wwPDB EM Validation Summary Report (i)

Aug 15, 2024 – 01:52 PM EDT

PDB ID	:	8T8P
EMDB ID	:	EMD-41101
Title	:	33-mer FliF MS-ring from Salmonella
Authors	:	Singh, P.K.; Iverson, T.M.
Deposited on	:	2023-06-23
Resolution	:	3.40 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 (i) 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 (i)) were used in the production of this report:

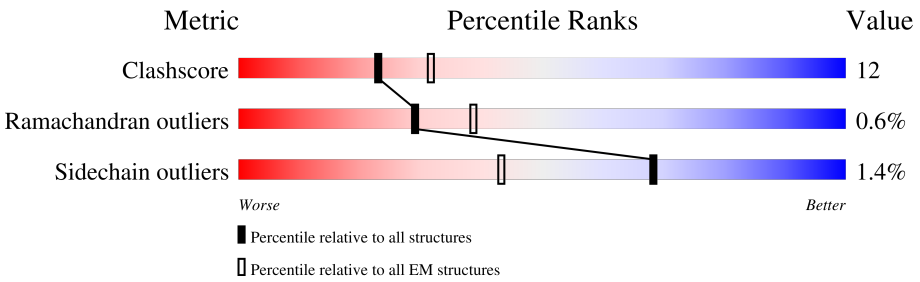
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 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)
Clashscore	158937	4297
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 <=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	• 29% 16% 55%
1	AA	560	13% 47% 9% 44%
1	B	560	13% 48% 8% 44%
1	BA	560	• 34% 10% • 55%
1	C	560	• 33% 12% 55%
1	CA	560	• 30% 15% • 55%
1	D	560	• 30% 15% 55%
1	DA	560	13% 47% 8% • 44%

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Mol	Chain	Length	Quality of chain
1	E	560	13% 47% 8% 44%
1	EA	560	34% 11% 55%
1	F	560	31% 14% 55%
1	FA	560	30% 15% 55%
1	G	560	32% 13% 55%
1	GA	560	13% 48% 8% 44%
1	H	560	13% 48% 7% 44%
1	HA	560	5% 32% 12% 55%
1	I	560	32% 13% 55%
1	J	560	30% 14% 55%
1	K	560	13% 46% 9% 44%
1	L	560	32% 13% 55%
1	M	560	29% 15% 55%
1	N	560	13% 48% 8% 44%
1	O	560	34% 11% 55%
1	P	560	29% 16% 55%
1	Q	560	14% 48% 7% 44%
1	R	560	33% 12% 55%
1	S	560	30% 15% 55%
1	T	560	14% 47% 8% 44%
1	V	560	33% 12% 55%
1	W	560	30% 15% 55%
1	X	560	14% 47% 8% 44%
1	Y	560	31% 14% 55%
1	Z	560	30% 15% 55%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 64845 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
			Total	C	N	O	S		
1	A	254	1945	1190	358	393	4	0	0
1	B	311	2005	1209	387	406	3	0	0
1	C	254	1945	1190	358	393	4	0	0
1	D	254	1945	1190	358	393	4	0	0
1	E	311	2005	1209	387	406	3	0	0
1	F	254	1945	1190	358	393	4	0	0
1	G	254	1945	1190	358	393	4	0	0
1	H	311	2005	1209	387	406	3	0	0
1	I	254	1945	1190	358	393	4	0	0
1	J	254	1945	1190	358	393	4	0	0
1	K	311	2005	1209	387	406	3	0	0
1	L	254	1945	1190	358	393	4	0	0
1	M	254	1945	1190	358	393	4	0	0
1	N	311	2005	1209	387	406	3	0	0
1	O	254	1945	1190	358	393	4	0	0
1	P	254	1945	1190	358	393	4	0	0
1	Q	311	2005	1209	387	406	3	0	0

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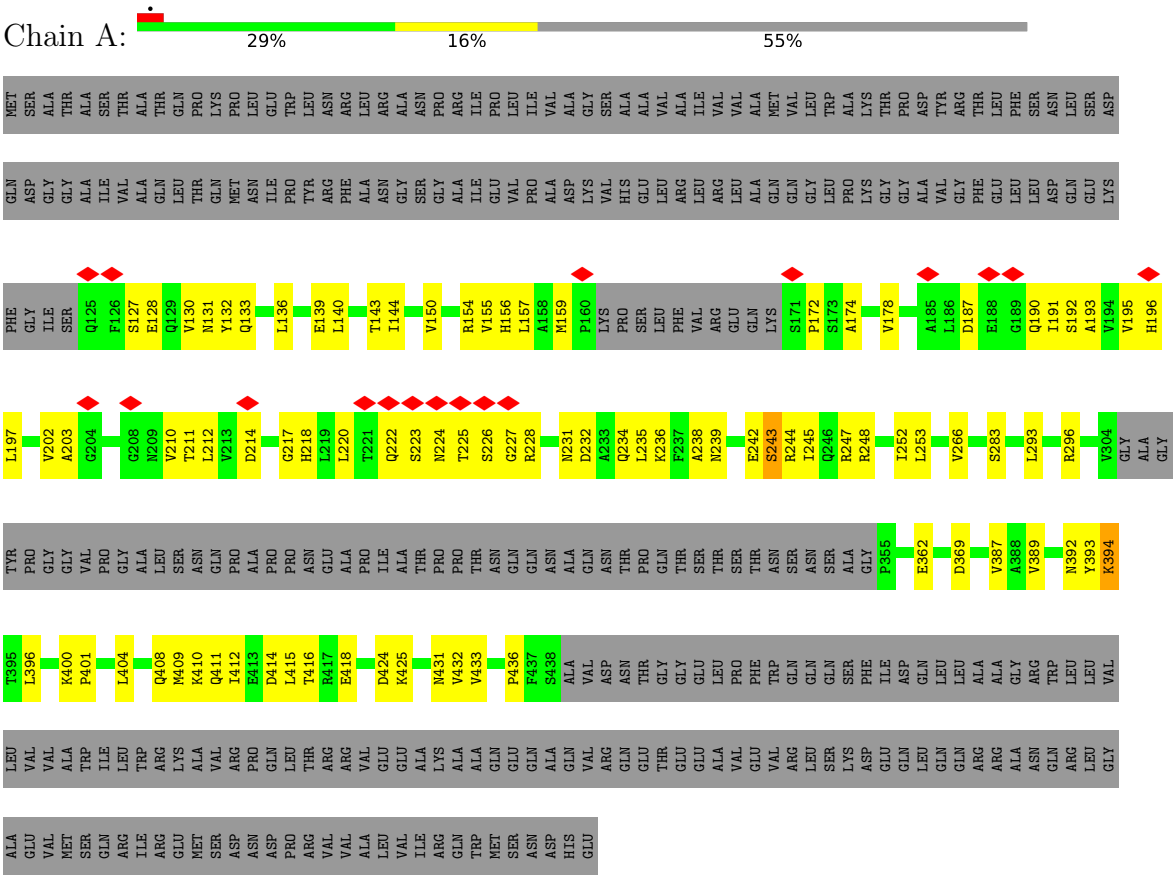
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	S	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	T	311	2005	1209	387	406	3	0	0
			Total	C	N	O	S		
1	V	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	W	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	X	311	2005	1209	387	406	3	0	0
			Total	C	N	O	S		
1	Y	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	Z	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	AA	311	2005	1209	387	406	3	0	0
			Total	C	N	O	S		
1	BA	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	CA	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	DA	311	2005	1209	387	406	3	0	0
			Total	C	N	O	S		
1	EA	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	FA	254	1945	1190	358	393	4	0	0
			Total	C	N	O	S		
1	GA	311	2005	1209	387	406	3	0	0
			Total	C	N	O	S		
1	HA	254	1945	1190	358	393	4	0	0

3 Residue-property plots (i)

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

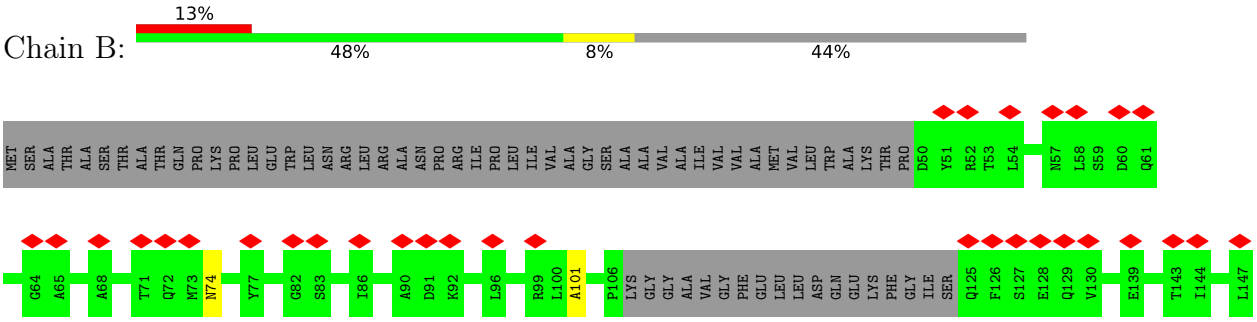
- Molecule 1: Flagellar M-ring protein

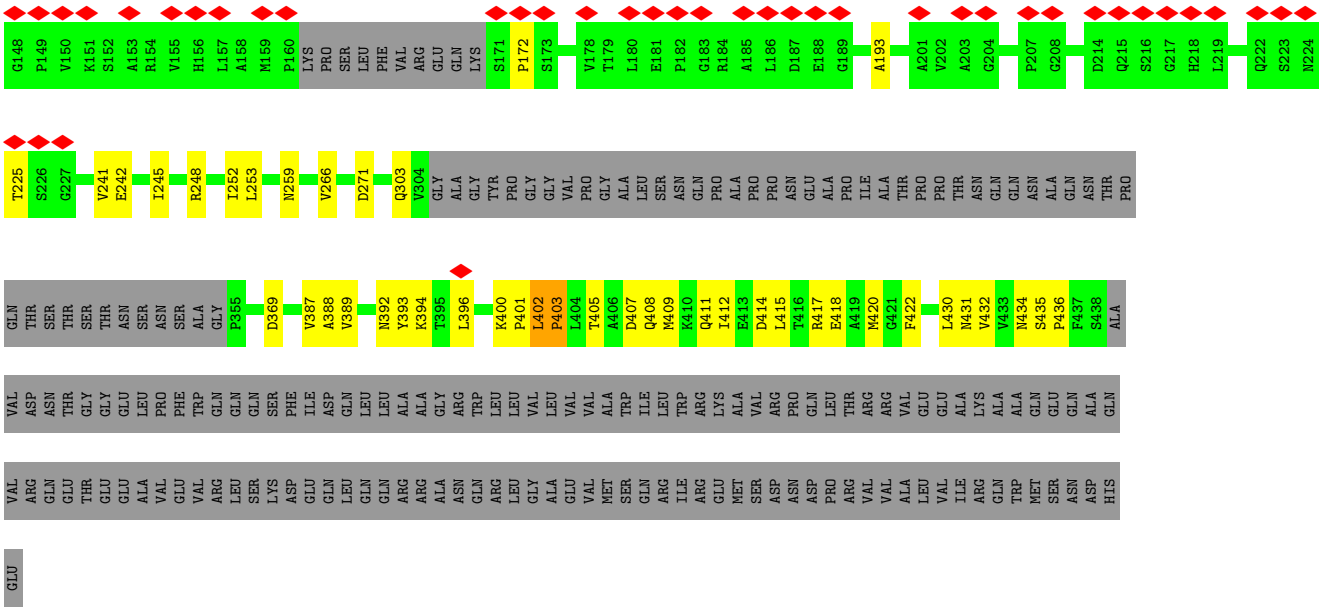
Chain A:



- Molecule 1: Flagellar M-ring protein

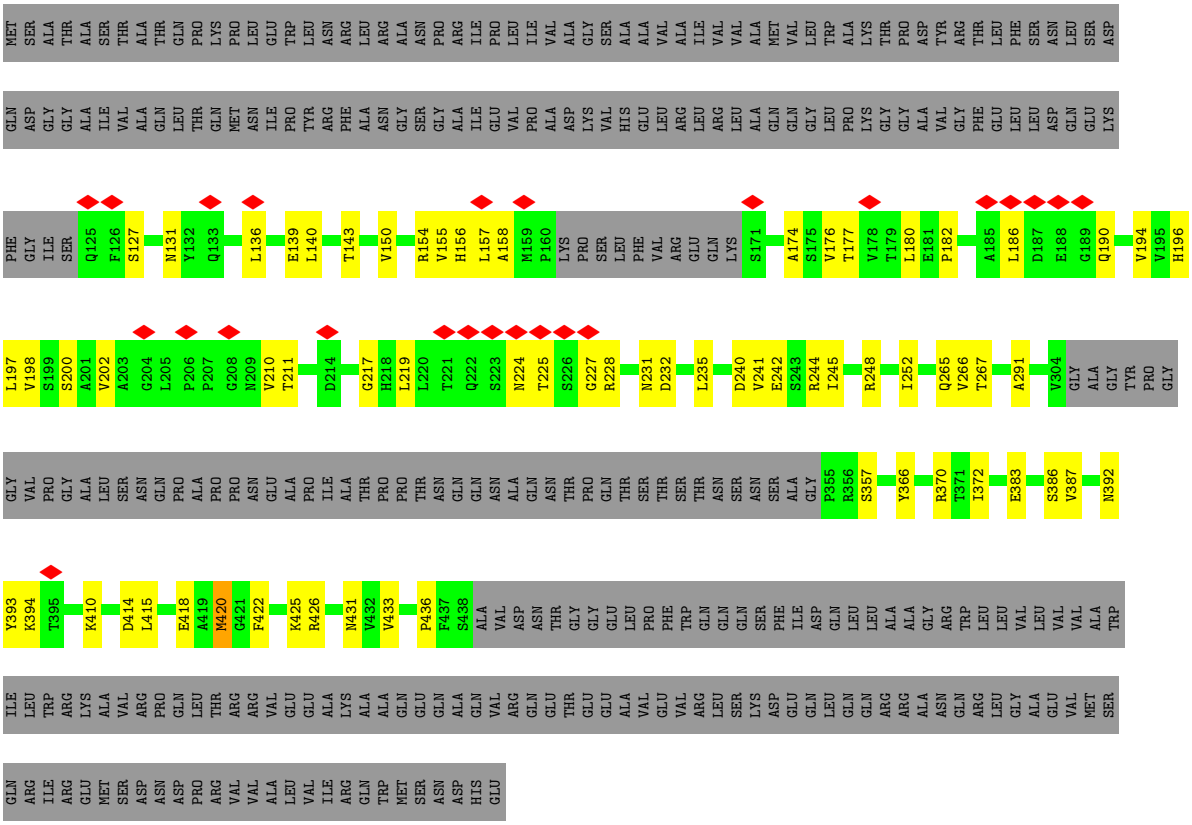
Chain B:





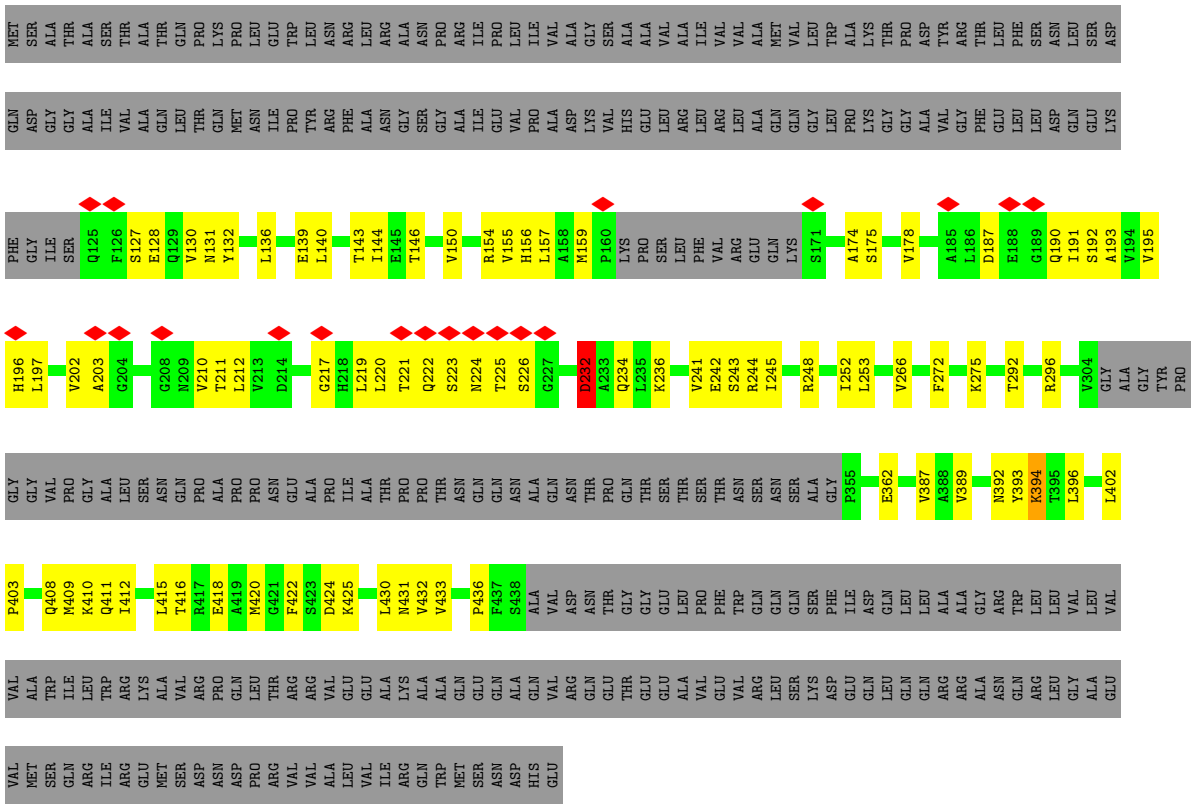
• Molecule 1: Flagellar M-ring protein

Chain C:



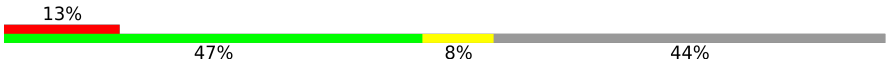
• Molecule 1: Flagellar M-ring protein

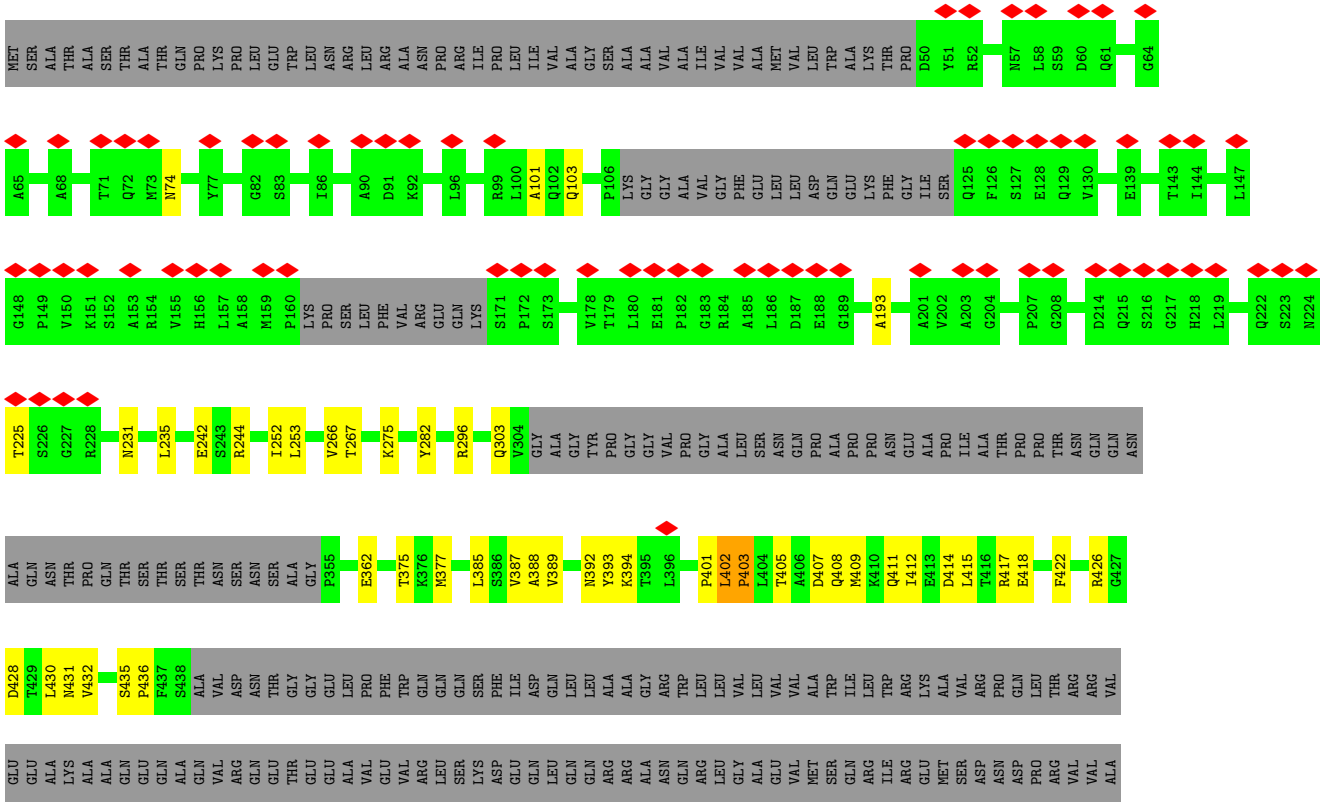
Chain D:



- Molecule 1: Flagellar M-ring protein

Chain E:





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

- Molecule 1: Flagellar M-ring protein

Chain F: 31% 14% • 55%

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

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

PHE GLY ILE SER Q125 F126 S127 N131 Y132 Q133 L136 E139 L140 T143 I144 K151 R154 V155 H156 L157 A158 M159 P160 LYS PRO SER LEU PHE VAL ARG GLU GLN LYS S171 A174 S175 V176 T177 V178 T179 L180 E181 P182 A185 L186 D187 E188 G189 Q190 I191 S192 A193

V194 V195 H196 S199 S200 A201 V202 A203 G204 L205 P206 P207 G208 N209 V210 T211 D214 G217 H218 L219 L220 T221 Q222 S223 N224 T225 S226 G227 R228 D229 L230 N231 D232 F237 D240 V241 E242 I245 R248 Q265 V266 T267 K275 L293 R296 S301 V304

GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY P355 R356 S357 T358 Q359 K376 E383 R384

L385 S386 V387 A388 V389 V390 V391 N392 Y393 K394 T395 L402 P403 D414 L415 M420 K425 R426 G427 D428 T429 L430 N431 V432 V433 N434 S435 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG

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

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

- Molecule 1: Flagellar M-ring protein

Chain G: 32% 13% • 55%

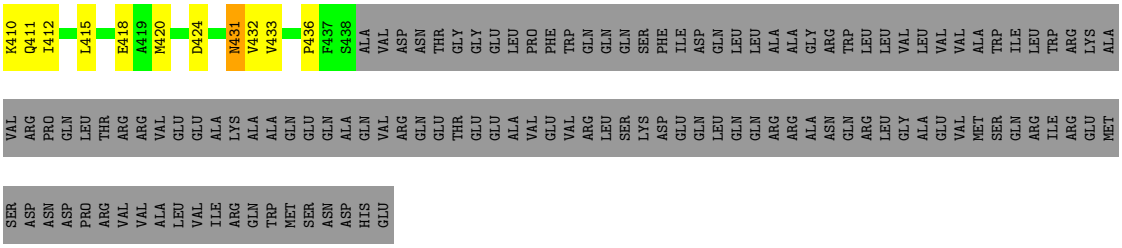
MET SER ALA THR ALA SER THR ALA THR GLN PRO LYS PRO LEU GLU TRP LEU ASN ARG LEU ARG ALA ASN PRO ARG ILE PRO LEU ILE VAL ALA GLY SER ALA ALA VAL ALA ILE VAL VAL ALA MET VAL LEU TRP ALA LYS THR PRO ASP TYR ARG THR LEU PHE SER ASN LEU SER ASP

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

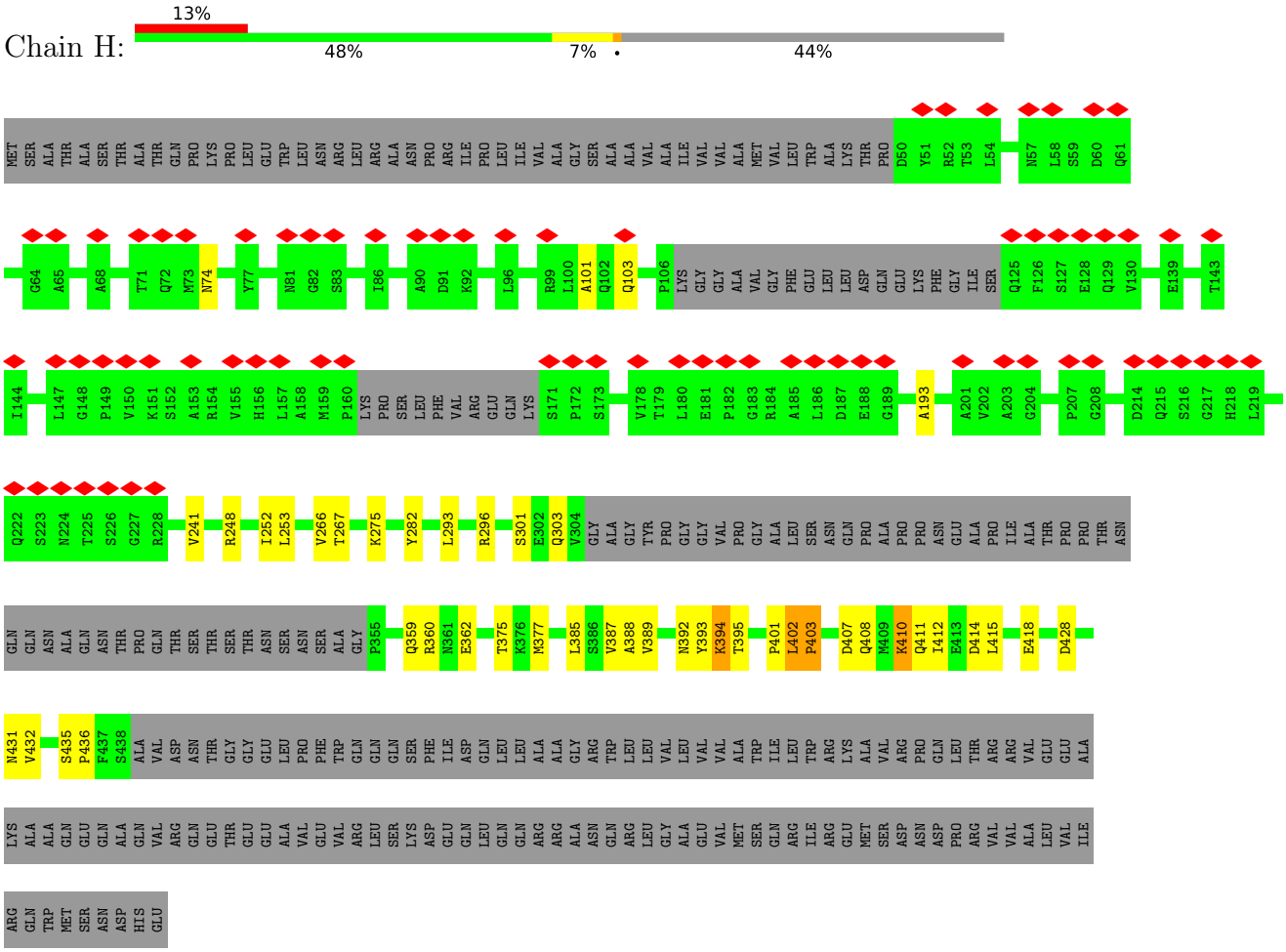
PHE GLY ILE SER Q125 F126 S127 E128 Q129 V130 N131 Y132 L136 E139 L140 T143 I144 V150 R154 V155 H156 L157 P160 LYS PRO SER LEU PHE VAL ARG GLU GLN LYS S171 A174 V178 A185 L186 D187 E188 G189 Q190 I191 S192 A193 V194 V195 H196 L197 A203

G204 G208 N209 V210 D214 G217 H218 L219 L220 T221 Q222 S223 N224 T225 S226 G227 D232 L235 N239 E242 S243 R244 R248 I252 L253 V266 T267 K275 T292 R296 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN

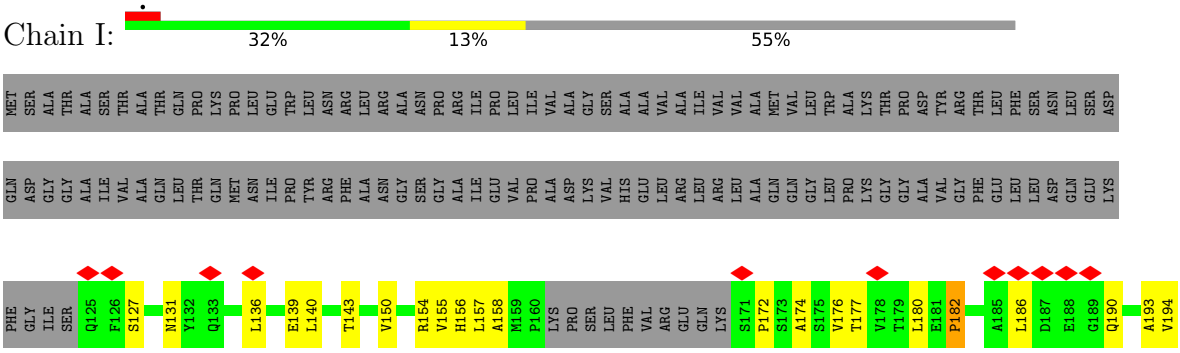
PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY P355 E362 M377 L385 S386 V387 A388 V389 N392 Y393 K394 T395 K400 P401 L402 P403 L404 Q408 M409

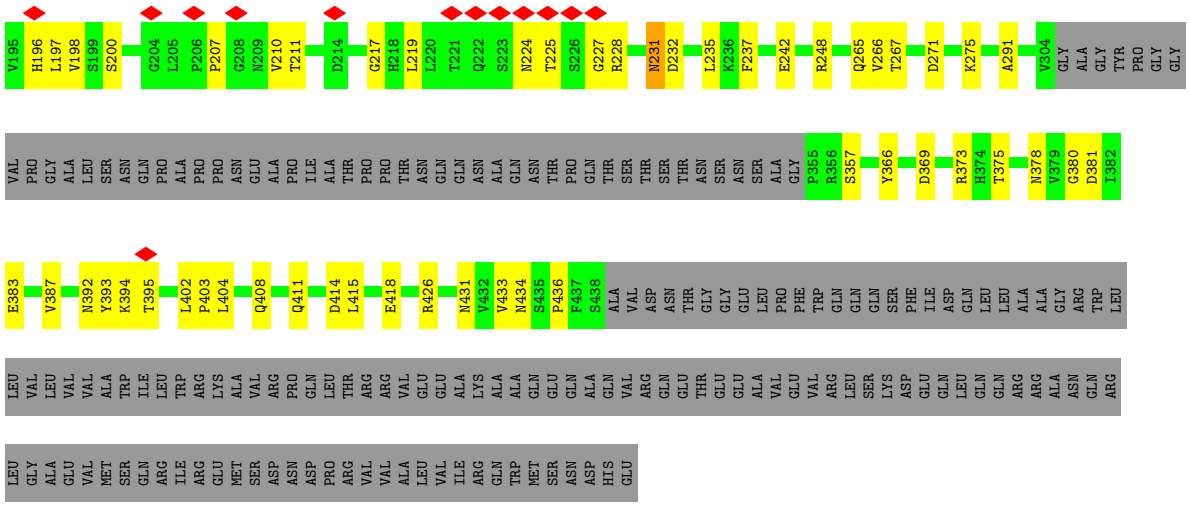


• Molecule 1: Flagellar M-ring protein



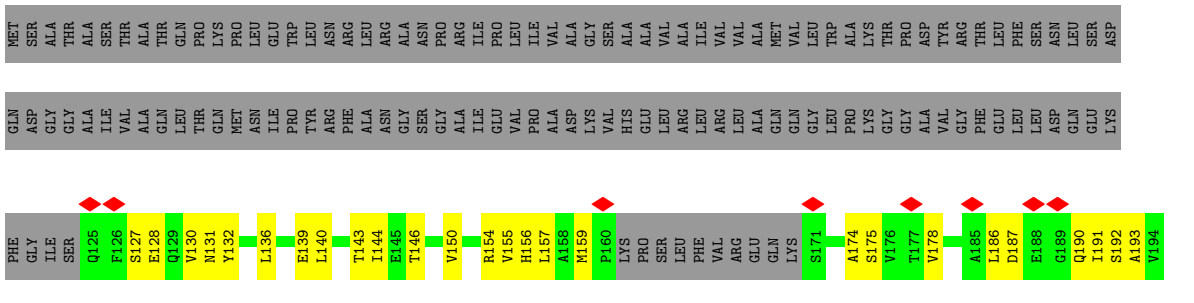
• Molecule 1: Flagellar M-ring protein





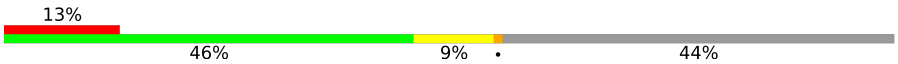
- Molecule 1: Flagellar M-ring protein

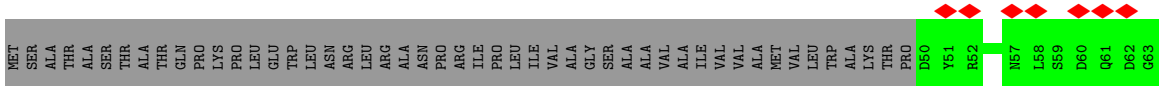
Chain J:

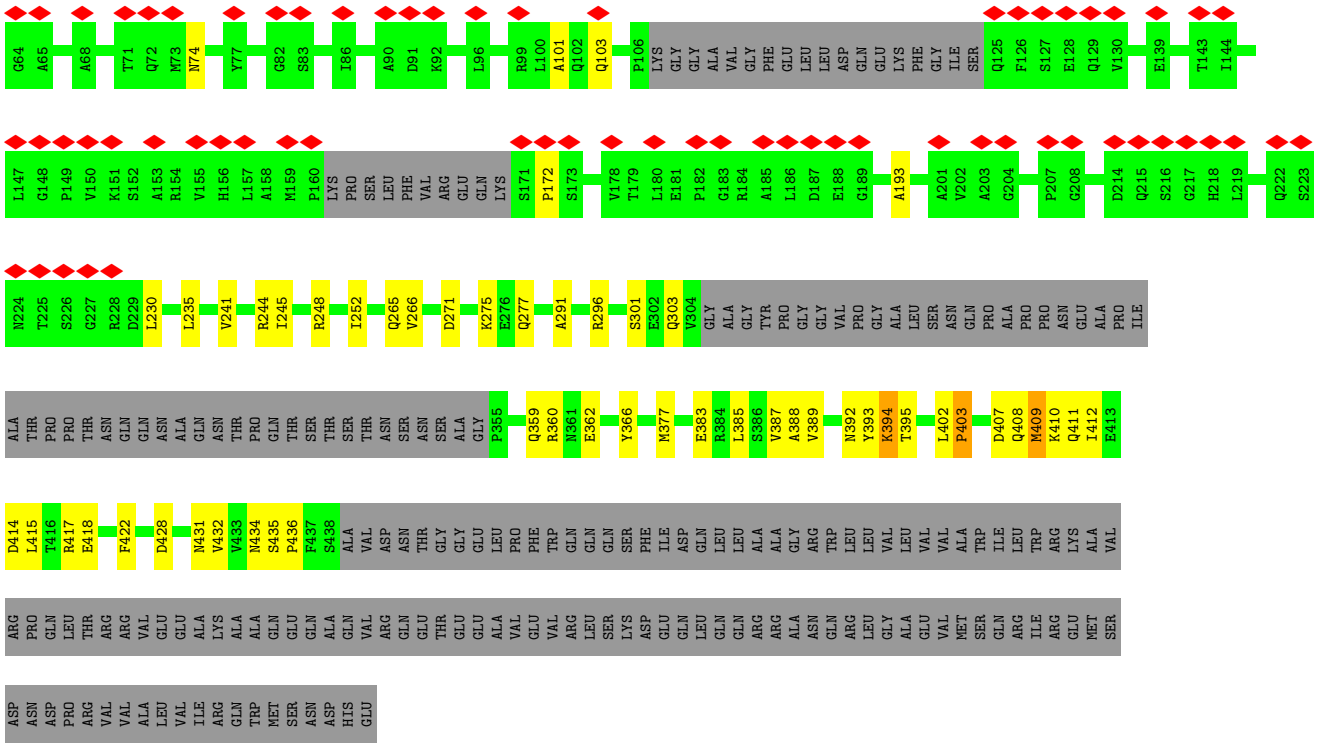


- Molecule 1: Flagellar M-ring protein

Chain K:

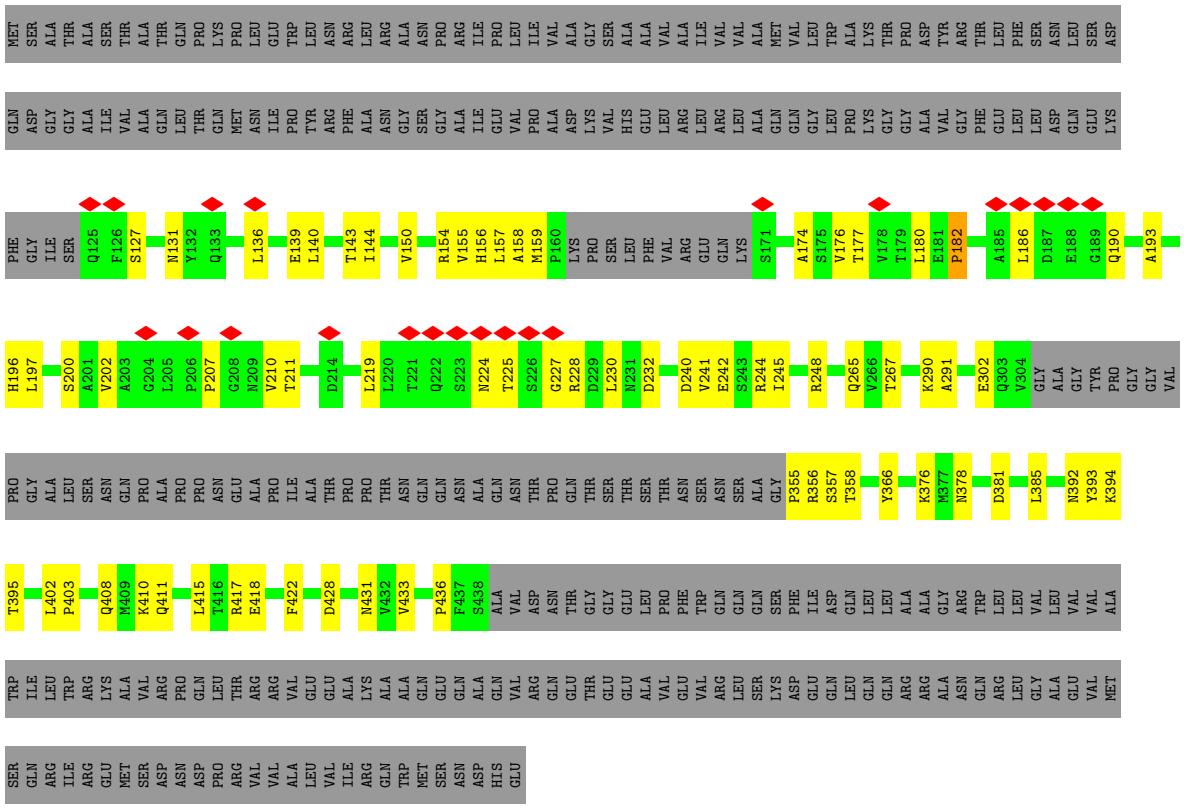






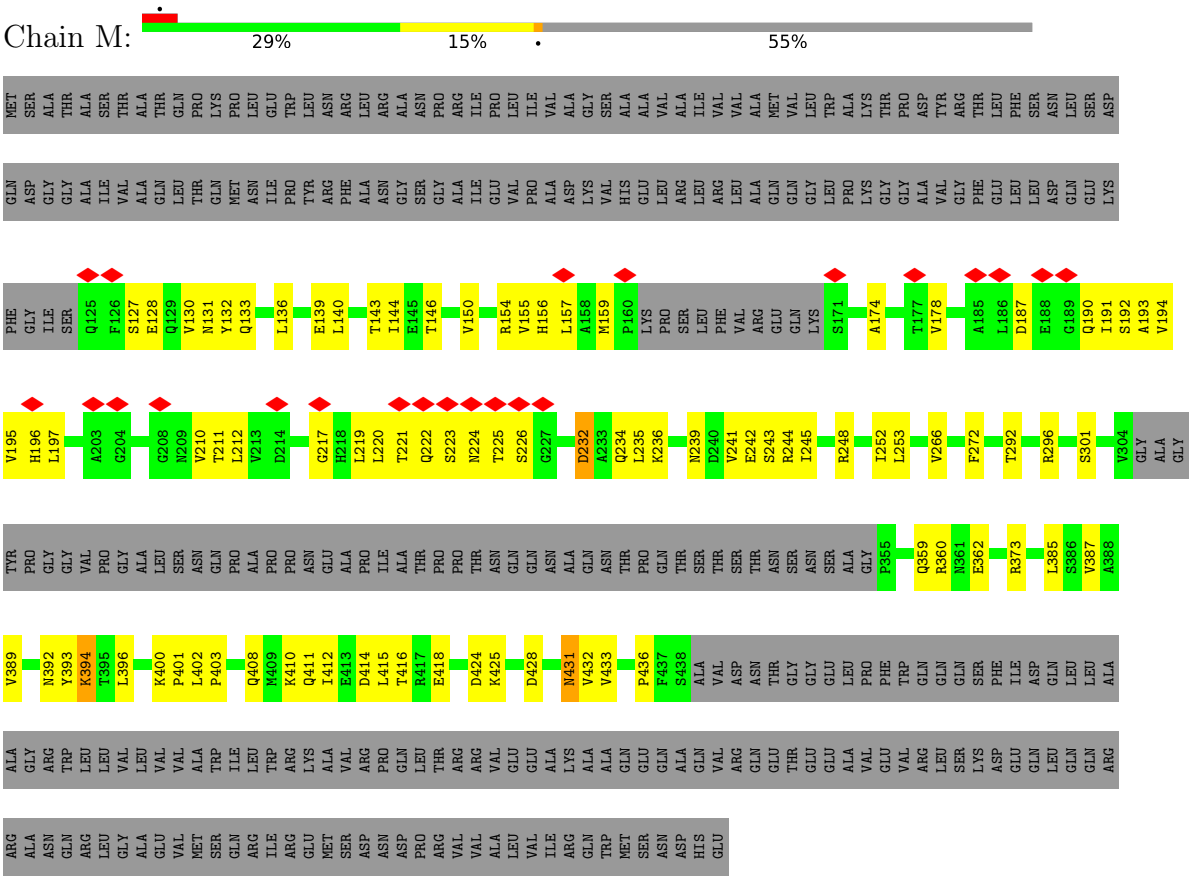
- Molecule 1: Flagellar M-ring protein

Chain L:



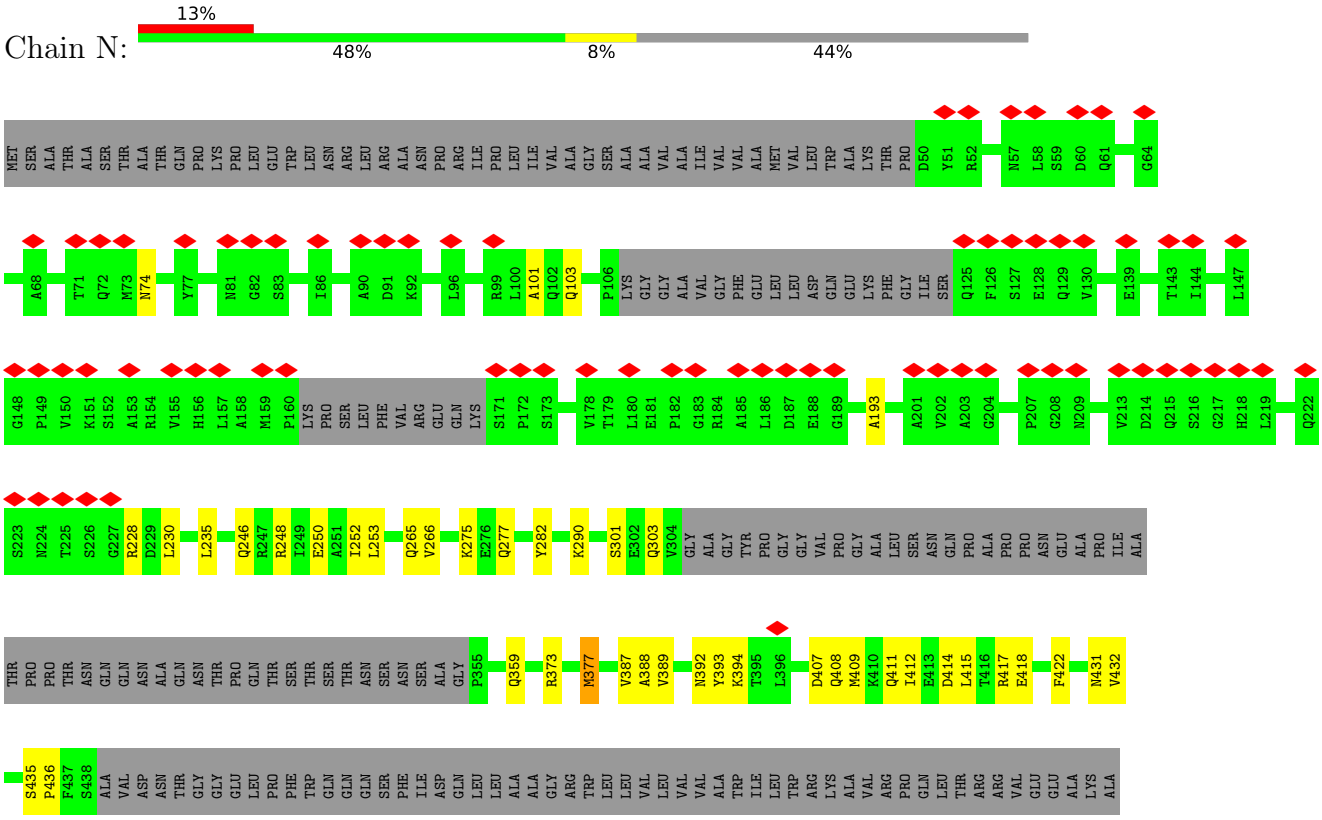
- Molecule 1: Flagellar M-ring protein

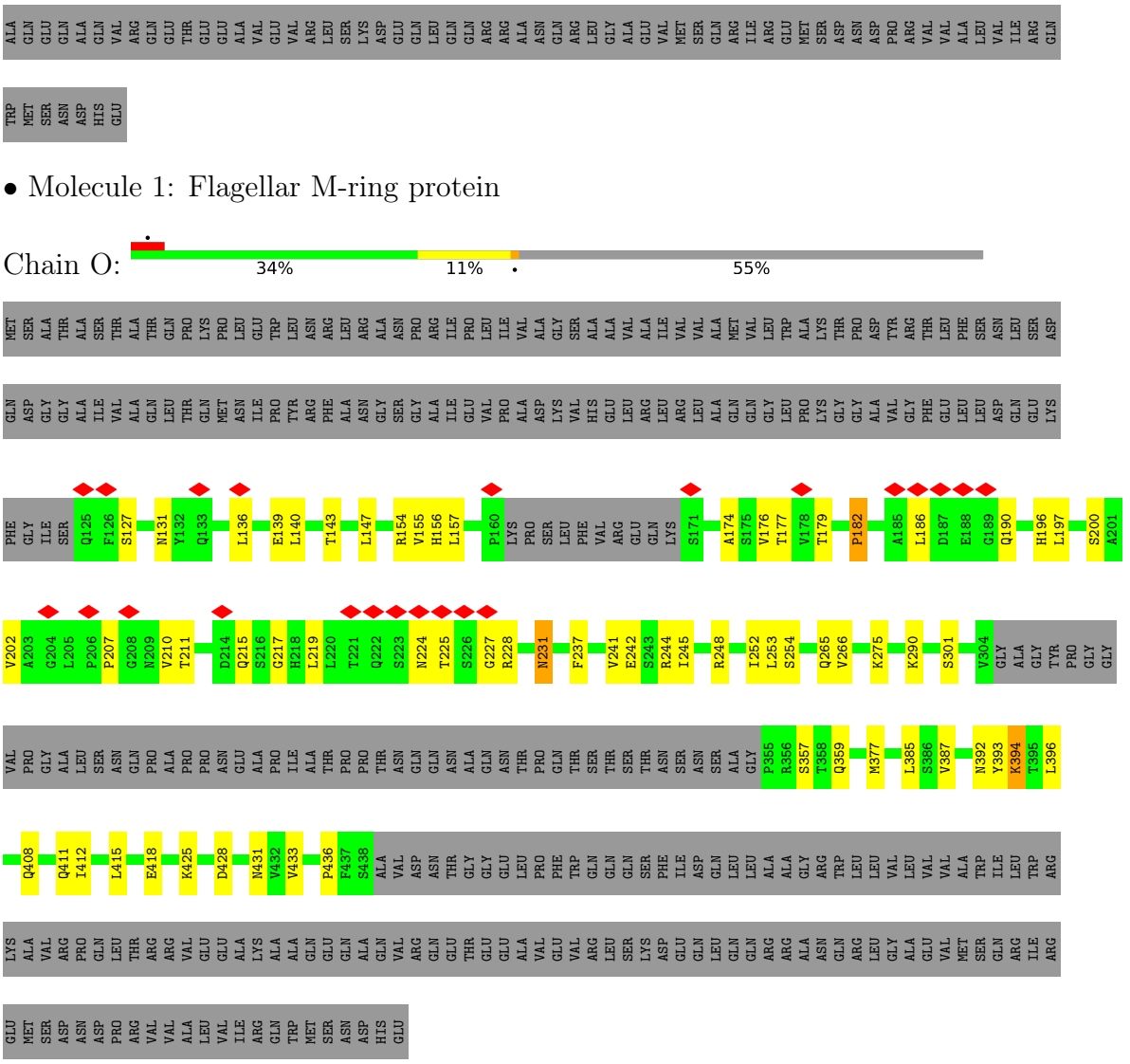
Chain M:



- Molecule 1: Flagellar M-ring protein

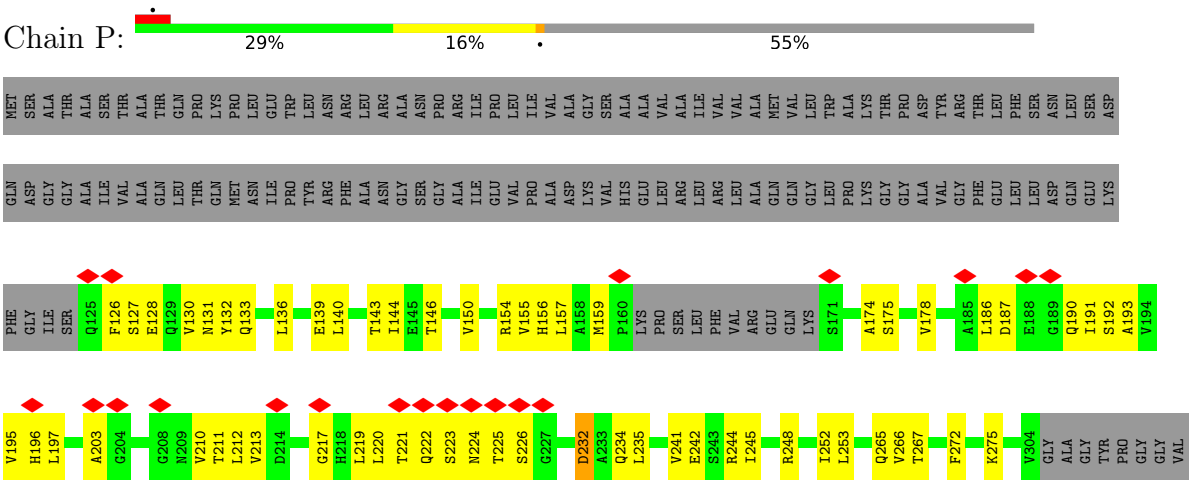
Chain N:

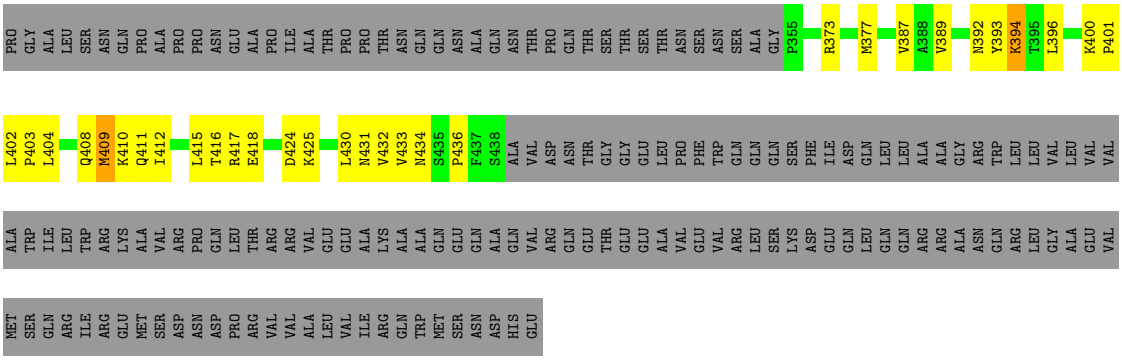




• Molecule 1: Flagellar M-ring protein

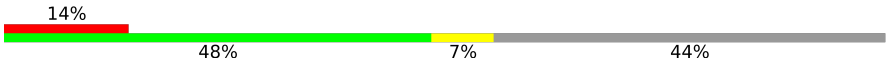
• Molecule 1: Flagellar M-ring protein

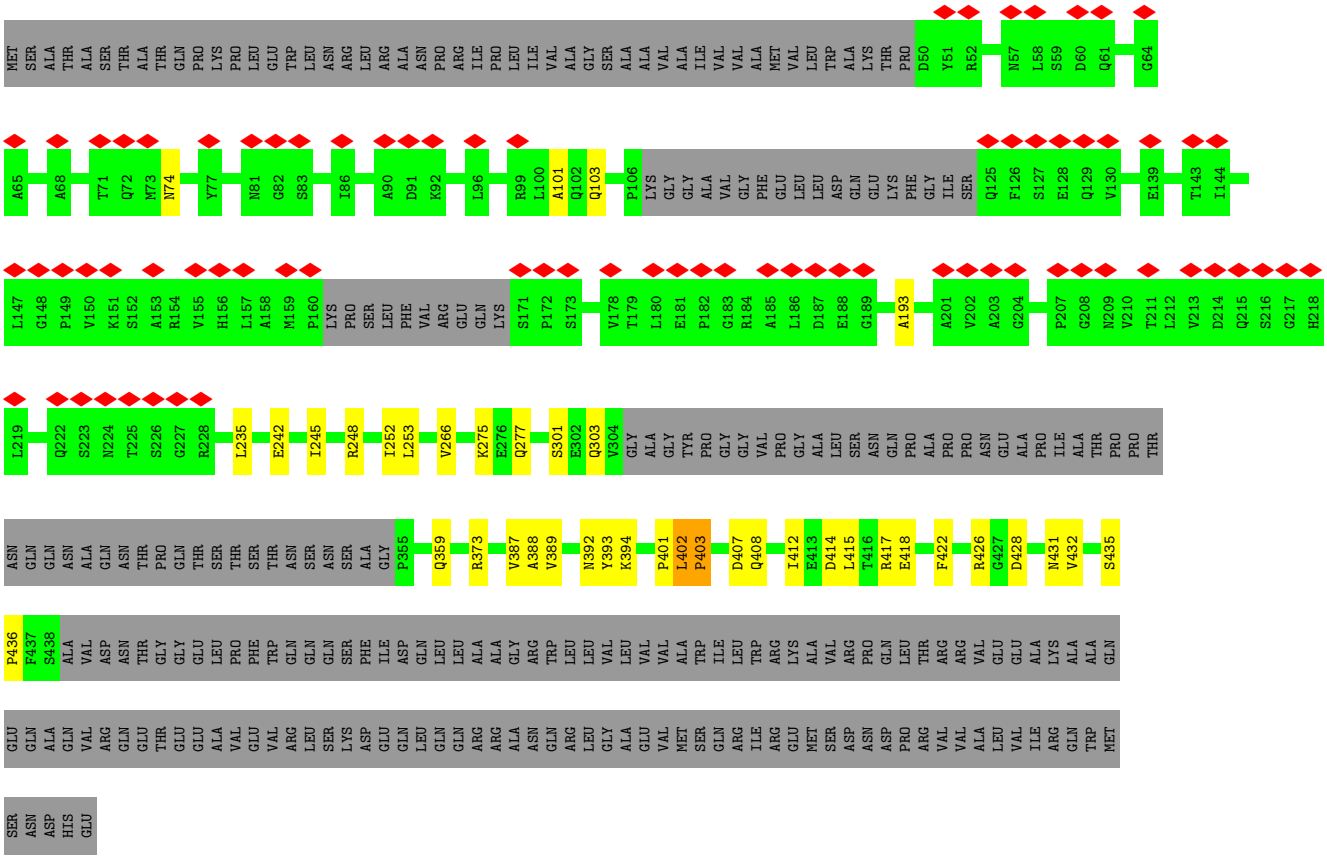




- Molecule 1: Flagellar M-ring protein

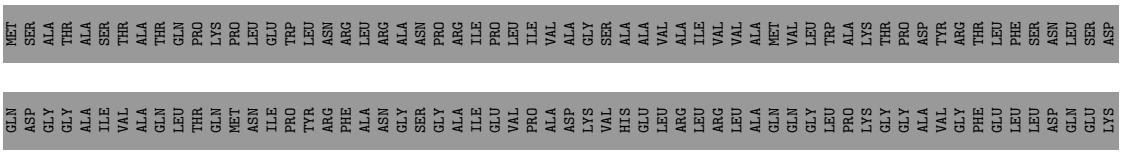
Chain Q:

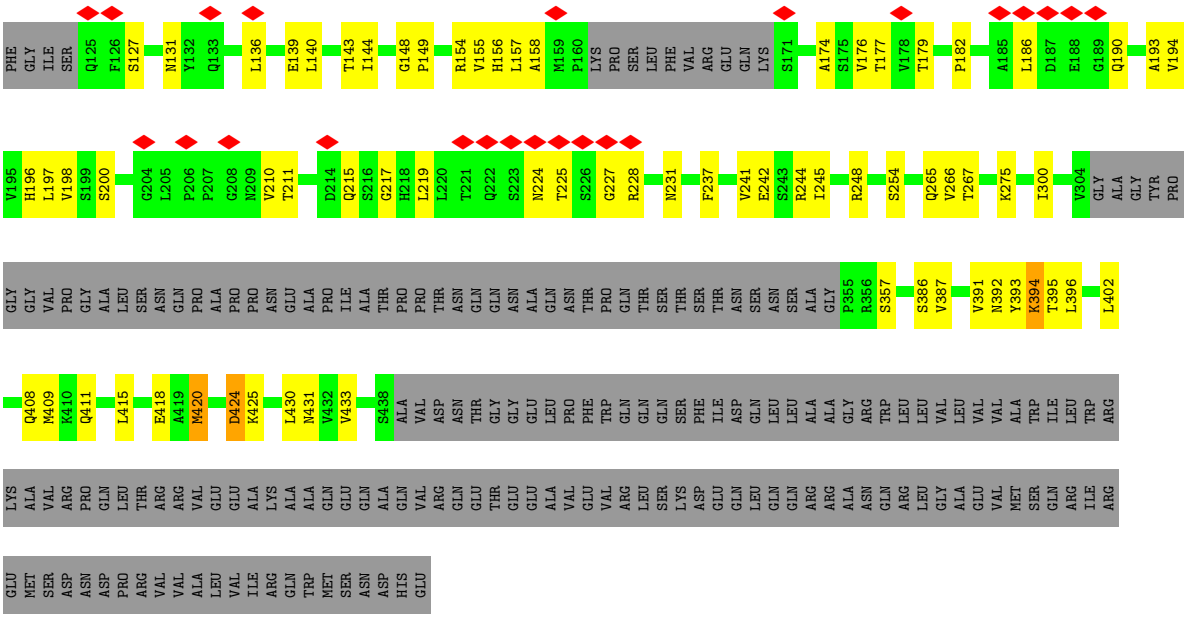




- Molecule 1: Flagellar M-ring protein

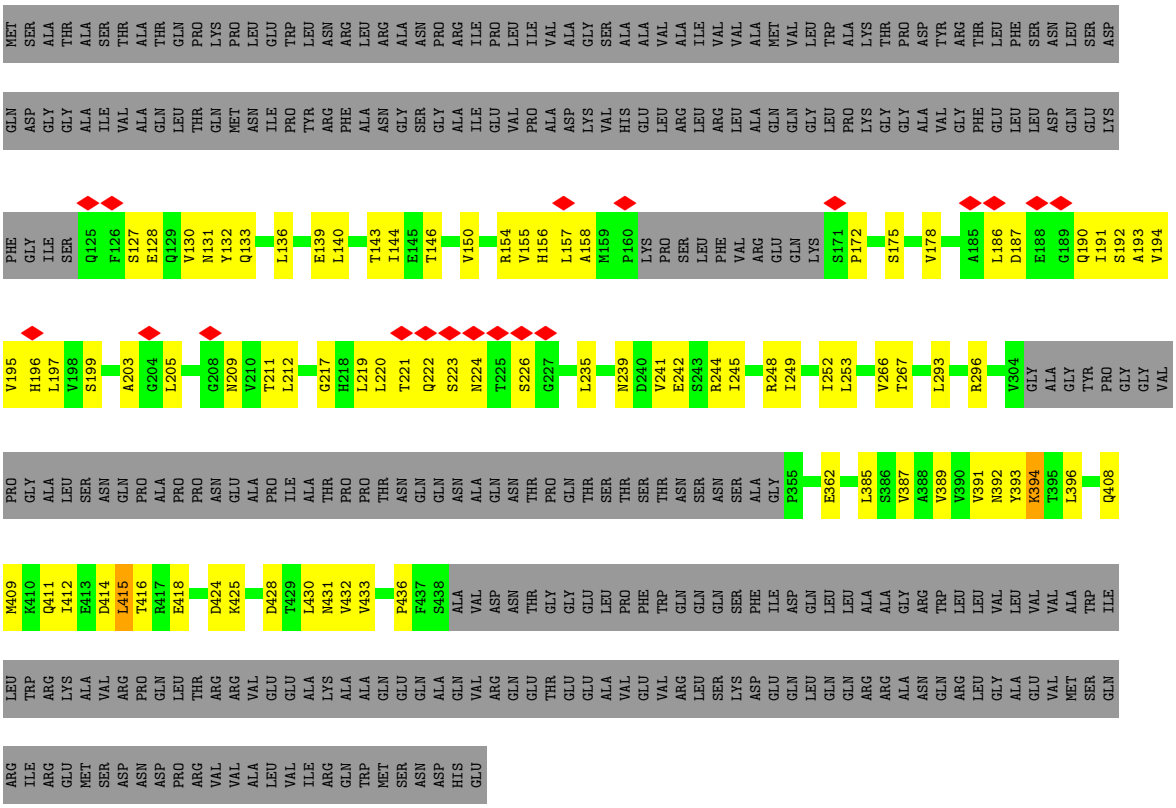
Chain R:





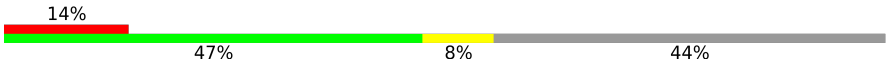
- Molecule 1: Flagellar M-ring protein

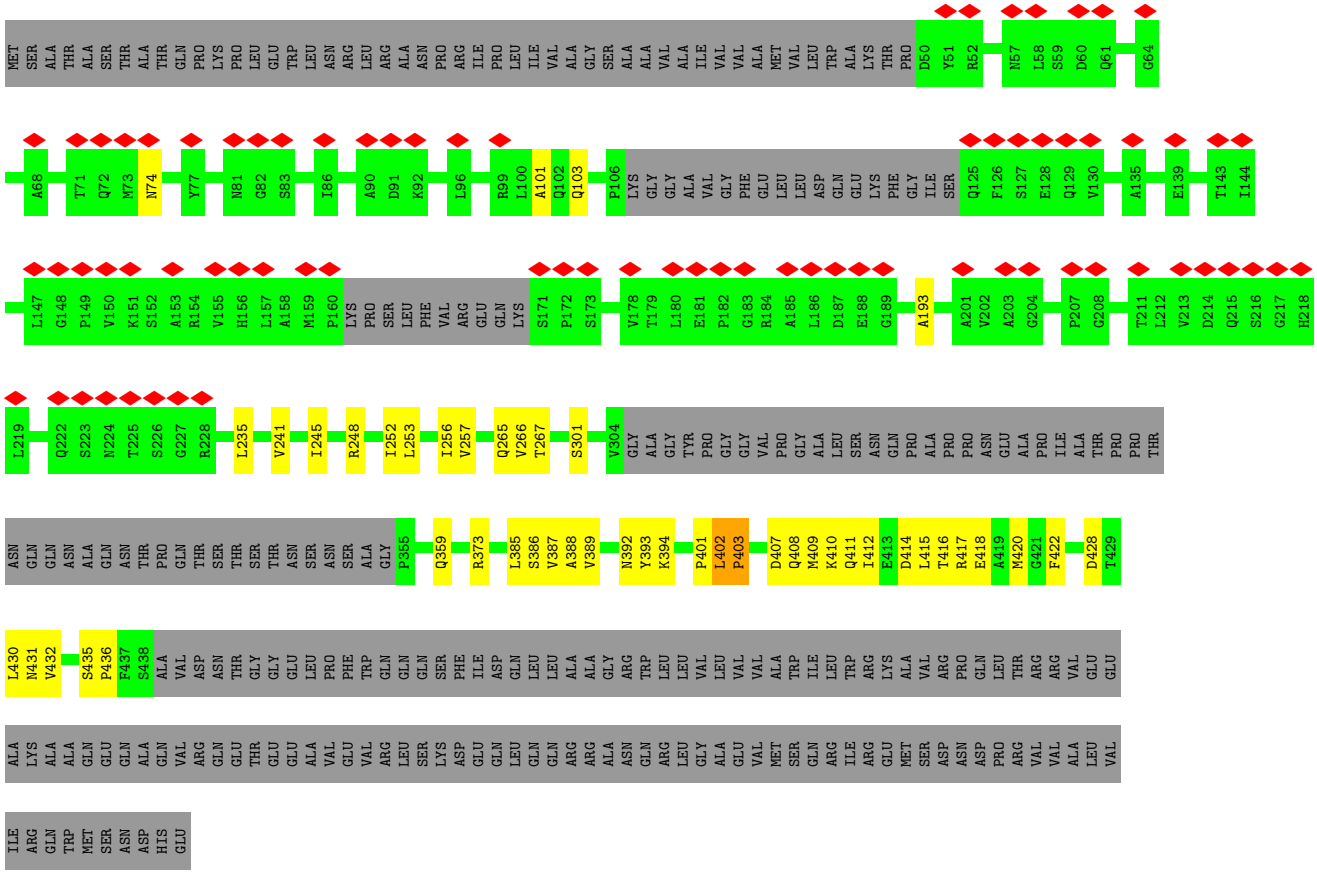
Chain S:



- Molecule 1: Flagellar M-ring protein

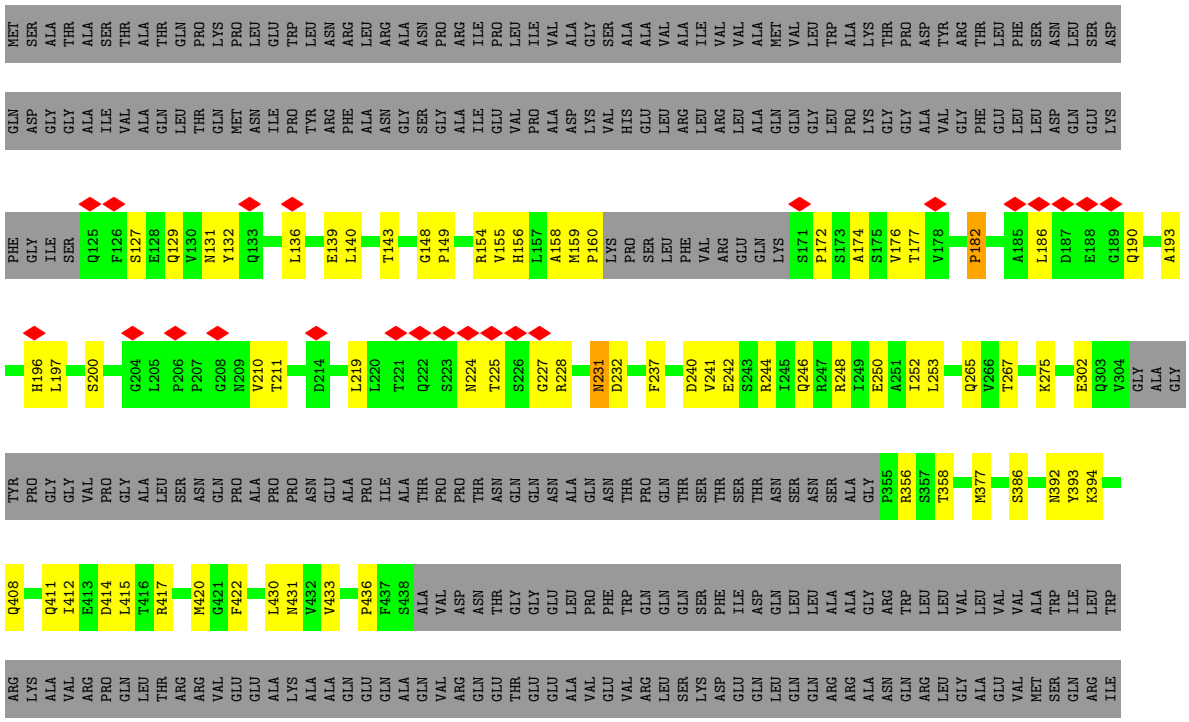
Chain T:





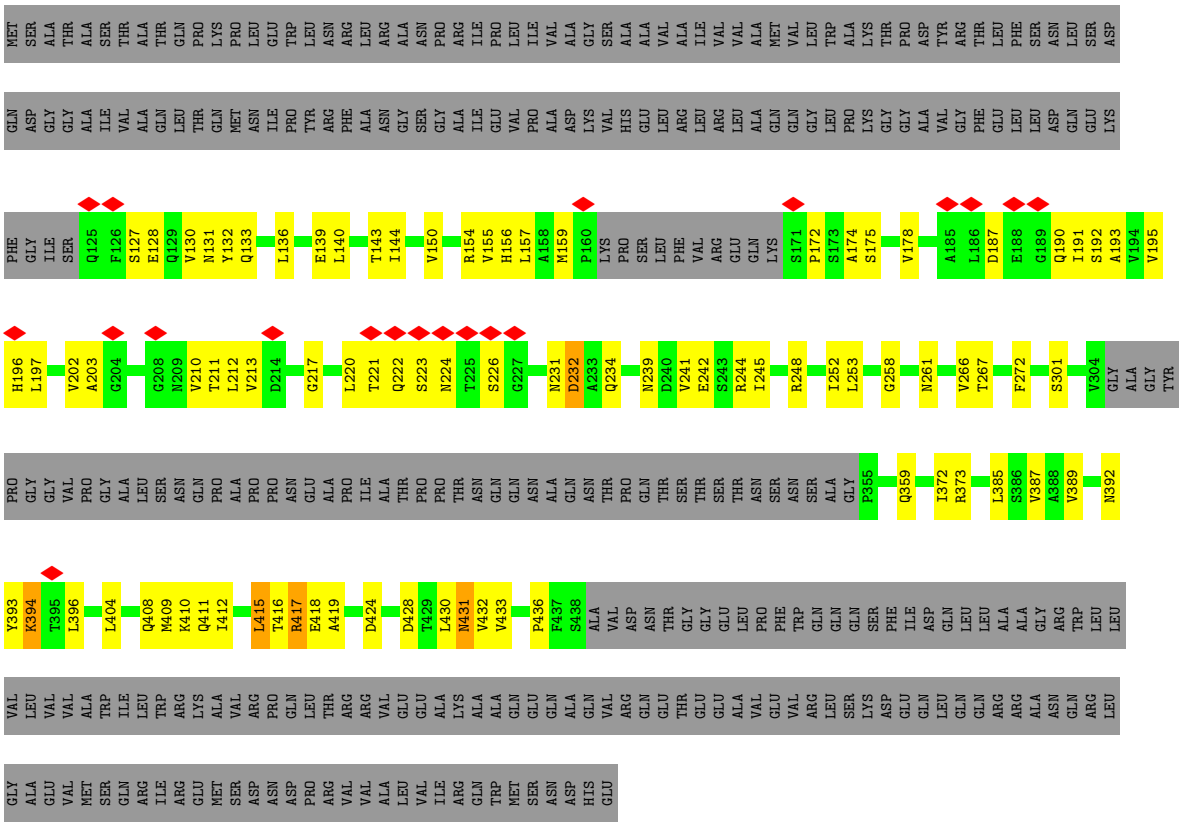
• Molecule 1: Flagellar M-ring protein

Chain V: 33% 12% 55%



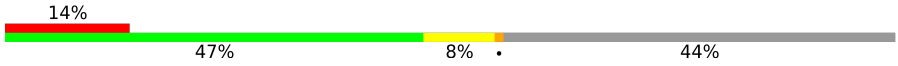
• Molecule 1: Flagellar M-ring protein

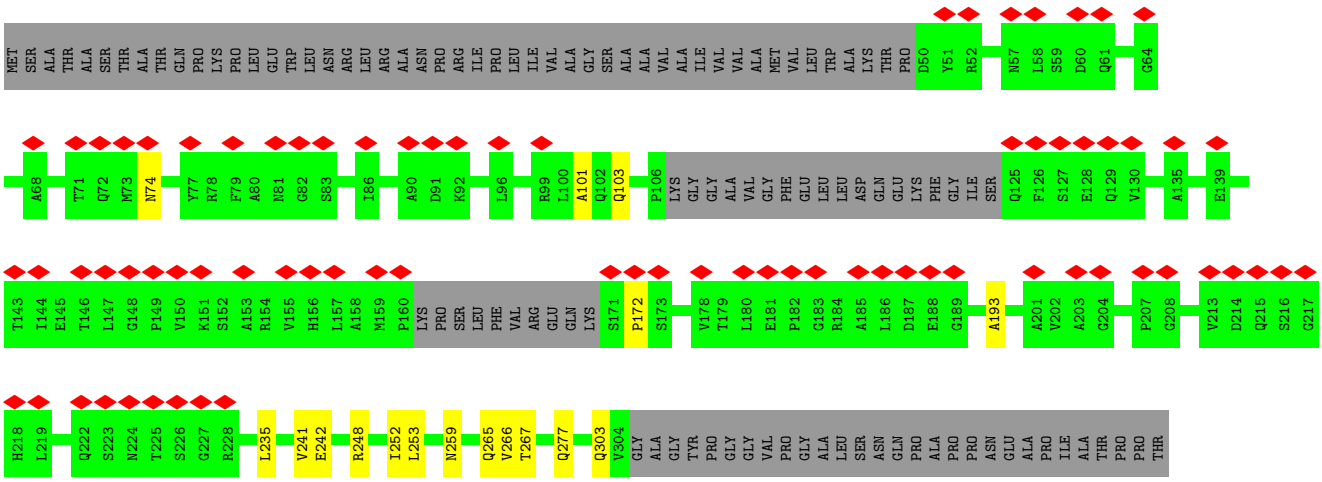
Chain W:

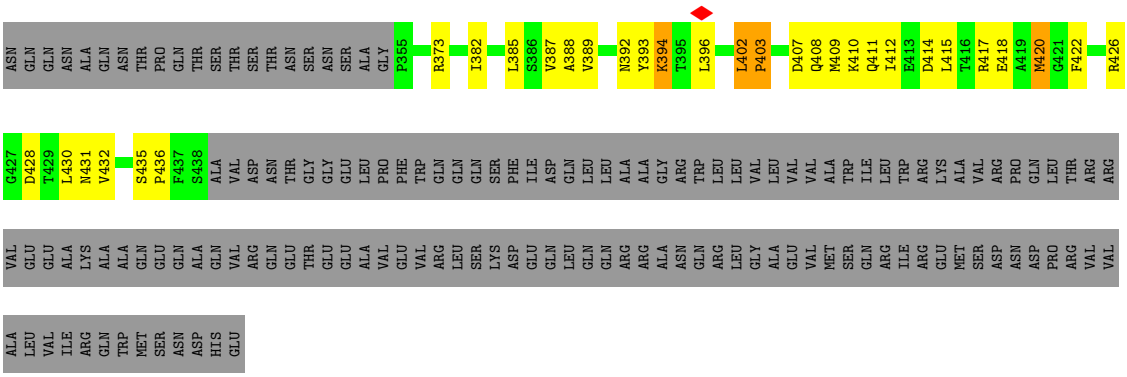


• Molecule 1: Flagellar M-ring protein

Chain X:

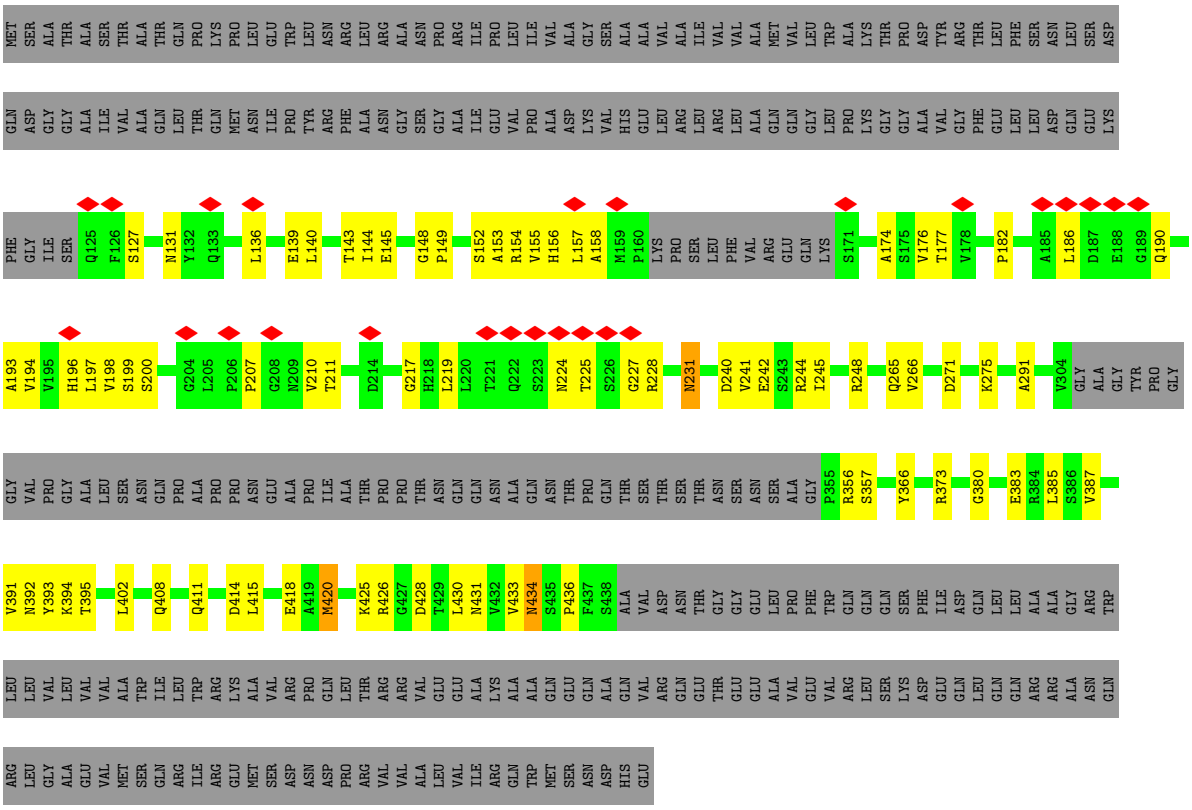






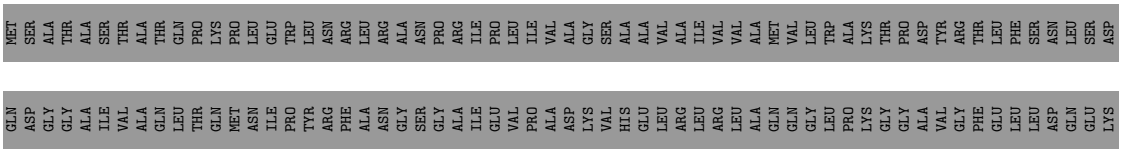
• Molecule 1: Flagellar M-ring protein

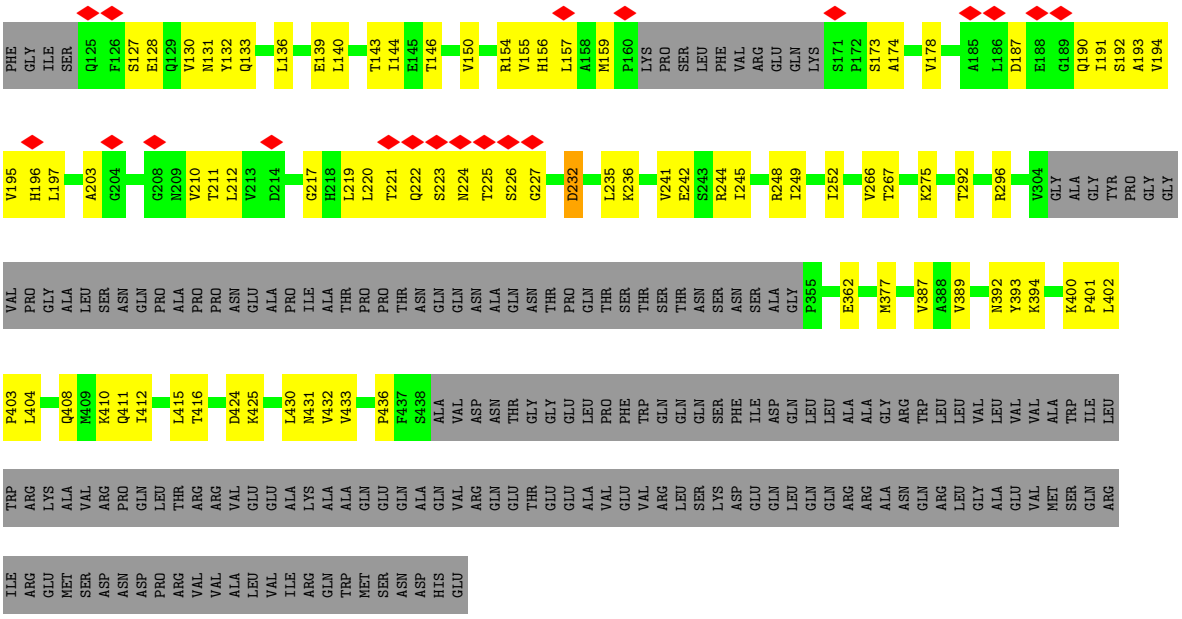
Chain Y:



• Molecule 1: Flagellar M-ring protein

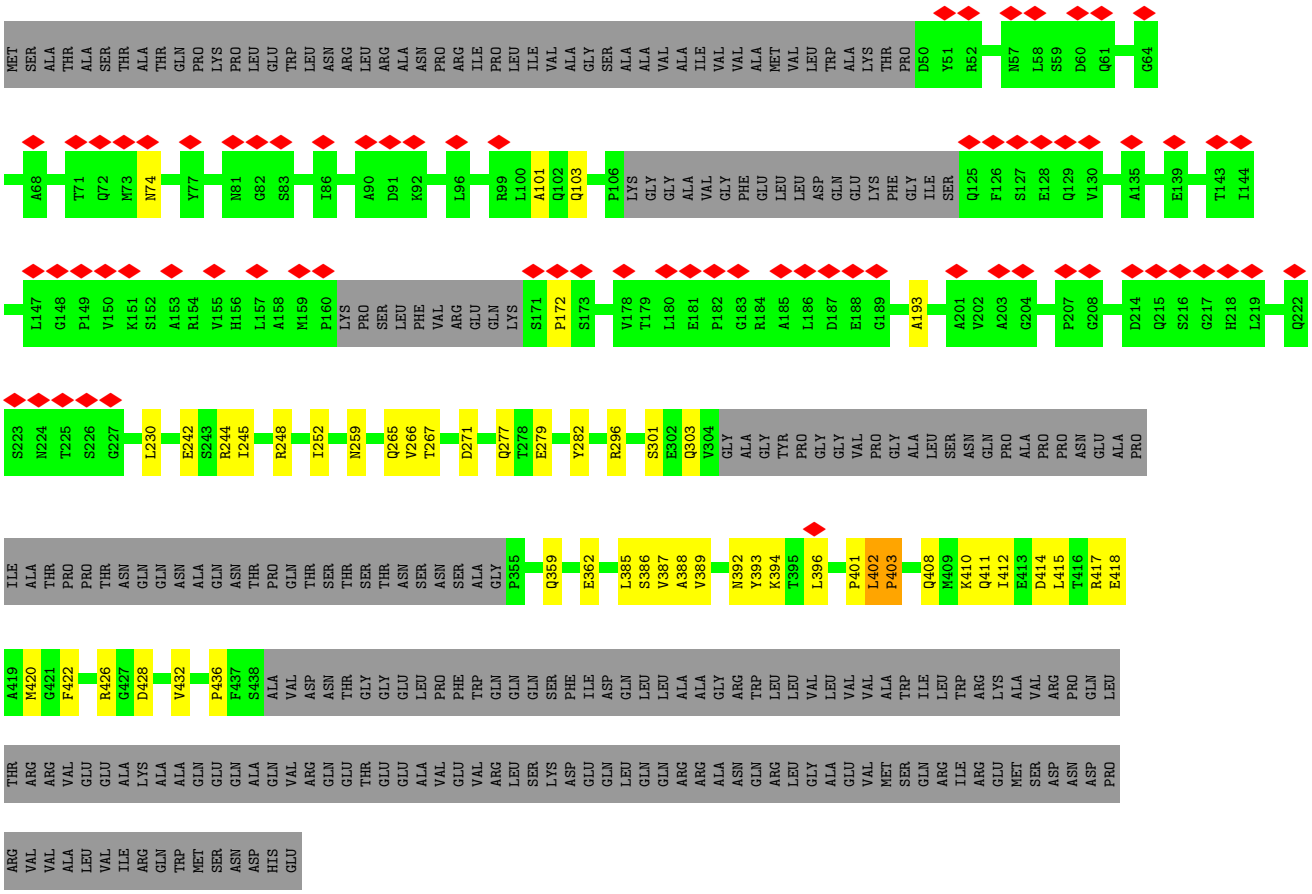
Chain Z:





- Molecule 1: Flagellar M-ring protein

Chain AA: 13% 47% 9% 44%



- Molecule 1: Flagellar M-ring protein

Chain BA: 34% 10% • 55%

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

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

PHE GLY ILE SER Q125 F126 S127 N131 Y132 Q133 L136 E139 L140 T143 V150 R154 V155 H156 L157 A158 M159 P160 LYS PRO SER LEU PHE VAL ARG GLU GLN LYS S171 A174 S175 V176 T177 V178 T179 L180 E181 P182 A185 L186 D187 E188 G189 Q190 V194 V195 H196

L197 V198 S199 S200 G204 L205 P206 P207 G208 N209 V210 D214 G217 H218 L219 L220 T221 Q222 S223 N224 T225 S226 G227 R228 N231 E242 S243 R244 R248 Q265 V266 T267 D271 N274 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN

PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY P355 R356 S357 G380 E383 R384 L385 S386 N392 Y393 K394 T395 L396 Q408 Q411 L415 E418 A419

M420 R426 G427 D428 T429 L430 N431 V432 V433 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU

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

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

- Molecule 1: Flagellar M-ring protein

Chain CA: 30% 15% • 55%

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

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

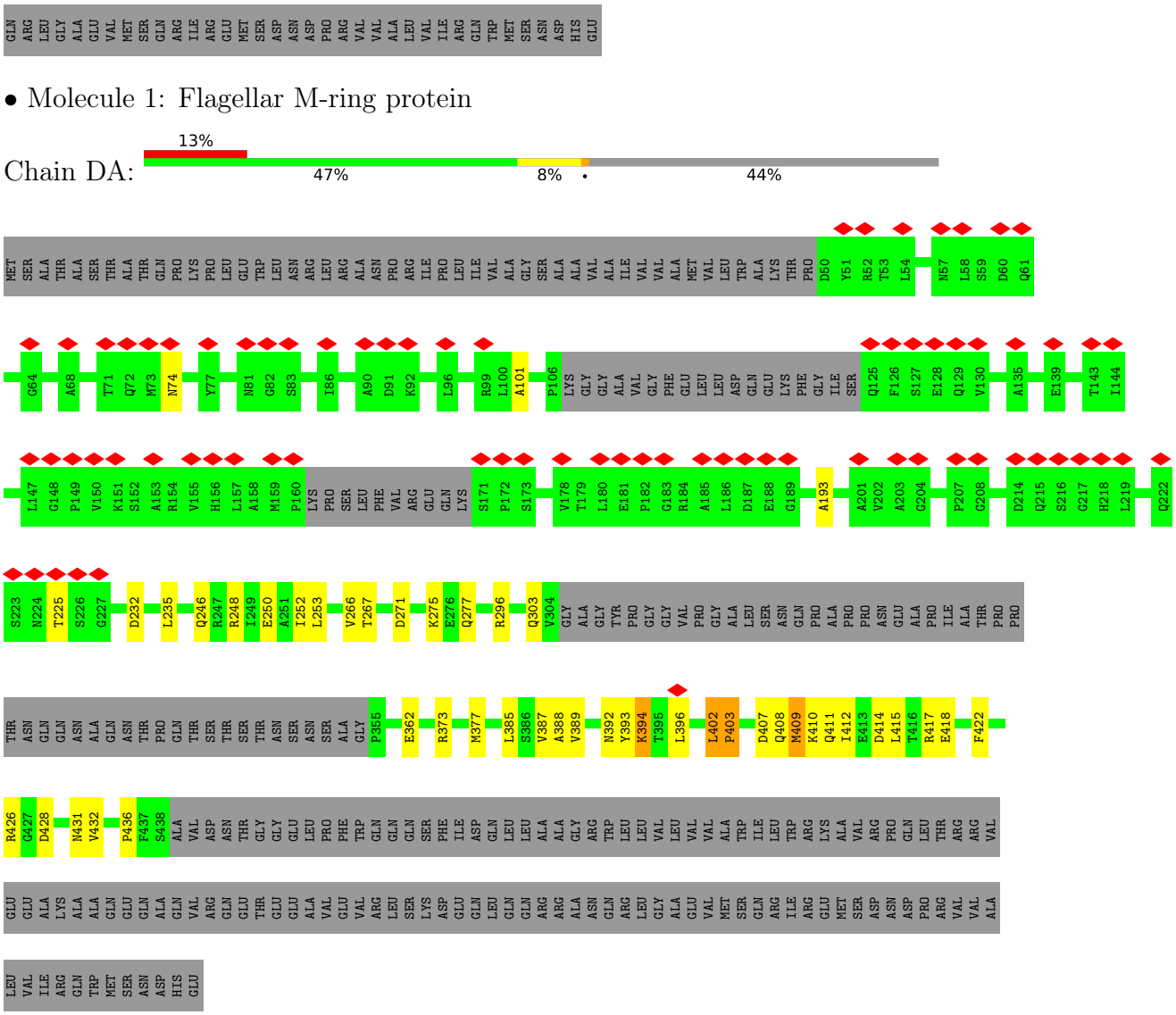
PHE GLY ILE SER Q125 F126 S127 E128 Q129 V130 N131 Y132 Q133 L136 E139 L140 T143 I144 V150 R154 V155 H156 L157 A158 M159 P160 LYS PRO SER LEU PHE VAL ARG GLU GLN LYS S171 A174 V178 A185 L186 D187 E188 G189 Q190 I191 S192 A193 V194 V195 H196 L197

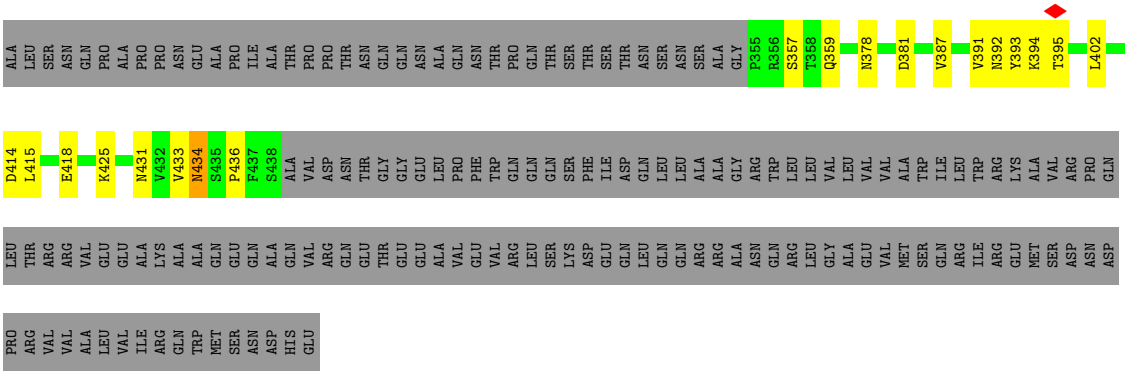
V202 A203 G204 G208 N209 V210 T211 L212 V213 D214 G217 H218 L219 L220 T221 Q222 S223 N224 T225 S226 G227 D232 A233 Q234 L235 K236 F237 A238 V241 E242 S243 R244 I245 R248 I249 I252 L253 G258 N261 V266 T267 F272 K275 R296 V304 GLY

ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY P355 E362 I372 M377 L385 S386 V387

A388 V389 N392 Y393 K394 T395 L396 Q408 M409 K410 Q411 I412 E413 D414 L415 T416 R417 E418 A419 D424 D428 T429 L430 N431 V432 V433 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG

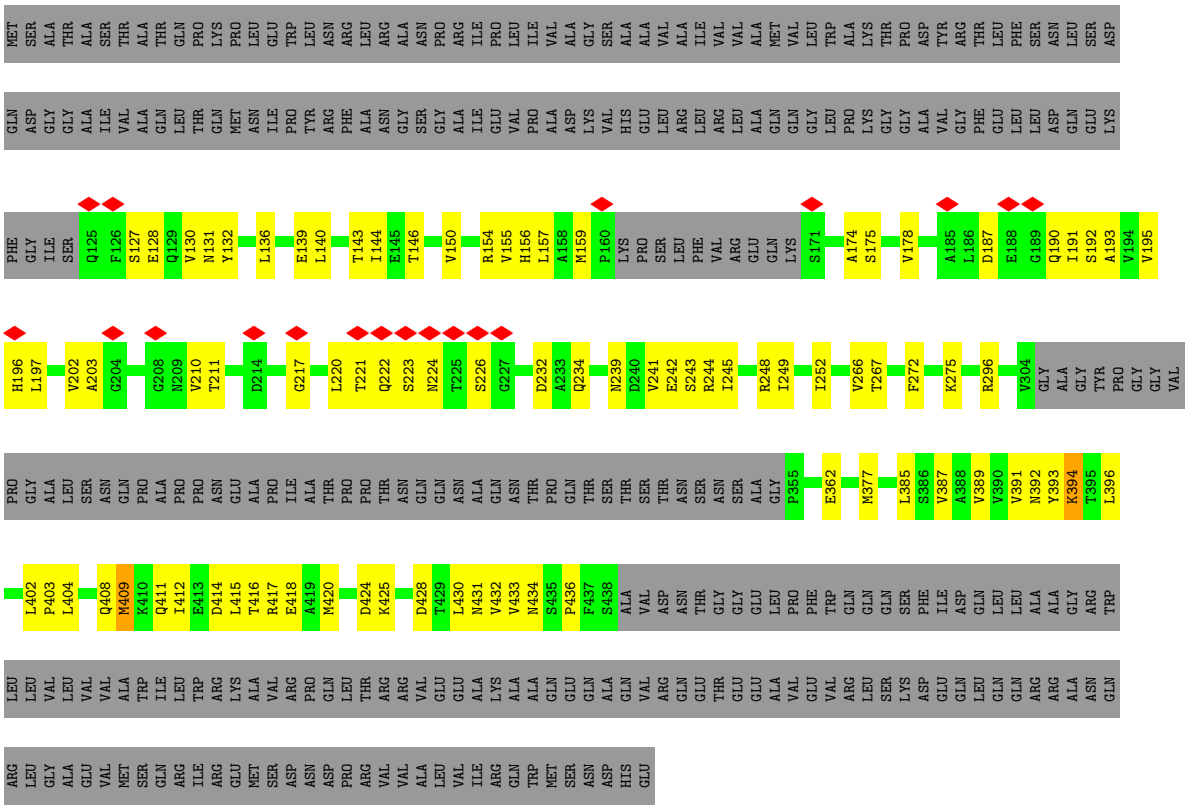
TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ALA ARG ALA ASN


GLN ARG LEU GLY ALA GLU VAL MET SER GLN ARG ILE ARG GLU MET SER ASP ASN ASP PRO ARG VAL VAL ALA LEU VAL ILE ARG GLN TRP MET SER ASN ASP HIS GLU
• Molecule 1: Flagellar M-ring protein
Chain DA:
13%
47%
8%
44%
MET SER ALA THR ALA SER THR ALA THR GLN PRO LYS PRO LEU GLU TRP LEU ASN ARG LEU ARG ALA ASN PRO ARG ILE PRO LEU ILE VAL ALA GLY SER ALA ALA VAL ALA ILE VAL VAL ALA MET VAL LEU TRP ALA LYS THR PRO D50 Y51 R52 T53 L54 N57 L58 S59 D60 Q61
G64 A68 T71 Q72 M73 N74 Y77 N81 G82 S83 I86 A90 D91 K92 L96 R99 L100 A101 P106 LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS PHE GLY ILE SER Q125 F126 S127 E128 Q129 V130 A135 E139 T143 I144
L147 G148 P149 V150 K151 S152 A153 R154 V155 H156 L157 A158 M159 P160 LYS PRO SER LEU PHE VAL ARG GLU GLN LYS S171 P172 S173 V178 T179 L180 E181 P182 G183 R184 A185 L186 D187 E188 G189 A193 A201 V202 A203 G204 P207 G208 D214 Q215 S216 G217 H218 L219 Q222
S223 N224 T225 S226 G227 D232 L235 Q246 R247 R248 I249 E250 A251 I252 L253 V266 T267 D271 K275 E276 Q277 R296 Q303 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO
THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY P355 E362 R373 M377 L385 S386 V387 A388 V389 N392 Y393 K394 T395 L396 L402 P403 D407 Q408 M409 K410 Q411 I412 E413 D414 L415 T416 R417 E418 F422
R426 G427 D428 M431 V432 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL
GLU GLU ALA LYS ALA ALA GLN GLU GLN GLN ALA GLN GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL MET SER GLN ARG ILE ARG GLU MET SER ASP ASN ASP PRO ARG VAL VAL ALA
LEU VAL ILE ARG GLN TRP MET SER ASN ASP HIS GLU
• Molecule 1: Flagellar M-ring protein
Chain EA:
34%
11%
55%
MET SER ALA THR ALA SER THR ALA THR GLN PRO LYS PRO LEU GLU TRP LEU ASN ARG LEU ARG ALA ASN PRO ARG ILE PRO LEU ILE VAL ALA GLY SER ALA ALA VAL ALA ILE VAL VAL ALA MET VAL LEU TRP ALA LYS THR PRO ASP TYR ARG THR LEU PHE SER ASN LEU SER ASP
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS
PHE GLY ILE SER Q125 F126 S127 N131 Y132 Q133 L136 E139 L140 T143 V150 R154 V155 H156 L157 A158 M159 P160 LYS PRO SER LEU PHE VAL ARG GLU GLN LYS S171 A174 S175 V176 T177 V178 T179 L180 A185 L186 D187 E188 G189 Q190 A193 V194 V195 H196 L197
V198 S199 S200 A201 V202 A203 G204 L205 P206 P207 G208 N209 V210 T211 D214 G217 H218 L219 L220 T221 Q222 S223 N224 T225 S226 G227 R228 N231 D232 F237 V241 E242 I245 R248 Q265 V266 K275 S301 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY



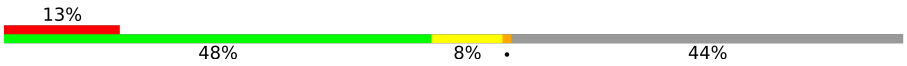
• Molecule 1: Flagellar M-ring protein

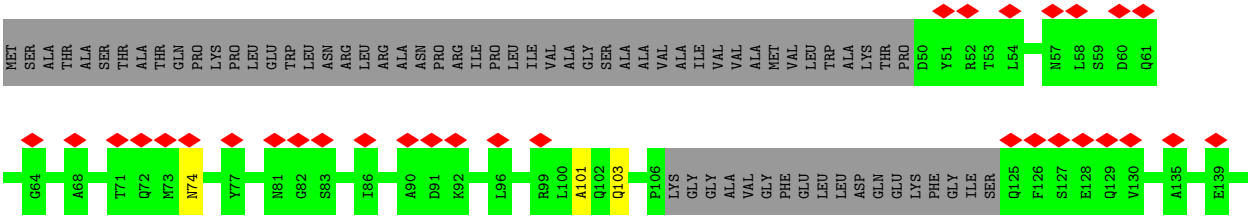
Chain FA:

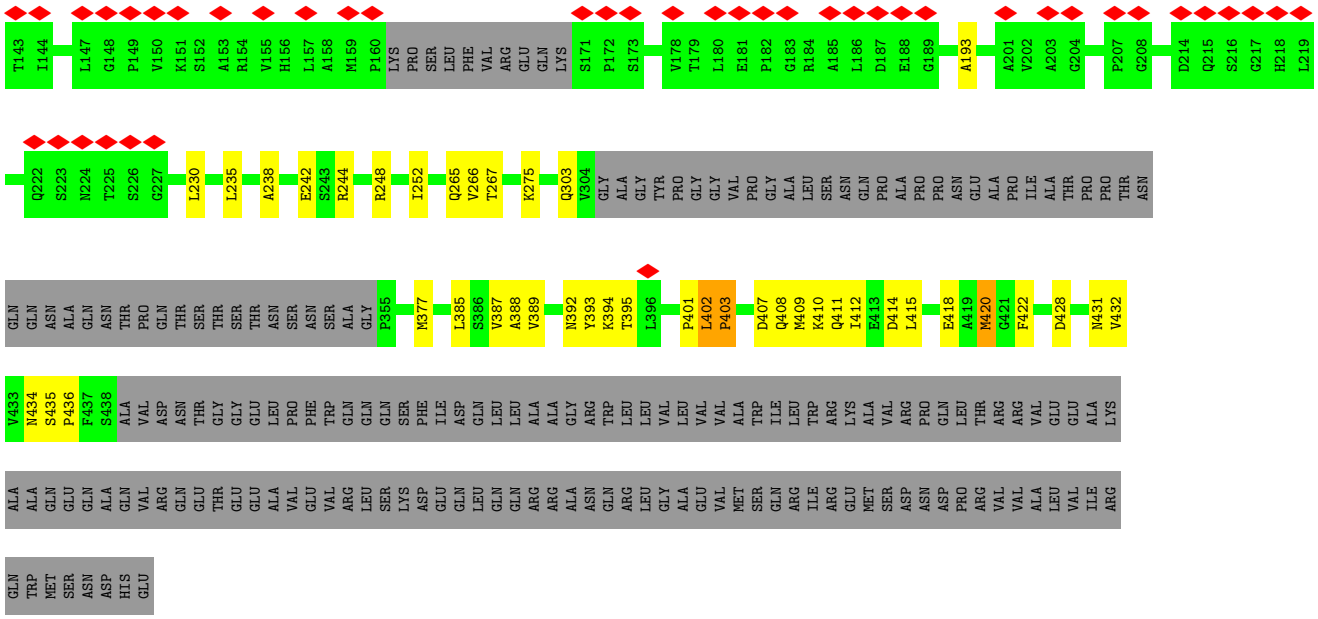


• Molecule 1: Flagellar M-ring protein

Chain GA:

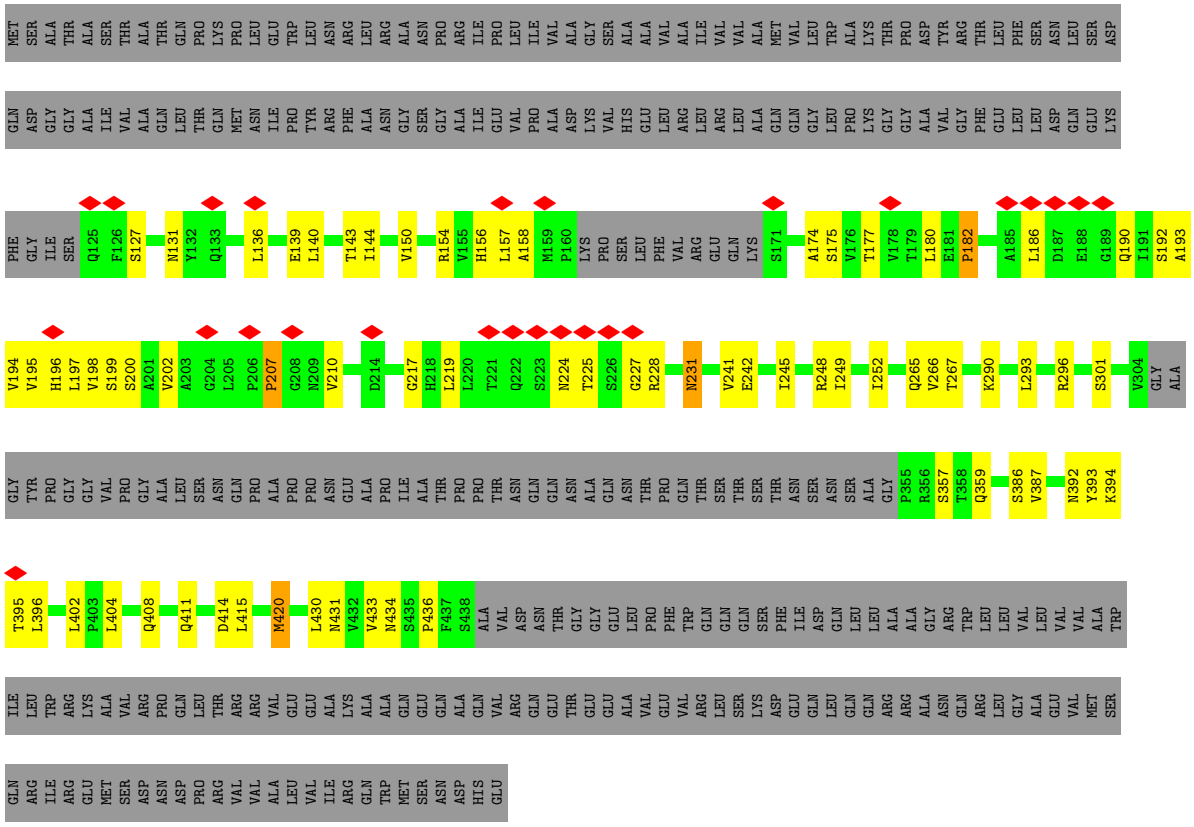






- Molecule 1: Flagellar M-ring protein

Chain HA:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C33	Depositor
Number of particles used	16411	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 ($e^-/Å^2$)	51.557	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.981	Depositor
Minimum map value	-0.272	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.173	Depositor
Map size (Å)	1046.784, 1046.784, 1046.784	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.363, 1.363, 1.363	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	0.25	0/1969	0.55	0/2668
1	AA	0.27	0/2017	0.56	3/2748 (0.1%)
1	B	0.28	1/2017 (0.0%)	0.62	2/2748 (0.1%)
1	BA	0.26	0/1969	0.55	1/2668 (0.0%)
1	C	0.26	0/1969	0.56	2/2668 (0.1%)
1	CA	0.26	0/1969	0.58	0/2668
1	D	0.25	0/1969	0.56	1/2668 (0.0%)
1	DA	0.25	0/2017	0.53	0/2748
1	E	0.25	0/2017	0.54	1/2748 (0.0%)
1	EA	0.26	0/1969	0.55	1/2668 (0.0%)
1	F	0.26	0/1969	0.56	0/2668
1	FA	0.25	0/1969	0.55	0/2668
1	G	0.26	0/1969	0.57	0/2668
1	GA	0.25	0/2017	0.53	1/2748 (0.0%)
1	H	0.25	0/2017	0.55	1/2748 (0.0%)
1	HA	0.26	0/1969	0.58	2/2668 (0.1%)
1	I	0.27	0/1969	0.58	4/2668 (0.1%)
1	J	0.26	0/1969	0.57	0/2668
1	K	0.28	1/2017 (0.0%)	0.60	1/2748 (0.0%)
1	L	0.26	0/1969	0.57	2/2668 (0.1%)
1	M	0.26	0/1969	0.58	0/2668
1	N	0.25	0/2017	0.53	0/2748
1	O	0.26	0/1969	0.58	3/2668 (0.1%)
1	P	0.26	0/1969	0.57	0/2668
1	Q	0.25	0/2017	0.53	1/2748 (0.0%)
1	R	0.25	0/1969	0.54	0/2668
1	S	0.26	0/1969	0.58	0/2668
1	T	0.25	0/2017	0.53	0/2748
1	V	0.53	2/1969 (0.1%)	0.74	3/2668 (0.1%)
1	W	0.26	0/1969	0.56	0/2668
1	X	0.28	0/2017	0.59	2/2748 (0.1%)
1	Y	0.25	0/1969	0.54	0/2668
1	Z	0.25	0/1969	0.55	0/2668
All	All	0.27	4/65505 (0.0%)	0.57	31/88924 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	182	PRO	CG-CD	-18.78	0.88	1.50
1	V	182	PRO	N-CD	7.22	1.57	1.47
1	K	172	PRO	CA-CB	-5.63	1.42	1.53
1	B	172	PRO	CA-CB	-5.62	1.42	1.53

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	182	PRO	N-CD-CG	-19.71	73.63	103.20
1	B	172	PRO	N-CA-CB	-14.47	85.93	103.30
1	K	172	PRO	N-CA-CB	-14.42	85.99	103.30
1	X	172	PRO	N-CA-CB	-13.88	86.64	103.30
1	V	182	PRO	CA-CB-CG	-11.00	83.09	104.00

There are no chirality outliers.

There are no planarity outliers.

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	1945	0	1931	78	0
1	AA	2005	0	1599	34	0
1	B	2005	0	1599	36	0
1	BA	1945	0	1931	58	0
1	C	1945	0	1931	58	0
1	CA	1945	0	1931	89	0
1	D	1945	0	1931	77	0
1	DA	2005	0	1599	38	0
1	E	2005	0	1599	36	0
1	EA	1945	0	1931	60	0
1	F	1945	0	1931	74	0
1	FA	1945	0	1931	82	0
1	G	1945	0	1931	73	0
1	GA	2005	0	1599	36	0
1	H	2005	0	1599	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HA	1945	0	1931	64	0
1	I	1945	0	1931	68	0
1	J	1945	0	1931	82	0
1	K	2005	0	1599	40	0
1	L	1945	0	1931	64	0
1	M	1945	0	1931	79	0
1	N	2005	0	1599	32	0
1	O	1945	0	1931	60	0
1	P	1945	0	1931	90	0
1	Q	2005	0	1599	35	0
1	R	1945	0	1931	64	0
1	S	1945	0	1931	76	0
1	T	2005	0	1599	35	0
1	V	1945	0	1931	74	0
1	W	1945	0	1931	79	0
1	X	2005	0	1599	39	0
1	Y	1945	0	1931	69	0
1	Z	1945	0	1931	76	0
All	All	64845	0	60071	1553	0

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

The worst 5 of 1553 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:FA:191:ILE:HG13	1:FA:220:LEU:HB3	1.57	0.87
1:R:228:ARG:HD3	1:R:231:ASN:HD21	1.38	0.85
1:GA:409:MET:HE1	1:GA:434:ASN:HB2	1.61	0.83
1:CA:219:LEU:HD21	1:HA:193:ALA:HA	1.59	0.82
1:CA:191:ILE:HG13	1:CA:220:LEU:HB3	1.65	0.79

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	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	34	67
1	AA	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	15	46
1	B	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	15	46
1	BA	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	C	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	CA	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	34	67
1	D	248/560 (44%)	239 (96%)	8 (3%)	1 (0%)	34	67
1	DA	303/560 (54%)	292 (96%)	8 (3%)	3 (1%)	15	46
1	E	303/560 (54%)	290 (96%)	10 (3%)	3 (1%)	15	46
1	EA	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	F	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	FA	248/560 (44%)	239 (96%)	8 (3%)	1 (0%)	34	67
1	G	248/560 (44%)	238 (96%)	9 (4%)	1 (0%)	34	67
1	GA	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	15	46
1	H	303/560 (54%)	290 (96%)	10 (3%)	3 (1%)	15	46
1	HA	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	I	248/560 (44%)	240 (97%)	7 (3%)	1 (0%)	34	67
1	J	248/560 (44%)	239 (96%)	8 (3%)	1 (0%)	34	67
1	K	303/560 (54%)	292 (96%)	8 (3%)	3 (1%)	15	46
1	L	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	M	248/560 (44%)	238 (96%)	9 (4%)	1 (0%)	34	67
1	N	303/560 (54%)	293 (97%)	8 (3%)	2 (1%)	22	55
1	O	248/560 (44%)	243 (98%)	4 (2%)	1 (0%)	34	67
1	P	248/560 (44%)	238 (96%)	9 (4%)	1 (0%)	34	67
1	Q	303/560 (54%)	290 (96%)	10 (3%)	3 (1%)	15	46
1	R	248/560 (44%)	243 (98%)	4 (2%)	1 (0%)	34	67
1	S	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	34	67
1	T	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	15	46
1	V	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	W	248/560 (44%)	240 (97%)	7 (3%)	1 (0%)	34	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	15	46
1	Y	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	34	67
1	Z	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	34	67
All	All	8789/18480 (48%)	8483 (96%)	252 (3%)	54 (1%)	29	57

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	ASN
1	B	394	LYS
1	B	403	PRO
1	C	394	LYS
1	E	394	LYS

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	218/467 (47%)	215 (99%)	3 (1%)	67	83
1	AA	142/467 (30%)	140 (99%)	2 (1%)	67	83
1	B	142/467 (30%)	138 (97%)	4 (3%)	43	70
1	BA	218/467 (47%)	216 (99%)	2 (1%)	78	90
1	C	218/467 (47%)	213 (98%)	5 (2%)	50	74
1	CA	218/467 (47%)	215 (99%)	3 (1%)	67	83
1	D	218/467 (47%)	215 (99%)	3 (1%)	67	83
1	DA	142/467 (30%)	139 (98%)	3 (2%)	53	76
1	E	142/467 (30%)	140 (99%)	2 (1%)	67	83
1	EA	218/467 (47%)	215 (99%)	3 (1%)	67	83
1	F	218/467 (47%)	212 (97%)	6 (3%)	43	70
1	FA	218/467 (47%)	215 (99%)	3 (1%)	67	83
1	G	218/467 (47%)	215 (99%)	3 (1%)	67	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	142/467 (30%)	140 (99%)	2 (1%)	67	83
1	H	142/467 (30%)	140 (99%)	2 (1%)	67	83
1	HA	218/467 (47%)	216 (99%)	2 (1%)	78	90
1	I	218/467 (47%)	216 (99%)	2 (1%)	78	90
1	J	218/467 (47%)	216 (99%)	2 (1%)	78	90
1	K	142/467 (30%)	140 (99%)	2 (1%)	67	83
1	L	218/467 (47%)	216 (99%)	2 (1%)	78	90
1	M	218/467 (47%)	213 (98%)	5 (2%)	50	74
1	N	142/467 (30%)	140 (99%)	2 (1%)	67	83
1	O	218/467 (47%)	215 (99%)	3 (1%)	67	83
1	P	218/467 (47%)	216 (99%)	2 (1%)	78	90
1	Q	142/467 (30%)	141 (99%)	1 (1%)	84	92
1	R	218/467 (47%)	214 (98%)	4 (2%)	59	79
1	S	218/467 (47%)	217 (100%)	1 (0%)	88	94
1	T	142/467 (30%)	140 (99%)	2 (1%)	67	83
1	V	218/467 (47%)	217 (100%)	1 (0%)	88	94
1	W	218/467 (47%)	213 (98%)	5 (2%)	50	74
1	X	142/467 (30%)	139 (98%)	3 (2%)	53	76
1	Y	218/467 (47%)	214 (98%)	4 (2%)	59	79
1	Z	218/467 (47%)	216 (99%)	2 (1%)	78	90
All	All	6358/15411 (41%)	6267 (99%)	91 (1%)	68	83

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	231	ASN
1	AA	259	ASN
1	W	415	LEU
1	Y	231	ASN
1	CA	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	434	ASN
1	X	434	ASN
1	FA	434	ASN
1	W	131	ASN
1	Y	131	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.

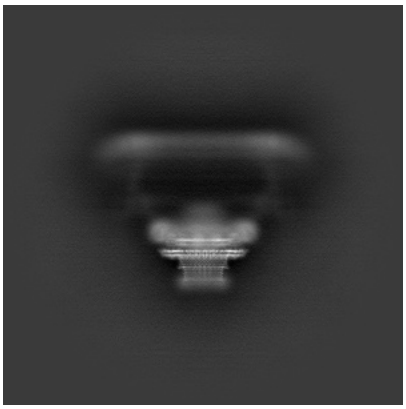
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-41101. These allow visual inspection of the internal detail of the map and identification of artifacts.

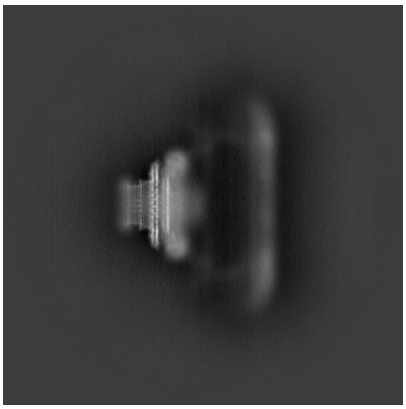
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

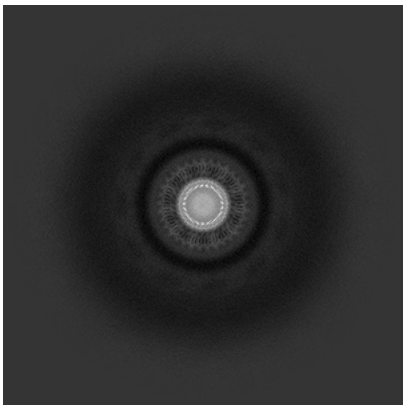
6.1.1 Primary map



X

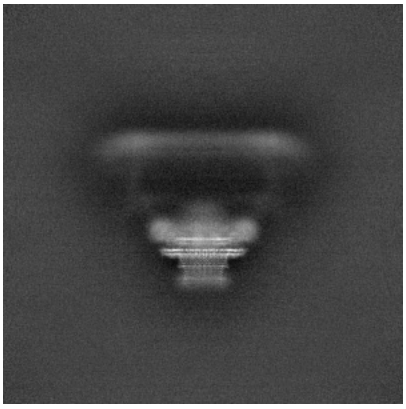


Y

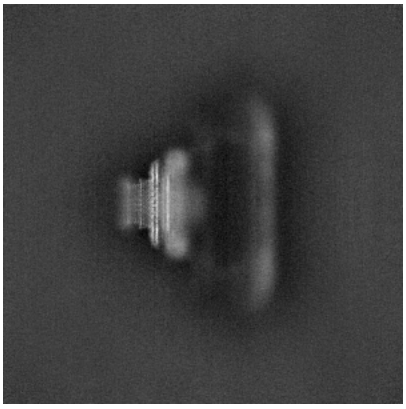


Z

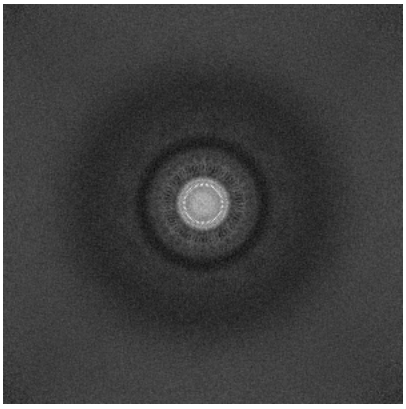
6.1.2 Raw map



X



Y

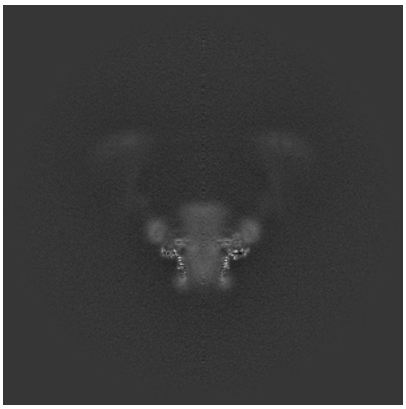


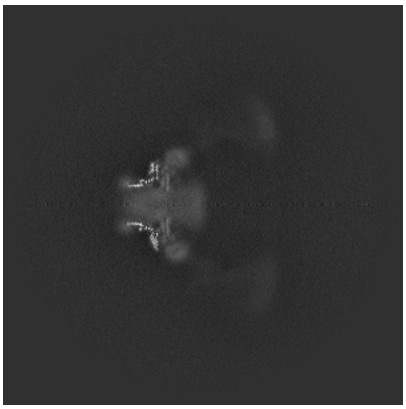
Z

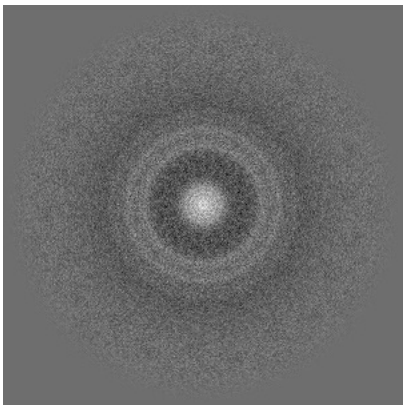
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

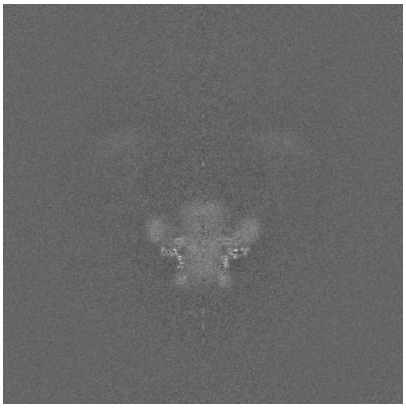
6.2.1 Primary map


X Index: 384

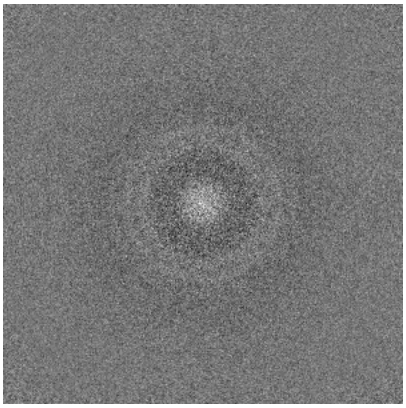

Y Index: 384


Z Index: 384

6.2.2 Raw map


X Index: 384

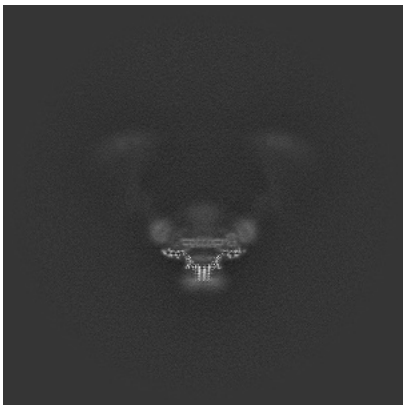
Y Index: 384

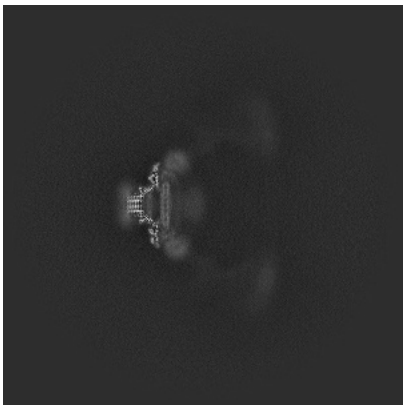

Z Index: 384

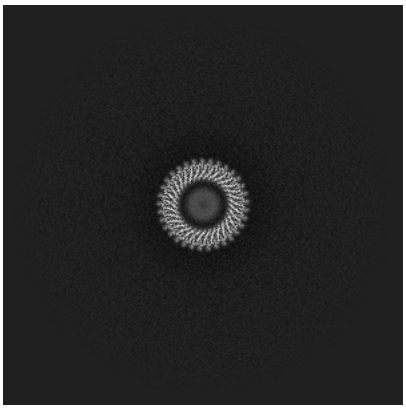
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

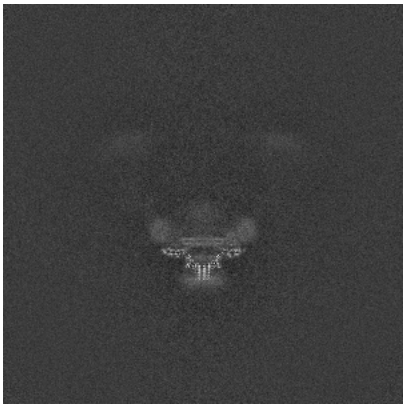
6.3.1 Primary map


X Index: 348

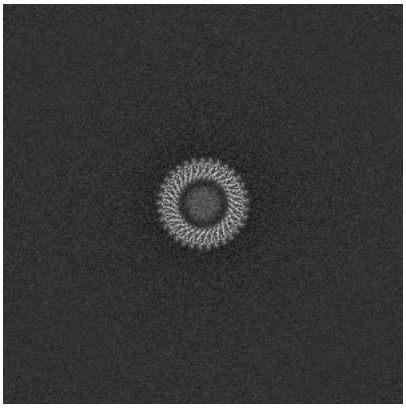

Y Index: 419


Z Index: 295

6.3.2 Raw map


X Index: 348

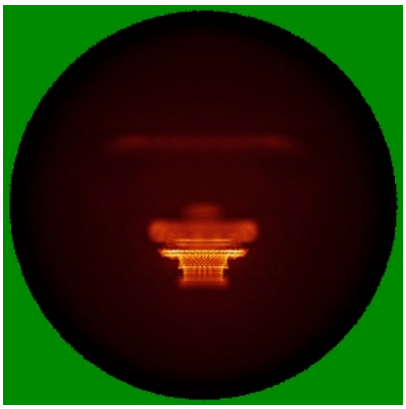
Y Index: 384

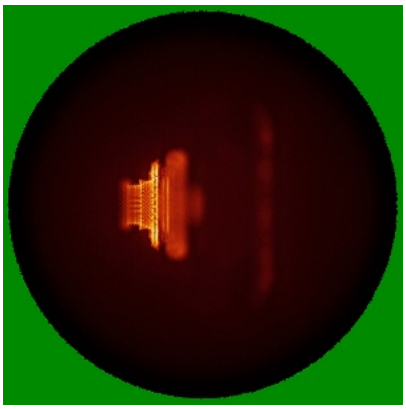

Z Index: 295

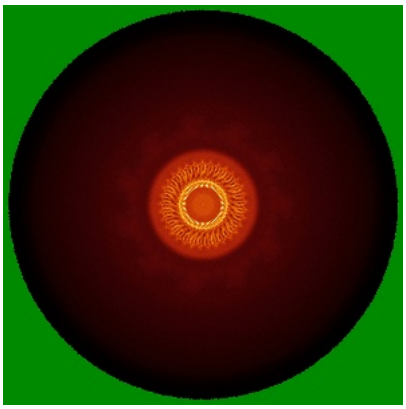
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

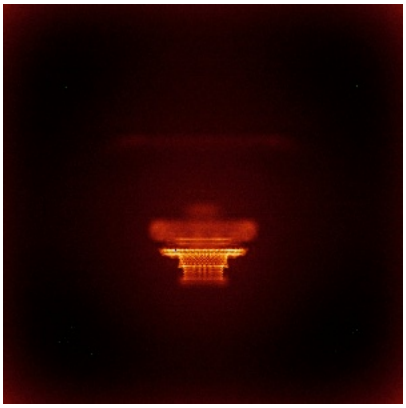
6.4.1 Primary map

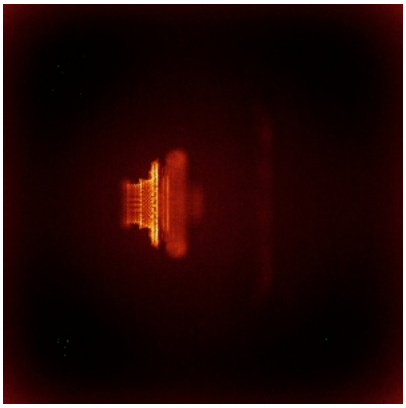

X

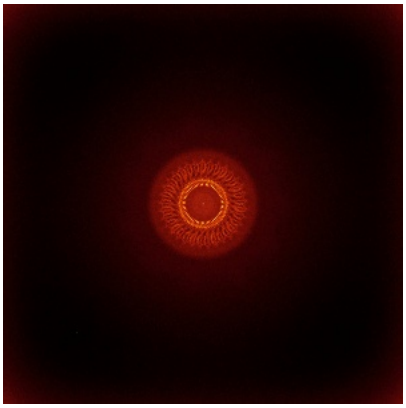

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.173. 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

X Y Z

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.

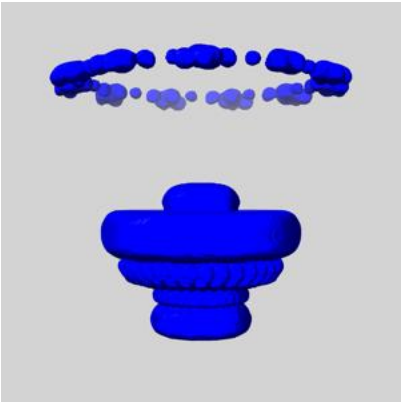
6.6 Mask visualisation (i)

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

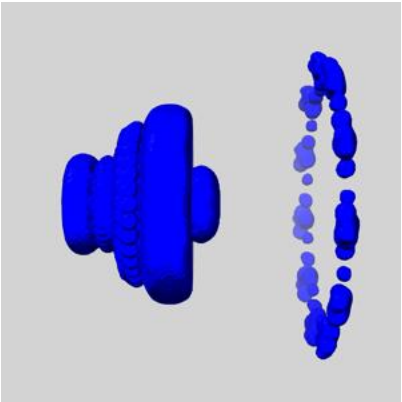
A mask typically either:

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

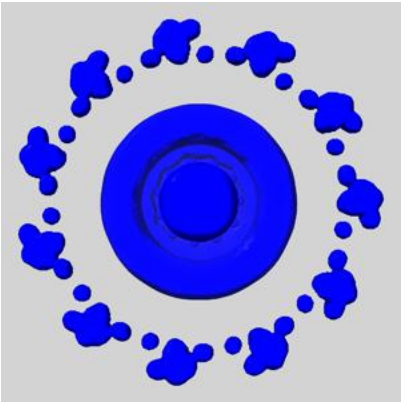
6.6.1 emd_41101_msk_1.map (i)



X



Y

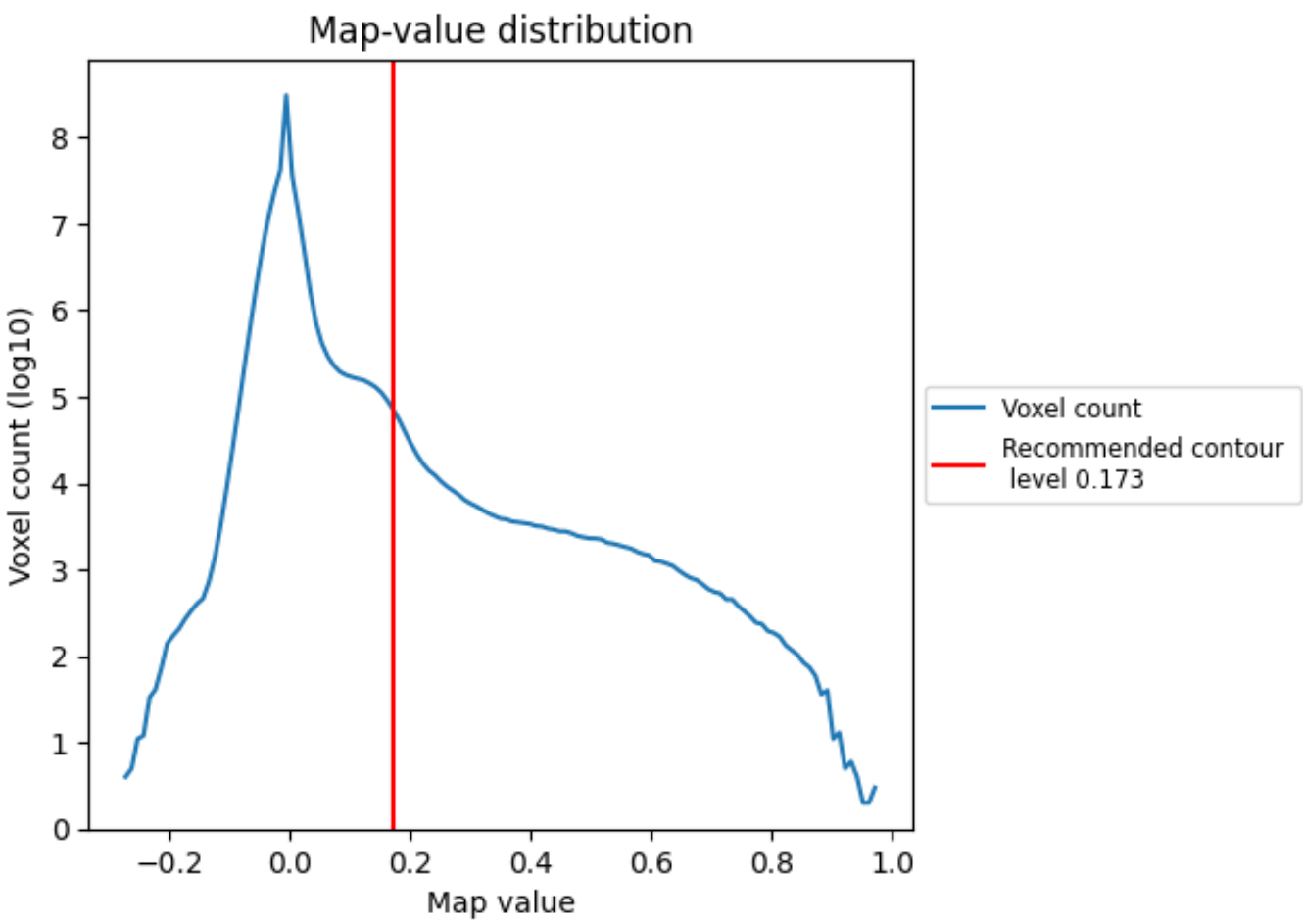


Z

7 Map analysis (i)

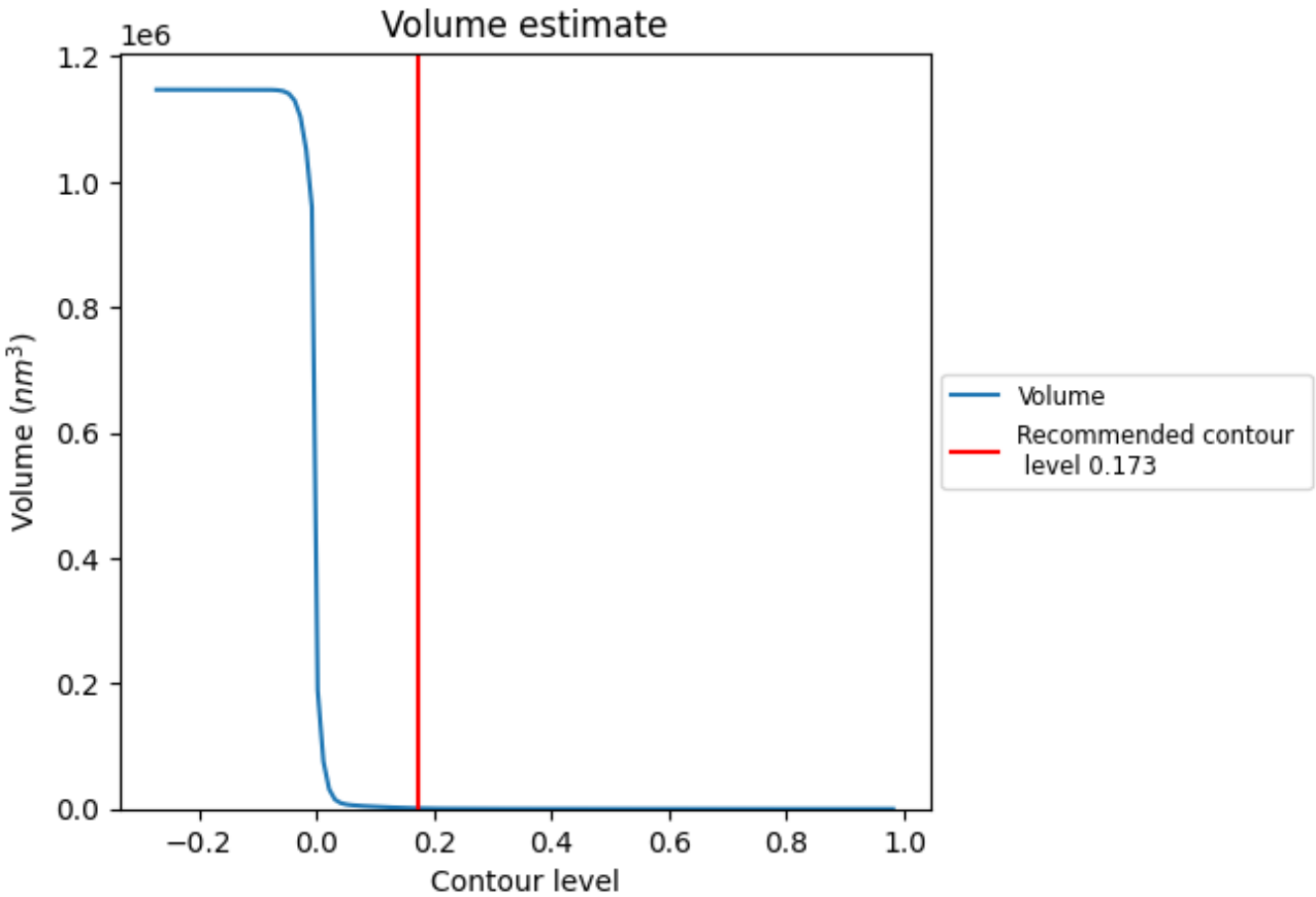
This section contains the results of statistical analysis of the map.

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.

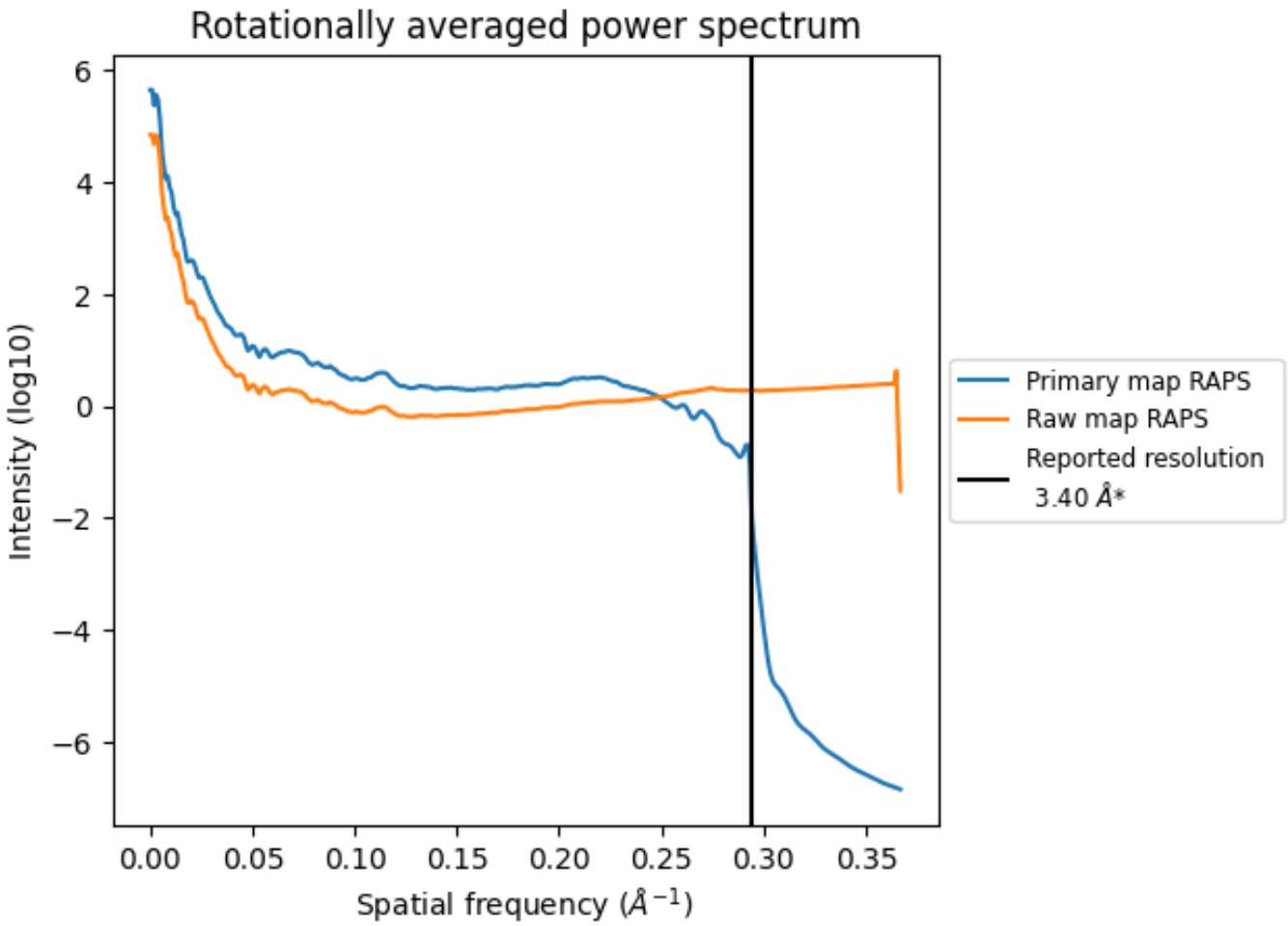
7.2 Volume estimate (i)



The volume at the recommended contour level is 1012 nm^3; this corresponds to an approximate mass of 914 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)

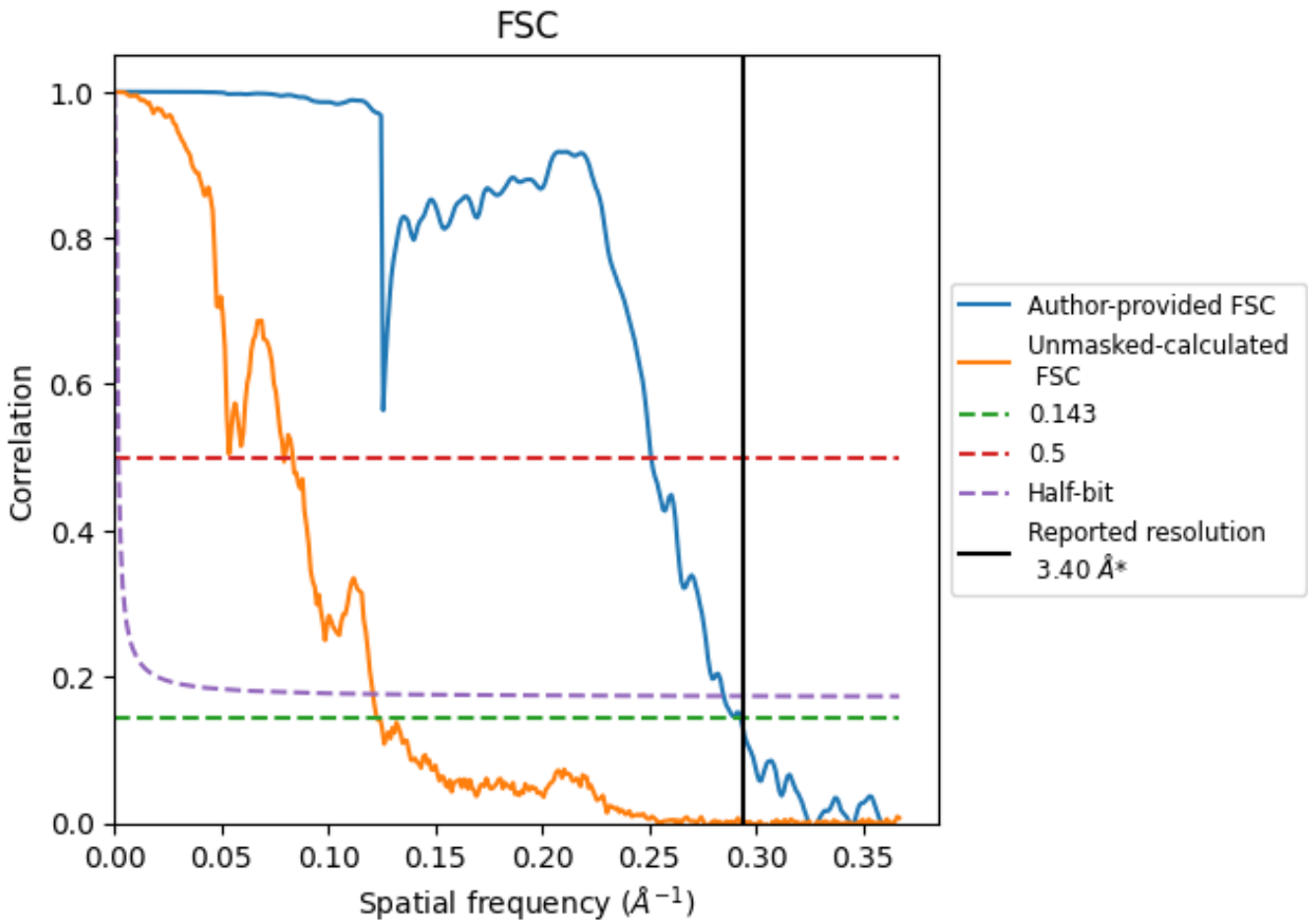


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

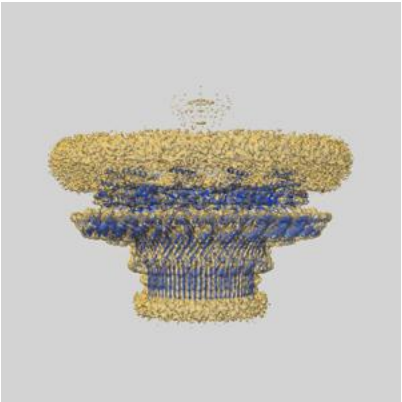
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.99	3.51
Unmasked-calculated*	8.14	12.64	8.28

*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 8.14 differs from the reported value 3.4 by more than 10 %

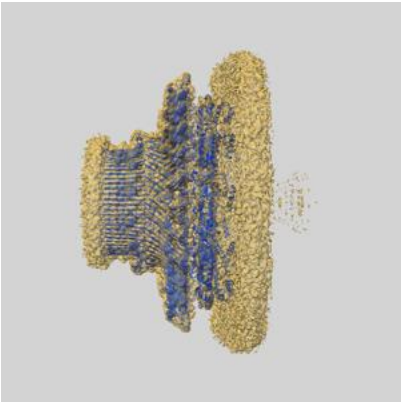
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-41101 and PDB model 8T8P. Per-residue inclusion information can be found in section 3 on page 6.

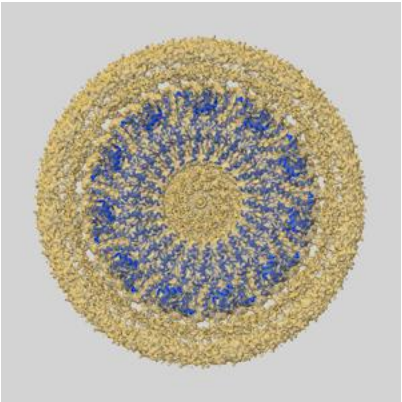
9.1 Map-model overlay (i)



X



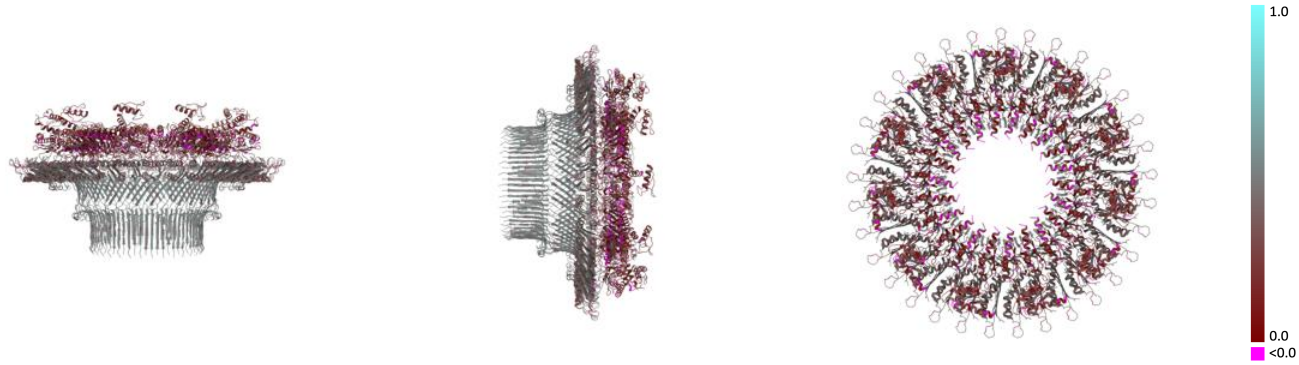
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.173 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.

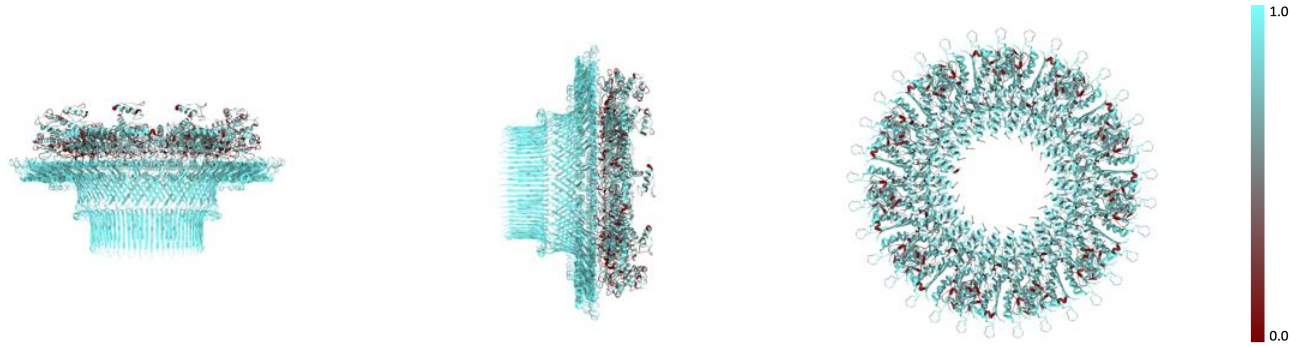
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

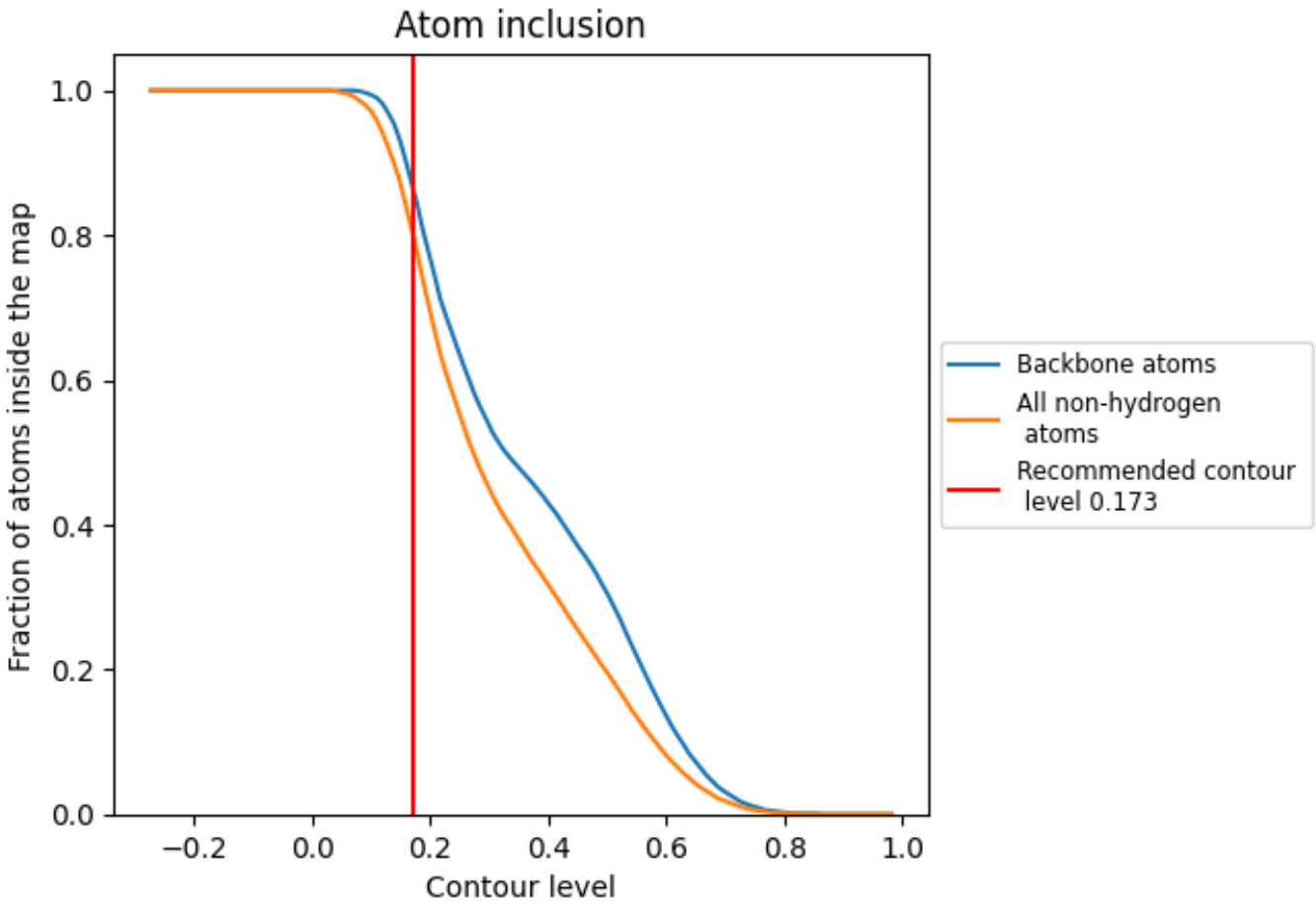
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.173).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.3530
A	0.8170	0.3420
AA	0.7580	0.3710
B	0.7590	0.3650
BA	0.8150	0.3460
C	0.8150	0.3470
CA	0.8160	0.3400
D	0.8210	0.3430
DA	0.7590	0.3660
E	0.7550	0.3680
EA	0.8100	0.3460
F	0.8170	0.3470
FA	0.8210	0.3420
G	0.8130	0.3430
GA	0.7550	0.3670
H	0.7540	0.3700
HA	0.8110	0.3440
I	0.8170	0.3470
J	0.8180	0.3430
K	0.7590	0.3700
L	0.8170	0.3480
M	0.8180	0.3410
N	0.7590	0.3690
O	0.8130	0.3480
P	0.8170	0.3420
Q	0.7580	0.3680
R	0.8100	0.3460
S	0.8210	0.3420
T	0.7520	0.3700
V	0.8130	0.3490
W	0.8230	0.3430
X	0.7500	0.3680
Y	0.8120	0.3460
Z	0.8240	0.3450