



wwPDB EM Model Validation Summary Report ⓘ

Mar 9, 2020 – 02:50 PM EDT

PDB ID : 6SD1
EMDB ID : EMD-10145
Title : Structure of the RBM3/collar region of the Salmonella flagella MS-ring protein
FliF with 33-fold symmetry applied
Authors : Johnson, S.; Fong, Y.H.; Deme, J.C.; Furlong, E.J.; Kuhlen, L.; Lea, S.M.
Deposited on : 2019-07-26
Resolution : 2.60 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

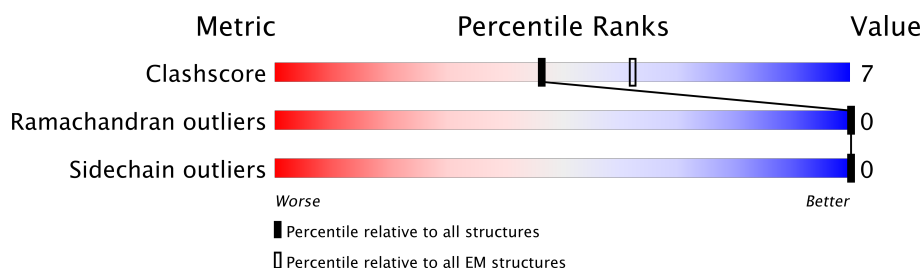
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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
















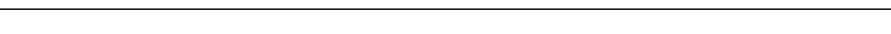
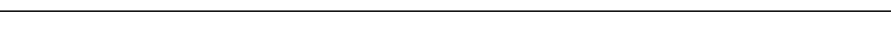
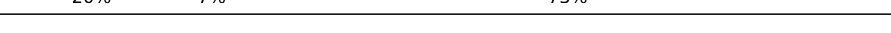








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	560	20% 7% 73%
1	B	560	19% 8% 73%
1	C	560	20% 7% 73%
1	D	560	20% 7% 73%
1	E	560	21% 6% 73%
1	F	560	21% 6% 73%
1	G	560	20% 7% 73%
1	H	560	20% 7% 73%
1	I	560	21% 6% 73%

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Mol	Chain	Length	Quality of chain
1	J	560	 21% 6% 73%
1	K	560	 22% 5% 73%
1	L	560	 21% 6% 73%
1	M	560	 20% 7% 73%
1	N	560	 21% 6% 73%
1	O	560	 20% 7% 73%
1	P	560	 20% 7% 73%
1	Q	560	 21% 6% 73%
1	R	560	 21% 6% 73%
1	S	560	 21% 6% 73%
1	T	560	 21% 6% 73%
1	U	560	 21% 6% 73%
1	V	560	 21% 6% 73%
1	W	560	 21% 6% 73%
1	X	560	 20% 7% 73%
1	Y	560	 20% 7% 73%
1	Z	560	 21% 6% 73%
1	a	560	 27% 73%
1	b	560	 27% 73%
1	c	560	 27% 73%
1	d	560	 27% 73%
1	e	560	 27% 73%
1	f	560	 27% 73%
1	g	560	 27% 73%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 39369 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar M-ring protein.

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

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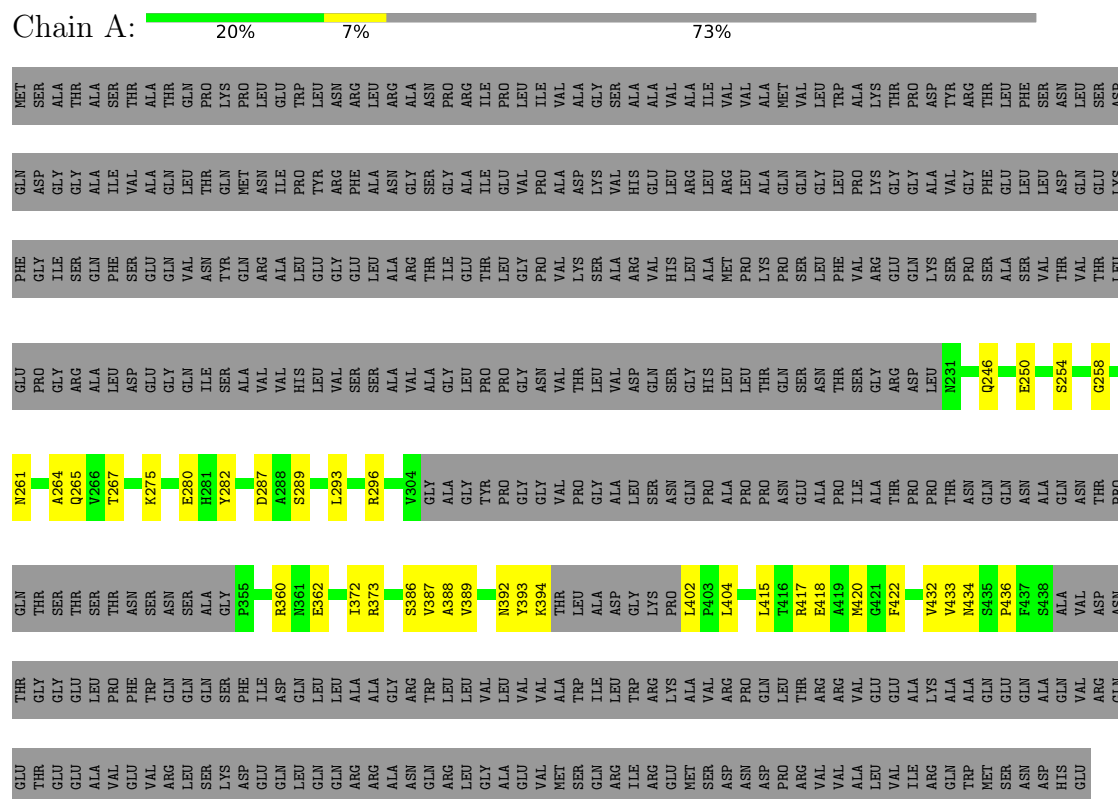
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	S	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	T	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	U	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	V	151	Total 1193	C 726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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

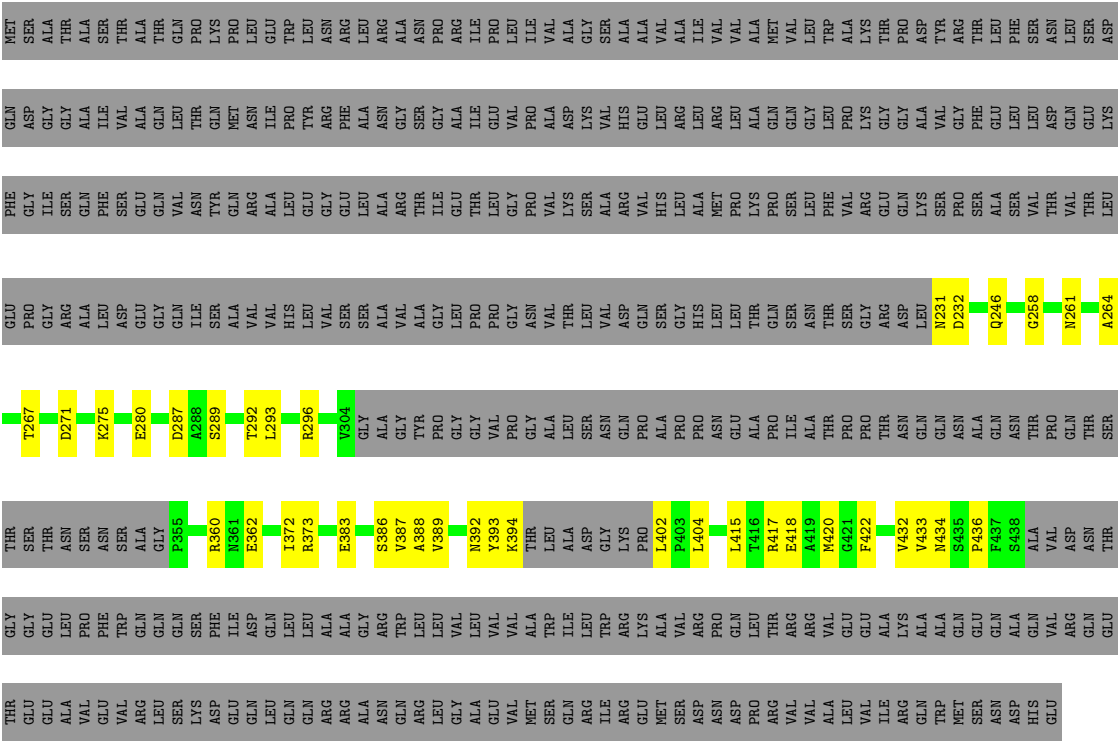
- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein

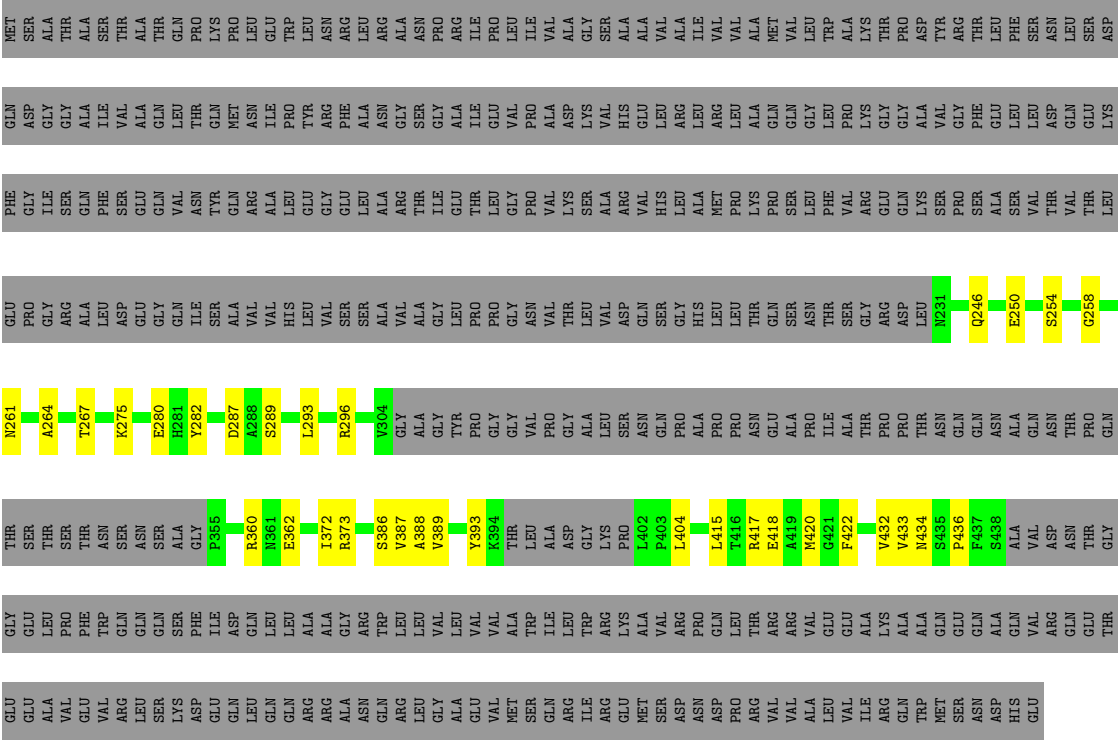






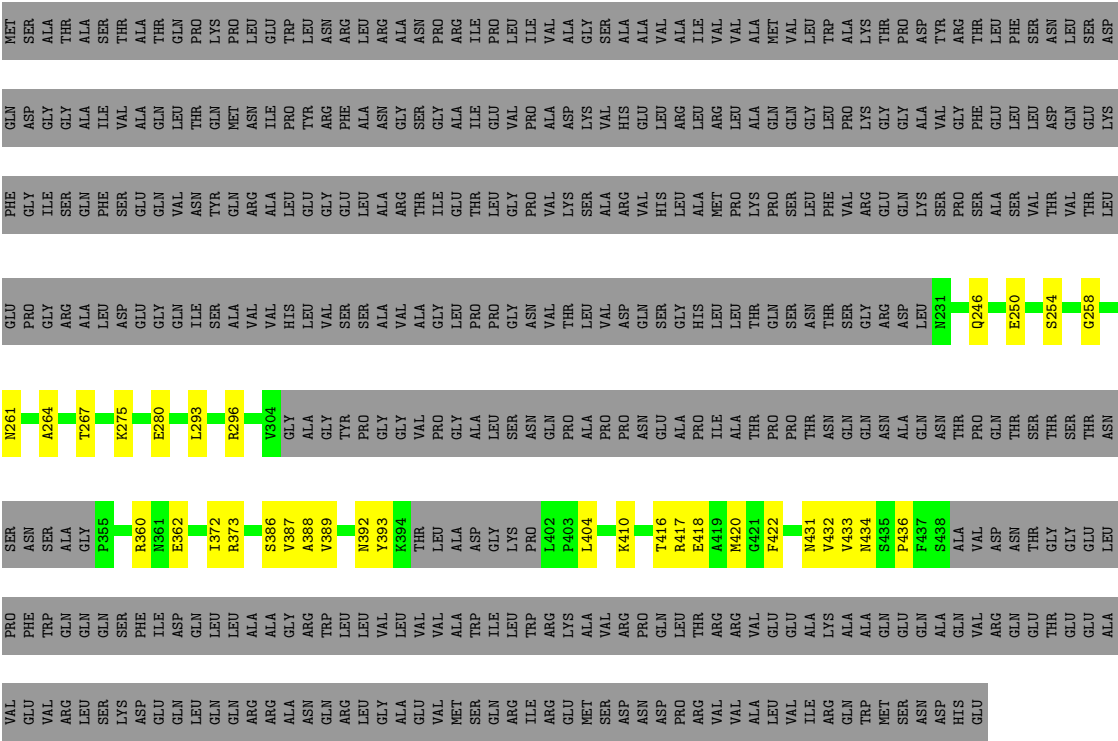
• Molecule 1: Flagellar M-ring protein

Chain I: 21% 6% 73%

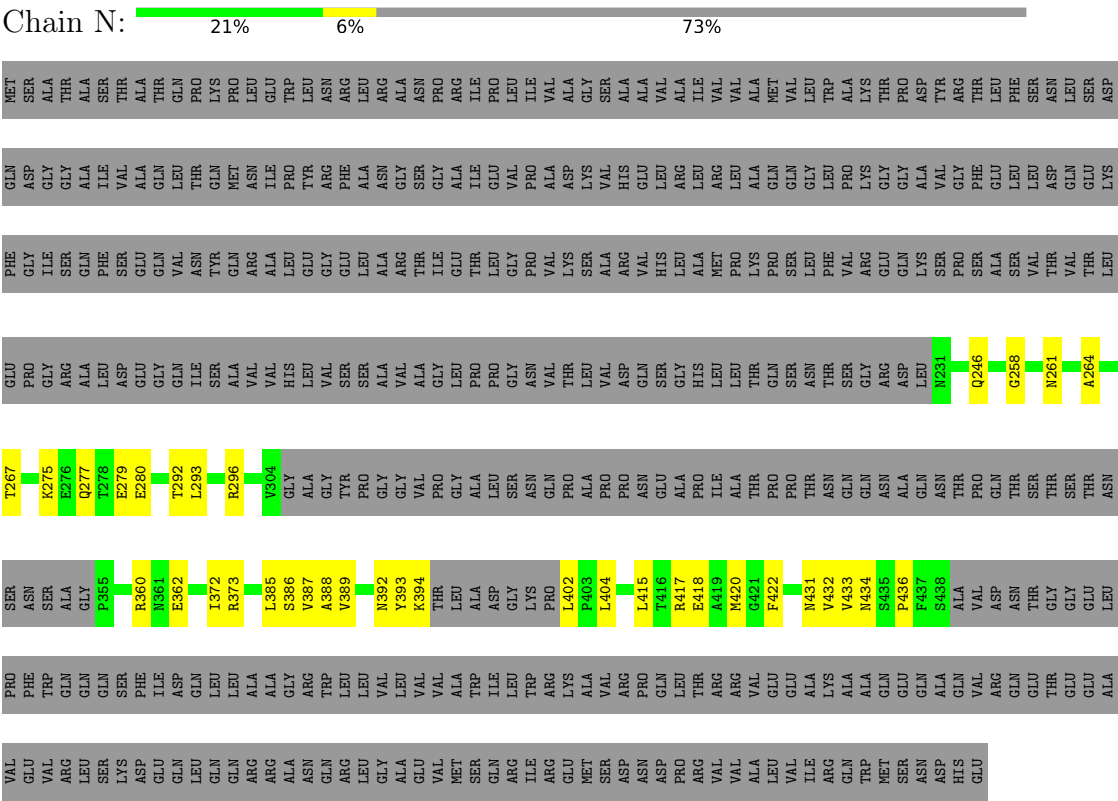


• Molecule 1: Flagellar M-ring protein

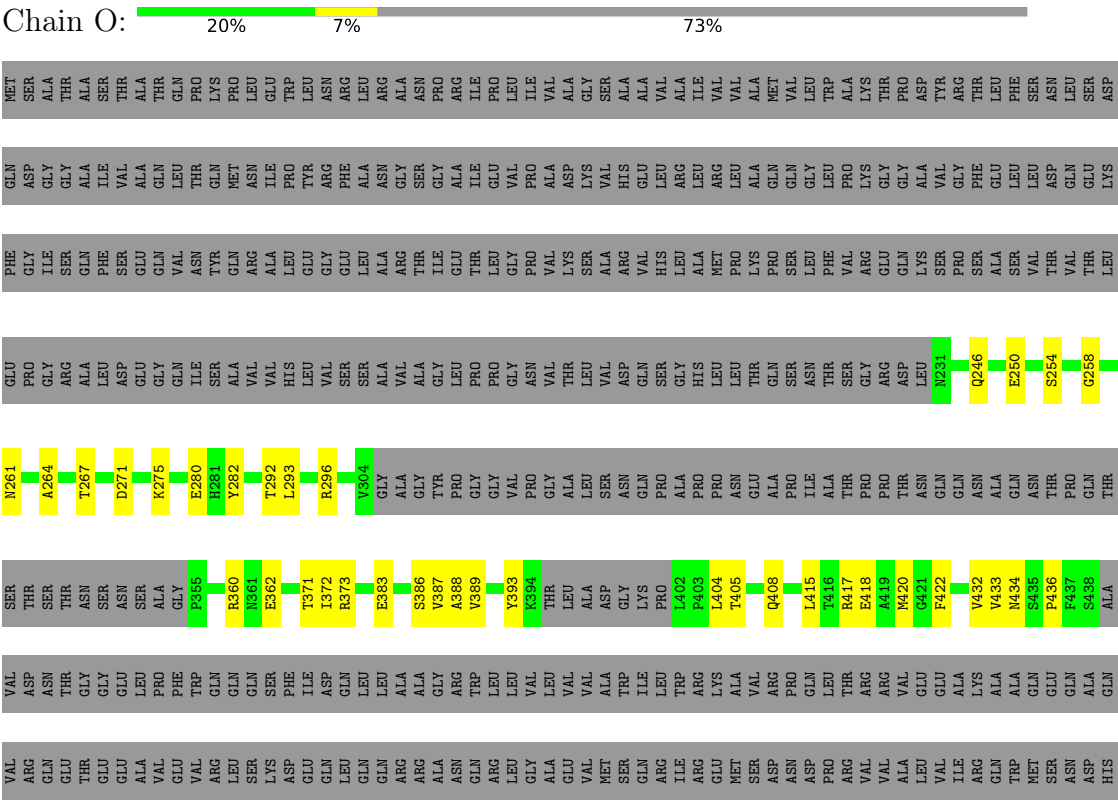
Chain J: 21% 6% 73%







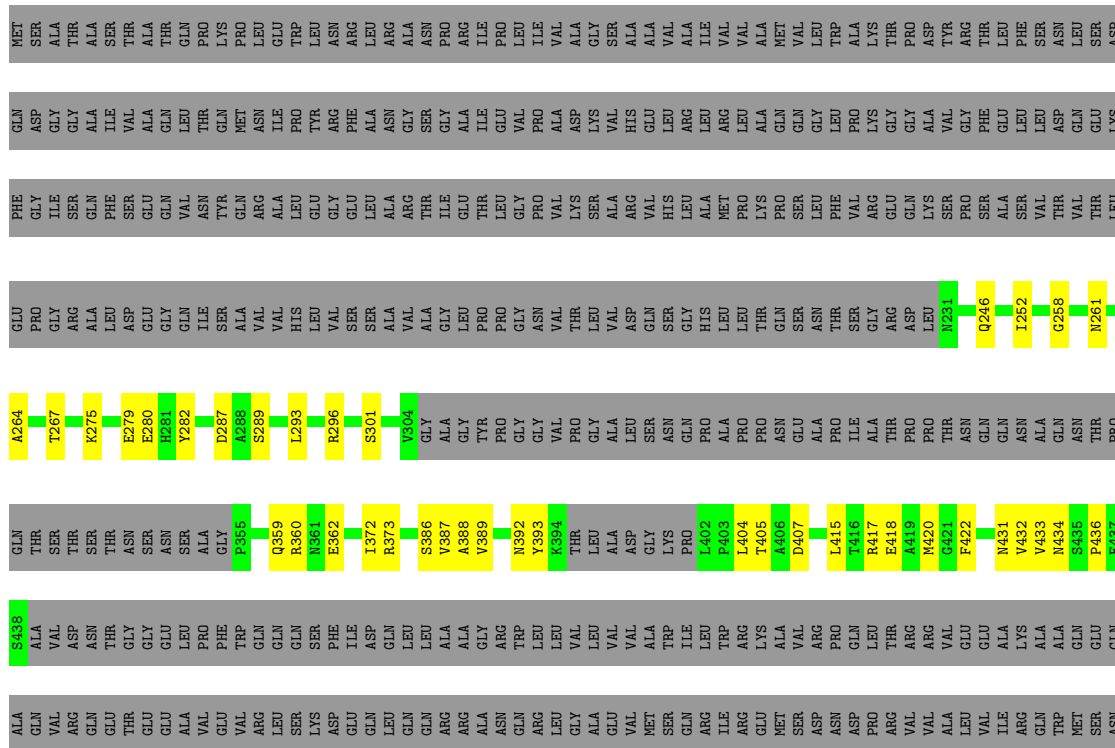
● Molecule 1: Flagellar M-ring protein



GLU


- Molecule 1: Flagellar M-ring protein

Chain P: 20% 7% 73%

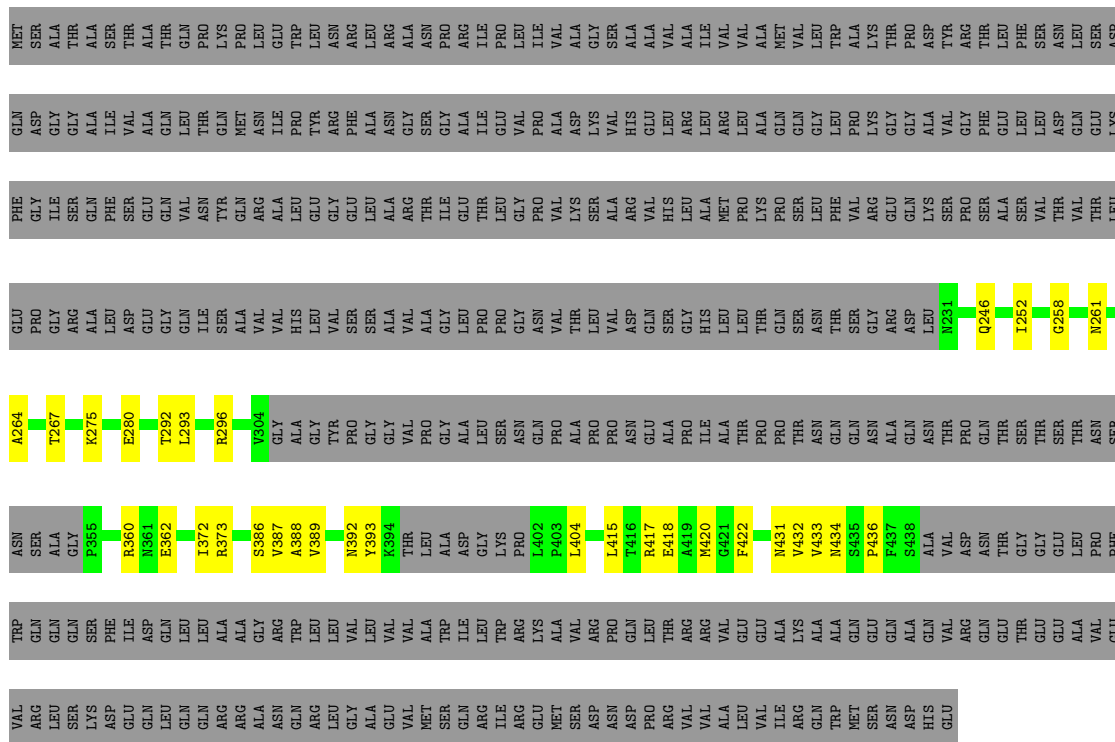


ASP

- Molecule 1: Flagellar M-ring protein

Chain Q:  21% 6% 73%





ASN	SER	ASN	SER	ALA	GLY	P365	R360	N361	E362	R373	S386	V387	A388	V389	N392	Y393	K394	THR	LEU	ALA	ASP	GLY	LYS	PRO	L402	P403	L404	L415	T416	R417	E418	A419	M420	G421	F422	N431	V432	V433	M434	S435	P436	F437	S438	ALA	VAL	ASP	ASN	THR	GLY	GLY	LEU	PRO
PHE	TRP	GLN	GLN	ALA	SER	PHE	ILE	ASP	LEU	ALA	ALA	GLY	ARG	TRP	LEU	VAL	VAL	VAL	TRP	TRP	ILE	LEU	TRP	ARG	LYS	ALA	VAL	ARG	PRO	GLN	LEU	THR	ARG	ARG	VAL	GLU	GLU	ALA	ALA	LYS	ALA	ALA	GLN	VAL	ARG	GLN	GLN	THR	GLY	GLY	ALA	VAL
GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	ARG	ALA	ASN	ARG	GLY	ALA	GLU	VAL	MET	SER	GLN	ARG	ILE	ARG	ILE	MET	SER	ASP	ASN	GLN	ARG	VAL	ILE	ALA	ARG	VAL	VAL	GLU	LEU	VAL	ILE	ARG	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU		

● Molecule 1: Flagellar M-ring protein

Chain T:			<div><div></div><div></div><div></div></div>										<div><div></div><div></div><div></div></div>																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
MET	GLN	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

● Molecule 1: Flagellar M-ring protein

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

● Molecule 1: Flagellar M-ring protein

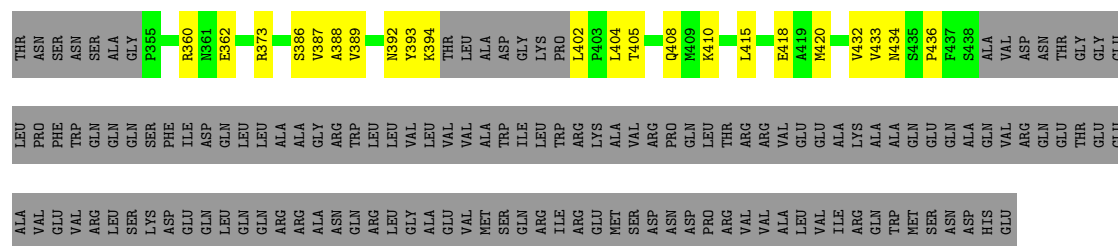


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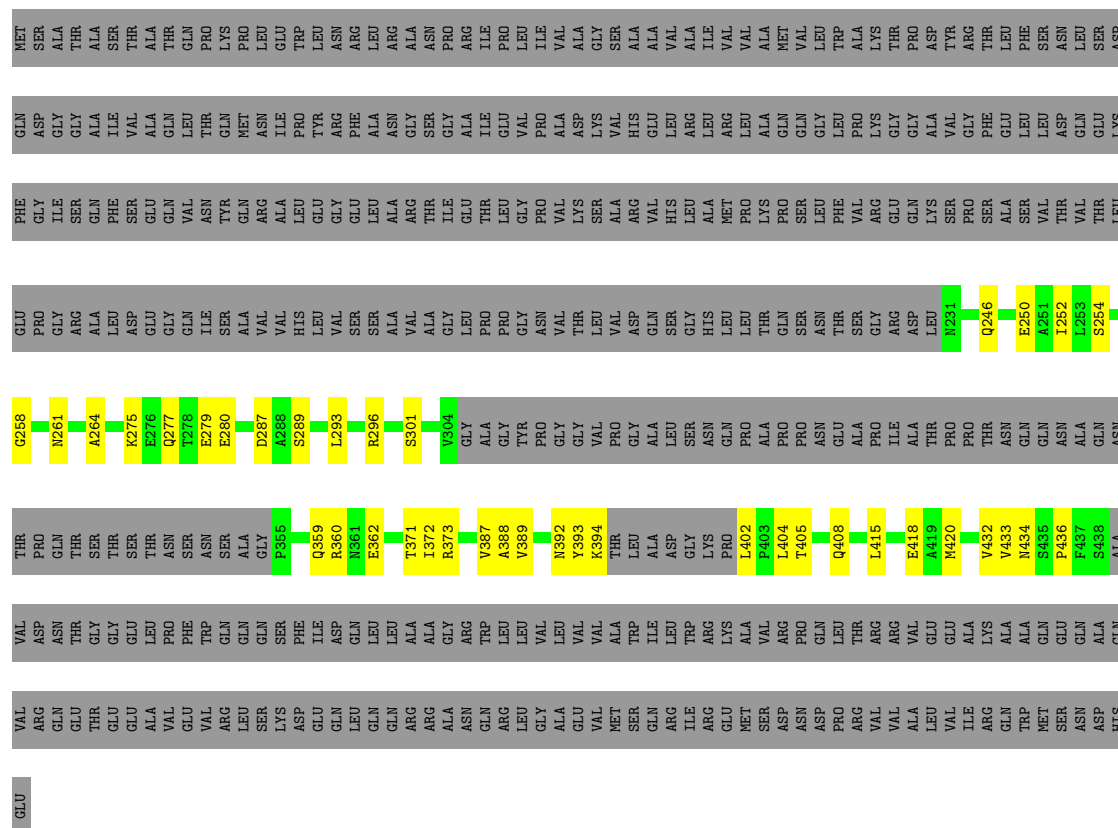
● Molecule 1: Flagellar M-ring protein



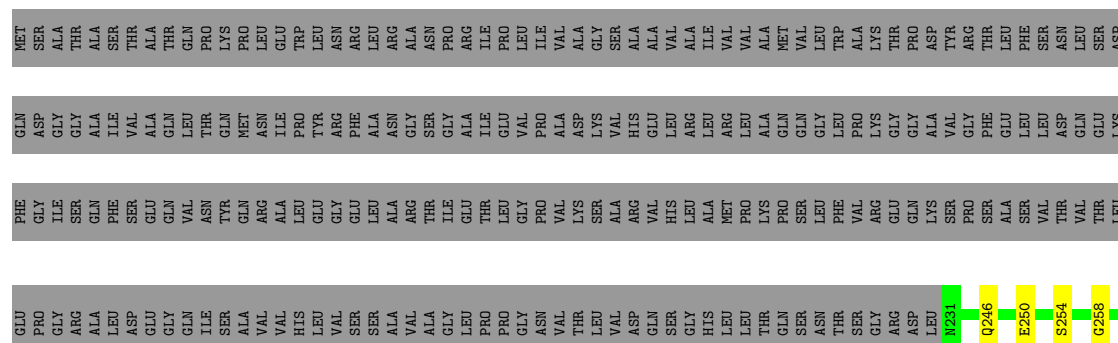
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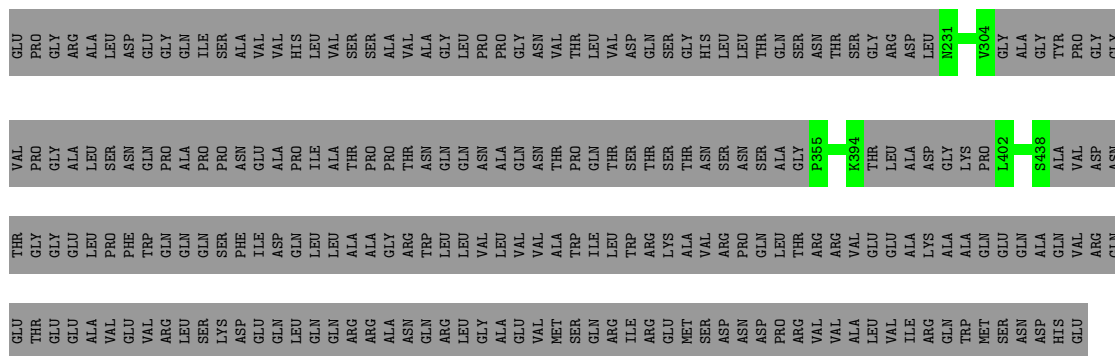
- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein







- Molecule 1: Flagellar M-ring protein

Chain b:  27% 73%



- Molecule 1: Flagellar M-ring protein

Chain c:  27% 73%



[illegible]

- Molecule 1: Flagellar M-ring protein

Chain d:  27% 73%

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

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

GLU	PRO	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	ALA	VAL	VAL	ASN	GLY	THR	VAL	VAL	THR	LEU	THR	VAL	ASP	GLN	SER	SER	GLY	HIS	LEU	LEU	THR	THR	SER	SER	GLY	ARG	ASP	LEU	M231	V046	GLY	ALA	GLY	Tyr	PRO	PRO	GLY
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THR	GLY	GLY	LEU	LEU	PRO	PHE	TRP	GLN	GLN	SER	PHE	ILE	ASP	GLN	LEU	LEU	ALA	ALA	GLY	ARG	TRP	LEU	VAL	VAL	VAL	ALA	TRP	ILE	LEU	TRP	LYS	ALA	VAL	ARG	PRO	GLN	LEU	THR	ARG	VAL	GLU	ALA	LYS	ALA	ALA	ALA	ALA	GLN	VAL	VAL	ARG	GLN
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GLU	THR	GLU	GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	GLN	GLN	GLN	ARG	ARG	ALA	ASN	GLN	GLN	GLU	VAL	VAL	MET	SER	GLN	ARG	ILE	ILE	ARG	ARG	GLU	MET	SER	ASP	ASN	ASP	ASP	PRO	ARG	VAL	VAL	ALA	ALA	LEU	VAL	ILE	ILE	ARG	GLN	TRP	TRP	MET	SER	ASN	ASP	HIS	GLU
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- Molecule 1: Flagellar M-ring protein

Chain e:  27% 73%

MET	SER	ALA	THR	ALA	SER	THR	ALA	THR	GLN	PRO	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ARG	LEU	ARG	ALA	ALA	ASN	PRO	ARG	ILE	PRO	PRO	ILE	ILE	VAL	GLY	GLY	SER	ALA	ALA	VAL	VAL	ALA	ALA	VAL	VAL	MET	VAL	LEU	LEU	TRP	THR	ALA	ALA	LYS	THR	ARG	THR	LEU	PHE	SER	ASN	LEU	LEU	SER	ASN	SER
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GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLU	GLY	GLN	ILE	SER	ALA	VAL	VAL	HIS	LEU	VAL	SER	SER	ALA	VAL	ALA	ALA	GLY	LEU	PRO	PRO	GLY	ASN	VAL	THR	THR	THR	CLN	SER	ASN	THR	SER	SER	GLY	ARG	ASP	LEU	M231	M230	GLY	ALA	GLY	Tyr	PRO	PRO	GLY	GLY
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[illegible]

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

GLU	THR	GLU	GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	GLN	GLN	GLN	ARG	ARG	ALA	ASN	GLN	ARG	GLN	LEU	GLY	ALA	GLU	VAL	VAL	SER	SER	GLN	ARG	ILE	ILE	ARG	GLU	MET	MET	ASP	ASP	ASN	ASP	PRO	ARG	VAL	VAL	ALA	ALA	LEU	VAL	ILE	ILE	ARG	GLN	TRP	MET	SER	SER	ASN	ASP	HIS	GLU
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- Molecule 1: Flagellar M-ring protein

Chain f:  27% 73%



- Molecule 1: Flagellar M-ring protein

Chain g: 27% 73%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C33	Depositor
Number of particles used	77849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/1205	0.42	0/1624
1	B	0.26	0/1205	0.42	0/1624
1	C	0.26	0/1205	0.42	0/1624
1	D	0.26	0/1205	0.42	0/1624
1	E	0.26	0/1205	0.43	0/1624
1	F	0.26	0/1205	0.43	0/1624
1	G	0.26	0/1205	0.42	0/1624
1	H	0.26	0/1205	0.42	0/1624
1	I	0.26	0/1205	0.42	0/1624
1	J	0.26	0/1205	0.42	0/1624
1	K	0.26	0/1205	0.42	0/1624
1	L	0.26	0/1205	0.43	0/1624
1	M	0.26	0/1205	0.42	0/1624
1	N	0.26	0/1205	0.42	0/1624
1	O	0.26	0/1205	0.42	0/1624
1	P	0.26	0/1205	0.42	0/1624
1	Q	0.26	0/1205	0.42	0/1624
1	R	0.26	0/1205	0.43	0/1624
1	S	0.26	0/1205	0.42	0/1624
1	T	0.26	0/1205	0.43	0/1624
1	U	0.26	0/1205	0.42	0/1624
1	V	0.26	0/1205	0.42	0/1624
1	W	0.26	0/1205	0.42	0/1624
1	X	0.26	0/1205	0.42	0/1624
1	Y	0.26	0/1205	0.42	0/1624
1	Z	0.26	0/1205	0.43	0/1624
1	a	0.26	0/1205	0.42	0/1624
1	b	0.26	0/1205	0.42	0/1624
1	c	0.26	0/1205	0.42	0/1624
1	d	0.26	0/1205	0.43	0/1624
1	e	0.26	0/1205	0.42	0/1624
1	f	0.26	0/1205	0.42	0/1624
1	g	0.26	0/1205	0.42	0/1624
All	All	0.26	0/39765	0.42	0/53592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1193	0	1173	29	0
1	B	1193	0	1173	29	0
1	C	1193	0	1173	26	0
1	D	1193	0	1173	25	0
1	E	1193	0	1173	26	0
1	F	1193	0	1173	26	0
1	G	1193	0	1173	32	0
1	H	1193	0	1173	26	0
1	I	1193	0	1173	23	0
1	J	1193	0	1173	24	0
1	K	1193	0	1173	22	0
1	L	1193	0	1173	24	0
1	M	1193	0	1173	26	0
1	N	1193	0	1173	25	0
1	O	1193	0	1173	26	0
1	P	1193	0	1173	27	0
1	Q	1193	0	1173	26	0
1	R	1193	0	1173	24	0
1	S	1193	0	1173	25	0
1	T	1193	0	1173	22	0
1	U	1193	0	1173	24	0
1	V	1193	0	1173	23	0
1	W	1193	0	1173	24	0
1	X	1193	0	1173	27	0
1	Y	1193	0	1173	27	0
1	Z	1193	0	1173	23	0
1	a	1193	0	1173	0	0
1	b	1193	0	1173	0	0
1	c	1193	0	1173	0	0
1	d	1193	0	1173	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	1193	0	1173	0	0
1	f	1193	0	1173	0	0
1	g	1193	0	1173	0	0
All	All	39369	0	38709	553	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 7.

The worst 5 of 553 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:Q:280:GLU:HG3	1:Q:372:ILE:HG12	1.80	0.64
1:B:250:GLU:O	1:B:254:SER:OG	2.15	0.63
1:H:360:ARG:NH1	1:H:362:GLU:OE1	2.31	0.63
1:P:405:THR:HG22	1:P:407:ASP:H	1.64	0.62
1:G:405:THR:HG22	1:G:407:ASP:H	1.64	0.61

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	B	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	C	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	D	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	E	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	F	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	G	145/560 (26%)	139 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	I	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	J	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	K	145/560 (26%)	136 (94%)	9 (6%)	0	100	100
1	L	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	M	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	N	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	O	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	P	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	Q	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	R	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	S	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	T	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	U	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	V	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	W	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	X	145/560 (26%)	137 (94%)	8 (6%)	0	100	100
1	Y	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	Z	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	a	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	b	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	c	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	d	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	e	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	f	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	g	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
All	All	4785/18480 (26%)	4579 (96%)	206 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/467 (29%)	134 (100%)	0	100	100
1	B	134/467 (29%)	134 (100%)	0	100	100
1	C	134/467 (29%)	134 (100%)	0	100	100
1	D	134/467 (29%)	134 (100%)	0	100	100
1	E	134/467 (29%)	134 (100%)	0	100	100
1	F	134/467 (29%)	134 (100%)	0	100	100
1	G	134/467 (29%)	134 (100%)	0	100	100
1	H	134/467 (29%)	134 (100%)	0	100	100
1	I	134/467 (29%)	134 (100%)	0	100	100
1	J	134/467 (29%)	134 (100%)	0	100	100
1	K	134/467 (29%)	134 (100%)	0	100	100
1	L	134/467 (29%)	134 (100%)	0	100	100
1	M	134/467 (29%)	134 (100%)	0	100	100
1	N	134/467 (29%)	134 (100%)	0	100	100
1	O	134/467 (29%)	134 (100%)	0	100	100
1	P	134/467 (29%)	134 (100%)	0	100	100
1	Q	134/467 (29%)	134 (100%)	0	100	100
1	R	134/467 (29%)	134 (100%)	0	100	100
1	S	134/467 (29%)	134 (100%)	0	100	100
1	T	134/467 (29%)	134 (100%)	0	100	100
1	U	134/467 (29%)	134 (100%)	0	100	100
1	V	134/467 (29%)	134 (100%)	0	100	100
1	W	134/467 (29%)	134 (100%)	0	100	100
1	X	134/467 (29%)	134 (100%)	0	100	100
1	Y	134/467 (29%)	134 (100%)	0	100	100
1	Z	134/467 (29%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	134/467 (29%)	134 (100%)	0	100	100
1	b	134/467 (29%)	134 (100%)	0	100	100
1	c	134/467 (29%)	134 (100%)	0	100	100
1	d	134/467 (29%)	134 (100%)	0	100	100
1	e	134/467 (29%)	134 (100%)	0	100	100
1	f	134/467 (29%)	134 (100%)	0	100	100
1	g	134/467 (29%)	134 (100%)	0	100	100
All	All	4422/15411 (29%)	4422 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	263	HIS
1	S	274	ASN
1	e	434	ASN
1	P	434	ASN
1	R	261	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.