



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 07:42 am GMT

PDB ID : 7BK0
EMDB ID : EMD-12195
Title : Salmonella FlhF ring (34mer) in intact basal body - C1
Authors : Johnson, S.; Furlong, E.; Lea, S.M.
Deposited on : 2021-01-14
Resolution : 3.80 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:

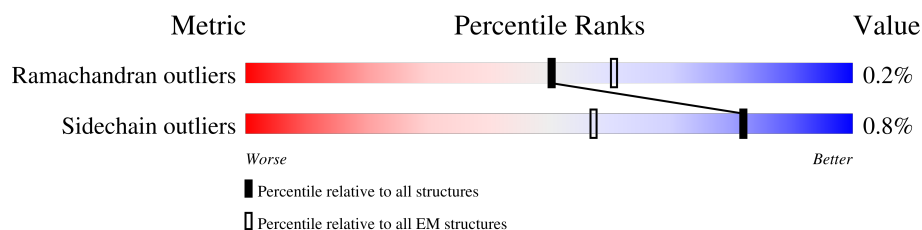
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	560	<div> <div>10%</div> <div>27%</div> <div>73%</div> </div>
1	B	560	<div> <div>23%</div> <div>44%</div> <div>55%</div> </div>
1	C	560	<div> <div>22%</div> <div>44%</div> <div>55%</div> </div>
1	D	560	<div> <div>11%</div> <div>27%</div> <div>73%</div> </div>
1	E	560	<div> <div>26%</div> <div>44%</div> <div>55%</div> </div>
1	F	560	<div> <div>10%</div> <div>27%</div> <div>73%</div> </div>
1	G	560	<div> <div>25%</div> <div>44%</div> <div>55%</div> </div>
1	H	560	<div> <div>26%</div> <div>44%</div> <div>55%</div> </div>
1	I	560	<div> <div>26%</div> <div>44%</div> <div>55%</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	U	560	
1	V	560	
1	W	560	
1	X	560	
1	Y	560	
1	Z	560	
1	a	560	
1	b	560	
1	c	560	
1	d	560	
1	e	560	
1	f	560	
1	g	560	
1	h	560	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 57536 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 M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	B	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	C	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	D	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	E	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	F	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	G	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	H	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	I	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	J	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	K	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	L	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	M	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	N	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	O	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	P	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	Q	250	Total 1931	C 1187	N 355	O 385	S 4	0	0

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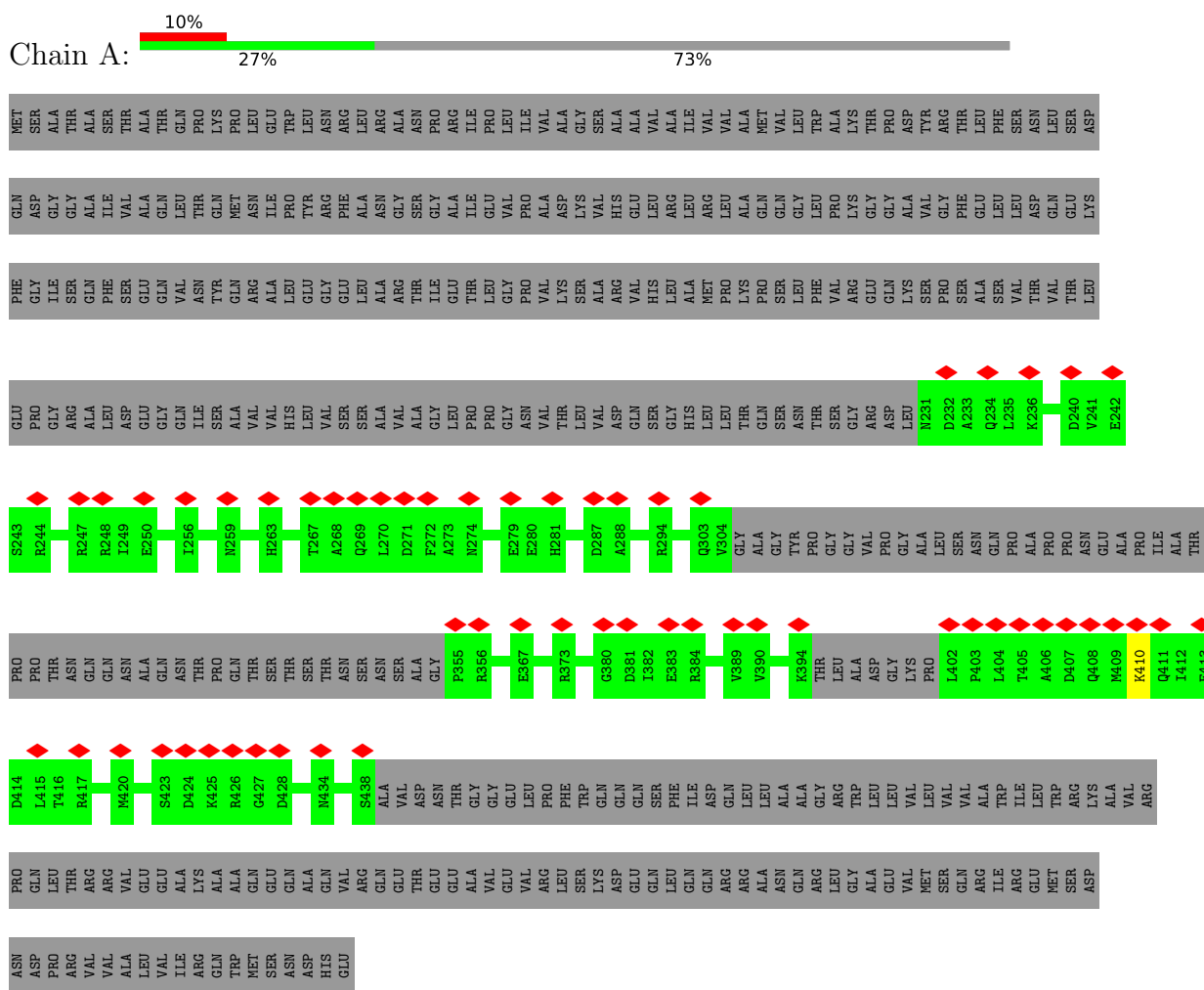
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	S	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	T	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	U	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	V	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	W	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	X	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	Y	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	Z	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	a	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	b	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	c	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	d	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	e	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	f	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	g	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	h	250	Total 1931	C 1187	N 355	O 385	S 4	0	0

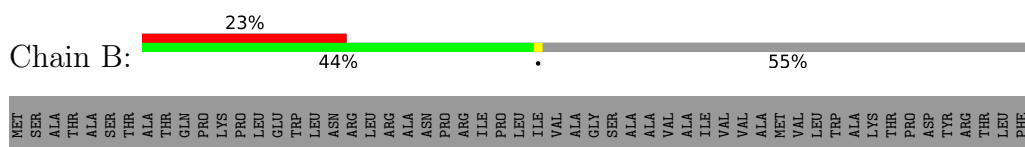
3 Residue-property plots

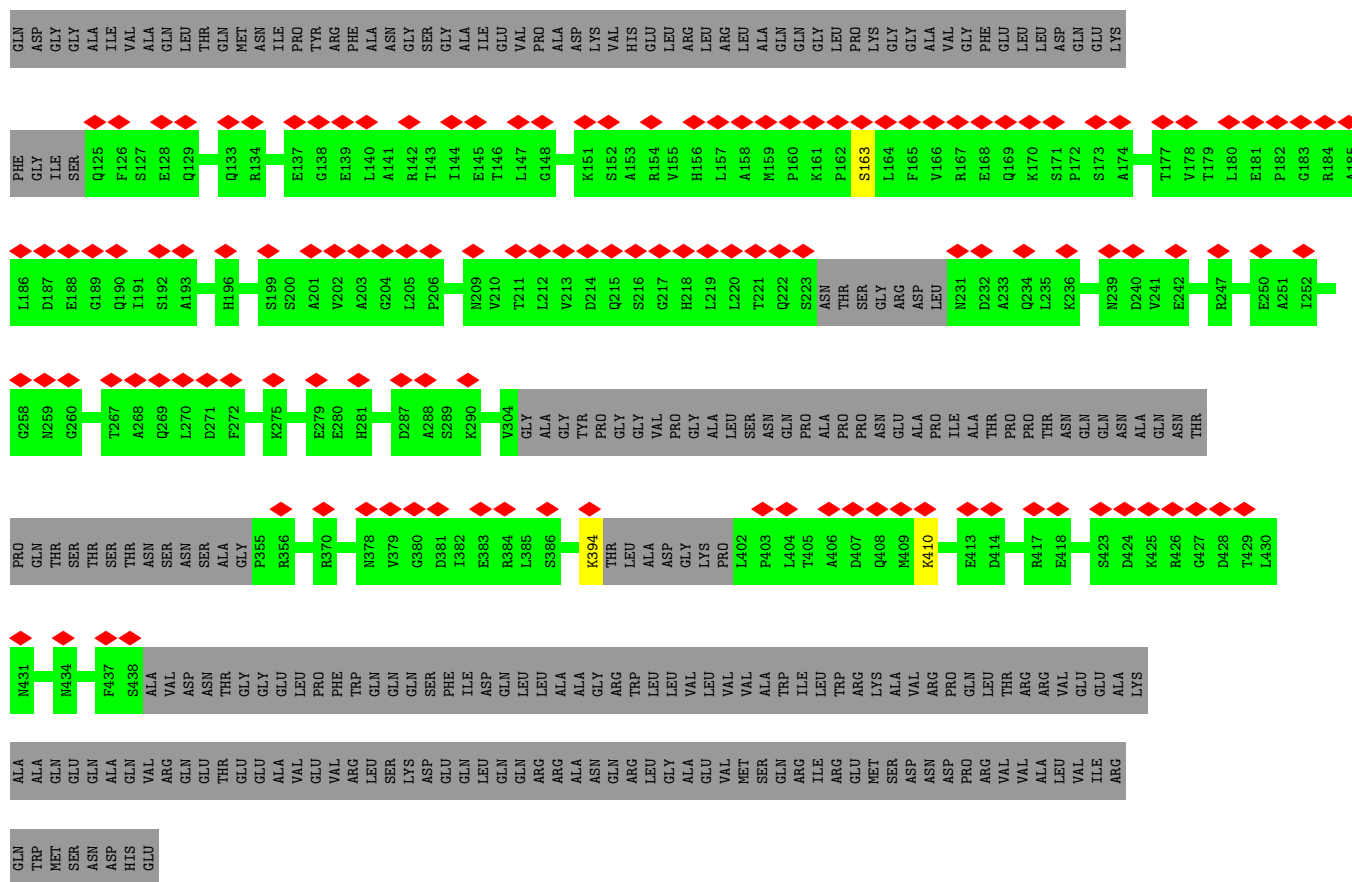
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Flagellar M-ring protein

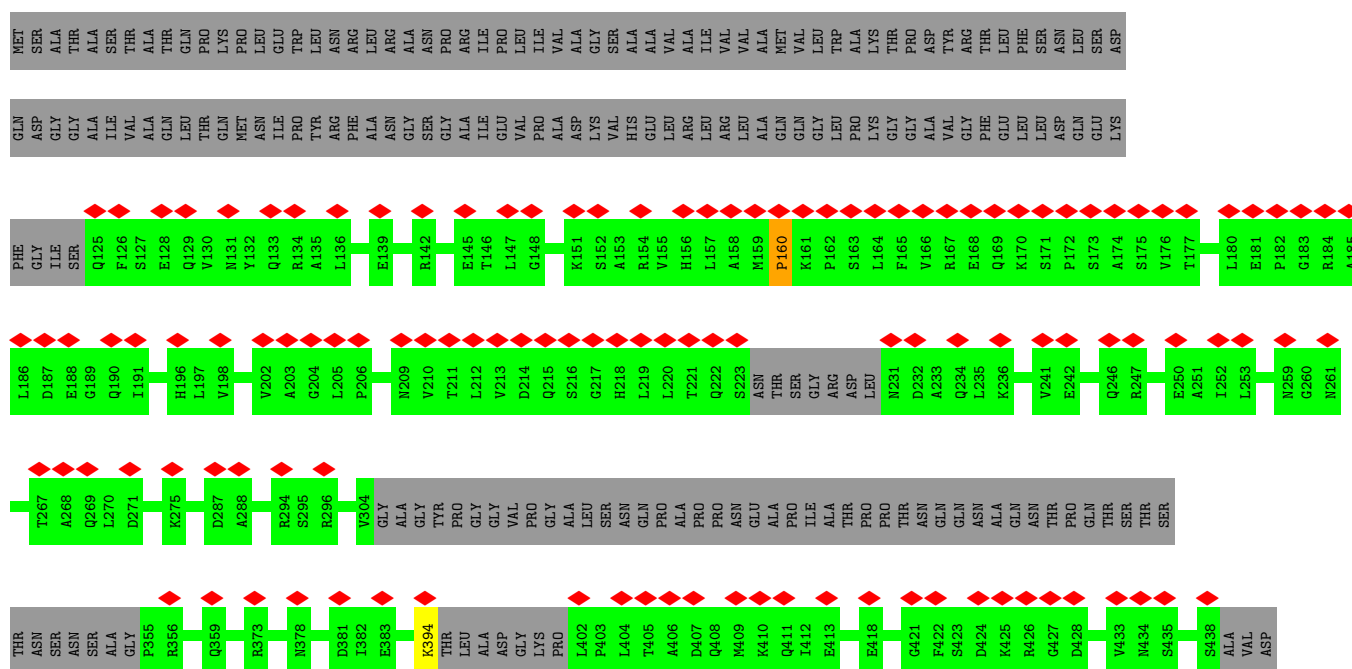


- Molecule 1: Flagellar M-ring protein

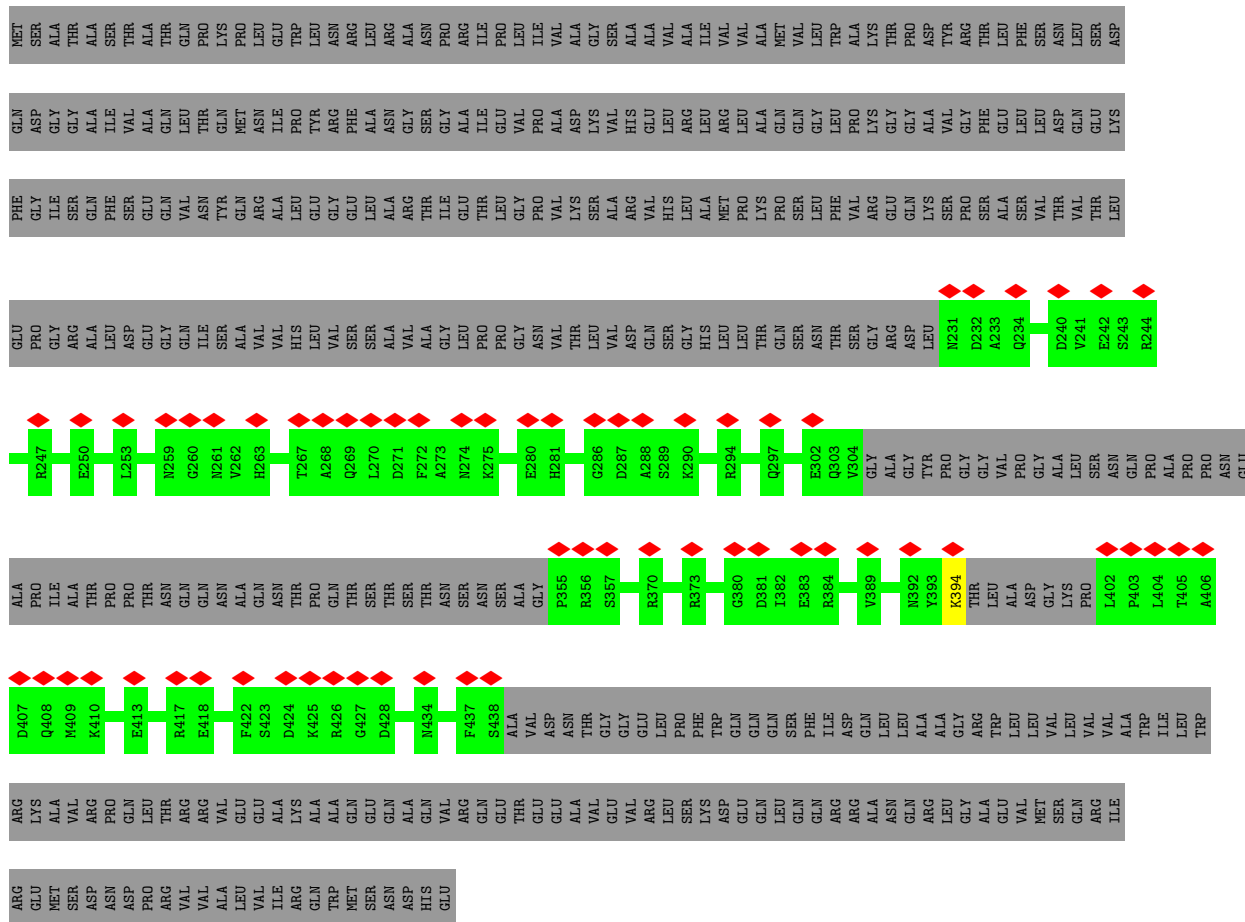




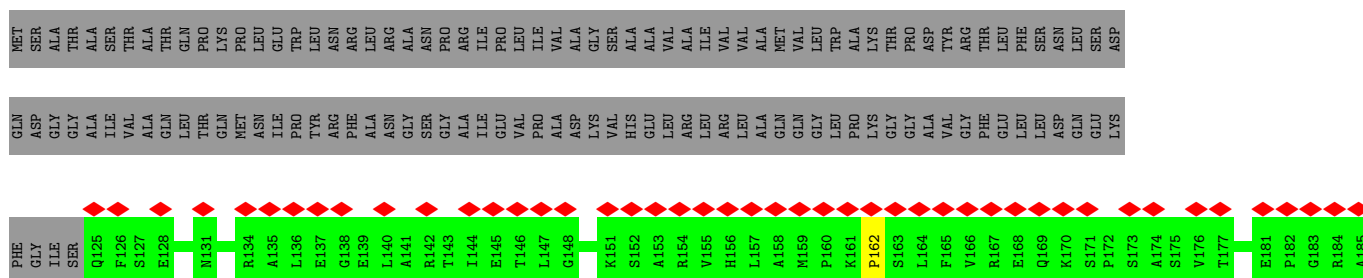
• Molecule 1: Flagellar M-ring protein

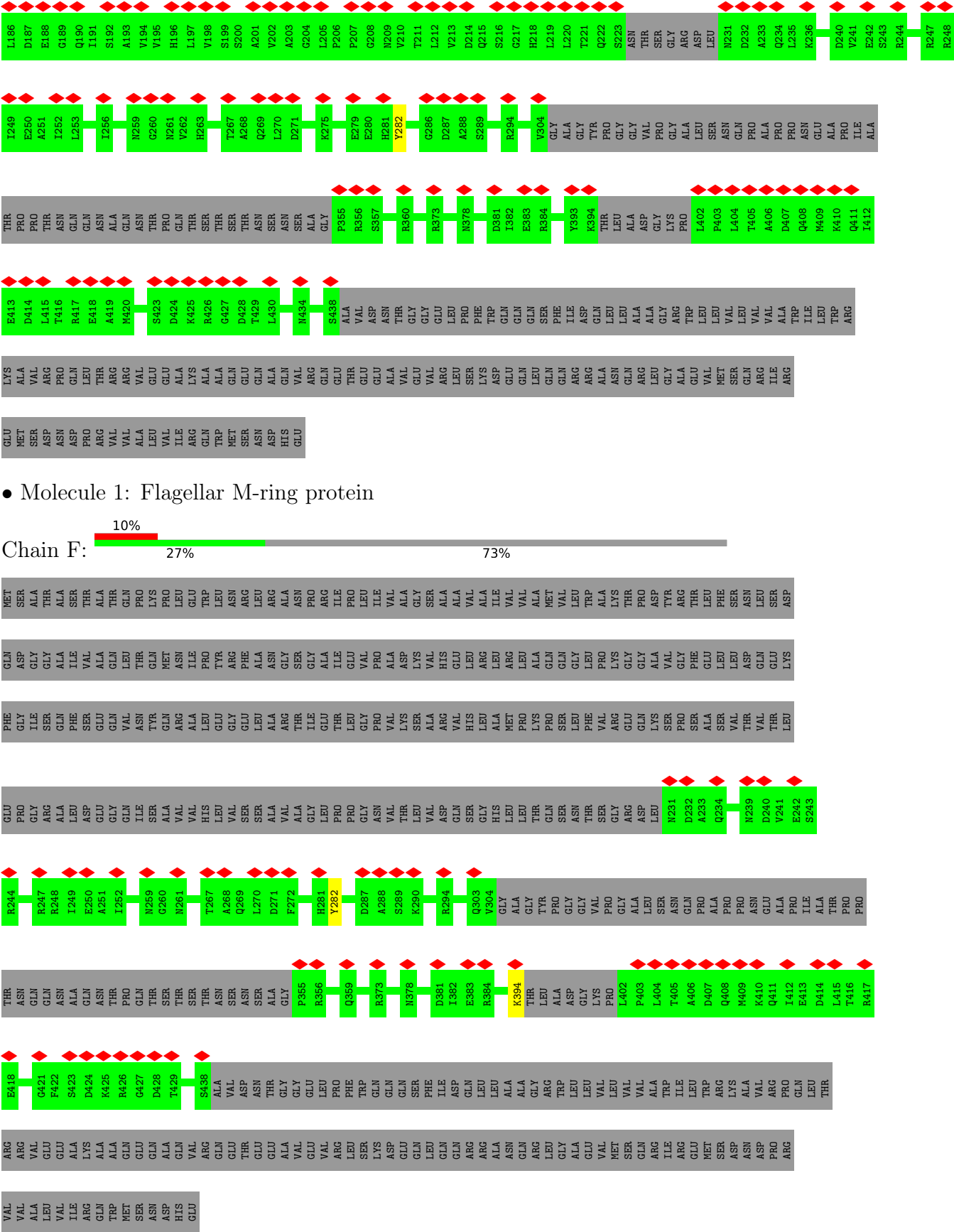


- Molecule 1: Flagellar M-ring protein

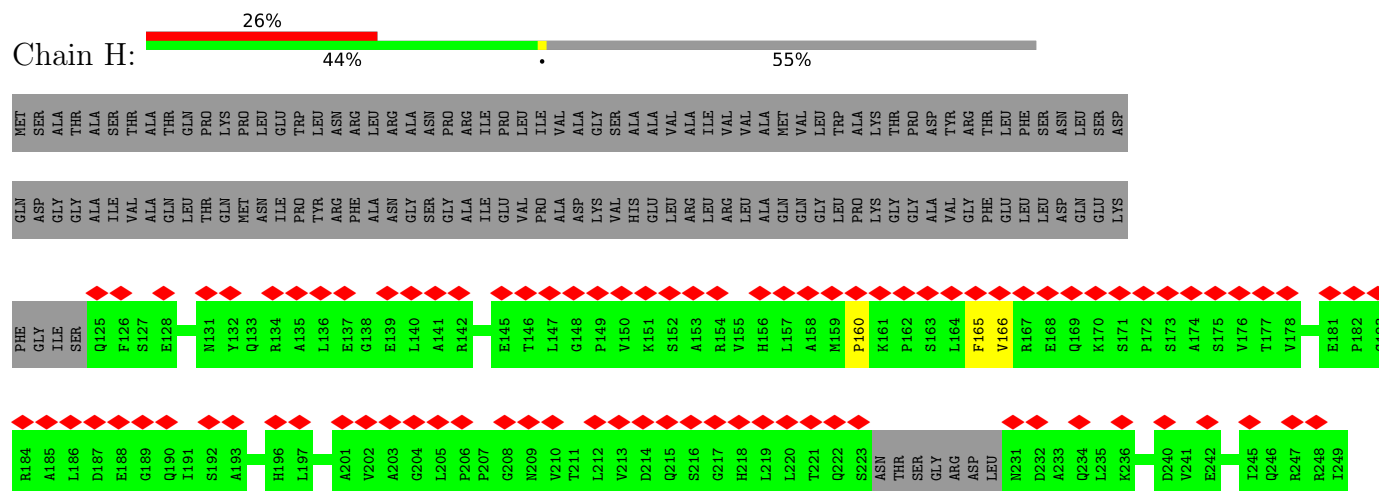


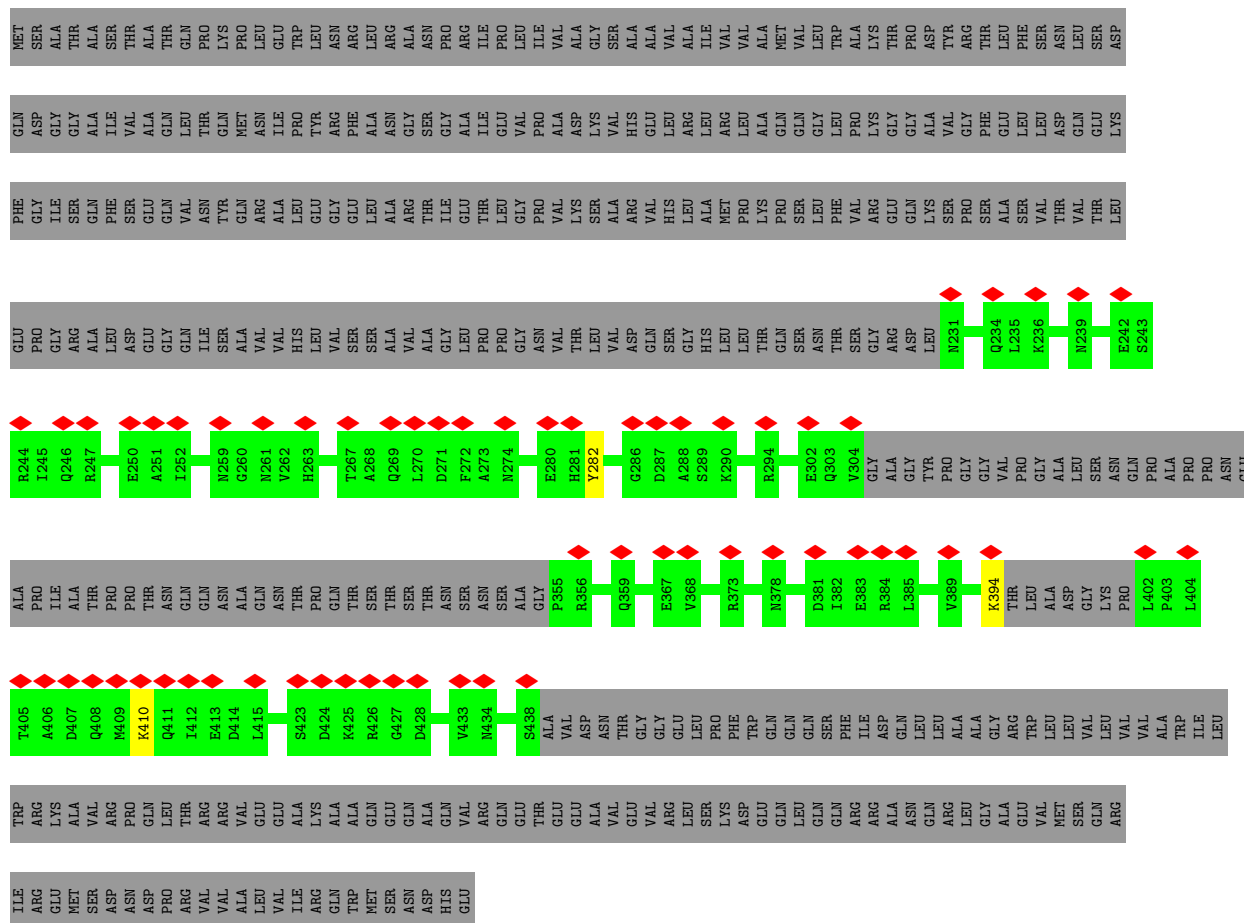
- Molecule 1: Flagellar M-ring protein



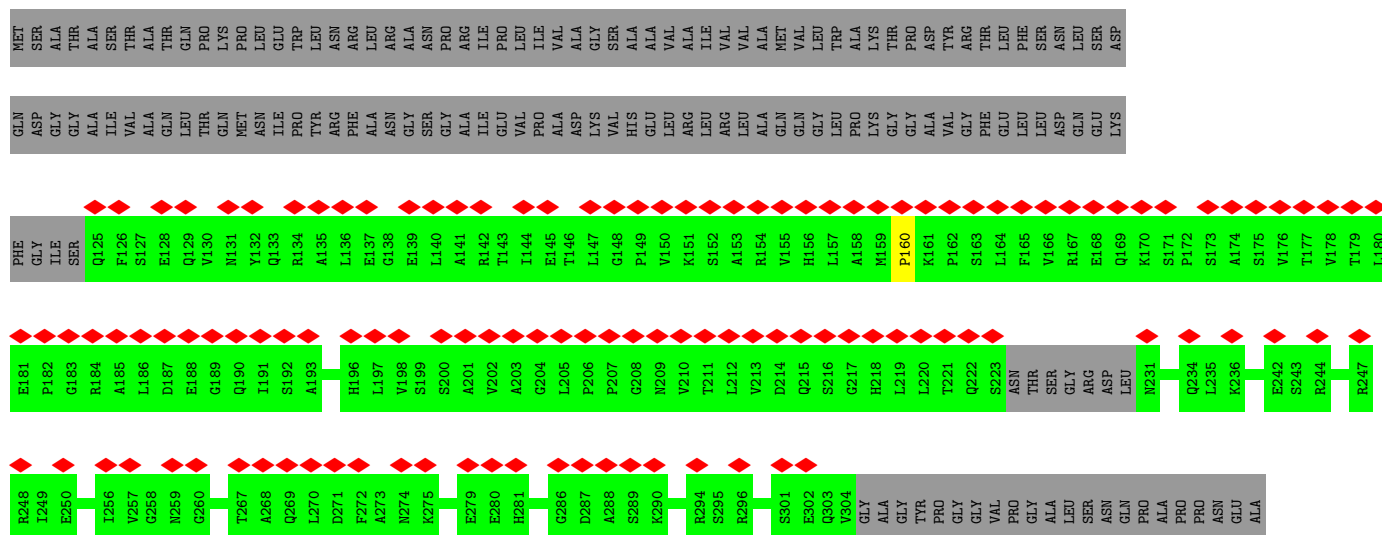
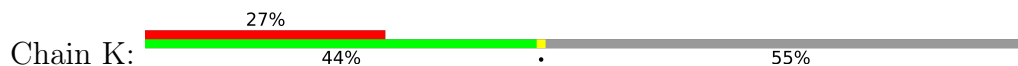


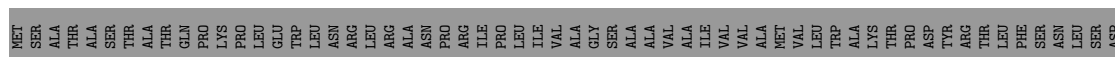
Chain G:



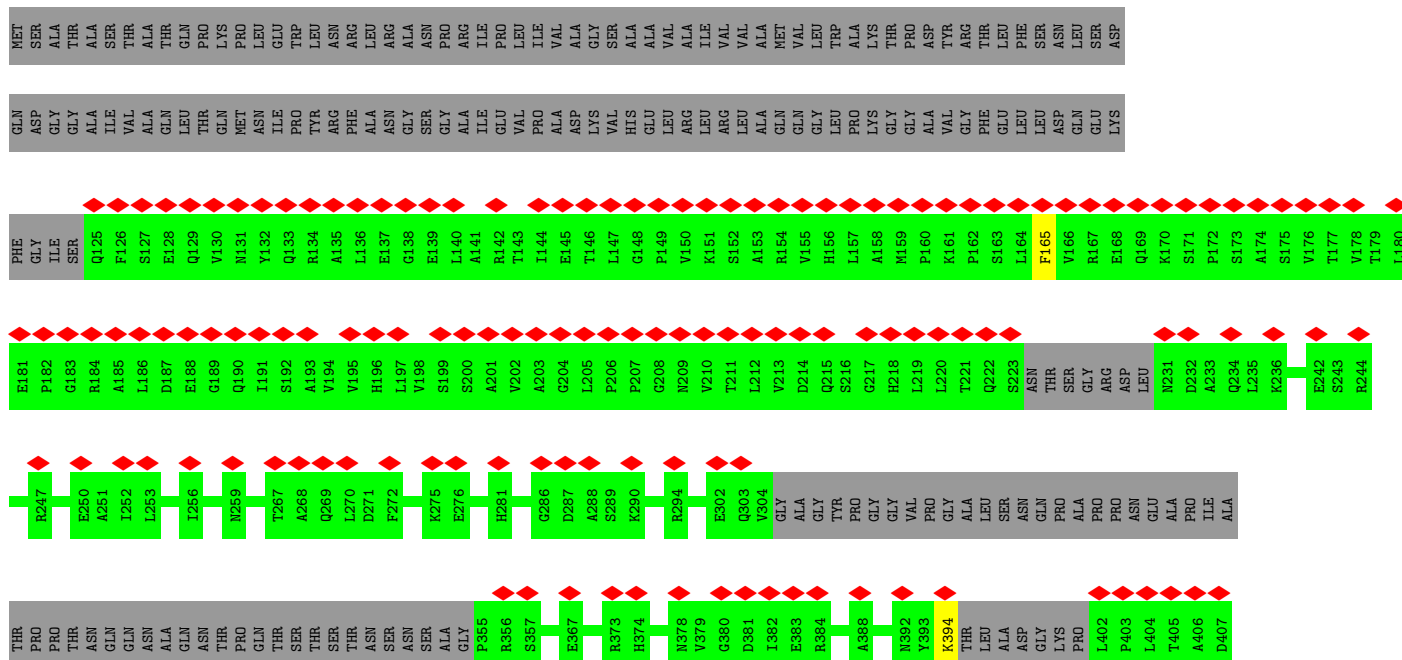


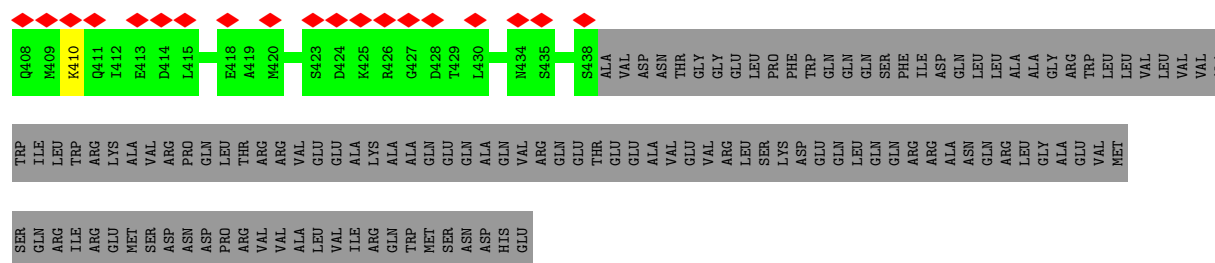
• Molecule 1: Flagellar M-ring protein



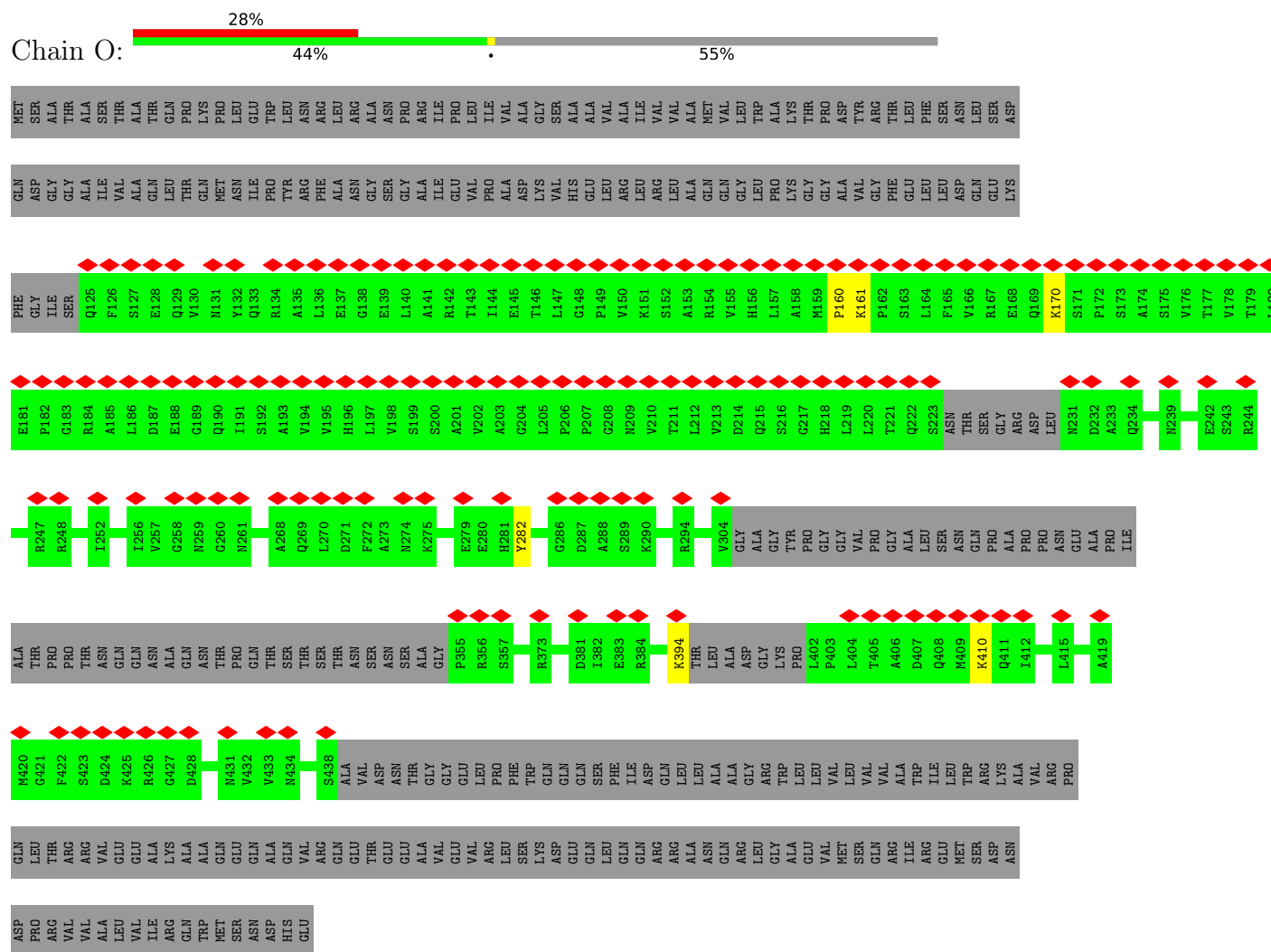


- Molecule 1: Flagellar M-ring protein

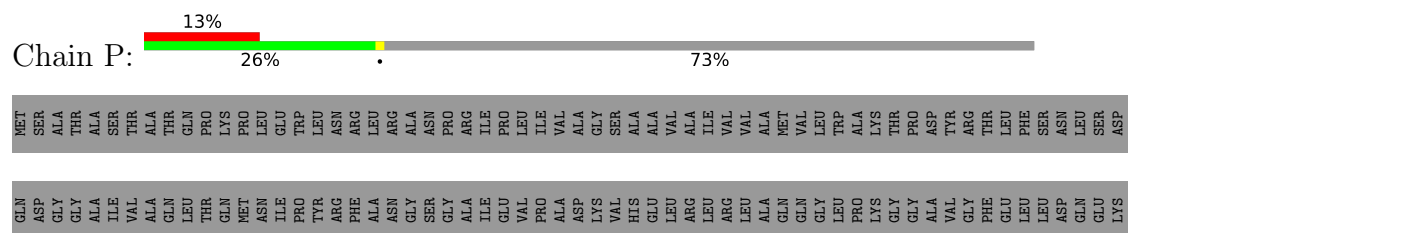




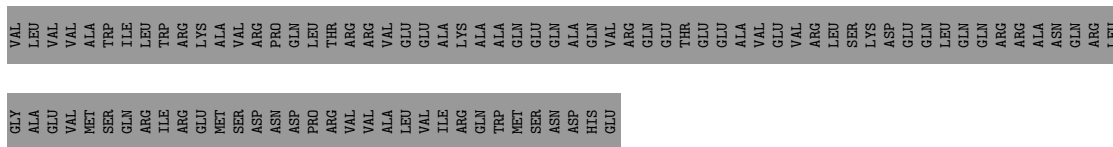
• Molecule 1: Flagellar M-ring protein



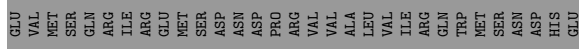
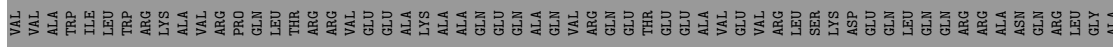
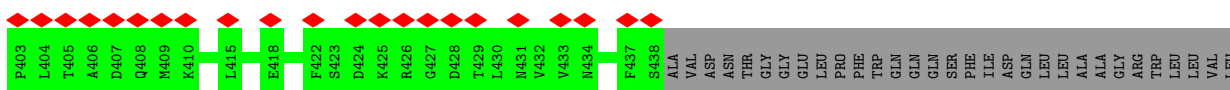
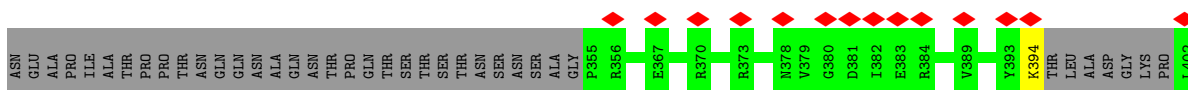
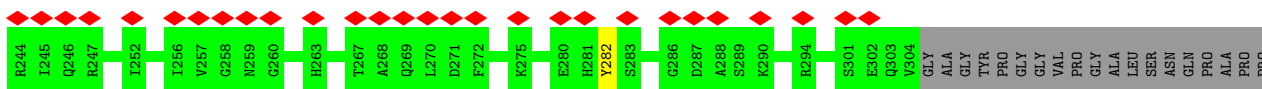
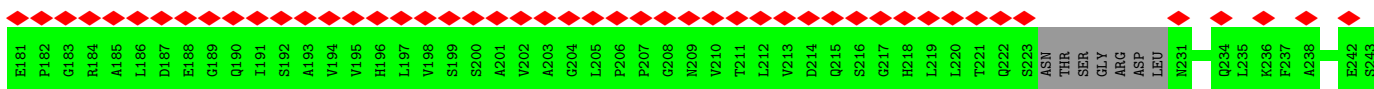
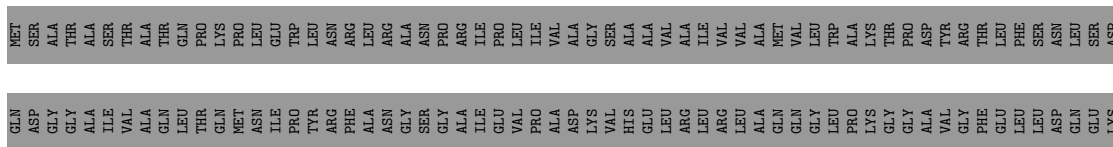
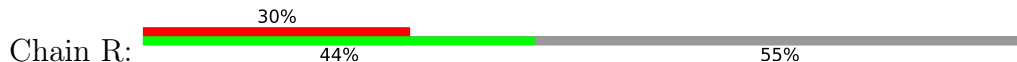
• Molecule 1: Flagellar M-ring protein



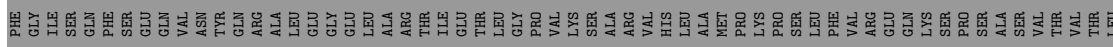
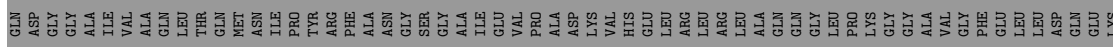
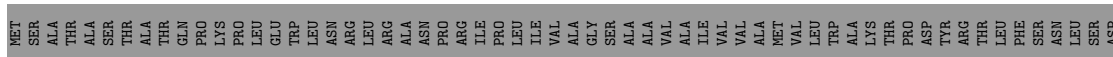




- Molecule 1: Flagellar M-ring protein

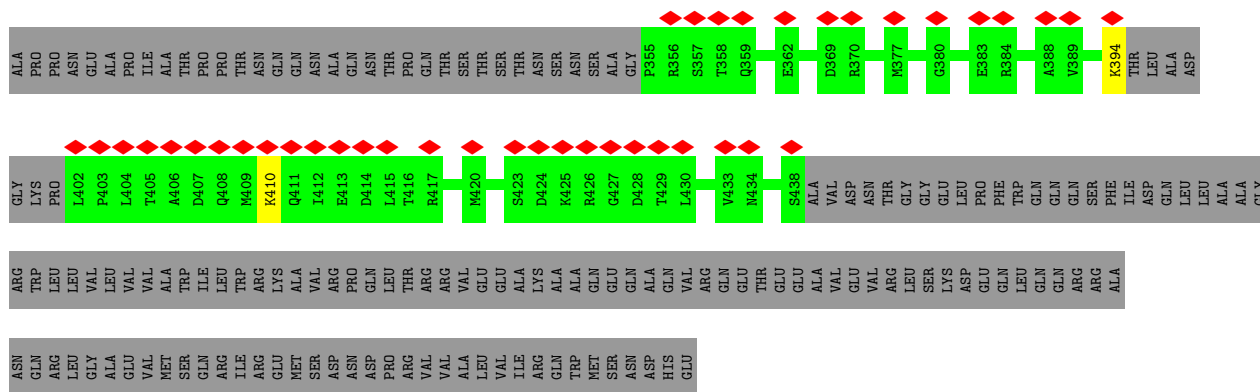


- Molecule 1: Flagellar M-ring protein

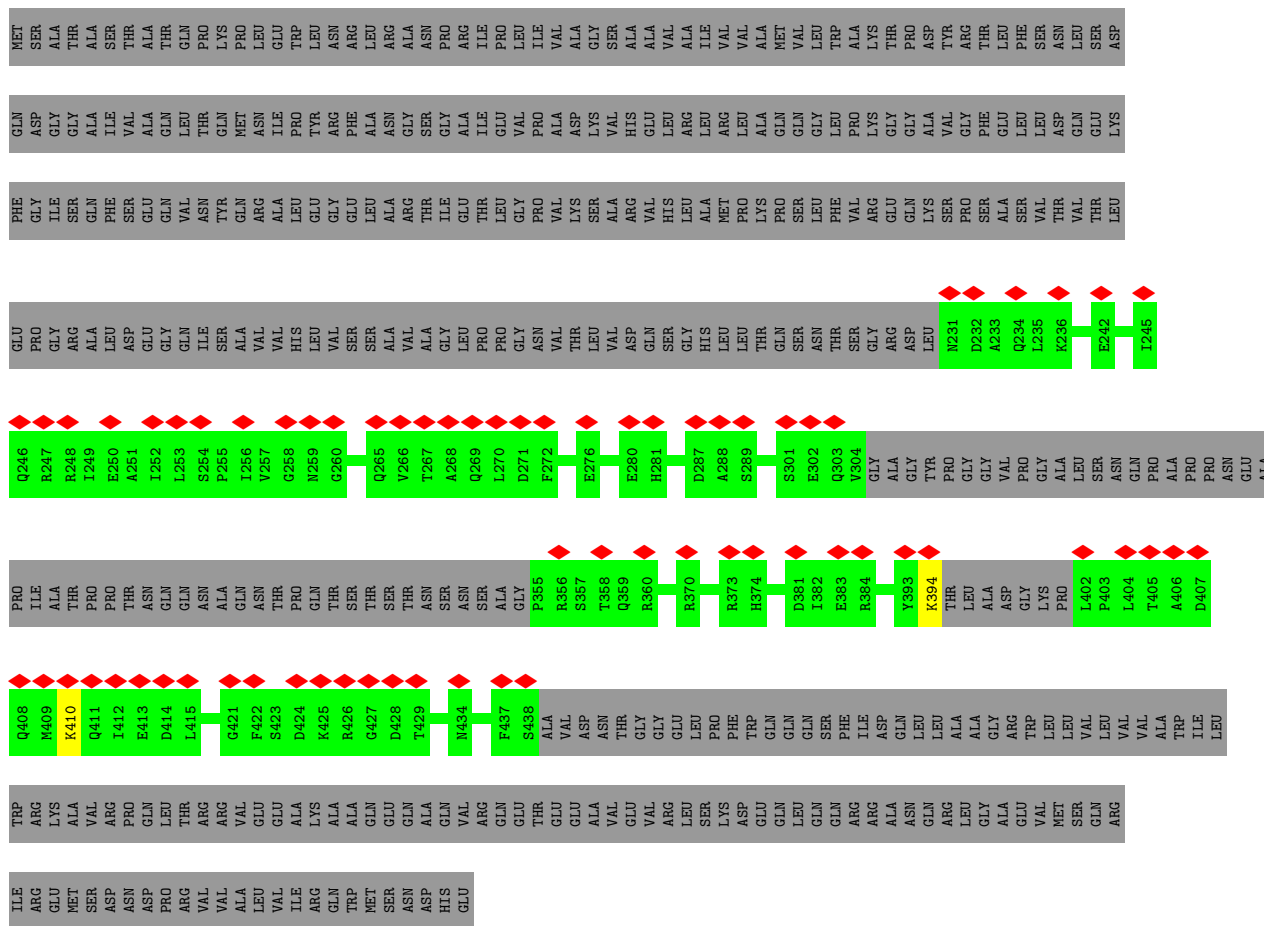




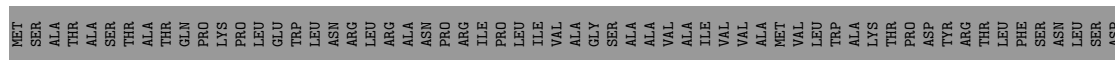


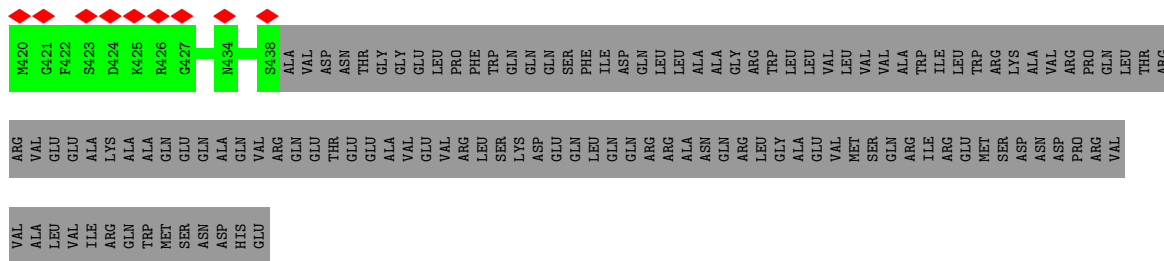


- Molecule 1: Flagellar M-ring protein

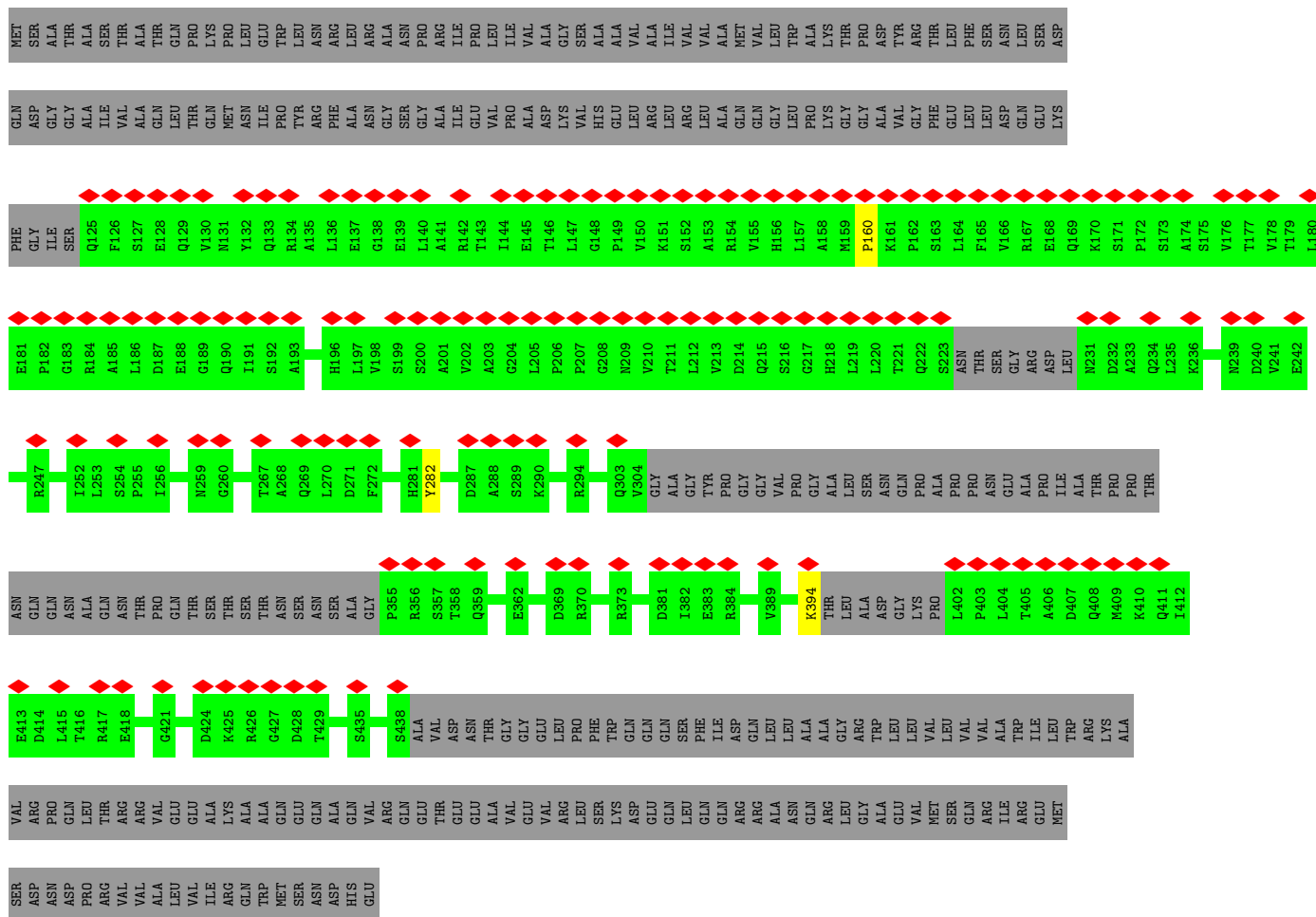


- Molecule 1: Flagellar M-ring protein

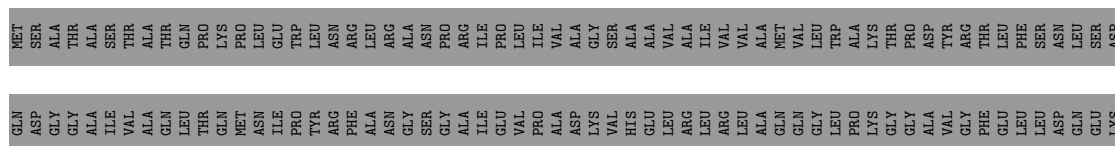




- Molecule 1: Flagellar M-ring protein

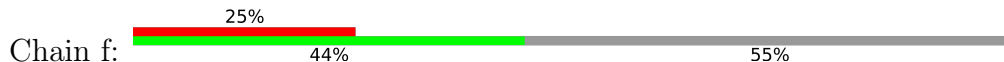


- Molecule 1: Flagellar M-ring protein



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









































- Molecule 1: Flagellar M-ring protein

[illegible][illegible]

E181	P192	G193	R194	A195	L196	D197	E198	G199	S192	A193	H196	L197	V202	A203	G204	L205	P206	P207	G208	N209	V210	T211	L212	V213	Q214	Q215	S216	G217	H218	L219	L220	T221	Q222	Q223	Q224	ASN	THR	SER	GLY	ARG	ASP	LEU	N231	Q234	L235	Q236	P237	A238	N239	D240	V241	E242	S243	E244	P247
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E250	A251	I252	I256	N259	G260	H261	V266	Q269	L270	D271	F272	E279	E280	H281	D287	A288	S289	K290	E302	Q303	V304	GLY	ALA	ALA	GLY	TYR	PRO	PRO	GLY	GLY	GLY	VAL	PRO	PRO	GLY	ALA	ALA	LEU	SER	ASN	ASN	GLN	PRO	ALA	ALA	PRO	PRO	PRO	PRO	ASN	GLU	ALA	ALA	PRO	ILE	ALA	ALA	THR	THR	PRO	PRO	THR	THR
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GLN	GLN	ASN	ALA	GLN	ASN	THR	PRO	GLN	THR	THR	THR	THR	ASN	SER	ASN	ALA	GLY	R355	R356	E367	R373	D381	I392	E393	R394	A388	V389	V390	V391	K394	THR	LEU	ALA	ASP	GLY	LYS	PRO	L402	P403	P404	L405	T406	D407	Q408	M409	K410	E413	D414	L415	E416
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[illegible]

ARG
VAL
VAL
ALA
LEU
VAL
ILE
ARG
GLN
TRP
MET
SER
ASN
ASP
HIS
GLU

- Molecule 1: Flagellar M-ring protein



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

[illegible]



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	0.025	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	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	0/1205	0.52	0/1624
1	B	0.38	0/1955	0.55	0/2645
1	C	0.39	0/1955	0.54	1/2645 (0.0%)
1	D	0.40	0/1205	0.53	0/1624
1	E	0.38	0/1955	0.55	1/2645 (0.0%)
1	F	0.39	0/1205	0.57	1/1624 (0.1%)
1	G	0.37	0/1955	0.54	0/2645
1	H	0.38	0/1955	0.56	0/2645
1	I	0.37	0/1955	0.53	0/2645
1	J	0.42	0/1205	0.53	1/1624 (0.1%)
1	K	0.36	0/1955	0.52	0/2645
1	L	0.36	0/1955	0.54	0/2645
1	M	0.40	0/1205	0.55	1/1624 (0.1%)
1	N	0.36	0/1955	0.55	0/2645
1	O	0.35	0/1955	0.53	1/2645 (0.0%)
1	P	0.37	0/1205	0.52	1/1624 (0.1%)
1	Q	0.35	0/1955	0.52	0/2645
1	R	0.35	0/1955	0.51	1/2645 (0.0%)
1	S	0.38	0/1205	0.50	1/1624 (0.1%)
1	T	0.35	0/1955	0.52	0/2645
1	U	0.35	0/1955	0.56	0/2645
1	V	0.38	0/1205	0.52	0/1624
1	W	0.35	0/1955	0.52	1/2645 (0.0%)
1	X	0.35	0/1955	0.52	1/2645 (0.0%)
1	Y	0.34	0/1955	0.53	0/2645
1	Z	0.40	0/1205	0.54	0/1624
1	a	0.36	0/1955	0.53	0/2645
1	b	0.38	0/1205	0.51	0/1624
1	c	0.37	0/1955	0.53	1/2645 (0.0%)
1	d	0.37	0/1955	0.54	0/2645
1	e	0.39	0/1205	0.52	1/1624 (0.1%)
1	f	0.37	0/1955	0.53	0/2645
1	g	0.37	0/1955	0.54	1/2645 (0.0%)
1	h	0.37	0/1955	0.51	0/2645

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.37	0/58220	0.53	14/78699 (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	1
1	E	0	1
1	G	0	1
1	H	0	1
1	L	0	1
1	N	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	282	TYR	C-N-CA	-6.68	105.00	121.70
1	g	282	TYR	C-N-CA	-6.66	105.05	121.70
1	M	282	TYR	C-N-CA	-6.35	105.82	121.70
1	R	282	TYR	C-N-CA	-5.97	106.76	121.70
1	F	282	TYR	C-N-CA	-5.91	106.92	121.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	163	SER	Peptide
1	E	162	PRO	Peptide
1	G	165	PHE	Peptide
1	H	165	PHE	Peptide
1	L	125	GLN	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	145/560 (26%)	143 (99%)	2 (1%)	0	100	100
1	B	242/560 (43%)	227 (94%)	15 (6%)	0	100	100
1	C	242/560 (43%)	230 (95%)	11 (4%)	1 (0%)	34	70
1	D	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	E	242/560 (43%)	226 (93%)	16 (7%)	0	100	100
1	F	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	G	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	34	70
1	H	242/560 (43%)	221 (91%)	19 (8%)	2 (1%)	19	57
1	I	242/560 (43%)	229 (95%)	12 (5%)	1 (0%)	34	70
1	J	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	K	242/560 (43%)	230 (95%)	11 (4%)	1 (0%)	34	70
1	L	242/560 (43%)	224 (93%)	18 (7%)	0	100	100
1	M	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	N	242/560 (43%)	223 (92%)	19 (8%)	0	100	100
1	O	242/560 (43%)	231 (96%)	10 (4%)	1 (0%)	34	70
1	P	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	Q	242/560 (43%)	224 (93%)	17 (7%)	1 (0%)	34	70
1	R	242/560 (43%)	229 (95%)	13 (5%)	0	100	100
1	S	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	T	242/560 (43%)	230 (95%)	12 (5%)	0	100	100
1	U	242/560 (43%)	231 (96%)	11 (4%)	0	100	100
1	V	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	W	242/560 (43%)	227 (94%)	14 (6%)	1 (0%)	34	70
1	X	242/560 (43%)	225 (93%)	17 (7%)	0	100	100
1	Y	242/560 (43%)	228 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	a	242/560 (43%)	227 (94%)	14 (6%)	1 (0%)	34	70
1	b	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	c	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	34	70
1	d	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	34	70
1	e	145/560 (26%)	144 (99%)	1 (1%)	0	100	100
1	f	242/560 (43%)	229 (95%)	12 (5%)	1 (0%)	34	70
1	g	242/560 (43%)	226 (93%)	15 (6%)	1 (0%)	34	70
1	h	242/560 (43%)	232 (96%)	10 (4%)	0	100	100
All	All	7161/19040 (38%)	6784 (95%)	363 (5%)	14 (0%)	50	79

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	160	PRO
1	O	160	PRO
1	g	160	PRO
1	K	160	PRO
1	a	160	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	B	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	C	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	D	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	E	217/467 (46%)	217 (100%)	0	100	100
1	F	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	G	217/467 (46%)	216 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	I	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	J	134/467 (29%)	132 (98%)	2 (2%)	65	81
1	K	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	L	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	M	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	N	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	O	217/467 (46%)	213 (98%)	4 (2%)	59	77
1	P	134/467 (29%)	131 (98%)	3 (2%)	52	72
1	Q	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	R	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	S	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	T	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	U	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	V	134/467 (29%)	132 (98%)	2 (2%)	65	81
1	W	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	X	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	Y	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	Z	134/467 (29%)	132 (98%)	2 (2%)	65	81
1	a	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	b	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	c	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	d	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	e	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	f	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	g	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	h	217/467 (46%)	216 (100%)	1 (0%)	88	94
All	All	6465/15878 (41%)	6414 (99%)	51 (1%)	82	89

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	394	LYS

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Mol	Chain	Res	Type
1	X	394	LYS
1	g	394	LYS
1	U	394	LYS
1	V	394	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	434	ASN
1	f	434	ASN
1	a	434	ASN
1	d	218	HIS
1	K	261	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.

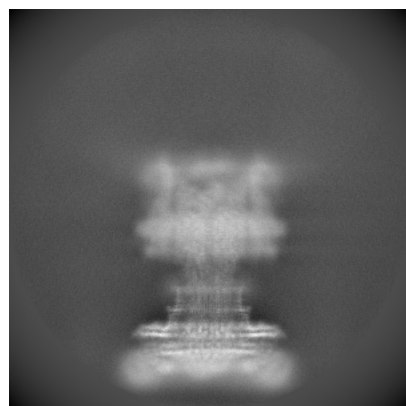
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12195. These allow visual inspection of the internal detail of the map and identification of artifacts.

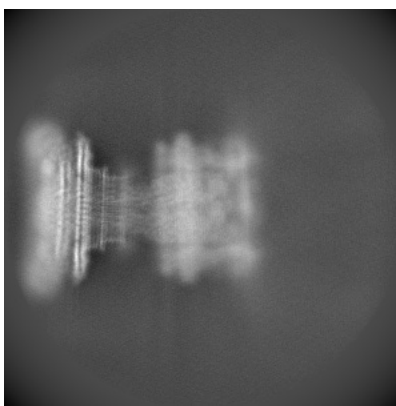
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

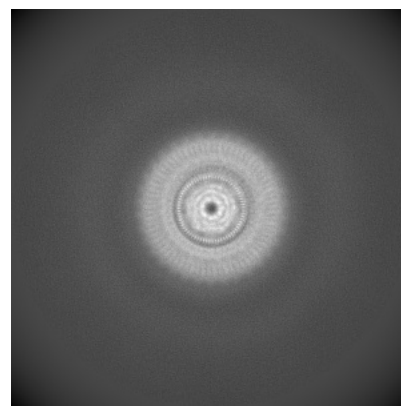
6.1.1 Primary map



X

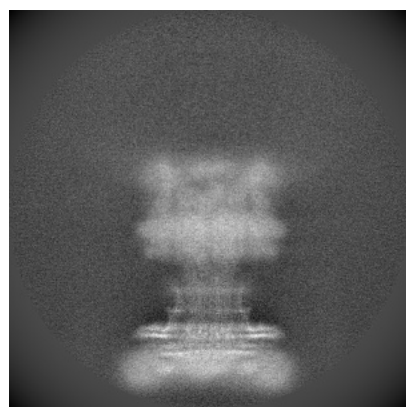


Y

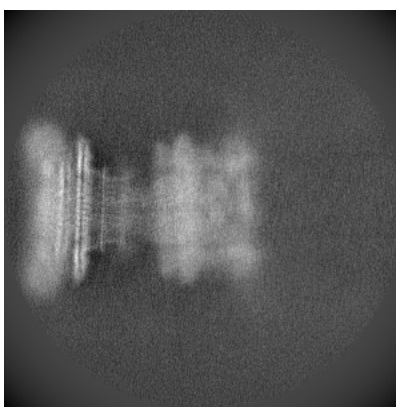


Z

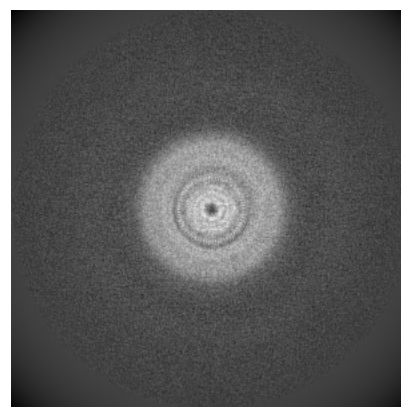
6.1.2 Raw map



X



Y

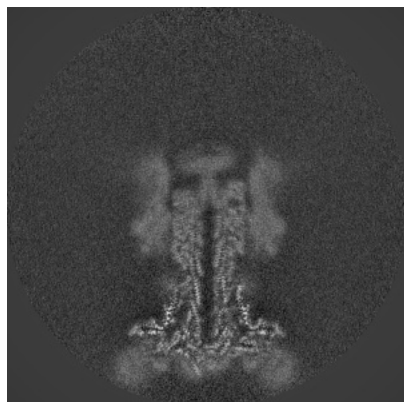


Z

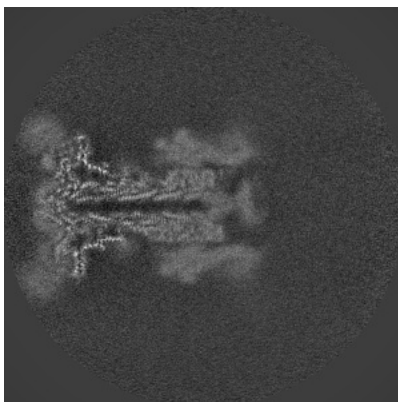
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

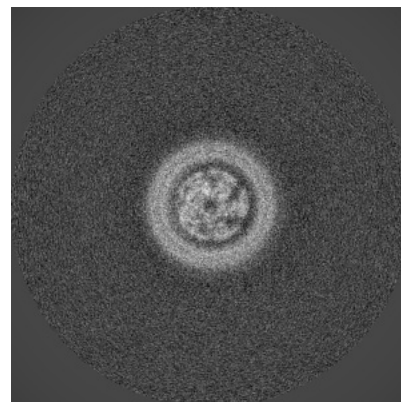
6.2.1 Primary map



X Index: 384

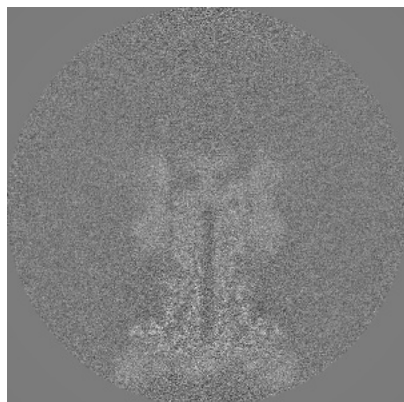


Y Index: 384

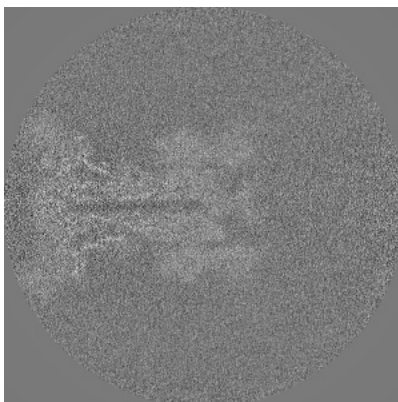


Z Index: 384

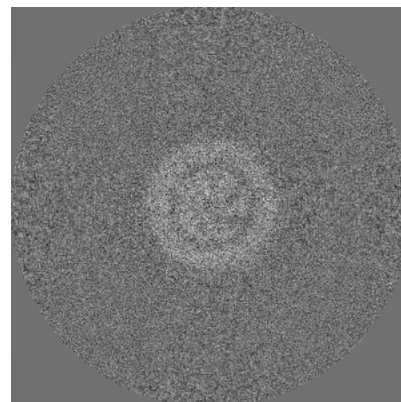
6.2.2 Raw map



X Index: 384



Y Index: 384

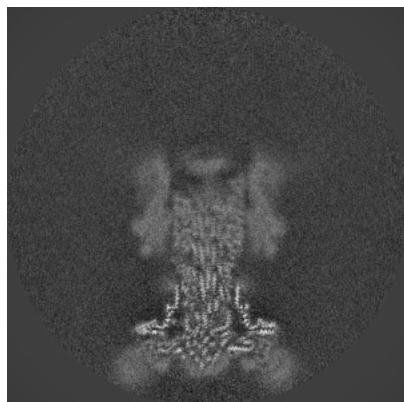


Z Index: 384

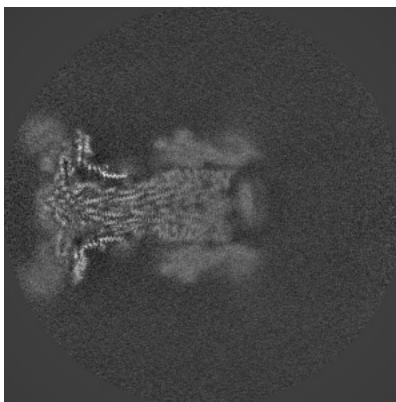
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

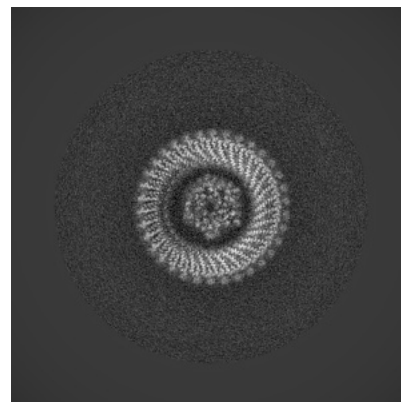
6.3.1 Primary map



X Index: 402

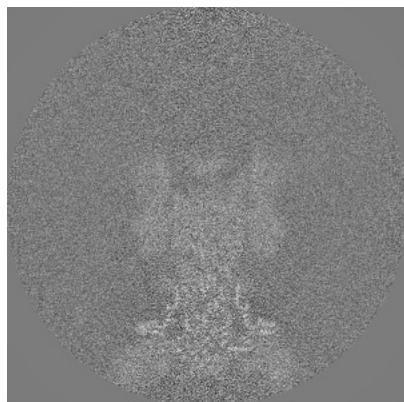


Y Index: 398

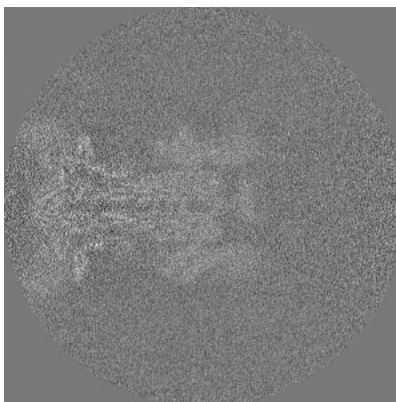


Z Index: 143

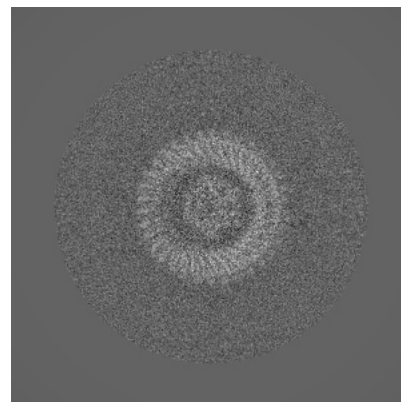
6.3.2 Raw map



X Index: 402



Y Index: 376

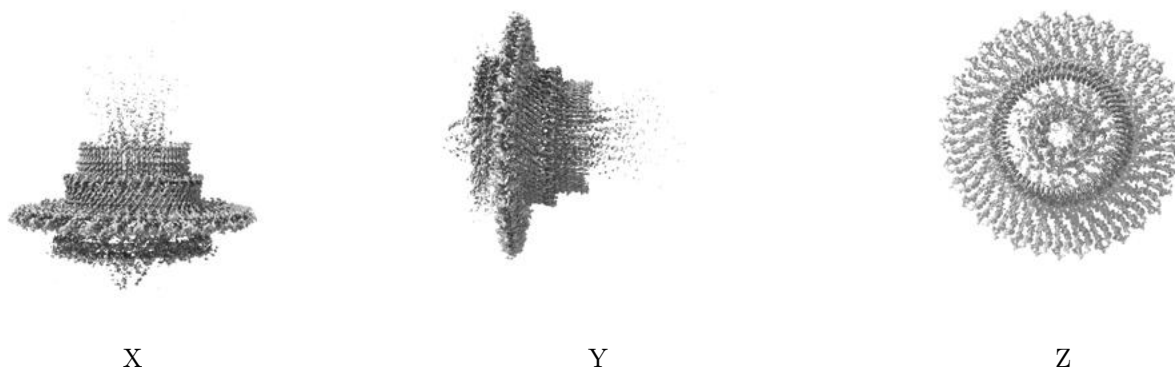


Z Index: 143

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

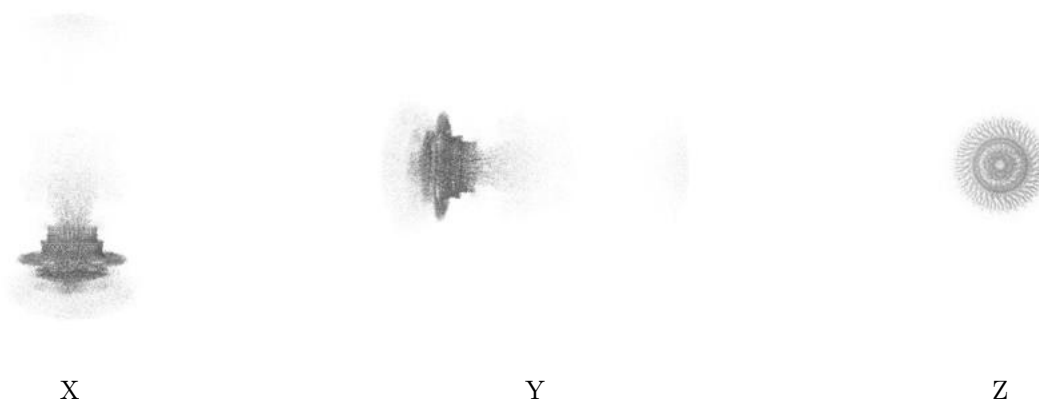
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

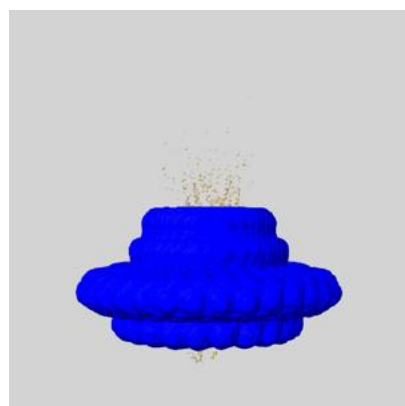
6.5 Mask visualisation [i](#)

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

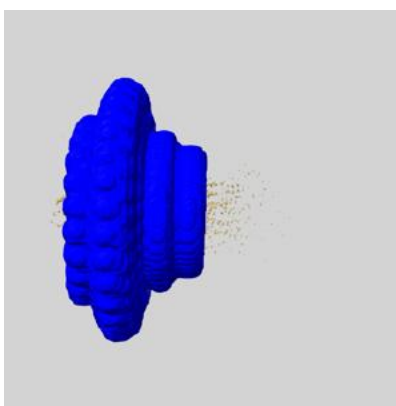
A mask typically either:

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

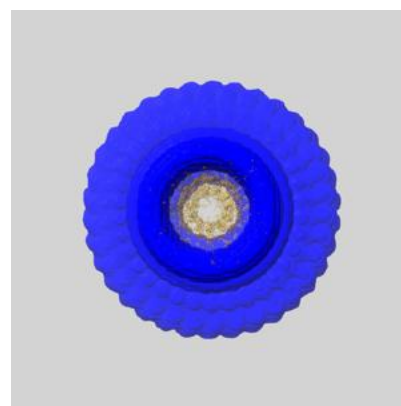
6.5.1 emd_12195_msk_1.map [i](#)



X



Y

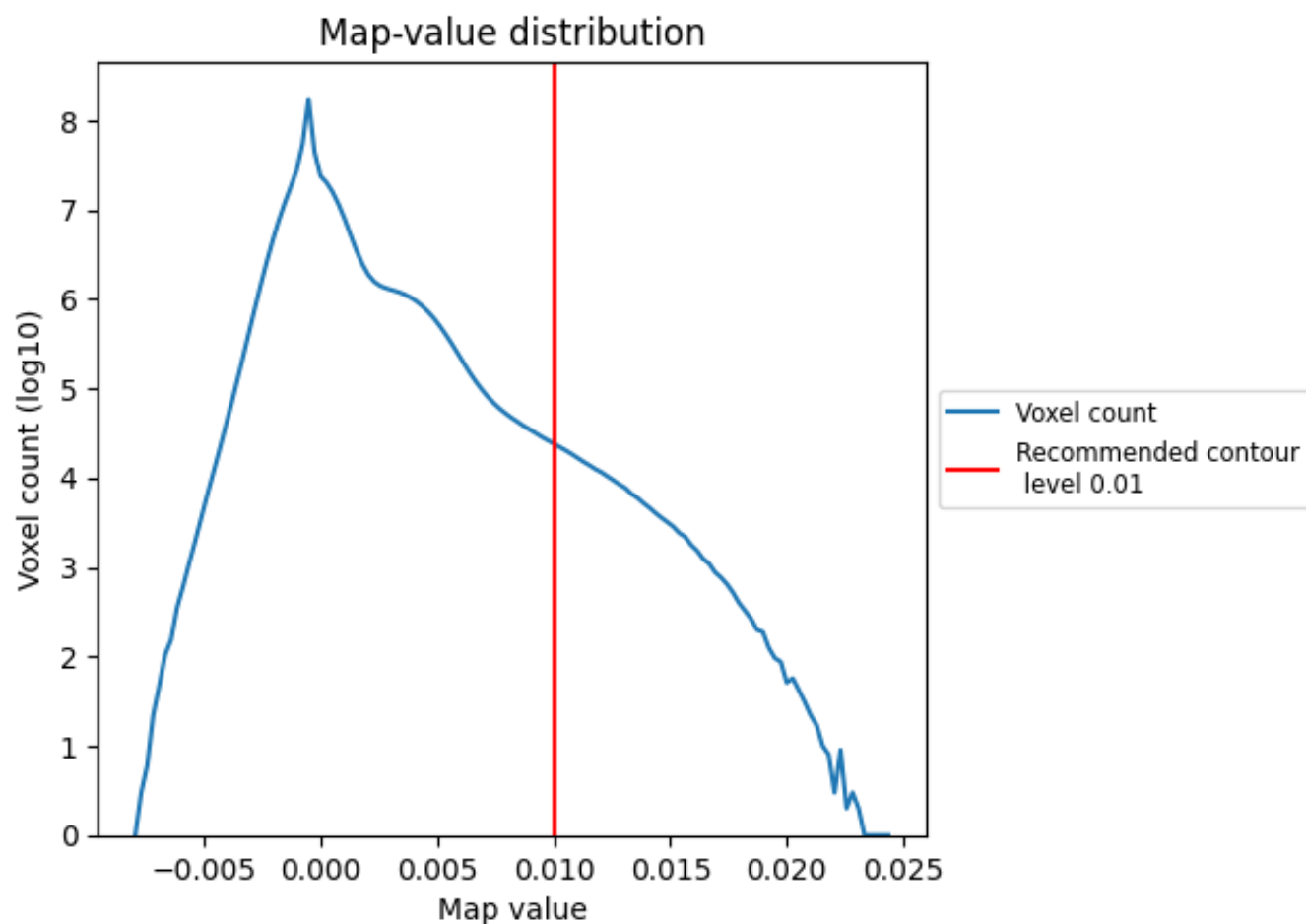


Z

7 Map analysis [i](#)

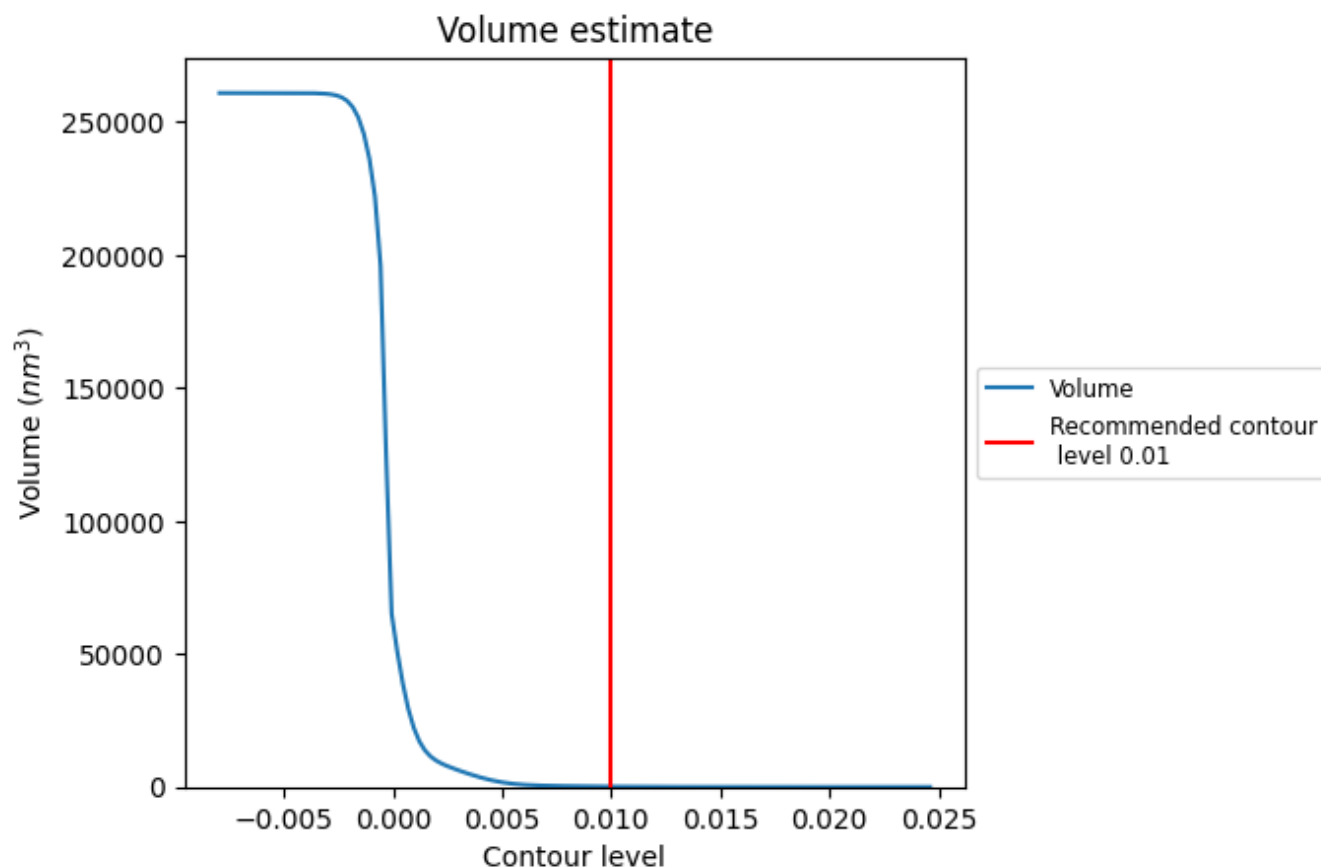
This section contains the results of statistical analysis of the map.

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.

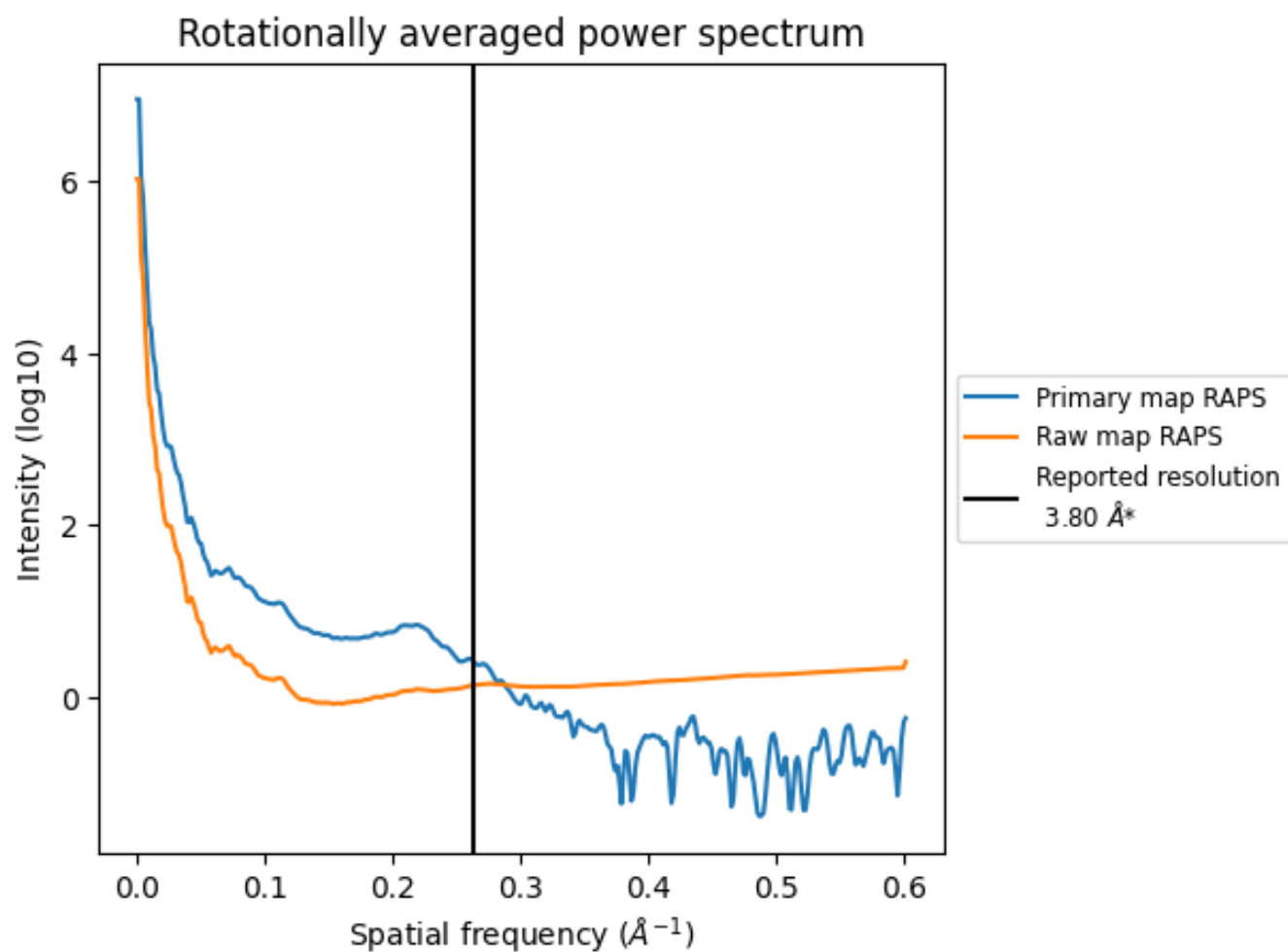
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm^3 ; this corresponds to an approximate mass of 125 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

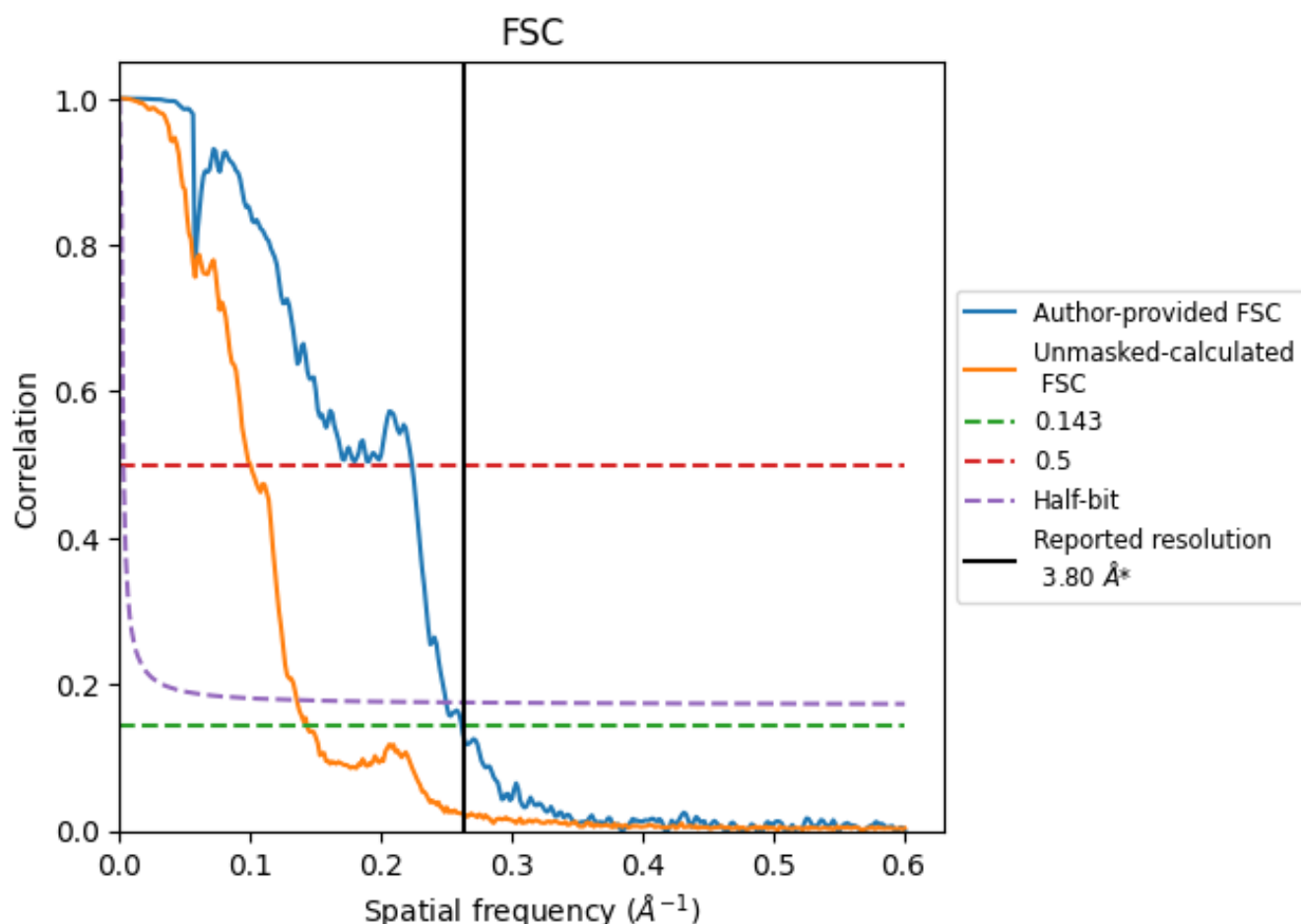


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

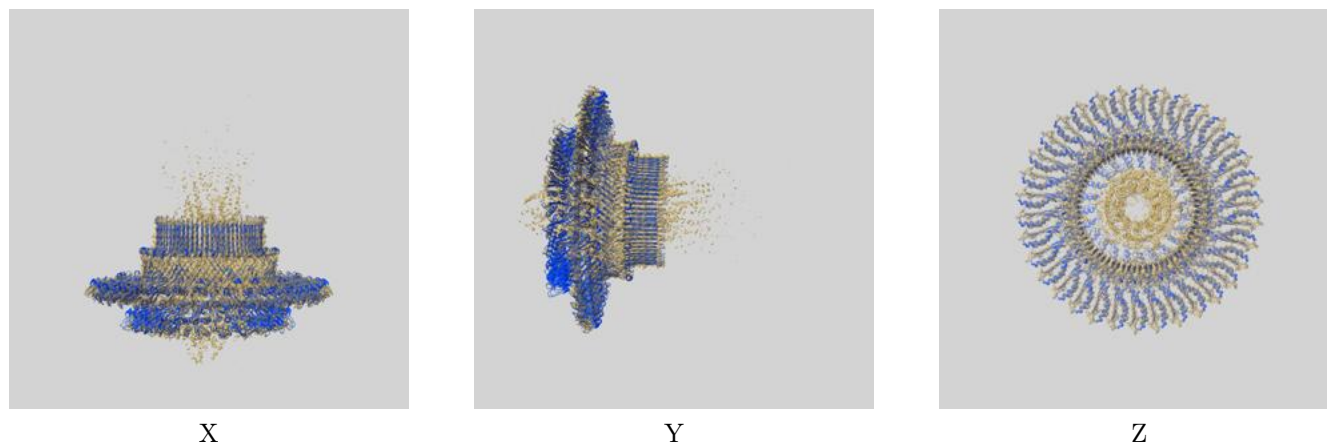
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.47	4.00
Unmasked-calculated*	6.96	9.98	7.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

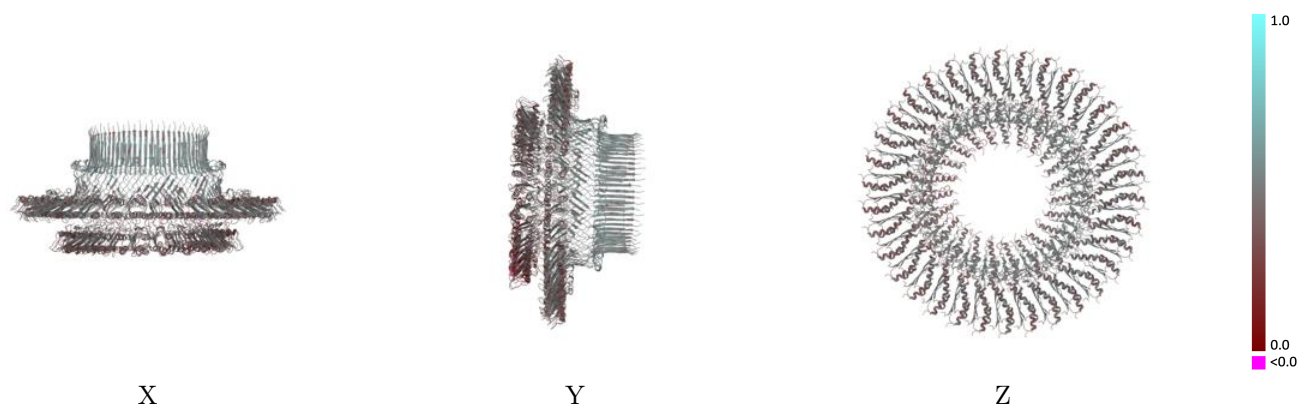
This section contains information regarding the fit between EMDB map EMD-12195 and PDB model 7BK0. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



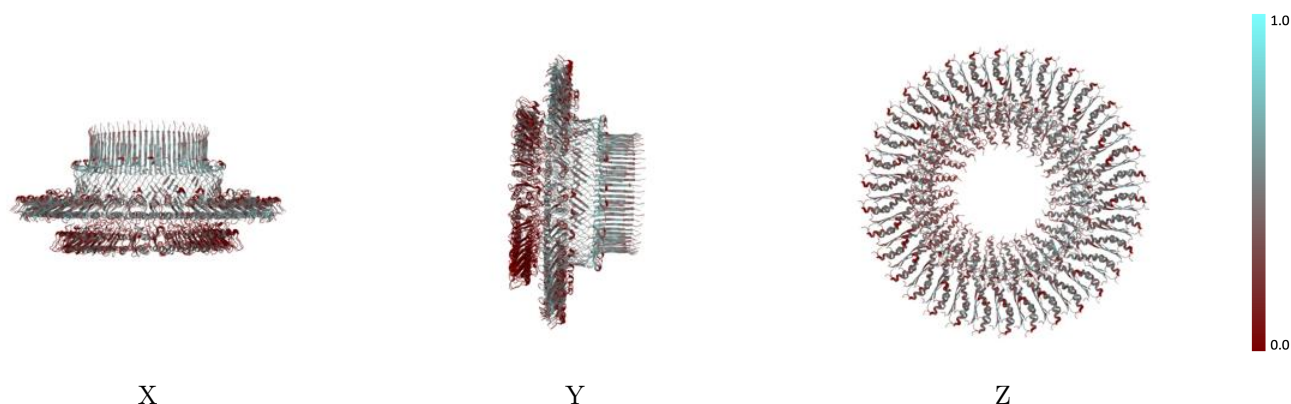
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



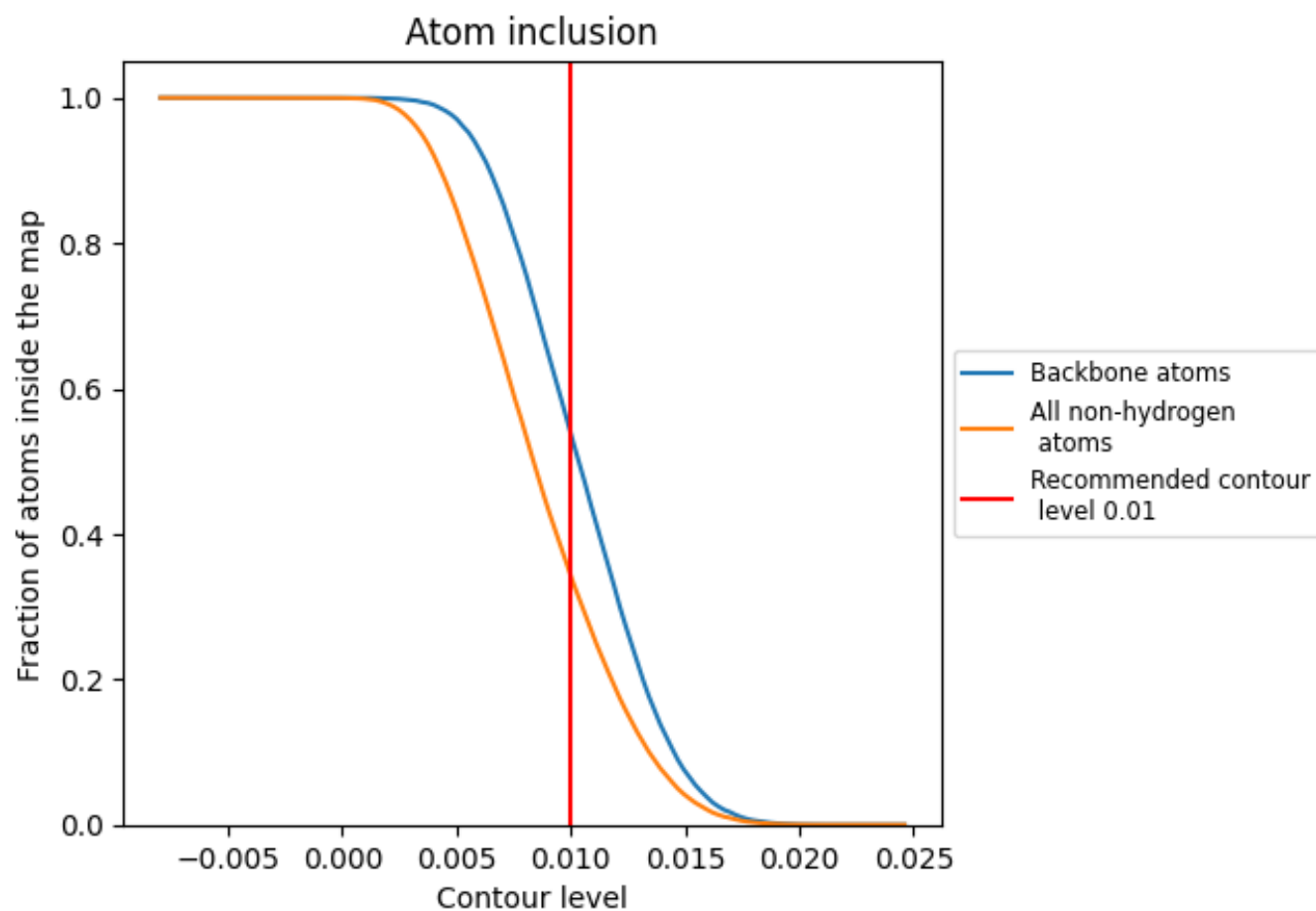
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 34% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3425	 0.4320
A	 0.4503	 0.4750
B	 0.3730	 0.4420
C	 0.3814	 0.4520
D	 0.4425	 0.4620
E	 0.3560	 0.4460
F	 0.4408	 0.4680
G	 0.3640	 0.4500
H	 0.3539	 0.4420
I	 0.3550	 0.4370
J	 0.4408	 0.4600
K	 0.3418	 0.4330
L	 0.3133	 0.4370
M	 0.4451	 0.4600
N	 0.3069	 0.4170
O	 0.2826	 0.4180
P	 0.4039	 0.4500
Q	 0.2673	 0.4070
R	 0.2673	 0.4030
S	 0.4091	 0.4570
T	 0.2435	 0.3790
U	 0.2499	 0.3740
V	 0.3774	 0.4360
W	 0.2361	 0.3850
X	 0.2567	 0.3930
Y	 0.2763	 0.4100
Z	 0.4177	 0.4510
a	 0.3117	 0.4260
b	 0.4391	 0.4550
c	 0.3238	 0.4320
d	 0.3487	 0.4350
e	 0.4477	 0.4670
f	 0.3492	 0.4350
g	 0.3624	 0.4430
h	 0.3745	 0.4520

