wwPDB EM Validation Summary Report (i)

Mar 5, 2026 – 09:58 AM UTC

PDB ID	:	8WKQ / pdb_00008wkq
EMDB ID	:	EMD-37605
Title	:	Cryo-EM structure of the MS ring (C1) with export apparatus and proximal rod within the flagellar motor-hook complex in the CW state.
Authors	:	Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on	:	2023-09-28
Resolution	:	3.80 Å(reported)
Based on initial models	:	., ?

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:

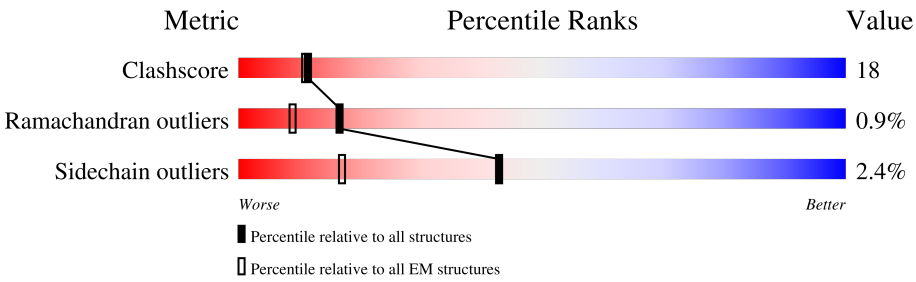
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

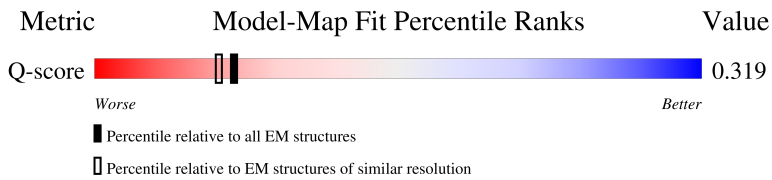
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	0	560	23% 6% 71%
1	1	560	21% 8% 71%
1	2	560	22% 7% 71%
1	3	560	23% 6% 71%

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Mol	Chain	Length	Quality of chain
1	4	560	22% 7% 71%
1	5	560	22% 7% 71%
1	6	560	22% 7% 71%
1	7	560	22% 7% 71%
1	8	560	23% 7% 71%
1	9	560	23% 6% 71%
1	AA	560	23% 6% 71%
1	AB	560	22% 7% 71%
1	AC	560	23% 7% 71%
1	AD	560	22% 7% 71%
1	AE	560	23% 6% 71%
1	AF	560	23% 6% 71%
1	AG	560	23% 7% 71%
1	AH	560	22% 7% 71%
1	AI	560	23% 7% 71%
1	AJ	560	23% 6% 71%
1	AK	560	23% 6% 71%
1	AL	560	23% 6% 71%
1	AM	560	23% 7% 71%
1	AN	560	22% 7% 71%
1	AO	560	22% 7% 71%
1	AP	560	22% 7% 71%
1	AQ	560	23% 6% 71%
1	UI	560	8% 15% 10% • 72%
1	UJ	560	10% 14% 11% • 72%

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Mol	Chain	Length	Quality of chain
1	UK	560	14% 15% 10% 72%
1	UL	560	16% 15% 10% 72%
1	UM	560	20% 15% 10% 72%
1	UN	560	16% 15% 10% 72%
1	UO	560	12% 15% 10% 72%
1	UP	560	10% 15% 9% 72%
1	WA	560	11% 8% 80%
1	WB	560	10% 8% 80%
1	WC	560	10% 8% 81%
1	WD	560	10% 8% 80%
1	WE	560	12% 6% 80%
1	WF	560	10% 9% 80%
1	WG	560	10% 9% 80%
1	WH	560	10% 6% 83%
1	WI	560	8% 7% 83%
1	WJ	560	9% 8% 82%
1	WK	560	8% 8% 82%
1	WL	560	8% 7% 85%
1	WM	560	8% 6% 85%
1	WN	560	8% 6% 85%
1	WO	560	9% 7% 83%
1	WP	560	10% 7% 82%
1	WQ	560	9% 9% 80%
1	WR	560	10% 8% 80%
1	WS	560	9% 10% 80%

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Mol	Chain	Length	Quality of chain
1	WT	560	10% 8% 80%
1	WU	560	11% 8% 80%
1	WV	560	10% 8% 80%
1	WW	560	9% 9% 80%
1	b	560	98%
1	c	560	97%
1	d	560	96%
1	e	560	97%
1	f	560	96%
1	g	560	97%
1	h	560	96%
1	i	560	97%
1	j	560	96%
1	k	560	97%
1	l	560	96%
1	t	560	22% 7% 71%
1	u	560	22% 7% 71%
1	v	560	23% 6% 71%
1	w	560	23% 6% 71%
1	x	560	23% 7% 71%
1	y	560	22% 7% 71%
1	z	560	22% 8% 71%
2	A	89	73% 26%
2	B	89	66% 34%
2	C	89	66% 34%

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Mol	Chain	Length	Quality of chain
2	D	89	63% 35%
3	E	264	62% 31%
4	F	245	52% 31% 16%
4	G	245	60% 24% 15%
4	H	245	63% 21% 15%
4	I	245	62% 22% 15%
4	J	245	55% 29% 15%
5	K	104	38% 18% 43%
5	L	104	69% 17% 12%
5	M	104	69% 15% 5% 11%
5	N	104	68% 20% 11%
5	O	104	64% 24% 11%
5	P	104	62% 24% 12%
6	Q	138	70% 28%
6	R	138	67% 20% 12%
6	S	138	5% 62% 27% 9%
6	T	138	8% 72% 19% 8%
6	U	138	15% 66% 22% 11%
7	V	134	40% 81% 19%
7	W	134	49% 81% 18%
7	X	134	55% 83% 16%
7	Y	134	63% 82% 16%
7	Z	134	67% 76% 22%
7	a	134	75% 80% 19%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 99073 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	UI	155	1172	733	211	226	2	0	0
1	UJ	155	1172	733	211	226	2	0	0
1	UK	155	1172	733	211	226	2	0	0
1	UL	155	1172	733	211	226	2	0	0
1	UM	155	1172	733	211	226	2	0	0
1	UN	155	1172	733	211	226	2	0	0
1	UO	155	1172	733	211	226	2	0	0
1	UP	155	1172	733	211	226	2	0	0
1	WA	113	849	534	148	166	1	0	0
1	WB	111	836	526	146	163	1	0	0
1	WC	108	812	510	142	159	1	0	0
1	WD	110	827	522	144	160	1	0	0
1	WE	112	843	531	147	164	1	0	0
1	WF	111	834	526	145	162	1	0	0
1	WG	112	843	531	147	164	1	0	0
1	WH	95	703	439	126	137	1	0	0
1	WI	95	703	439	126	137	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	WJ	99	737	462	131	143	1	0	0
			Total	C	N	O	S		
1	WK	98	729	456	130	142	1	0	0
			Total	C	N	O	S		
1	WL	85	622	389	110	122	1	0	0
			Total	C	N	O	S		
1	WM	82	596	372	107	116	1	0	0
			Total	C	N	O	S		
1	WN	84	611	380	109	121	1	0	0
			Total	C	N	O	S		
1	WO	96	714	448	127	138	1	0	0
			Total	C	N	O	S		
1	WP	100	741	464	132	144	1	0	0
			Total	C	N	O	S		
1	WQ	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
1	WR	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
1	WS	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
1	WT	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
1	WU	112	843	531	147	164	1	0	0
			Total	C	N	O	S		
1	WV	110	827	521	144	161	1	0	0
			Total	C	N	O	S		
1	WW	111	834	526	145	162	1	0	0
			Total	C	N	O			
1	b	13	81	50	15	16		0	0
			Total	C	N	O			
1	c	16	103	64	19	20		0	0
			Total	C	N	O			
1	d	20	133	83	23	27		0	0
			Total	C	N	O			
1	e	16	103	64	19	20		0	0
			Total	C	N	O			
1	f	21	140	88	24	28		0	0
			Total	C	N	O			
1	g	16	103	64	19	20		0	0
			Total	C	N	O			
1	h	21	140	88	24	28		0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
1	i	16	103	64	19	20		0	0
			Total	C	N	O			
1	j	20	133	83	23	27		0	0
			Total	C	N	O			
1	k	16	103	64	19	20		0	0
			Total	C	N	O			
1	l	21	140	88	24	28		0	0
			Total	C	N	O	S		
1	t	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	u	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	v	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	w	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	x	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	y	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	z	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	1	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	2	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	3	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	4	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	5	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	6	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	7	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	8	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	9	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
1	0	164	1275	776	237	259	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	164	1275	776	237	259	3	0	0
1	AB	164	1275	776	237	259	3	0	0
1	AC	164	1275	776	237	259	3	0	0
1	AD	164	1275	776	237	259	3	0	0
1	AE	164	1275	776	237	259	3	0	0
1	AF	164	1275	776	237	259	3	0	0
1	AG	164	1275	776	237	259	3	0	0
1	AH	164	1275	776	237	259	3	0	0
1	AI	164	1275	776	237	259	3	0	0
1	AJ	164	1275	776	237	259	3	0	0
1	AK	164	1275	776	237	259	3	0	0
1	AL	164	1275	776	237	259	3	0	0
1	AM	164	1275	776	237	259	3	0	0
1	AN	164	1275	776	237	259	3	0	0
1	AO	164	1275	776	237	259	3	0	0
1	AP	164	1275	776	237	259	3	0	0
1	AQ	164	1275	776	237	259	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	89	670	449	100	114	7	0	0
2	B	89	670	449	100	114	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	89	670	449	100	114	7	0	0
2	D	89	670	449	100	114	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	253	1945	1305	307	318	15	0	0

- Molecule 4 is a protein called Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	207	1605	1072	249	272	12	0	0
4	G	209	1626	1086	252	276	12	0	0
4	H	208	1614	1077	251	274	12	0	0
4	I	208	1614	1077	251	274	12	0	0
4	J	209	1623	1084	251	276	12	0	0

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	59	429	265	74	83	7	0	0
5	L	91	672	415	121	129	7	0	0
5	M	93	686	424	123	132	7	0	0
5	N	93	686	424	123	132	7	0	0
5	O	93	686	424	123	132	7	0	0
5	P	92	679	420	122	130	7	0	0

- Molecule 6 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Q	134	1030	633	189	203	5	0	0
6	R	121	942	583	172	182	5	0	0
6	S	125	967	598	177	187	5	0	0
6	T	127	982	606	182	189	5	0	0
6	U	123	950	588	172	185	5	0	0

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

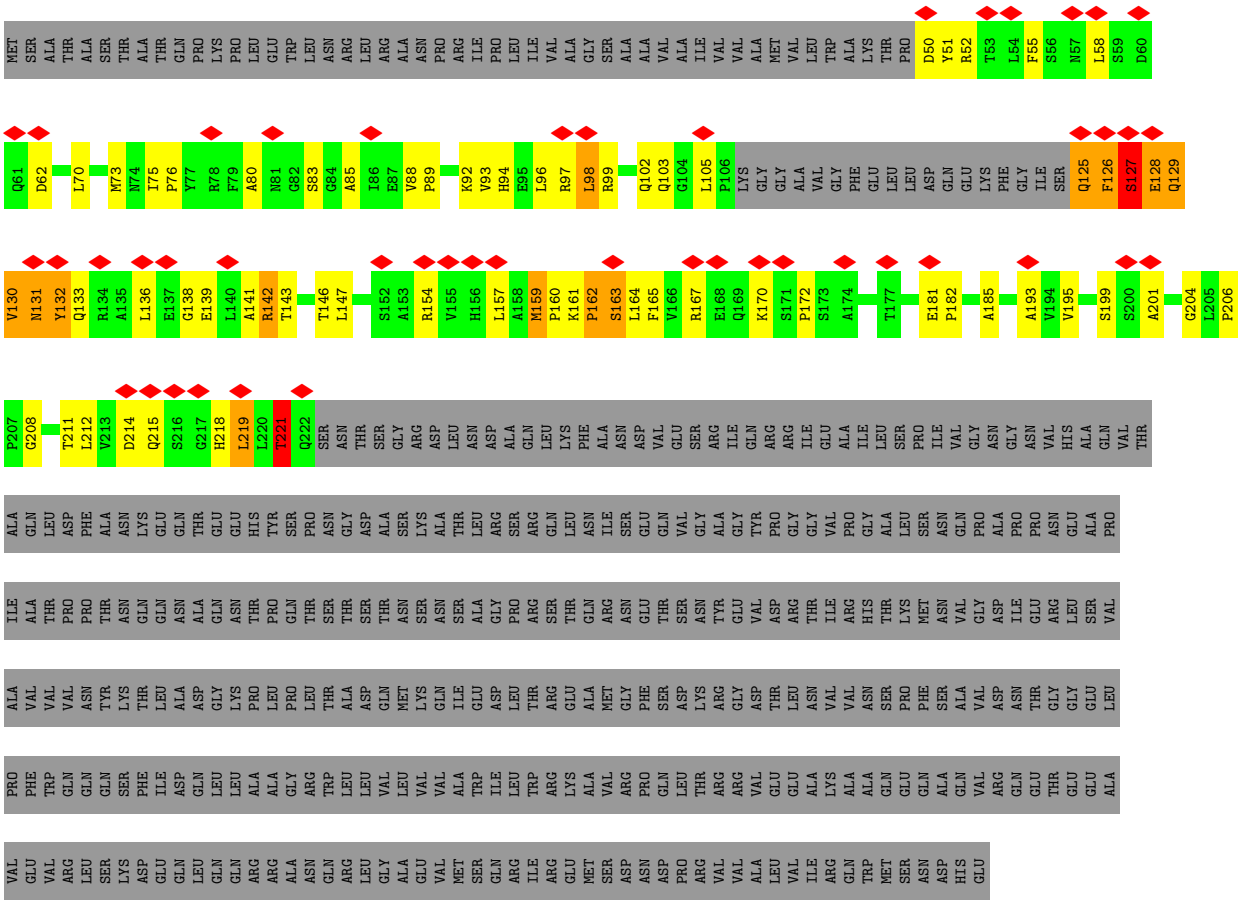
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	V	133	969	604	167	193	5	0	0
7	W	132	964	601	166	192	5	0	0
7	X	133	969	604	167	193	5	0	0
7	Y	133	969	604	167	193	5	0	0
7	Z	133	969	604	167	193	5	0	0
7	a	133	969	604	167	193	5	0	0

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.

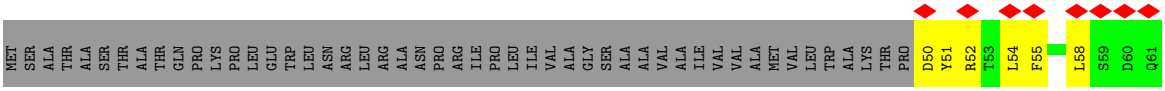
• Molecule 1: Flagellar M-ring protein

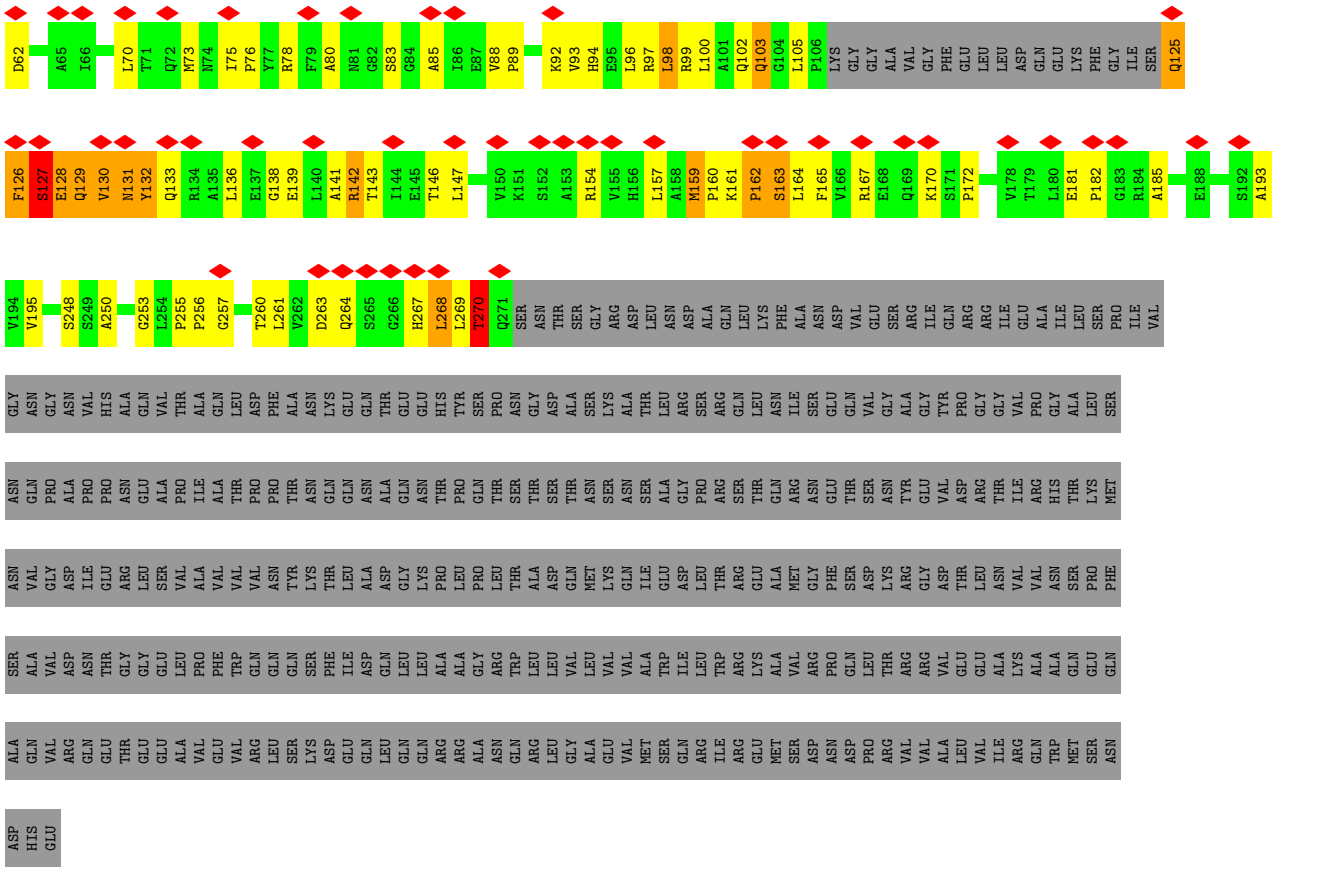
Chain UI: 8% 15% 10% • 72%



• Molecule 1: Flagellar M-ring protein

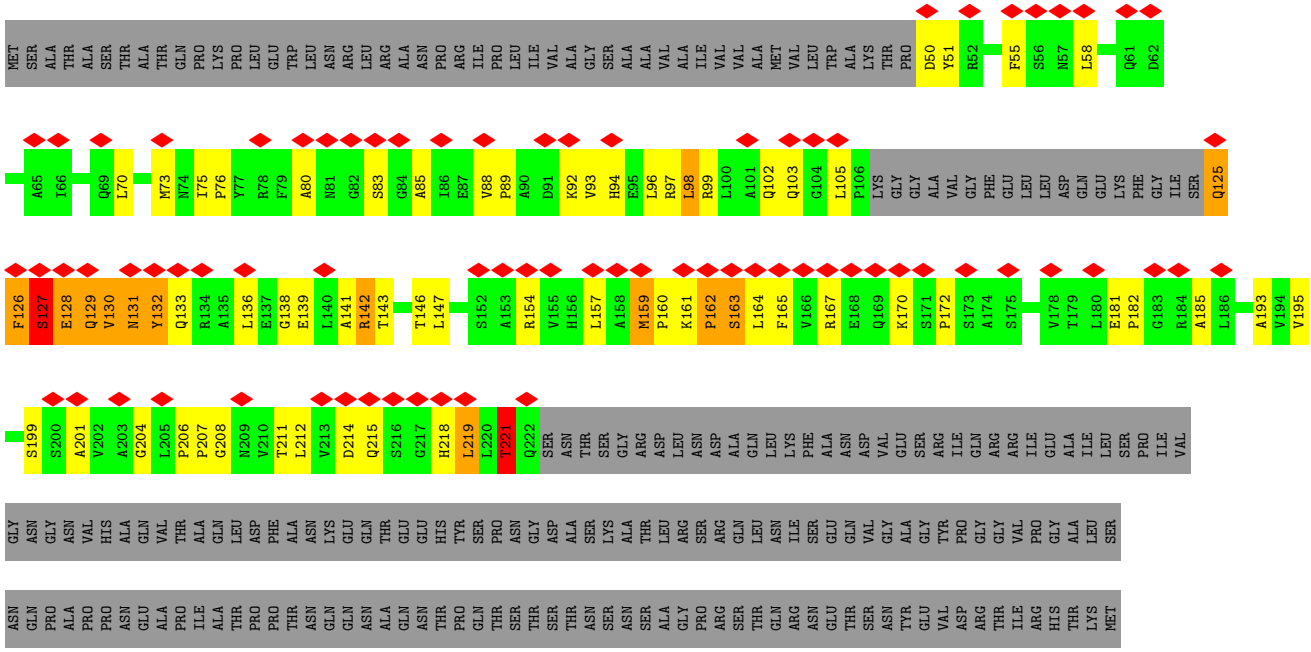
Chain UJ: 10% 14% 11% • 72%

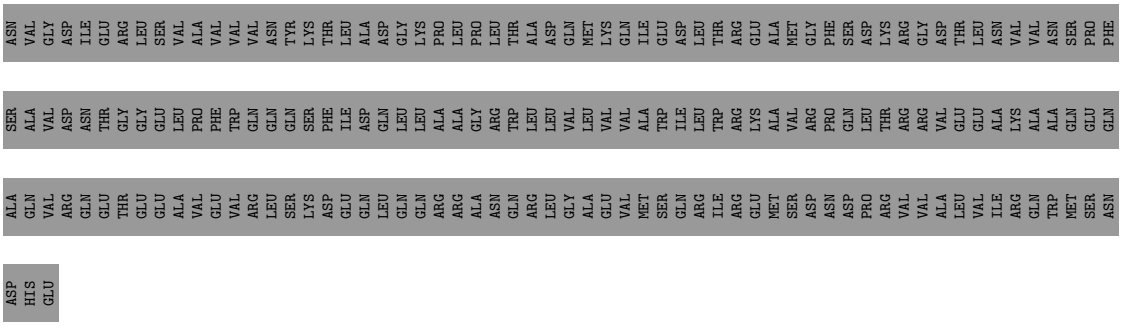




- Molecule 1: Flagellar M-ring protein

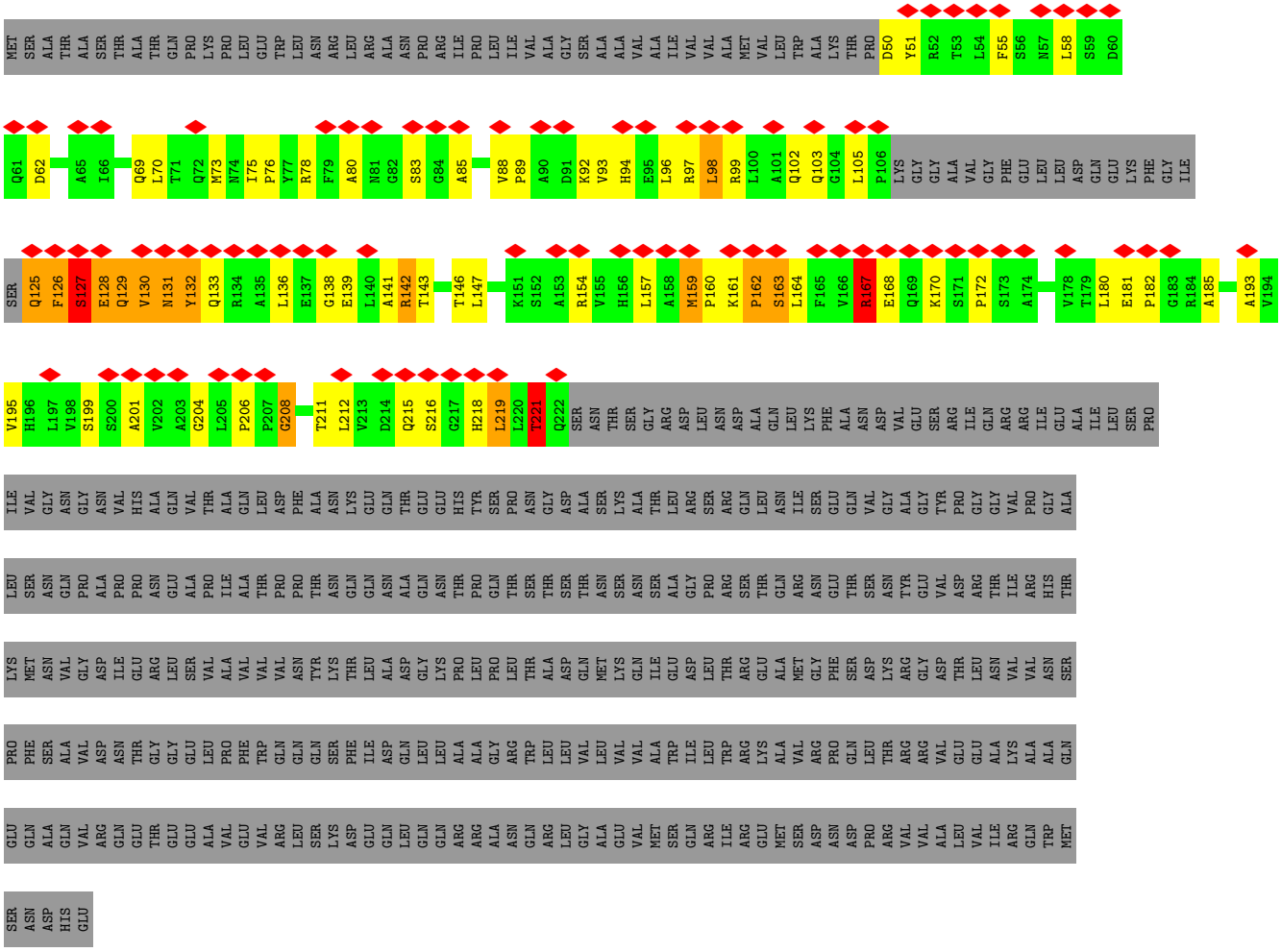
Chain UK:





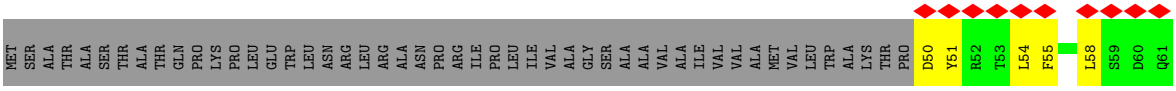
- Molecule 1: Flagellar M-ring protein

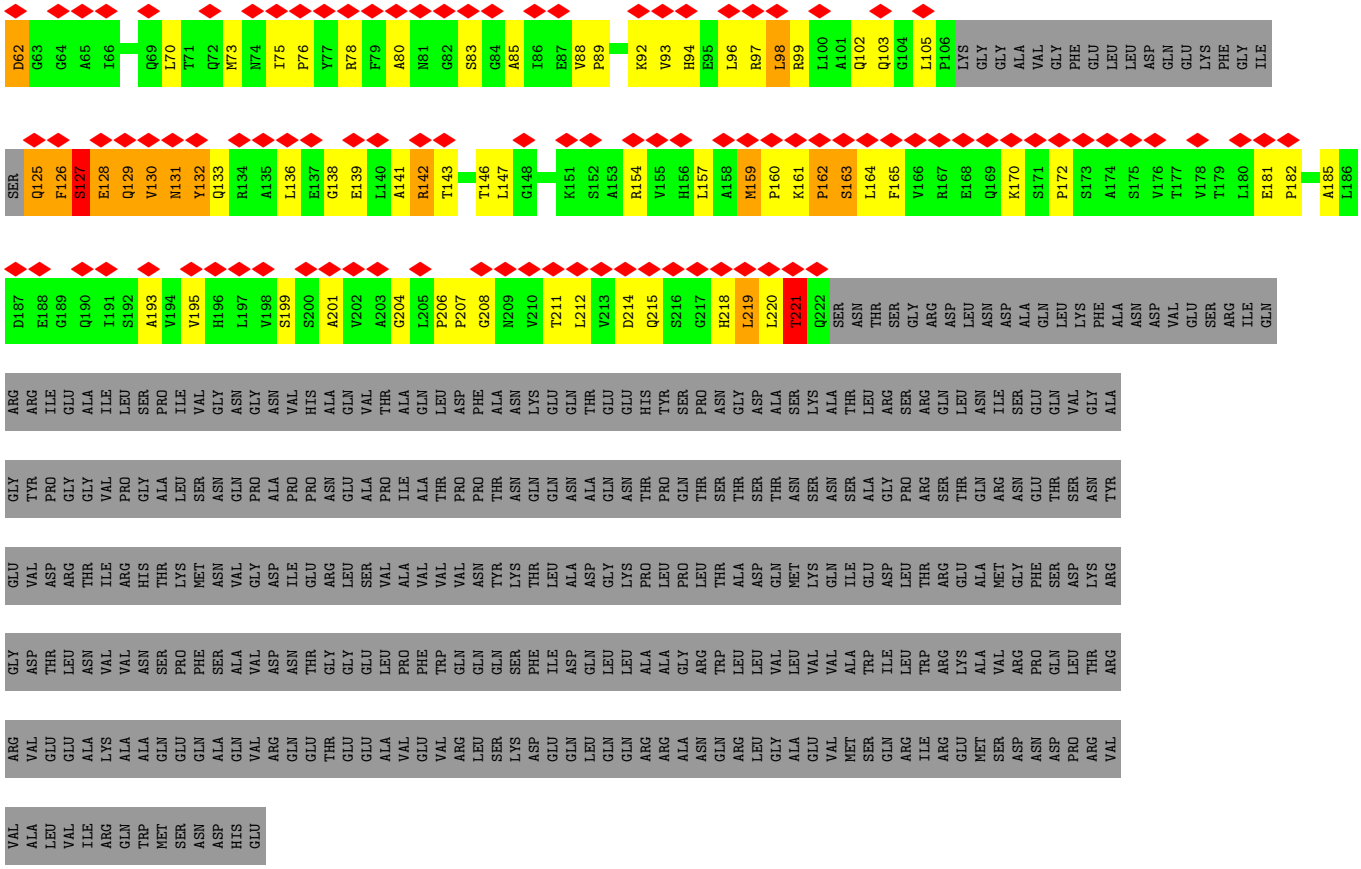
Chain UL:



- Molecule 1: Flagellar M-ring protein

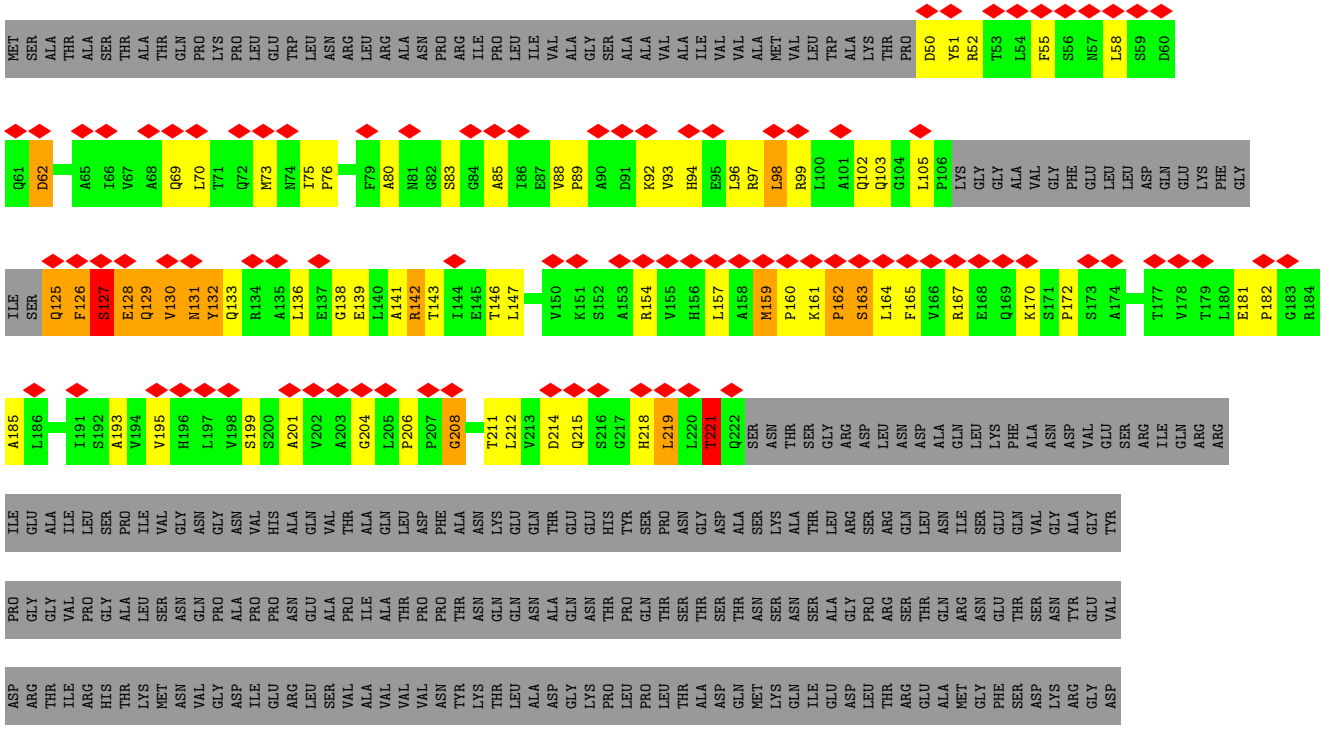
Chain UM:

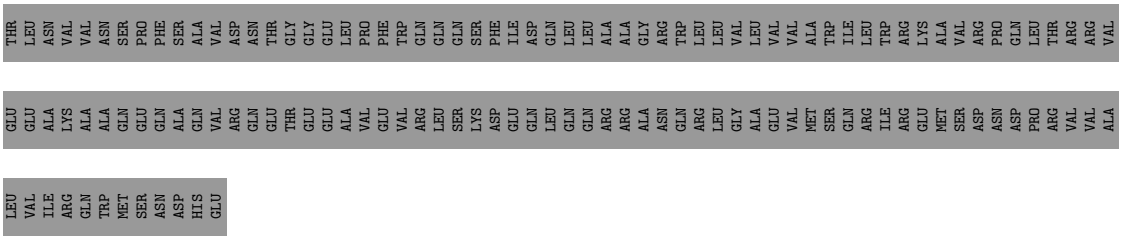




- Molecule 1: Flagellar M-ring protein

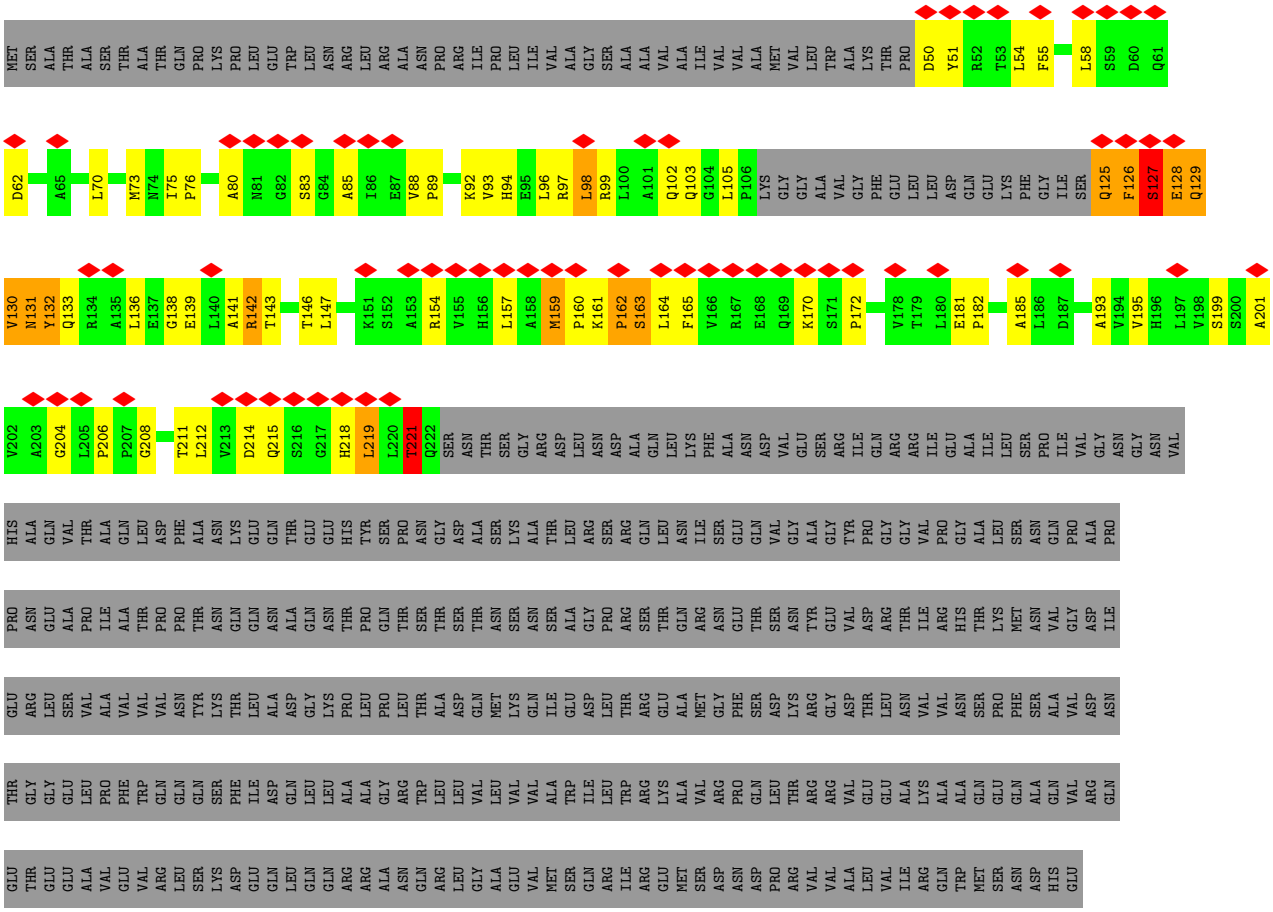
Chain UN:





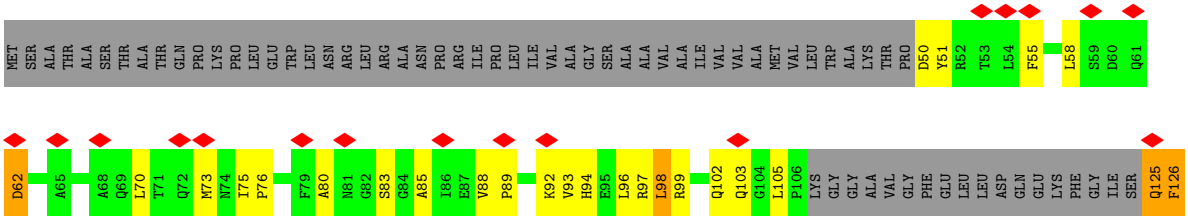
• Molecule 1: Flagellar M-ring protein

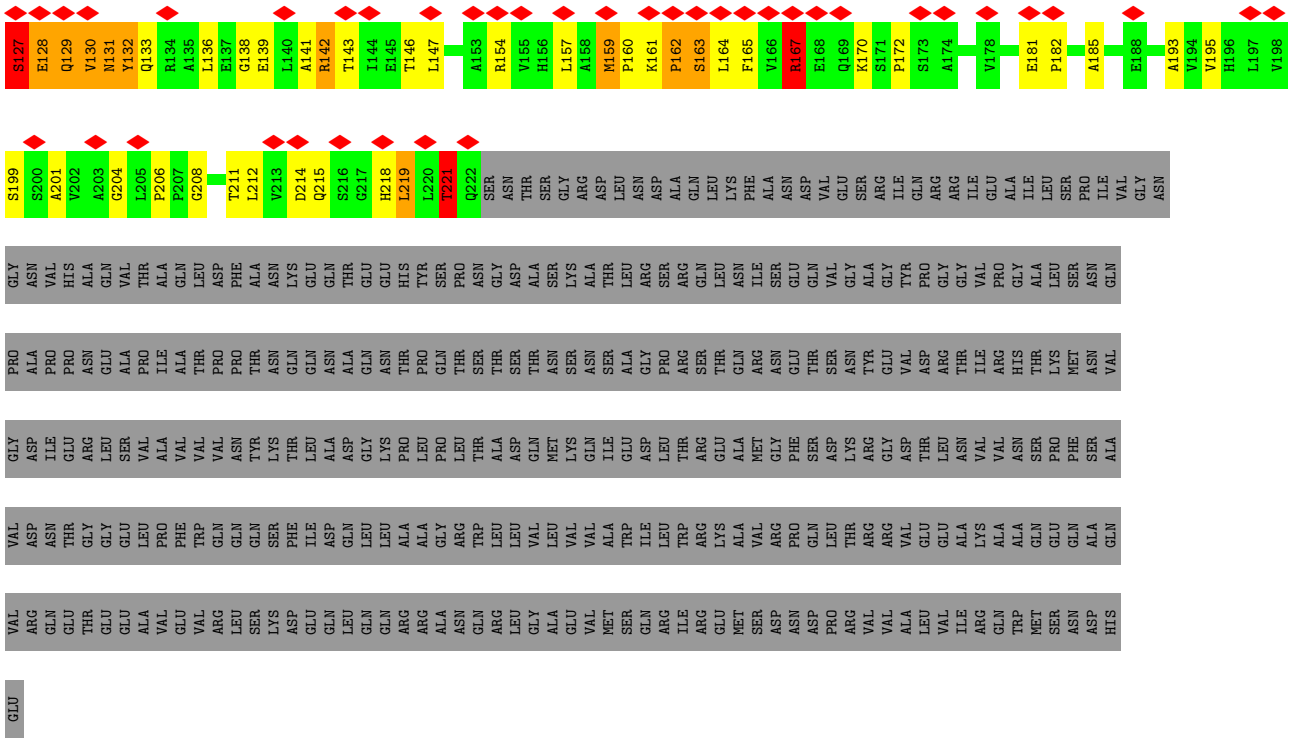
Chain UO:



• Molecule 1: Flagellar M-ring protein

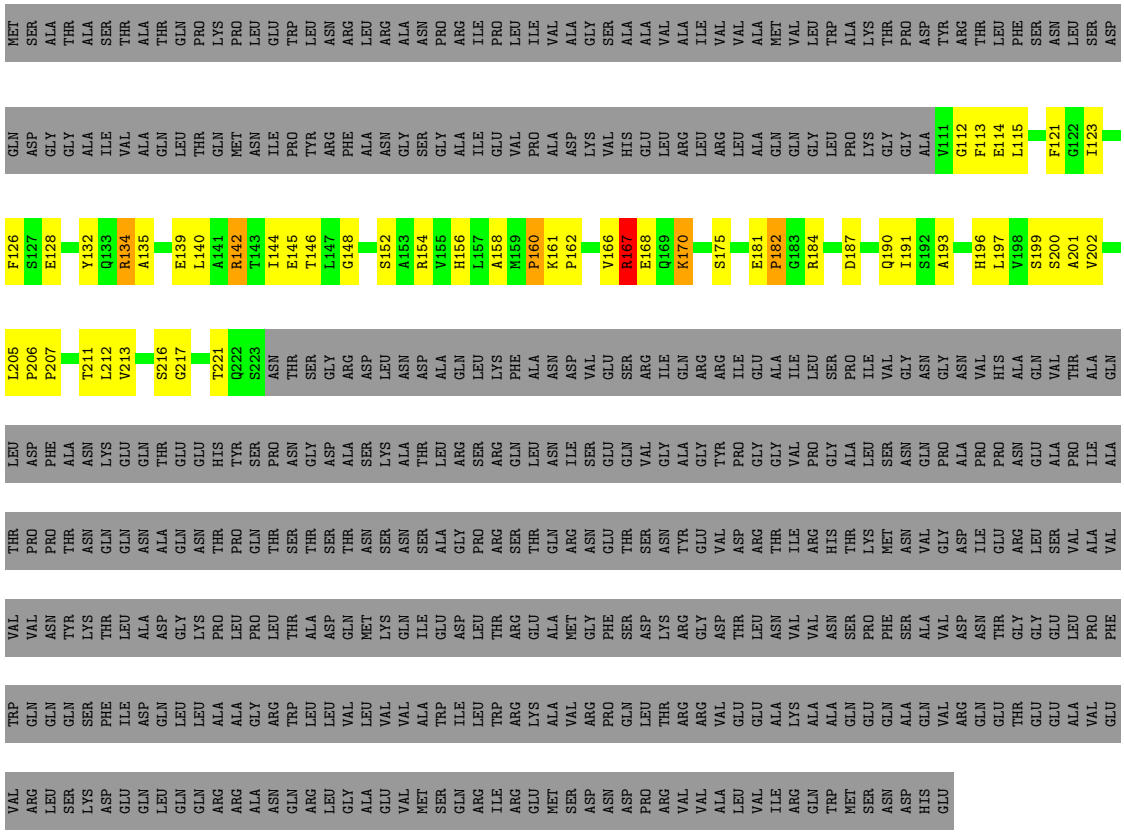
Chain UP:





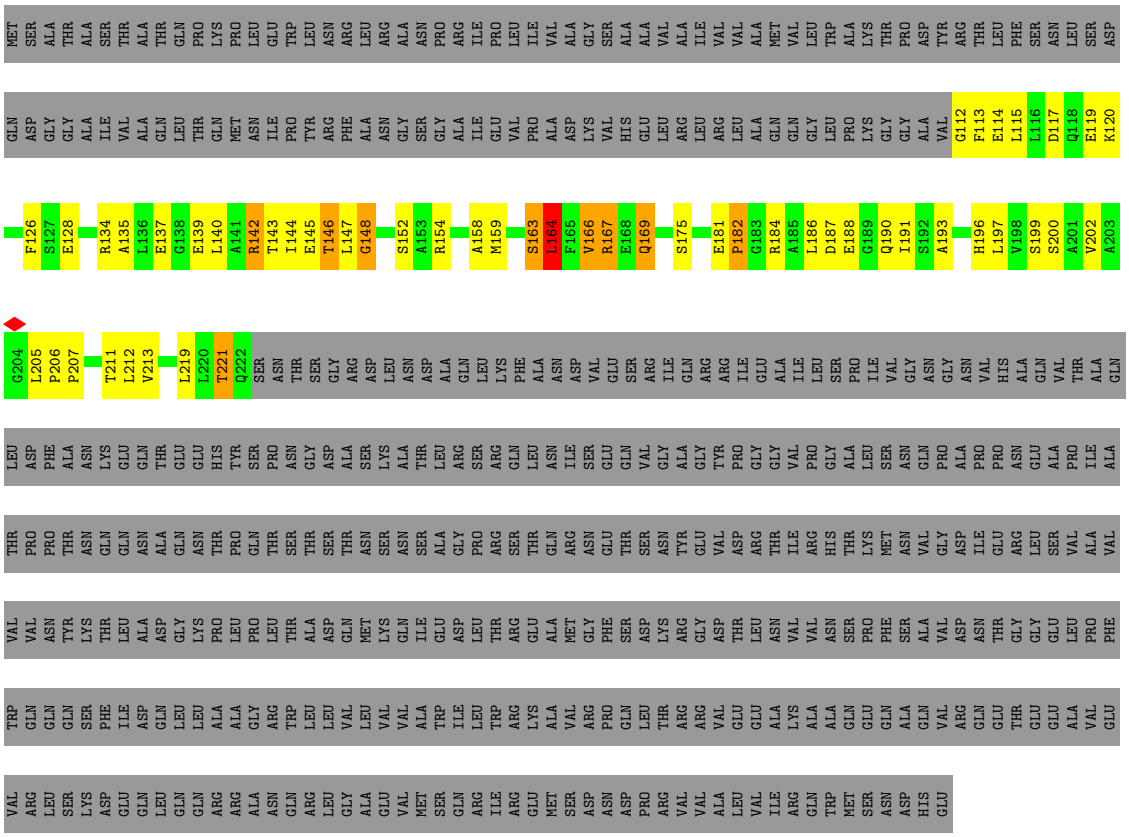
- Molecule 1: Flagellar M-ring protein

Chain WA:



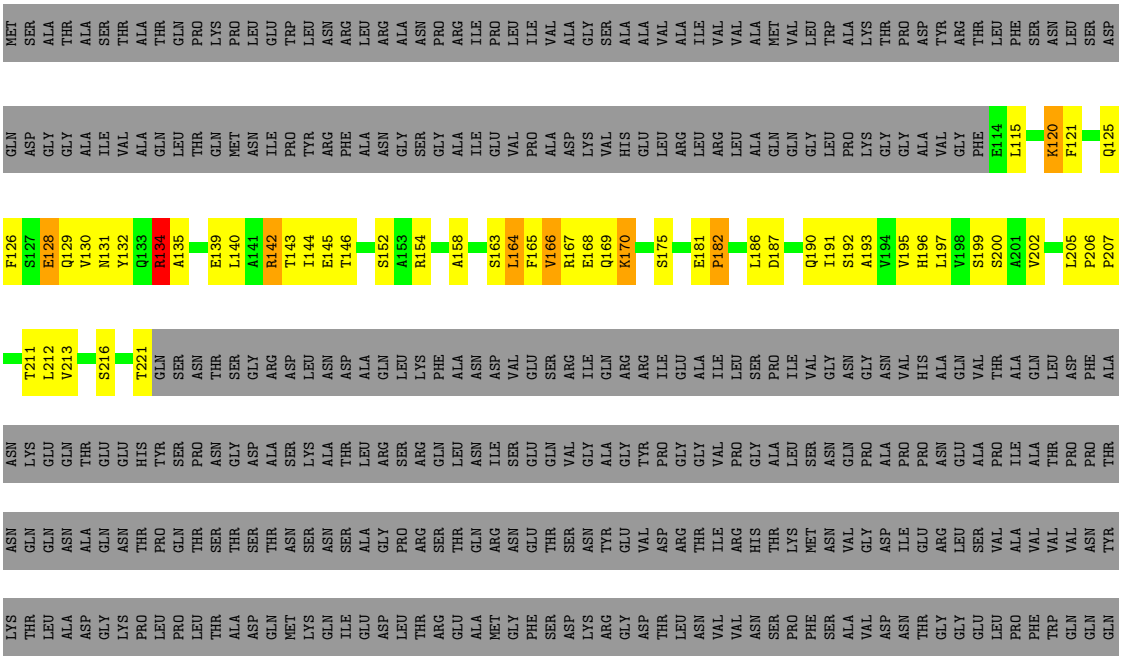
- Molecule 1: Flagellar M-ring protein

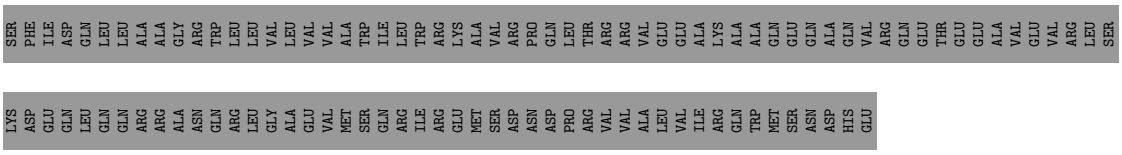
Chain WB: 10% 8% • 80%



- Molecule 1: Flagellar M-ring protein

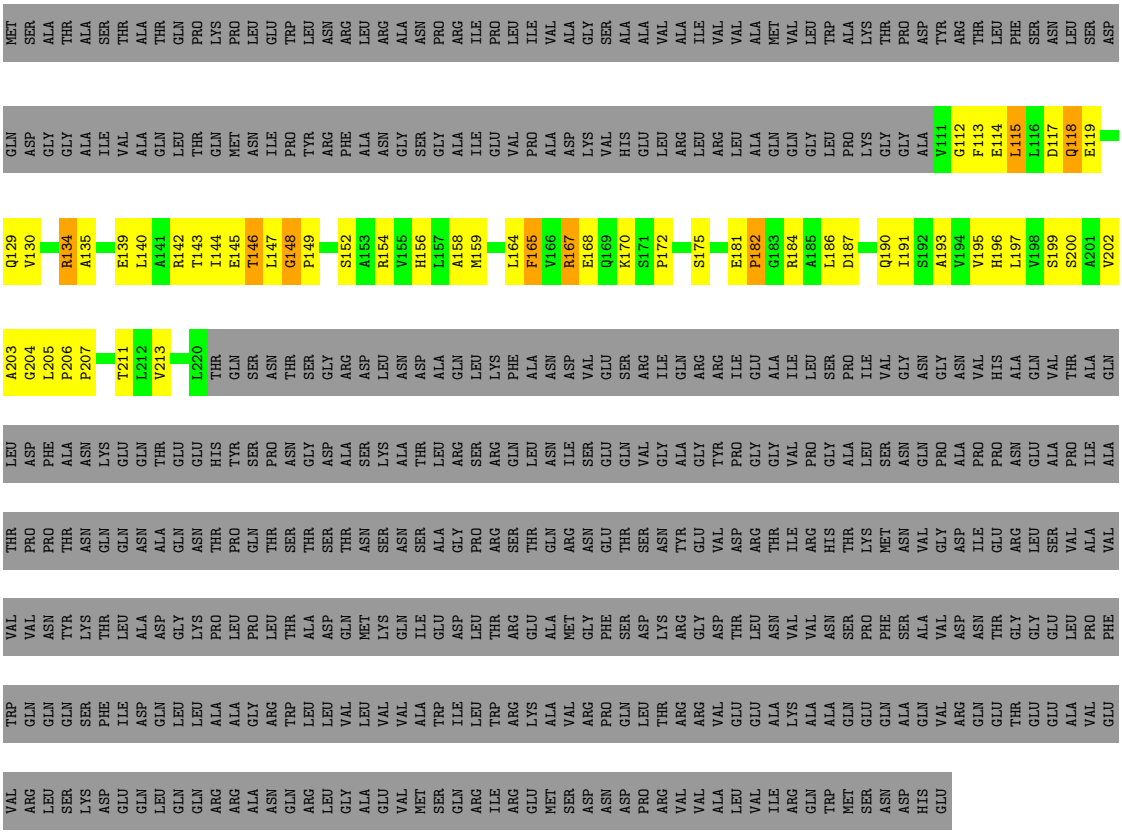
Chain WC: 10% 8% • 81%





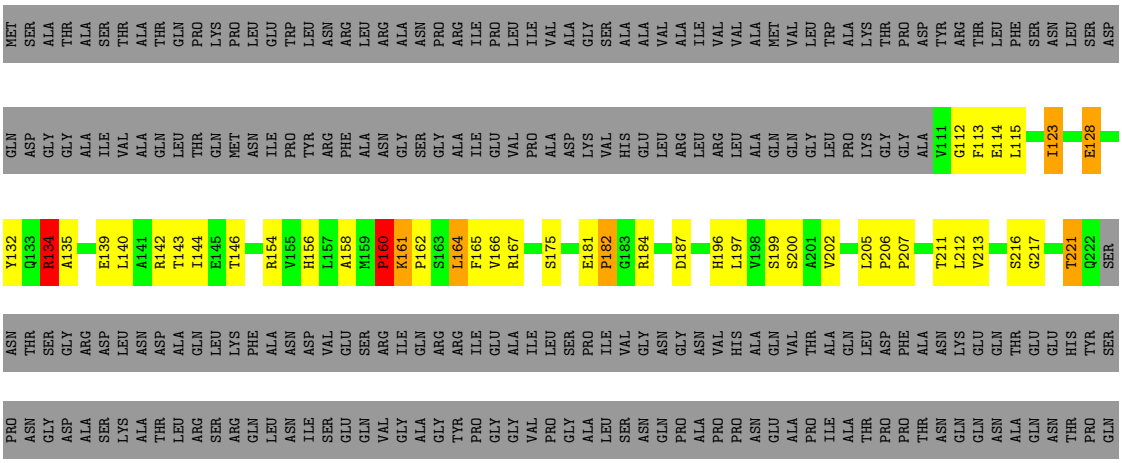
• Molecule 1: Flagellar M-ring protein

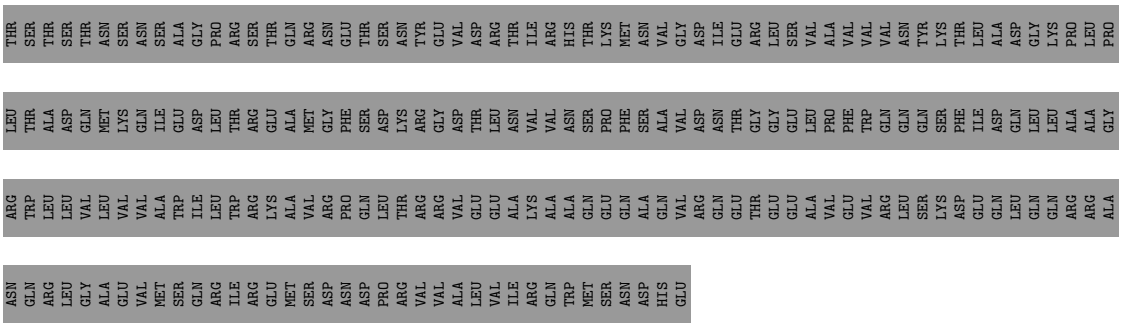
Chain WD: 10% 8% • 80%



• Molecule 1: Flagellar M-ring protein

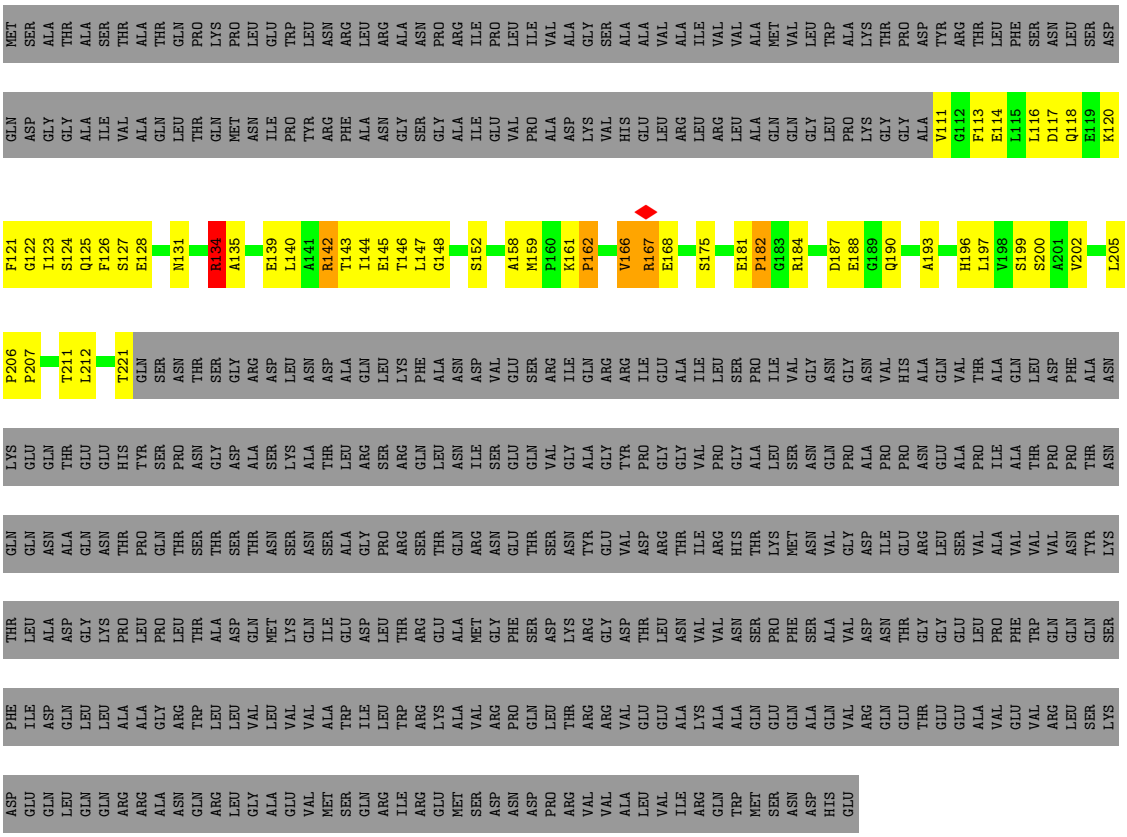
Chain WE: 12% 6% • 80%





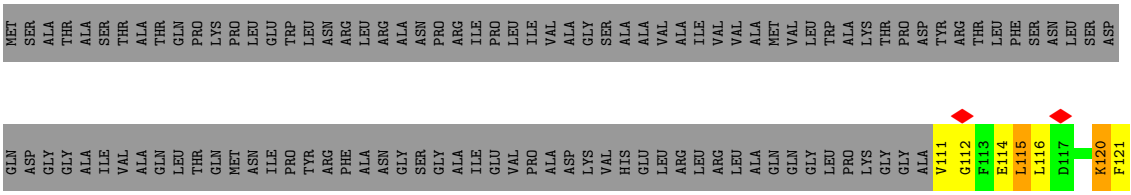
- Molecule 1: Flagellar M-ring protein

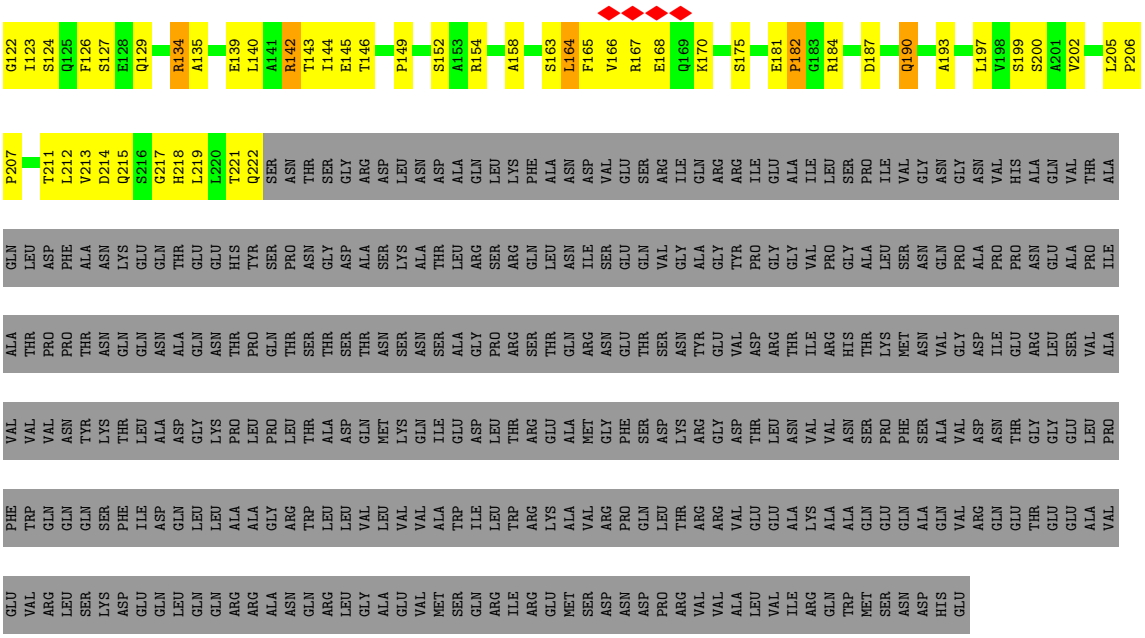
Chain WF: 10% 9% • 80%



- Molecule 1: Flagellar M-ring protein

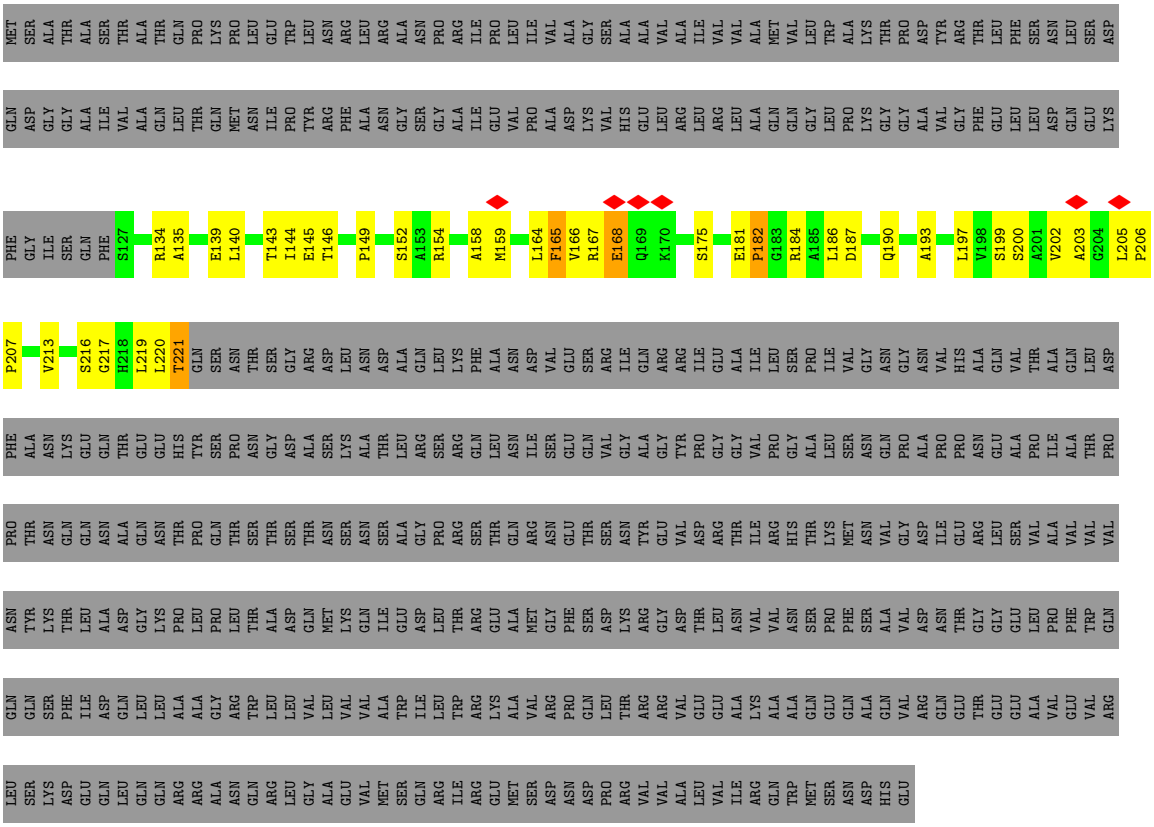
Chain WG: • 10% 9% • 80%





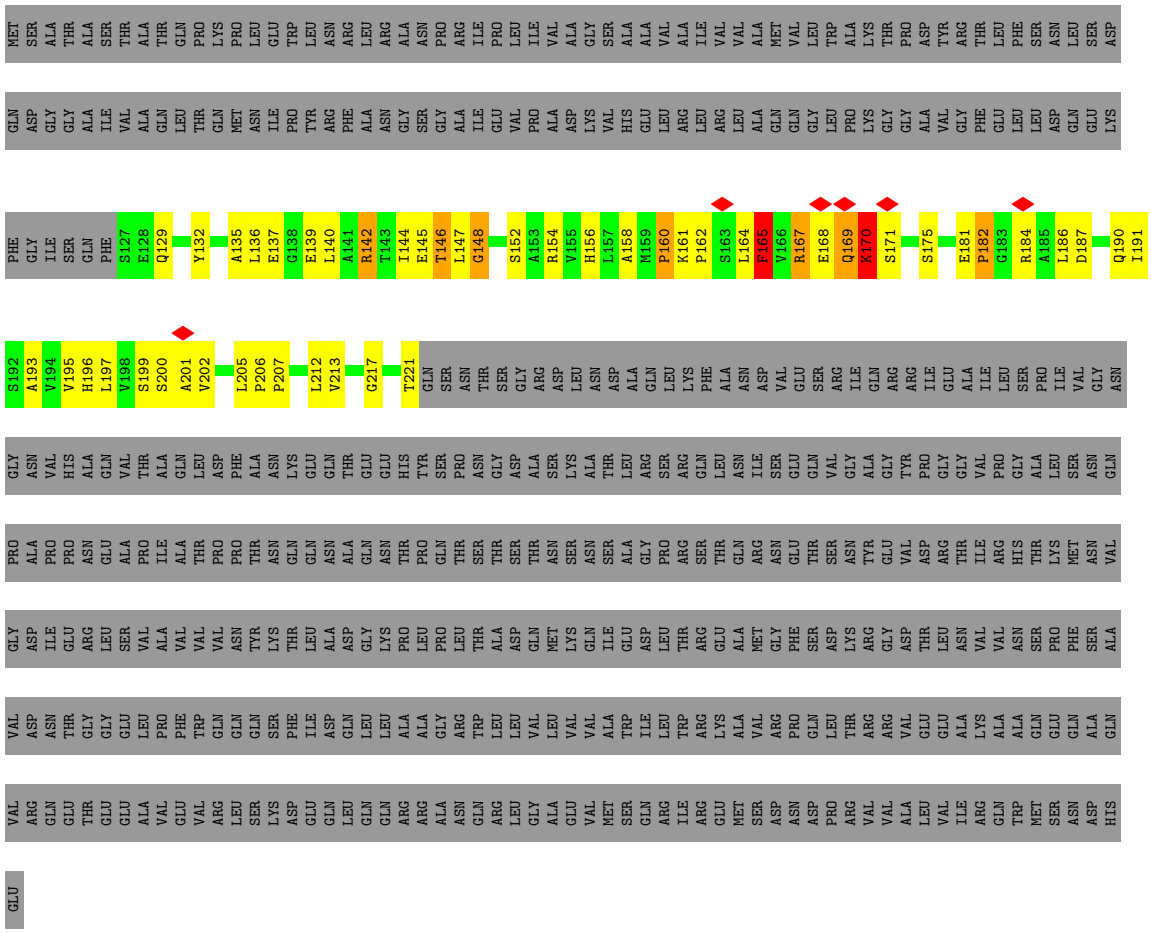
- Molecule 1: Flagellar M-ring protein

Chain WH:



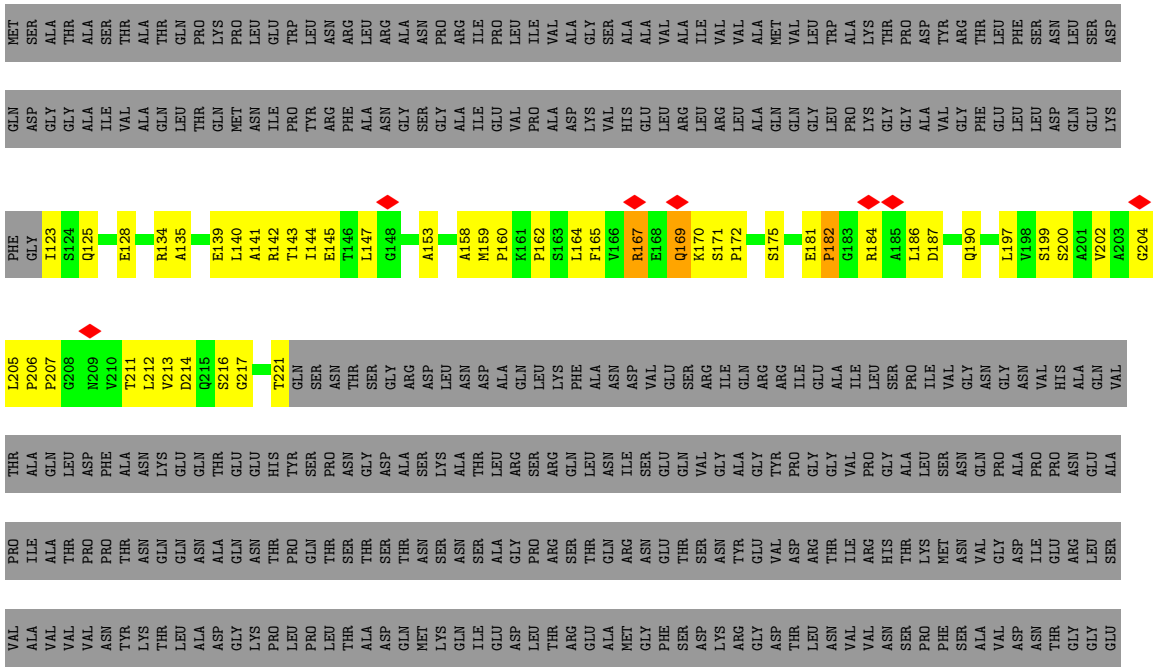
- Molecule 1: Flagellar M-ring protein

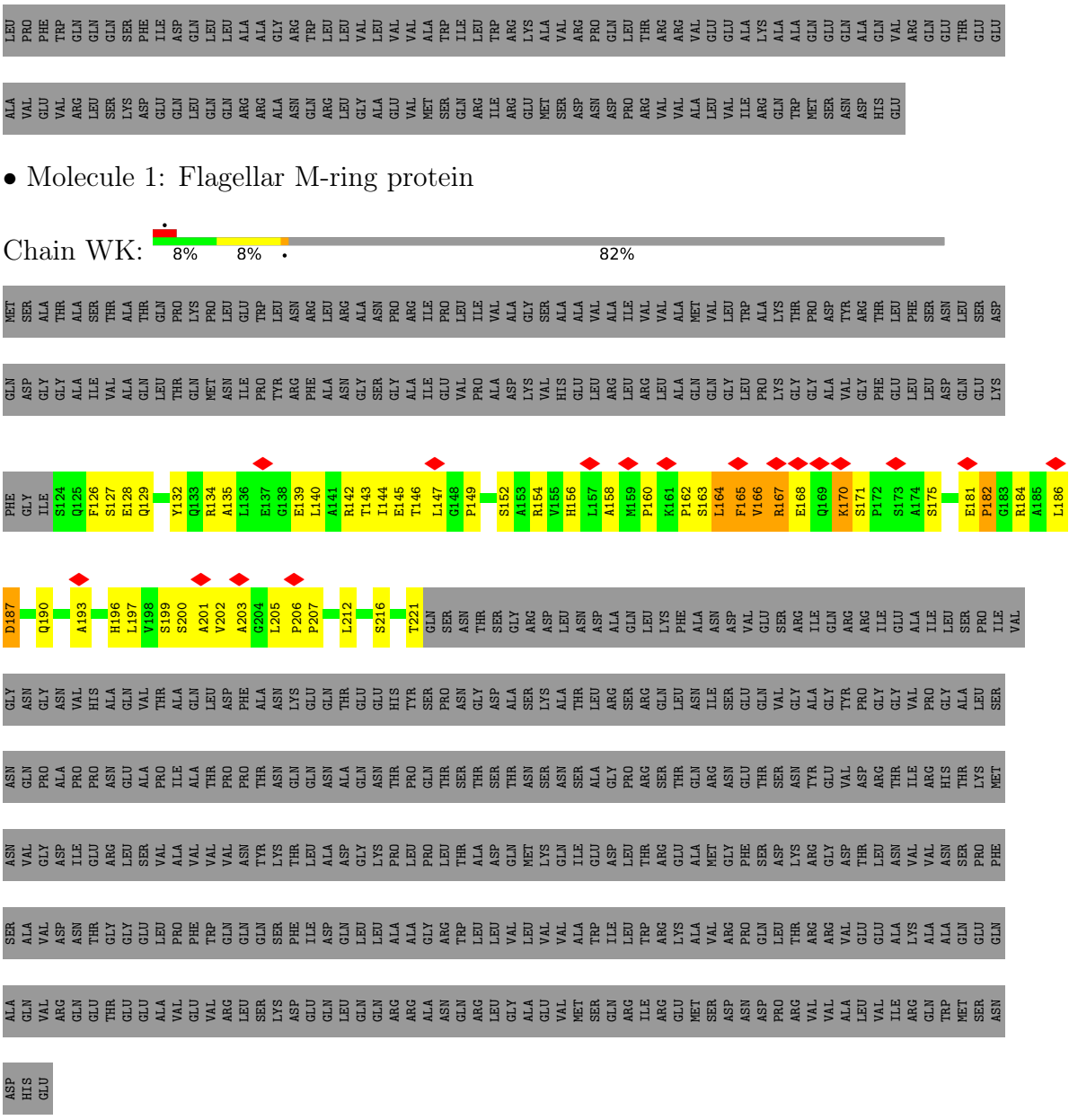
Chain WI:



- Molecule 1: Flagellar M-ring protein

Chain WJ:



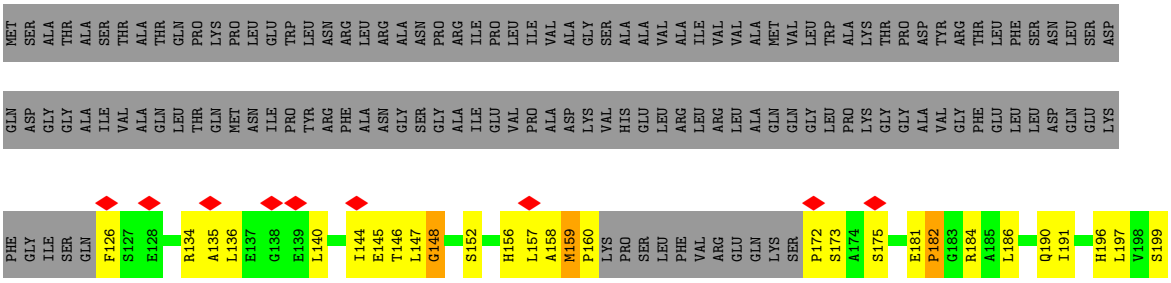


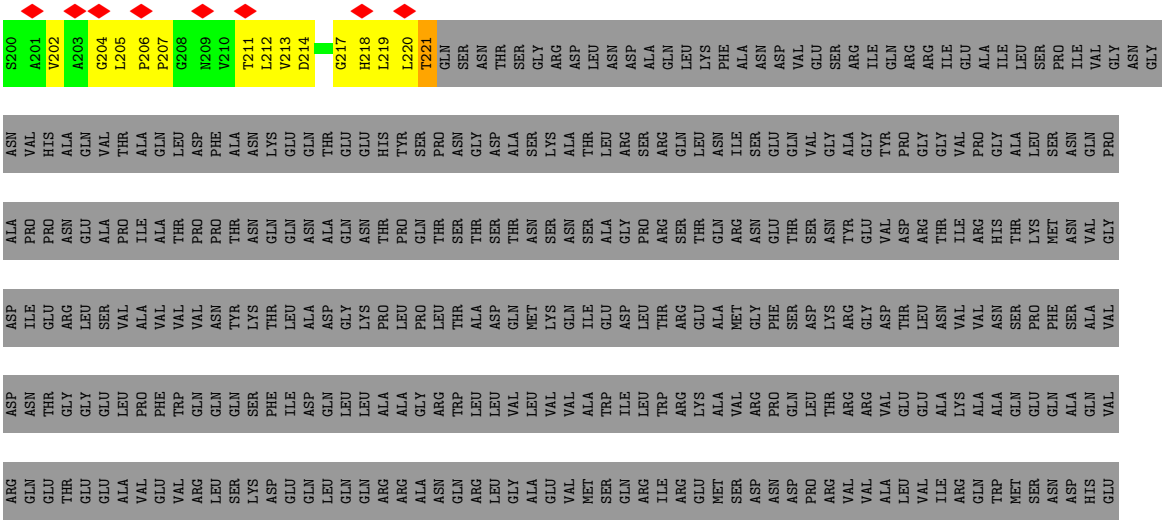
• Molecule 1: Flagellar M-ring protein

Chain WK: 8% 8% • 82%

• Molecule 1: Flagellar M-ring protein

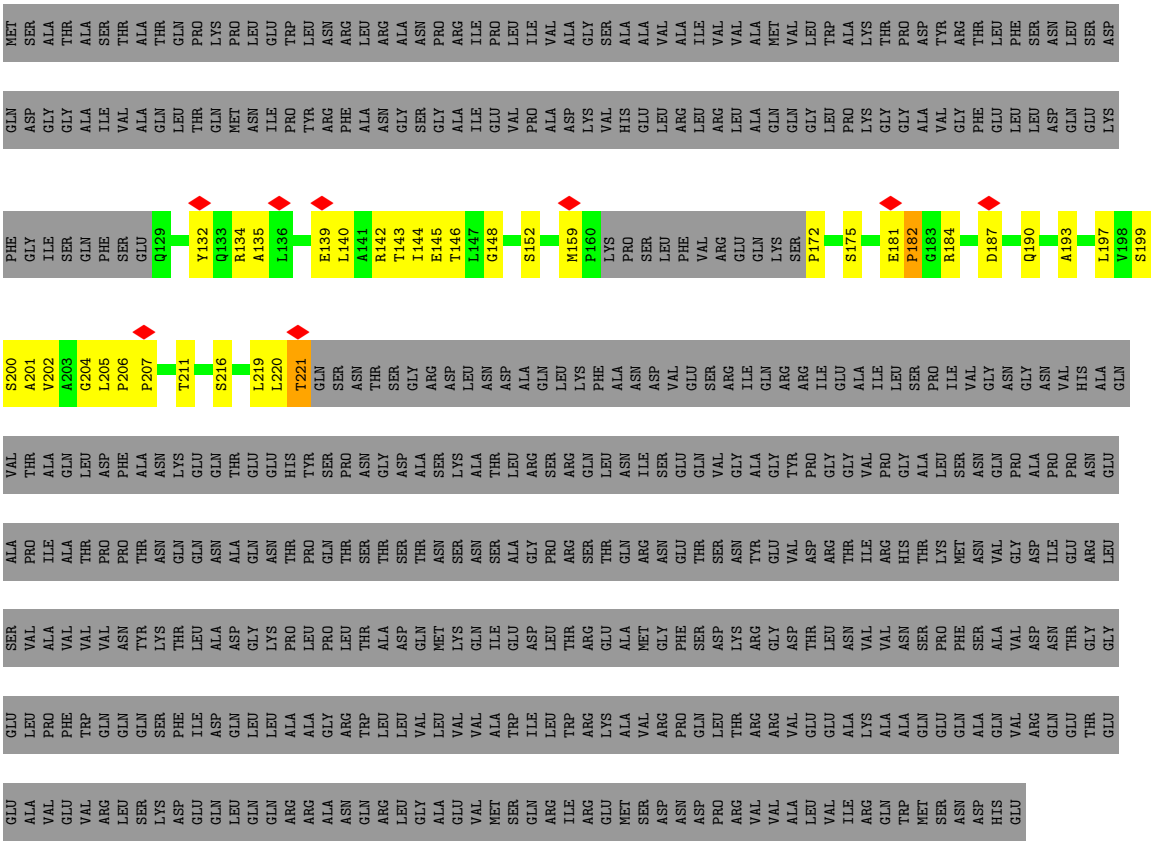
Chain WL: 8% 7% • 85%





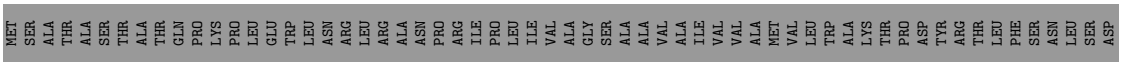
- Molecule 1: Flagellar M-ring protein

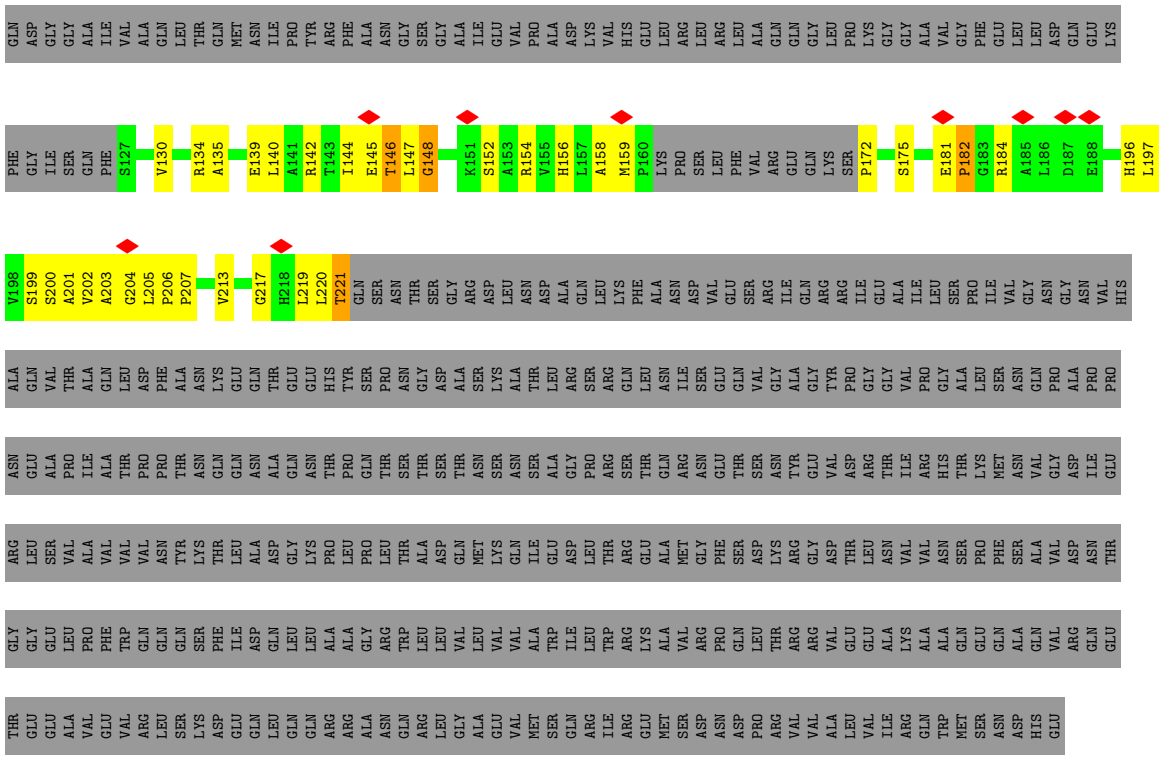
Chain WM:



- Molecule 1: Flagellar M-ring protein

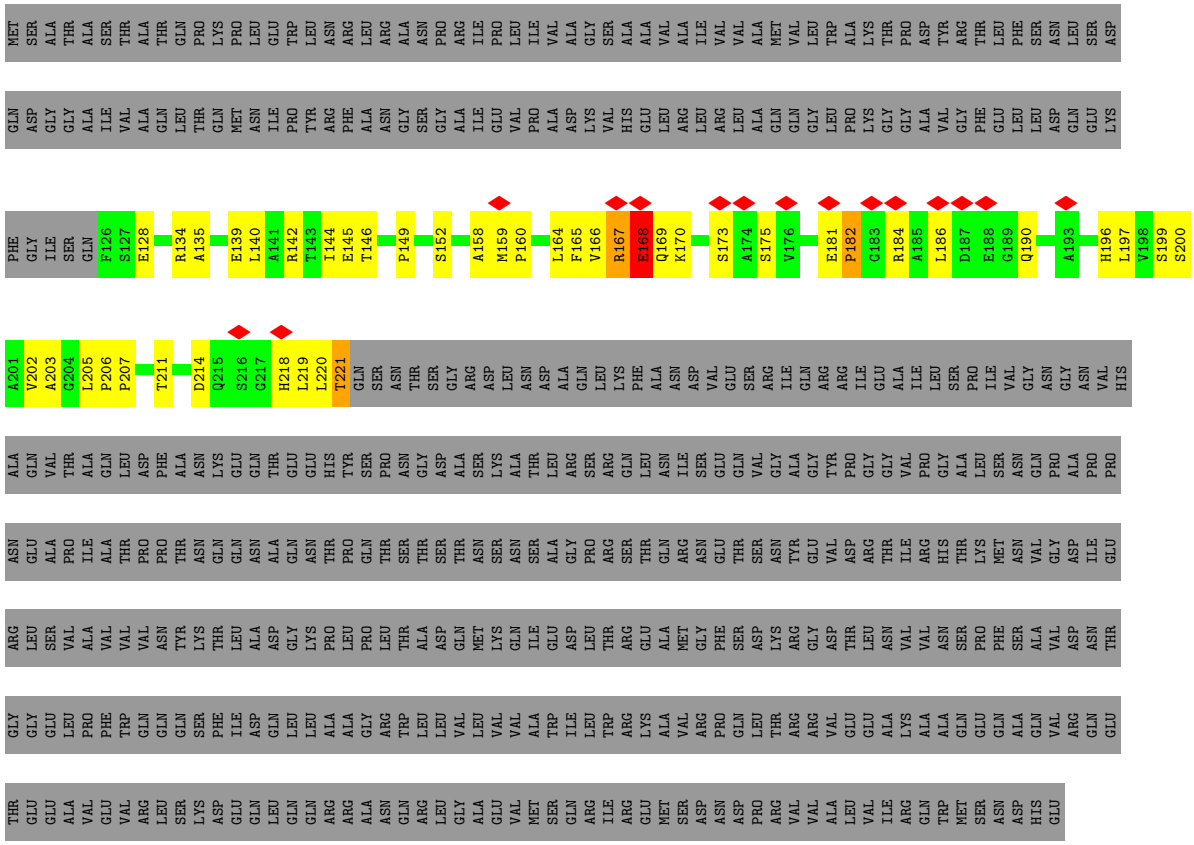
Chain WN:





- Molecule 1: Flagellar M-ring protein

Chain WO:



• Molecule 1: Flagellar M-ring protein

Chain WP: 10% 7% • 82%

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 G122 I123 F126 S127 E128 R134 A135 E139 L140 A141 R142 T143 I144 E145 T146 L147 G148 K151 S152 A153 R154 A158 M159 P160 K161 P162 S163 L164 F165 V166 Q169 S175 E181 P182 G183 R184 A185 L186 D187 E188 G189 Q190 I191 S192 A193 H196 L197 V198 S199 S200

A201 V202 L205 P206 P207 T211 L212 V213 D214 Q215 S216 G217 H218 T221 GLN SER ASN THR SER GLY ARG ASP LEU ASN ASP ALA GLN LEU LYS PHE ALA ASN ASP VAL GLU SER ARG ILE GLN ARG ARG ILE GLU ALA ILE LEU SER PRO ILE VAL GLY ASN GLY ASN VAL HIS ALA

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

LEU SER VAL ALA VAL VAL VAL ASN TYR LYS THR LEU ALA ASP GLY LYS PRO LEU PRO LEU THR ALA ASP GLN MET LYS GLN ILE GLU ASP LEU THR ARG GLU ALA MET GLY PHE SER ASP LYS ARG GLY ASP THR LEU ASN VAL VAL ASN SER PRO PHE SER 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 ARG ALA ASN GLN ARG LEU GLY ALA GLU 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 WQ: 9% 9% • 80%

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

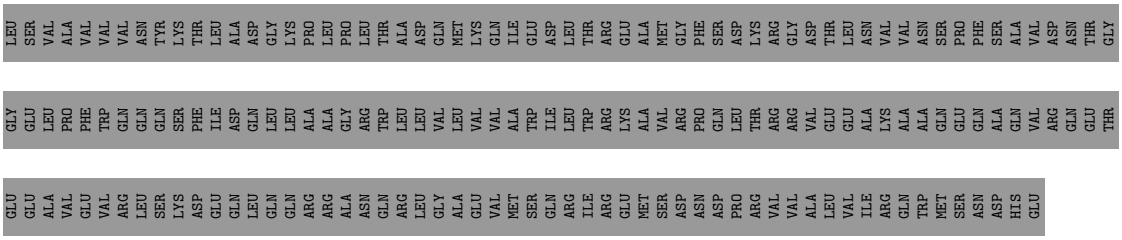
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA V111 G112 F113 E114 E119 K120 F121 G122 I123

S124 Q125 F126 S127 E128 R134 A135 E139 L140 A141 R142 T143 I144 E145 T146 L147 G148 K151 S152 A158 M159 P160 S163 L164 F165 V166 R167 E168 Q169 K170 S171 P172 S175 E181 P182 G183 R184 A185 L186 D187 E188 G189 Q190 A193 H196 L197 V198 S199 S200 A201 V202

A203 G204 L205 P206 P207 T211 L212 V213 D214 Q215 S216 G217 H218 L219 L220 T221 GLN SER ASN THR SER GLY ARG ASP LEU ASN ASP ALA GLN LEU LYS PHE ALA ASN ASP VAL GLU SER ARG ILE GLN ARG ARG ILE GLU ALA ILE LEU SER PRO ILE VAL GLY ASN GLY ASN VAL HIS ALA

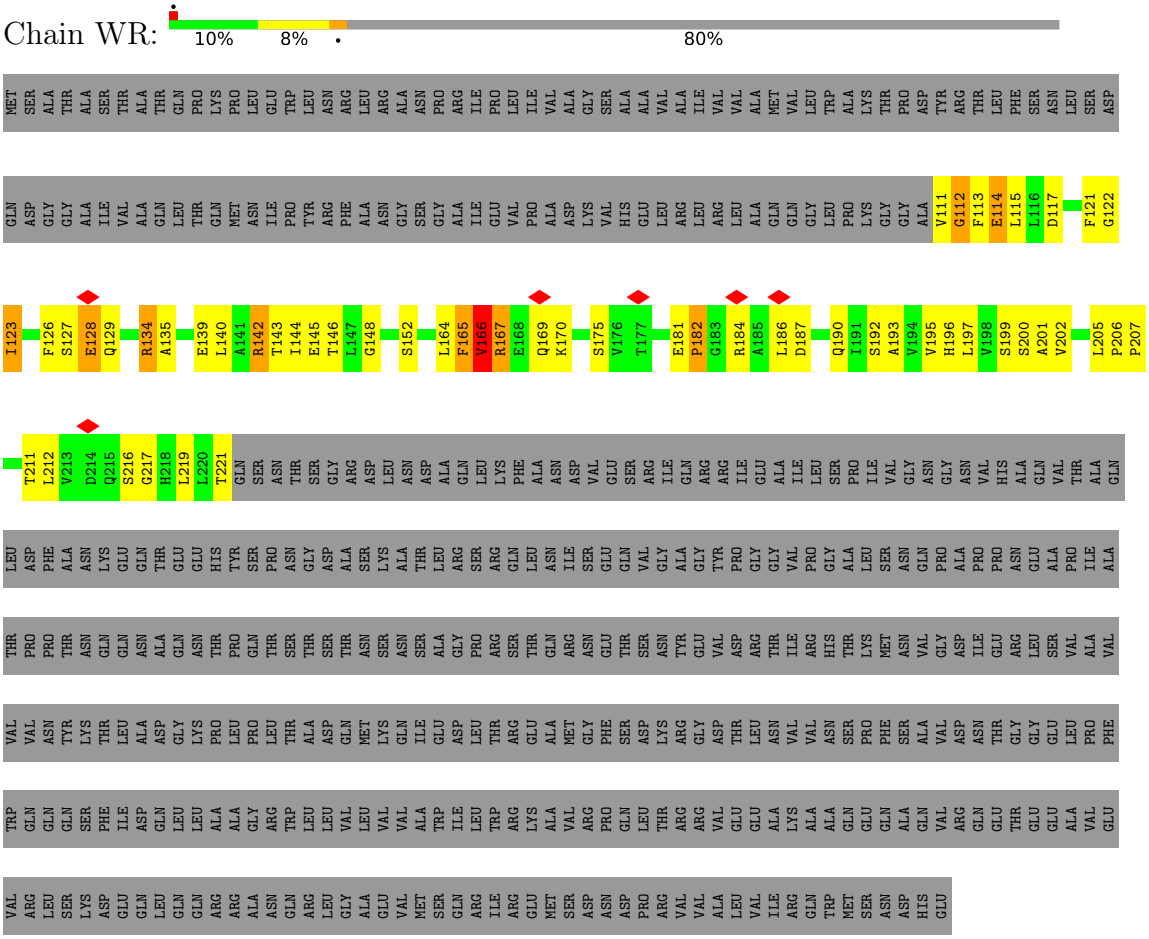
GLN VAL THR ALA GLN LEU ASP PHE ALA ASN LYS GLU GLN THR GLU GLU HIS TYR SER PRO ASN GLY ASP ALA SER LYS ALA THR LEU ARG SER ARG GLN LEU ASN ILE SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN

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



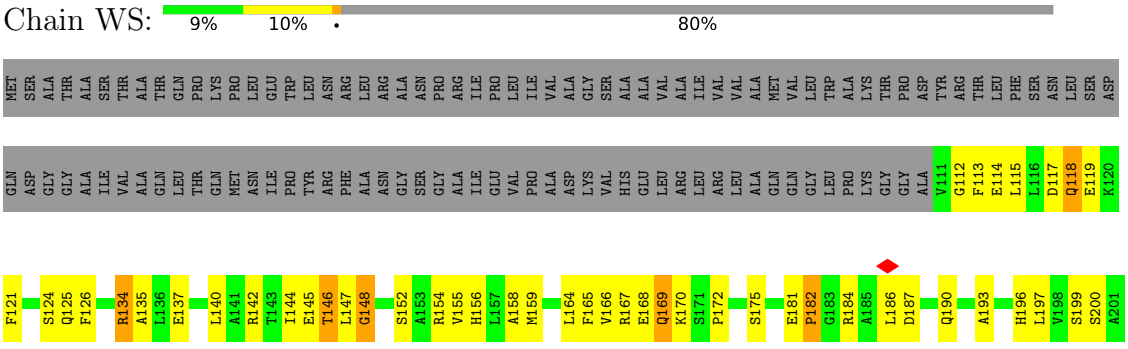
• Molecule 1: Flagellar M-ring protein

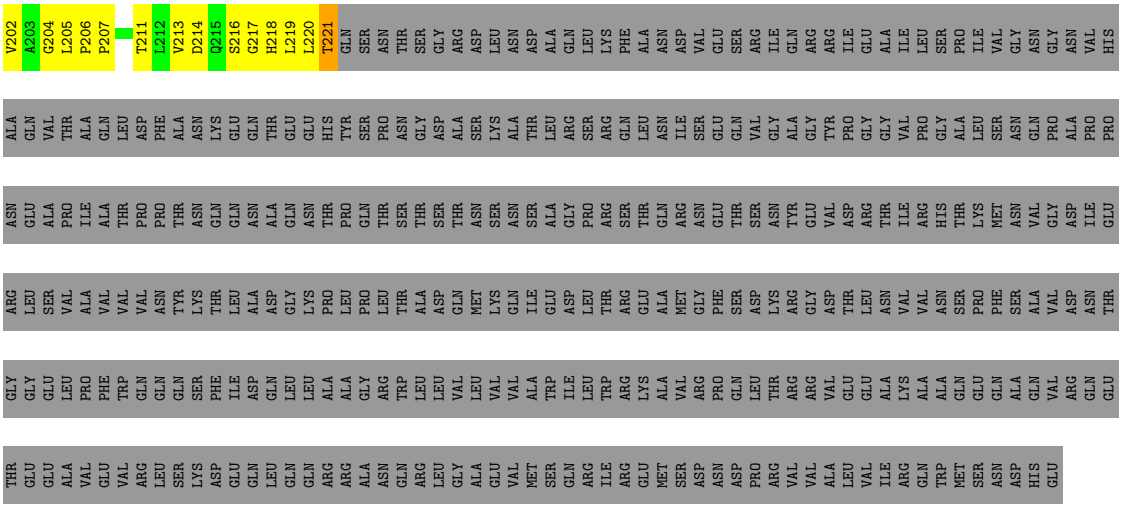
Chain WR:



• Molecule 1: Flagellar M-ring protein

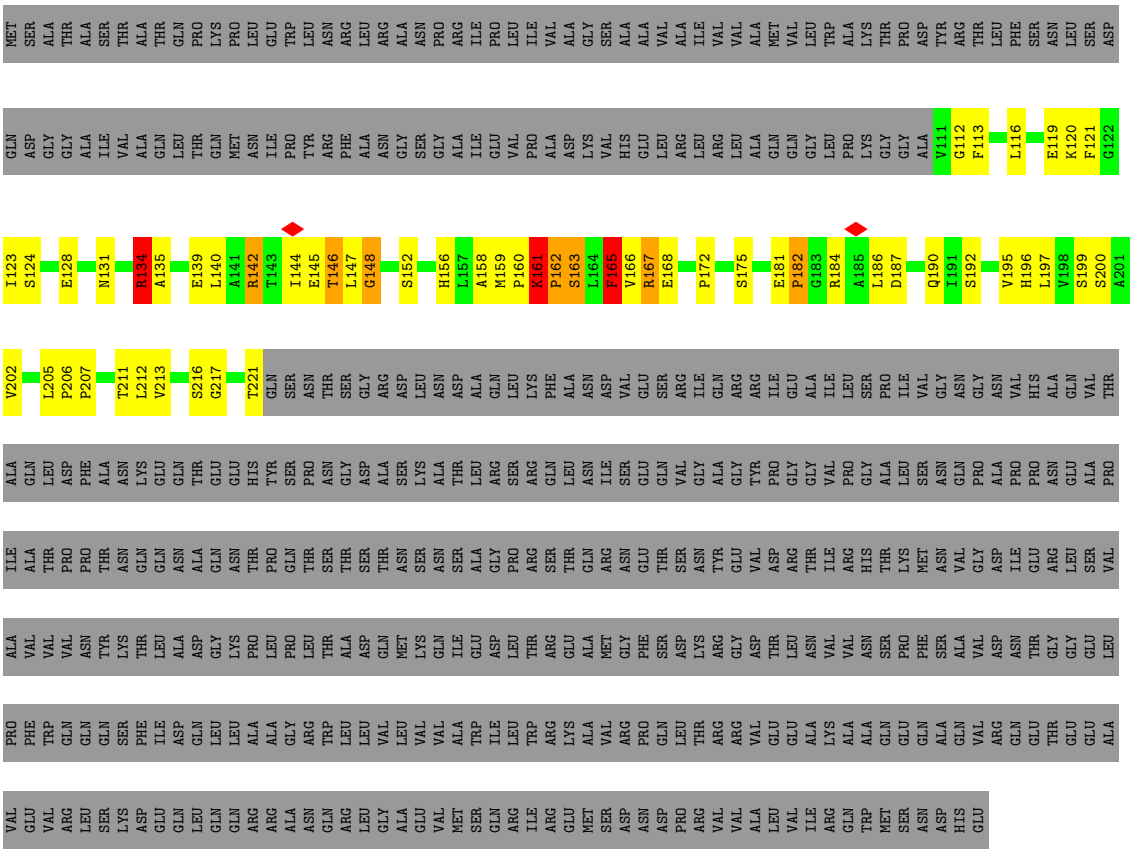
Chain WS:





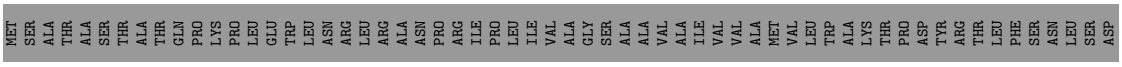
- Molecule 1: Flagellar M-ring protein

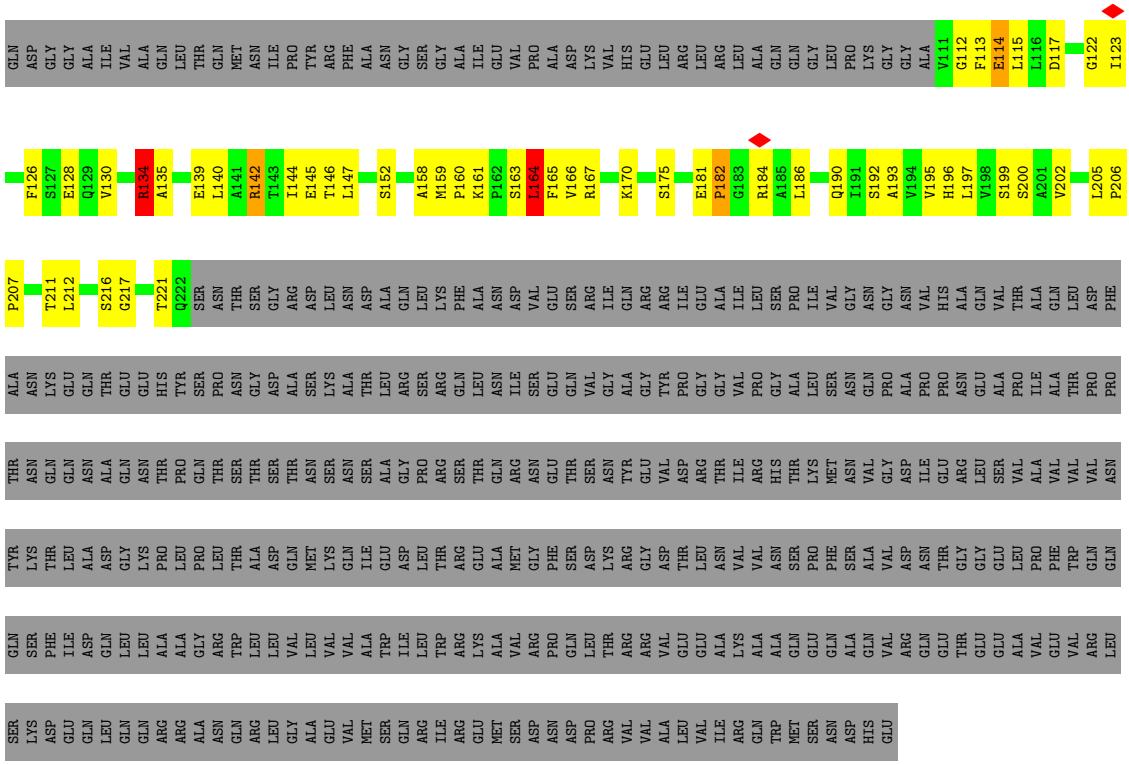
Chain WT: 10% 8% •• 80%



- Molecule 1: Flagellar M-ring protein

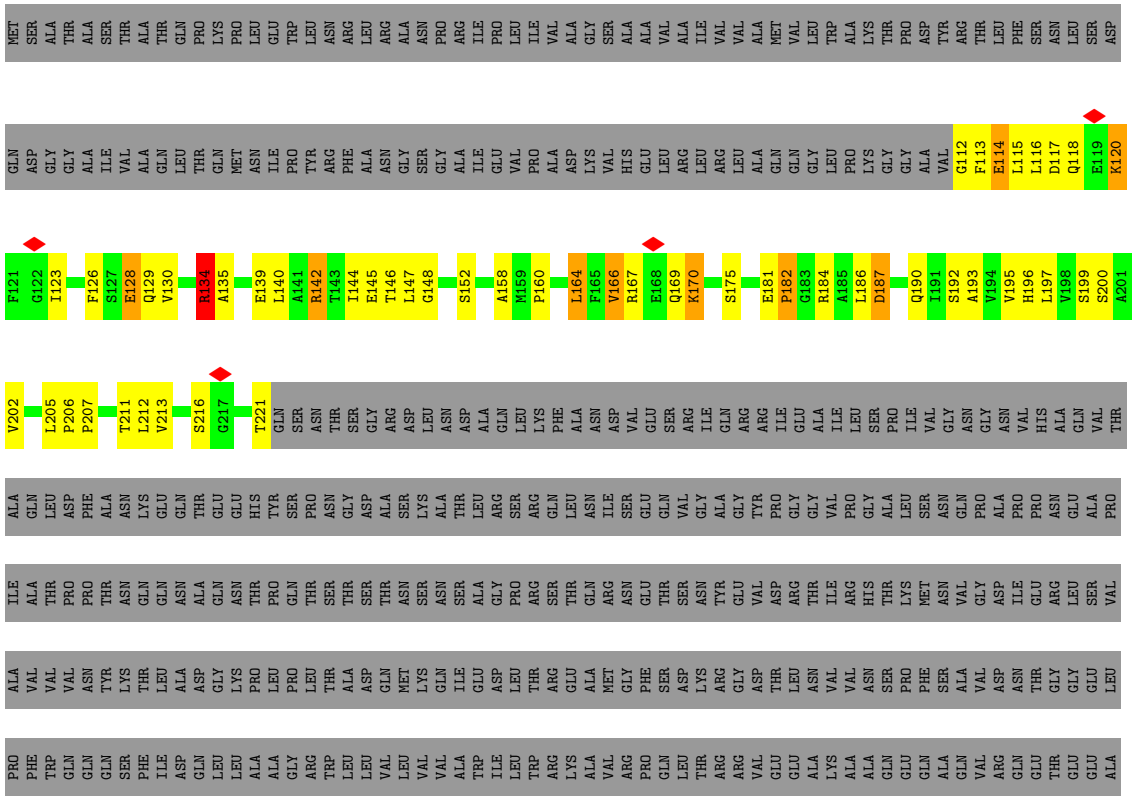
Chain WU: 11% 8% • 80%

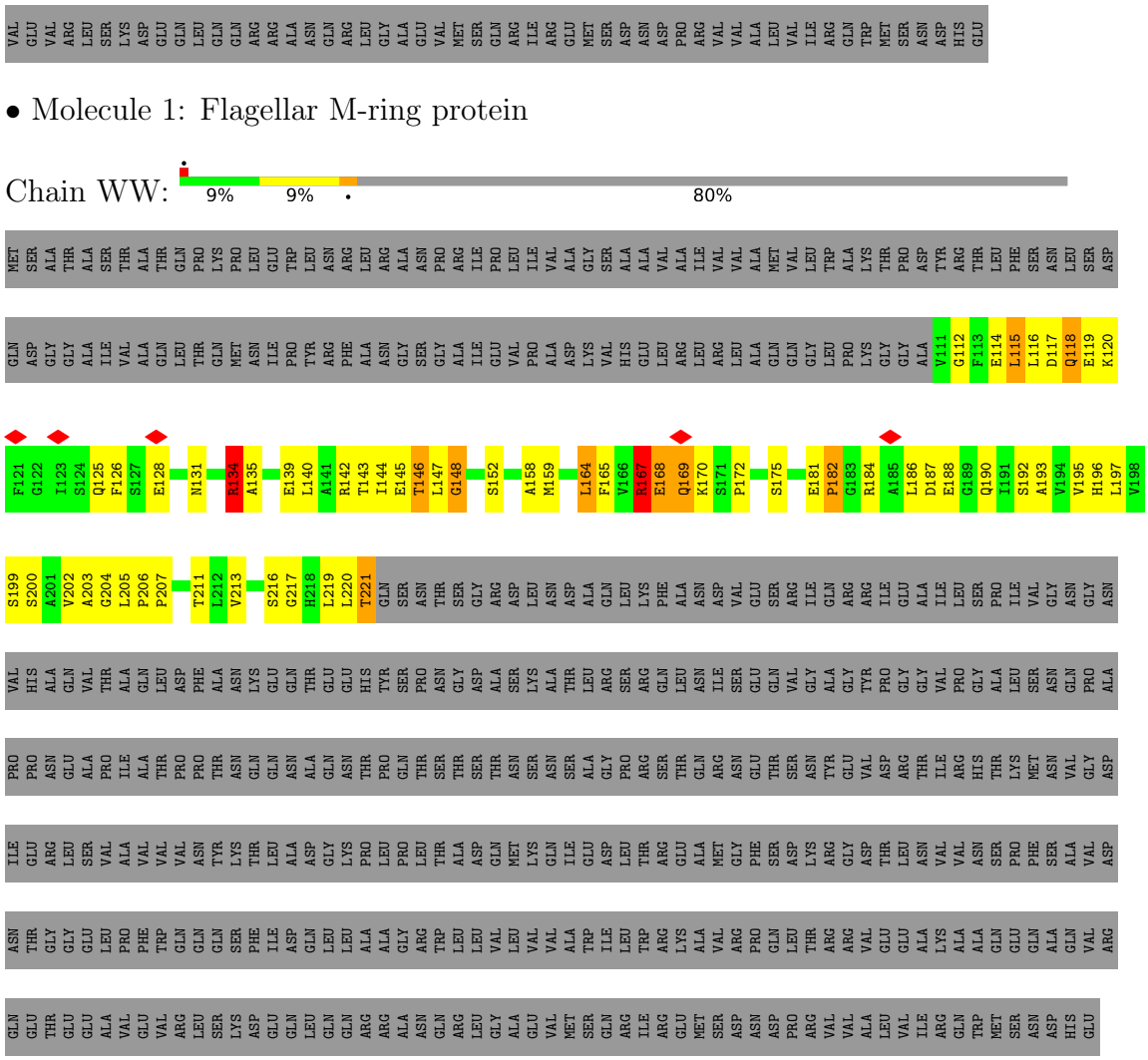


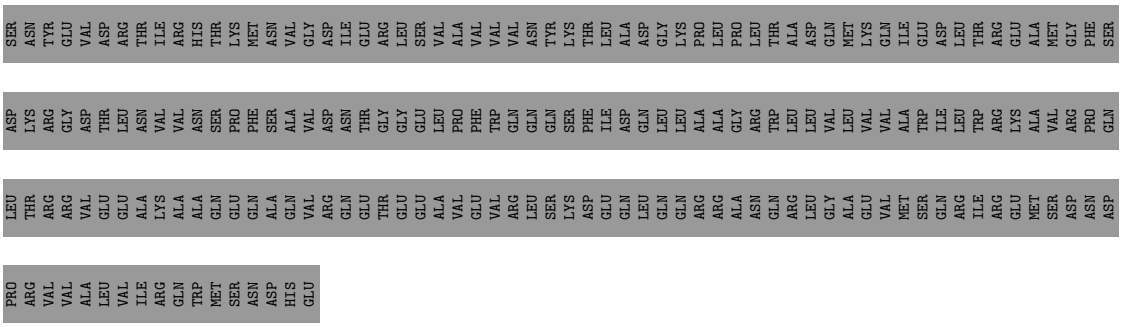


• Molecule 1: Flagellar M-ring protein

Chain WV: 10% 8% 80%

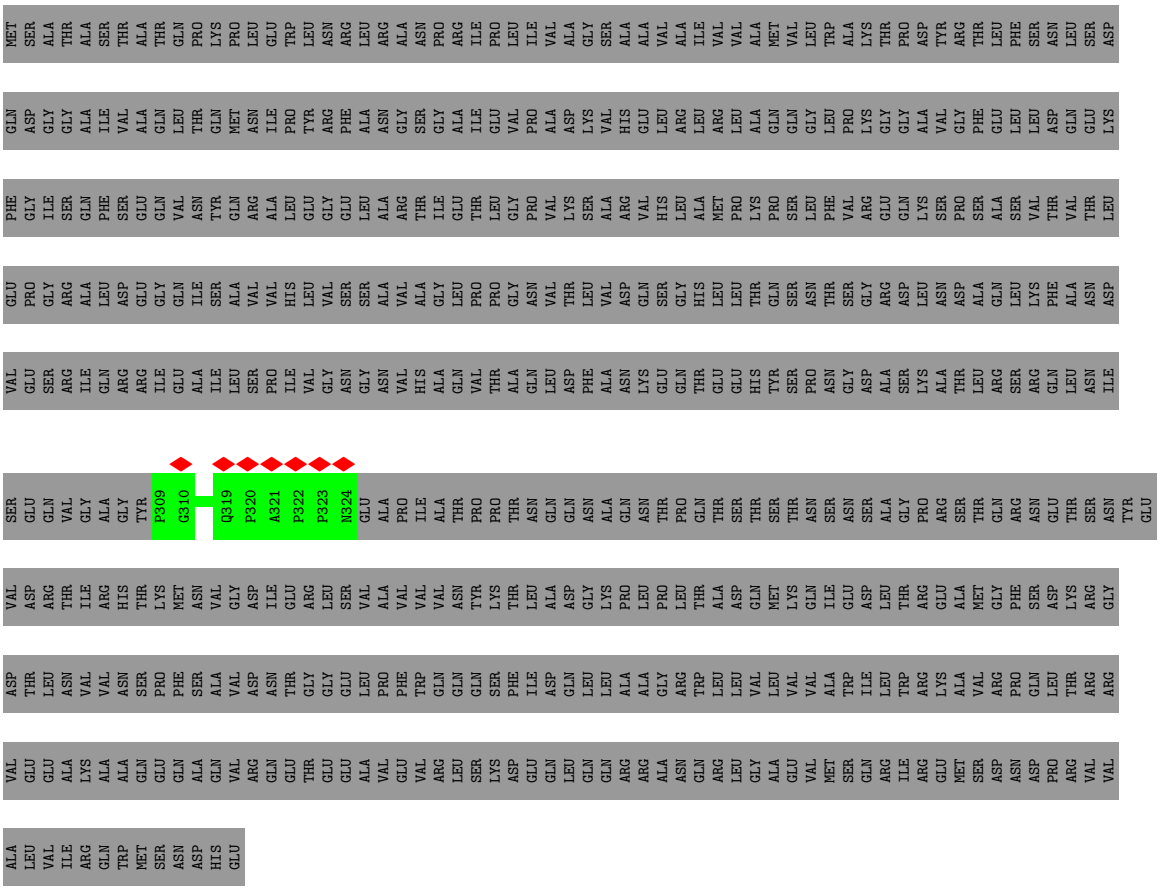



• Molecule 1: Flagellar M-ring protein
Chain WW:
9%
9%
80%
• Molecule 1: Flagellar M-ring protein
Chain b:
98%



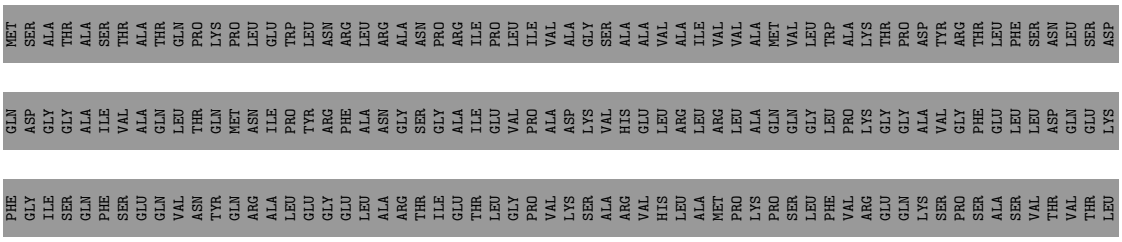
• Molecule 1: Flagellar M-ring protein

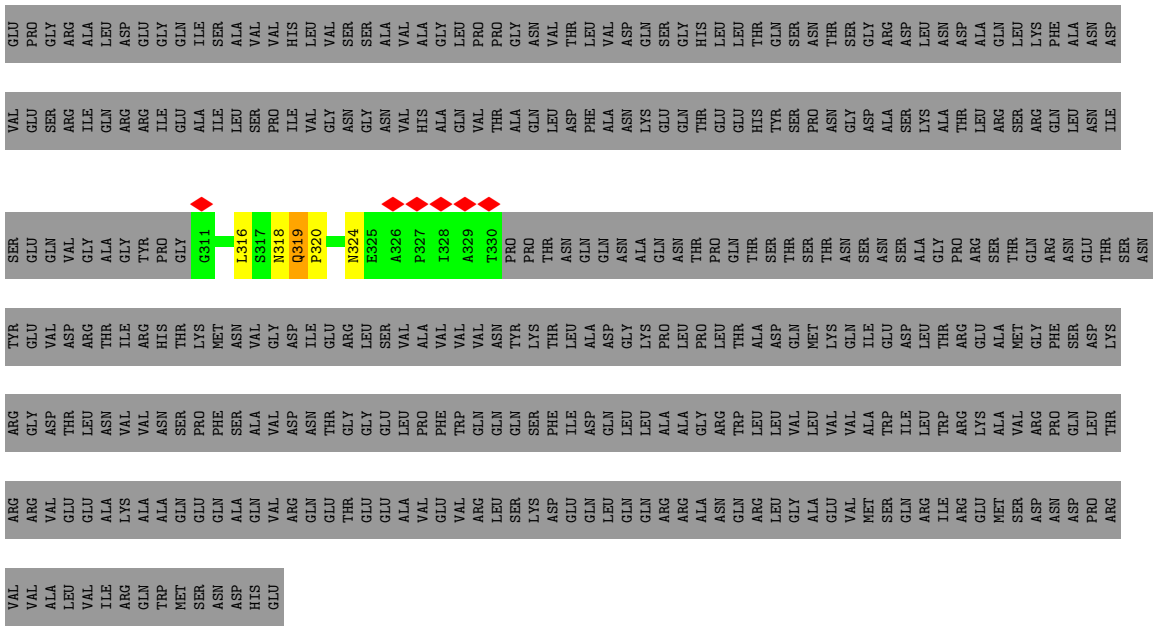
Chain c: 97%



• Molecule 1: Flagellar M-ring protein

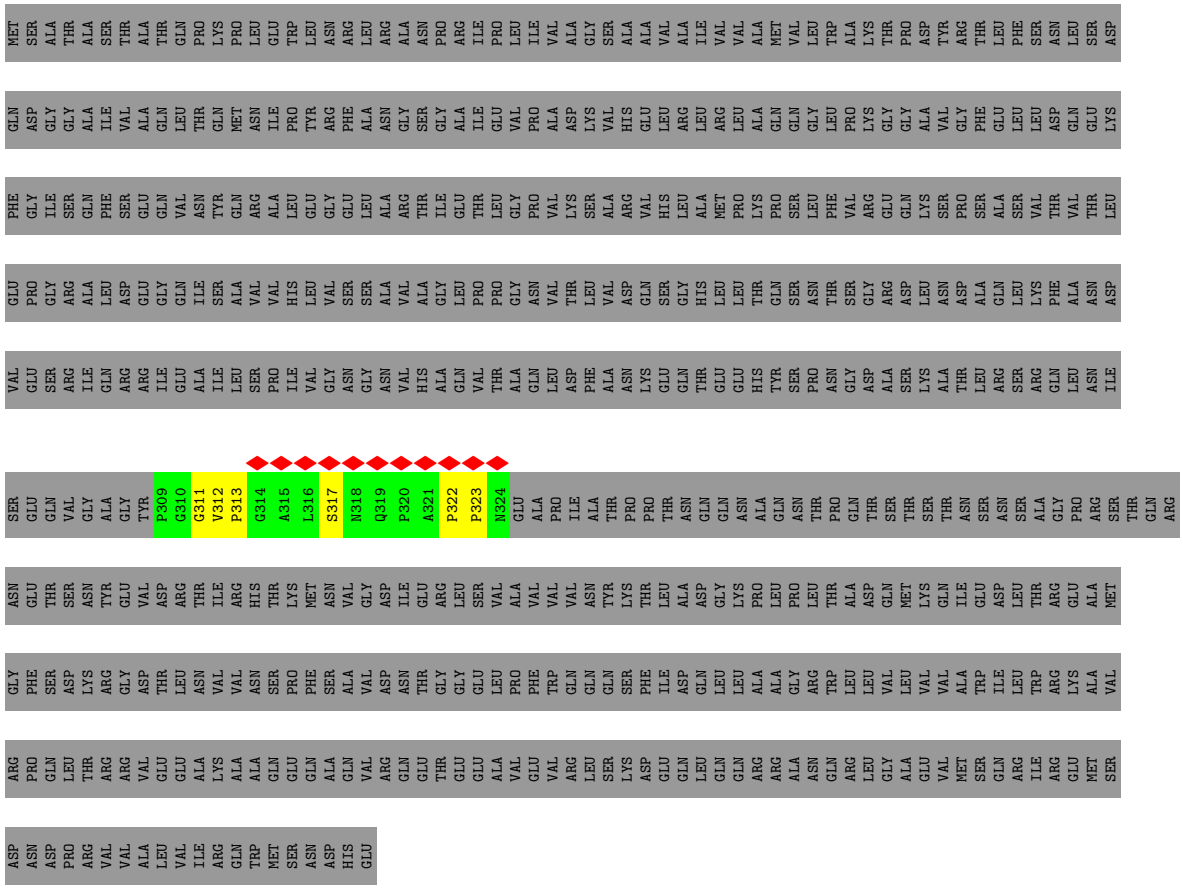
Chain d: 96%





• Molecule 1: Flagellar M-ring protein

Chain e: 97%



• Molecule 1: Flagellar M-ring protein

Chain f: 96%

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY G311 Q319 N324 E325 A326 P327 I328 A329 T330 P331 PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG ASN GLU THR SER ASN TYR GLU VAL ASP

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

LEU ASN VAL VAL ASN SER PRO PHE SER 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 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: 97%

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

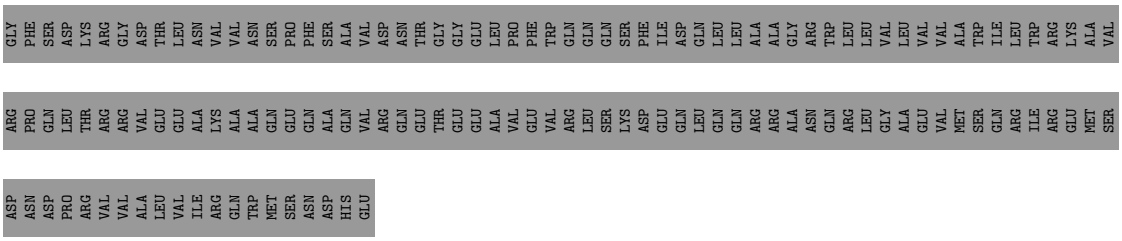
PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU

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

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

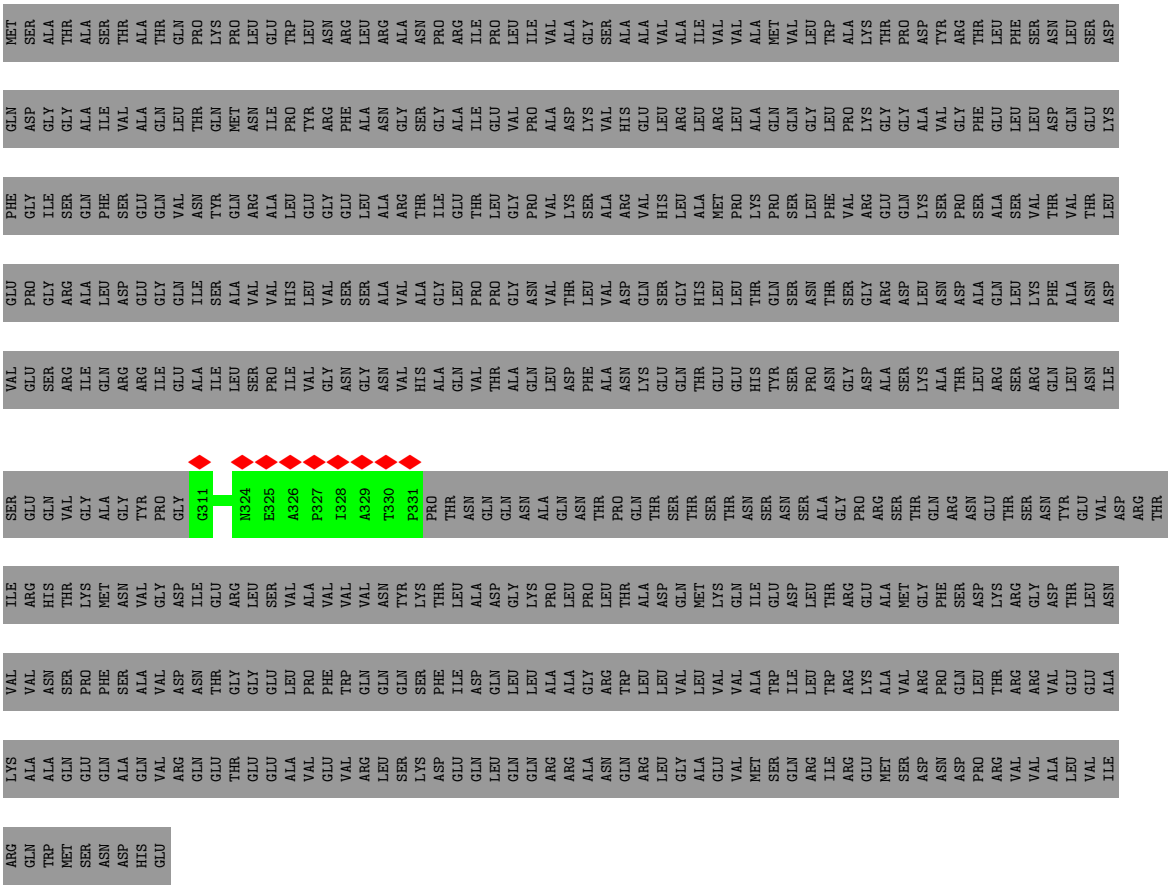
SER GLU GLN VAL GLY ALA GLY TYR P309 G310 G311 V312 P313 G314 A315 L316 S317 N318 Q319 P320 A321 P322 P323 N324 GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN THR GLN ARG

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



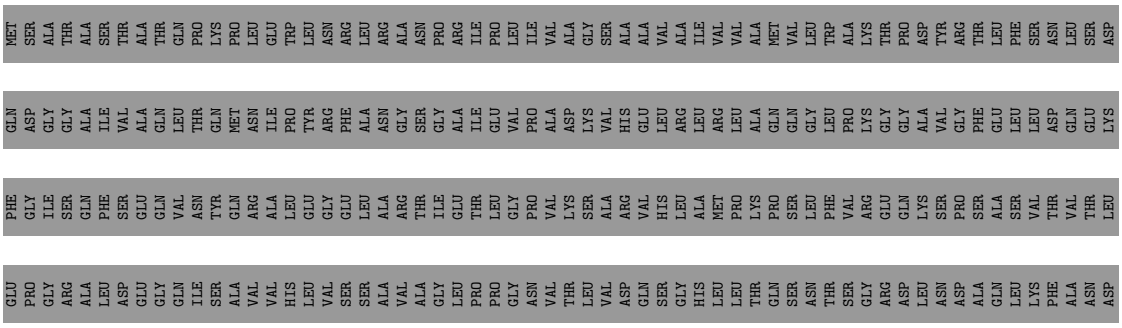
• Molecule 1: Flagellar M-ring protein

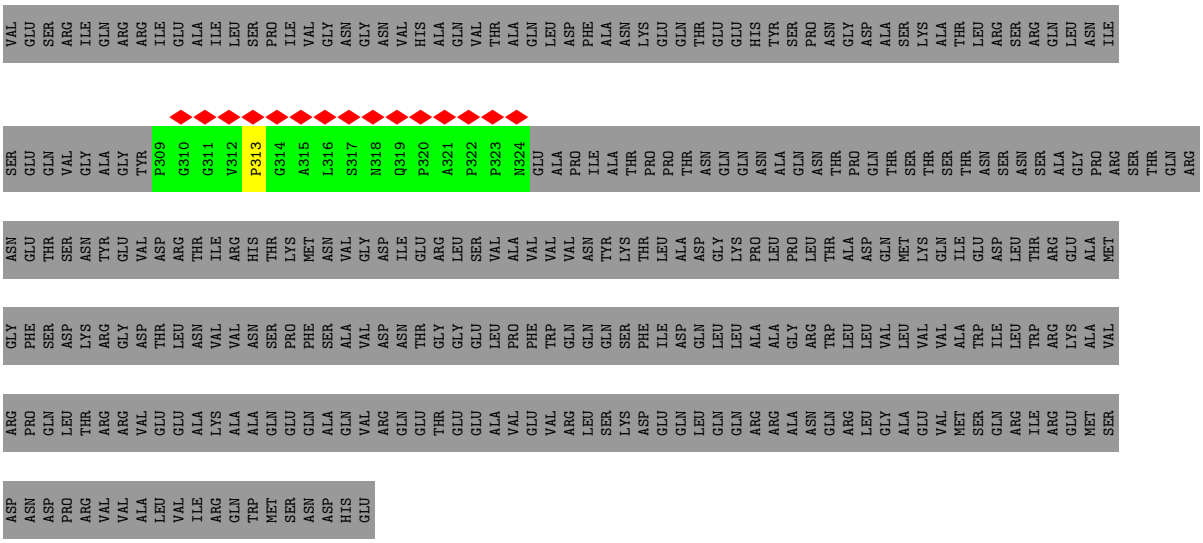
Chain h: 96%



• Molecule 1: Flagellar M-ring protein

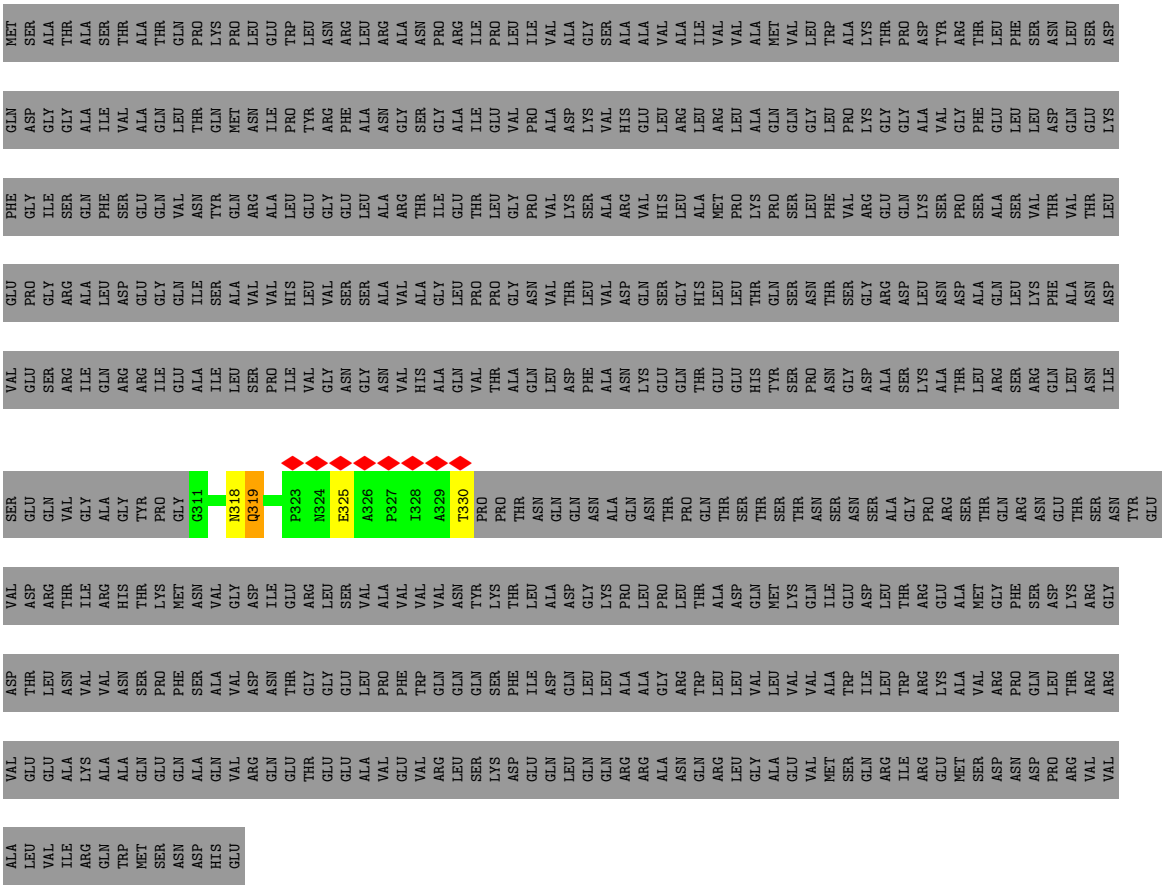
Chain i: 97%





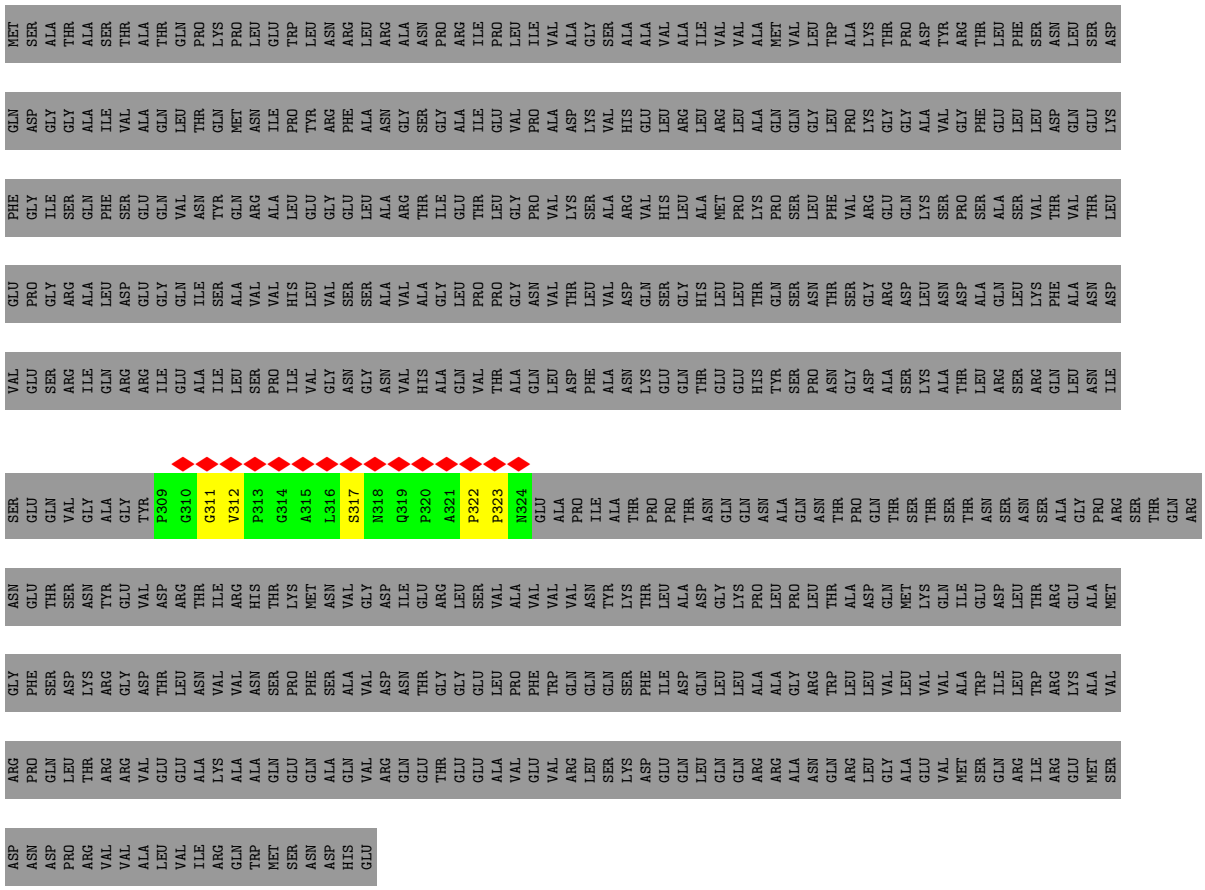
- Molecule 1: Flagellar M-ring protein

Chain j: 96%



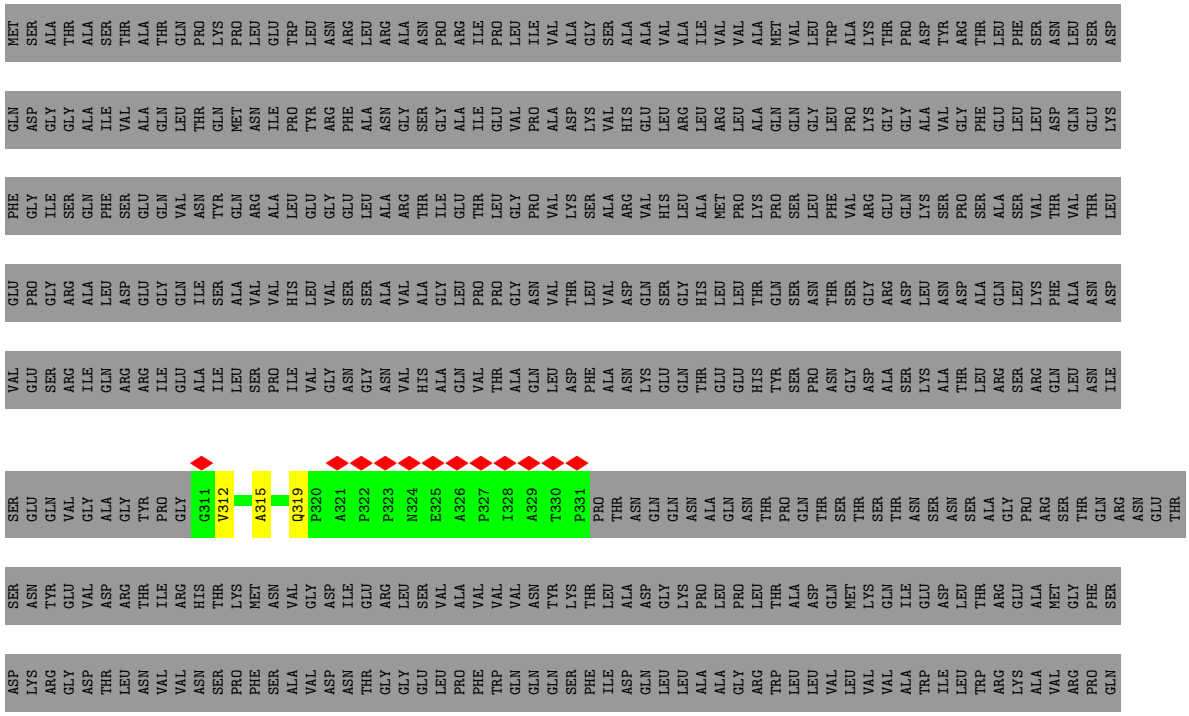
- Molecule 1: Flagellar M-ring protein

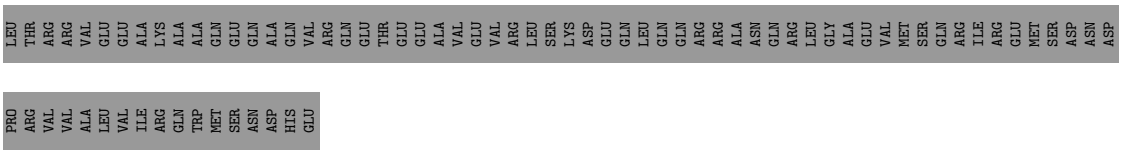
Chain k: 97%



- Molecule 1: Flagellar M-ring protein

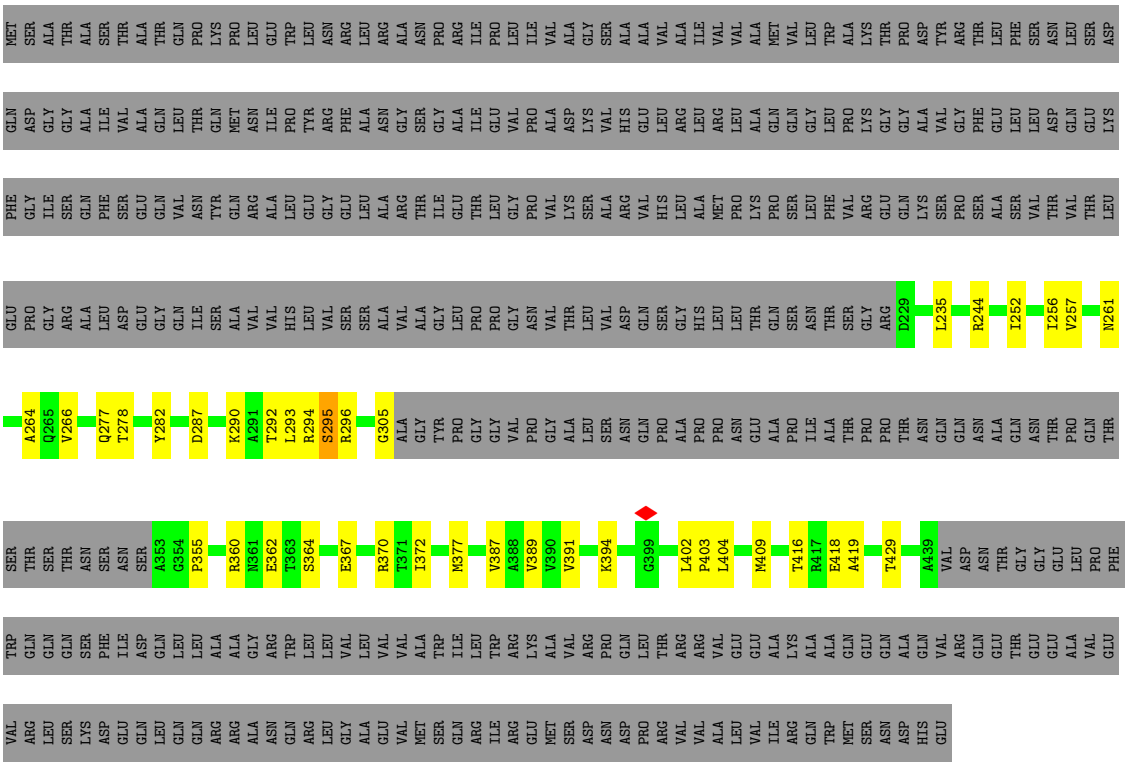
Chain l: 96%





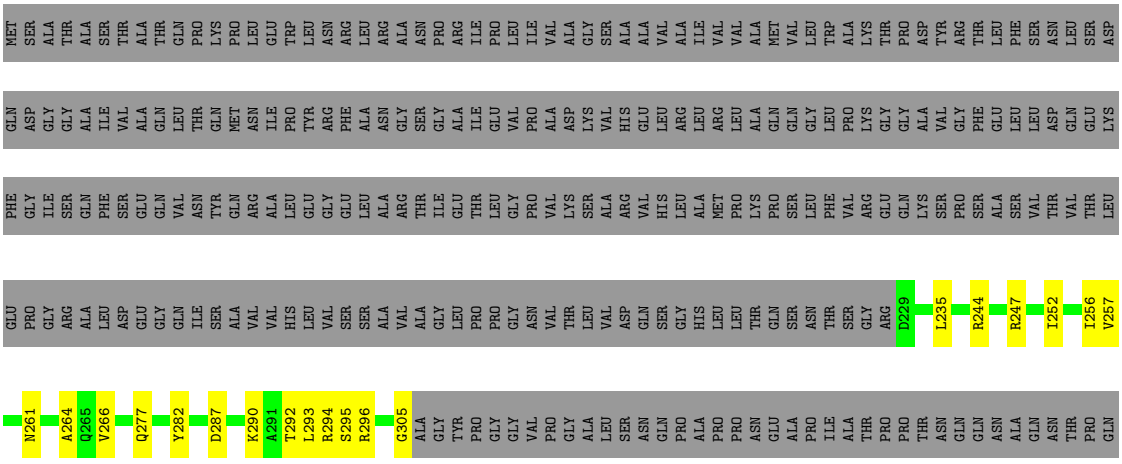
• Molecule 1: Flagellar M-ring protein

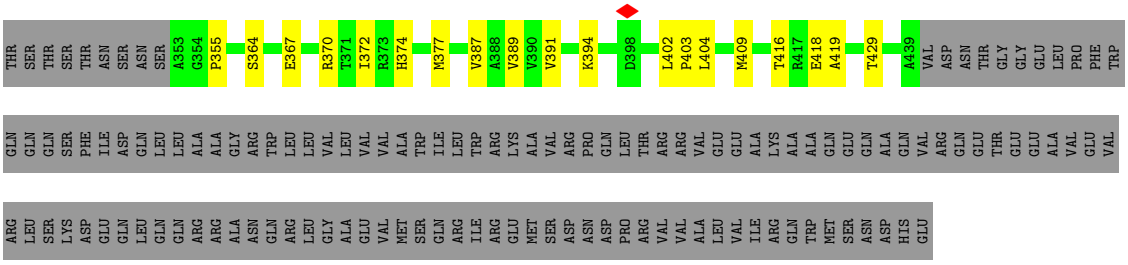
Chain t:



• Molecule 1: Flagellar M-ring protein

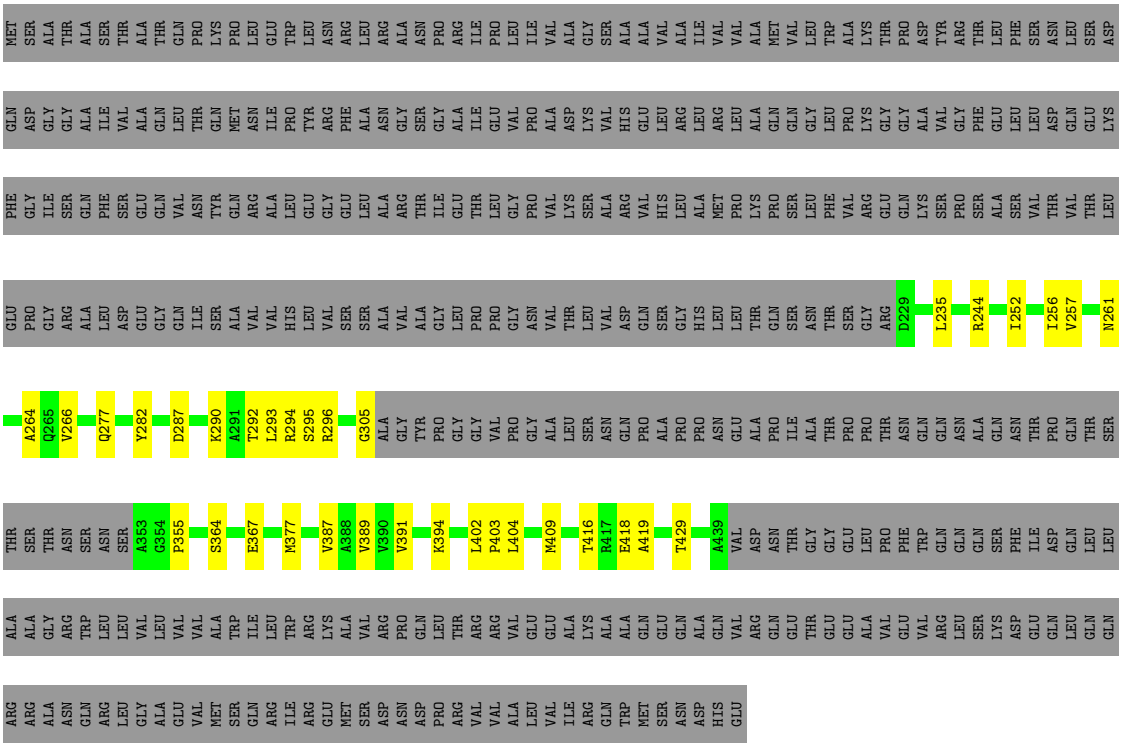
Chain u:





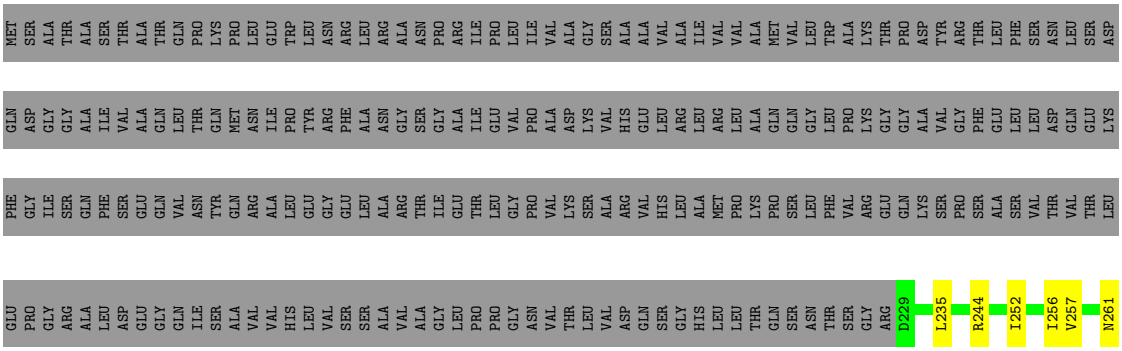
• Molecule 1: Flagellar M-ring protein

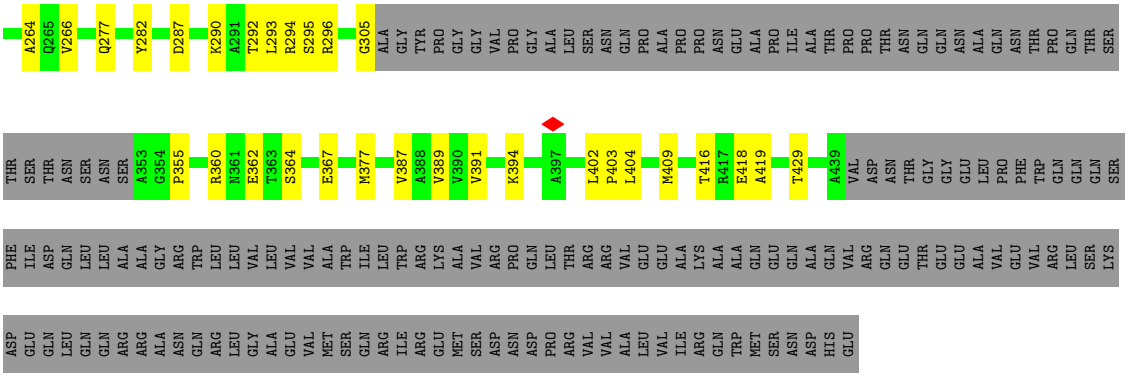
Chain v: 23% 6% 71%



• Molecule 1: Flagellar M-ring protein

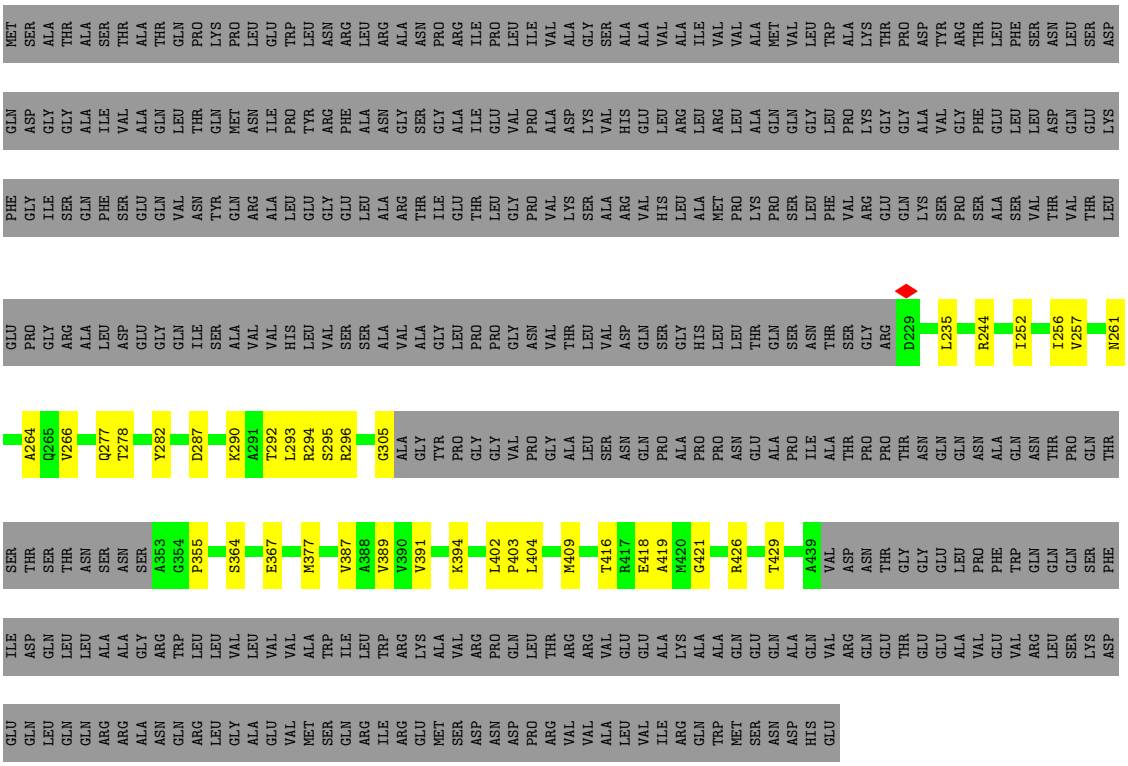
Chain w: 23% 6% 71%





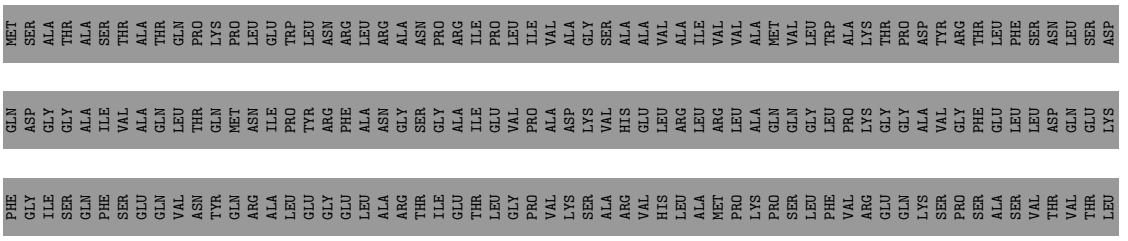
- Molecule 1: Flagellar M-ring protein

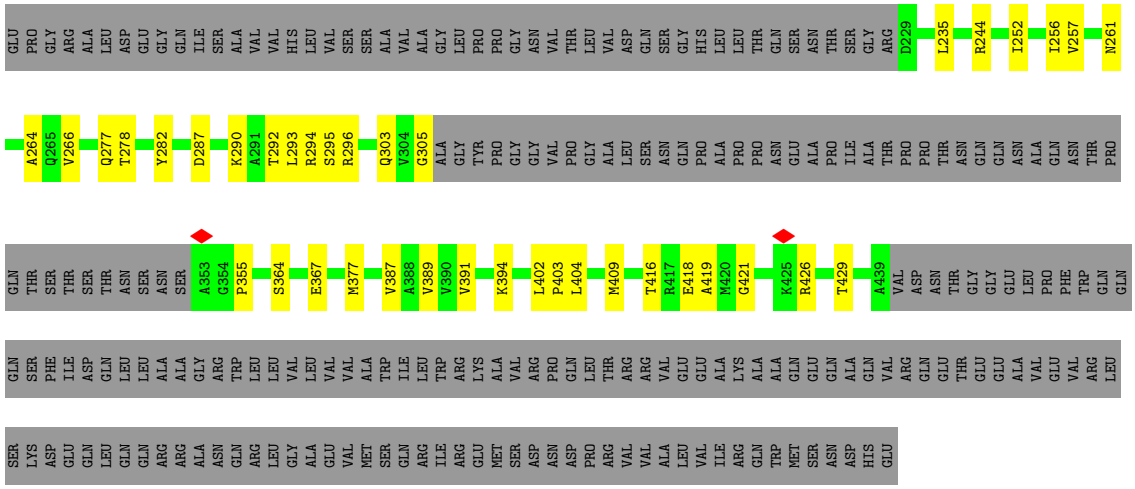
Chain x: 23% 7% 71%



- Molecule 1: Flagellar M-ring protein

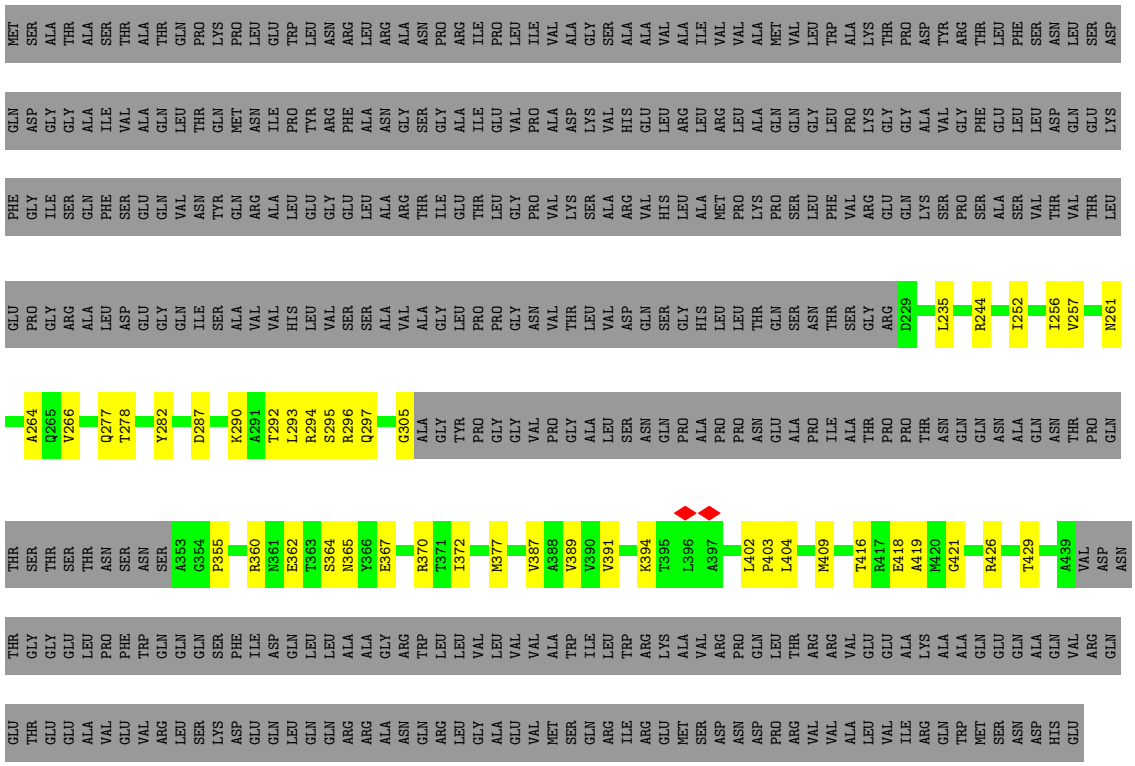
Chain y: 22% 7% 71%





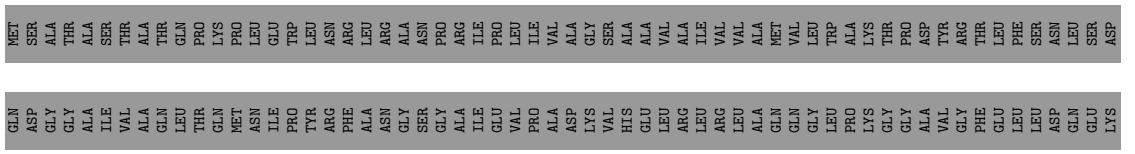
- Molecule 1: Flagellar M-ring protein

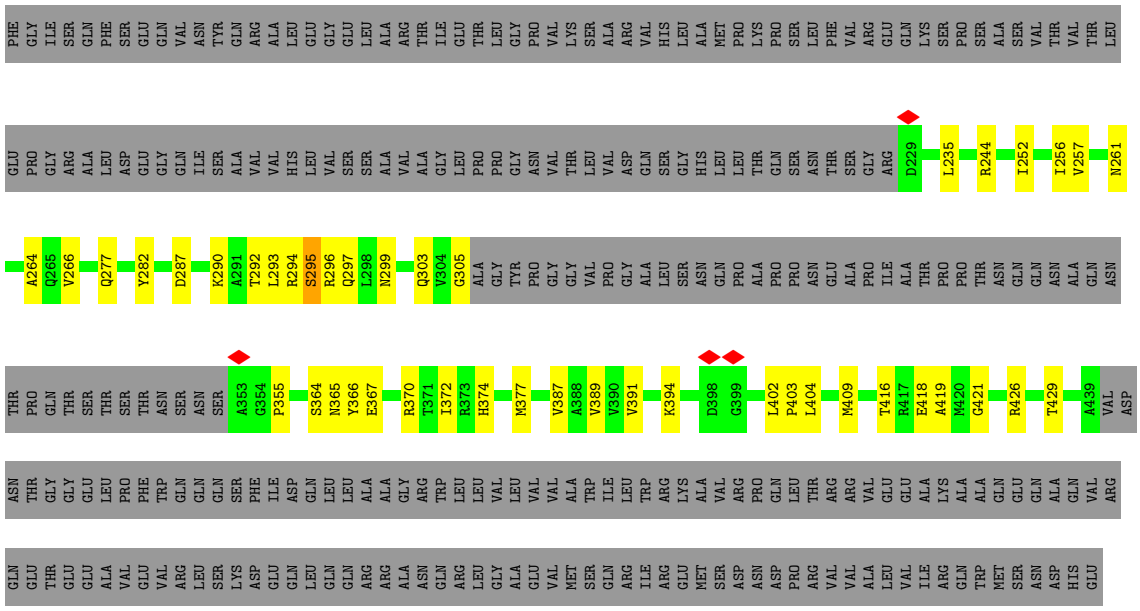
Chain z:



- Molecule 1: Flagellar M-ring protein

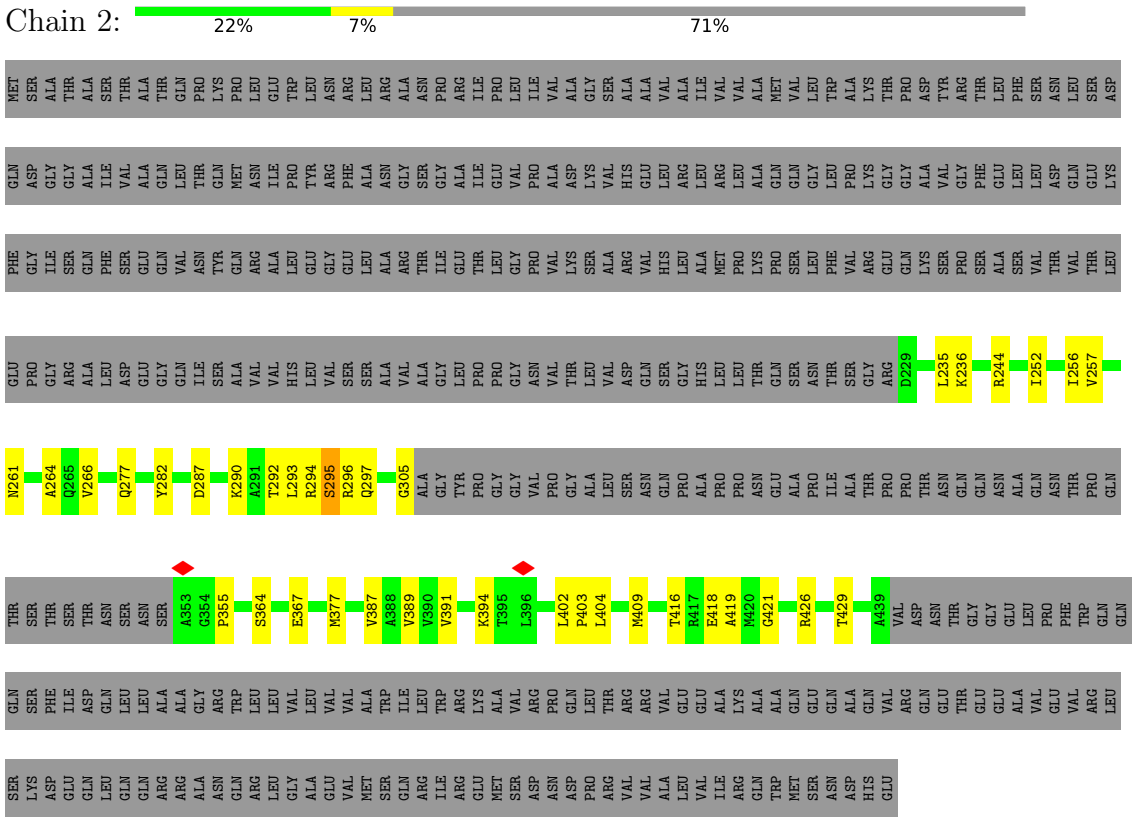
Chain 1:





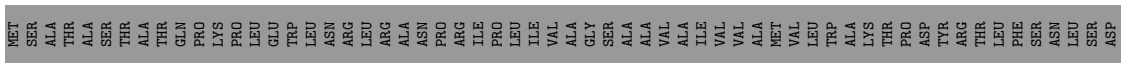
- Molecule 1: Flagellar M-ring protein

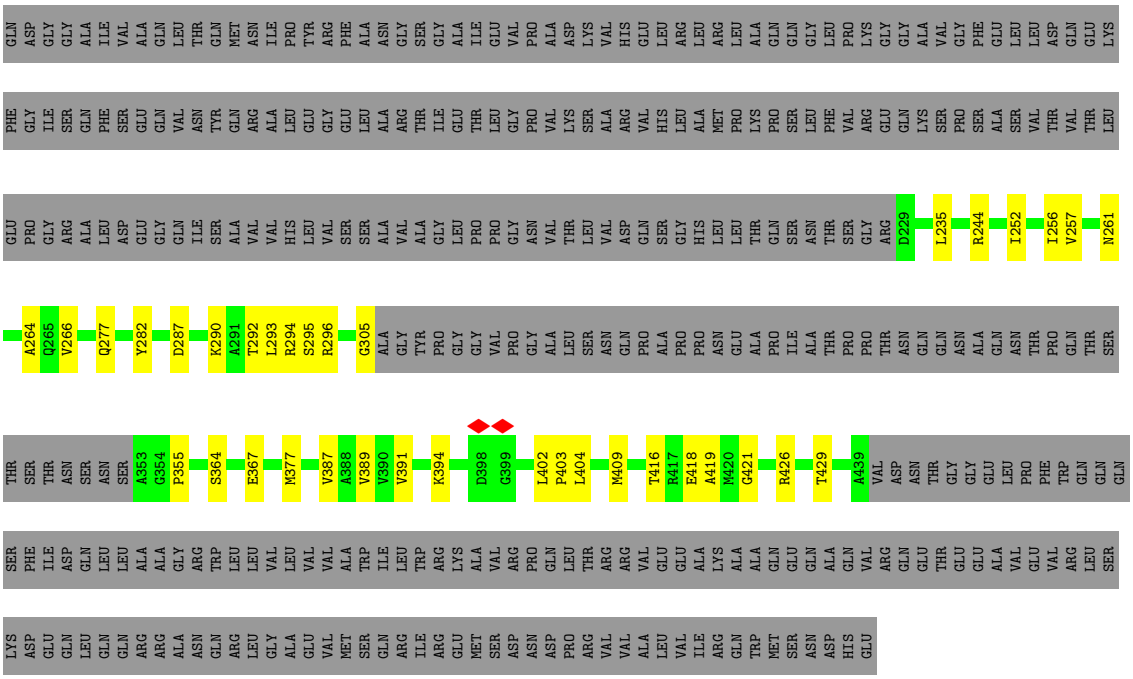
Chain 2:



- Molecule 1: Flagellar M-ring protein

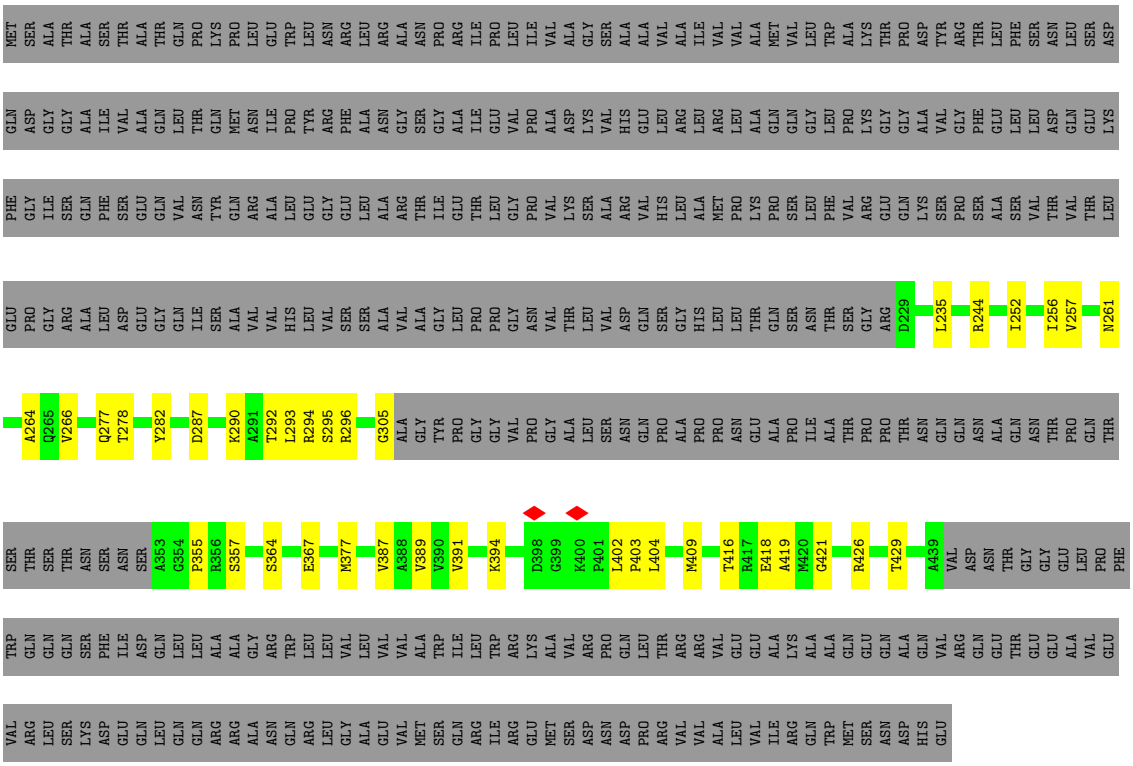
Chain 3:





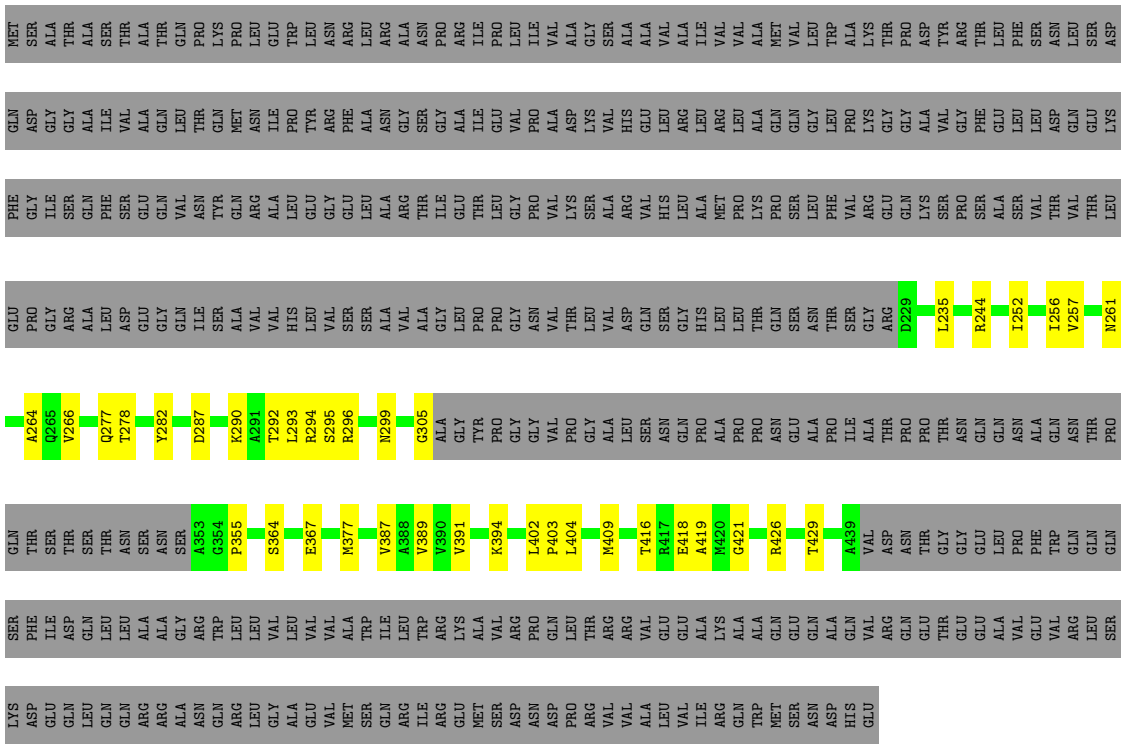
- Molecule 1: Flagellar M-ring protein

Chain 4: 22% 7% 71%



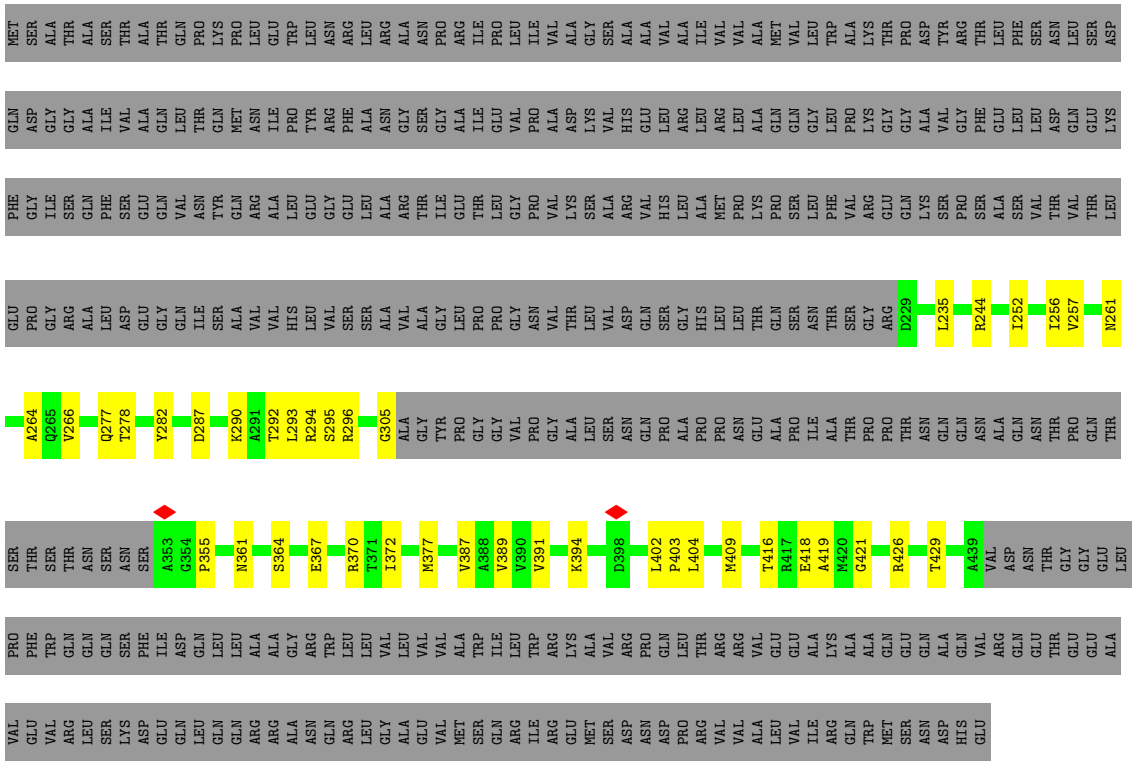
- Molecule 1: Flagellar M-ring protein

Chain 5: 22% 7% 71%



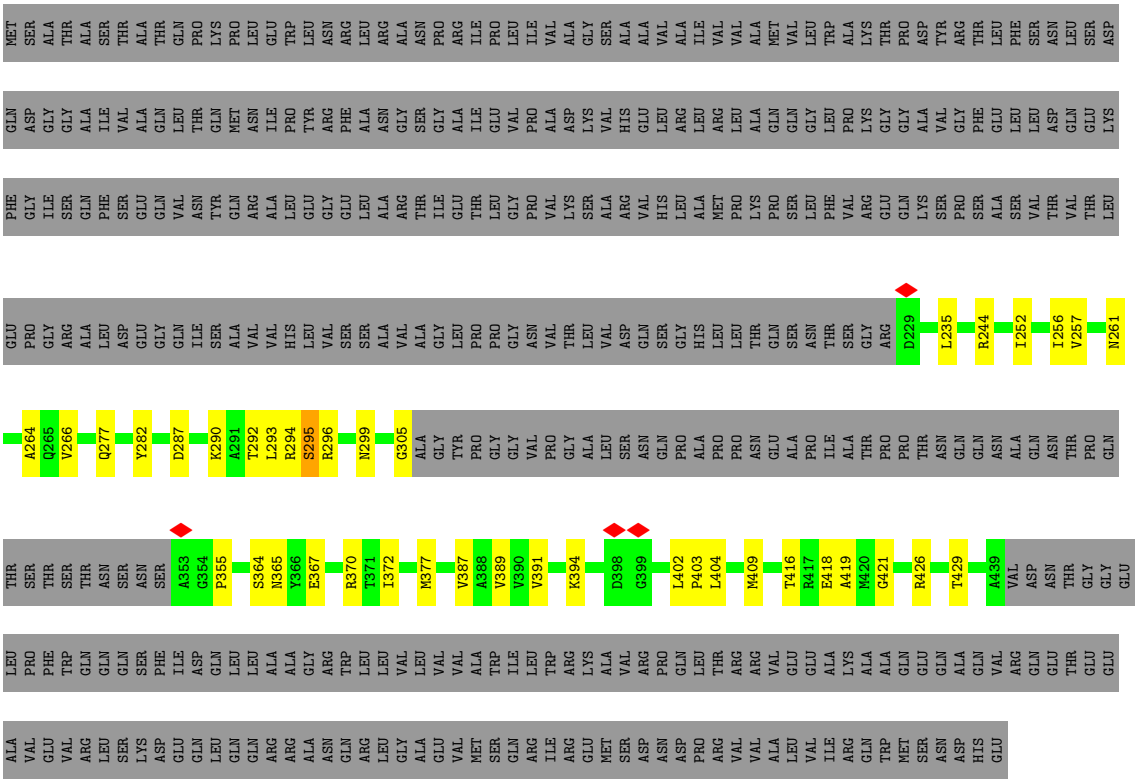
- Molecule 1: Flagellar M-ring protein

Chain 6: 22% 7% 71%



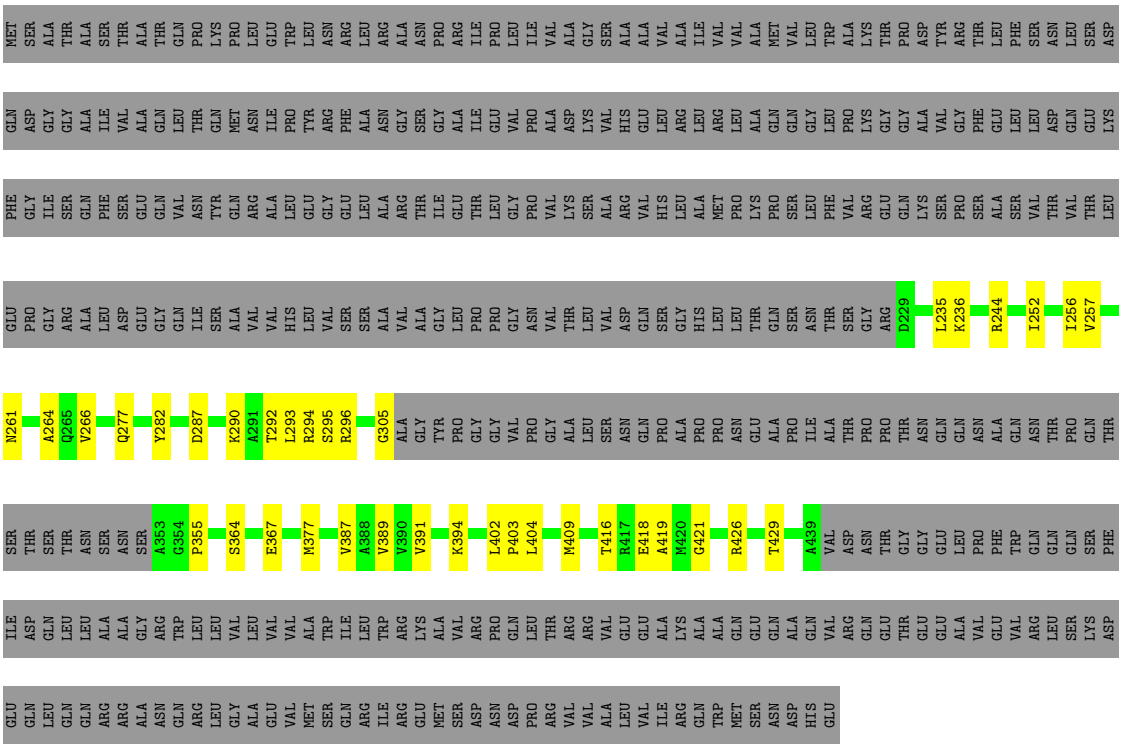
- Molecule 1: Flagellar M-ring protein

Chain 7: 22% 7% 71%



- Molecule 1: Flagellar M-ring protein

Chain 8: 23% 7% 71%



- Molecule 1: Flagellar M-ring protein

Chain 9: 23% 6% 71%

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 L235 R244 I252 I256 V257 N261

A264 Q265 V266 Q277 Y282 D287 K290 A291 T292 L293 R294 S295 R296 G305 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 A353 G354 P355 S364 E367 M377 V387 A388 V389 V390 V391 K394 A397 D398 G399 L402 P403 L404 M409 T416 R417 E418 A419 M420 G421 R426 T429 A439 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 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 0: 23% 6% 71%

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 L235 R244 I252 I256 V257 N261

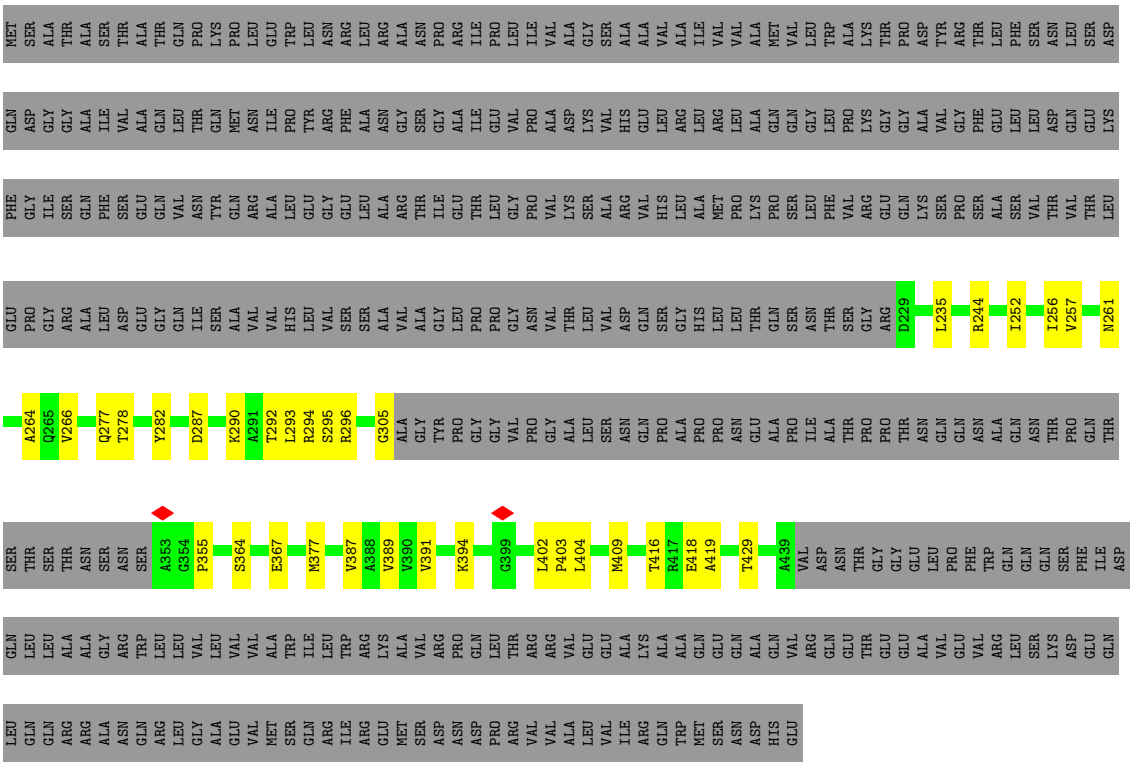
A264 Q265 V266 E276 Q277 T278 Y282 D287 K290 A291 T292 L293 R294 S295 R296 G305 ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN

THR SER THR SER THR ASN SER ASN SER A353 G354 P355 S364 E367 M377 V387 A388 V389 V390 V391 K394 A397 D398 G399 L402 P403 L404 M409 T416 R417 E418 A419 T429 A439 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 ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS

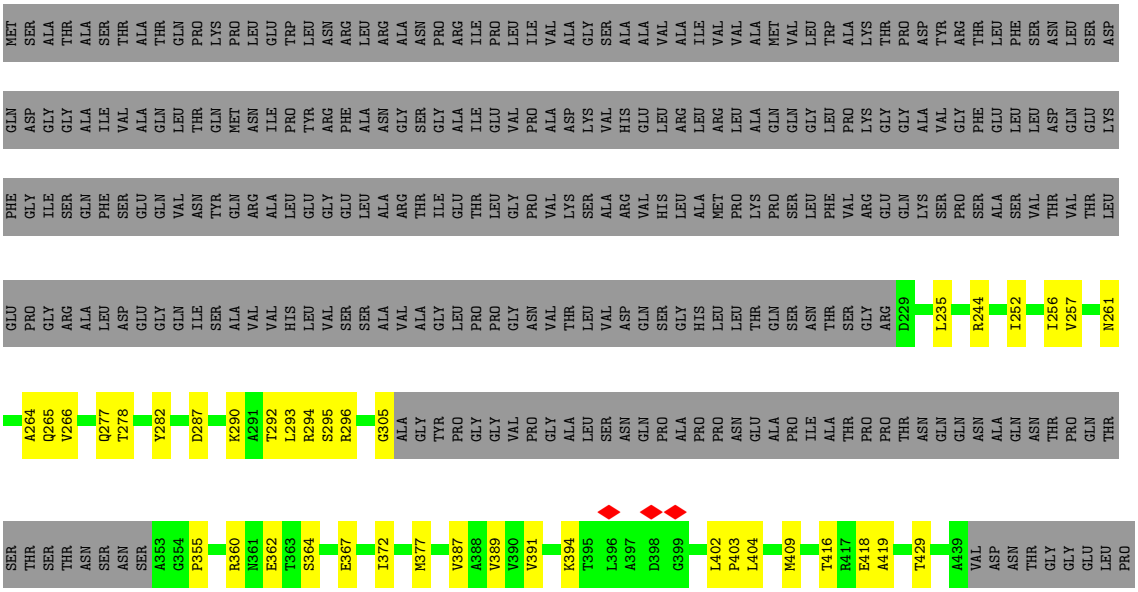
• Molecule 1: Flagellar M-ring protein

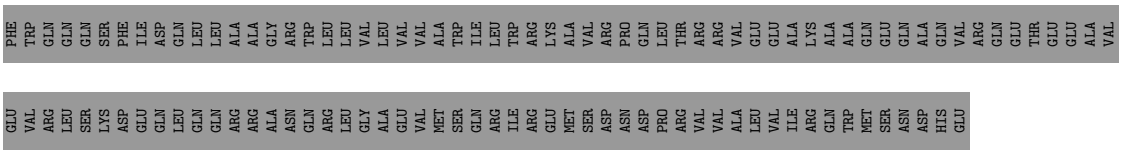
Chain AA:



• Molecule 1: Flagellar M-ring protein

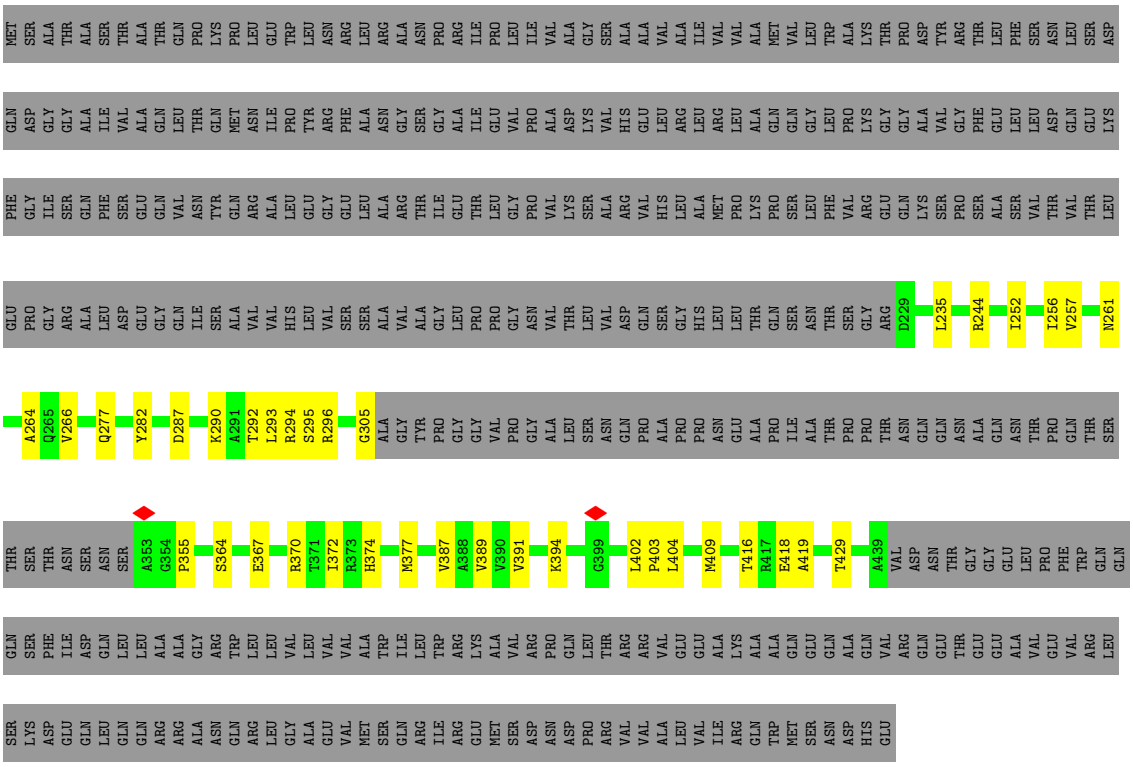
Chain AB:





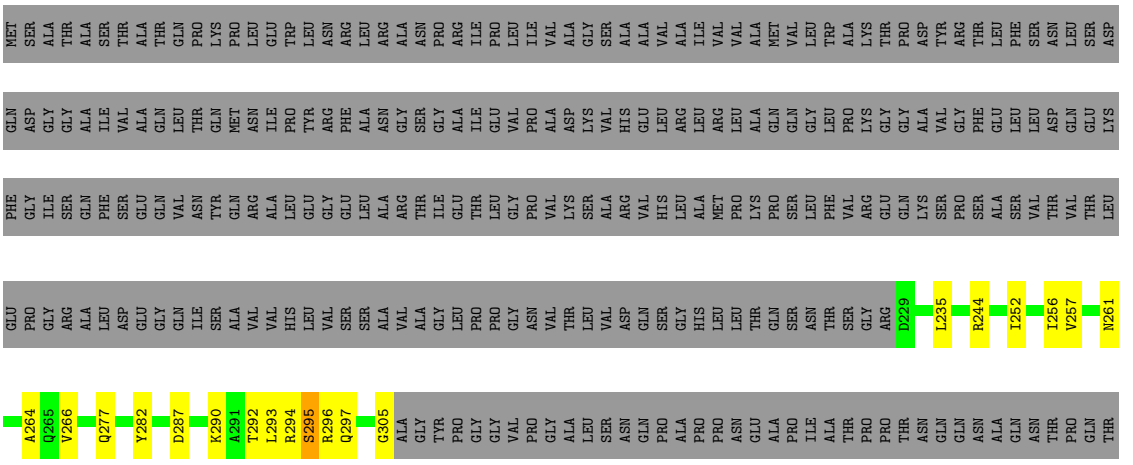
• Molecule 1: Flagellar M-ring protein

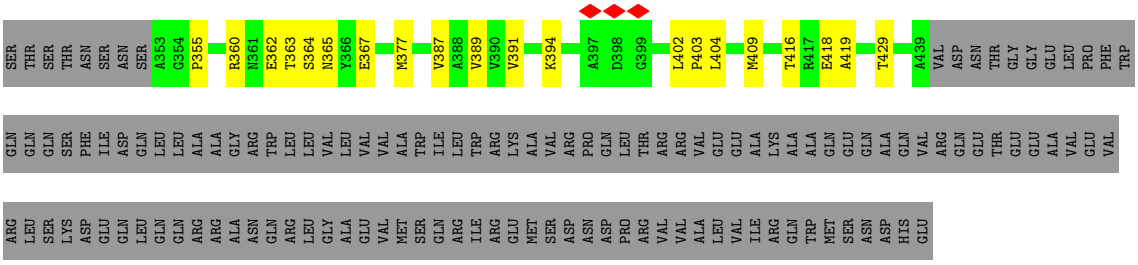
Chain AC: 23% 7% 71%



• Molecule 1: Flagellar M-ring protein

Chain AD: 22% 7% 71%





• Molecule 1: Flagellar M-ring protein

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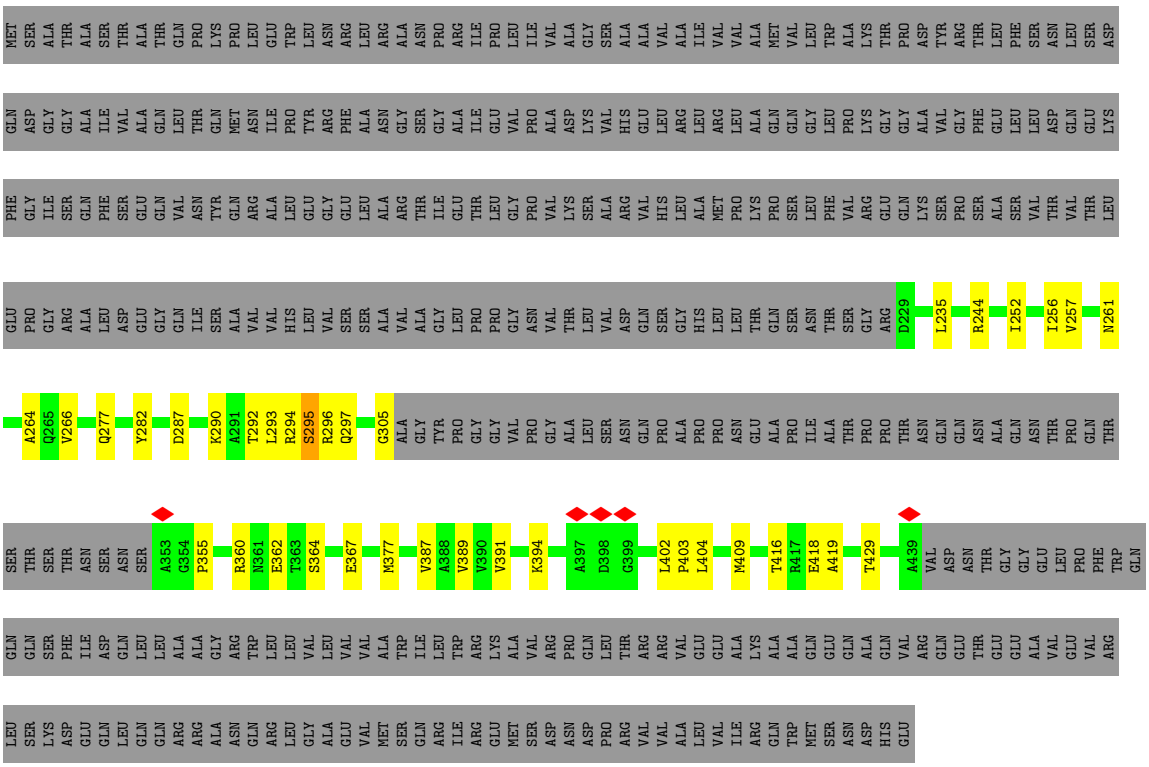
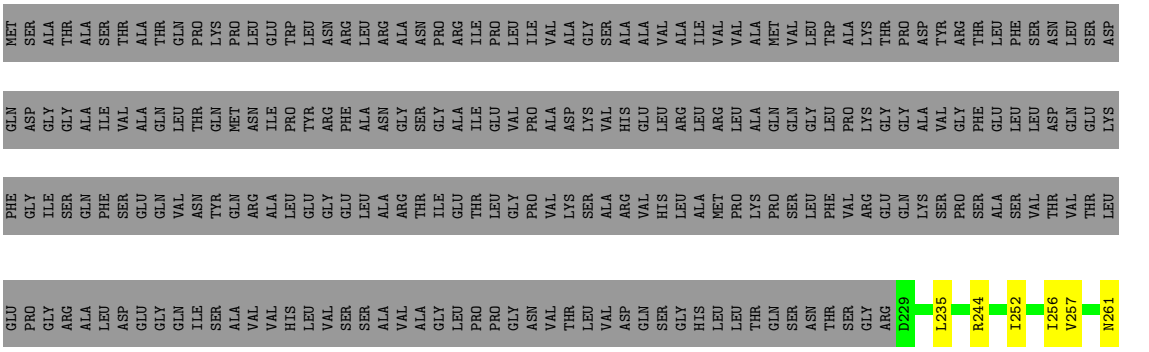
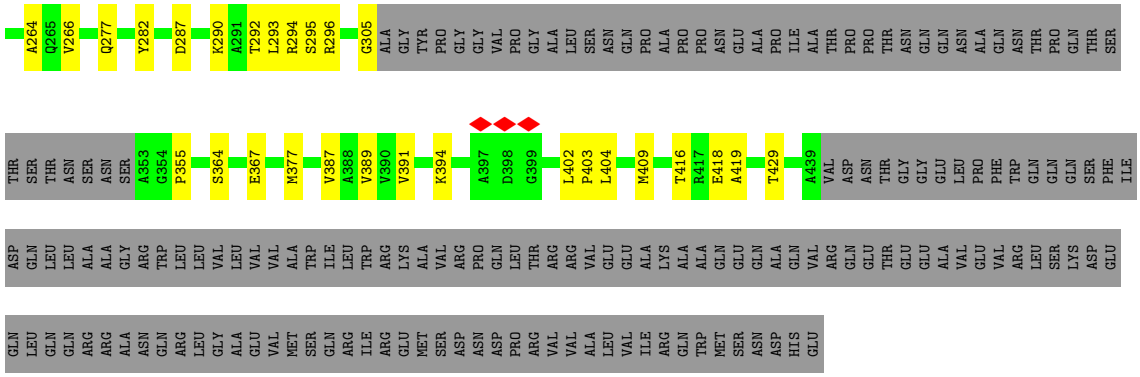


• Molecule 1: Flagellar M-ring protein

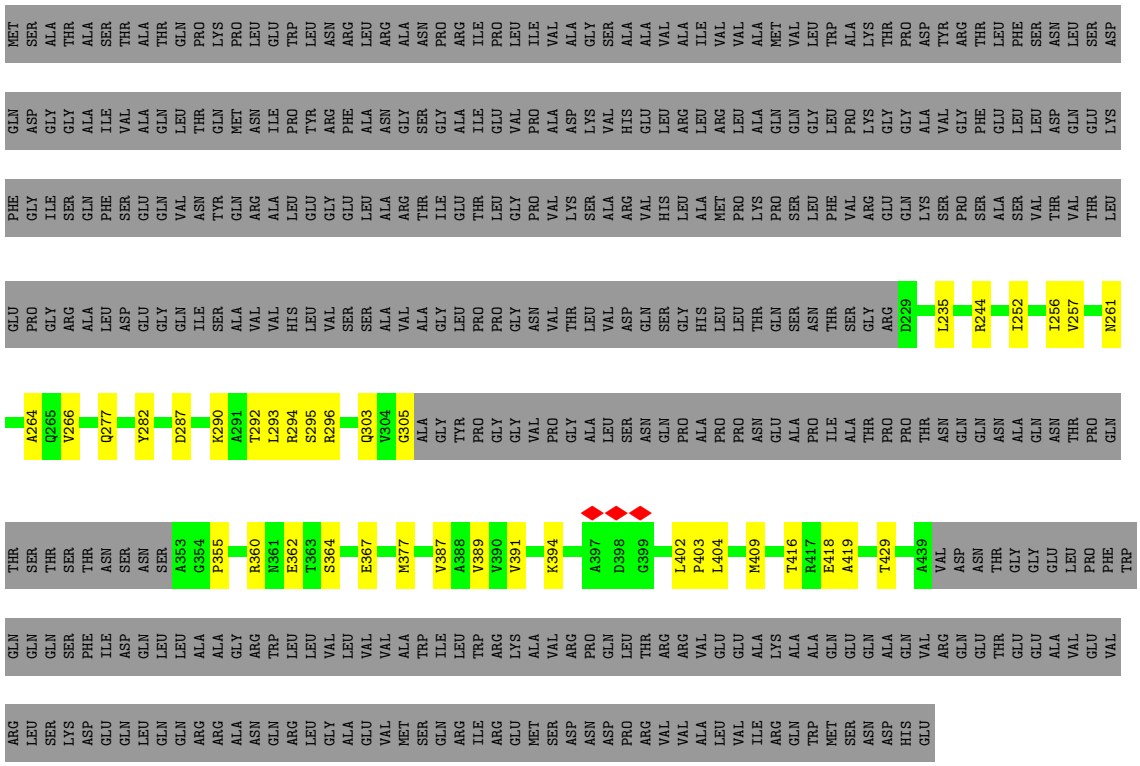
Chain AF:





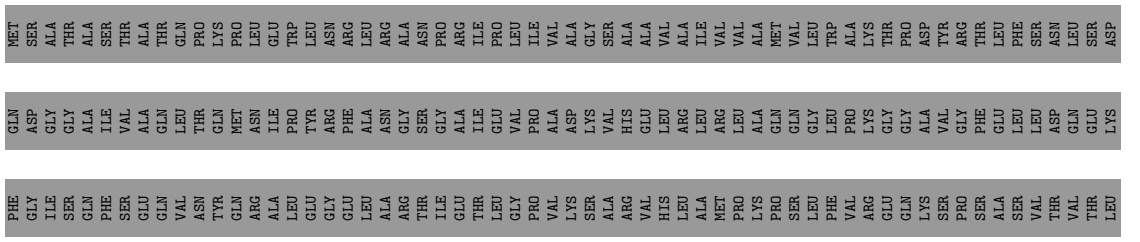
- Molecule 1: Flagellar M-ring protein

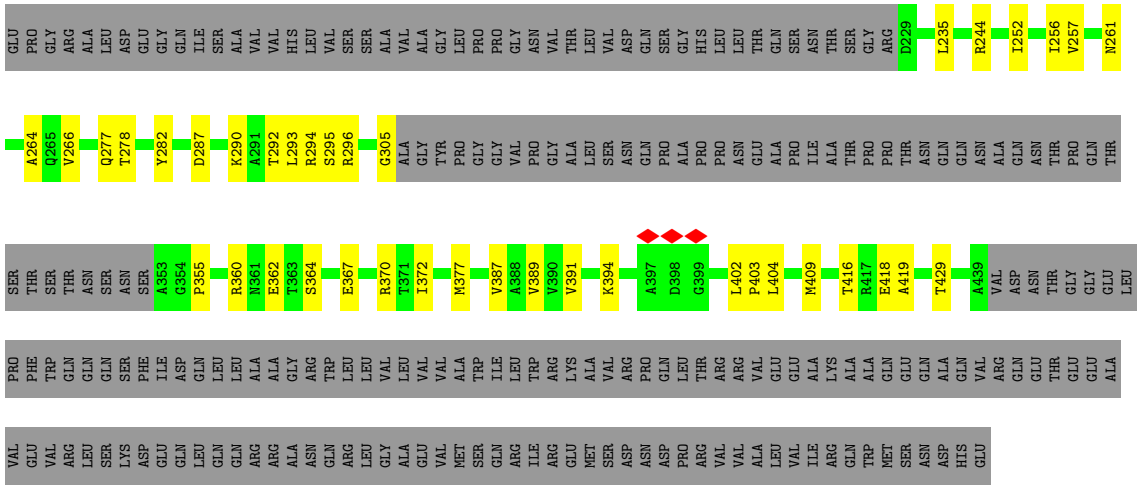
Chain AG:



- Molecule 1: Flagellar M-ring protein

Chain AH:





• Molecule 1: Flagellar M-ring protein

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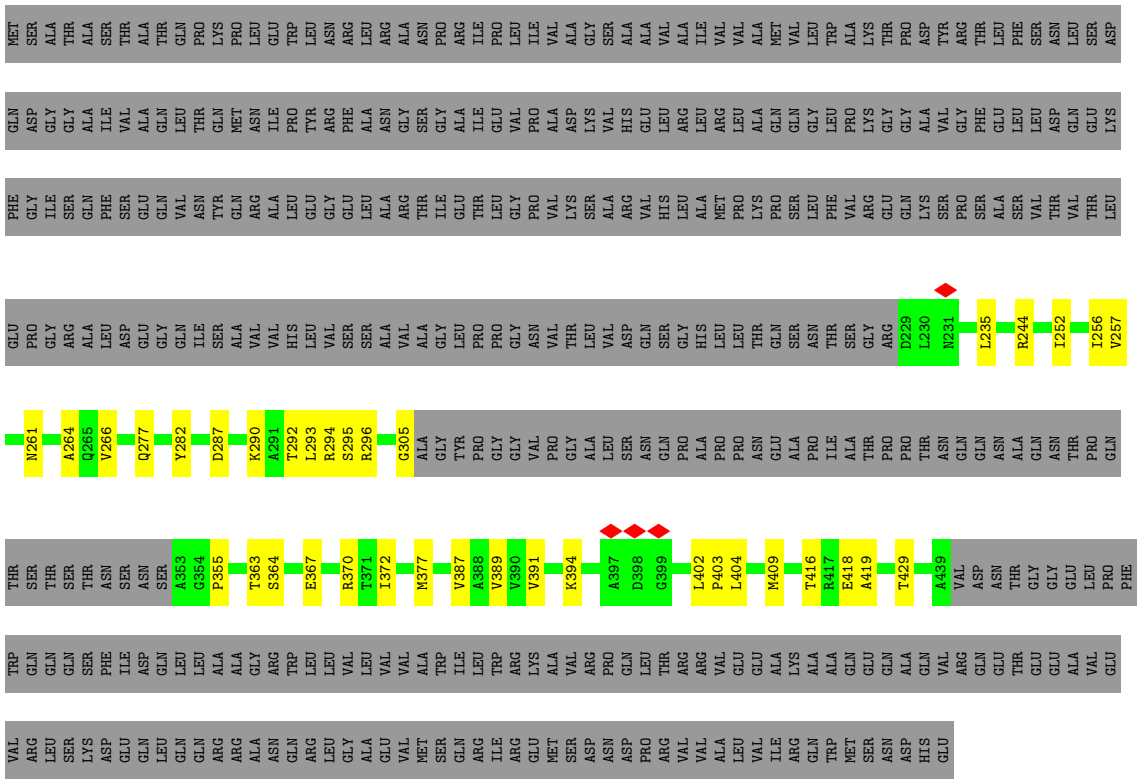
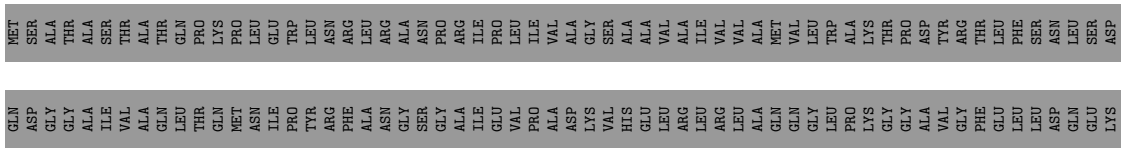
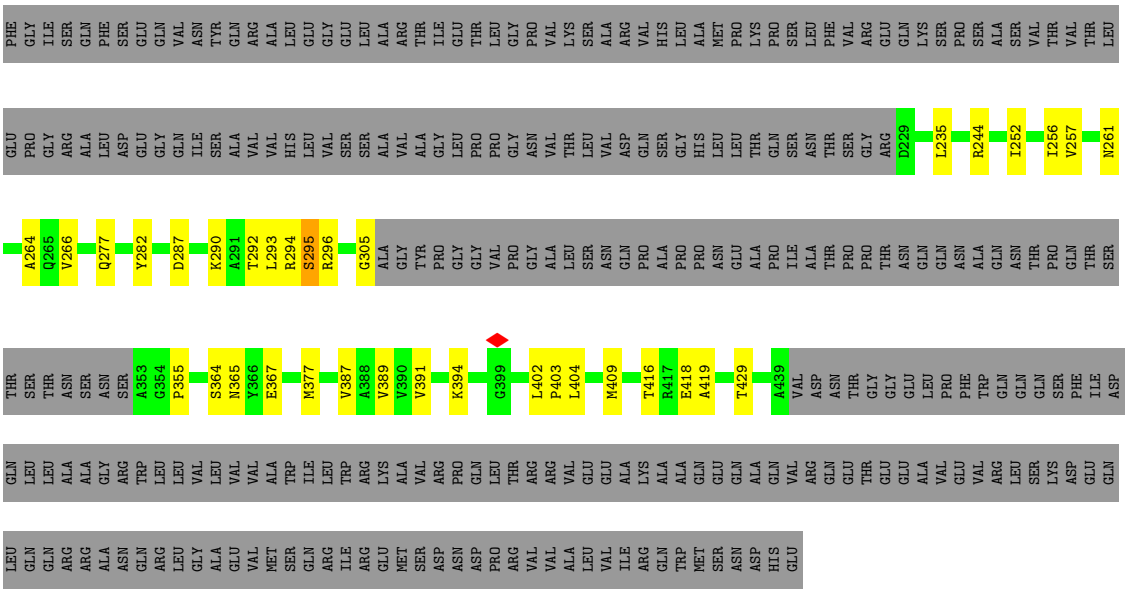


• Molecule 1: Flagellar M-ring protein

Chain AJ:





- Molecule 1: Flagellar M-ring protein

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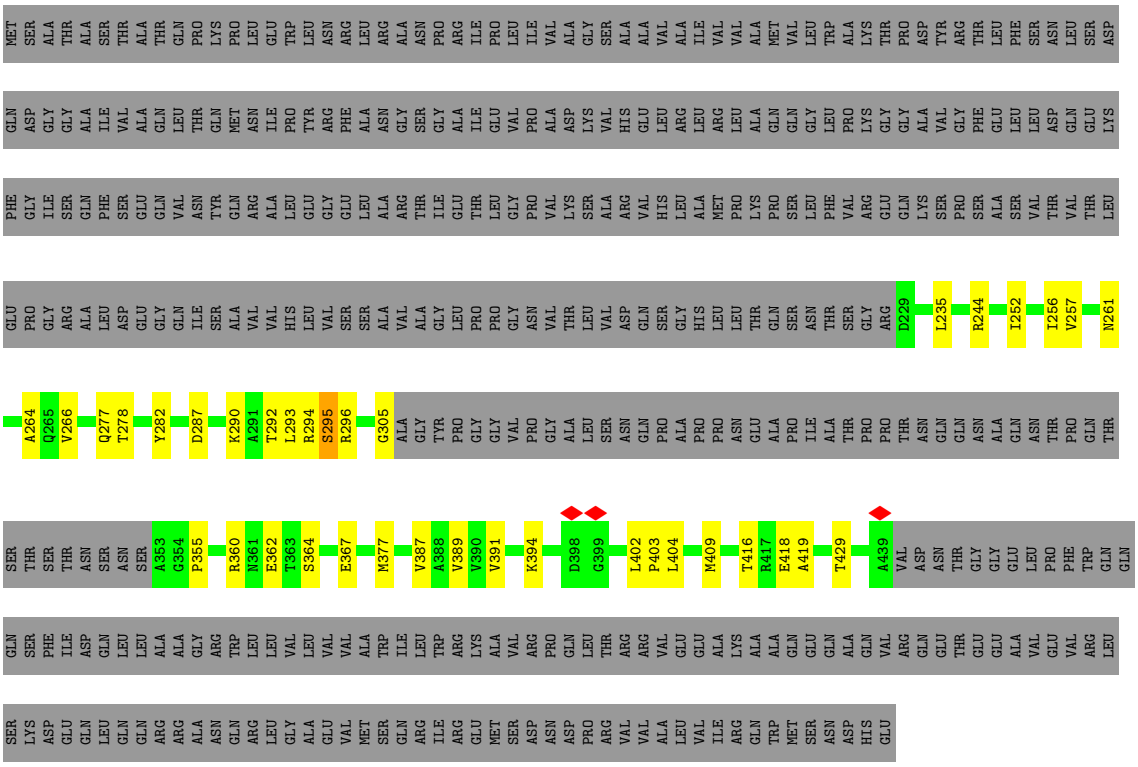
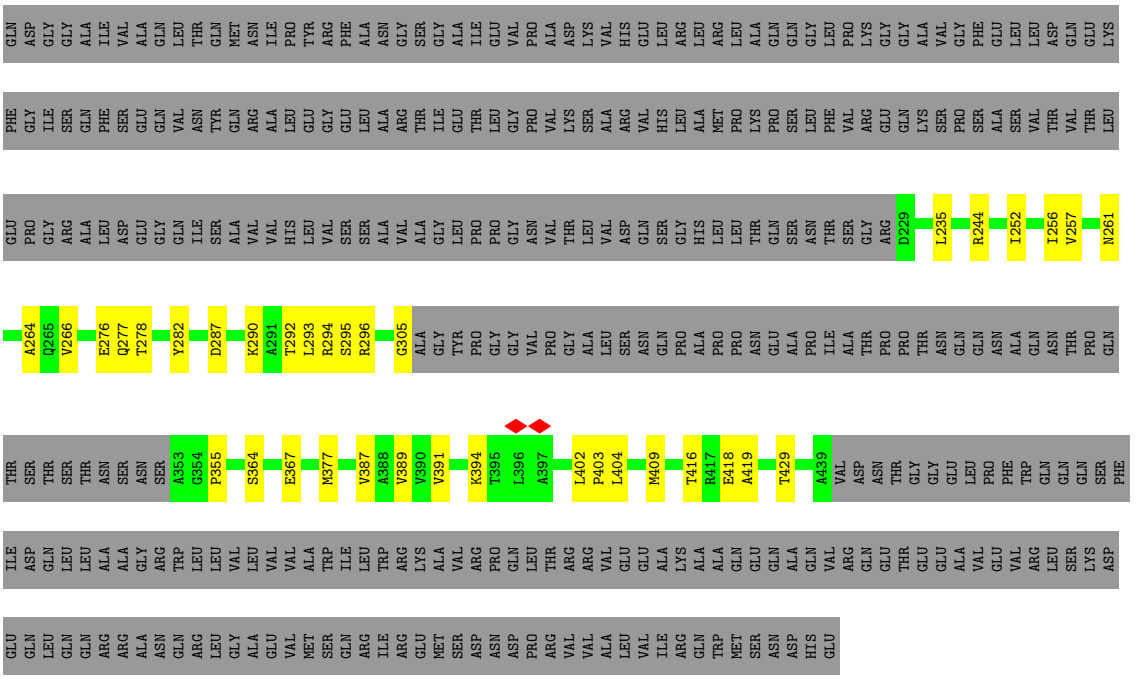


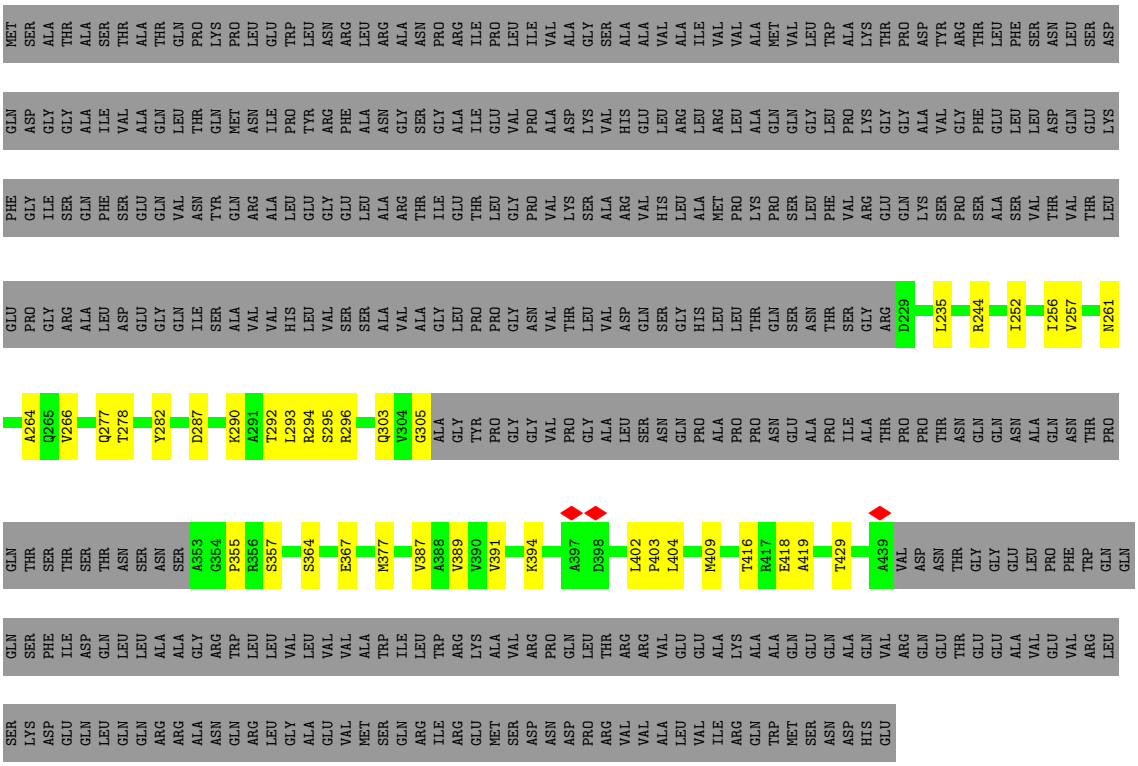
- Molecule 1: Flagellar M-ring protein

Chain AL:



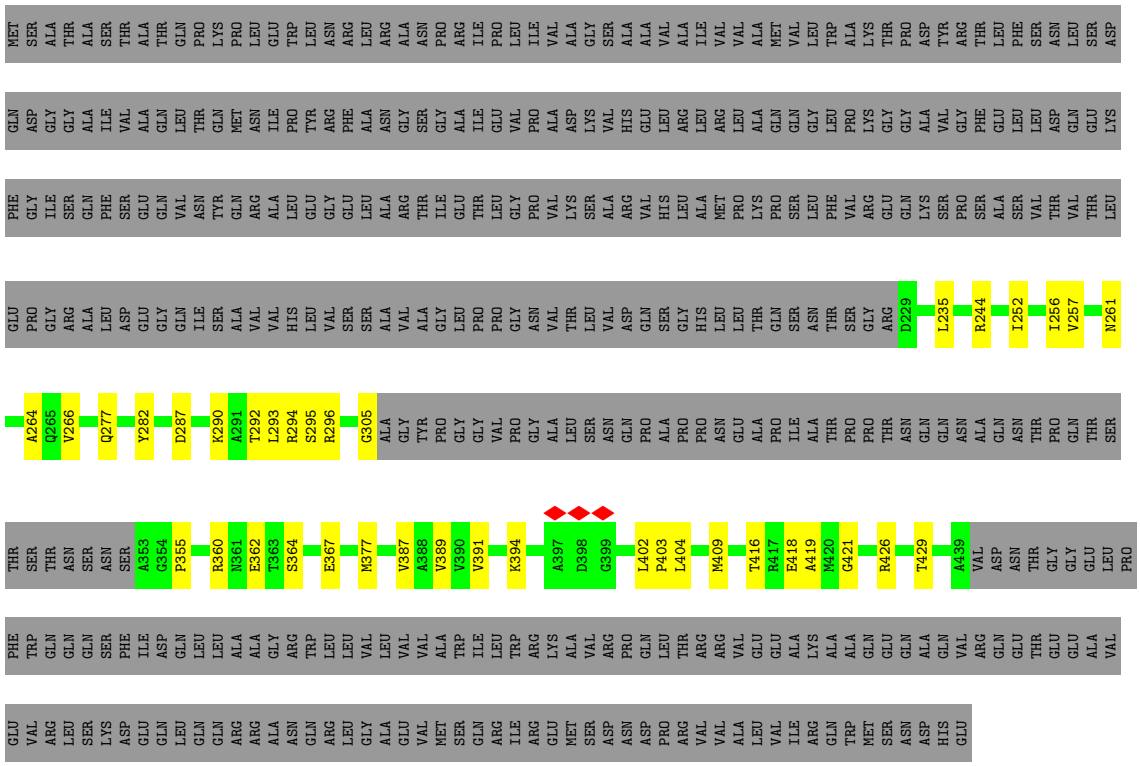
• Molecule 1: Flagellar M-ring protein

Chain AM:



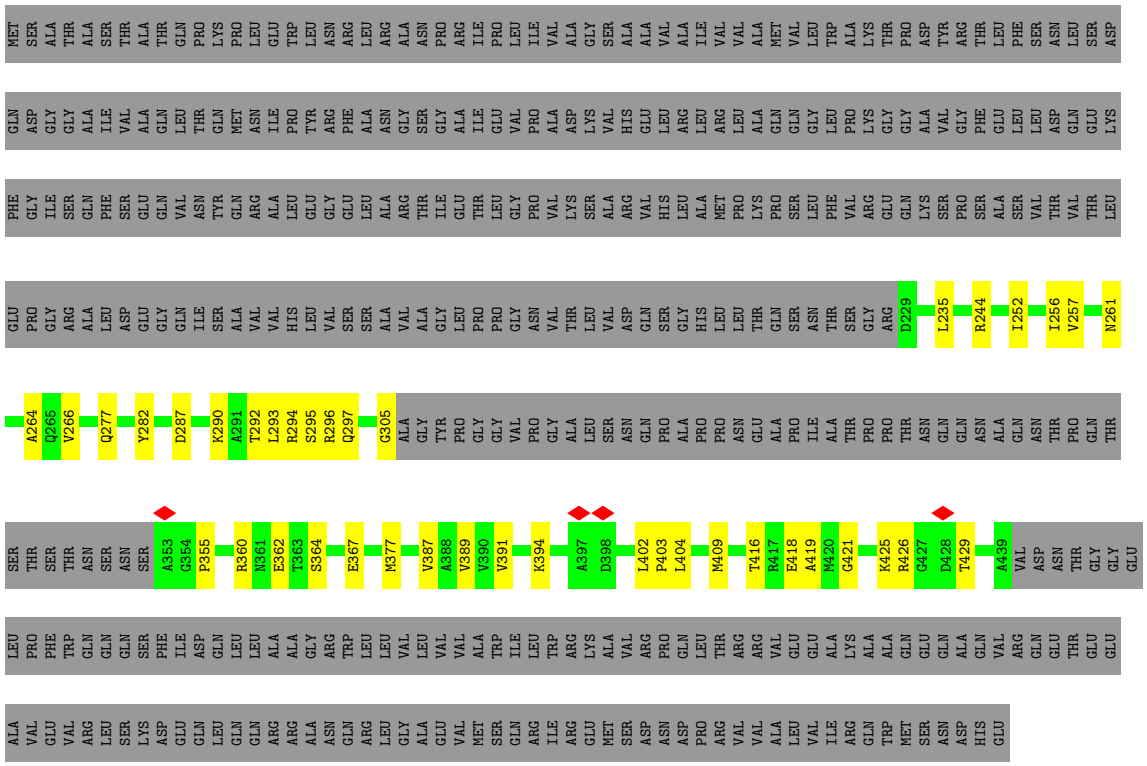
• Molecule 1: Flagellar M-ring protein

Chain AN:



• Molecule 1: Flagellar M-ring protein

Chain AO:



• Molecule 1: Flagellar M-ring protein

Chain AP: 22% 7% 71%

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 L235 R244 I252 I256 V257 N261

A264 Q265 V266 E276 Q277 T278 Y282 D287 K290 A291 T292 L293 R294 S295 R296 Q297 G305 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 A353 G354 P355 Q359 S364 E367 M377 V387 A388 V389 V390 V391 K394 A397 L402 P403 L404 M409 T416 R417 E418 A419 M420 G421 R426 T429 A439 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 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 AQ: 23% 6% 71%

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 L235 R244 I252 I256 V257 N261

A264 Q265 V266 E276 Q277 T278 Y282 D287 K290 A291 T292 L293 R294 S295 R296 G305 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

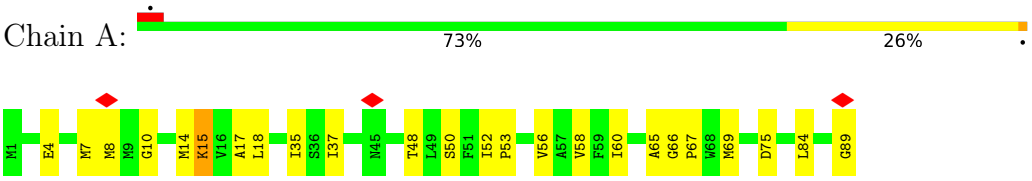
THR SER THR SER THR ASN SER ASN SER A353 G354 P355 S364 E367 H374 M377 V387 A388 V389 V390 V391 K394 G399 L402 P403 L404 M409 T416 R417 E418 A419 T429 A439 VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER

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 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 2: Flagellar biosynthetic protein FliQ

Chain A:



• Molecule 2: Flagellar biosynthetic protein FliQ

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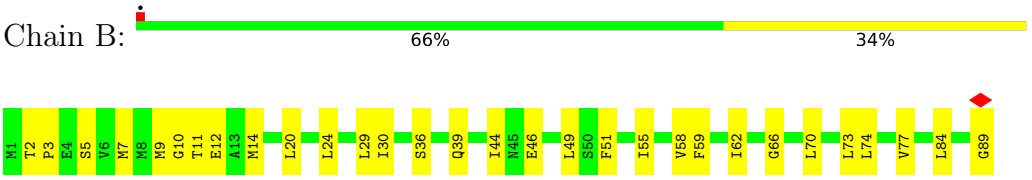

• Molecule 2: Flagellar biosynthetic protein FliQ

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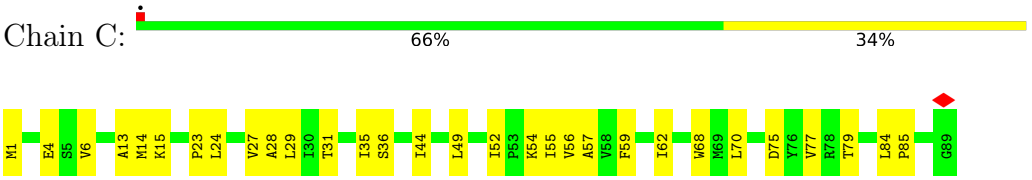
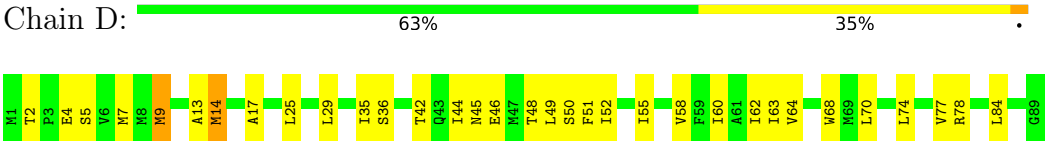


• Molecule 2: Flagellar biosynthetic protein FliQ

Chain D:



• Molecule 3: Flagellar biosynthetic protein FliR

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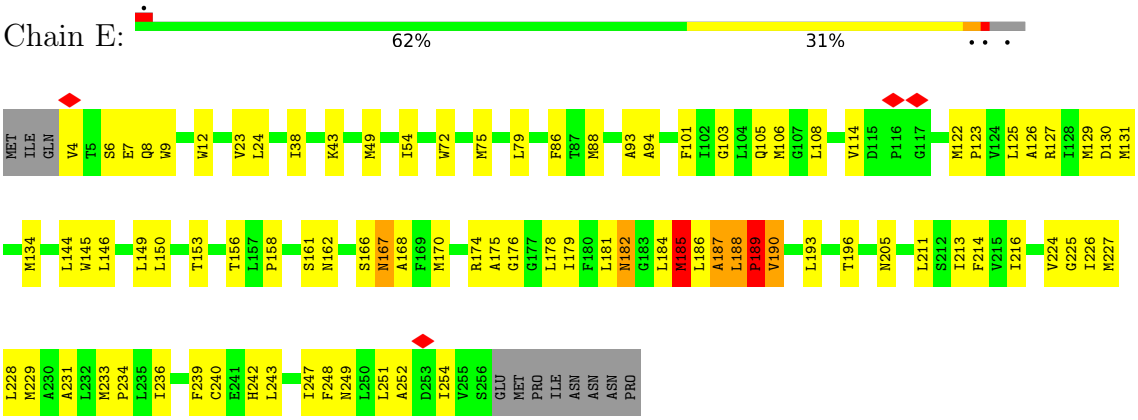
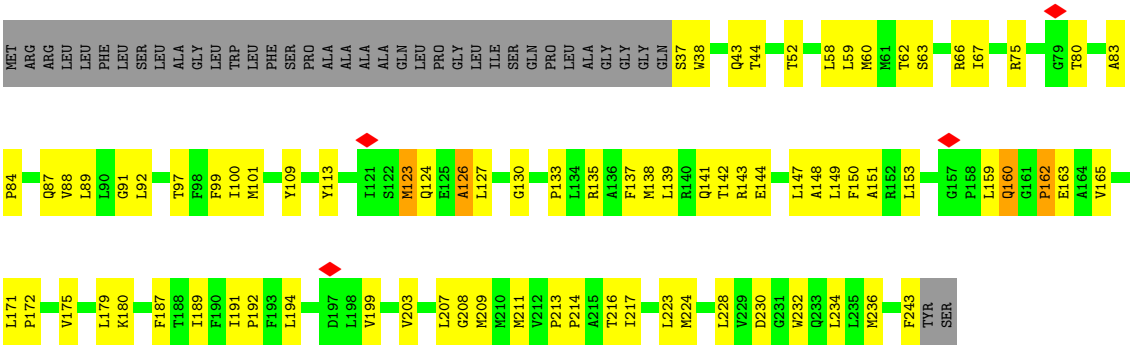


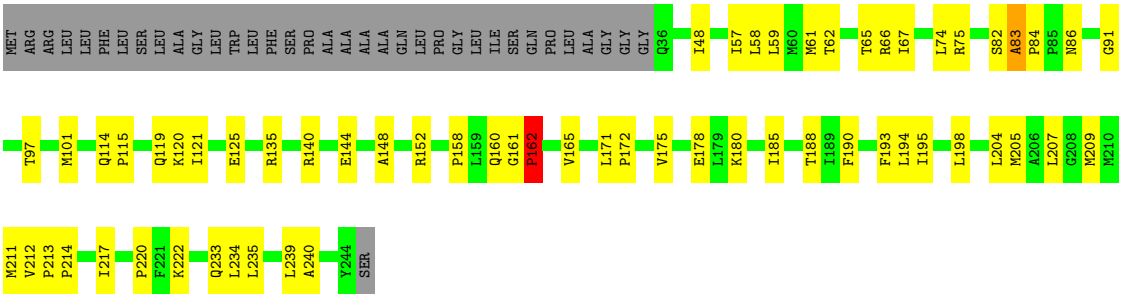
• Molecule 4: Flagellar biosynthetic protein FliP

Chain F:



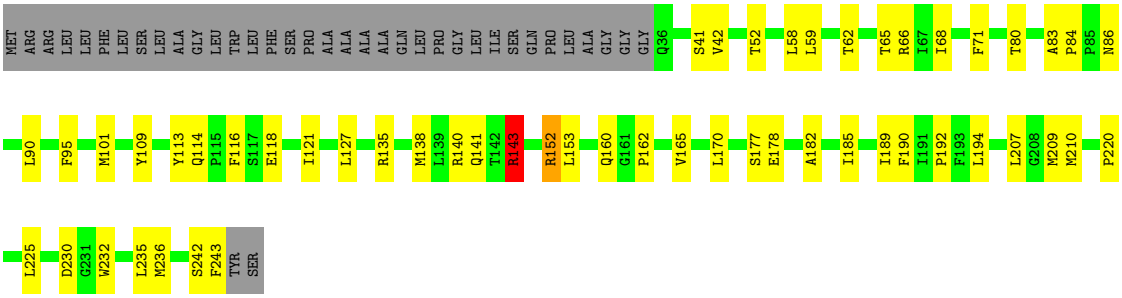
• Molecule 4: Flagellar biosynthetic protein FliP

Chain G: 60% 24% 15%



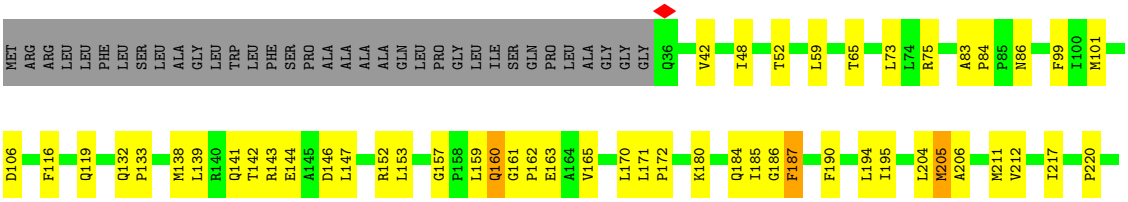
• Molecule 4: Flagellar biosynthetic protein FliP

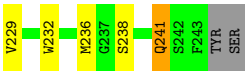
Chain H: 63% 21% 15%



• Molecule 4: Flagellar biosynthetic protein FliP

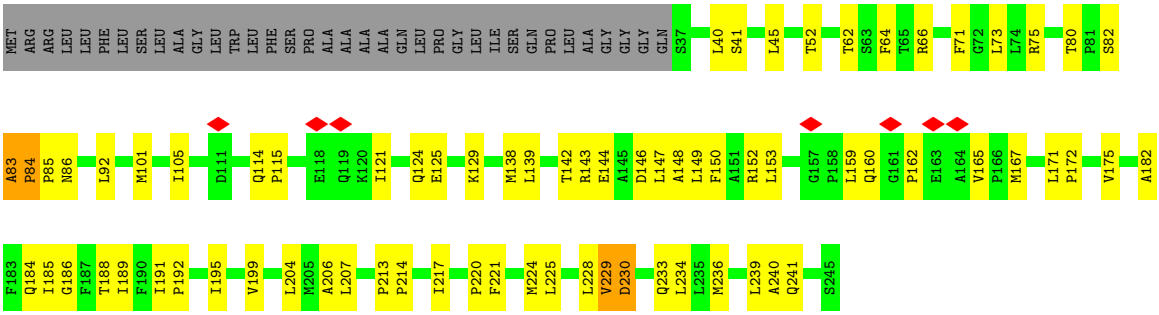
Chain I: 62% 22% • 15%





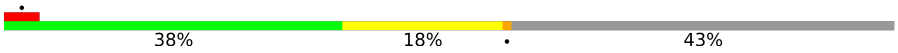
• Molecule 4: Flagellar biosynthetic protein FliP

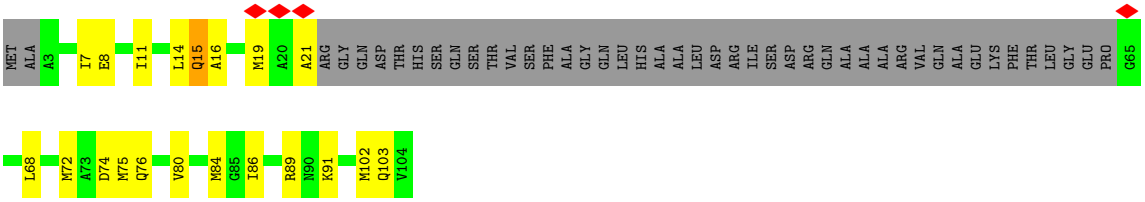
Chain J:



• Molecule 5: Flagellar hook-basal body complex protein FliE

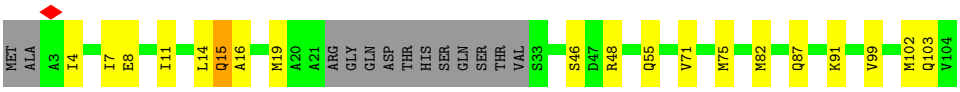
Chain K:





• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain L:



• Molecule 5: Flagellar hook-basal body complex protein FliE

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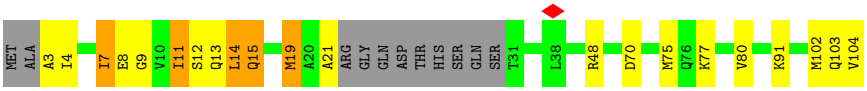

• Molecule 5: Flagellar hook-basal body complex protein FliE

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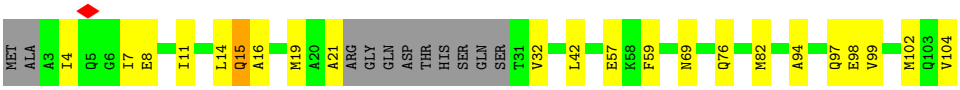

• Molecule 5: Flagellar hook-basal body complex protein FliE

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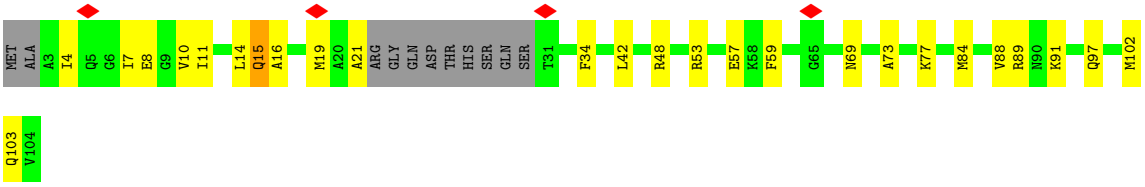

• Molecule 5: Flagellar hook-basal body complex protein FliE

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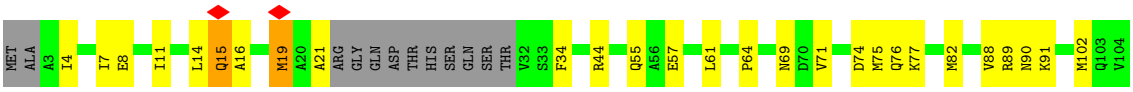
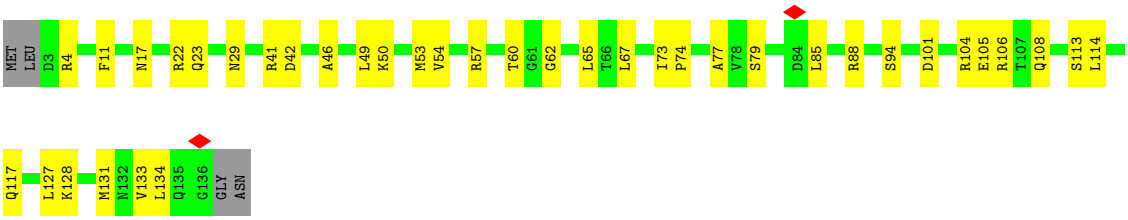


• Molecule 6: Flagellar basal body rod protein FlgB

Chain Q:



• Molecule 6: Flagellar basal body rod protein FlgB

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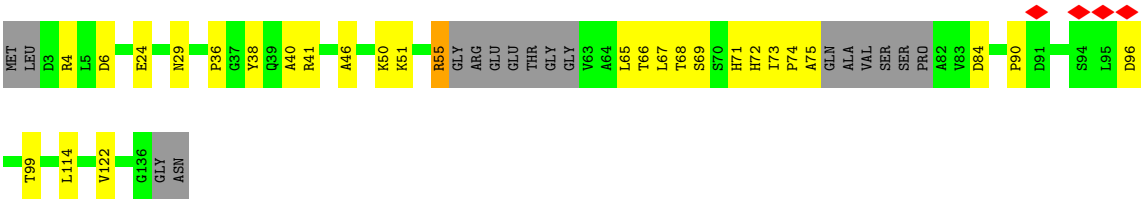
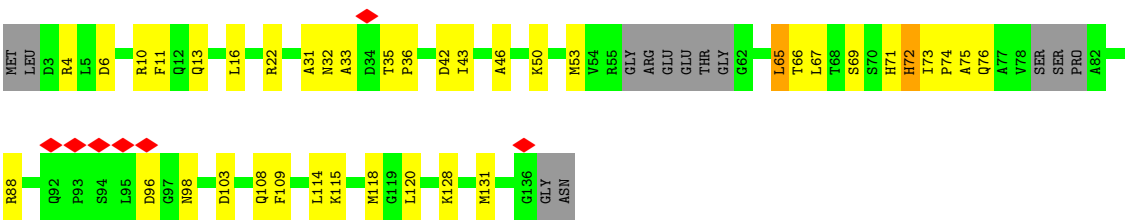


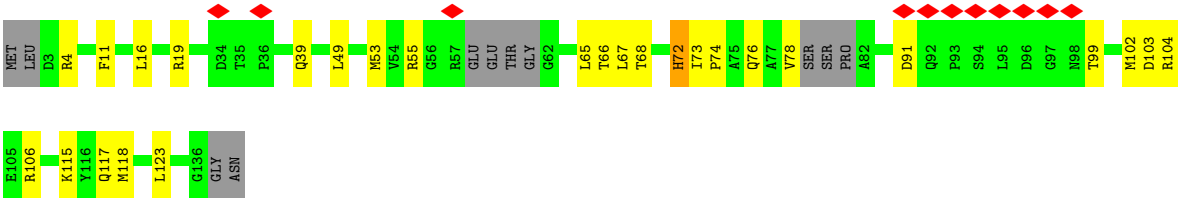
• Molecule 6: Flagellar basal body rod protein FlgB

Chain S:



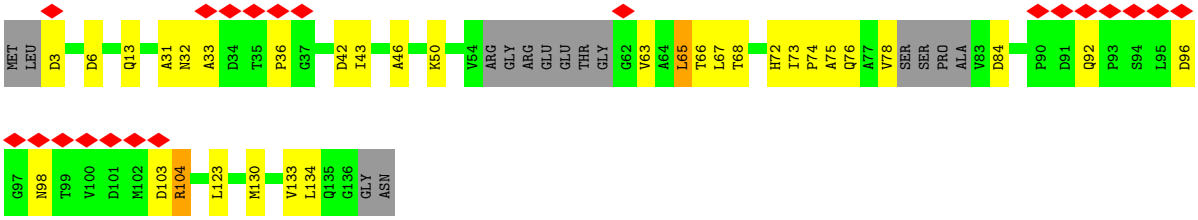
• Molecule 6: Flagellar basal body rod protein FlgB

Chain T:



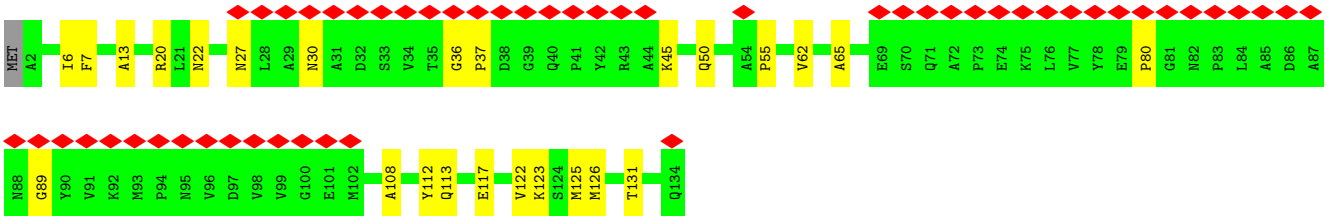
• Molecule 6: Flagellar basal body rod protein FlgB

Chain U:



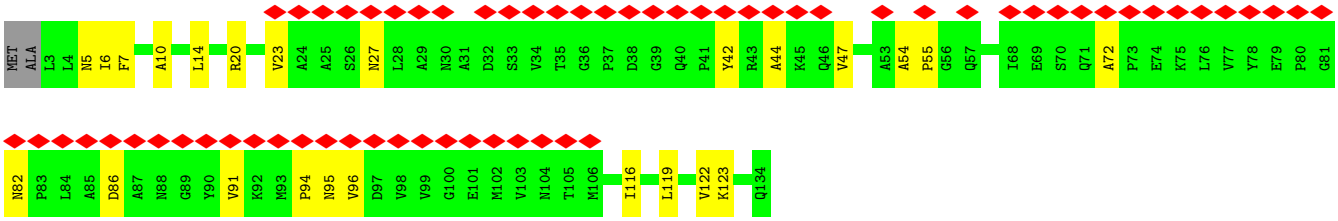
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain V:



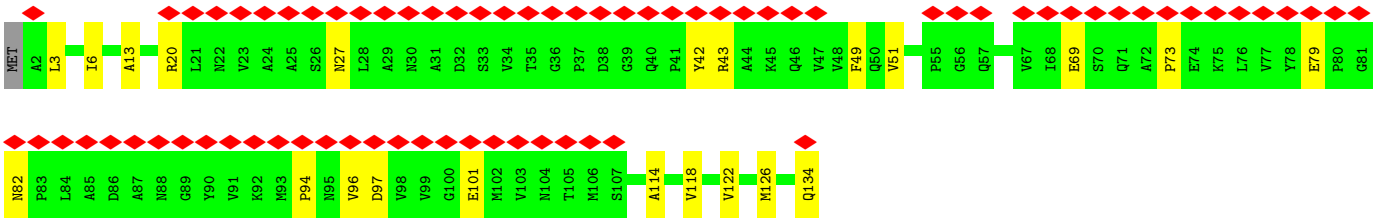
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain W:



• Molecule 7: Flagellar basal-body rod protein FlgC

Chain X:

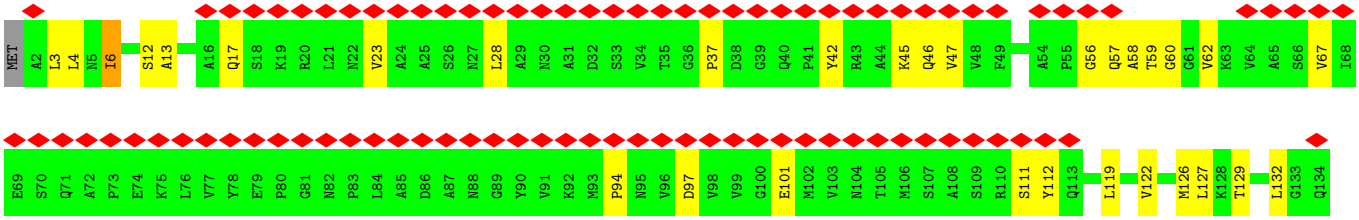


• Molecule 7: Flagellar basal-body rod protein FlgC

Chain Y:

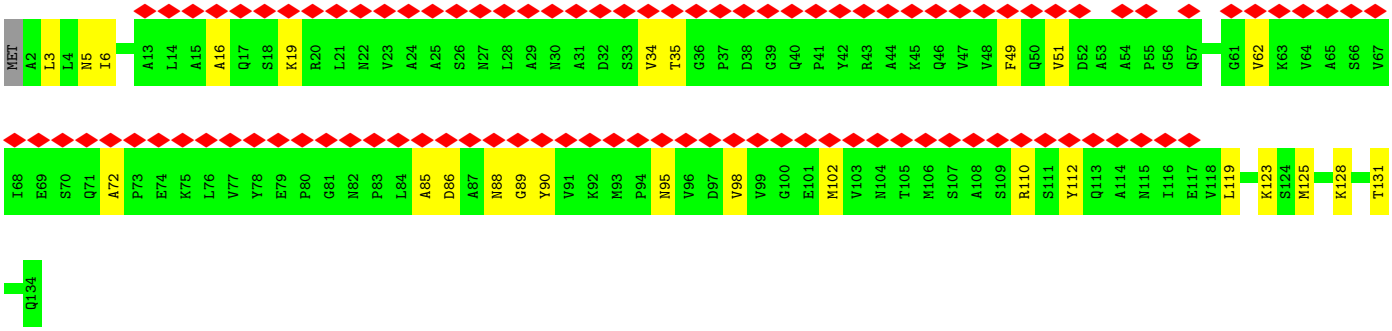
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain Z:



• Molecule 7: Flagellar basal-body rod protein FlgC

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0	0.22	0/1289	0.44	1/1741 (0.1%)
1	1	0.22	0/1289	0.44	1/1741 (0.1%)
1	2	0.23	0/1289	0.44	1/1741 (0.1%)
1	3	0.23	0/1289	0.44	1/1741 (0.1%)
1	4	0.23	0/1289	0.44	1/1741 (0.1%)
1	5	0.23	0/1289	0.44	1/1741 (0.1%)
1	6	0.22	0/1289	0.44	1/1741 (0.1%)
1	7	0.23	0/1289	0.44	1/1741 (0.1%)
1	8	0.23	0/1289	0.44	1/1741 (0.1%)
1	9	0.23	0/1289	0.44	1/1741 (0.1%)
1	AA	0.22	0/1289	0.44	1/1741 (0.1%)
1	AB	0.23	0/1289	0.44	1/1741 (0.1%)
1	AC	0.22	0/1289	0.44	1/1741 (0.1%)
1	AD	0.23	0/1289	0.44	1/1741 (0.1%)
1	AE	0.23	0/1289	0.44	1/1741 (0.1%)
1	AF	0.22	0/1289	0.44	1/1741 (0.1%)
1	AG	0.23	0/1289	0.44	1/1741 (0.1%)
1	AH	0.23	0/1289	0.44	1/1741 (0.1%)
1	AI	0.22	0/1289	0.44	1/1741 (0.1%)
1	AJ	0.22	0/1289	0.44	1/1741 (0.1%)
1	AK	0.22	0/1289	0.44	1/1741 (0.1%)
1	AL	0.23	0/1289	0.44	1/1741 (0.1%)
1	AM	0.22	0/1289	0.44	1/1741 (0.1%)
1	AN	0.22	0/1289	0.44	1/1741 (0.1%)
1	AO	0.22	0/1289	0.44	1/1741 (0.1%)
1	AP	0.23	0/1289	0.44	1/1741 (0.1%)
1	AQ	0.23	0/1289	0.44	1/1741 (0.1%)
1	UI	1.26	19/1191 (1.6%)	1.29	19/1618 (1.2%)
1	UJ	1.27	20/1191 (1.7%)	1.29	19/1618 (1.2%)
1	UK	1.25	19/1191 (1.6%)	1.29	19/1618 (1.2%)
1	UL	1.24	18/1191 (1.5%)	1.30	19/1618 (1.2%)
1	UM	1.27	20/1191 (1.7%)	1.29	19/1618 (1.2%)
1	UN	1.26	20/1191 (1.7%)	1.28	18/1618 (1.1%)
1	UO	1.25	19/1191 (1.6%)	1.28	19/1618 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	UP	1.27	20/1191 (1.7%)	1.28	19/1618 (1.2%)
1	WA	0.89	0/863	1.20	2/1172 (0.2%)
1	WB	0.91	0/850	1.21	1/1154 (0.1%)
1	WC	0.89	0/825	1.15	0/1121
1	WD	0.91	0/841	1.16	0/1142
1	WE	0.88	0/857	1.17	1/1164 (0.1%)
1	WF	0.89	0/848	1.17	0/1152
1	WG	0.88	0/857	1.16	0/1164
1	WH	0.90	0/714	1.15	1/973 (0.1%)
1	WI	0.88	0/714	1.20	2/973 (0.2%)
1	WJ	0.90	0/749	1.19	1/1020 (0.1%)
1	WK	0.90	0/741	1.16	0/1009
1	WL	0.89	0/631	1.16	1/860 (0.1%)
1	WM	0.88	0/604	1.15	1/824 (0.1%)
1	WN	0.89	0/619	1.17	1/844 (0.1%)
1	WO	0.89	0/726	1.19	3/989 (0.3%)
1	WP	0.89	0/753	1.16	0/1025
1	WQ	0.90	0/848	1.19	0/1152
1	WR	0.89	0/848	1.14	0/1152
1	WS	0.91	0/848	1.19	1/1152 (0.1%)
1	WT	0.89	0/848	1.18	0/1152
1	WU	0.89	0/857	1.16	1/1164 (0.1%)
1	WV	0.91	0/841	1.17	0/1142
1	WW	0.91	0/848	1.19	2/1152 (0.2%)
1	b	0.71	0/83	0.97	0/114
1	c	0.17	0/107	0.37	0/148
1	d	0.27	0/137	0.52	0/191
1	e	0.20	0/107	0.45	0/148
1	f	1.32	1/145 (0.7%)	1.50	3/203 (1.5%)
1	g	0.22	0/107	0.57	0/148
1	h	0.13	0/145	0.29	0/203
1	i	0.15	0/107	0.41	0/148
1	j	0.26	0/137	0.66	0/191
1	k	0.17	0/107	0.30	0/148
1	l	0.26	0/145	0.45	0/203
1	t	0.22	0/1289	0.44	1/1741 (0.1%)
1	u	0.22	0/1289	0.44	1/1741 (0.1%)
1	v	0.22	0/1289	0.44	1/1741 (0.1%)
1	w	0.23	0/1289	0.44	1/1741 (0.1%)
1	x	0.23	0/1289	0.44	1/1741 (0.1%)
1	y	0.22	0/1289	0.44	1/1741 (0.1%)
1	z	0.23	0/1289	0.44	1/1741 (0.1%)
2	A	0.27	0/681	0.49	0/930

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	B	0.16	0/681	0.42	0/930
2	C	0.23	0/681	0.44	0/930
2	D	0.26	0/681	0.55	0/930
3	E	0.45	3/1994 (0.2%)	0.61	3/2724 (0.1%)
4	F	0.33	0/1643	0.61	4/2237 (0.2%)
4	G	0.26	0/1665	0.46	2/2267 (0.1%)
4	H	0.22	0/1652	0.42	0/2249
4	I	0.22	0/1652	0.41	1/2249 (0.0%)
4	J	0.30	0/1662	0.53	1/2263 (0.0%)
5	K	0.52	0/428	0.84	0/572
5	L	0.41	0/675	0.64	0/905
5	M	0.42	0/689	0.70	0/925
5	N	0.42	0/689	0.64	0/925
5	O	0.42	0/689	0.66	0/925
5	P	0.43	0/682	0.67	0/915
6	Q	0.44	0/1042	0.59	0/1408
6	R	0.36	0/951	0.47	0/1282
6	S	0.40	0/976	0.59	0/1316
6	T	0.39	0/991	0.64	3/1335 (0.2%)
6	U	0.40	0/959	0.53	0/1293
7	V	0.16	0/981	0.31	0/1334
7	W	0.14	0/976	0.32	0/1327
7	X	0.52	2/981 (0.2%)	0.98	3/1334 (0.2%)
7	Y	0.16	0/981	0.37	0/1334
7	Z	0.15	0/981	0.35	0/1334
7	a	0.19	0/981	0.37	0/1334
All	All	0.59	161/100455 (0.2%)	0.76	223/136142 (0.2%)

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	UI	0	2
1	UJ	0	2
1	UK	0	3
1	UL	0	3
1	UM	0	2
1	UN	0	2
1	UO	0	2
1	UP	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	WA	0	3
1	WB	0	4
1	WC	0	3
1	WD	0	1
1	WE	0	2
1	WF	0	3
1	WG	0	3
1	WI	0	1
1	WJ	0	3
1	WK	0	2
1	WL	0	2
1	WM	0	1
1	WN	0	1
1	WO	0	1
1	WP	0	3
1	WQ	0	2
1	WR	0	3
1	WS	0	1
1	WT	0	2
1	WU	0	2
1	WV	0	3
1	WW	0	2
4	H	0	1
6	Q	0	1
6	U	0	1
7	Y	0	1
7	a	0	1
All	All	0	72

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	331	PRO	CG-CD	-13.84	1.03	1.50
1	UJ	125	GLN	C-N	13.62	1.51	1.33
1	UP	125	GLN	C-N	13.60	1.51	1.33
1	UK	125	GLN	C-N	13.59	1.51	1.33
1	UO	125	GLN	C-N	13.55	1.51	1.33

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	73	PRO	CB-CG-CD	23.05	179.86	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	73	PRO	N-CD-CG	-18.80	75.00	103.20
1	f	331	PRO	N-CD-CG	-16.10	79.05	103.20
7	X	73	PRO	CA-CB-CG	-14.26	77.40	104.50
1	UO	126	PHE	O-C-N	13.87	136.82	122.12

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	UI	221	THR	Mainchain
1	UI	50	ASP	Mainchain
1	UJ	270	THR	Mainchain
1	UJ	50	ASP	Mainchain
1	UK	50	ASP	Mainchain

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	0	1275	0	1254	34	0
1	1	1275	0	1254	59	0
1	2	1275	0	1254	40	0
1	3	1275	0	1254	31	0
1	4	1275	0	1254	45	0
1	5	1275	0	1254	39	0
1	6	1275	0	1254	50	0
1	7	1275	0	1254	54	0
1	8	1275	0	1254	34	0
1	9	1275	0	1254	32	0
1	AA	1275	0	1254	30	0
1	AB	1275	0	1254	44	0
1	AC	1275	0	1254	47	0
1	AD	1275	0	1254	47	0
1	AE	1275	0	1254	46	0
1	AF	1275	0	1254	29	0
1	AG	1275	0	1254	33	0
1	AH	1275	0	1254	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	1275	0	1254	48	0
1	AJ	1275	0	1254	42	0
1	AK	1275	0	1254	41	0
1	AL	1275	0	1254	39	0
1	AM	1275	0	1254	39	0
1	AN	1275	0	1254	31	0
1	AO	1275	0	1254	34	0
1	AP	1275	0	1254	39	0
1	AQ	1275	0	1254	33	0
1	UI	1172	0	1181	64	0
1	UJ	1172	0	1181	81	0
1	UK	1172	0	1181	75	0
1	UL	1172	0	1181	74	0
1	UM	1172	0	1181	70	0
1	UN	1172	0	1181	71	0
1	UO	1172	0	1181	64	0
1	UP	1172	0	1181	68	0
1	WA	849	0	860	82	0
1	WB	836	0	846	82	0
1	WC	812	0	826	72	0
1	WD	827	0	840	98	0
1	WE	843	0	855	90	0
1	WF	834	0	847	64	0
1	WG	843	0	855	72	0
1	WH	703	0	722	69	0
1	WI	703	0	722	78	0
1	WJ	737	0	755	93	0
1	WK	729	0	744	86	0
1	WL	622	0	632	61	0
1	WM	596	0	612	49	0
1	WN	611	0	623	59	0
1	WO	714	0	731	54	0
1	WP	741	0	758	75	0
1	WQ	834	0	847	75	0
1	WR	834	0	847	64	0
1	WS	834	0	847	83	0
1	WT	834	0	847	77	0
1	WU	843	0	855	68	0
1	WV	827	0	838	67	0
1	WW	834	0	847	89	0
1	b	81	0	78	6	0
1	c	103	0	99	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	133	0	129	7	0
1	e	103	0	99	4	0
1	f	140	0	136	4	0
1	g	103	0	99	3	0
1	h	140	0	136	0	0
1	i	103	0	99	1	0
1	j	133	0	129	10	0
1	k	103	0	99	3	0
1	l	140	0	136	2	0
1	t	1275	0	1254	45	0
1	u	1275	0	1254	34	0
1	v	1275	0	1254	28	0
1	w	1275	0	1254	30	0
1	x	1275	0	1254	33	0
1	y	1275	0	1254	37	0
1	z	1275	0	1254	51	0
2	A	670	0	739	35	0
2	B	670	0	739	38	0
2	C	670	0	739	35	0
2	D	670	0	739	42	0
3	E	1945	0	2063	124	0
4	F	1605	0	1701	87	0
4	G	1626	0	1718	63	0
4	H	1614	0	1709	57	0
4	I	1614	0	1709	77	0
4	J	1623	0	1715	93	0
5	K	429	0	445	40	0
5	L	672	0	684	53	0
5	M	686	0	700	54	0
5	N	686	0	700	47	0
5	O	686	0	700	53	0
5	P	679	0	693	51	0
6	Q	1030	0	1025	29	0
6	R	942	0	943	37	0
6	S	967	0	968	61	0
6	T	982	0	984	46	0
6	U	950	0	946	60	0
7	V	969	0	981	23	0
7	W	964	0	976	16	0
7	X	969	0	981	16	0
7	Y	969	0	981	18	0
7	Z	969	0	981	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	a	969	0	981	21	0
All	All	99073	0	99719	3548	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 18.

The worst 5 of 3548 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:WD:168:GLU:CD	1:WD:170:LYS:HE3	1.40	1.43
1:WC:121:PHE:HZ	2:C:15:LYS:NZ	1.21	1.35
1:UP:103:GLN:HG2	1:WW:182:PRO:CB	1.58	1.33
1:UP:103:GLN:CG	1:WW:182:PRO:HB3	1.56	1.32
5:L:11:ILE:HG22	1:AH:372:ILE:CD1	1.58	1.32

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	0	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	1	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	2	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	3	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	4	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	5	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	6	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	7	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	9	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AA	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AB	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AC	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AD	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AE	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AF	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AG	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AH	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AI	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AJ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AK	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AL	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AM	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AN	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AO	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AP	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AQ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	9	38
1	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	9	38
1	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	9	38
1	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	9	38
1	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	9	38
1	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	9	38
1	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	9	38
1	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	9	38
1	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	27
1	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	18
1	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	45
1	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	2	22
1	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	26
1	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	6	33
1	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	30
1	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	14
1	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	12	43
1	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	25
1	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	28
1	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	27
1	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	21
1	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	31
1	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	17
1	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	21
1	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	14
1	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	16
1	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	14
1	WU	110/560 (20%)	101 (92%)	8 (7%)	1 (1%)	14	45
1	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	32
1	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	18
1	b	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
1	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
1	d	18/560 (3%)	18 (100%)	0	0	100	100
1	e	14/560 (2%)	14 (100%)	0	0	100	100
1	f	19/560 (3%)	19 (100%)	0	0	100	100
1	g	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
1	h	19/560 (3%)	19 (100%)	0	0	100	100
1	i	14/560 (2%)	14 (100%)	0	0	100	100
1	j	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
1	k	14/560 (2%)	14 (100%)	0	0	100	100
1	l	19/560 (3%)	19 (100%)	0	0	100	100
1	t	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	v	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	w	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	x	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	y	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	z	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
2	A	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
2	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
2	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
2	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
3	E	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	4	29
4	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
4	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	12	43
4	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
4	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	24	57
4	J	207/245 (84%)	201 (97%)	4 (2%)	2 (1%)	12	43
5	K	55/104 (53%)	53 (96%)	2 (4%)	0	100	100
5	L	87/104 (84%)	87 (100%)	0	0	100	100
5	M	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
5	N	89/104 (86%)	89 (100%)	0	0	100	100
5	O	89/104 (86%)	89 (100%)	0	0	100	100
5	P	88/104 (85%)	88 (100%)	0	0	100	100
6	Q	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
6	R	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
6	S	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
6	T	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
6	U	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
7	V	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
7	W	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
7	X	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
7	Y	131/134 (98%)	127 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Z	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	48
7	a	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
All	All	12674/46523 (27%)	12203 (96%)	362 (3%)	109 (1%)	16	45

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	WO	168	GLU
1	WR	123	ILE
1	WR	165	PHE
1	WR	166	VAL
1	WS	187	ASP

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	0	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	1	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	2	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	3	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	4	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	5	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	6	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	7	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	8	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	9	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AA	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AB	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AC	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AD	141/467 (30%)	140 (99%)	1 (1%)	76	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AE	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AF	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AG	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AH	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AI	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AJ	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AK	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AL	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AM	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AN	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AO	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AP	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	AQ	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	UI	128/467 (27%)	122 (95%)	6 (5%)	23	48
1	UJ	128/467 (27%)	121 (94%)	7 (6%)	19	45
1	UK	128/467 (27%)	122 (95%)	6 (5%)	23	48
1	UL	128/467 (27%)	122 (95%)	6 (5%)	23	48
1	UM	128/467 (27%)	122 (95%)	6 (5%)	23	48
1	UN	128/467 (27%)	122 (95%)	6 (5%)	23	48
1	UO	128/467 (27%)	122 (95%)	6 (5%)	23	48
1	UP	128/467 (27%)	121 (94%)	7 (6%)	19	45
1	WA	95/467 (20%)	91 (96%)	4 (4%)	26	50
1	WB	93/467 (20%)	86 (92%)	7 (8%)	12	38
1	WC	91/467 (20%)	83 (91%)	8 (9%)	9	33
1	WD	92/467 (20%)	88 (96%)	4 (4%)	26	50
1	WE	94/467 (20%)	87 (93%)	7 (7%)	13	38
1	WF	93/467 (20%)	84 (90%)	9 (10%)	8	29
1	WG	94/467 (20%)	85 (90%)	9 (10%)	8	29
1	WH	79/467 (17%)	75 (95%)	4 (5%)	21	46
1	WI	79/467 (17%)	75 (95%)	4 (5%)	21	46
1	WJ	83/467 (18%)	80 (96%)	3 (4%)	31	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	WK	82/467 (18%)	76 (93%)	6 (7%)	13	39
1	WL	69/467 (15%)	67 (97%)	2 (3%)	37	58
1	WM	66/467 (14%)	64 (97%)	2 (3%)	36	57
1	WN	68/467 (15%)	66 (97%)	2 (3%)	37	58
1	WO	80/467 (17%)	76 (95%)	4 (5%)	22	47
1	WP	83/467 (18%)	80 (96%)	3 (4%)	31	54
1	WQ	93/467 (20%)	90 (97%)	3 (3%)	34	56
1	WR	93/467 (20%)	85 (91%)	8 (9%)	10	33
1	WS	93/467 (20%)	89 (96%)	4 (4%)	26	50
1	WT	93/467 (20%)	86 (92%)	7 (8%)	12	38
1	WU	94/467 (20%)	88 (94%)	6 (6%)	16	42
1	WV	92/467 (20%)	81 (88%)	11 (12%)	5	21
1	WW	93/467 (20%)	85 (91%)	8 (9%)	10	33
1	b	8/467 (2%)	8 (100%)	0	100	100
1	c	11/467 (2%)	11 (100%)	0	100	100
1	d	14/467 (3%)	12 (86%)	2 (14%)	3	17
1	e	11/467 (2%)	11 (100%)	0	100	100
1	f	15/467 (3%)	15 (100%)	0	100	100
1	g	11/467 (2%)	11 (100%)	0	100	100
1	h	15/467 (3%)	15 (100%)	0	100	100
1	i	11/467 (2%)	11 (100%)	0	100	100
1	j	14/467 (3%)	13 (93%)	1 (7%)	13	39
1	k	11/467 (2%)	11 (100%)	0	100	100
1	l	15/467 (3%)	15 (100%)	0	100	100
1	t	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	u	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	v	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	w	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	x	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	y	141/467 (30%)	140 (99%)	1 (1%)	76	77
1	z	141/467 (30%)	140 (99%)	1 (1%)	76	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	74/74 (100%)	72 (97%)	2 (3%)	39	59
2	B	74/74 (100%)	74 (100%)	0	100	100
2	C	74/74 (100%)	74 (100%)	0	100	100
2	D	74/74 (100%)	72 (97%)	2 (3%)	39	59
3	E	210/221 (95%)	208 (99%)	2 (1%)	68	74
4	F	177/204 (87%)	175 (99%)	2 (1%)	65	73
4	G	179/204 (88%)	174 (97%)	5 (3%)	38	58
4	H	178/204 (87%)	176 (99%)	2 (1%)	65	73
4	I	178/204 (87%)	175 (98%)	3 (2%)	53	67
4	J	179/204 (88%)	178 (99%)	1 (1%)	78	79
5	K	45/79 (57%)	43 (96%)	2 (4%)	25	49
5	L	68/79 (86%)	66 (97%)	2 (3%)	37	58
5	M	70/79 (89%)	65 (93%)	5 (7%)	13	39
5	N	70/79 (89%)	67 (96%)	3 (4%)	26	50
5	O	70/79 (89%)	68 (97%)	2 (3%)	37	58
5	P	69/79 (87%)	65 (94%)	4 (6%)	18	44
6	Q	110/113 (97%)	109 (99%)	1 (1%)	70	74
6	R	101/113 (89%)	100 (99%)	1 (1%)	68	74
6	S	103/113 (91%)	99 (96%)	4 (4%)	28	52
6	T	104/113 (92%)	103 (99%)	1 (1%)	68	74
6	U	102/113 (90%)	100 (98%)	2 (2%)	48	65
7	V	104/105 (99%)	104 (100%)	0	100	100
7	W	104/105 (99%)	104 (100%)	0	100	100
7	X	104/105 (99%)	104 (100%)	0	100	100
7	Y	104/105 (99%)	103 (99%)	1 (1%)	68	74
7	Z	104/105 (99%)	102 (98%)	2 (2%)	50	66
7	a	104/105 (99%)	104 (100%)	0	100	100
All	All	10879/38698 (28%)	10618 (98%)	261 (2%)	43	62

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	295	SER

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Mol	Chain	Res	Type
1	5	295	SER
1	AQ	295	SER
1	WG	190	GLN
1	WG	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	234	GLN
1	AJ	281	HIS
1	AC	234	GLN
1	AF	234	GLN
1	AL	303	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

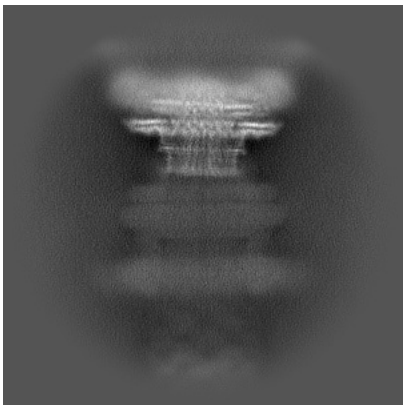
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37605. These allow visual inspection of the internal detail of the map and identification of artifacts.

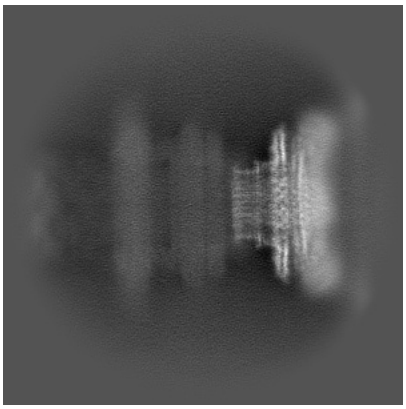
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

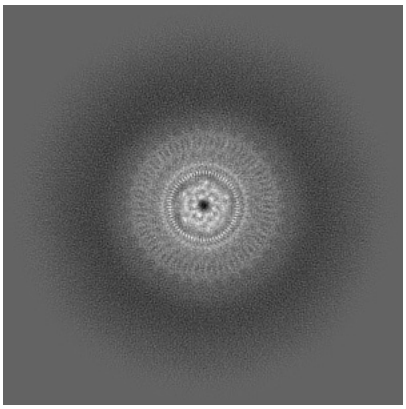
6.1.1 Primary map



X

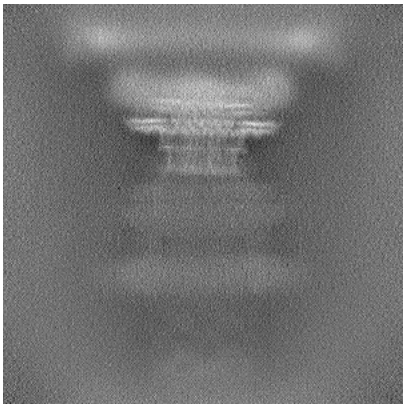


Y

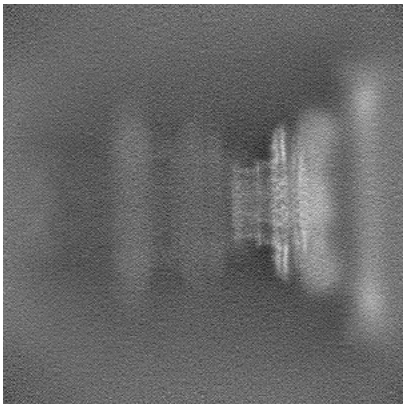


Z

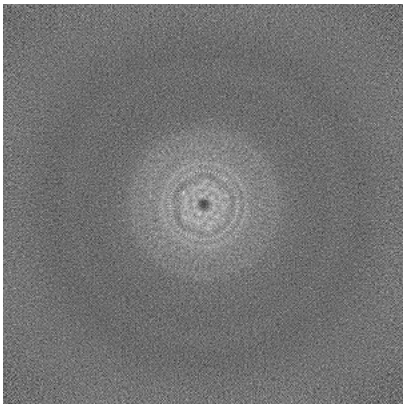
6.1.2 Raw map



X



Y

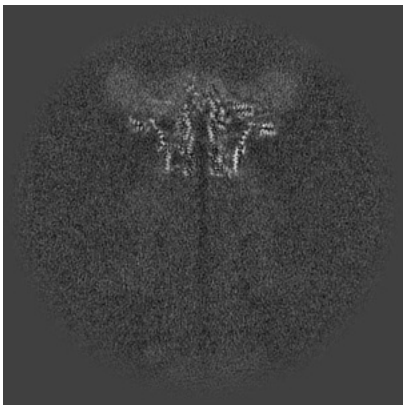


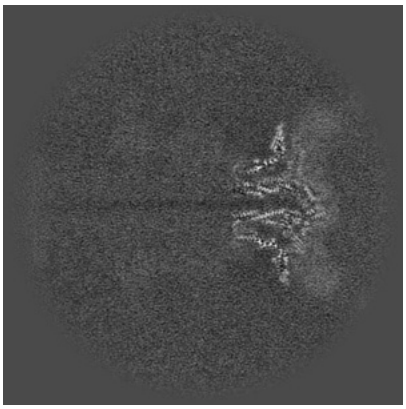
Z

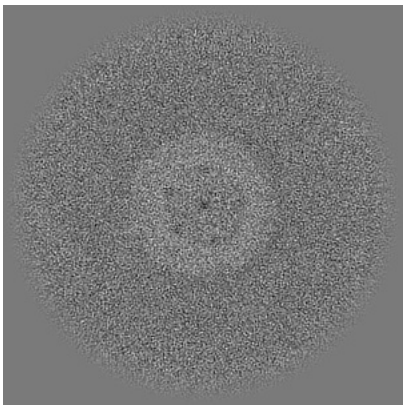
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

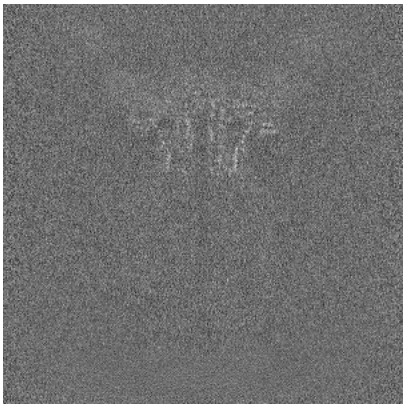
6.2.1 Primary map

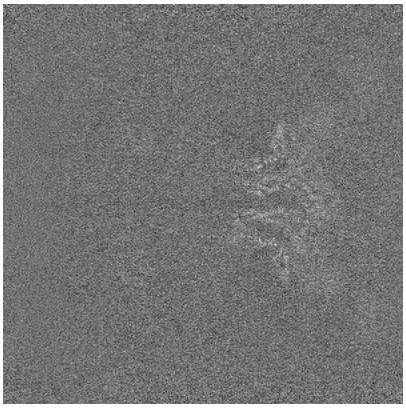

X Index: 256

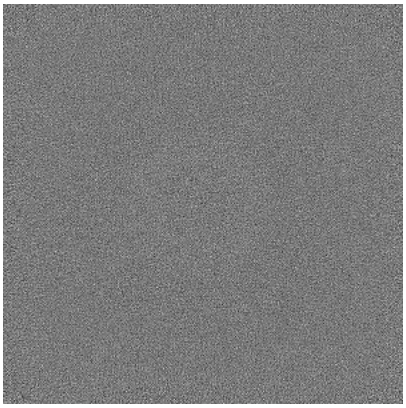

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

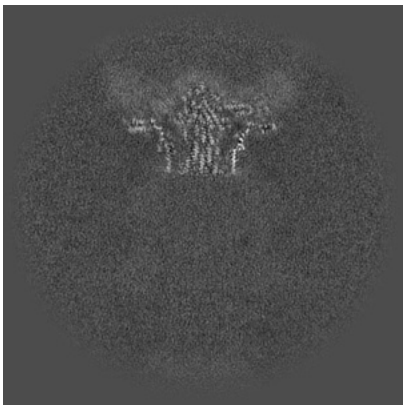

Y Index: 256


Z Index: 256

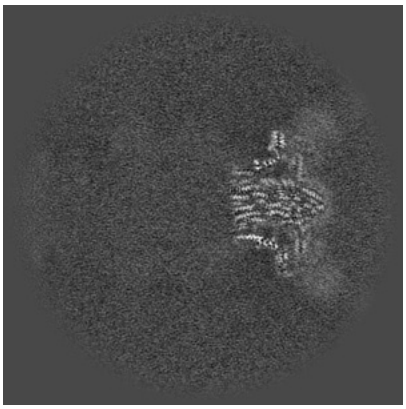
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

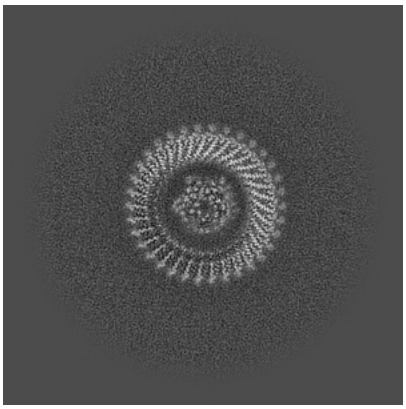
6.3.1 Primary map



X Index: 244

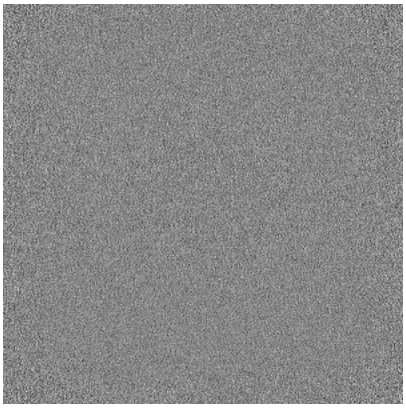


Y Index: 265

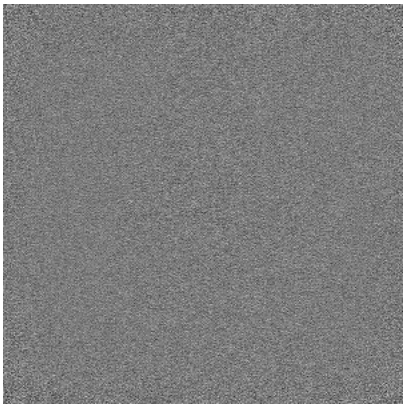


Z Index: 358

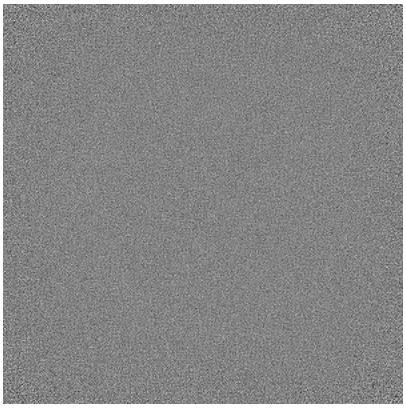
6.3.2 Raw map



X Index: 0



Y Index: 0

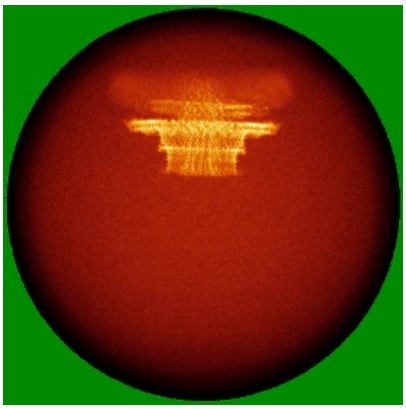


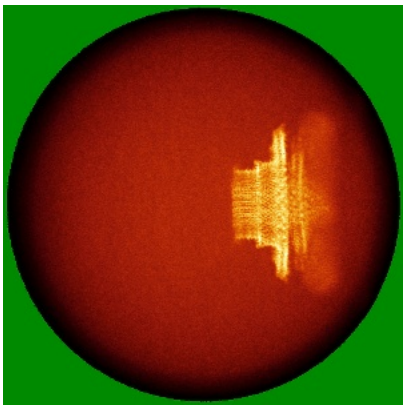
Z Index: 0

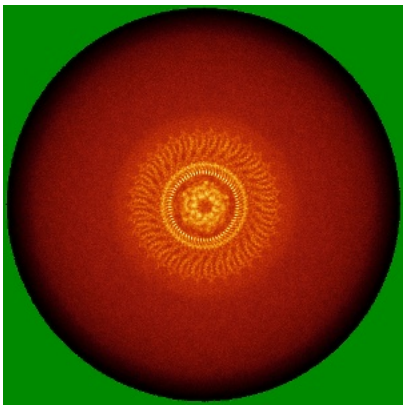
The images above show the largest variance slices of the map in three orthogonal directions.

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

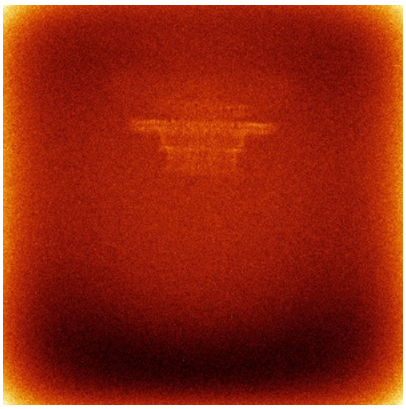
6.4.1 Primary map

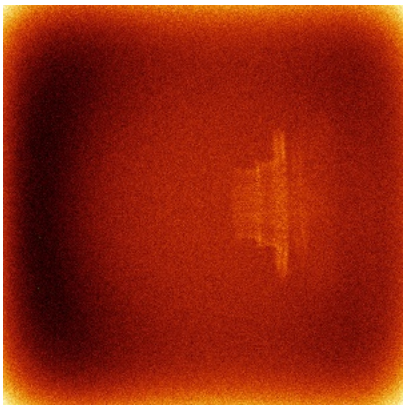

X

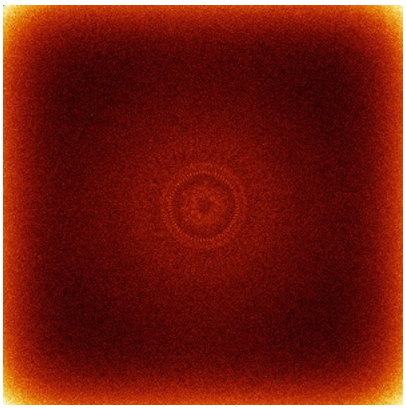

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

This section was not generated.

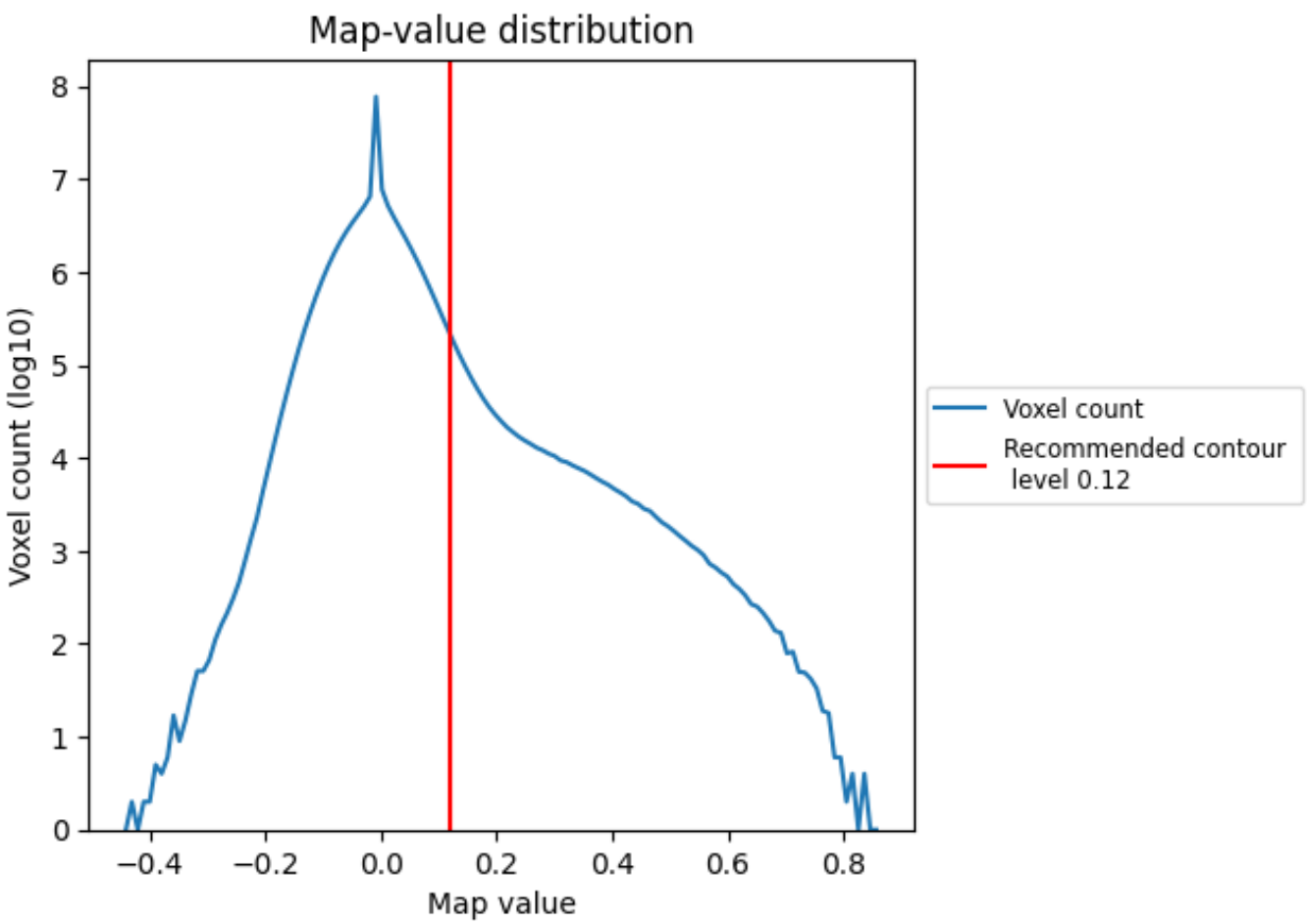
6.6 Mask visualisation (i)

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

7 Map analysis (i)

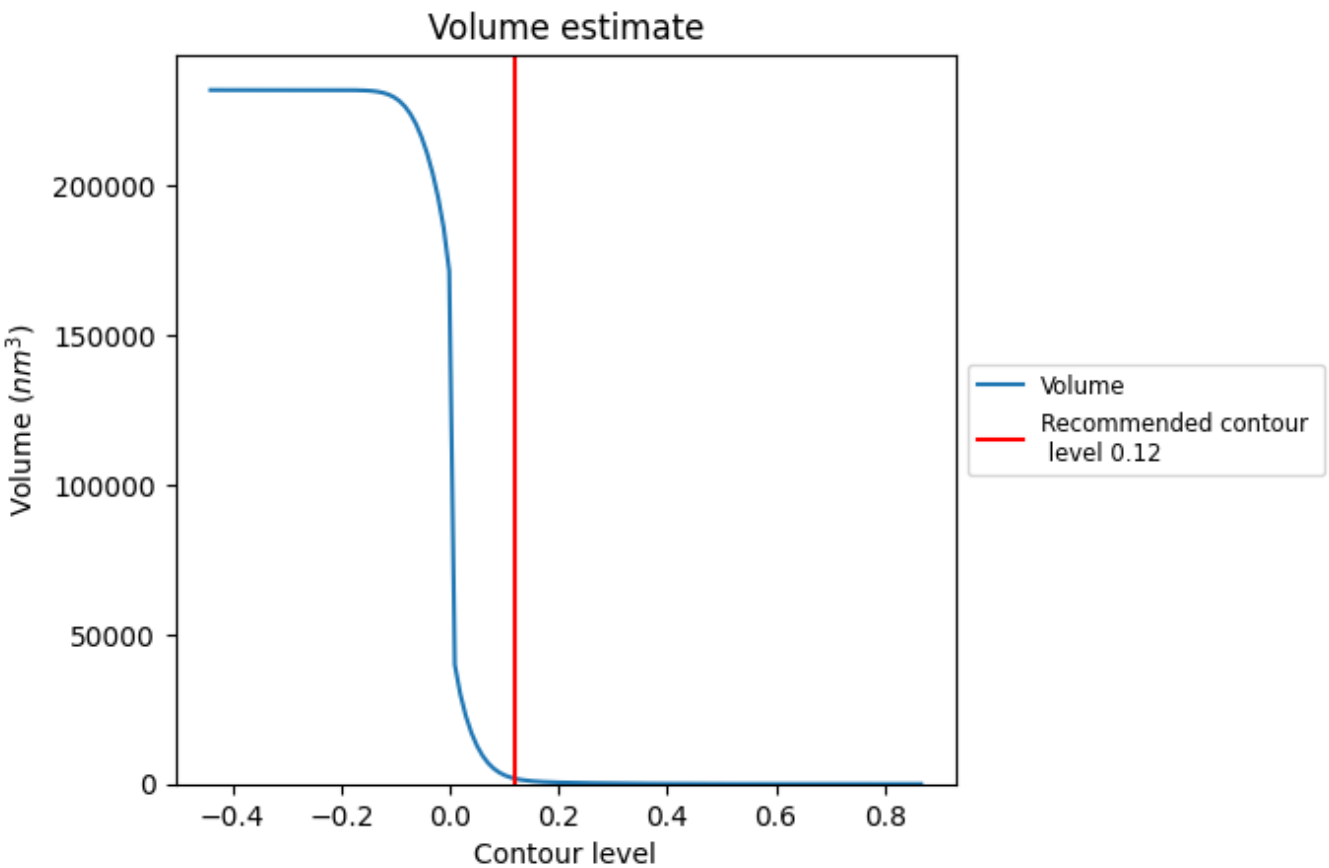
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

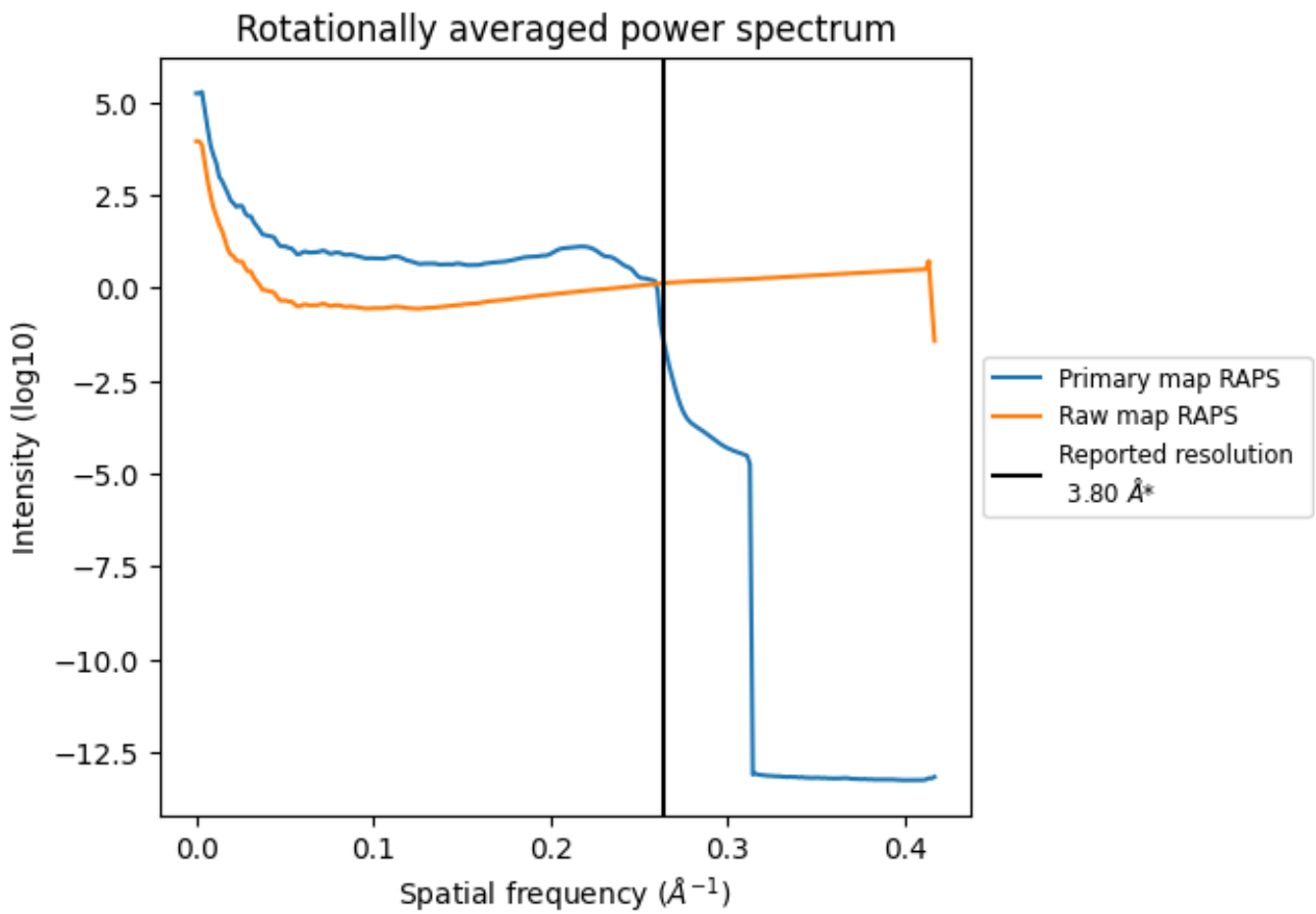
7.2 Volume estimate (i)



The volume at the recommended contour level is 1782 nm^3; this corresponds to an approximate mass of 1610 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)

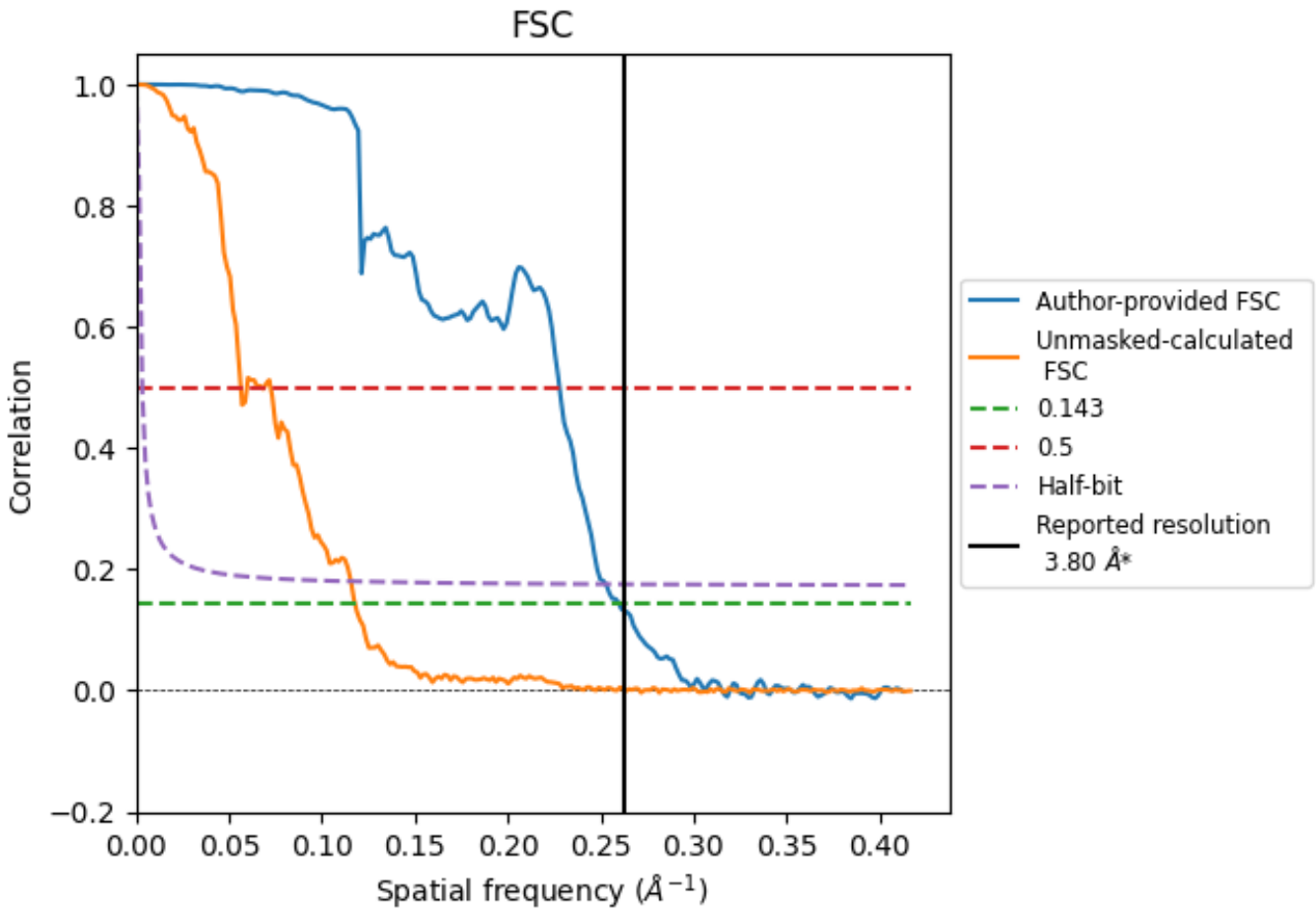


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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	3.85	4.39	3.96
Unmasked-calculated*	8.49	17.76	8.65

*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 8.49 differs from the reported value 3.8 by more than 10 %

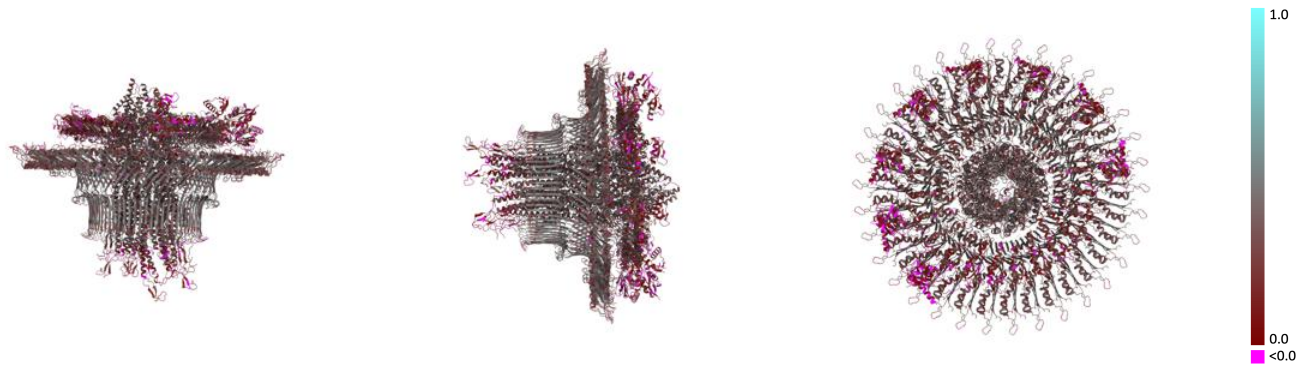
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37605 and PDB model 8WKQ. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay (i)

This section was not generated.

9.2 Q-score mapped to coordinate model (i)



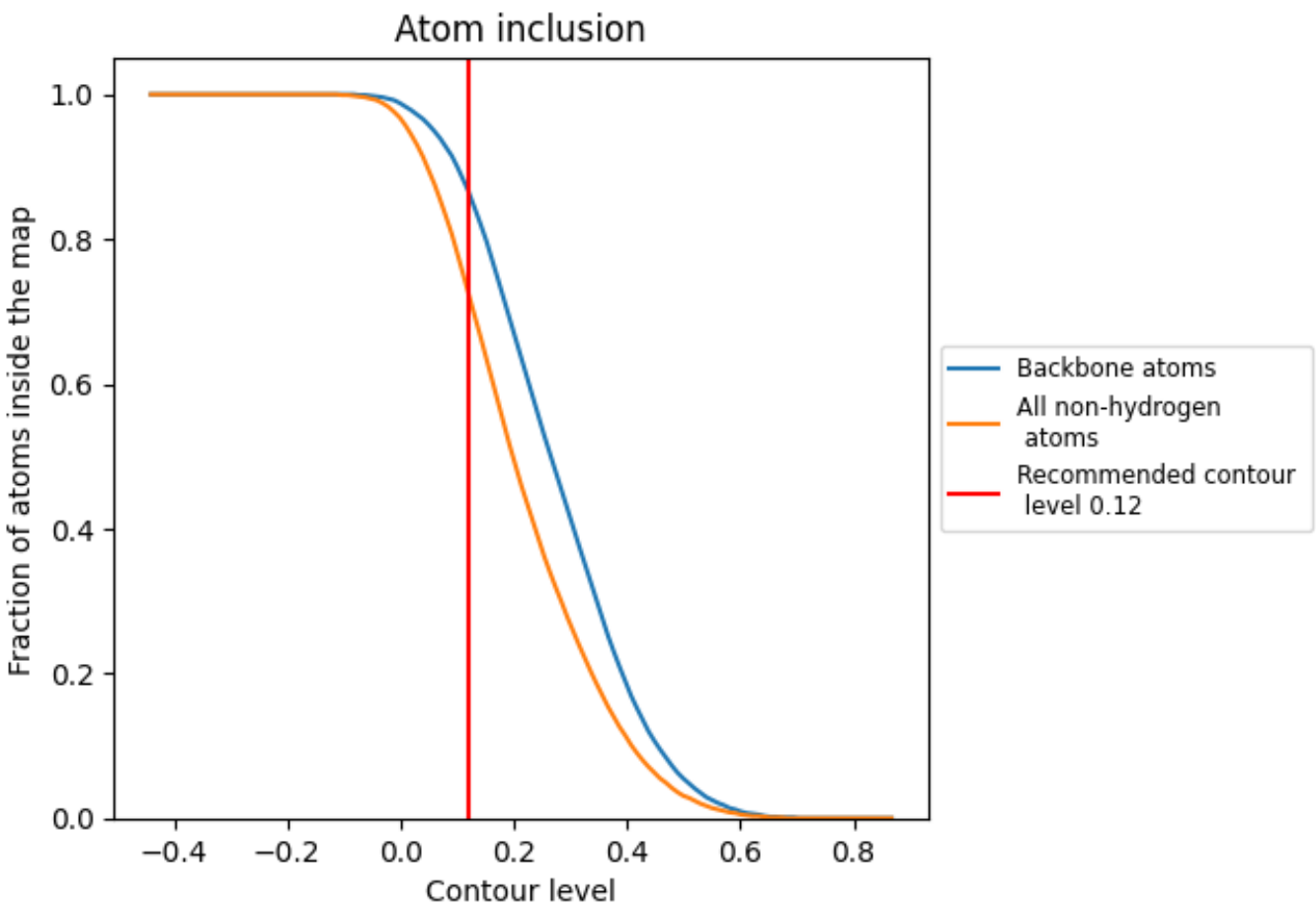
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.3190
0	0.8170	0.3700
1	0.8140	0.3590
2	0.8250	0.3680
3	0.8290	0.3720
4	0.8250	0.3740
5	0.8190	0.3730
6	0.8280	0.3770
7	0.8200	0.3750
8	0.8340	0.3860
9	0.8330	0.3850
A	0.7670	0.3160
AA	0.8140	0.3660
AB	0.8210	0.3660
AC	0.8210	0.3690
AD	0.8240	0.3640
AE	0.8180	0.3720
AF	0.8290	0.3590
AG	0.8120	0.3470
AH	0.8200	0.3540
AI	0.8010	0.3490
AJ	0.8220	0.3610
AK	0.8270	0.3650
AL	0.8140	0.3620
AM	0.8110	0.3650
AN	0.8040	0.3640
AO	0.8250	0.3750
AP	0.8220	0.3740
AQ	0.8160	0.3700
B	0.8150	0.3480
C	0.8200	0.3510
D	0.8090	0.3460
E	0.7840	0.3500
F	0.7940	0.3610
G	0.8120	0.3750

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Chain	Atom inclusion	Q-score
H	0.7990	0.3690
I	0.7870	0.3680
J	0.7640	0.3640
K	0.7300	0.3590
L	0.7890	0.3540
M	0.7750	0.3500
N	0.7680	0.3580
O	0.7610	0.3430
P	0.7660	0.3520
Q	0.7750	0.3790
R	0.7740	0.3690
S	0.7420	0.3670
T	0.7260	0.3610
U	0.6610	0.3390
UI	0.5160	0.2040
UJ	0.4890	0.1640
UK	0.4160	0.1540
UL	0.3670	0.1180
UM	0.2850	0.0510
UN	0.3590	0.0800
UO	0.4200	0.1310
UP	0.4760	0.1390
V	0.5020	0.3110
W	0.4120	0.2850
WA	0.7920	0.3380
WB	0.7910	0.3290
WC	0.8040	0.3460
WD	0.7890	0.3400
WE	0.7680	0.3210
WF	0.7780	0.3230
WG	0.7460	0.2860
WH	0.7690	0.2810
WI	0.7200	0.2360
WJ	0.6920	0.2170
WK	0.6500	0.1970
WL	0.6770	0.1880
WM	0.7090	0.2250
WN	0.6880	0.1660
WO	0.6630	0.1650
WP	0.7480	0.2330
WQ	0.7300	0.2510
WR	0.7300	0.2820

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Chain	Atom inclusion	Q-score
WS	0.7870	0.2910
WT	0.7950	0.3240
WU	0.7600	0.2930
WV	0.7590	0.2860
WW	0.7790	0.3220
X	0.3500	0.2540
Y	0.2900	0.2230
Z	0.2590	0.2420
a	0.2050	0.2240
b	0.6670	0.3370
c	0.5050	0.3570
d	0.5640	0.3320
e	0.2430	0.2510
f	0.4930	0.2610
g	0.0870	0.1150
h	0.4360	0.2610
i	0.0680	0.1250
j	0.4510	0.2720
k	0.0780	0.1940
l	0.3360	0.2730
t	0.8270	0.3780
u	0.8270	0.3630
v	0.8240	0.3710
w	0.8280	0.3750
x	0.8300	0.3680
y	0.8260	0.3730
z	0.8250	0.3740