	 0.2503	 0.4530
c	 0.3406	 0.4800
d	 0.3547	 0.4830



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Chain	Atom inclusion	Q-score
e	 0.3563	 0.4810
f	 0.3193	 0.4700
g	 0.2902	 0.4570
h	 0.3676	 0.4870
i	 0.3681	 0.4890
j	 0.3707	 0.4900
k	 0.3557	 0.4820
l	 0.3734	 0.5050
m	 0.3820	 0.5090
n	 0.3929	 0.5120
o	 0.3696	 0.5030
p	 0.3788	 0.5060
q	 0.3752	 0.5000
r	 0.3733	 0.4940
s	 0.3572	 0.4830
t	 0.3396	 0.4720
u	 0.3375	 0.4610
v	 0.3577	 0.4830
w	 0.3536	 0.4730
x	 0.2918	 0.4650
y	 0.2191	 0.3990
z	 0.1781	 0.3420