



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:14 AM UTC

PDB ID : 7BIN / pdb_00007bin
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 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:

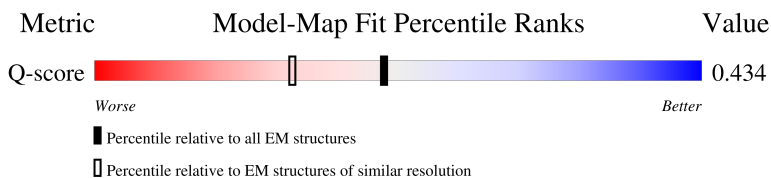
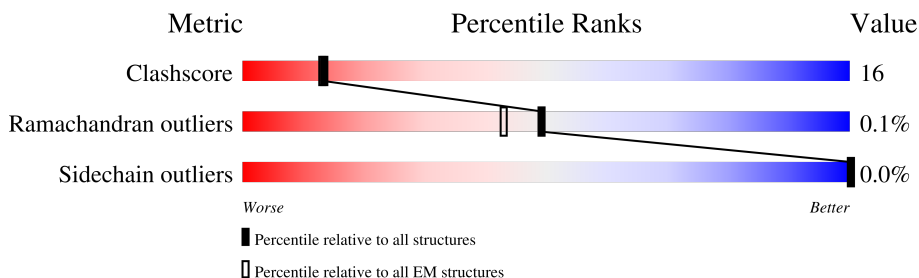
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.20 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	15020 (2.70 - 3.70)

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	245	83% 48% 36% 15%
1	B	245	82% 52% 32% 15%
1	C	245	78% 49% 35% 15%
1	D	245	81% 46% 38% 15%

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Mol	Chain	Length	Quality of chain
1	E	245	82% 50% 34% 15%
2	F	264	98% 56% 41%
3	G	89	100% 60% 40%
3	H	89	100% 72% 28%
3	I	89	100% 62% 37%
3	J	89	100% 64% 35%
4	K	104	35% 23% 14% 62%
4	L	104	61% 61% 12% 28%
4	M	104	57% 60% 12% 28%
4	N	104	55% 49% 23% 28%
4	O	104	56% 55% 17% 28%
4	P	104	64% 41% 31% 28%
5	Q	138	88% 66% 30%
5	R	138	59% 60% 27% 13%
5	S	138	56% 62% 27% 12%
5	T	138	48% 52% 25% 23%
5	U	138	64% 57% 28% 14%
6	V	134	76% 71% 28%
6	W	134	60% 73% 25%
6	X	134	57% 66% 32%
6	Y	134	54% 73% 25%
6	Z	134	55% 69% 30%
6	a	134	75% 69% 29%
7	b	251	79% 65% 33%
7	c	251	65% 63% 35%




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Mol	Chain	Length	Quality of chain
7	d	251	62% 62% 37%
7	e	251	59% 57% 41%
7	f	251	66% 65% 33%
8	1	260	80% 69% 31%
8	2	260	82% 70% 30%
8	3	260	88% 70% 30%
8	4	260	99% 66% 34%
8	g	260	71% 70% 30%
8	h	260	55% 72% 28%
8	i	260	58% 67% 33%
8	j	260	55% 73% 27%
8	k	260	58% 73% 27%
8	l	260	52% 70% 25%
8	m	260	52% 66% 30%
8	n	260	49% 70% 26%
8	o	260	52% 71% 25%
8	p	260	53% 68% 28%
8	q	260	55% 75% 22%
8	r	260	56% 69% 31%
8	s	260	60% 74% 26%
8	t	260	60% 72% 28%
8	u	260	61% 70% 30%
8	v	260	63% 75% 25%
8	w	260	59% 69% 31%
8	x	260	71% 74% 26%

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Mol	Chain	Length	Quality of chain
8	y	260	 79%
8	z	260	 70% 30%
8	z	260	 85% 69% 31%

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	1623	1084	251	276	12	0	0
1	B	209	1623	1084	251	276	12	0	0
1	C	209	1623	1084	251	276	12	0	0
1	D	209	1623	1084	251	276	12	0	0
1	E	209	1623	1084	251	276	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	1986	1329	314	327	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	670	449	100	114	7	0	0
3	H	89	670	449	100	114	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		

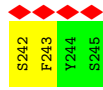
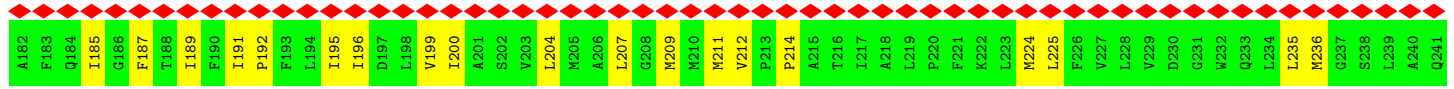
- Molecule 8 is a protein called Flagellar basal-body rod protein FlgG.

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		

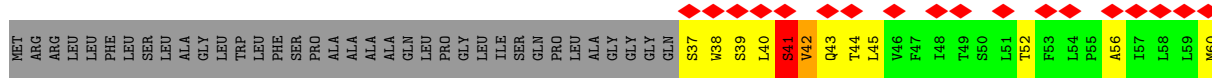
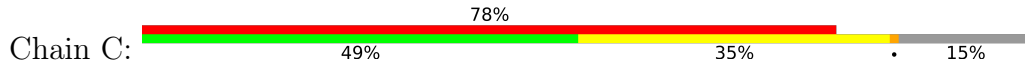
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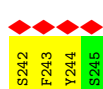
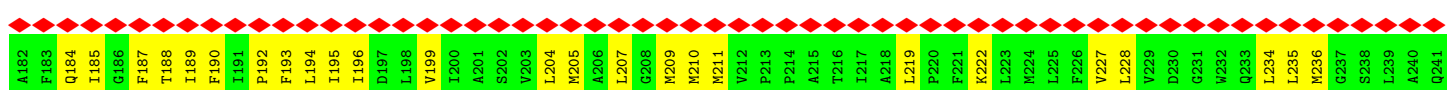
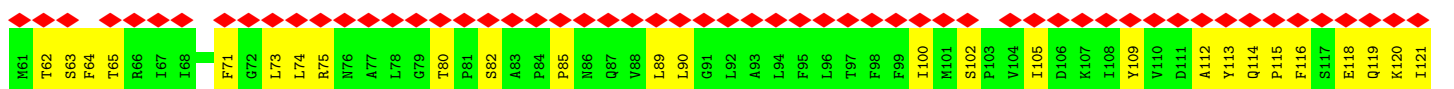
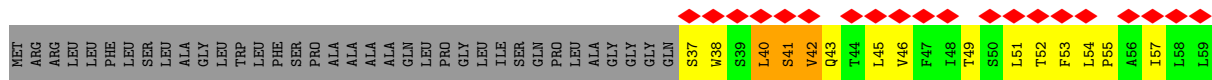
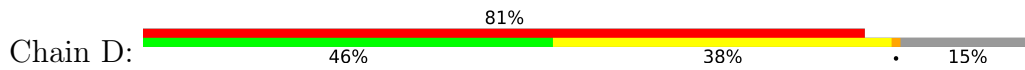
Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	249	Total	C	N	O	S	0	0
			1871	1157	328	381	5		
8	p	249	Total	C	N	O	S	0	0
			1871	1157	328	381	5		
8	q	251	Total	C	N	O	S	0	0
			1886	1167	330	384	5		
8	r	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	s	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
8	t	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		



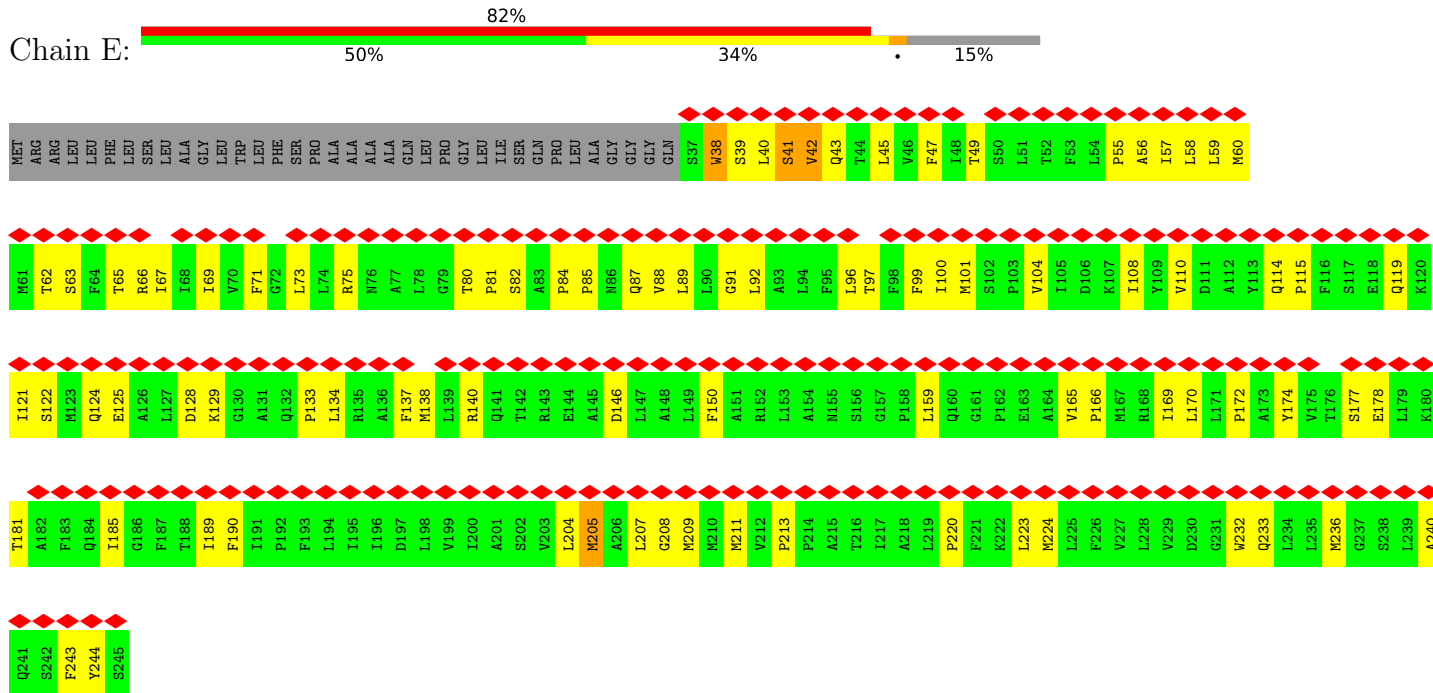
• Molecule 1: Flagellar biosynthetic protein FlpP



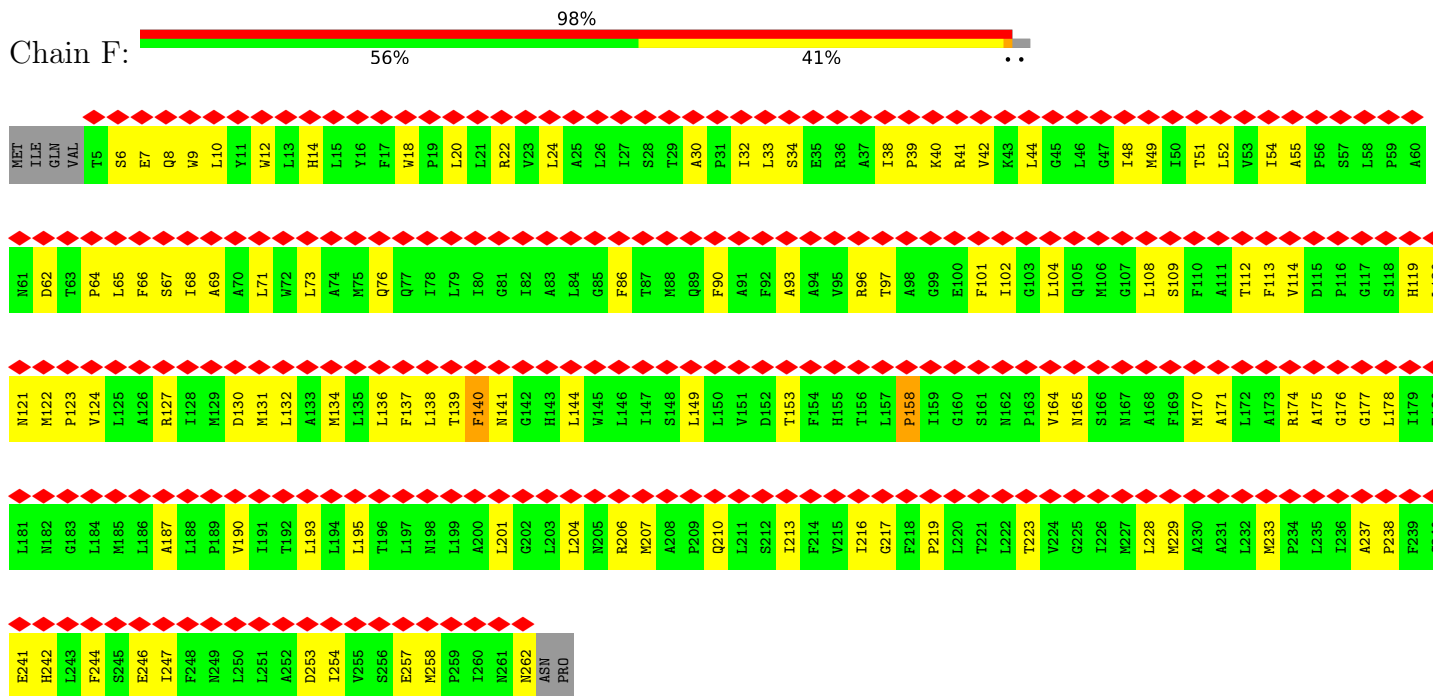
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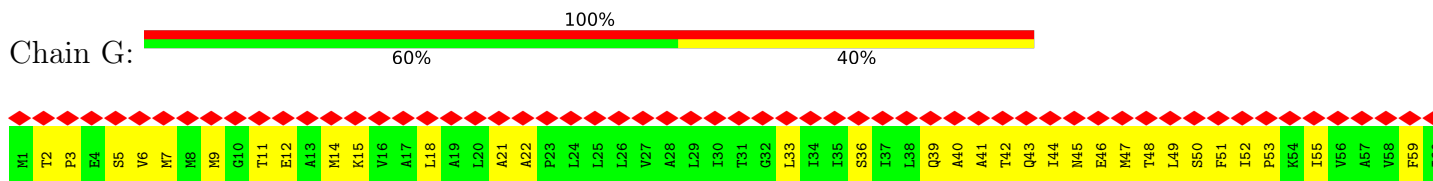
• Molecule 1: Flagellar biosynthetic protein FliP

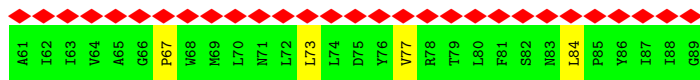


• Molecule 2: Flagellar biosynthetic protein FliR

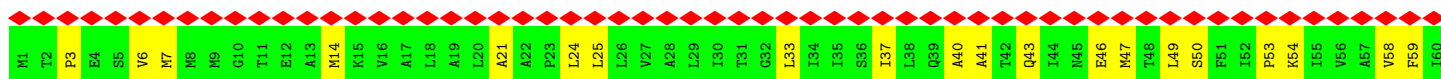
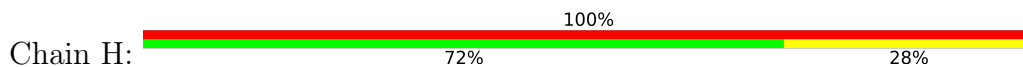


• Molecule 3: Flagellar biosynthetic protein FliQ

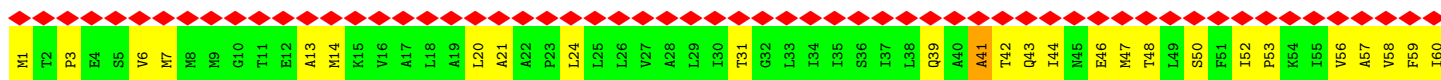




• Molecule 3: Flagellar biosynthetic protein FliQ



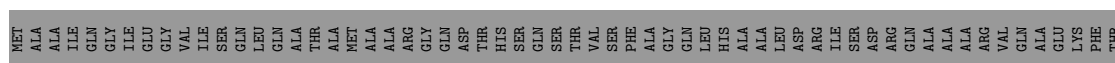
• Molecule 3: Flagellar biosynthetic protein FliQ



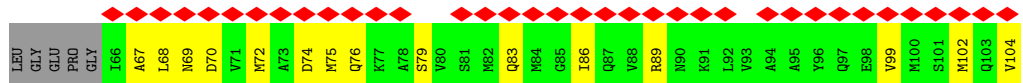
• Molecule 3: Flagellar biosynthetic protein FliQ



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

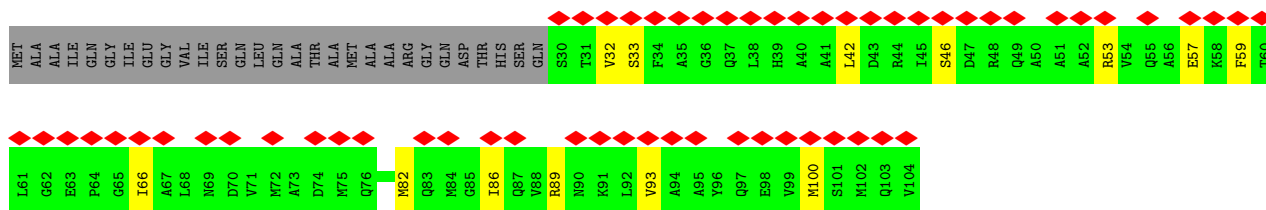


• Molecule 4: Flagellar hook-basal body complex protein FliE

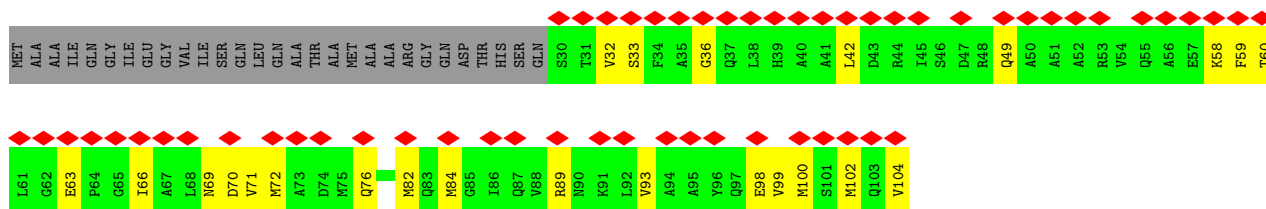




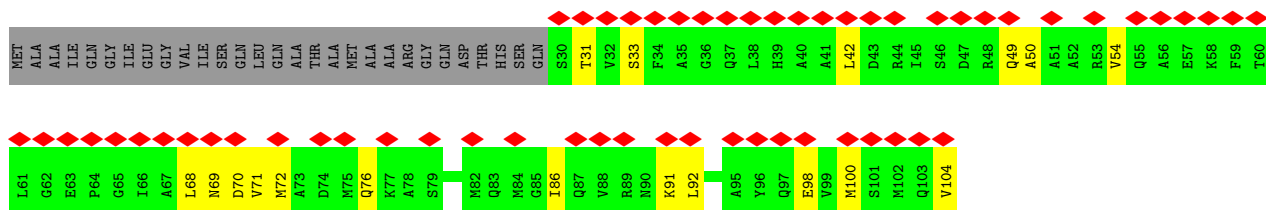
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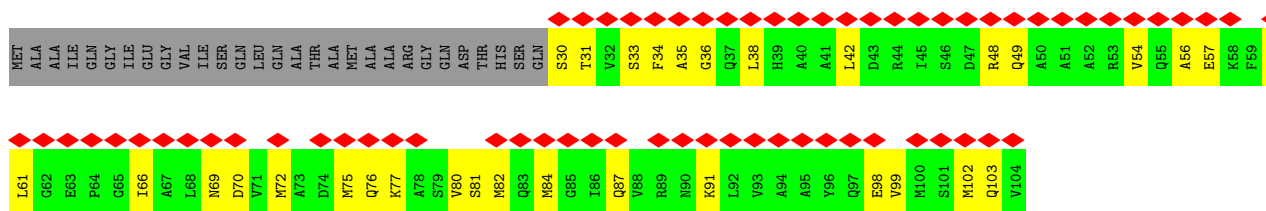
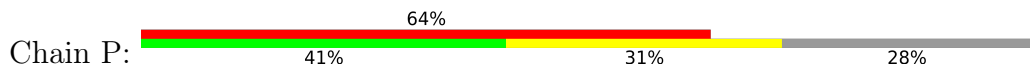
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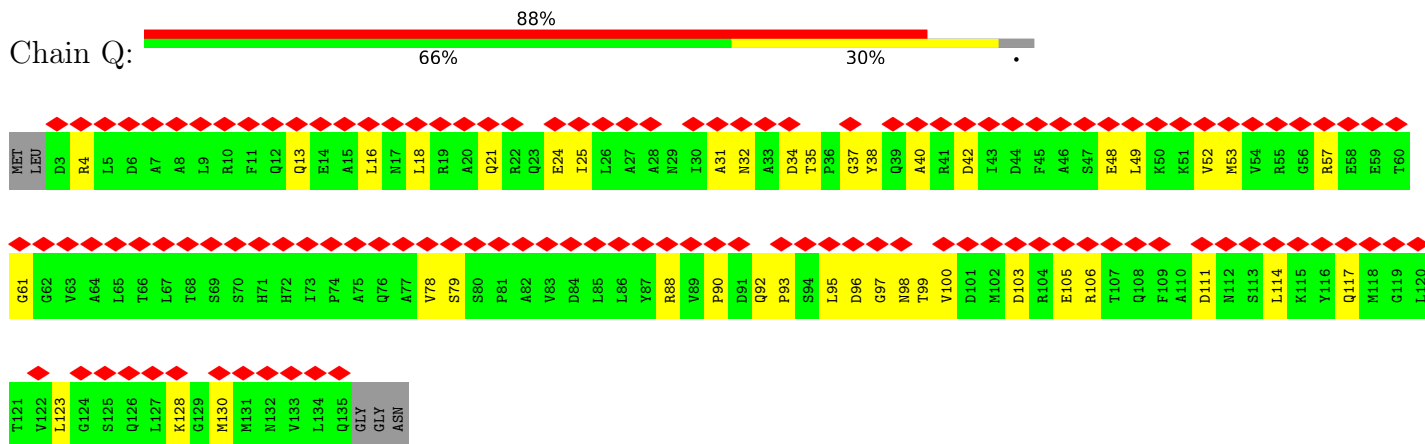
• Molecule 4: Flagellar hook-basal body complex protein FliE



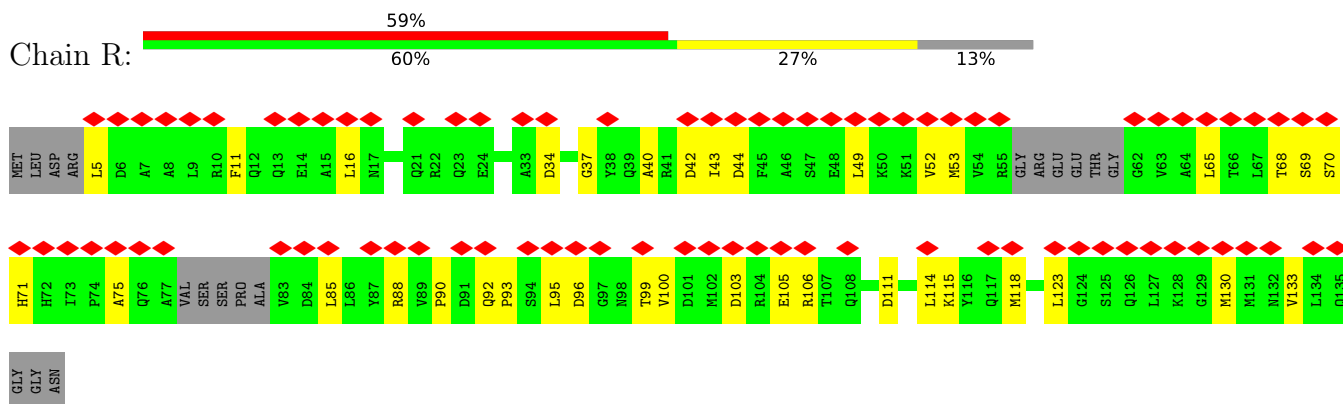
• Molecule 4: Flagellar hook-basal body complex protein FliE



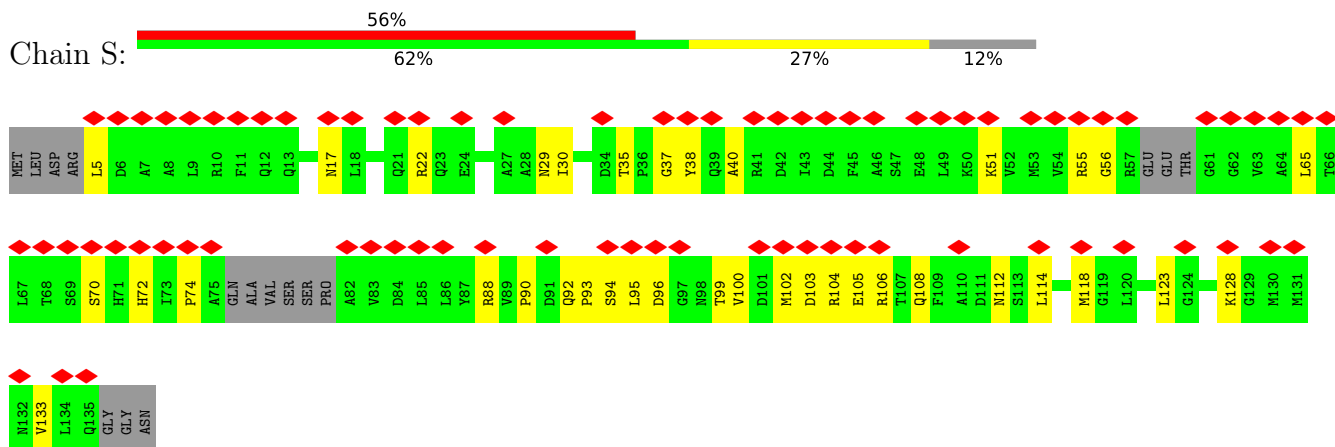
• Molecule 5: Flagellar basal body rod protein FlgB



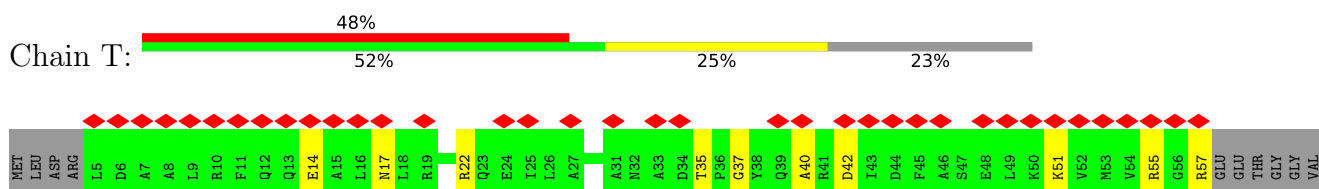
• Molecule 5: Flagellar basal body rod protein FlgB

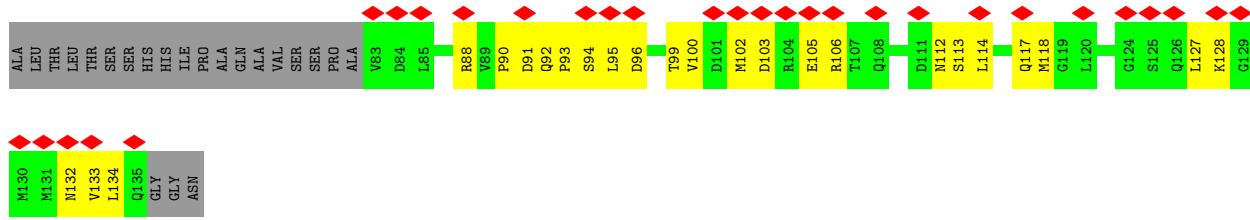


• Molecule 5: Flagellar basal body rod protein FlgB

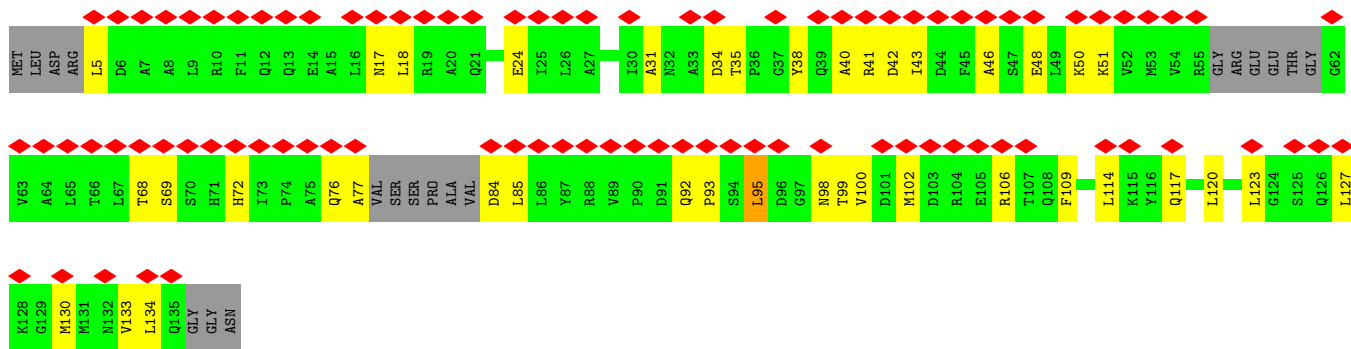


• Molecule 5: Flagellar basal body rod protein FlgB

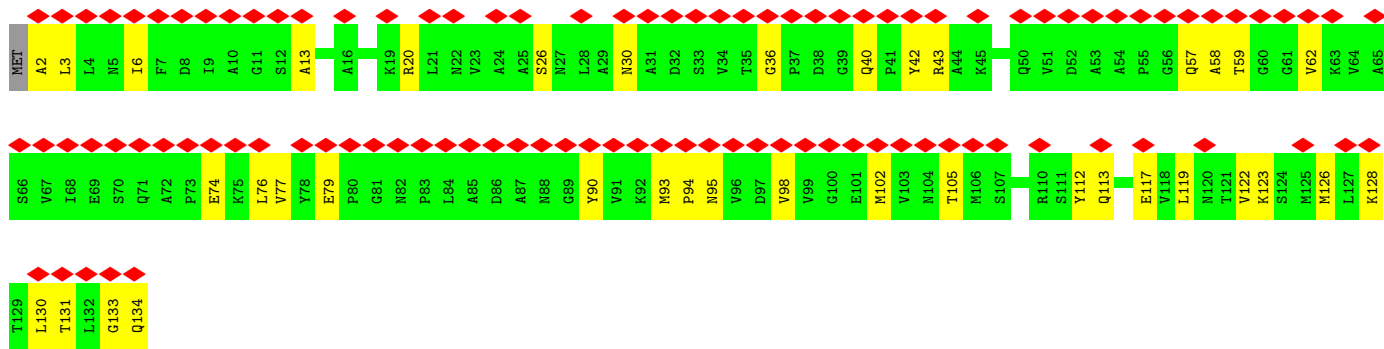
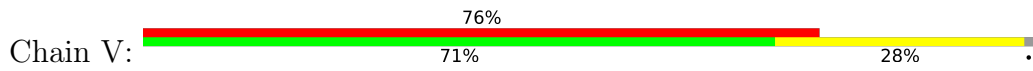




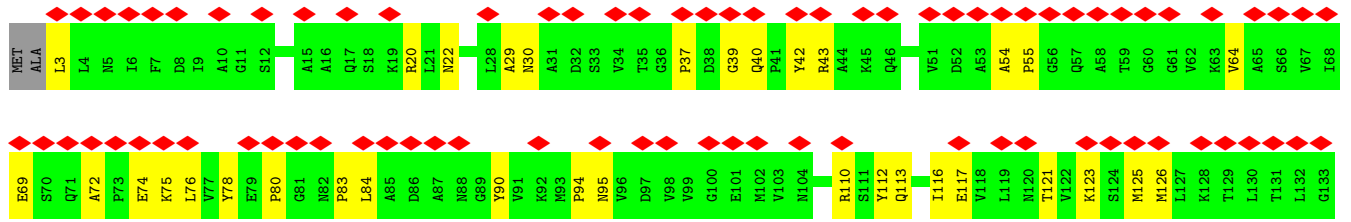
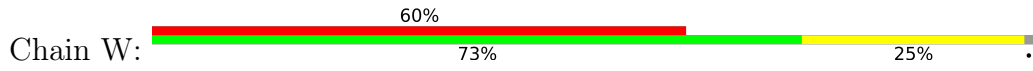
• Molecule 5: Flagellar basal body rod protein FlgB



• Molecule 6: Flagellar basal-body rod protein FlgC

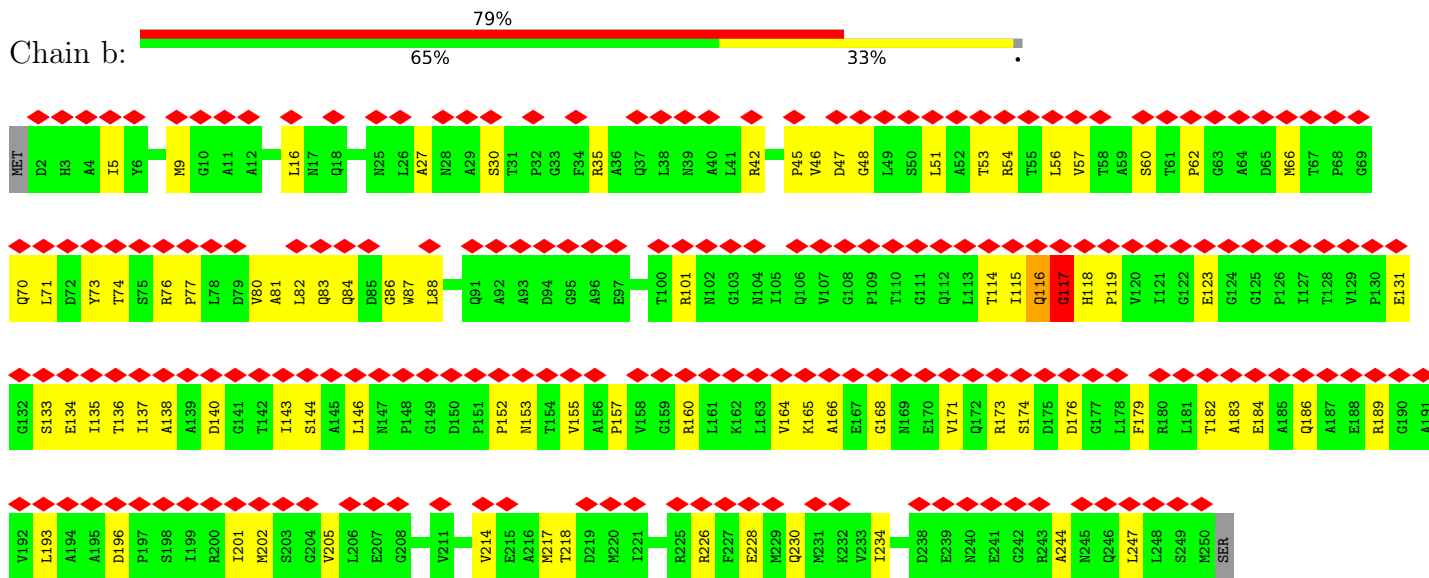


• Molecule 6: Flagellar basal-body rod protein FlgC

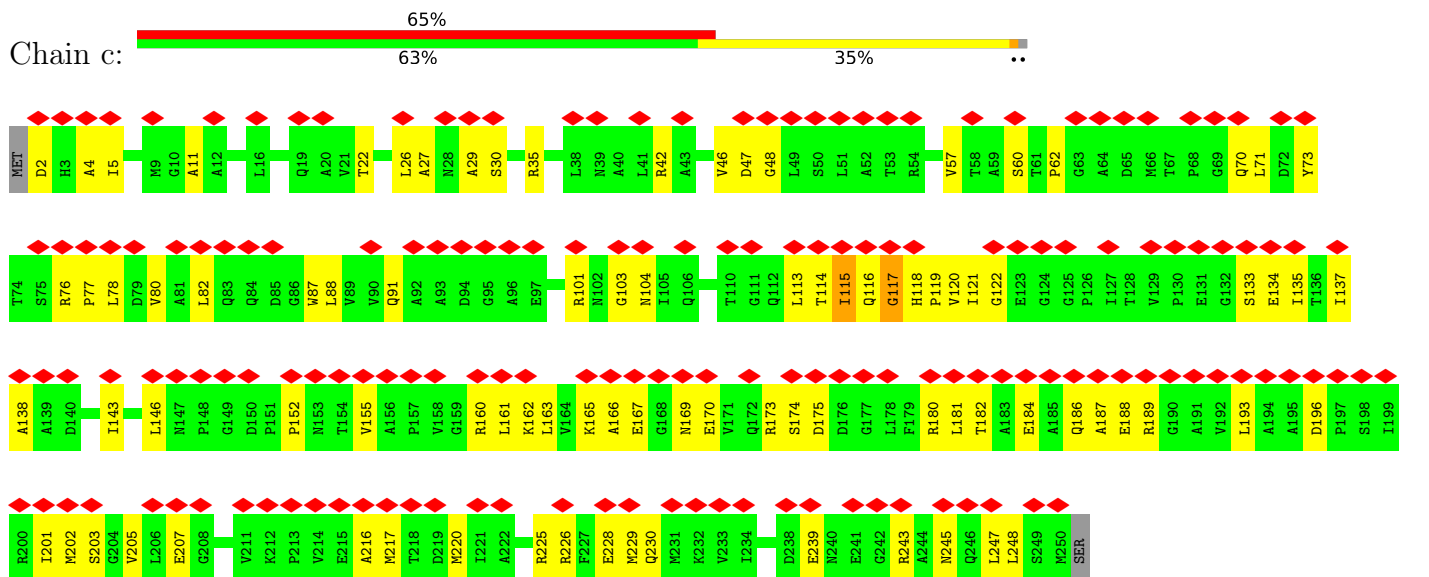




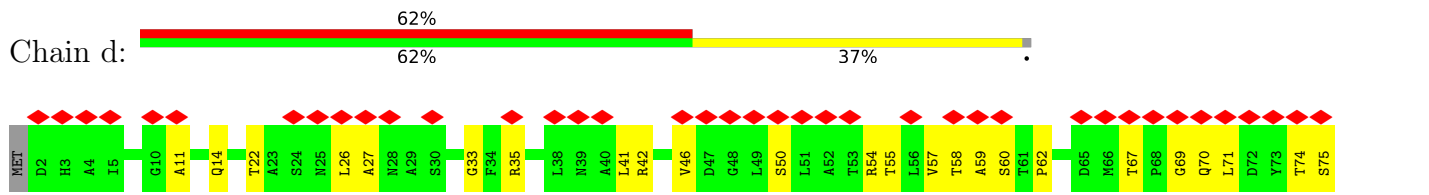
• Molecule 7: Flagellar basal-body rod protein FlgF

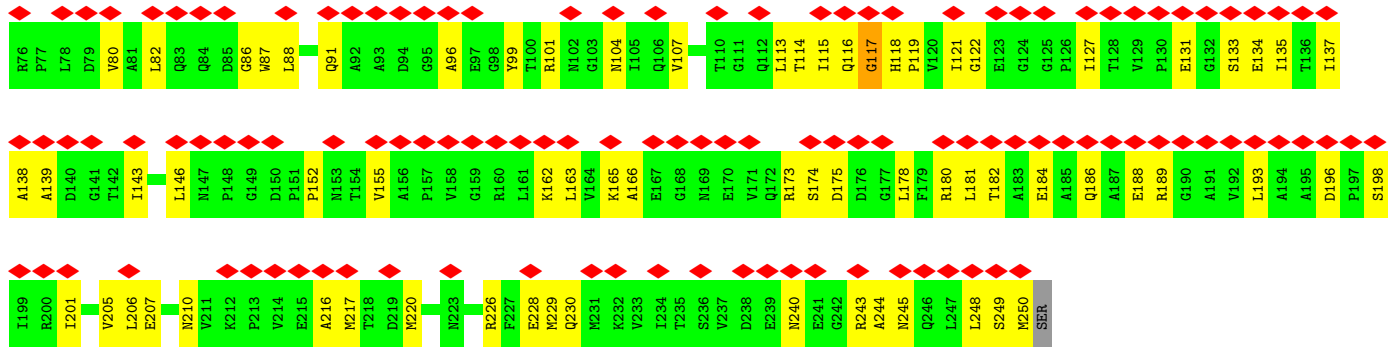


• Molecule 7: Flagellar basal-body rod protein FlgF

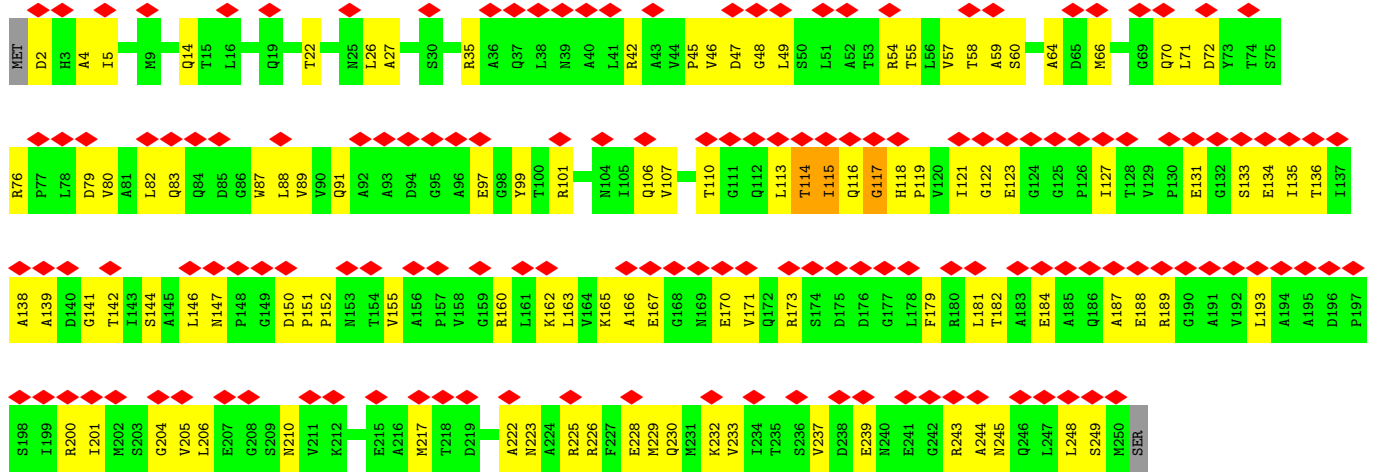


• Molecule 7: Flagellar basal-body rod protein FlgF

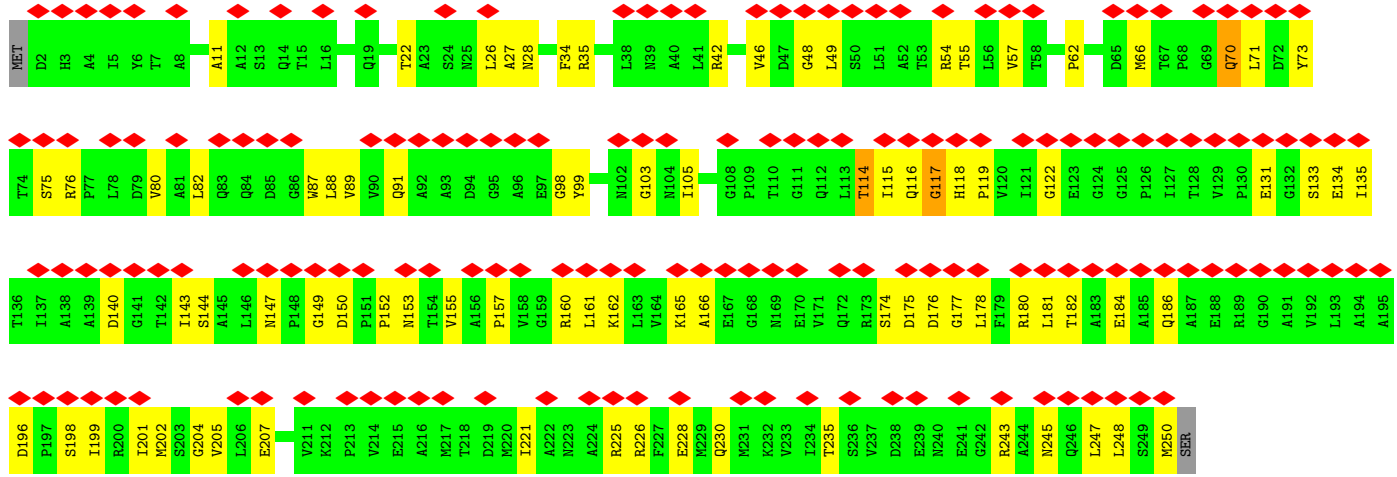




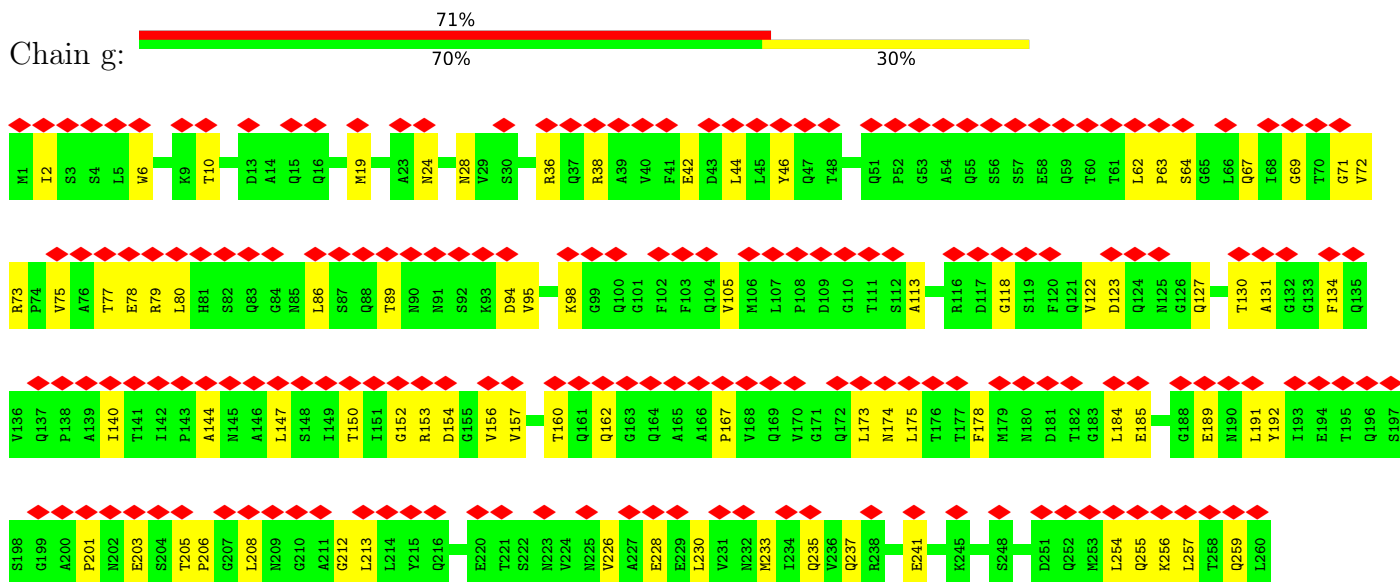
• Molecule 7: Flagellar basal-body rod protein FlgF



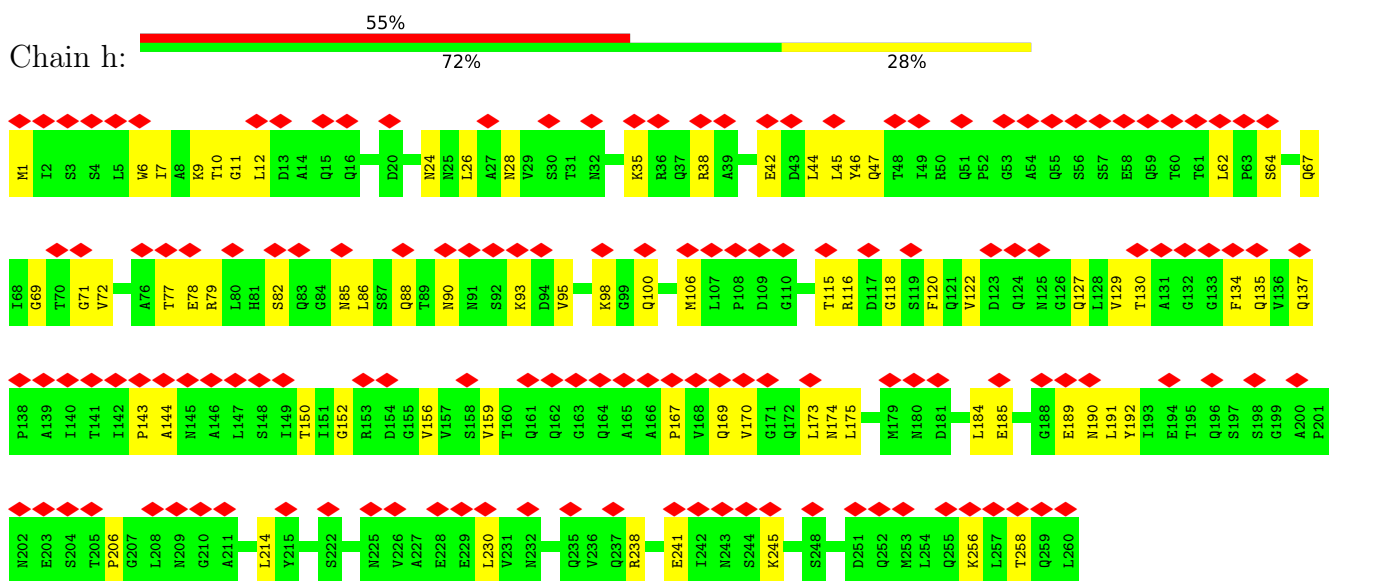
• Molecule 7: Flagellar basal-body rod protein FlgF



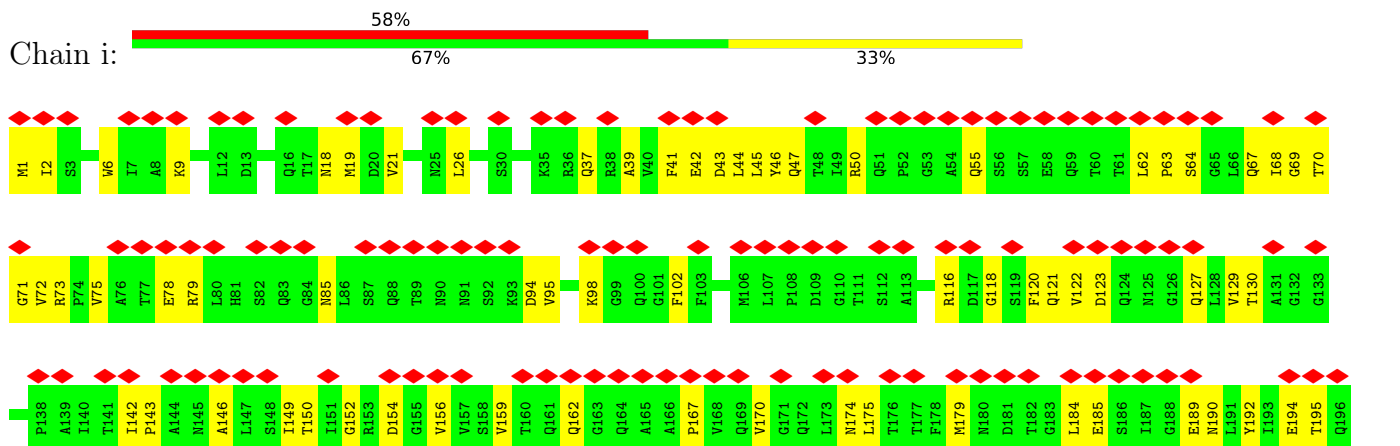
• Molecule 8: Flagellar basal-body rod protein FlgG

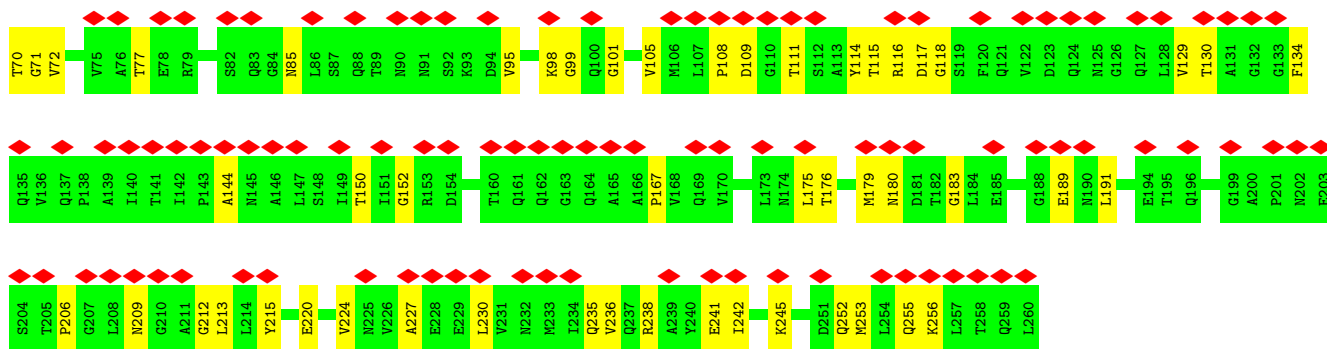


• Molecule 8: Flagellar basal-body rod protein FlgG

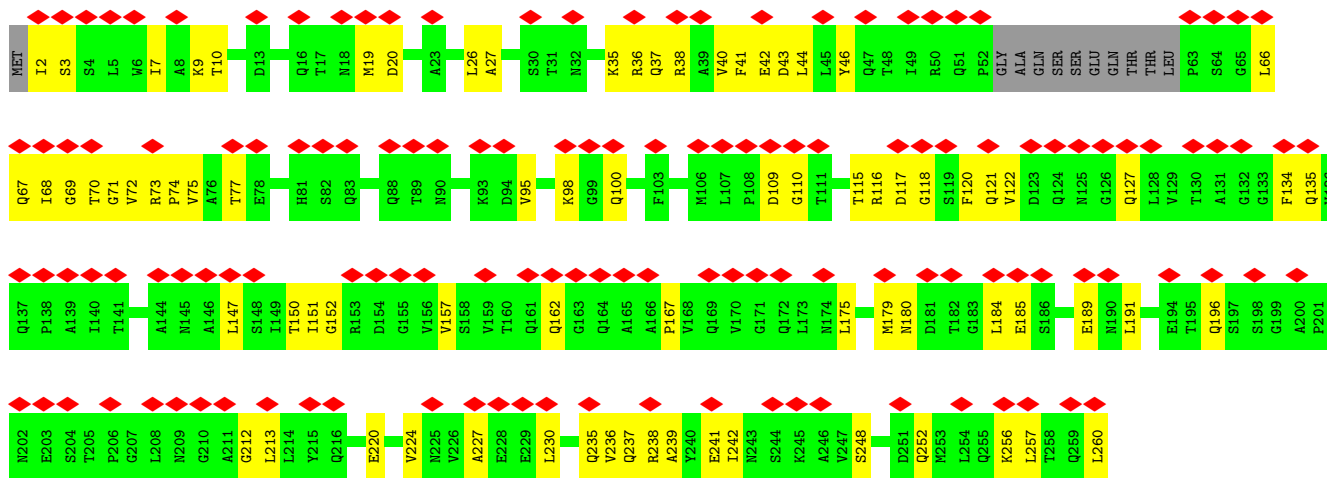


• Molecule 8: Flagellar basal-body rod protein FlgG

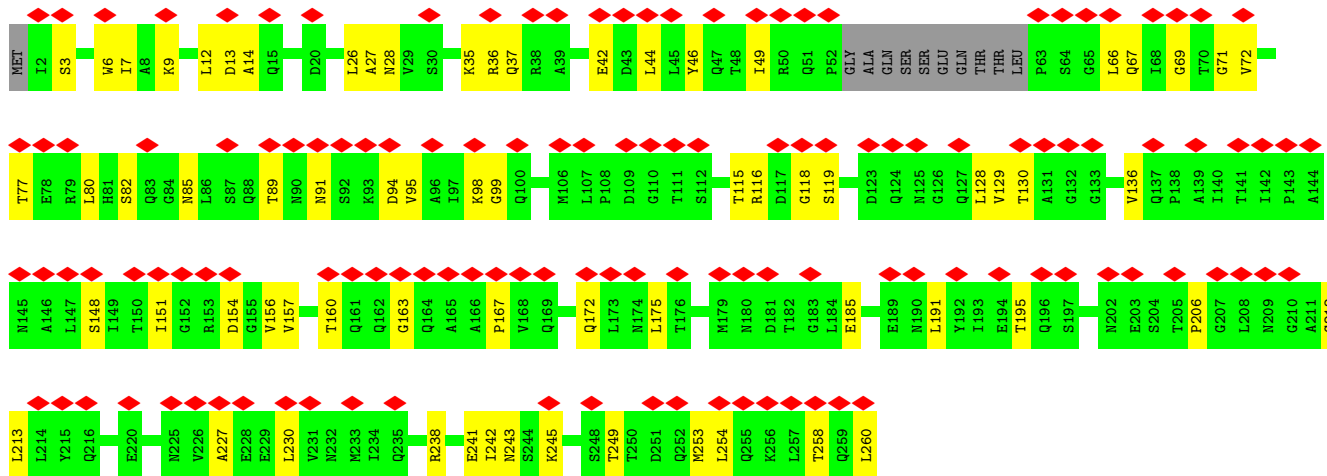




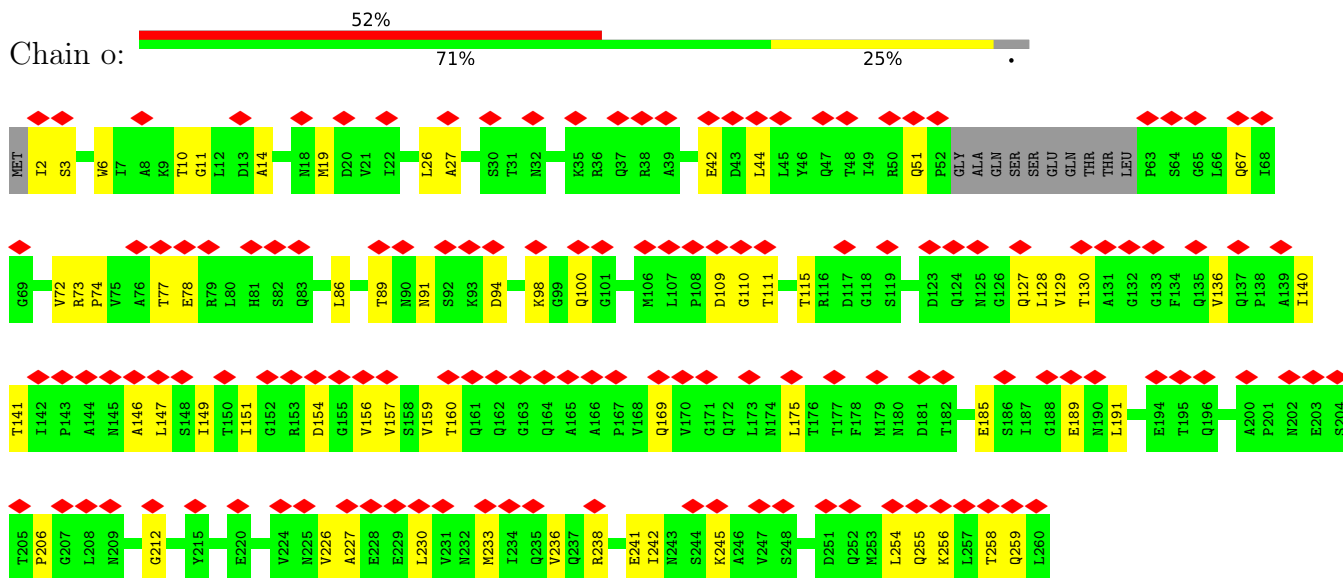
• Molecule 8: Flagellar basal-body rod protein FlgG



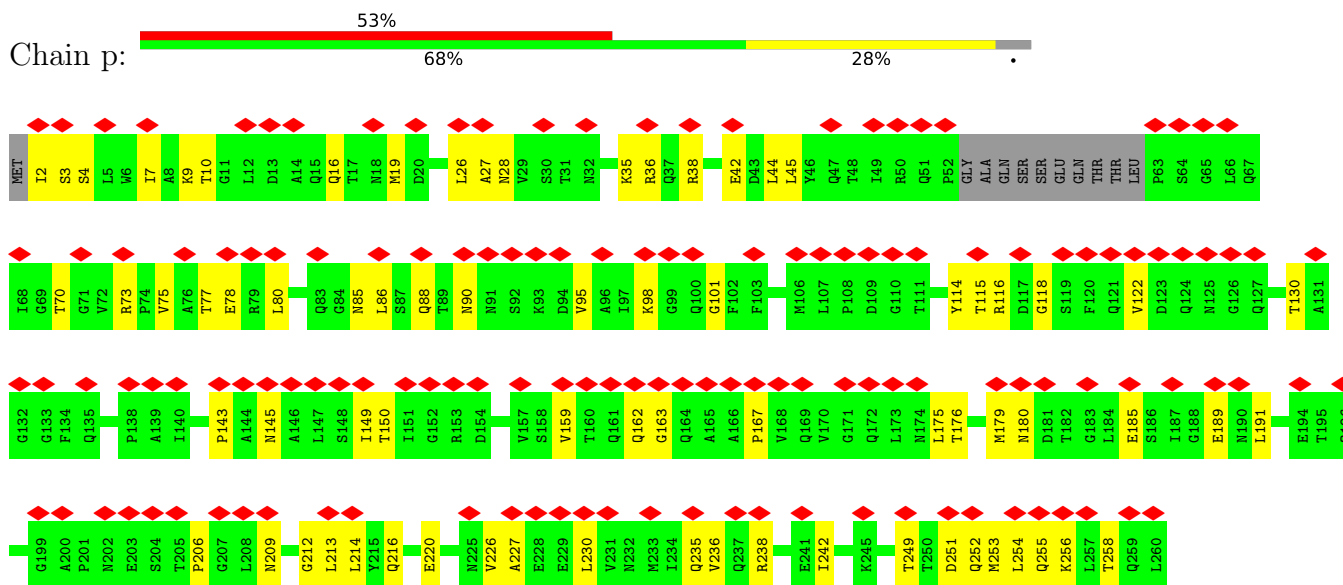
• Molecule 8: Flagellar basal-body rod protein FlgG



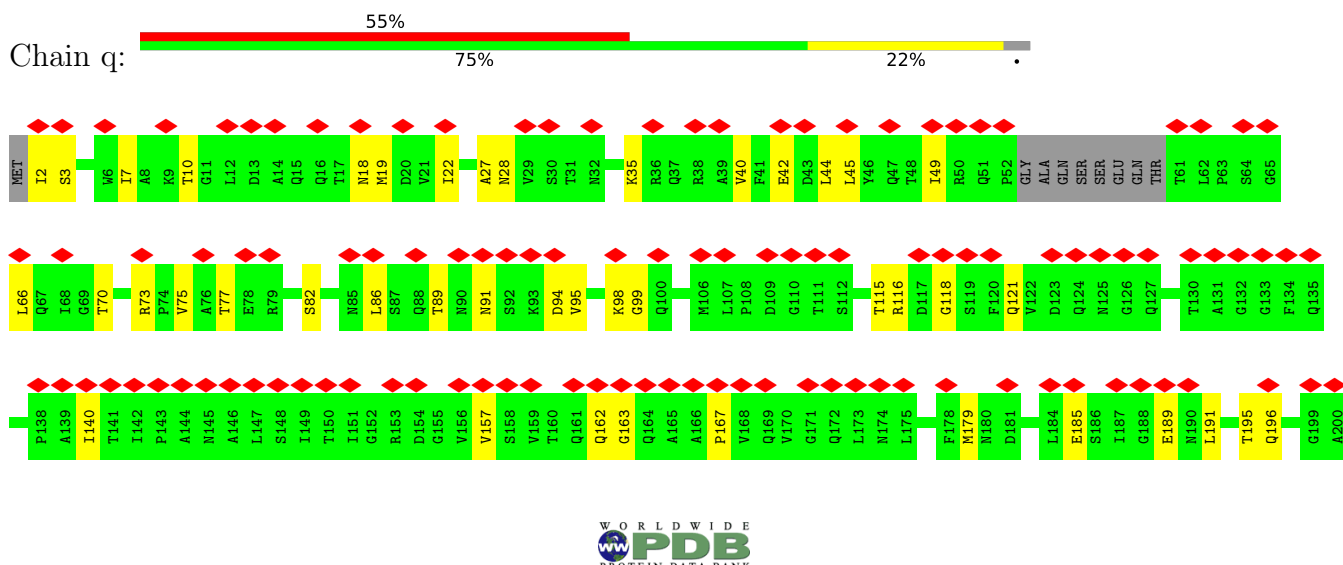
• Molecule 8: Flagellar basal-body rod protein FlgG

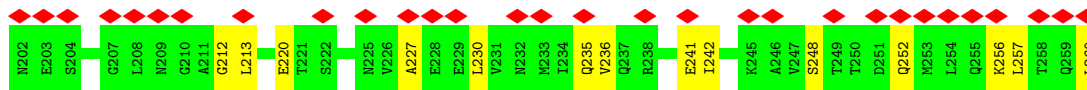


• Molecule 8: Flagellar basal-body rod protein FlgG

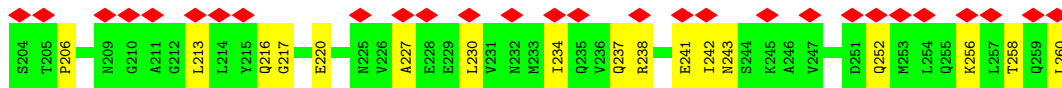
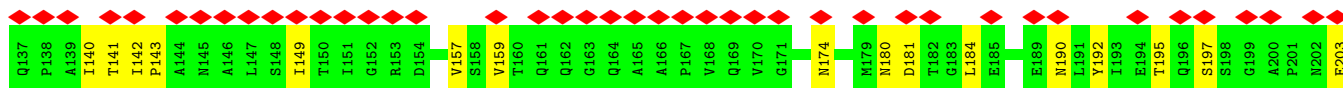
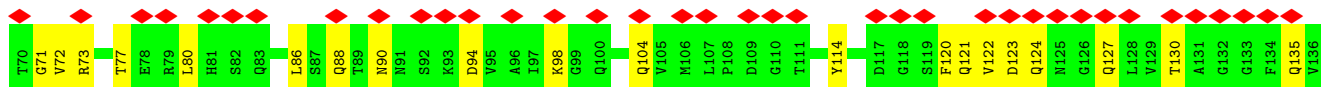
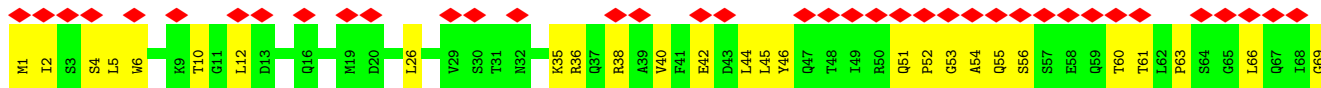


• Molecule 8: Flagellar basal-body rod protein FlgG

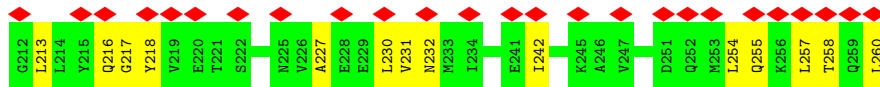
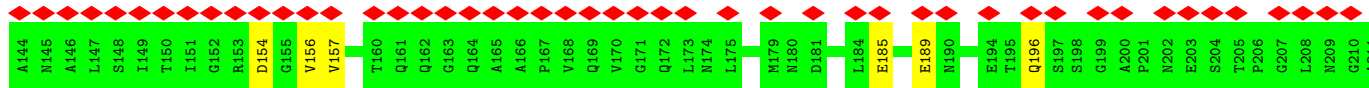
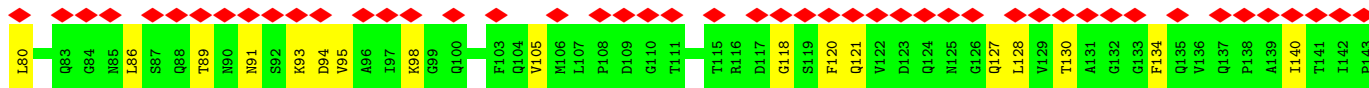
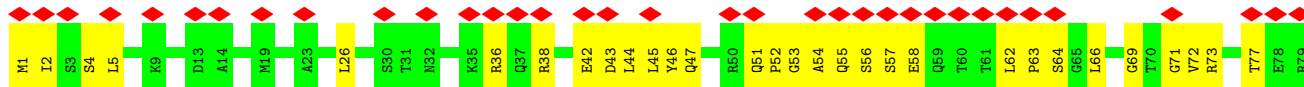
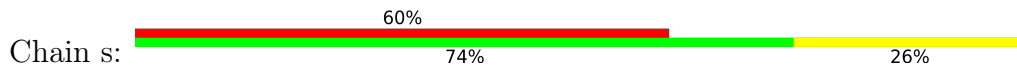




• Molecule 8: Flagellar basal-body rod protein FlgG

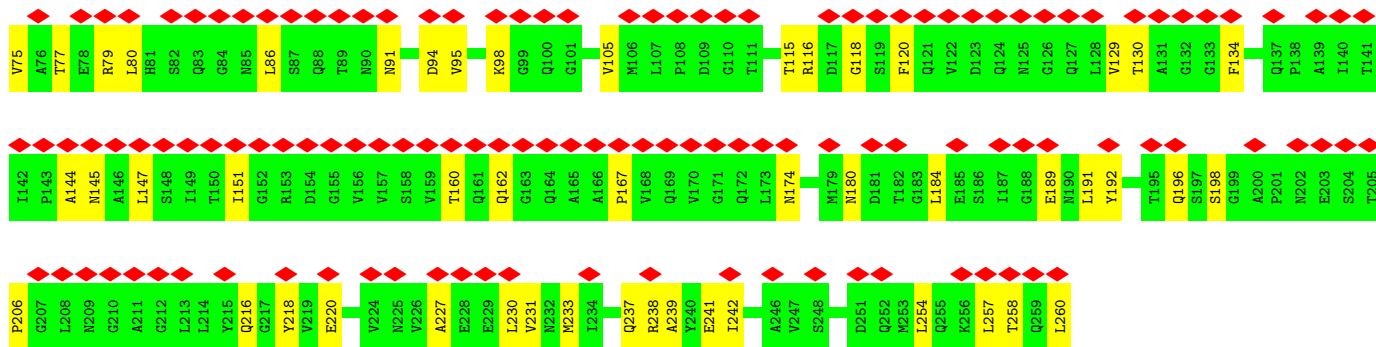


• Molecule 8: Flagellar basal-body rod protein FlgG

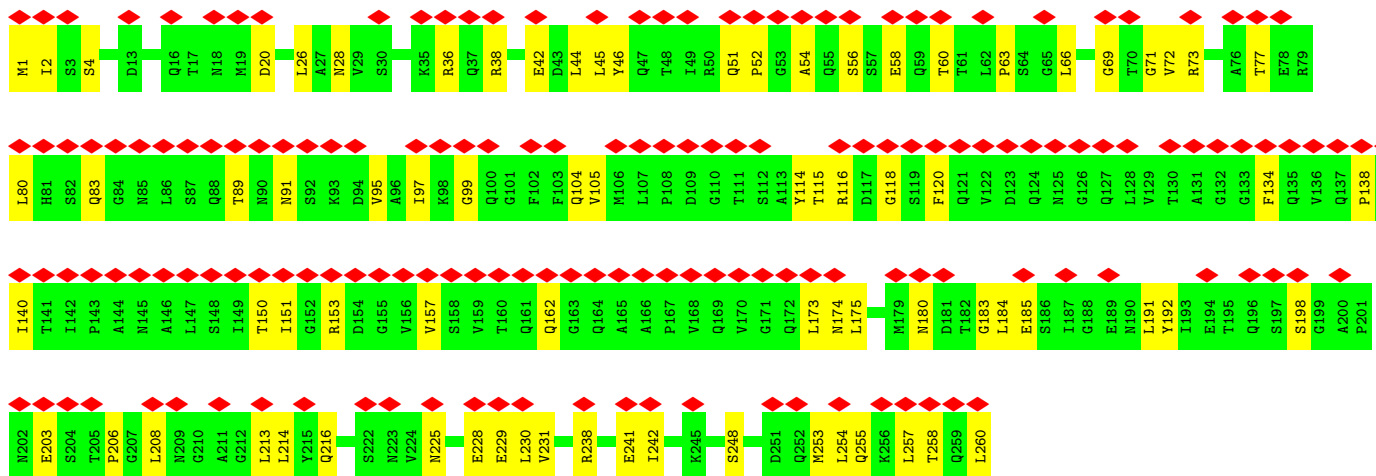


• Molecule 8: Flagellar basal-body rod protein FlgG

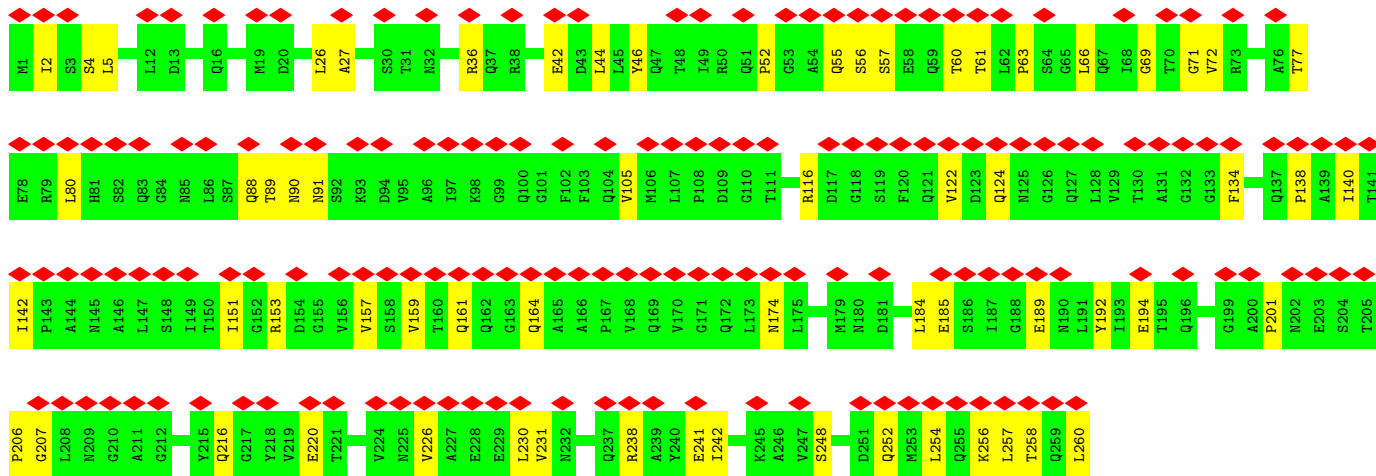
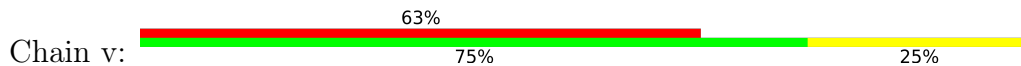




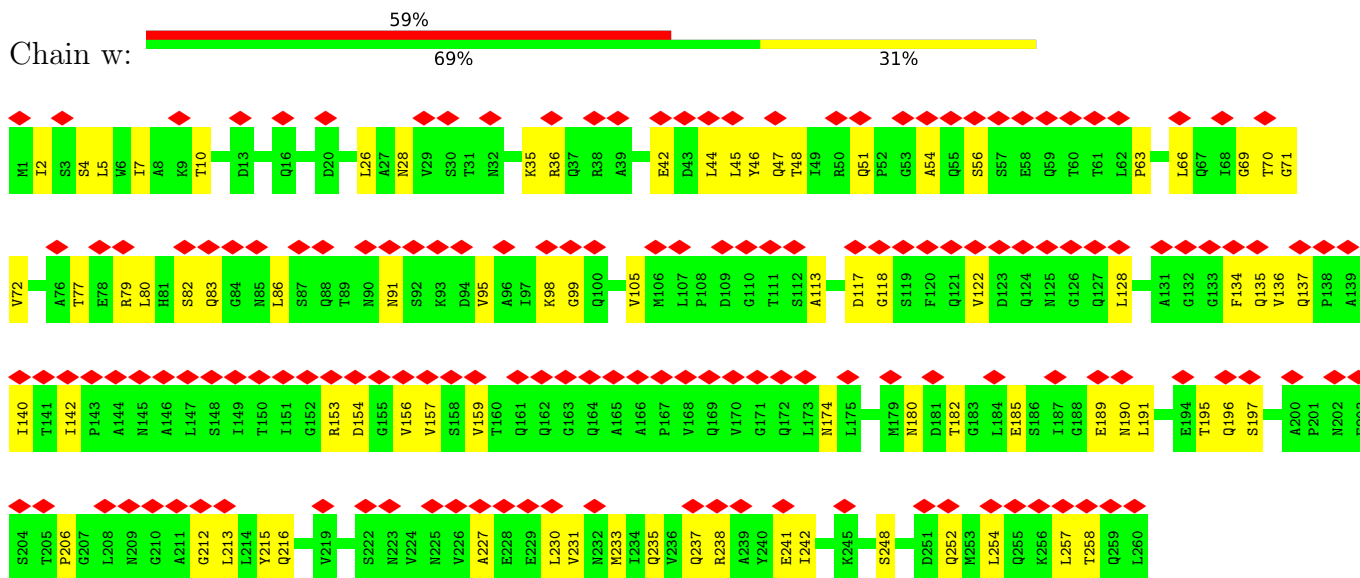
• Molecule 8: Flagellar basal-body rod protein FlgG



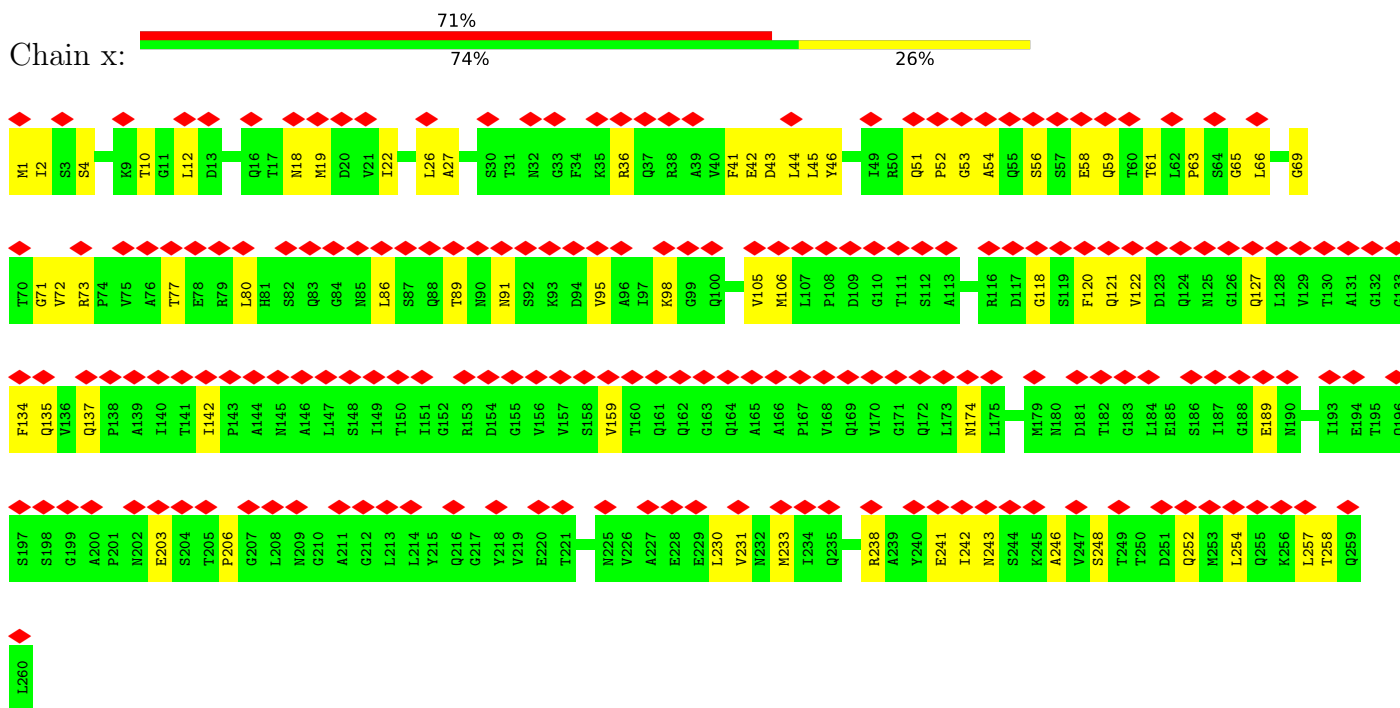
• Molecule 8: Flagellar basal-body rod protein FlgG



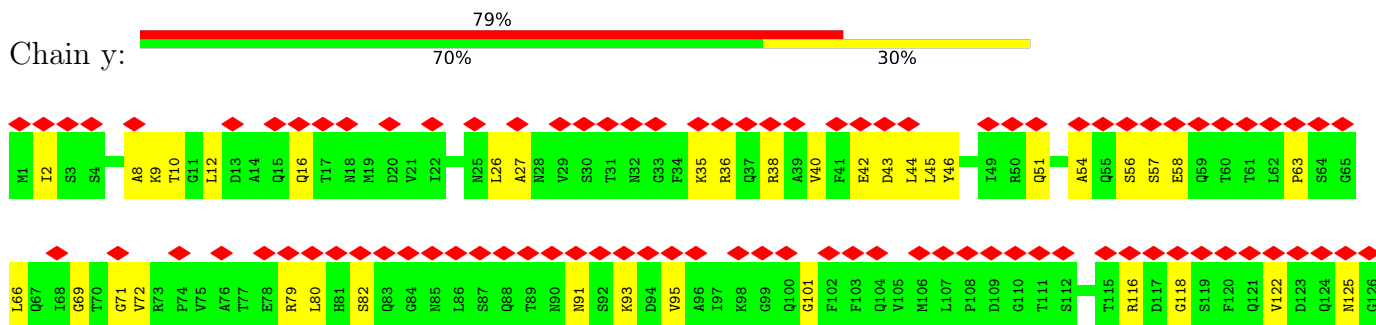
• Molecule 8: Flagellar basal-body rod protein FlgG

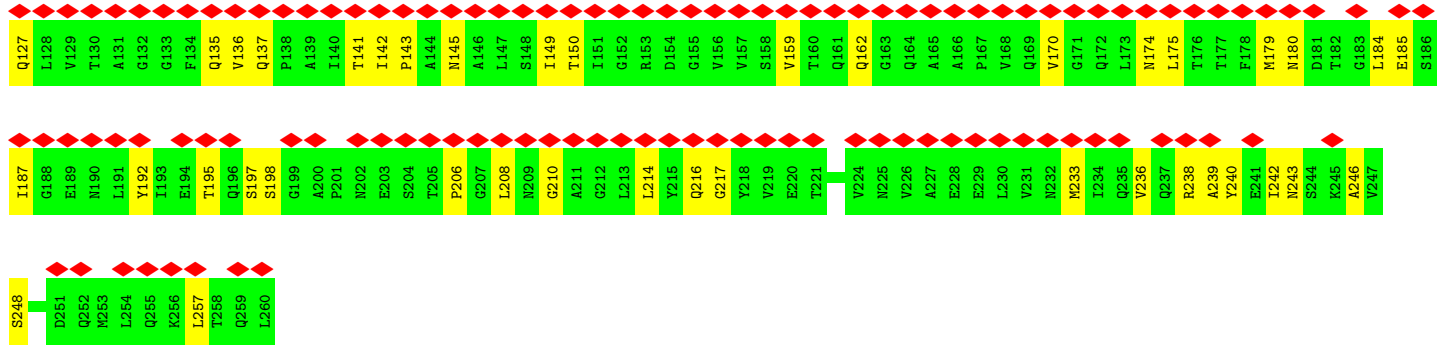


• Molecule 8: Flagellar basal-body rod protein FlgG

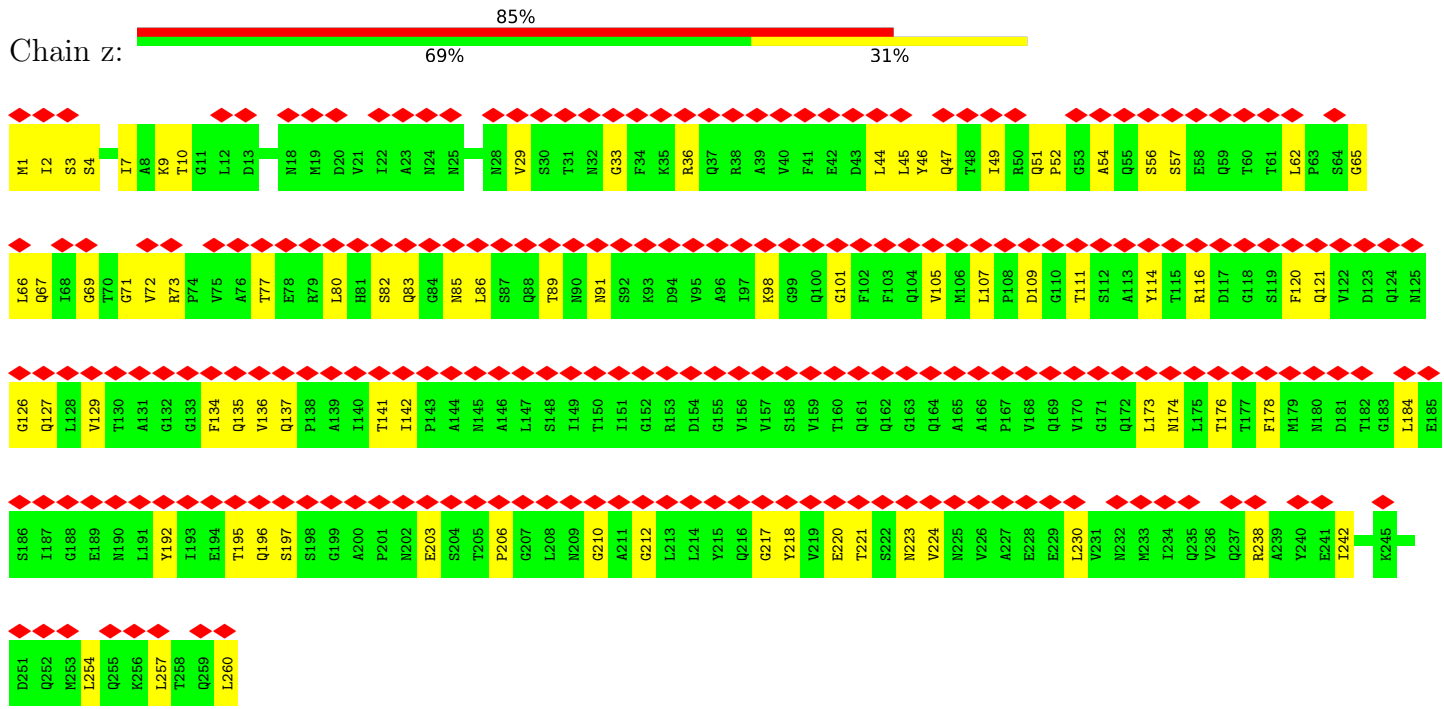


• Molecule 8: Flagellar basal-body rod protein FlgG

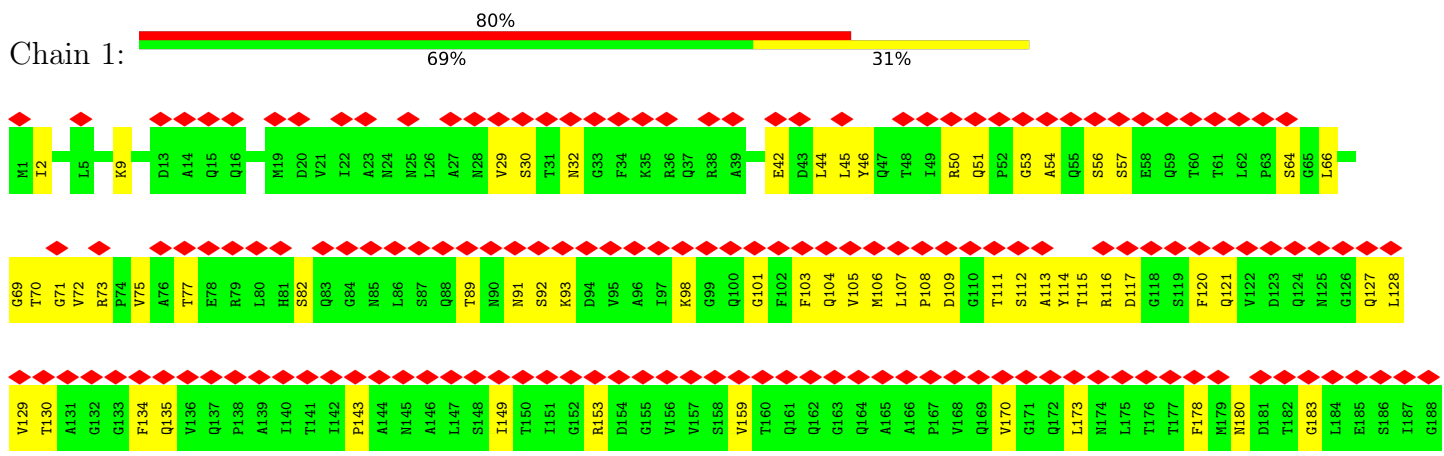


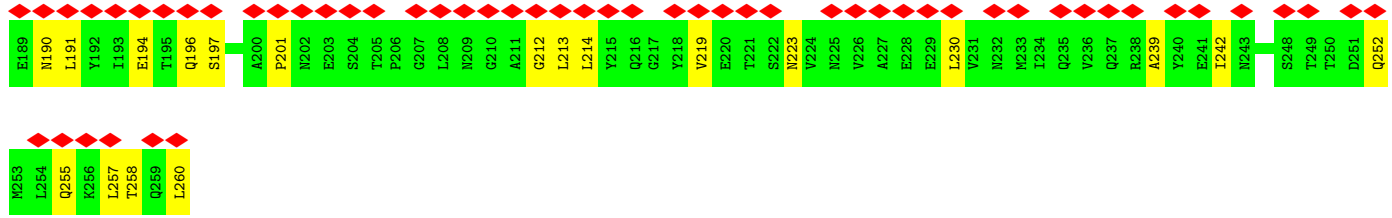


• Molecule 8: Flagellar basal-body rod protein FlgG

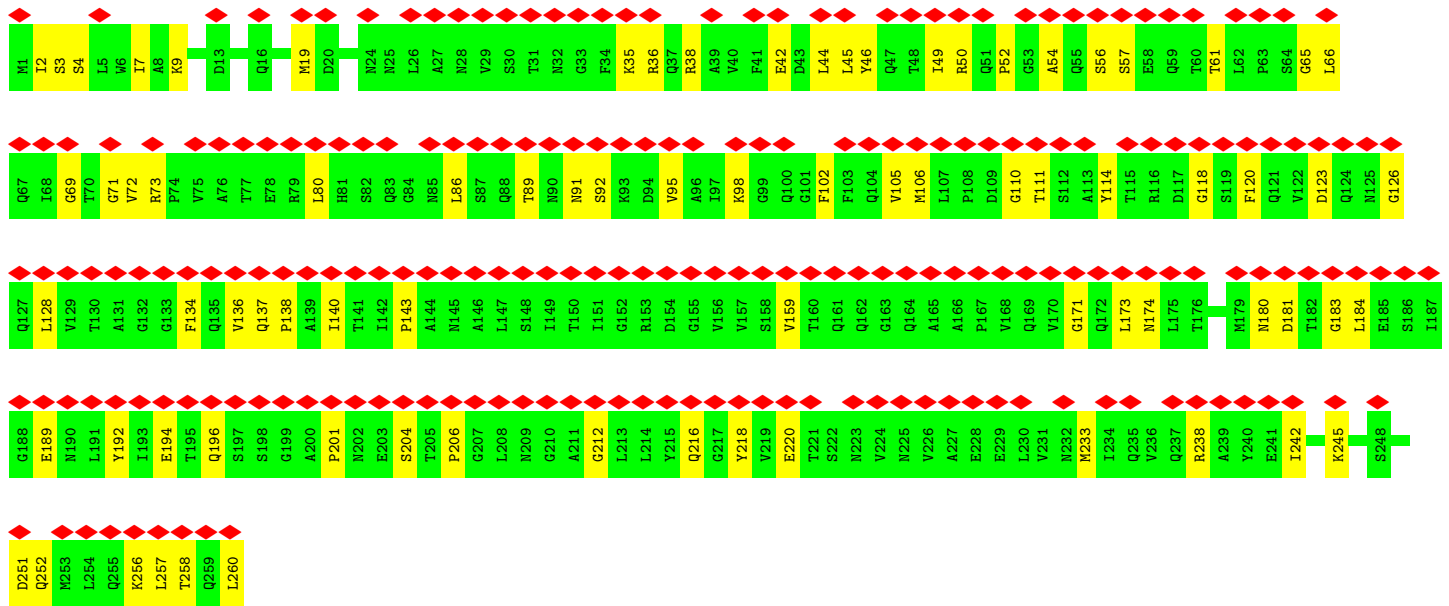
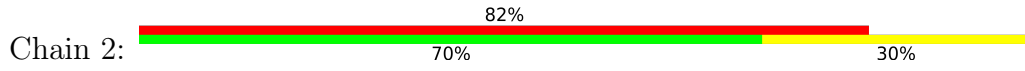


• Molecule 8: Flagellar basal-body rod protein FlgG

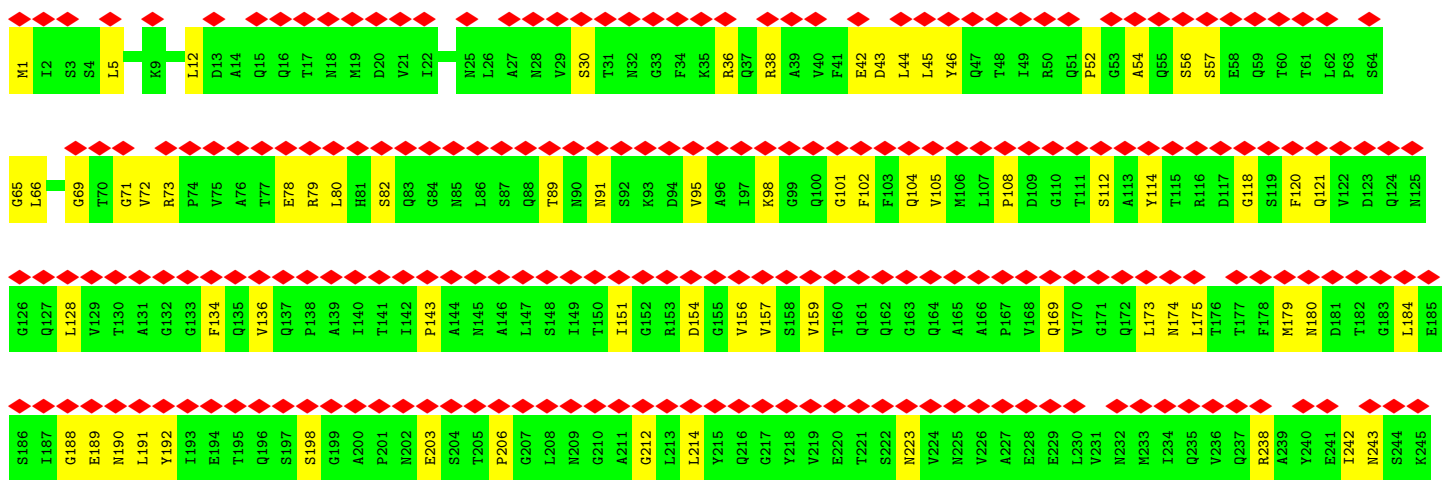
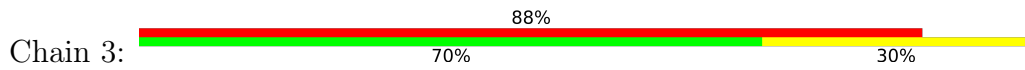


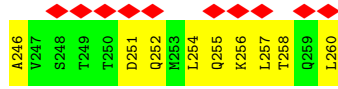


• Molecule 8: Flagellar basal-body rod protein FlgG

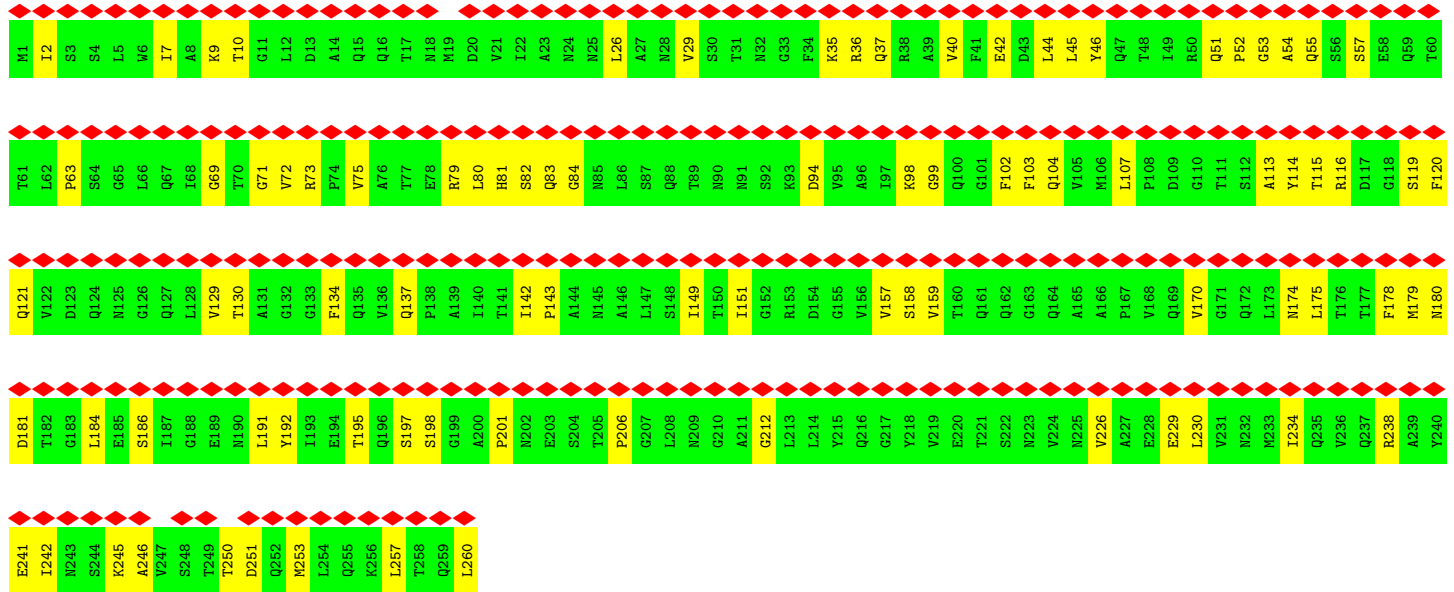


• Molecule 8: Flagellar basal-body rod protein FlgG





• 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/1662	0.63	2/2263 (0.1%)
1	B	0.35	0/1662	0.62	0/2263
1	C	0.36	0/1662	0.64	1/2263 (0.0%)
1	D	0.36	0/1662	0.62	2/2263 (0.1%)
1	E	1.11	1/1662 (0.1%)	0.64	2/2263 (0.1%)
2	F	0.31	0/2035	0.60	2/2777 (0.1%)
3	G	0.28	0/681	0.60	0/930
3	H	0.29	0/681	0.56	0/930
3	I	0.31	0/681	0.51	0/930
3	J	1.86	6/681 (0.9%)	0.56	0/930
4	K	0.31	0/296	0.53	0/395
4	L	0.28	0/567	0.39	0/761
4	M	0.31	0/567	0.45	0/761
4	N	0.30	0/567	0.42	0/761
4	O	0.29	0/567	0.44	0/761
4	P	0.30	0/567	0.43	0/761
5	Q	0.34	0/1035	0.52	0/1399
5	R	0.34	0/941	0.49	0/1269
5	S	0.38	0/951	0.52	0/1281
5	T	0.37	0/842	0.48	0/1132
5	U	0.33	0/934	0.46	0/1259
6	V	0.40	0/981	0.66	0/1334
6	W	0.37	0/976	0.56	0/1327
6	X	0.40	0/976	0.56	0/1327
6	Y	0.38	0/976	0.54	0/1327
6	Z	0.37	0/976	0.54	0/1327
6	a	0.36	0/976	0.56	0/1327
7	b	0.35	0/1836	0.57	0/2502
7	c	0.39	0/1836	0.58	0/2502
7	d	0.40	0/1836	0.58	0/2502
7	e	0.38	0/1836	0.55	0/2502
7	f	0.36	0/1836	0.54	0/2502
8	1	0.31	0/1973	0.48	0/2682
8	2	0.30	0/1973	0.47	0/2682

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	3	0.29	0/1973	0.47	0/2682
8	4	0.23	0/1973	0.47	0/2682
8	g	0.34	0/1973	0.46	0/2682
8	h	0.37	0/1973	0.46	0/2682
8	i	0.37	0/1973	0.47	0/2682
8	j	0.38	0/1973	0.47	0/2682
8	k	0.37	0/1973	0.47	0/2682
8	l	0.37	0/1894	0.45	0/2573
8	m	0.39	0/1894	0.47	0/2573
8	n	0.37	0/1894	0.45	0/2573
8	o	0.38	0/1894	0.46	0/2573
8	p	0.38	0/1894	0.47	0/2573
8	q	0.37	0/1909	0.45	0/2595
8	r	0.37	0/1973	0.50	0/2682
8	s	0.37	0/1973	0.53	0/2682
8	t	0.37	0/1973	0.52	1/2682 (0.0%)
8	u	0.36	0/1973	0.50	0/2682
8	v	0.38	0/1973	0.49	0/2682
8	w	0.37	0/1973	0.50	0/2682
8	x	0.33	0/1973	0.47	0/2682
8	y	0.30	0/1973	0.45	0/2682
8	z	0.29	0/1973	0.44	0/2682
All	All	0.42	7/82837 (0.0%)	0.52	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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	MET	SD-CE	43.51	2.88	1.79
3	J	51	PHE	CD1-CE1	21.93	2.04	1.38
3	J	51	PHE	CE2-CZ	21.65	2.03	1.38
3	J	51	PHE	CD2-CE2	21.09	2.02	1.38
3	J	51	PHE	CE1-CZ	20.92	2.01	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	205	MET	CG-SD-CE	14.35	132.46	100.90
8	t	167	PRO	CA-N-CD	-8.81	99.66	112.00
1	C	41	SER	N-CA-C	-6.43	100.19	109.31
1	A	224	MET	CB-CG-SD	-6.32	93.75	112.70
1	D	113	TYR	CA-C-N	-5.64	113.57	119.83

There are no chirality outliers.

5 of 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

5.2 Too-close contacts [i](#)

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	1623	0	1715	92	0
1	B	1623	0	1715	92	0
1	C	1623	0	1715	101	0
1	D	1623	0	1715	101	0
1	E	1623	0	1715	120	0
2	F	1986	0	2099	108	0
3	G	670	0	739	32	0
3	H	670	0	739	27	0
3	I	670	0	739	33	0
3	J	670	0	739	58	0
4	K	296	0	308	18	0
4	L	563	0	571	11	0
4	M	563	0	571	13	0
4	N	563	0	571	24	0
4	O	563	0	571	20	0
4	P	563	0	571	39	0
5	Q	1023	0	1020	43	0
5	R	932	0	934	30	0
5	S	942	0	945	37	0
5	T	835	0	838	34	0
5	U	925	0	925	40	0
6	V	969	0	979	43	0
6	W	964	0	976	32	0
6	X	964	0	976	47	0
6	Y	964	0	976	35	0
6	Z	964	0	976	44	0
6	a	964	0	976	41	0
7	b	1812	0	1800	80	0
7	c	1812	0	1800	89	0
7	d	1812	0	1800	98	0
7	e	1812	0	1800	91	0
7	f	1812	0	1800	82	0
8	1	1949	0	1926	72	0
8	2	1949	0	1926	70	0
8	3	1949	0	1926	75	0
8	4	1949	0	1926	82	0
8	g	1949	0	1926	71	0
8	h	1949	0	1926	83	0
8	i	1949	0	1926	86	0
8	j	1949	0	1926	76	0
8	k	1949	0	1926	64	0
8	l	1871	0	1849	61	0
8	m	1871	0	1849	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	n	1871	0	1849	66	0
8	o	1871	0	1849	64	0
8	p	1871	0	1849	74	0
8	q	1886	0	1866	53	0
8	r	1949	0	1926	76	0
8	s	1949	0	1926	69	0
8	t	1949	0	1926	72	0
8	u	1949	0	1926	81	0
8	v	1949	0	1926	53	0
8	w	1949	0	1926	95	0
8	x	1949	0	1926	65	0
8	y	1949	0	1926	75	0
8	z	1949	0	1926	66	0
All	All	81721	0	82093	2639	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 16.

The worst 5 of 2639 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)
1:B:96:LEU:HD22	1:B:236:MET:CE	1.21	1.65
1:E:96:LEU:HD22	1:E:236:MET:CE	1.29	1.53
3:J:51:PHE:CE1	3:J:51:PHE:CZ	2.01	1.48
3:J:51:PHE:CZ	3:J:51:PHE:CE2	2.03	1.47
3:J:51:PHE:CE1	3:J:51:PHE:CD1	2.04	1.45

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	207/245 (84%)	182 (88%)	23 (11%)	2 (1%)	12	45
1	B	207/245 (84%)	183 (88%)	22 (11%)	2 (1%)	12	45
1	C	207/245 (84%)	177 (86%)	29 (14%)	1 (0%)	24	59
1	D	207/245 (84%)	181 (87%)	25 (12%)	1 (0%)	24	59
1	E	207/245 (84%)	183 (88%)	22 (11%)	2 (1%)	12	45
2	F	254/264 (96%)	223 (88%)	30 (12%)	1 (0%)	30	62
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%)	16	50
6	W	130/134 (97%)	108 (83%)	22 (17%)	0	100	100
6	X	130/134 (97%)	107 (82%)	22 (17%)	1 (1%)	16	50
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%)	30	62
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	49	79

5 of 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

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%)	78	84
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%)	109 (100%)	0	100	100
5	R	100/113 (88%)	100 (100%)	0	100	100
5	S	100/113 (88%)	100 (100%)	0	100	100
5	T	89/113 (79%)	89 (100%)	0	100	100
5	U	99/113 (88%)	98 (99%)	1 (1%)	68	80
6	V	104/105 (99%)	103 (99%)	1 (1%)	68	80
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%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	215 (100%)	0	100	100
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%)	81	85
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%)	208 (100%)	0	100	100
8	r	215/215 (100%)	215 (100%)	0	100	100
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
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%)	215 (100%)	0	100	100
8	z	215/215 (100%)	215 (100%)	0	100	100
All	All	8918/9331 (96%)	8914 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	236	MET
5	U	117	GLN
6	V	59	THR
8	n	172	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
8	t	67	GLN
8	z	252	GLN
8	v	24	ASN
8	w	172	GLN
8	3	67	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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

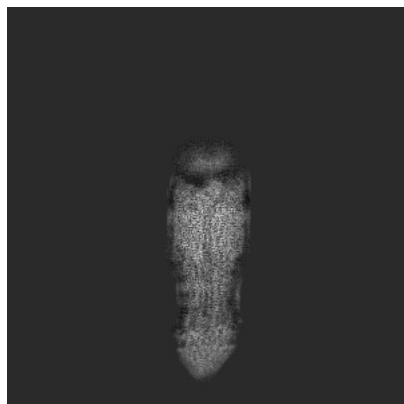
6 Map visualisation [i](#)

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.

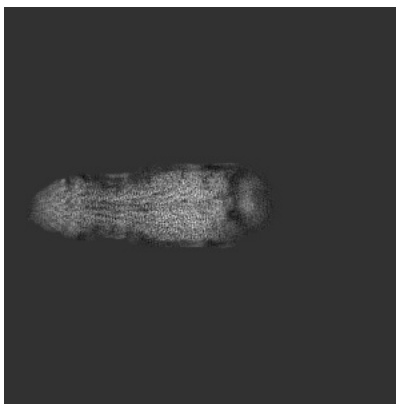
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

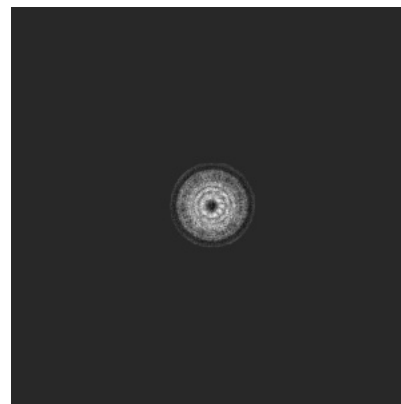
6.1.1 Primary map



X

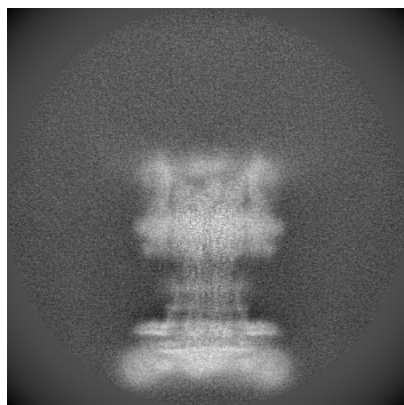


Y

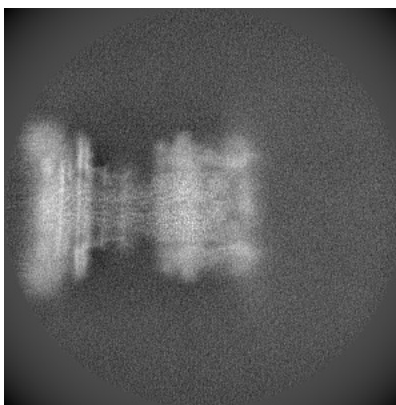


Z

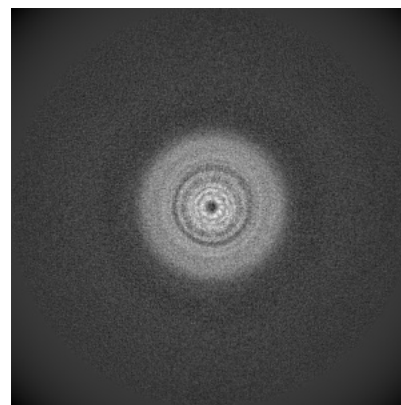
6.1.2 Raw map



X



Y

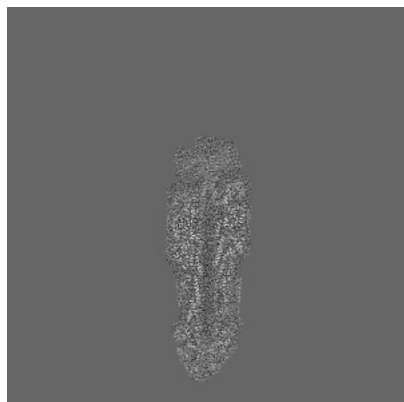


Z

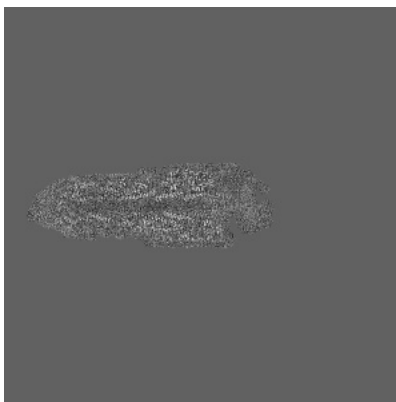
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

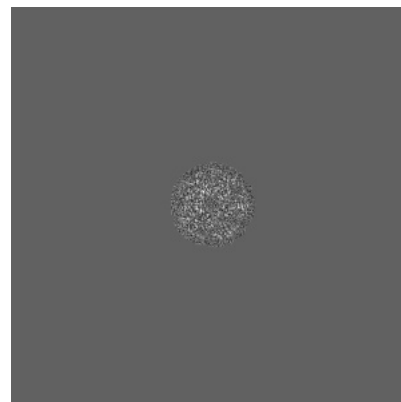
6.2.1 Primary map



X Index: 384

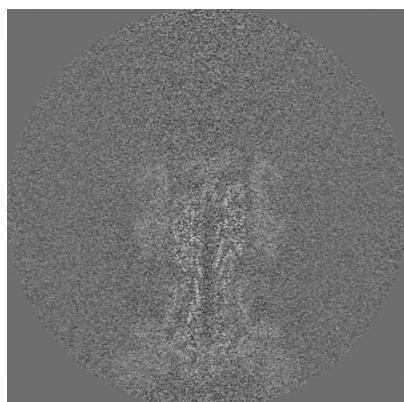


Y Index: 384

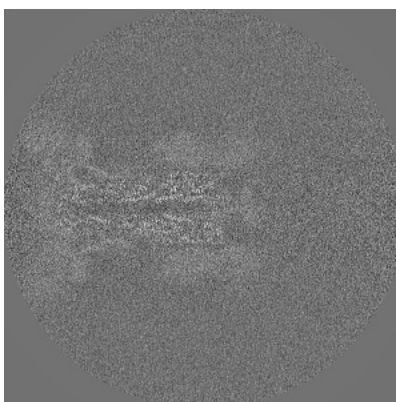


Z Index: 384

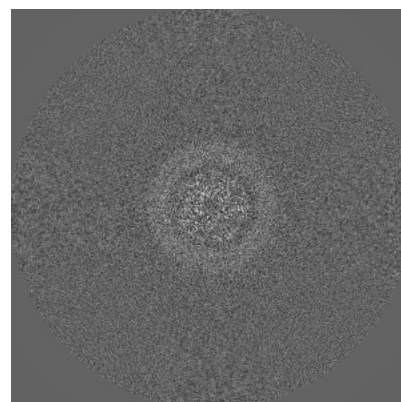
6.2.2 Raw map



X Index: 384



Y Index: 384

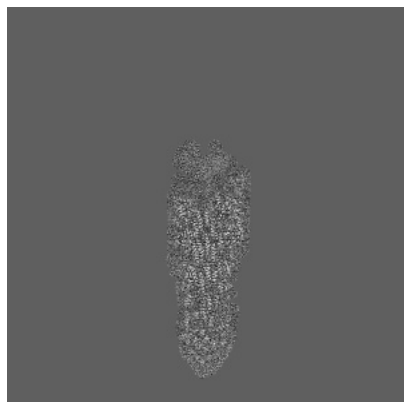


Z Index: 384

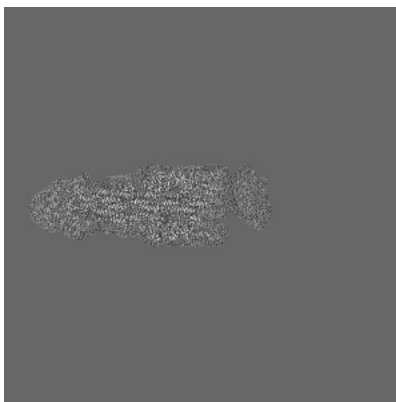
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

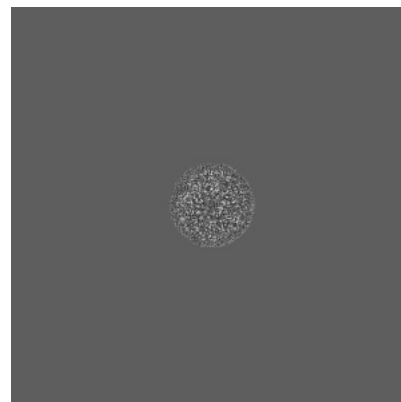
6.3.1 Primary map



X Index: 404

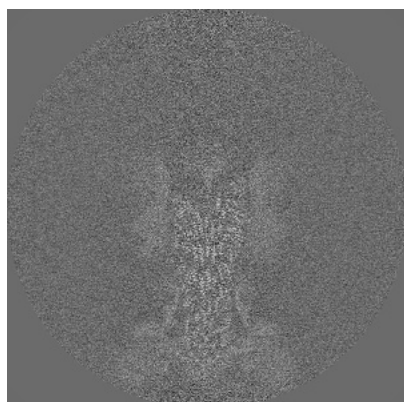


Y Index: 366

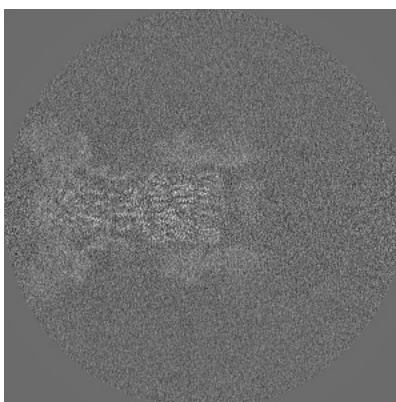


Z Index: 355

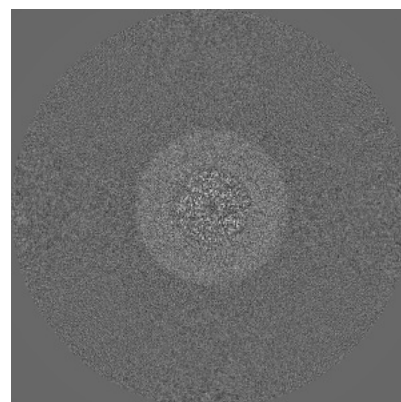
6.3.2 Raw map



X Index: 403



Y Index: 371

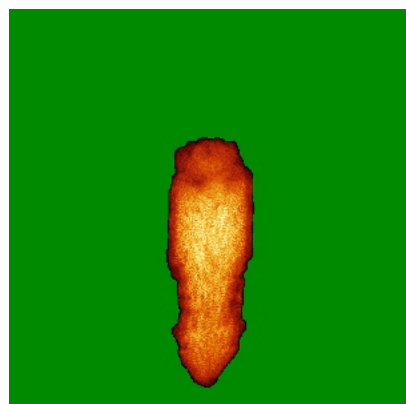


Z Index: 354

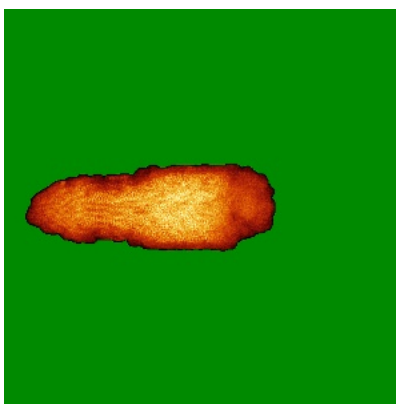
The images above show the largest variance slices of the map in three orthogonal directions.

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

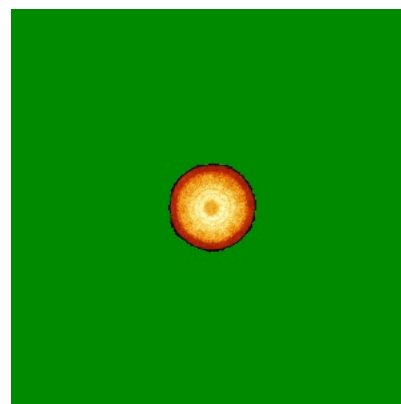
6.4.1 Primary map



X

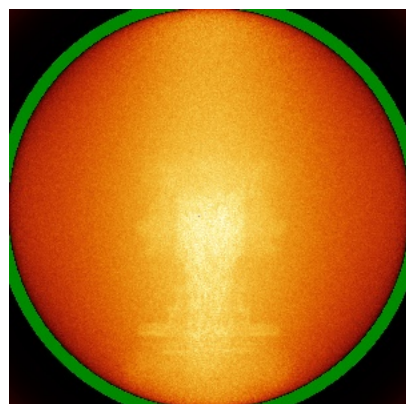


Y

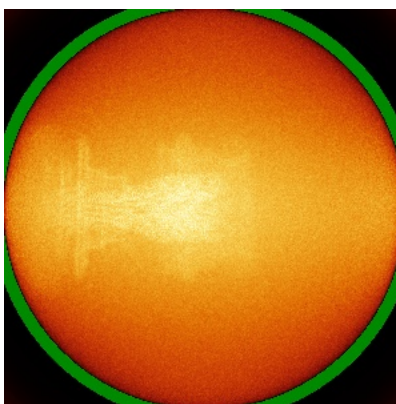


Z

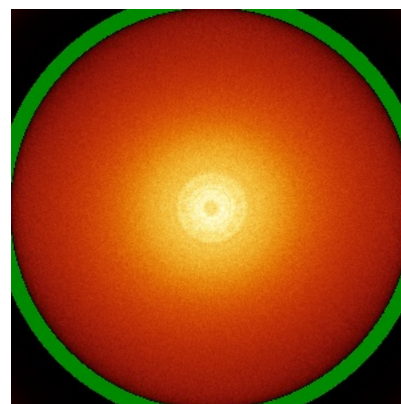
6.4.2 Raw map



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 0.02. 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.

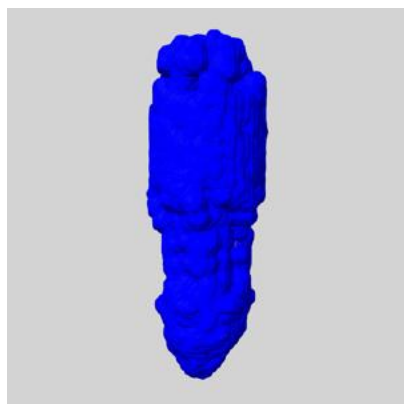
6.6 Mask visualisation [i](#)

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

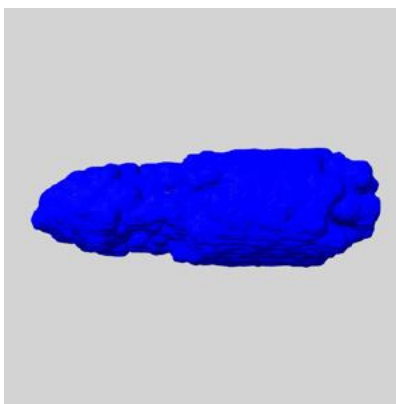
A mask typically either:

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

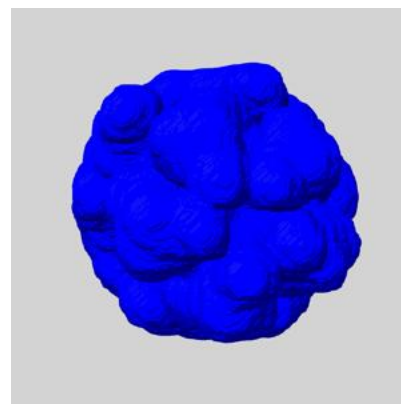
6.6.1 emd_12192_msk_1.map [i](#)



X



Y

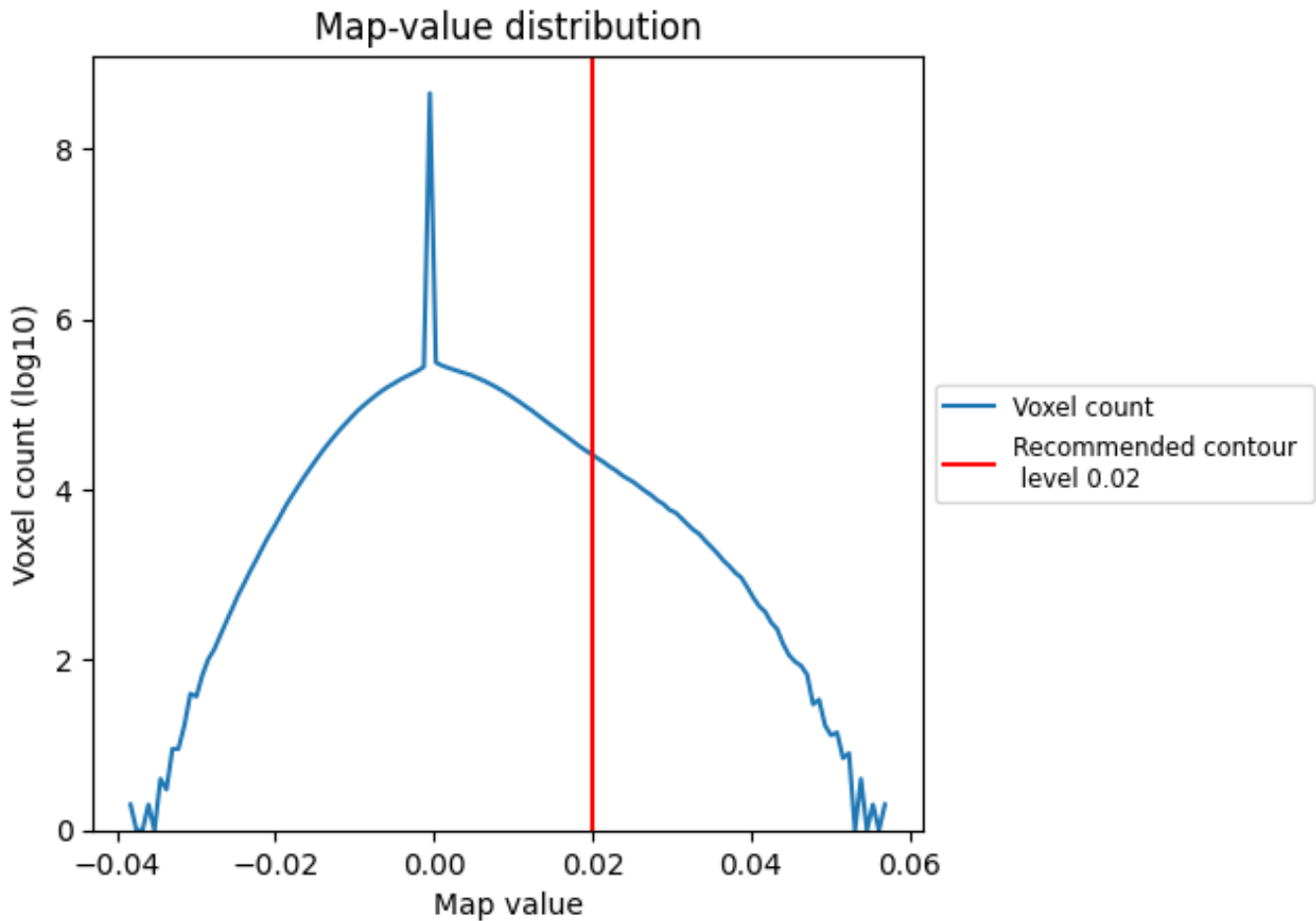


Z

7 Map analysis [i](#)

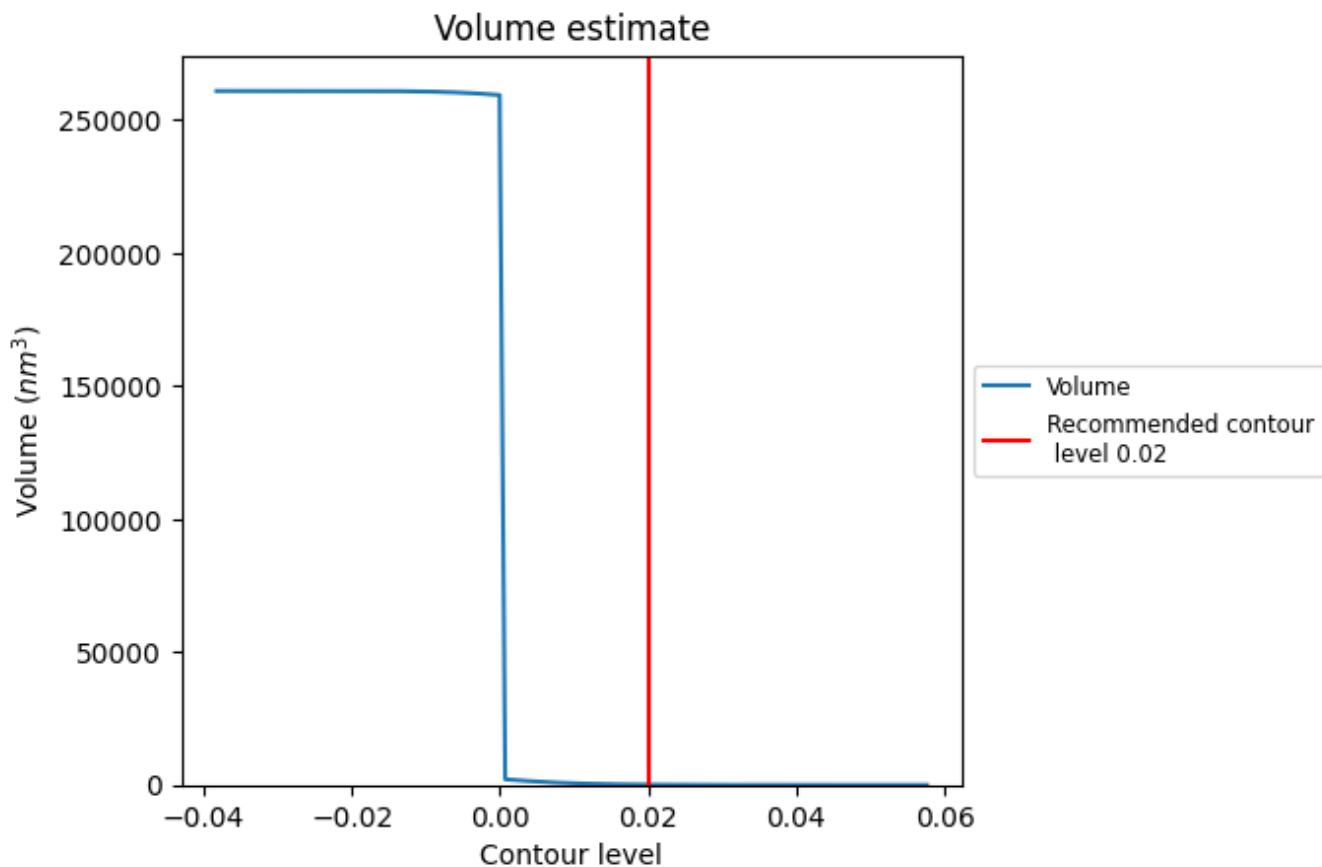
This section contains the results of statistical analysis of the map.

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.

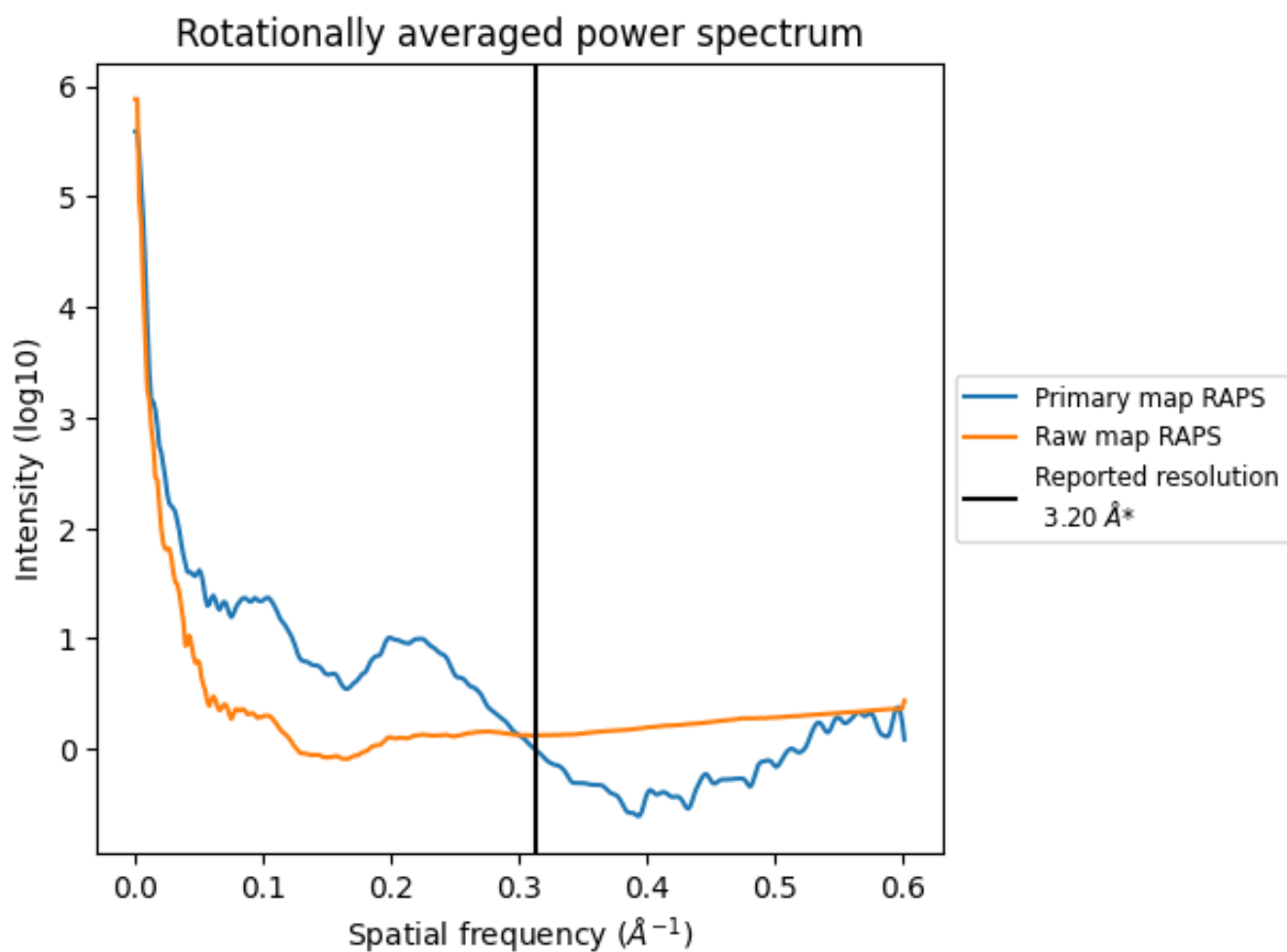
7.2 Volume estimate [i](#)



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](#)

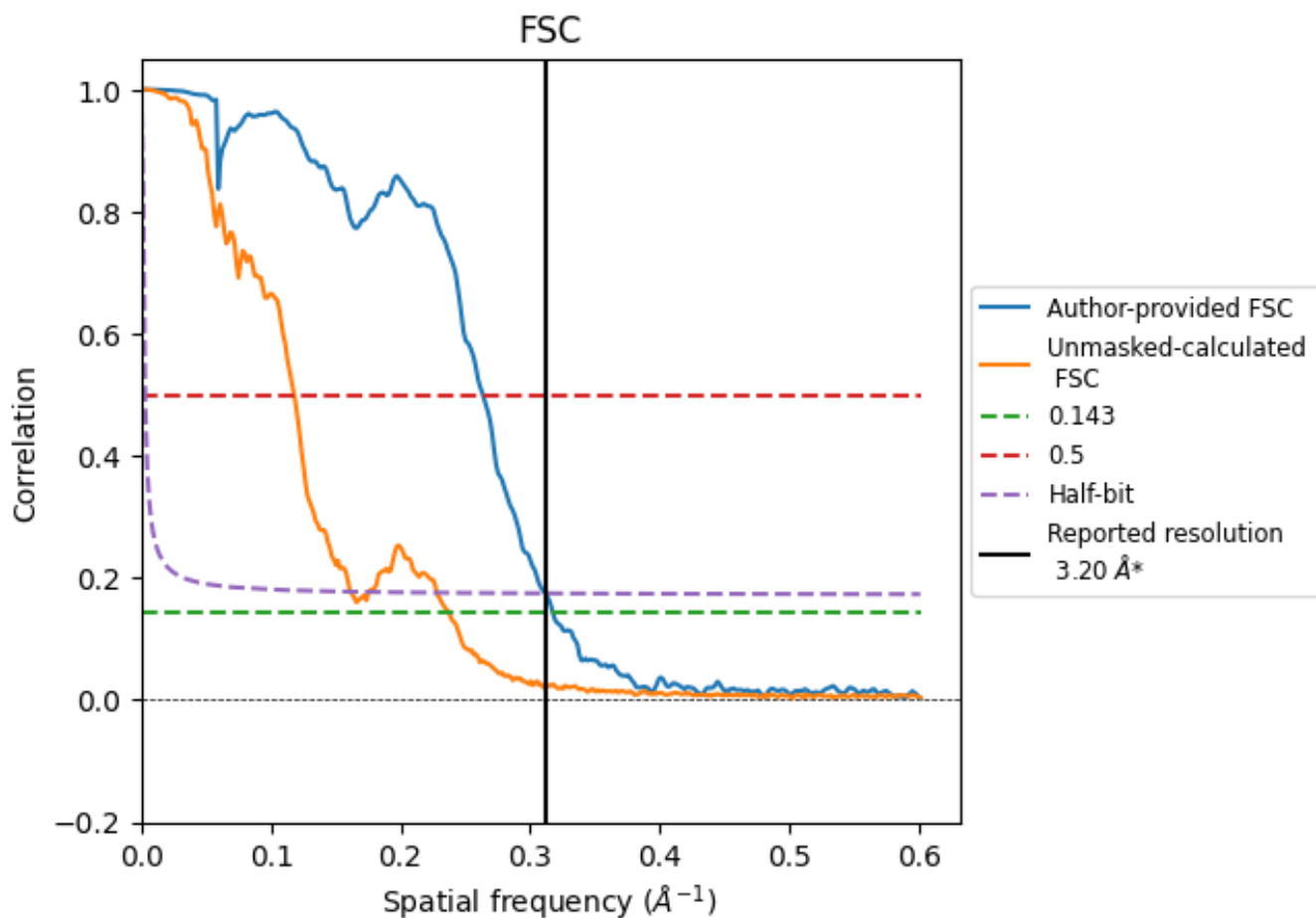


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 Å⁻¹

8.2 Resolution estimates [i](#)

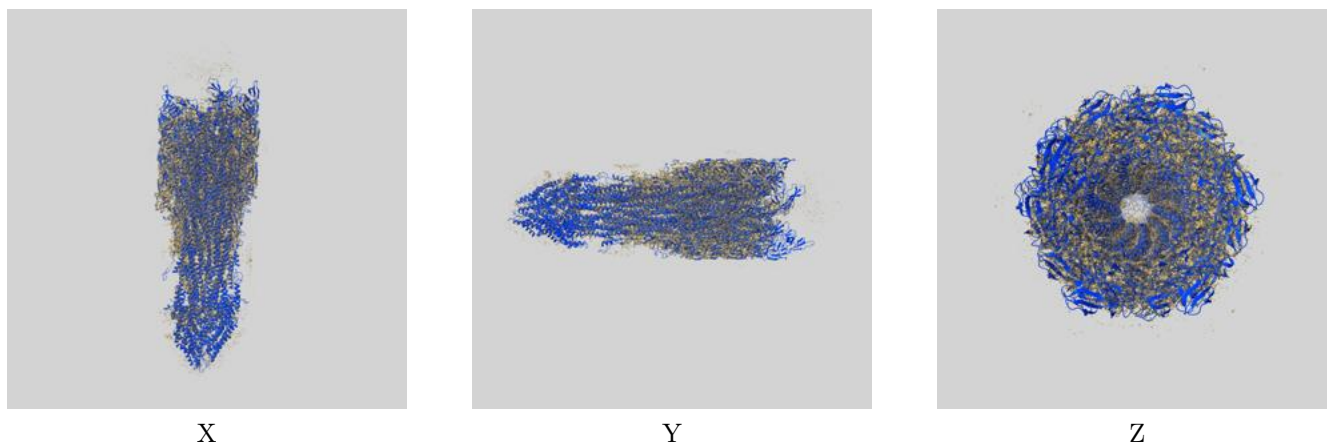
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.80	3.21
Unmasked-calculated*	4.22	8.47	6.20

*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](#)

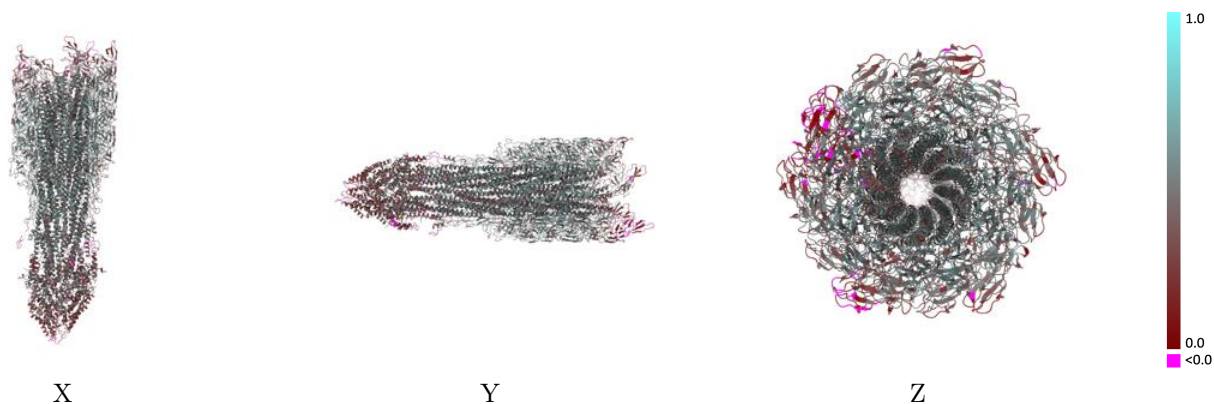
This section contains information regarding the fit between EMDB map EMD-12192 and PDB model 7BIN. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



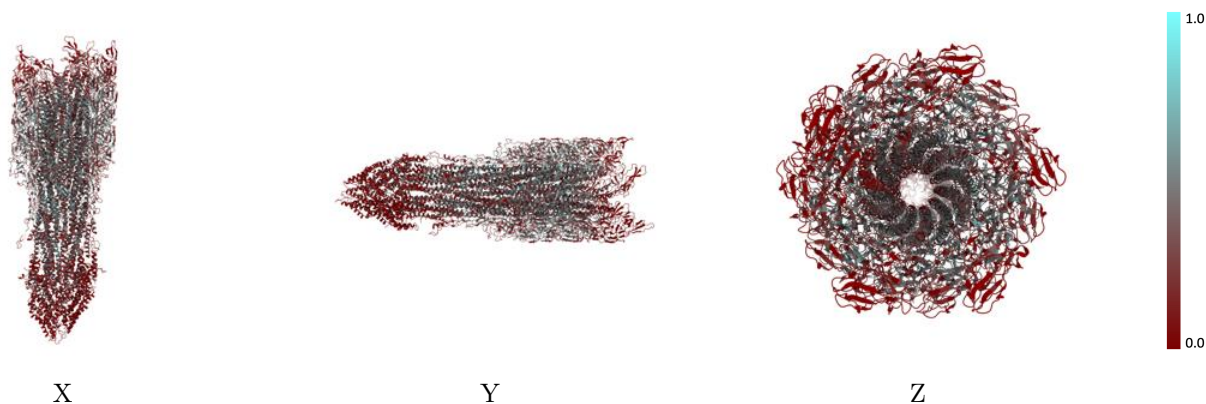
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



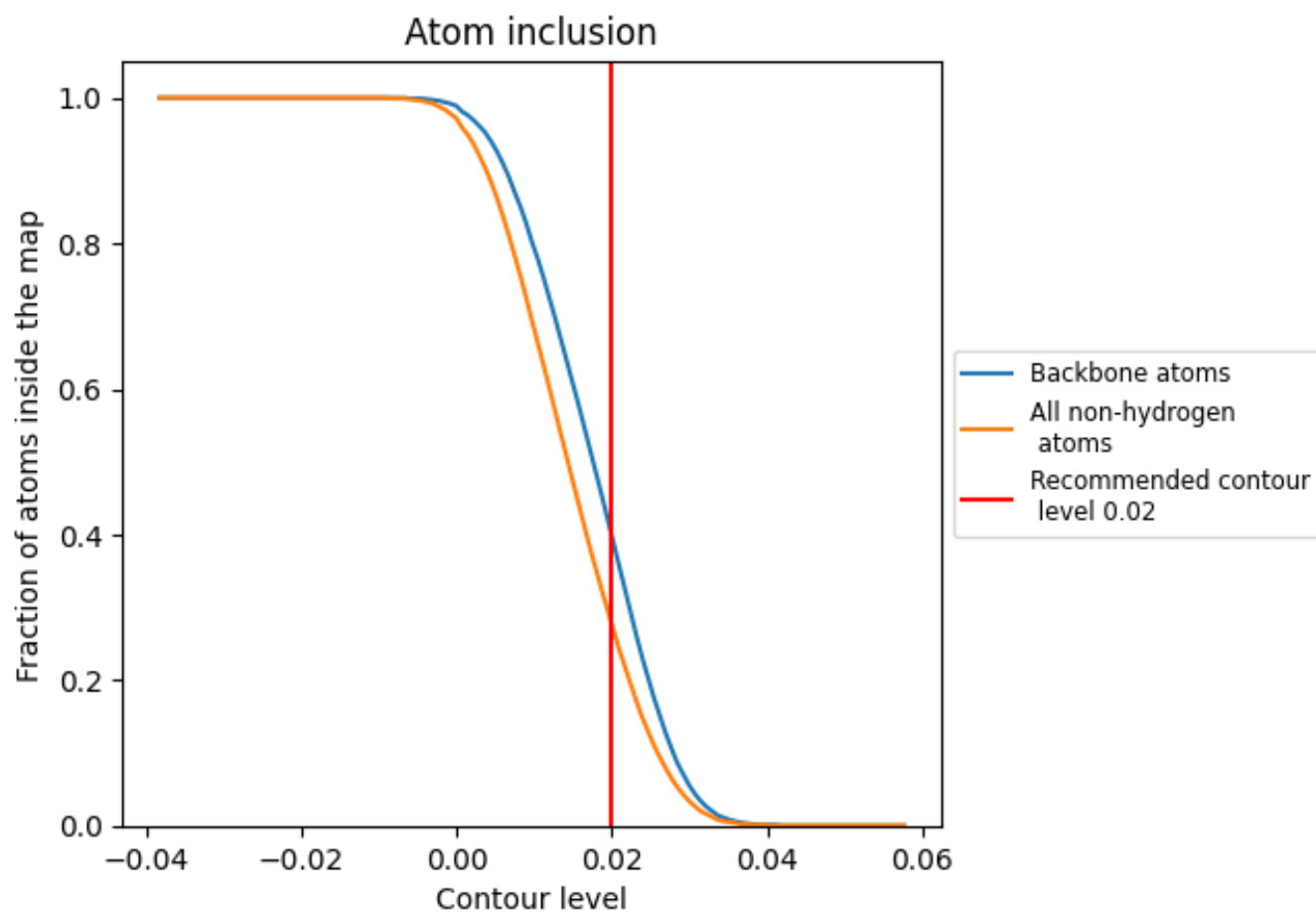
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.2230	 0.4130
3	 0.1750	 0.4010
4	 0.0460	 0.2250
A	 0.1000	 0.3440
B	 0.1450	 0.3610
C	 0.1660	 0.3820
D	 0.1480	 0.3630
E	 0.0810	 0.3210
F	 0.0450	 0.2890
G	 0.0440	 0.2750
H	 0.0660	 0.2870
I	 0.0510	 0.2790
J	 0.0230	 0.2350
K	 0.1840	 0.3990
L	 0.2310	 0.4310
M	 0.2780	 0.4570
N	 0.2870	 0.4400
O	 0.2640	 0.4330
P	 0.2170	 0.4120
Q	 0.2010	 0.4150
R	 0.3030	 0.4100
S	 0.3210	 0.4200
T	 0.3540	 0.4770
U	 0.2760	 0.3970
V	 0.2290	 0.3980
W	 0.3200	 0.4540
X	 0.3530	 0.4680
Y	 0.3710	 0.4790
Z	 0.3540	 0.4610
a	 0.2650	 0.4250
b	 0.2500	 0.4530
c	 0.3410	 0.4800
d	 0.3550	 0.4830



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Chain	Atom inclusion	Q-score
e	 0.3560	 0.4810
f	 0.3190	 0.4700
g	 0.2900	 0.4570
h	 0.3680	 0.4870
i	 0.3680	 0.4890
j	 0.3710	 0.4900
k	 0.3560	 0.4820
l	 0.3730	 0.5050
m	 0.3820	 0.5090
n	 0.3930	 0.5120
o	 0.3700	 0.5030
p	 0.3790	 0.5060
q	 0.3750	 0.5000
r	 0.3730	 0.4940
s	 0.3570	 0.4830
t	 0.3400	 0.4720
u	 0.3380	 0.4610
v	 0.3580	 0.4830
w	 0.3540	 0.4730
x	 0.2920	 0.4650
y	 0.2190	 0.3990
z	 0.1780	 0.3420