



## Full wwPDB EM Validation Report ⓘ

Oct 14, 2025 – 05:41 PM JST

PDB ID : 8Z5V / pdb\_00008z5v  
EMDB ID : EMD-39783  
Title : Cryo-EM structure of the MS ring (C34) within the polar flagellar motor  
Authors : Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2024-04-18  
Resolution : 2.93 Å (reported)  
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

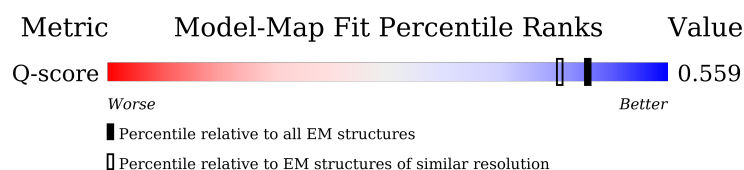
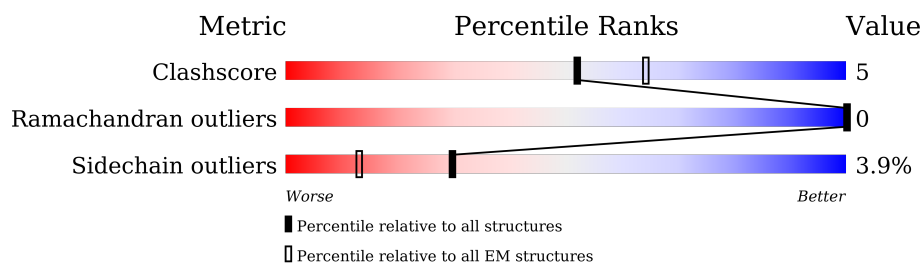
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.93 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.
















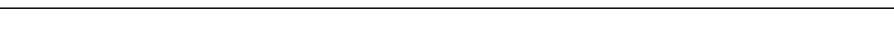
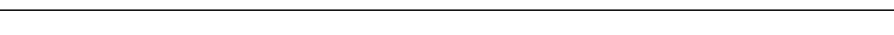
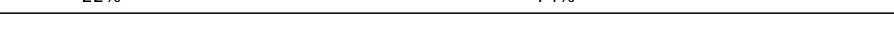

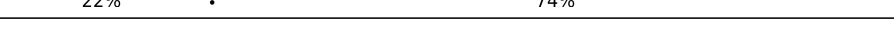







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13037 ( 2.43 - 3.43 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	580	
1	B	580	
1	C	580	
1	D	580	

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Mol	Chain	Length	Quality of chain
1	E	580	 22% . 74%
1	F	580	 22% . 74%
1	G	580	 22% . 74%
1	H	580	 22% . 74%
1	I	580	 22% . 74%
1	J	580	 22% . 74%
1	K	580	 22% . 74%
1	L	580	 22% . 74%
1	M	580	 22% . 74%
1	N	580	 22% . 74%
1	O	580	 22% . 74%
1	P	580	 22% . 74%
1	Q	580	 22% . 74%
1	R	580	 22% . 74%
1	S	580	 22% . 74%
1	T	580	 21% . 74%
1	U	580	 22% . 74%
1	V	580	 22% . 74%
1	W	580	 22% . 74%
1	X	580	 22% . 74%
1	Y	580	 22% . 74%
1	Z	580	 21% . 74%
1	a	580	 21% . 74%
1	b	580	 22% . 74%
1	c	580	 21% . 74%

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Mol	Chain	Length	Quality of chain
1	d	580	<div><div></div><div>21%</div><div></div><div>74%</div></div>
1	e	580	<div><div></div><div>22%</div><div></div><div>74%</div></div>
1	f	580	<div><div></div><div>21%</div><div></div><div>74%</div></div>
1	g	580	<div><div></div><div>21%</div><div></div><div>74%</div></div>
1	h	580	<div><div></div><div>21%</div><div></div><div>74%</div></div>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 39814 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	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	B	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	C	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	D	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	E	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	F	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	G	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	H	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	I	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	J	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	K	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	L	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	M	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	N	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	O	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	P	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	Q	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		

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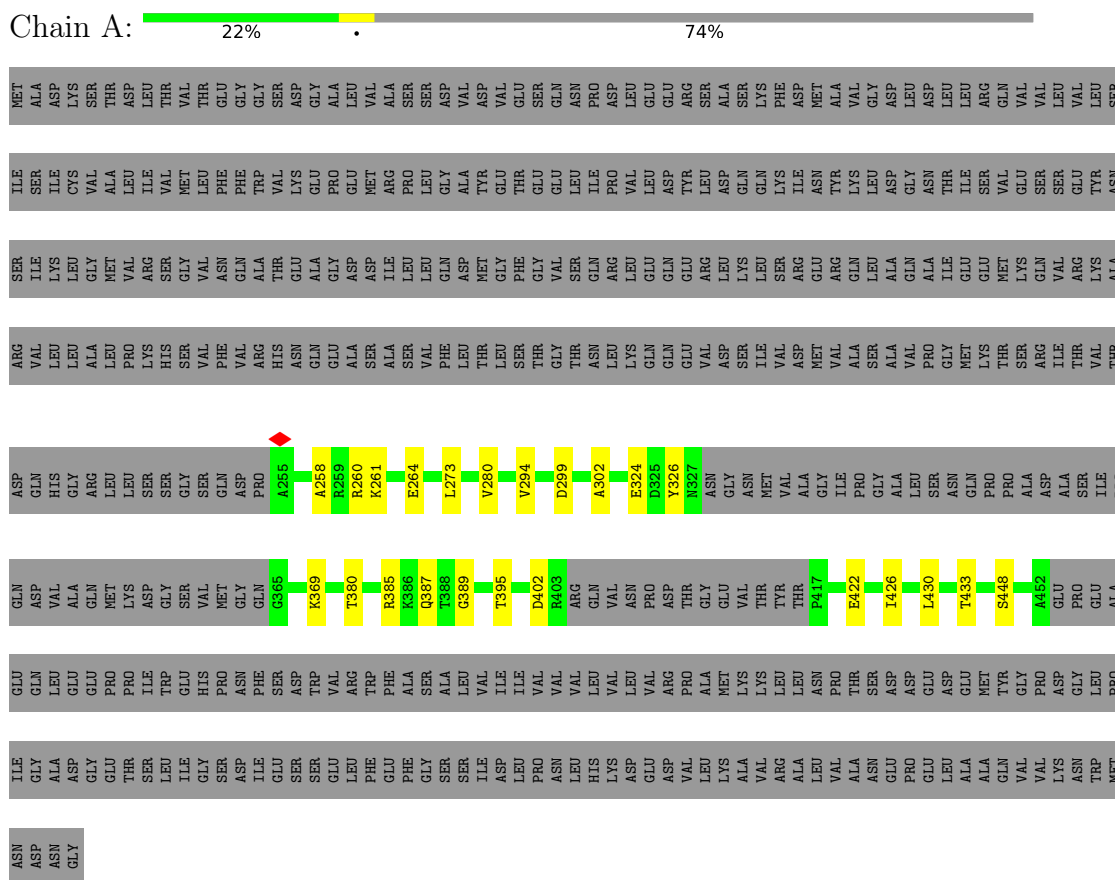
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	S	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	T	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	U	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	V	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	W	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	X	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	Y	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	Z	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	a	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	b	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	c	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	d	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	e	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	f	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	g	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		
1	h	148	Total	C	N	O	S	0	0
			1171	719	215	235	2		

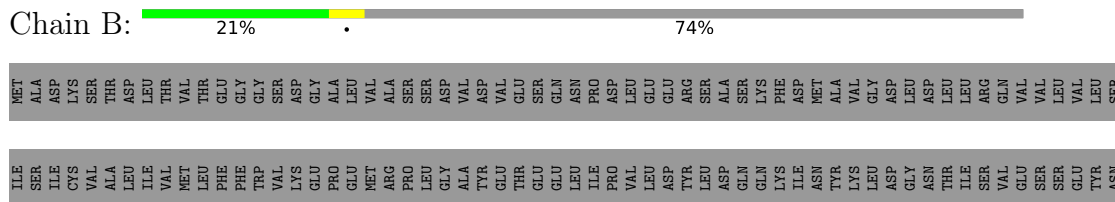
### 3 Residue-property plots

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

#### • Molecule 1: Flagellar M-ring protein



#### • Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein

[illegible]

- Molecule 1: Flagellar M-ring protein



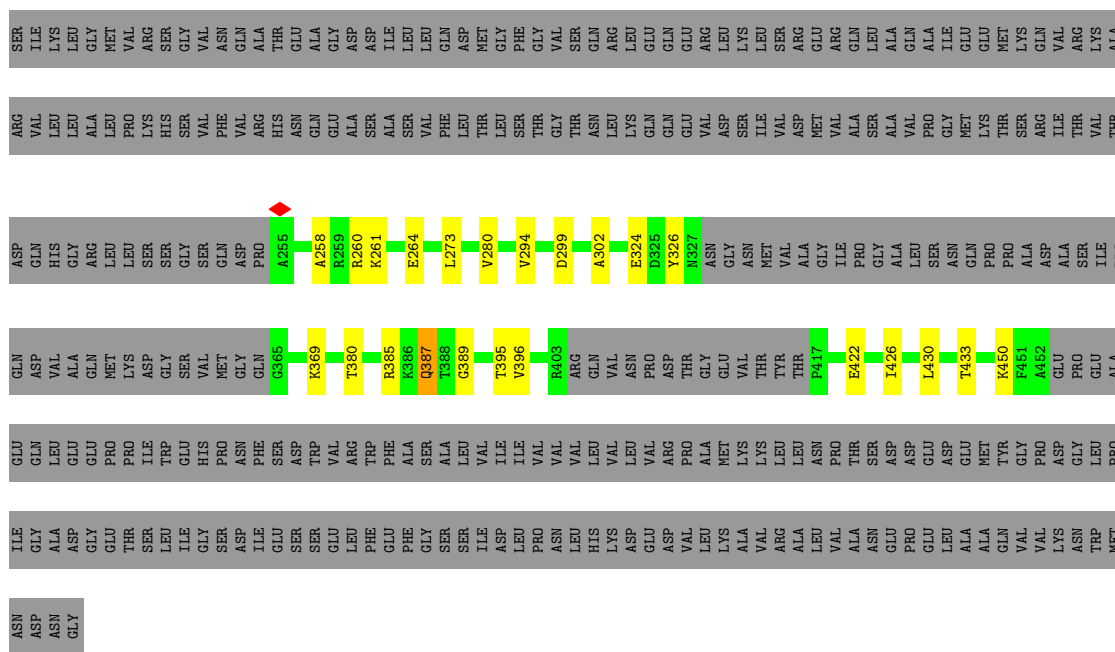




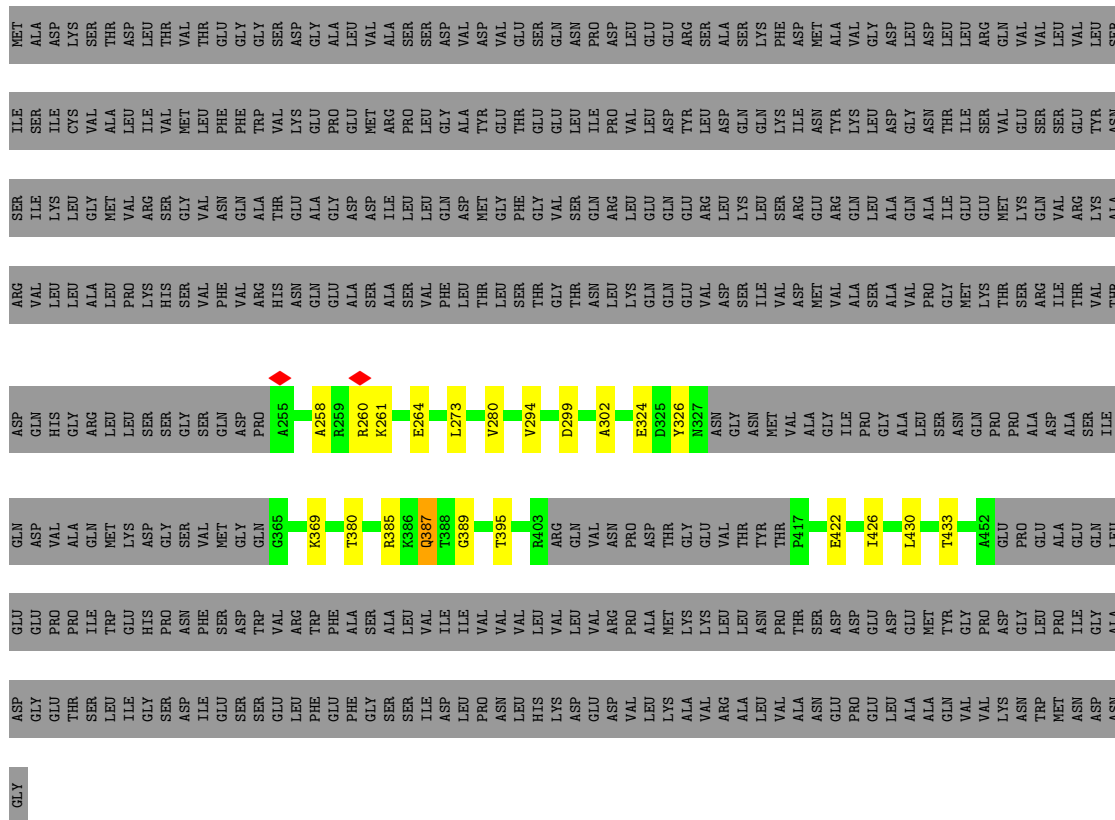
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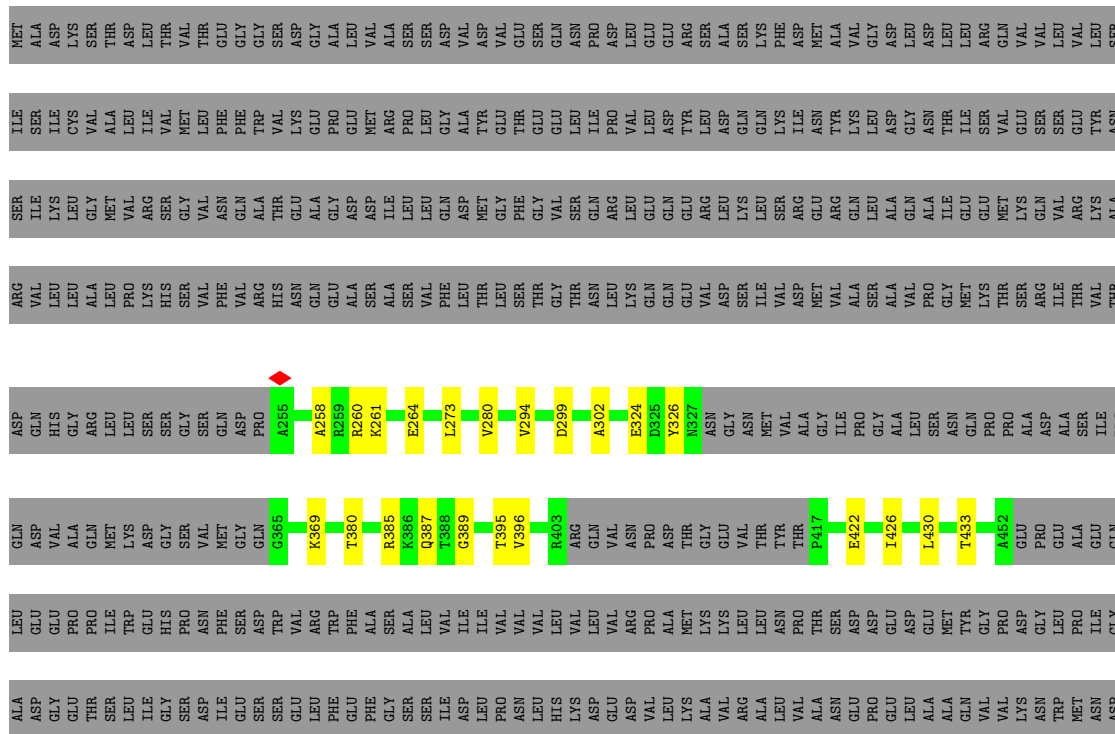


- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein





GLN	ASP	VAL	GLN	ASP	GLN	ASP	ARG	SER	ILE	FILE	MET
ASP	HIS	LEU	VAL	LEU	VAL	LEU	VAL	ILE	SER	SER	ALA
ALA	ARG	ALA	LEU	ALA	LEU	GLY	ALA	GLY	LEU	CYS	LYS
GLN	MET	MET	LEU	LEU	LEU	VAL	PRO	VAL	VAL	ALA	THR
LYS	ASP	LYS	PRO	LEU	PRO	VAL	VAL	VAL	ASP	LEU	ASP
ASP	GLY	HIS	SER	SER	SER	ARG	LYS	ARG	VAL	ILE	LEU
GLY	SER	SER	SER	GLY	SER	GLY	SER	GLY	VAL	VAL	THR
VAL	SER	VAL	VAL	SER	PHE	VAL	PHE	ASN	ASN	THR	THR
MET	MET	GLN	VAL	GLN	VAL	GLN	VAL	GLN	PHE	PHE	GLU
GLY	ASP	ASP	VAL	ASP	VAL	GLN	VAL	GLN	GLY	GLY	GLY
GLN	PRO	ARG	ARG	ARG	ARG	ASN	ASN	ALA	ALA	VAL	TRP
G365	A295	HIS	HIS	ASN	GLY	GLU	GLU	GLU	VAL	LYS	ASP
K369	A258	GLN	GLN	ALA	ALA	ALA	GLN	GLY	GLY	PRO	ALA
T380	R259	GLU	ALA	ALA	ALA	ALA	ALA	ASP	ASP	GLU	LEU
R385	R260	SER	SER	SER	ALA	ALA	ALA	ASP	ILE	ARG	VAL
K386	K261	SER	ALA	ALA	ALA	ALA	ALA	LEU	LEU	PRO	SER
Q387	E264	SER	VAL	VAL	VAL	VAL	PHE	LEU	LEU	LEU	ASP
T388	L273	LEU	LEU	LEU	LEU	LEU	GLN	GLN	GLY	ALA	VAL
G389	V280	THR	THR	THR	THR	THR	THR	MET	THR	THR	ASP
T395	V294	SER	SER	SER	SER	GLY	GLY	VAL	GLU	GLU	VAL
R403	D299	THR	THR	THR	THR	GLY	GLY	VAL	GLU	GLU	ASN
ARG	A302	VAL	ASN	ASN	ASN	ASN	ASN	GLN	ILE	ILE	PRO
GLN	VAL	VAL	LYS	LYS	LYS	LEU	LEU	ARG	PRO	VAL	ASP
ASN	ASP	ASP	ASP	ASP	GLN	GLN	GLN	GLU	LEU	VAL	LEU
PRO	E324	ASP	GLN	GLN	GLN	GLN	GLN	GLU	LEU	ASP	GLU
ASP	B325	GLN	GLN	GLN	GLN	GLN	GLN	GLU	GLU	THR	GLU
THR	Y326	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR	THR	ARG
GLY	R327	ASN	VAL	VAL	VAL	VAL	VAL	GLU	LEU	ASP	ASP
GLU	ASN	ASP	ASP	ASP	ASP	ASP	ASP	LEU	LEU	GLY	LEU
VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU	ALA	ASP	GLY
THR	ASN	ASN	SER	SER	SER	SER	ILE	LEU	GLN	ASP	GLY
THR	MET	MET	ILE	ILE	ILE	ILE	VAL	SER	GLN	THR	THR
THR	THR	THR	VAL	VAL	VAL	VAL	VAL	ARG	GLN	VAL	GLN
THR	P417	VAL	ASP	ASP	ASP	ASP	ASP	ARG	ASN	ILE	ASP
E422	E422	GLY	MET	MET	MET	MET	MET	GLY	THR	THR	THR
I426	I426	ILE	ILE	ILE	ILE	ILE	ALA	GLN	VAL	VAL	VAL
L430	L430	PRO	SER	SER	SER	SER	VAL	ALA	ALA	ASP	ASP
T433	T433	ASN	GLY	GLY	GLY	GLY	GLY	ILE	THR	THR	THR
A452	A452	GLN	MET	MET	MET	MET	MET	GLU	GLU	ILE	ILE
GLU	GLU	PRO	THR	THR	THR	THR	THR	MET	VAL	VAL	ARG
PRO	PRO	ALA	SER	SER	SER	SER	SER	LYS	GLU	GLU	GLN
GLU	GLU	ASP	ARG	ARG	ARG	ARG	ARG	GLN	THR	THR	VAL
ALA	ALA	ALA	ILE	ILE	ILE	ILE	ILE	VAL	SER	SER	VAL
GLU	GLU	SER	THR	THR	THR	THR	THR	ARG	GLU	GLU	VAL
GLN	GLN	ILE	VAL	VAL	VAL	VAL	VAL	LYS	THR	THR	SER
LEU	LEU	THR	THR	THR	THR	THR	THR	ALA	ASN	ASN	THR

[illegible]

- Molecule 1: Flagellar M-ring protein

Chain Q:  22% 1% 77%

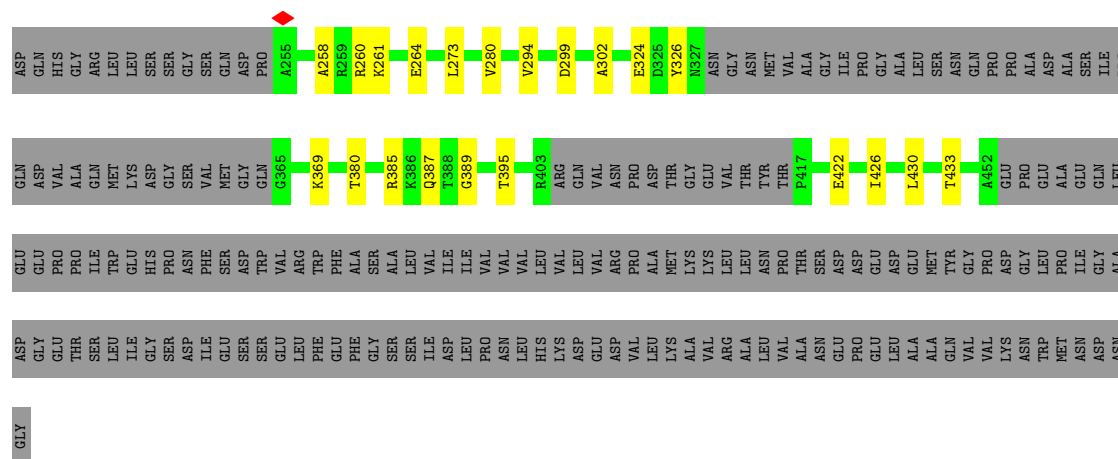
[illegible]

- Molecule 1: Flagellar M-ring protein

Chain R:  22% 1% 77%

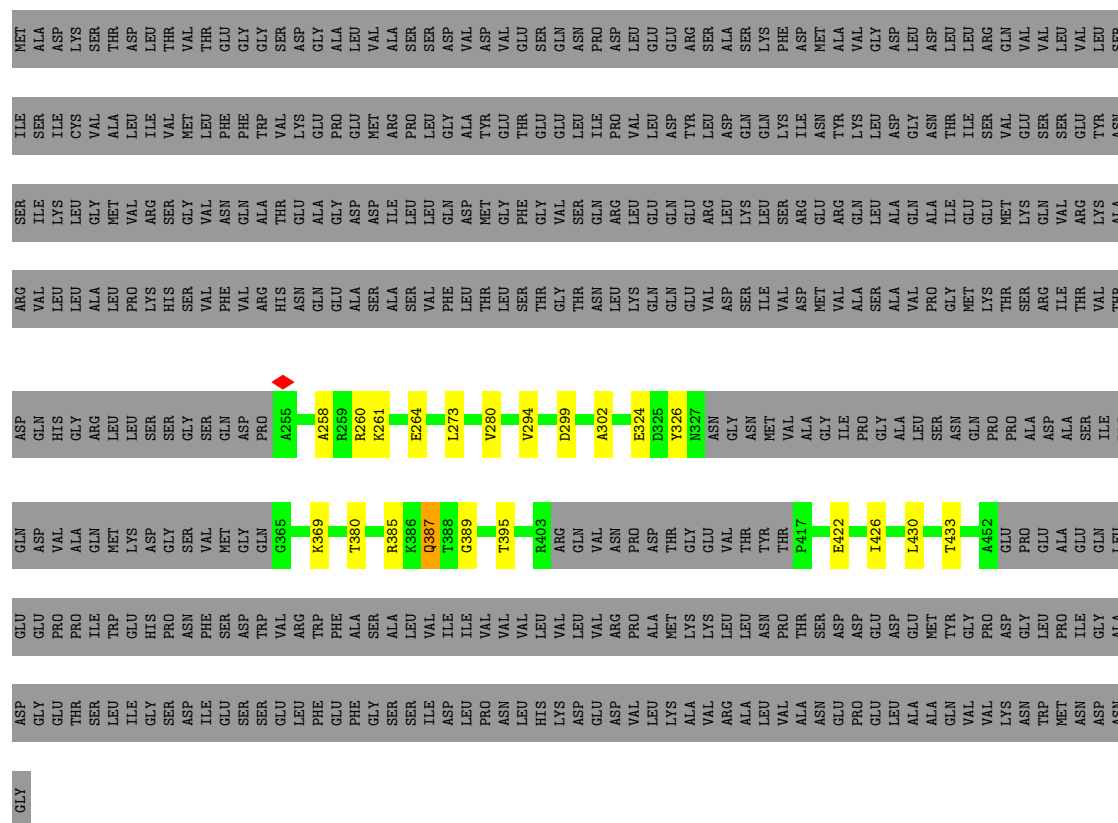
ARG	VAL	VAL	ARG	SER	ILE	ILE	MET
LEU	LEU	LEU	LYS	ILE	SER	SER	ALA
LEU	LEU	LEU	LEU	LYS	ILE	ASP	ASP
LEU	ALA	ALA	GLY	VAL	CYS	LYS	SER
PRO	VAL	VAL	MET	VAL	ALA	THR	THR
LYS	ARG	VAL	VAL	VAL	LEU	ASP	ASP
HIS	HIS	THR	ARG	ARG	ILE	LEU	LEU
SER	SER	THR	GLY	GLY	MET	THR	THR
VAL	VAL	VAL	VAL	VAL	LEU	THR	THR
PHE	PHE	ASN	ASN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





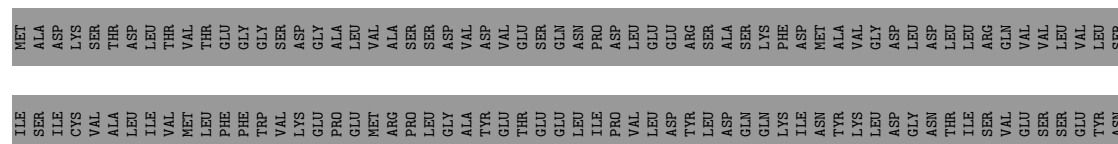
- Molecule 1: Flagellar M-ring protein

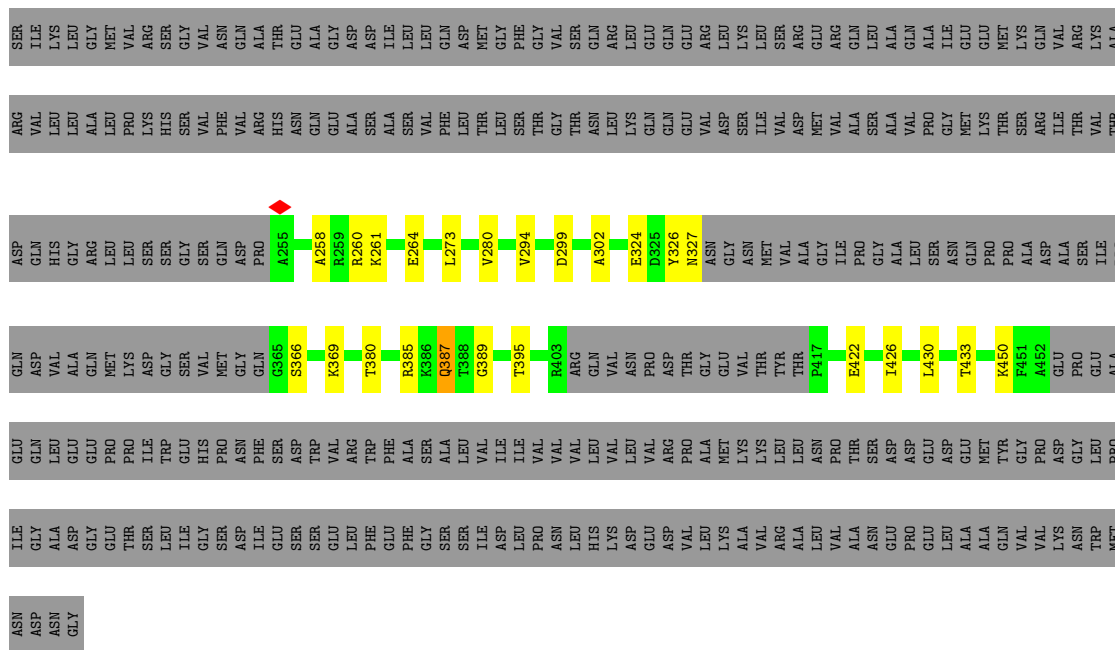
Chain S:  22% . 74%



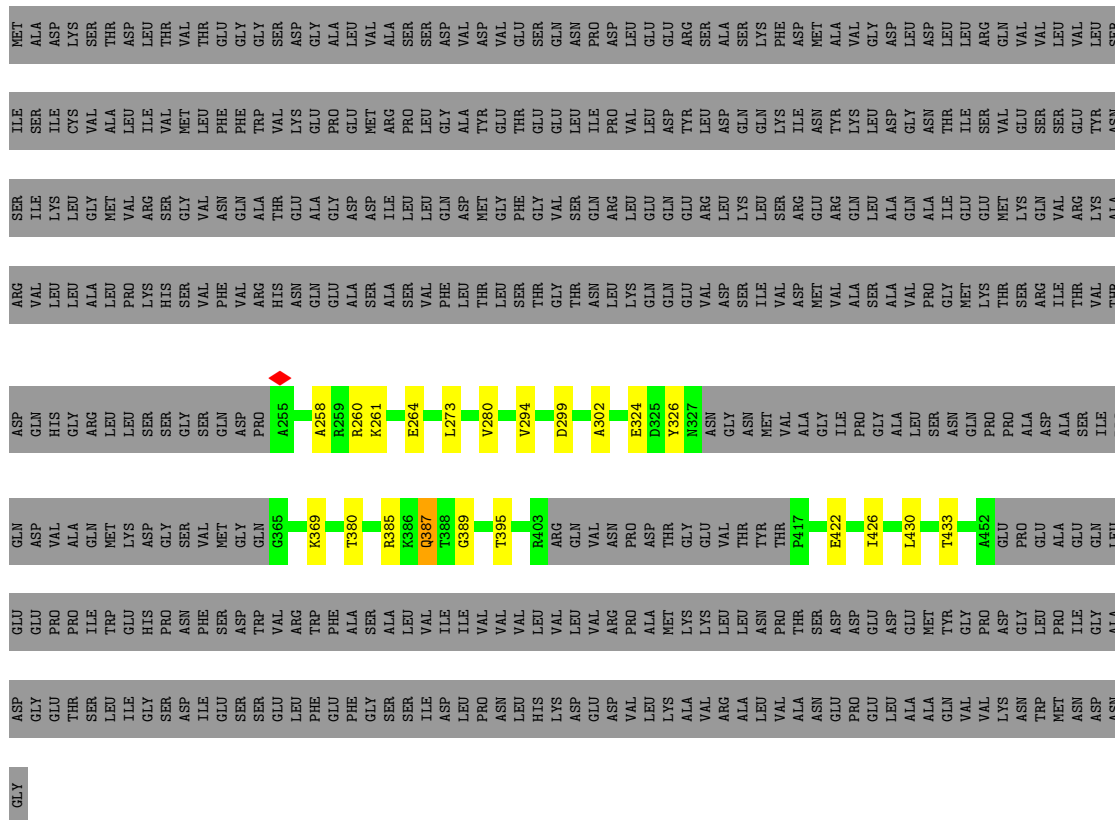
- Molecule 1: Flagellar M-ring protein

Chain T:  21% . 74%





- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein



[illegible]

- Molecule 1: Flagellar M-ring protein

Chain W:  22% . 74%

ASP	GLU	GLN	ASP	ARG	SER	ILE	MET
GLY	GLU	ASP	GLN	VAL	ILE	SER	ALA
THR	PRO	VAL	HIS	LEU	LEU	LYS	ASP
SER	ILE	GLN	ARG	ALA	GLY	CYS	LYS
LEU	TRP	MET	LEU	LEU	MET	ALA	THR
ILE	GLU	LYS	LEU	PRO	VAL	LEU	ASP
GLY	HIS	ASP	SER	LYS	ARG	ILE	LEU
SER	PRO	GLY	SER	HIS	SER	VAL	LEU
ASN	PHE	SER	GLY	SER	GLY	MET	VAL
ILE	GLU	VAL	SER	VAL	ASN	LEU	THR
GLU	SER	MET	GLN	PHE	VAL	PHE	GLY
SER	ASP	GLY	ASP	VAL	GLN	TRP	GLY
TRP	TRP	GLN	PRO	ARG	ALA	GLY	SER
VAL	VAL	GLN	ASP	HIS	THR	VAL	GLY
ARG	ARG	ASP	A255	HIS	THR	LYS	ASP
TRP	PHE	K369	A258	GLN	ALA	GLY	GLY
ALA	ALA	T380	R259	ALA	ASP	PRO	ALA
PHE	GLY	SER	R260	SER	ASP	GLU	GLY
SER	SER	ALA	K261	ALA	ASP	GLY	GLY
SER	SER	LEU	K386	VAL	LEU	ARG	GLY
ILE	VAL	LEU	K387	VAL	LEU	ILE	SER
ASP	ILE	ILE	T388	PHE	GLN	GLY	SER
LEU	VAL	VAL	G389	LEU	ASP	ALA	ASP
PRO	VAL	VAL	T395	THR	MET	ALA	VAL
ASN	VAL	VAL	T396	LEU	GLY	THR	VAL
HIS	LEU	VAL	R403	THR	VAL	GLU	SER
LYS	VAL	ARG	D299	GLY	VAL	GLU	GLN
ASP	LEU	GLN	A302	THR	SER	LEU	ASN
GLU	VAL	VAL	ASN	ASN	GLN	ILE	PRO
ASP	ARG	ASP	ASN	LEU	ARG	PRO	ASP
LEU	PRO	PRO	E324	LYS	LEU	VAL	LEU
ALA	ALA	ALA	D325	GLN	GLY	VAL	GLY
LYS	MET	THR	Y326	GLN	GLN	LEU	GLU
ALA	LYS	GLY	N327	GLU	ASP	ASP	ARG
VAL	VAL	GLU	ASN	VAL	LEU	LEU	SER
ARG	LEU	VAL	GLY	ASP	LEU	ALA	GLY
ALA	LEU	THR	ASN	SER	LEU	GLN	LYS
LEU	ASN	THR	MET	ILE	LEU	LYS	SER
VAL	PRO	THR	VAL	VAL	SER	PHE	ASP
ALA	THR	P417	VAL	ASP	ARG	ILE	ASP
ASN	SER	GLY	ALA	MET	GLY	ASN	MET
GLU	ASP	E422	GLY	VAL	ARG	VAL	GLY
PRO	ASP	ASP	ILE	ALA	GLN	LYS	VAL
GLU	GLU	I426	PRO	SER	LEU	GLY	GLY
LEU	ASP	ALA	GLY	ALA	ALA	ASP	ASP
ALA	GLU	L430	LEU	VAL	GLN	LEU	LEU
GLN	MET	T433	SER	PRO	ALA	ASN	ASP
VAL	GLY	GLY	ASN	GLY	ILE	LEU	LEU
VAL	PRO	A452	GLN	MET	GLU	ILE	ARG
LYS	ASP	GLU	PRO	THR	MET	VAL	GLN
ASN	GLY	PRO	PRO	SER	GLY	GLY	VAL
TRP	LEU	GLU	ALA	ARG	GLN	ASP	VAL
MET	PRO	ALA	ASP	ILE	VAL	SER	VAL
ASN	ILE	GLU	SER	THR	ARG	LEU	VAL
GLY	GLY	LEU	ILE	VAL	LYS	GLY	VAL
ALA	ALA	THR	ILE	THR	ALA	THR	SER

[illegible]

	ASN GLY	ALA ASP GLY GLU THR SER LEU ILE GLY SER ASP TLE GLJ PHE PHE SER SER TLE ASP LEU PRO VAL VAL LEU HIS LYS ASP GLJ ASP VAL LEU LYS ALA VAL ARG ALA LEU VAL ALA GLN GLU PRO GLJ LEU ALA GLN VAL VAL LYS ASN TRP MET ASN ASP	LEU GLJ PRO PRO TIE TRP GLJ HIS PRO ASN PHE SER ASP TRP VAL VAL ARG TRP PHE ALA SER ALA LEU VAL TIE TIE VAL VAL VAL LEU VAL LEU VAL ARG PRO ALA MET LYS LYS LEU LEU ASN PHO THR SER ASP ASP GLJ ASP GLY MET TYR GLY PRO ASP GLY MET GLY PRO GLY LEU PRO TIE GLY ASP
--	------------	--	---

- Molecule 1: Flagellar M-ring protein

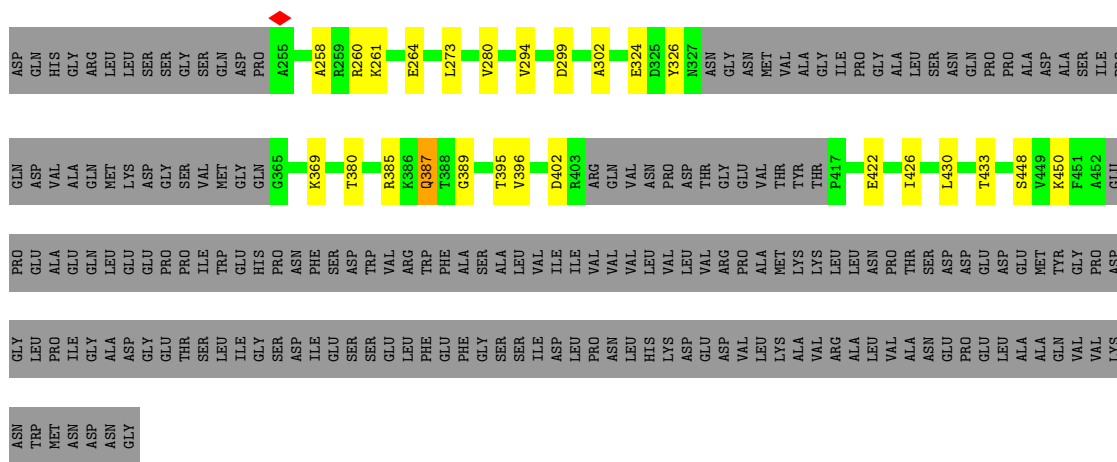
Chain Z:  21% . 74%

[illegible]

- Molecule 1: Flagellar M-ring protein

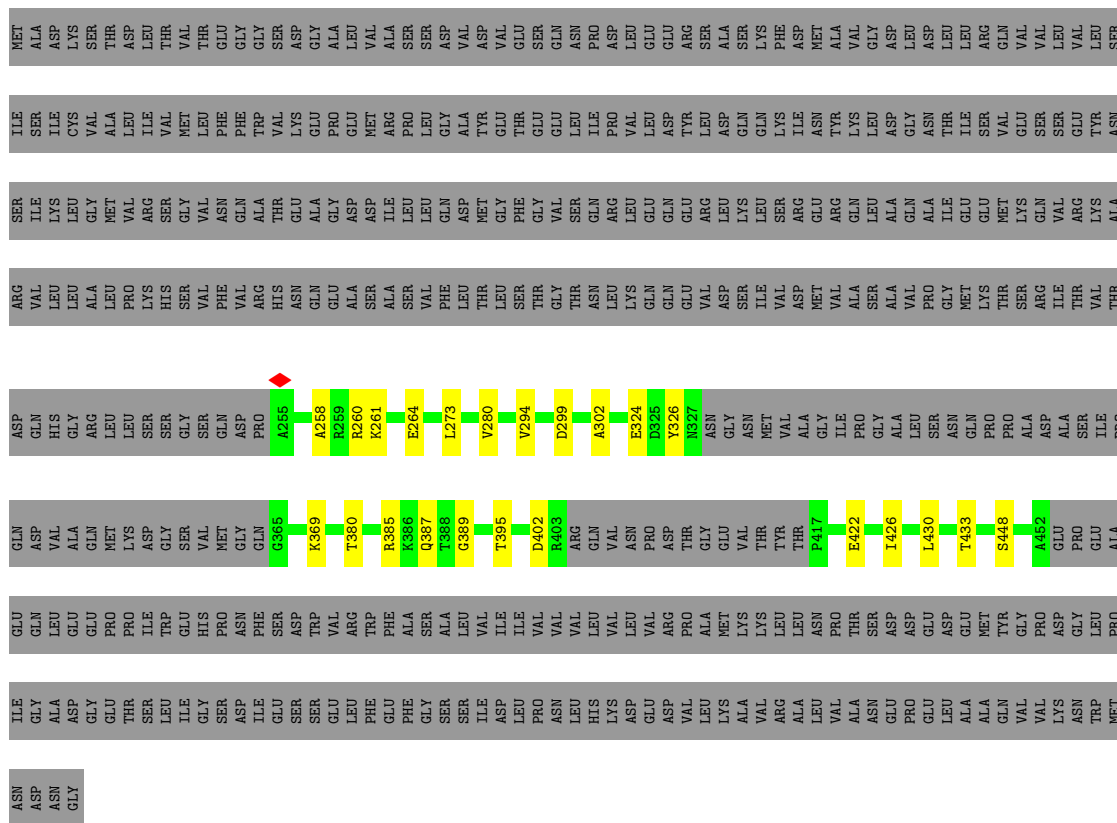
Chain a:  21% . 74%

[illegible]



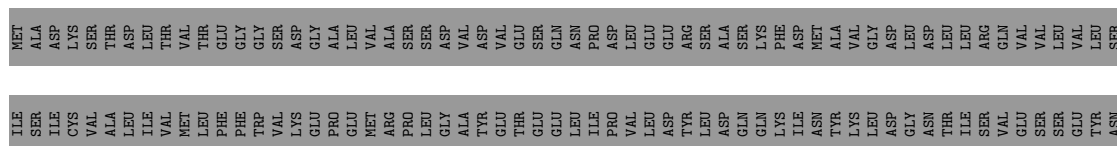
- Molecule 1: Flagellar M-ring protein

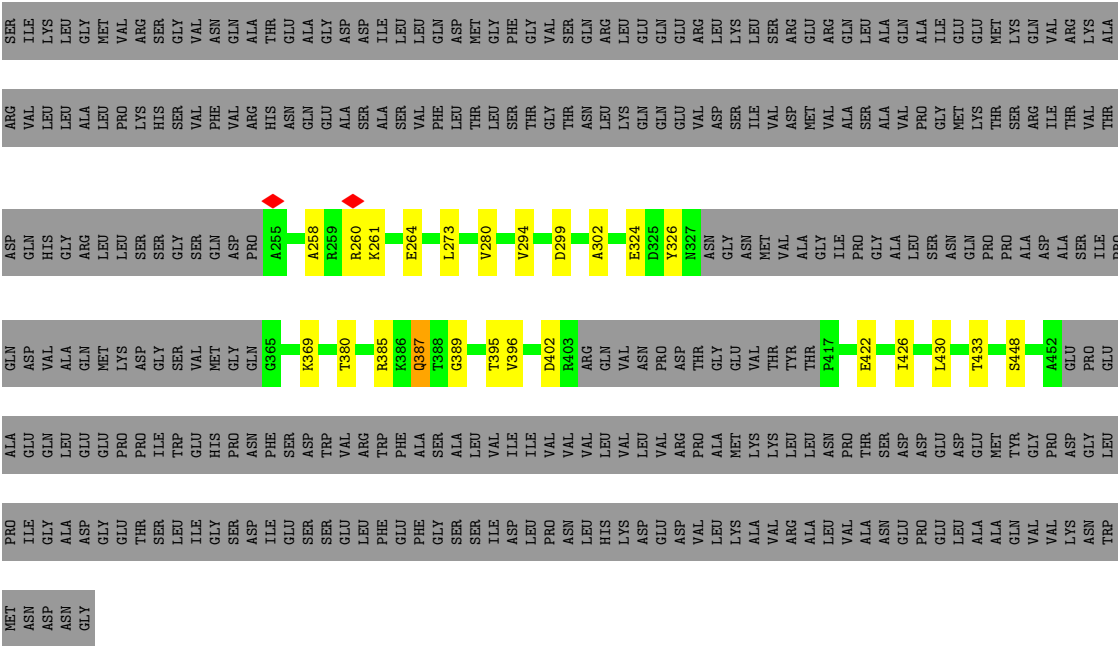
Chain b:  22% 1% 74%



- Molecule 1: Flagellar M-ring protein

Chain c:  21% . 74%





• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein







GLN	ASP	GLN	ASP	ASP	GLN	ASP	ARG	SER	ILE	ILE	MET
ASP	VAL	VAL	VAL	HIS	GLY	HIS	VAL	ILE	SER	ILE	ALA
VAL	GLN	ALA	GLY	ARG	GLN	ARG	ALA	GLY	CYS	VAL	LYS
MET	MET	LEU	LEU	LEU	LEU	LEU	PRO	MET	ALA	THR	THR
LYS	ASP	SER	SER	SER	LEU	SER	LYS	ARG	LEU	LEU	ASP
ASP	GLY	SER	SER	GLY	GLY	SER	HIS	SER	VAL	THR	THR
GLY	MET	SER	SER	GLY	GLN	SER	PHE	VAL	LEU	THR	GLU
GLN	ASP	ASP	VAL	GLN	ASP	ASP	VAL	GLN	PHE	GLY	GLY
G385	A255	A255	ARG	HIS	THR	THR	ASN	THR	VAL	VAL	SER
K369	A258	A258	GLN	ASN	GLY	GLY	GLN	GLY	GLY	GLY	ASP
T380	R259	R259	ALA	ALA	ALA	ALA	ALA	ASP	PRO	GLU	ALA
R386	R260	R260	SER	SER	SER	SER	SER	ASP	GLY	PRO	GLY
Q387	E264	E264	ALA	ALA	ALA	ALA	ALA	ILE	ARG	ALA	ALA
T388	L273	L273	PHE	PHE	PHE	PHE	PHE	GLN	GLN	LYS	VAL
G389	V280	V280	LEU	LEU	THR	THR	THR	ASP	ALA	GLY	VAL
T395	V294	V294	LEU	LEU	LEU	LEU	LEU	MET	TYR	TYR	ASP
D402	D299	D299	THR	THR	GLY	THR	THR	SER	LEU	ASN	ASN
R403	A302	A302	ASN	ASN	THR	THR	ASN	GLN	ILE	PRO	PRO
ARG	E324	E324	LYS	LYS	LYS	LYS	LYS	GLN	VAL	ASP	ASP
GLN	R325	R325	GLN	GLN	GLN	GLN	GLN	GLY	VAL	LEU	LEU
ASN	Y326	Y326	GLN	GLN	GLN	GLN	GLN	GLY	ASP	GLY	GLY
PRO	R327	R327	GLU	GLU	GLU	GLU	GLU	ARG	TYR	ARG	ARG
ASP	ASN	ASN	VAL	VAL	VAL	VAL	VAL	ARG	LEU	SER	SER
THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ALA	ALA
GLY	ASN	ASN	GLY	GLY	GLY	GLY	GLY	LYS	GLN	LYS	LYS
GLU	ASN	ASN	SER	SER	SER	SER	ILE	SER	ILE	PHE	PHE
VAL	ASN	ASN	THR	THR	THR	THR	THR	ARG	ASP	ASP	ASP
THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ARG	ILE	ILE	ILE
THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ARG	ASP	ASP	ASP
P417	ILE	ILE	PRO	PRO	PRO	PRO	PRO	GLY	TYR	TYR	TYR
E422	E422	E422	GLY	GLY	GLY	GLY	GLY	ILE	LYS	LYS	LYS
I426	GLY	GLY	SER	SER	SER	SER	SER	LEU	LEU	LEU	LEU
L430	ALA	ALA	VAL	VAL	VAL	VAL	VAL	GLN	ASP	ASP	ASP
T433	ASN	ASN	GLN	GLN	GLN	GLN	GLN	ILE	ASN	ASN	ASN
S448	PRO	PRO	THR	THR	THR	THR	THR	GLY	VAL	VAL	VAL
V449	ASP	ASP	ALA	ALA	ALA	ALA	ALA	GLY	GLY	GLY	GLY
K450	ALA	ALA	ARG	ARG	ARG	ARG	ARG	THR	THR	THR	THR
F451	ALA	ALA	ILE	ILE	ILE	ILE	ILE	GLY	GLY	GLY	GLY
A452	SER	SER	THR	THR	THR	THR	THR	ARG	GLY	GLY	GLY
GLU	ILE	ILE	THR	THR	THR	THR	THR	LYS	TYR	TYR	TYR
PRO	ALA	ALA	VAL	VAL	VAL	VAL	VAL	ALA	ASN	ASN	ASN

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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	58418	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 ( $e^-/\text{\AA}^2$ )	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	3.077	Depositor
Minimum map value	-1.858	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0.16	0/1182	0.27	0/1588
1	B	0.16	0/1182	0.27	0/1588
1	C	0.16	0/1182	0.27	0/1588
1	D	0.16	0/1182	0.27	0/1588
1	E	0.16	0/1182	0.27	0/1588
1	F	0.16	0/1182	0.27	0/1588
1	G	0.16	0/1182	0.27	0/1588
1	H	0.16	0/1182	0.27	0/1588
1	I	0.16	0/1182	0.27	0/1588
1	J	0.16	0/1182	0.27	0/1588
1	K	0.16	0/1182	0.27	0/1588
1	L	0.16	0/1182	0.27	0/1588
1	M	0.16	0/1182	0.27	0/1588
1	N	0.16	0/1182	0.27	0/1588
1	O	0.16	0/1182	0.27	0/1588
1	P	0.16	0/1182	0.27	0/1588
1	Q	0.16	0/1182	0.27	0/1588
1	R	0.16	0/1182	0.27	0/1588
1	S	0.16	0/1182	0.27	0/1588
1	T	0.16	0/1182	0.27	0/1588
1	U	0.16	0/1182	0.27	0/1588
1	V	0.16	0/1182	0.27	0/1588
1	W	0.16	0/1182	0.27	0/1588
1	X	0.16	0/1182	0.27	0/1588
1	Y	0.16	0/1182	0.27	0/1588
1	Z	0.16	0/1182	0.27	0/1588
1	a	0.16	0/1182	0.27	0/1588
1	b	0.16	0/1182	0.27	0/1588
1	c	0.16	0/1182	0.27	0/1588
1	d	0.16	0/1182	0.27	0/1588
1	e	0.16	0/1182	0.27	0/1588
1	f	0.16	0/1182	0.27	0/1588
1	g	0.16	0/1182	0.27	0/1588
1	h	0.16	0/1182	0.27	0/1588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.16	0/40188	0.27	0/53992

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	1171	0	1164	12	0
1	B	1171	0	1164	15	0
1	C	1171	0	1164	12	0
1	D	1171	0	1164	12	0
1	E	1171	0	1164	11	0
1	F	1171	0	1164	13	0
1	G	1171	0	1164	13	0
1	H	1171	0	1164	12	0
1	I	1171	0	1164	12	0
1	J	1171	0	1164	13	0
1	K	1171	0	1164	14	0
1	L	1171	0	1164	13	0
1	M	1171	0	1164	13	0
1	N	1171	0	1164	12	0
1	O	1171	0	1164	13	0
1	P	1171	0	1164	13	0
1	Q	1171	0	1164	14	0
1	R	1171	0	1164	12	0
1	S	1171	0	1164	13	0
1	T	1171	0	1164	15	0
1	U	1171	0	1164	13	0
1	V	1171	0	1164	13	0
1	W	1171	0	1164	13	0
1	X	1171	0	1164	14	0
1	Y	1171	0	1164	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	1171	0	1164	14	0
1	a	1171	0	1164	16	0
1	b	1171	0	1164	13	0
1	c	1171	0	1164	15	0
1	d	1171	0	1164	15	0
1	e	1171	0	1164	12	0
1	f	1171	0	1164	14	0
1	g	1171	0	1164	14	0
1	h	1171	0	1164	13	0
All	All	39814	0	39576	415	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 5.

All (415) 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:a:258:ALA:HA	1:a:261:LYS:HD2	1.70	0.74
1:U:258:ALA:HA	1:U:261:LYS:HD2	1.70	0.73
1:X:258:ALA:HA	1:X:261:LYS:HD2	1.70	0.73
1:Y:258:ALA:HA	1:Y:261:LYS:HD2	1.70	0.73
1:d:258:ALA:HA	1:d:261:LYS:HD2	1.70	0.73
1:R:258:ALA:HA	1:R:261:LYS:HD2	1.70	0.73
1:V:258:ALA:HA	1:V:261:LYS:HD2	1.70	0.73
1:b:258:ALA:HA	1:b:261:LYS:HD2	1.70	0.73
1:g:258:ALA:HA	1:g:261:LYS:HD2	1.70	0.73
1:S:258:ALA:HA	1:S:261:LYS:HD2	1.70	0.73
1:e:258:ALA:HA	1:e:261:LYS:HD2	1.70	0.73
1:P:258:ALA:HA	1:P:261:LYS:HD2	1.70	0.73
1:B:258:ALA:HA	1:B:261:LYS:HD2	1.70	0.73
1:O:258:ALA:HA	1:O:261:LYS:HD2	1.70	0.73
1:M:258:ALA:HA	1:M:261:LYS:HD2	1.70	0.72
1:h:258:ALA:HA	1:h:261:LYS:HD2	1.70	0.72
1:J:258:ALA:HA	1:J:261:LYS:HD2	1.70	0.72
1:E:258:ALA:HA	1:E:261:LYS:HD2	1.70	0.72
1:W:258:ALA:HA	1:W:261:LYS:HD2	1.70	0.72
1:T:258:ALA:HA	1:T:261:LYS:HD2	1.70	0.72
1:Z:258:ALA:HA	1:Z:261:LYS:HD2	1.70	0.72
1:c:258:ALA:HA	1:c:261:LYS:HD2	1.70	0.72
1:D:258:ALA:HA	1:D:261:LYS:HD2	1.70	0.72
1:G:258:ALA:HA	1:G:261:LYS:HD2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:258:ALA:HA	1:L:261:LYS:HD2	1.70	0.72
1:A:258:ALA:HA	1:A:261:LYS:HD2	1.70	0.71
1:f:258:ALA:HA	1:f:261:LYS:HD2	1.70	0.71
1:H:258:ALA:HA	1:H:261:LYS:HD2	1.70	0.71
1:C:258:ALA:HA	1:C:261:LYS:HD2	1.70	0.71
1:Q:258:ALA:HA	1:Q:261:LYS:HD2	1.71	0.71
1:K:258:ALA:HA	1:K:261:LYS:HD2	1.70	0.71
1:N:258:ALA:HA	1:N:261:LYS:HD2	1.70	0.71
1:F:258:ALA:HA	1:F:261:LYS:HD2	1.70	0.71
1:I:258:ALA:HA	1:I:261:LYS:HD2	1.70	0.71
1:I:324:GLU:HG3	1:I:369:LYS:HD2	1.77	0.67
1:N:324:GLU:HG3	1:N:369:LYS:HD2	1.77	0.67
1:F:324:GLU:HG3	1:F:369:LYS:HD2	1.77	0.67
1:J:324:GLU:HG3	1:J:369:LYS:HD2	1.77	0.67
1:M:324:GLU:HG3	1:M:369:LYS:HD2	1.77	0.67
1:P:324:GLU:HG3	1:P:369:LYS:HD2	1.77	0.67
1:G:324:GLU:HG3	1:G:369:LYS:HD2	1.77	0.67
1:L:324:GLU:HG3	1:L:369:LYS:HD2	1.77	0.67
1:Q:324:GLU:HG3	1:Q:369:LYS:HD2	1.77	0.67
1:C:324:GLU:HG3	1:C:369:LYS:HD2	1.77	0.67
1:K:324:GLU:HG3	1:K:369:LYS:HD2	1.77	0.67
1:T:324:GLU:HG3	1:T:369:LYS:HD2	1.77	0.67
1:H:324:GLU:HG3	1:H:369:LYS:HD2	1.77	0.67
1:O:324:GLU:HG3	1:O:369:LYS:HD2	1.77	0.67
1:B:324:GLU:HG3	1:B:369:LYS:HD2	1.77	0.66
1:D:324:GLU:HG3	1:D:369:LYS:HD2	1.77	0.66
1:R:324:GLU:HG3	1:R:369:LYS:HD2	1.77	0.66
1:S:324:GLU:HG3	1:S:369:LYS:HD2	1.77	0.66
1:E:324:GLU:HG3	1:E:369:LYS:HD2	1.77	0.66
1:U:324:GLU:HG3	1:U:369:LYS:HD2	1.77	0.66
1:W:324:GLU:HG3	1:W:369:LYS:HD2	1.77	0.66
1:h:324:GLU:HG3	1:h:369:LYS:HD2	1.77	0.66
1:A:324:GLU:HG3	1:A:369:LYS:HD2	1.77	0.66
1:V:324:GLU:HG3	1:V:369:LYS:HD2	1.77	0.66
1:X:324:GLU:HG3	1:X:369:LYS:HD2	1.77	0.66
1:g:324:GLU:HG3	1:g:369:LYS:HD2	1.77	0.66
1:a:324:GLU:HG3	1:a:369:LYS:HD2	1.77	0.66
1:Z:324:GLU:HG3	1:Z:369:LYS:HD2	1.77	0.66
1:d:324:GLU:HG3	1:d:369:LYS:HD2	1.77	0.65
1:e:324:GLU:HG3	1:e:369:LYS:HD2	1.77	0.65
1:Y:324:GLU:HG3	1:Y:369:LYS:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:324:GLU:HG3	1:b:369:LYS:HD2	1.77	0.65
1:c:324:GLU:HG3	1:c:369:LYS:HD2	1.77	0.65
1:f:324:GLU:HG3	1:f:369:LYS:HD2	1.77	0.65
1:b:324:GLU:OE2	1:b:326:TYR:OH	2.26	0.54
1:Y:324:GLU:OE2	1:Y:326:TYR:OH	2.26	0.54
1:Z:324:GLU:OE2	1:Z:326:TYR:OH	2.26	0.54
1:a:324:GLU:OE2	1:a:326:TYR:OH	2.26	0.54
1:c:324:GLU:OE2	1:c:326:TYR:OH	2.26	0.54
1:d:324:GLU:OE2	1:d:326:TYR:OH	2.26	0.54
1:X:324:GLU:OE2	1:X:326:TYR:OH	2.26	0.54
1:e:324:GLU:OE2	1:e:326:TYR:OH	2.26	0.54
1:f:324:GLU:OE2	1:f:326:TYR:OH	2.26	0.53
1:P:273:LEU:HD23	1:P:294:VAL:HG11	1.91	0.53
1:W:324:GLU:OE2	1:W:326:TYR:OH	2.26	0.53
1:D:273:LEU:HD23	1:D:294:VAL:HG11	1.91	0.53
1:H:273:LEU:HD23	1:H:294:VAL:HG11	1.91	0.53
1:J:273:LEU:HD23	1:J:294:VAL:HG11	1.91	0.53
1:L:273:LEU:HD23	1:L:294:VAL:HG11	1.91	0.53
1:N:273:LEU:HD23	1:N:294:VAL:HG11	1.91	0.53
1:R:273:LEU:HD23	1:R:294:VAL:HG11	1.91	0.53
1:V:324:GLU:OE2	1:V:326:TYR:OH	2.26	0.53
1:g:324:GLU:OE2	1:g:326:TYR:OH	2.26	0.53
1:B:273:LEU:HD23	1:B:294:VAL:HG11	1.91	0.53
1:F:273:LEU:HD23	1:F:294:VAL:HG11	1.91	0.53
1:O:273:LEU:HD23	1:O:294:VAL:HG11	1.91	0.53
1:P:324:GLU:OE2	1:P:326:TYR:OH	2.26	0.53
1:h:324:GLU:OE2	1:h:326:TYR:OH	2.26	0.53
1:C:273:LEU:HD23	1:C:294:VAL:HG11	1.91	0.53
1:E:273:LEU:HD23	1:E:294:VAL:HG11	1.91	0.53
1:G:273:LEU:HD23	1:G:294:VAL:HG11	1.91	0.53
1:K:273:LEU:HD23	1:K:294:VAL:HG11	1.91	0.53
1:T:273:LEU:HD23	1:T:294:VAL:HG11	1.91	0.53
1:U:324:GLU:OE2	1:U:326:TYR:OH	2.26	0.53
1:A:273:LEU:HD23	1:A:294:VAL:HG11	1.91	0.53
1:M:273:LEU:HD23	1:M:294:VAL:HG11	1.91	0.53
1:A:324:GLU:OE2	1:A:326:TYR:OH	2.26	0.53
1:I:273:LEU:HD23	1:I:294:VAL:HG11	1.91	0.53
1:Q:273:LEU:HD23	1:Q:294:VAL:HG11	1.91	0.53
1:T:324:GLU:OE2	1:T:326:TYR:OH	2.26	0.53
1:g:273:LEU:HD23	1:g:294:VAL:HG11	1.91	0.53
1:h:273:LEU:HD23	1:h:294:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:324:GLU:OE2	1:Q:326:TYR:OH	2.26	0.53
1:V:273:LEU:HD23	1:V:294:VAL:HG11	1.91	0.53
1:e:273:LEU:HD23	1:e:294:VAL:HG11	1.91	0.53
1:J:324:GLU:OE2	1:J:326:TYR:OH	2.26	0.52
1:S:273:LEU:HD23	1:S:294:VAL:HG11	1.91	0.52
1:S:324:GLU:OE2	1:S:326:TYR:OH	2.26	0.52
1:f:273:LEU:HD23	1:f:294:VAL:HG11	1.91	0.52
1:B:324:GLU:OE2	1:B:326:TYR:OH	2.26	0.52
1:C:324:GLU:OE2	1:C:326:TYR:OH	2.26	0.52
1:R:324:GLU:OE2	1:R:326:TYR:OH	2.26	0.52
1:W:273:LEU:HD23	1:W:294:VAL:HG11	1.91	0.52
1:c:273:LEU:HD23	1:c:294:VAL:HG11	1.91	0.52
1:K:324:GLU:OE2	1:K:326:TYR:OH	2.26	0.52
1:U:273:LEU:HD23	1:U:294:VAL:HG11	1.91	0.52
1:a:273:LEU:HD23	1:a:294:VAL:HG11	1.91	0.52
1:X:273:LEU:HD23	1:X:294:VAL:HG11	1.91	0.52
1:Y:273:LEU:HD23	1:Y:294:VAL:HG11	1.91	0.52
1:d:273:LEU:HD23	1:d:294:VAL:HG11	1.91	0.52
1:D:324:GLU:OE2	1:D:326:TYR:OH	2.26	0.52
1:Z:273:LEU:HD23	1:Z:294:VAL:HG11	1.91	0.52
1:E:324:GLU:OE2	1:E:326:TYR:OH	2.26	0.52
1:F:324:GLU:OE2	1:F:326:TYR:OH	2.26	0.52
1:O:324:GLU:OE2	1:O:326:TYR:OH	2.26	0.52
1:N:324:GLU:OE2	1:N:326:TYR:OH	2.26	0.52
1:b:273:LEU:HD23	1:b:294:VAL:HG11	1.91	0.52
1:L:324:GLU:OE2	1:L:326:TYR:OH	2.26	0.51
1:G:324:GLU:OE2	1:G:326:TYR:OH	2.26	0.51
1:H:324:GLU:OE2	1:H:326:TYR:OH	2.26	0.51
1:I:324:GLU:OE2	1:I:326:TYR:OH	2.26	0.51
1:M:324:GLU:OE2	1:M:326:TYR:OH	2.26	0.51
1:L:430:LEU:HA	1:L:433:THR:HB	1.94	0.50
1:P:430:LEU:HA	1:P:433:THR:HB	1.94	0.50
1:S:430:LEU:HA	1:S:433:THR:HB	1.94	0.50
1:H:430:LEU:HA	1:H:433:THR:HB	1.94	0.50
1:J:430:LEU:HA	1:J:433:THR:HB	1.94	0.50
1:N:430:LEU:HA	1:N:433:THR:HB	1.94	0.50
1:Q:430:LEU:HA	1:Q:433:THR:HB	1.94	0.50
1:U:430:LEU:HA	1:U:433:THR:HB	1.94	0.50
1:M:430:LEU:HA	1:M:433:THR:HB	1.94	0.50
1:O:430:LEU:HA	1:O:433:THR:HB	1.94	0.50
1:R:430:LEU:HA	1:R:433:THR:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:430:LEU:HA	1:I:433:THR:HB	1.94	0.50
1:W:430:LEU:HA	1:W:433:THR:HB	1.94	0.50
1:G:430:LEU:HA	1:G:433:THR:HB	1.94	0.49
1:K:430:LEU:HA	1:K:433:THR:HB	1.94	0.49
1:T:430:LEU:HA	1:T:433:THR:HB	1.94	0.49
1:V:430:LEU:HA	1:V:433:THR:HB	1.94	0.49
1:F:430:LEU:HA	1:F:433:THR:HB	1.94	0.49
1:X:430:LEU:HA	1:X:433:THR:HB	1.94	0.49
1:Y:430:LEU:HA	1:Y:433:THR:HB	1.94	0.49
1:E:430:LEU:HA	1:E:433:THR:HB	1.94	0.49
1:Z:430:LEU:HA	1:Z:433:THR:HB	1.94	0.49
1:C:430:LEU:HA	1:C:433:THR:HB	1.94	0.49
1:a:430:LEU:HA	1:a:433:THR:HB	1.94	0.49
1:D:430:LEU:HA	1:D:433:THR:HB	1.94	0.49
1:J:299:ASP:O	1:J:389:GLY:HA2	2.13	0.49
1:M:299:ASP:O	1:M:389:GLY:HA2	2.13	0.49
1:b:430:LEU:HA	1:b:433:THR:HB	1.94	0.49
1:c:430:LEU:HA	1:c:433:THR:HB	1.94	0.49
1:A:430:LEU:HA	1:A:433:THR:HB	1.94	0.49
1:B:430:LEU:HA	1:B:433:THR:HB	1.94	0.49
1:G:299:ASP:O	1:G:389:GLY:HA2	2.13	0.49
1:P:299:ASP:O	1:P:389:GLY:HA2	2.13	0.49
1:g:430:LEU:HA	1:g:433:THR:HB	1.94	0.49
1:D:299:ASP:O	1:D:389:GLY:HA2	2.13	0.49
1:R:299:ASP:O	1:R:389:GLY:HA2	2.13	0.49
1:b:299:ASP:O	1:b:389:GLY:HA2	2.13	0.49
1:e:430:LEU:HA	1:e:433:THR:HB	1.94	0.49
1:f:430:LEU:HA	1:f:433:THR:HB	1.94	0.49
1:A:299:ASP:O	1:A:389:GLY:HA2	2.13	0.48
1:O:299:ASP:O	1:O:389:GLY:HA2	2.13	0.48
1:S:299:ASP:O	1:S:389:GLY:HA2	2.13	0.48
1:V:299:ASP:O	1:V:389:GLY:HA2	2.13	0.48
1:Z:299:ASP:O	1:Z:389:GLY:HA2	2.13	0.48
1:d:430:LEU:HA	1:d:433:THR:HB	1.94	0.48
1:h:430:LEU:HA	1:h:433:THR:HB	1.94	0.48
1:L:299:ASP:O	1:L:389:GLY:HA2	2.13	0.48
1:X:299:ASP:O	1:X:389:GLY:HA2	2.13	0.48
1:d:299:ASP:O	1:d:389:GLY:HA2	2.13	0.48
1:E:299:ASP:O	1:E:389:GLY:HA2	2.13	0.48
1:f:299:ASP:O	1:f:389:GLY:HA2	2.13	0.48
1:g:299:ASP:O	1:g:389:GLY:HA2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:ASP:O	1:H:389:GLY:HA2	2.13	0.48
1:I:299:ASP:O	1:I:389:GLY:HA2	2.13	0.48
1:T:299:ASP:O	1:T:389:GLY:HA2	2.13	0.48
1:U:299:ASP:O	1:U:389:GLY:HA2	2.13	0.48
1:e:299:ASP:O	1:e:389:GLY:HA2	2.13	0.48
1:B:299:ASP:O	1:B:389:GLY:HA2	2.13	0.48
1:K:299:ASP:O	1:K:389:GLY:HA2	2.13	0.48
1:F:299:ASP:O	1:F:389:GLY:HA2	2.13	0.48
1:Y:299:ASP:O	1:Y:389:GLY:HA2	2.13	0.48
1:c:299:ASP:O	1:c:389:GLY:HA2	2.13	0.48
1:h:299:ASP:O	1:h:389:GLY:HA2	2.13	0.48
1:a:299:ASP:O	1:a:389:GLY:HA2	2.13	0.48
1:C:299:ASP:O	1:C:389:GLY:HA2	2.13	0.47
1:N:299:ASP:O	1:N:389:GLY:HA2	2.13	0.47
1:B:260:ARG:O	1:B:264:GLU:HG2	2.15	0.47
1:J:260:ARG:O	1:J:264:GLU:HG2	2.15	0.47
1:Q:299:ASP:O	1:Q:389:GLY:HA2	2.13	0.47
1:g:260:ARG:O	1:g:264:GLU:HG2	2.15	0.47
1:E:260:ARG:O	1:E:264:GLU:HG2	2.15	0.47
1:W:299:ASP:O	1:W:389:GLY:HA2	2.13	0.47
1:G:260:ARG:O	1:G:264:GLU:HG2	2.15	0.47
1:H:260:ARG:O	1:H:264:GLU:HG2	2.15	0.47
1:d:260:ARG:O	1:d:264:GLU:HG2	2.15	0.47
1:D:260:ARG:O	1:D:264:GLU:HG2	2.15	0.47
1:K:260:ARG:O	1:K:264:GLU:HG2	2.15	0.47
1:M:260:ARG:O	1:M:264:GLU:HG2	2.15	0.47
1:U:260:ARG:O	1:U:264:GLU:HG2	2.15	0.47
1:W:260:ARG:O	1:W:264:GLU:HG2	2.15	0.47
1:Y:260:ARG:O	1:Y:264:GLU:HG2	2.15	0.47
1:a:260:ARG:O	1:a:264:GLU:HG2	2.15	0.47
1:A:260:ARG:O	1:A:264:GLU:HG2	2.15	0.47
1:N:260:ARG:O	1:N:264:GLU:HG2	2.15	0.47
1:R:260:ARG:O	1:R:264:GLU:HG2	2.15	0.47
1:S:260:ARG:O	1:S:264:GLU:HG2	2.15	0.47
1:c:260:ARG:O	1:c:264:GLU:HG2	2.15	0.47
1:T:260:ARG:O	1:T:264:GLU:HG2	2.15	0.47
1:f:260:ARG:O	1:f:264:GLU:HG2	2.15	0.47
1:P:260:ARG:O	1:P:264:GLU:HG2	2.15	0.46
1:Q:260:ARG:O	1:Q:264:GLU:HG2	2.15	0.46
1:V:260:ARG:O	1:V:264:GLU:HG2	2.15	0.46
1:h:260:ARG:O	1:h:264:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:260:ARG:O	1:e:264:GLU:HG2	2.15	0.46
1:O:260:ARG:O	1:O:264:GLU:HG2	2.15	0.46
1:Z:260:ARG:O	1:Z:264:GLU:HG2	2.15	0.46
1:X:260:ARG:O	1:X:264:GLU:HG2	2.15	0.46
1:C:260:ARG:O	1:C:264:GLU:HG2	2.15	0.46
1:L:260:ARG:O	1:L:264:GLU:HG2	2.15	0.46
1:I:260:ARG:O	1:I:264:GLU:HG2	2.15	0.46
1:b:260:ARG:O	1:b:264:GLU:HG2	2.15	0.46
1:F:260:ARG:O	1:F:264:GLU:HG2	2.15	0.46
1:a:369:LYS:HE3	1:a:369:LYS:HB3	1.85	0.45
1:P:369:LYS:HE3	1:P:369:LYS:HB3	1.85	0.45
1:T:369:LYS:HB3	1:T:369:LYS:HE3	1.85	0.45
1:G:387:GLN:HE21	1:G:387:GLN:HB2	1.63	0.45
1:L:369:LYS:HE3	1:L:369:LYS:HB3	1.85	0.45
1:d:258:ALA:O	1:d:261:LYS:HG2	2.18	0.44
1:e:258:ALA:O	1:e:261:LYS:HG2	2.18	0.44
1:T:258:ALA:O	1:T:261:LYS:HG2	2.18	0.44
1:b:369:LYS:HE3	1:b:369:LYS:HB3	1.85	0.44
1:S:258:ALA:O	1:S:261:LYS:HG2	2.18	0.44
1:Y:258:ALA:O	1:Y:261:LYS:HG2	2.18	0.44
1:Z:258:ALA:O	1:Z:261:LYS:HG2	2.18	0.44
1:d:387:GLN:HE21	1:d:387:GLN:HB2	1.63	0.44
1:J:258:ALA:O	1:J:261:LYS:HG2	2.18	0.44
1:U:369:LYS:HB3	1:U:369:LYS:HE3	1.85	0.44
1:X:258:ALA:O	1:X:261:LYS:HG2	2.18	0.44
1:C:258:ALA:O	1:C:261:LYS:HG2	2.18	0.44
1:F:258:ALA:O	1:F:261:LYS:HG2	2.18	0.44
1:M:258:ALA:O	1:M:261:LYS:HG2	2.18	0.44
1:U:258:ALA:O	1:U:261:LYS:HG2	2.18	0.44
1:G:258:ALA:O	1:G:261:LYS:HG2	2.18	0.44
1:I:258:ALA:O	1:I:261:LYS:HG2	2.18	0.44
1:a:387:GLN:HE21	1:a:387:GLN:HB2	1.63	0.44
1:L:387:GLN:HE21	1:L:387:GLN:HB2	1.63	0.44
1:c:258:ALA:O	1:c:261:LYS:HG2	2.18	0.44
1:A:258:ALA:O	1:A:261:LYS:HG2	2.18	0.44
1:O:258:ALA:O	1:O:261:LYS:HG2	2.18	0.44
1:g:387:GLN:HE21	1:g:387:GLN:HB2	1.63	0.44
1:N:258:ALA:O	1:N:261:LYS:HG2	2.18	0.43
1:a:258:ALA:O	1:a:261:LYS:HG2	2.18	0.43
1:f:258:ALA:O	1:f:261:LYS:HG2	2.18	0.43
1:B:258:ALA:O	1:B:261:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:258:ALA:O	1:P:261:LYS:HG2	2.18	0.43
1:E:258:ALA:O	1:E:261:LYS:HG2	2.18	0.43
1:K:258:ALA:O	1:K:261:LYS:HG2	2.18	0.43
1:Q:258:ALA:O	1:Q:261:LYS:HG2	2.18	0.43
1:R:258:ALA:O	1:R:261:LYS:HG2	2.18	0.43
1:B:369:LYS:HE3	1:B:369:LYS:HB3	1.85	0.43
1:W:258:ALA:O	1:W:261:LYS:HG2	2.18	0.43
1:g:258:ALA:O	1:g:261:LYS:HG2	2.18	0.43
1:h:258:ALA:O	1:h:261:LYS:HG2	2.18	0.43
1:X:387:GLN:HE21	1:X:387:GLN:HB2	1.63	0.43
1:D:258:ALA:O	1:D:261:LYS:HG2	2.18	0.43
1:L:258:ALA:O	1:L:261:LYS:HG2	2.18	0.43
1:c:369:LYS:HE3	1:c:369:LYS:HB3	1.85	0.43
1:K:387:GLN:HE21	1:K:387:GLN:HB2	1.63	0.43
1:Q:369:LYS:HE3	1:Q:369:LYS:HB3	1.85	0.43
1:V:258:ALA:O	1:V:261:LYS:HG2	2.18	0.43
1:H:258:ALA:O	1:H:261:LYS:HG2	2.18	0.43
1:V:369:LYS:HE3	1:V:369:LYS:HB3	1.85	0.43
1:b:258:ALA:O	1:b:261:LYS:HG2	2.18	0.43
1:F:387:GLN:HE21	1:F:387:GLN:HB2	1.63	0.43
1:H:369:LYS:HE3	1:H:369:LYS:HB3	1.85	0.42
1:B:387:GLN:HE21	1:B:387:GLN:HB2	1.63	0.42
1:Q:402:ASP:OD1	1:Q:448:SER:OG	2.33	0.42
1:U:387:GLN:HE21	1:U:387:GLN:HB2	1.63	0.42
1:M:369:LYS:HE3	1:M:369:LYS:HB3	1.85	0.42
1:M:450:LYS:HE2	1:M:450:LYS:HB2	1.85	0.42
1:Q:302:ALA:HB3	1:R:385:ARG:HB3	2.02	0.42
1:Q:387:GLN:HE21	1:Q:387:GLN:HB2	1.63	0.42
1:T:450:LYS:HE2	1:T:450:LYS:HB2	1.85	0.42
1:W:302:ALA:HB3	1:X:385:ARG:HB3	2.02	0.42
1:c:302:ALA:HB3	1:d:385:ARG:HB3	2.02	0.42
1:P:302:ALA:HB3	1:Q:385:ARG:HB3	2.02	0.42
1:P:387:GLN:HE21	1:P:387:GLN:HB2	1.63	0.42
1:R:302:ALA:HB3	1:S:385:ARG:HB3	2.02	0.42
1:V:302:ALA:HB3	1:W:385:ARG:HB3	2.02	0.42
1:b:302:ALA:HB3	1:c:385:ARG:HB3	2.02	0.42
1:d:302:ALA:HB3	1:e:385:ARG:HB3	2.02	0.42
1:A:385:ARG:HB3	1:h:302:ALA:HB3	2.02	0.42
1:A:302:ALA:HB3	1:B:385:ARG:HB3	2.02	0.42
1:X:302:ALA:HB3	1:Y:385:ARG:HB3	2.02	0.42
1:F:450:LYS:HB2	1:F:450:LYS:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:ALA:HB3	1:L:385:ARG:HB3	2.02	0.41
1:L:302:ALA:HB3	1:M:385:ARG:HB3	2.02	0.41
1:L:426:ILE:O	1:L:430:LEU:HG	2.20	0.41
1:d:369:LYS:HE3	1:d:369:LYS:HB3	1.85	0.41
1:d:426:ILE:O	1:d:430:LEU:HG	2.21	0.41
1:h:426:ILE:O	1:h:430:LEU:HG	2.20	0.41
1:B:302:ALA:HB3	1:C:385:ARG:HB3	2.02	0.41
1:J:387:GLN:HE21	1:J:387:GLN:HB2	1.63	0.41
1:O:426:ILE:O	1:O:430:LEU:HG	2.20	0.41
1:Y:426:ILE:O	1:Y:430:LEU:HG	2.20	0.41
1:g:426:ILE:O	1:g:430:LEU:HG	2.20	0.41
1:F:302:ALA:HB3	1:G:385:ARG:HB3	2.02	0.41
1:H:426:ILE:O	1:H:430:LEU:HG	2.20	0.41
1:S:426:ILE:O	1:S:430:LEU:HG	2.21	0.41
1:T:387:GLN:HE21	1:T:387:GLN:HB2	1.63	0.41
1:W:426:ILE:O	1:W:430:LEU:HG	2.21	0.41
1:X:426:ILE:O	1:X:430:LEU:HG	2.21	0.41
1:Z:426:ILE:O	1:Z:430:LEU:HG	2.21	0.41
1:a:302:ALA:HB3	1:b:385:ARG:HB3	2.02	0.41
1:c:426:ILE:O	1:c:430:LEU:HG	2.20	0.41
1:f:402:ASP:OD1	1:f:448:SER:OG	2.33	0.41
1:g:302:ALA:HB3	1:h:385:ARG:HB3	2.02	0.41
1:A:402:ASP:OD1	1:A:448:SER:OG	2.33	0.41
1:C:426:ILE:O	1:C:430:LEU:HG	2.20	0.41
1:D:426:ILE:O	1:D:430:LEU:HG	2.20	0.41
1:E:302:ALA:HB3	1:F:385:ARG:HB3	2.02	0.41
1:G:426:ILE:O	1:G:430:LEU:HG	2.20	0.41
1:K:426:ILE:O	1:K:430:LEU:HG	2.21	0.41
1:P:426:ILE:O	1:P:430:LEU:HG	2.21	0.41
1:S:302:ALA:HB3	1:T:385:ARG:HB3	2.02	0.41
1:U:302:ALA:HB3	1:V:385:ARG:HB3	2.02	0.41
1:W:369:LYS:HB3	1:W:369:LYS:HE3	1.85	0.41
1:W:387:GLN:HE21	1:W:387:GLN:HB2	1.63	0.41
1:a:450:LYS:HE2	1:a:450:LYS:HB2	1.85	0.41
1:G:302:ALA:HB3	1:H:385:ARG:HB3	2.02	0.41
1:M:302:ALA:HB3	1:N:385:ARG:HB3	2.02	0.41
1:O:302:ALA:HB3	1:P:385:ARG:HB3	2.02	0.41
1:Q:426:ILE:O	1:Q:430:LEU:HG	2.20	0.41
1:V:426:ILE:O	1:V:430:LEU:HG	2.20	0.41
1:Y:302:ALA:HB3	1:Z:385:ARG:HB3	2.02	0.41
1:a:426:ILE:O	1:a:430:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:302:ALA:HB3	1:f:385:ARG:HB3	2.02	0.41
1:h:450:LYS:HE2	1:h:450:LYS:HB2	1.85	0.41
1:I:450:LYS:HB2	1:I:450:LYS:HE2	1.85	0.41
1:N:426:ILE:O	1:N:430:LEU:HG	2.20	0.41
1:O:387:GLN:HE21	1:O:387:GLN:HB2	1.63	0.41
1:X:369:LYS:HB3	1:X:369:LYS:HE3	1.85	0.41
1:Z:387:GLN:HE21	1:Z:387:GLN:HB2	1.63	0.41
1:g:402:ASP:OD1	1:g:448:SER:OG	2.33	0.41
1:I:426:ILE:O	1:I:430:LEU:HG	2.20	0.41
1:J:302:ALA:HB3	1:K:385:ARG:HB3	2.02	0.41
1:S:369:LYS:HB3	1:S:369:LYS:HE3	1.85	0.41
1:V:450:LYS:HE2	1:V:450:LYS:HB2	1.85	0.41
1:M:426:ILE:O	1:M:430:LEU:HG	2.20	0.41
1:R:426:ILE:O	1:R:430:LEU:HG	2.21	0.41
1:T:426:ILE:O	1:T:430:LEU:HG	2.20	0.41
1:a:402:ASP:OD1	1:a:448:SER:OG	2.33	0.41
1:A:426:ILE:O	1:A:430:LEU:HG	2.20	0.41
1:C:369:LYS:HE3	1:C:369:LYS:HB3	1.85	0.41
1:D:302:ALA:HB3	1:E:385:ARG:HB3	2.02	0.41
1:E:426:ILE:O	1:E:430:LEU:HG	2.21	0.41
1:H:302:ALA:HB3	1:I:385:ARG:HB3	2.02	0.41
1:R:369:LYS:HB3	1:R:369:LYS:HE3	1.85	0.41
1:U:426:ILE:O	1:U:430:LEU:HG	2.20	0.41
1:b:402:ASP:OD1	1:b:448:SER:OG	2.33	0.41
1:c:387:GLN:HE21	1:c:387:GLN:HB2	1.63	0.41
1:e:426:ILE:O	1:e:430:LEU:HG	2.21	0.41
1:D:450:LYS:HB2	1:D:450:LYS:HE2	1.85	0.41
1:J:294:VAL:HG22	1:J:396:VAL:HG22	2.03	0.41
1:T:302:ALA:HB3	1:U:385:ARG:HB3	2.02	0.41
1:Y:369:LYS:HB3	1:Y:369:LYS:HE3	1.85	0.41
1:d:294:VAL:HG22	1:d:396:VAL:HG22	2.03	0.41
1:f:302:ALA:HB3	1:g:385:ARG:HB3	2.02	0.41
1:G:450:LYS:HE2	1:G:450:LYS:HB2	1.85	0.40
1:J:426:ILE:O	1:J:430:LEU:HG	2.20	0.40
1:f:426:ILE:O	1:f:430:LEU:HG	2.20	0.40
1:h:402:ASP:OD1	1:h:448:SER:OG	2.33	0.40
1:K:294:VAL:HG22	1:K:396:VAL:HG22	2.03	0.40
1:N:302:ALA:HB3	1:O:385:ARG:HB3	2.02	0.40
1:O:294:VAL:HG22	1:O:396:VAL:HG22	2.03	0.40
1:d:327:ASN:HB2	1:d:366:SER:HB3	2.04	0.40
1:B:426:ILE:O	1:B:430:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ALA:HB3	1:D:385:ARG:HB3	2.02	0.40
1:Y:327:ASN:HB2	1:Y:366:SER:HB3	2.04	0.40
1:Z:294:VAL:HG22	1:Z:396:VAL:HG22	2.03	0.40
1:Z:302:ALA:HB3	1:a:385:ARG:HB3	2.02	0.40
1:b:426:ILE:O	1:b:430:LEU:HG	2.20	0.40
1:e:327:ASN:HB2	1:e:366:SER:HB3	2.04	0.40
1:F:426:ILE:O	1:F:430:LEU:HG	2.20	0.40
1:Z:327:ASN:HB2	1:Z:366:SER:HB3	2.04	0.40
1:a:294:VAL:HG22	1:a:396:VAL:HG22	2.03	0.40
1:c:294:VAL:HG22	1:c:396:VAL:HG22	2.03	0.40
1:f:294:VAL:HG22	1:f:396:VAL:HG22	2.03	0.40
1:g:294:VAL:HG22	1:g:396:VAL:HG22	2.03	0.40
1:B:327:ASN:HB2	1:B:366:SER:HB3	2.04	0.40
1:B:450:LYS:HB2	1:B:450:LYS:HE2	1.85	0.40
1:I:302:ALA:HB3	1:J:385:ARG:HB3	2.02	0.40
1:K:450:LYS:HB2	1:K:450:LYS:HE2	1.85	0.40
1:N:294:VAL:HG22	1:N:396:VAL:HG22	2.03	0.40
1:S:387:GLN:HE21	1:S:387:GLN:HB2	1.63	0.40
1:T:327:ASN:HB2	1:T:366:SER:HB3	2.04	0.40
1:X:327:ASN:HB2	1:X:366:SER:HB3	2.04	0.40
1:c:402:ASP:OD1	1:c:448:SER:OG	2.33	0.40
1:f:387:GLN:HE21	1:f:387:GLN:HB2	1.63	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	B	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	C	142/580 (24%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	E	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	F	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	G	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	H	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	I	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	J	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	K	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	L	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	M	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	N	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	O	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	P	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	Q	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	R	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	S	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	T	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	U	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	V	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	W	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	X	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	Y	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	Z	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	a	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	b	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	c	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	d	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	e	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	f	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	g	142/580 (24%)	138 (97%)	4 (3%)	0	100	100
1	h	142/580 (24%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4828/19720 (24%)	4692 (97%)	136 (3%)	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	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	B	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	C	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	D	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	E	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	F	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	G	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	H	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	I	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	J	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	K	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	L	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	M	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	N	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	O	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	P	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	Q	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	R	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	S	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	T	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	U	128/500 (26%)	123 (96%)	5 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	W	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	X	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	Y	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	Z	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	a	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	b	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	c	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	d	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	e	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	f	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	g	128/500 (26%)	123 (96%)	5 (4%)	27	52
1	h	128/500 (26%)	123 (96%)	5 (4%)	27	52
All	All	4352/17000 (26%)	4182 (96%)	170 (4%)	30	52

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	VAL
1	A	380	THR
1	A	387	GLN
1	A	395	THR
1	A	422	GLU
1	B	280	VAL
1	B	380	THR
1	B	387	GLN
1	B	395	THR
1	B	422	GLU
1	C	280	VAL
1	C	380	THR
1	C	387	GLN
1	C	395	THR
1	C	422	GLU
1	D	280	VAL
1	D	380	THR
1	D	387	GLN
1	D	395	THR

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Mol	Chain	Res	Type
1	D	422	GLU
1	E	280	VAL
1	E	380	THR
1	E	387	GLN
1	E	395	THR
1	E	422	GLU
1	F	280	VAL
1	F	380	THR
1	F	387	GLN
1	F	395	THR
1	F	422	GLU
1	G	280	VAL
1	G	380	THR
1	G	387	GLN
1	G	395	THR
1	G	422	GLU
1	H	280	VAL
1	H	380	THR
1	H	387	GLN
1	H	395	THR
1	H	422	GLU
1	I	280	VAL
1	I	380	THR
1	I	387	GLN
1	I	395	THR
1	I	422	GLU
1	J	280	VAL
1	J	380	THR
1	J	387	GLN
1	J	395	THR
1	J	422	GLU
1	K	280	VAL
1	K	380	THR
1	K	387	GLN
1	K	395	THR
1	K	422	GLU
1	L	280	VAL
1	L	380	THR
1	L	387	GLN
1	L	395	THR
1	L	422	GLU
1	M	280	VAL

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Mol	Chain	Res	Type
1	M	380	THR
1	M	387	GLN
1	M	395	THR
1	M	422	GLU
1	N	280	VAL
1	N	380	THR
1	N	387	GLN
1	N	395	THR
1	N	422	GLU
1	O	280	VAL
1	O	380	THR
1	O	387	GLN
1	O	395	THR
1	O	422	GLU
1	P	280	VAL
1	P	380	THR
1	P	387	GLN
1	P	395	THR
1	P	422	GLU
1	Q	280	VAL
1	Q	380	THR
1	Q	387	GLN
1	Q	395	THR
1	Q	422	GLU
1	R	280	VAL
1	R	380	THR
1	R	387	GLN
1	R	395	THR
1	R	422	GLU
1	S	280	VAL
1	S	380	THR
1	S	387	GLN
1	S	395	THR
1	S	422	GLU
1	T	280	VAL
1	T	380	THR
1	T	387	GLN
1	T	395	THR
1	T	422	GLU
1	U	280	VAL
1	U	380	THR
1	U	387	GLN

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Mol	Chain	Res	Type
1	U	395	THR
1	U	422	GLU
1	V	280	VAL
1	V	380	THR
1	V	387	GLN
1	V	395	THR
1	V	422	GLU
1	W	280	VAL
1	W	380	THR
1	W	387	GLN
1	W	395	THR
1	W	422	GLU
1	X	280	VAL
1	X	380	THR
1	X	387	GLN
1	X	395	THR
1	X	422	GLU
1	Y	280	VAL
1	Y	380	THR
1	Y	387	GLN
1	Y	395	THR
1	Y	422	GLU
1	Z	280	VAL
1	Z	380	THR
1	Z	387	GLN
1	Z	395	THR
1	Z	422	GLU
1	a	280	VAL
1	a	380	THR
1	a	387	GLN
1	a	395	THR
1	a	422	GLU
1	b	280	VAL
1	b	380	THR
1	b	387	GLN
1	b	395	THR
1	b	422	GLU
1	c	280	VAL
1	c	380	THR
1	c	387	GLN
1	c	395	THR
1	c	422	GLU

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Mol	Chain	Res	Type
1	d	280	VAL
1	d	380	THR
1	d	387	GLN
1	d	395	THR
1	d	422	GLU
1	e	280	VAL
1	e	380	THR
1	e	387	GLN
1	e	395	THR
1	e	422	GLU
1	f	280	VAL
1	f	380	THR
1	f	387	GLN
1	f	395	THR
1	f	422	GLU
1	g	280	VAL
1	g	380	THR
1	g	387	GLN
1	g	395	THR
1	g	422	GLU
1	h	280	VAL
1	h	380	THR
1	h	387	GLN
1	h	395	THR
1	h	422	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	A	387	GLN
1	A	445	ASN
1	B	305	GLN
1	B	387	GLN
1	B	445	ASN
1	C	305	GLN
1	C	387	GLN
1	C	445	ASN
1	D	305	GLN
1	D	387	GLN
1	D	445	ASN
1	E	305	GLN

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Mol	Chain	Res	Type
1	E	387	GLN
1	E	445	ASN
1	F	305	GLN
1	F	387	GLN
1	F	445	ASN
1	G	305	GLN
1	G	387	GLN
1	G	445	ASN
1	H	305	GLN
1	H	387	GLN
1	H	445	ASN
1	I	305	GLN
1	I	387	GLN
1	I	445	ASN
1	J	305	GLN
1	J	387	GLN
1	J	445	ASN
1	K	305	GLN
1	K	387	GLN
1	K	445	ASN
1	L	305	GLN
1	L	387	GLN
1	L	445	ASN
1	M	305	GLN
1	M	387	GLN
1	M	445	ASN
1	N	305	GLN
1	N	387	GLN
1	N	445	ASN
1	O	305	GLN
1	O	387	GLN
1	O	445	ASN
1	P	305	GLN
1	P	387	GLN
1	P	445	ASN
1	Q	305	GLN
1	Q	387	GLN
1	Q	445	ASN
1	R	305	GLN
1	R	387	GLN
1	R	445	ASN
1	S	305	GLN

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Mol	Chain	Res	Type
1	S	387	GLN
1	S	445	ASN
1	T	305	GLN
1	T	387	GLN
1	T	445	ASN
1	U	305	GLN
1	U	387	GLN
1	U	445	ASN
1	V	305	GLN
1	V	387	GLN
1	V	445	ASN
1	W	305	GLN
1	W	387	GLN
1	W	445	ASN
1	X	305	GLN
1	X	387	GLN
1	X	445	ASN
1	Y	305	GLN
1	Y	387	GLN
1	Y	445	ASN
1	Z	305	GLN
1	Z	387	GLN
1	Z	445	ASN
1	a	305	GLN
1	a	387	GLN
1	a	445	ASN
1	b	305	GLN
1	b	387	GLN
1	b	445	ASN
1	c	305	GLN
1	c	387	GLN
1	c	445	ASN
1	d	305	GLN
1	d	387	GLN
1	d	445	ASN
1	e	305	GLN
1	e	387	GLN
1	e	445	ASN
1	f	305	GLN
1	f	387	GLN
1	f	445	ASN
1	g	305	GLN

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Mol	Chain	Res	Type
1	g	387	GLN
1	g	445	ASN
1	h	305	GLN
1	h	387	GLN
1	h	445	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 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.

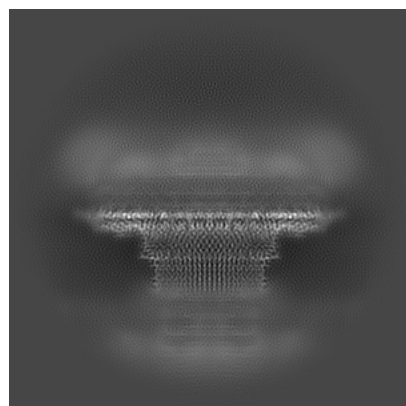
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39783. These allow visual inspection of the internal detail of the map and identification of artifacts.

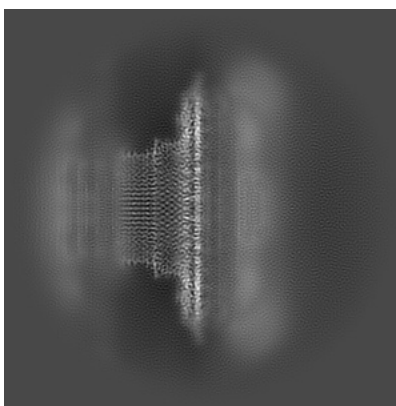
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

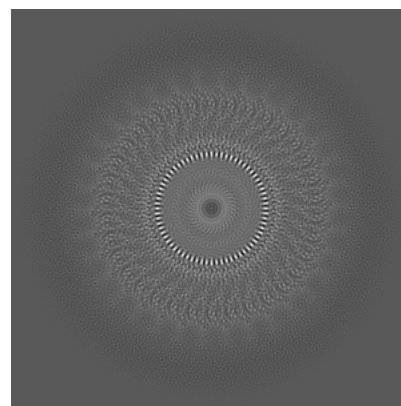
#### 6.1.1 Primary map



X

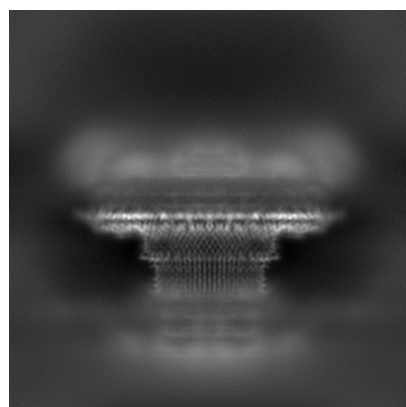


Y

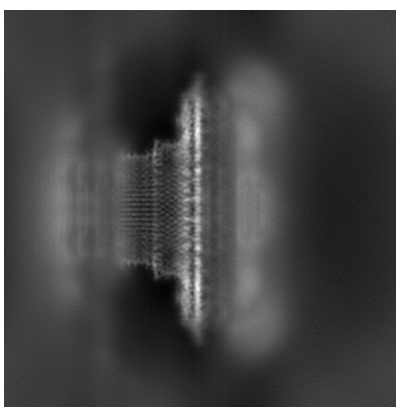


Z

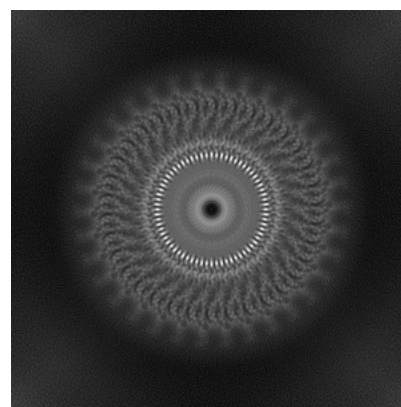
#### 6.1.2 Raw map



X



Y

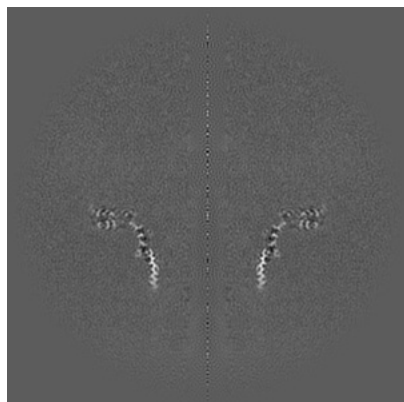


Z

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

## 6.2 Central slices [i](#)

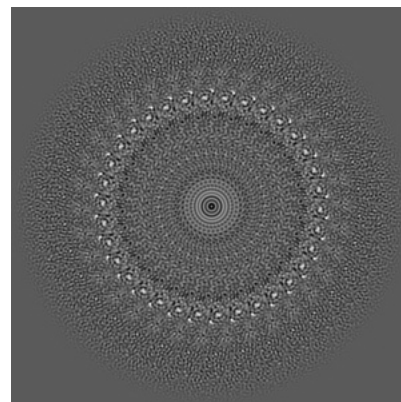
### 6.2.1 Primary map



X Index: 160

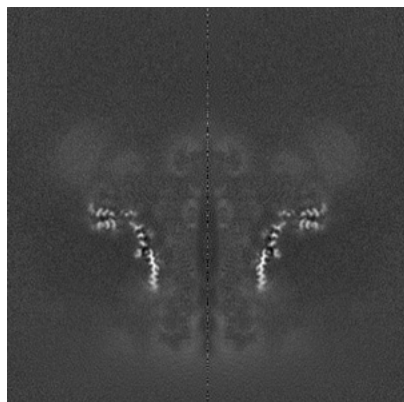


Y Index: 160

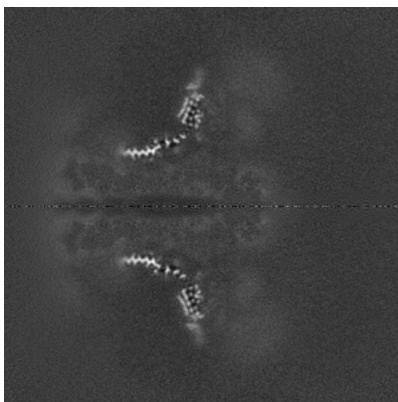


Z Index: 160

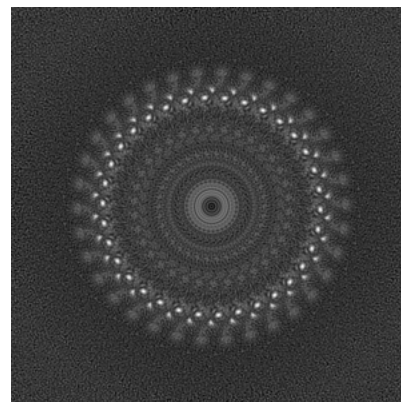
### 6.2.2 Raw map



X Index: 160



Y Index: 160

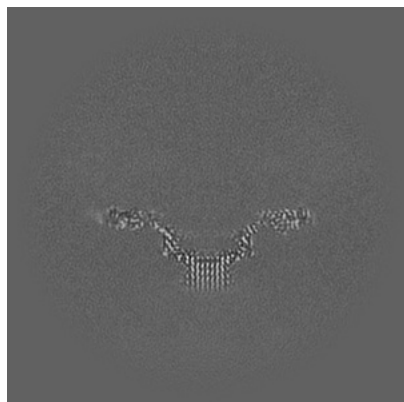


Z Index: 160

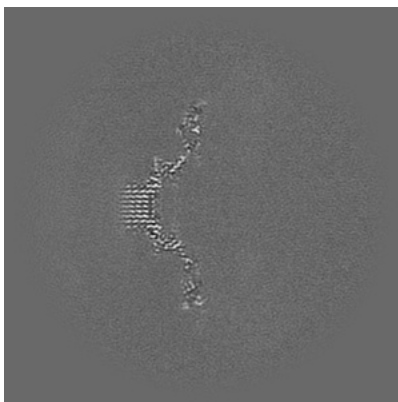
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

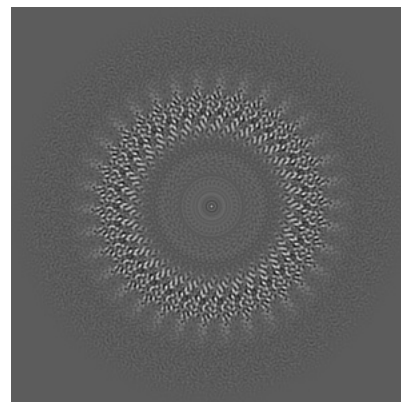
### 6.3.1 Primary map



X Index: 118

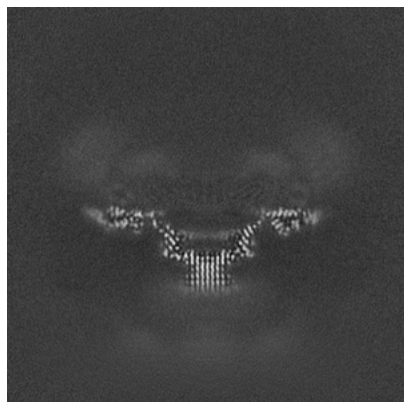


Y Index: 118

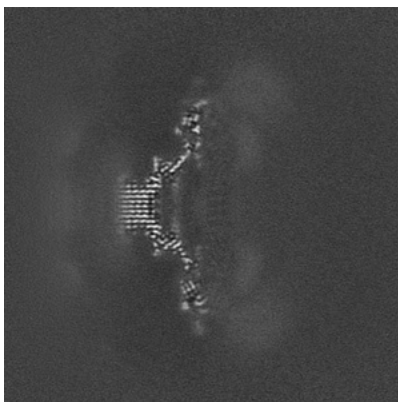


Z Index: 153

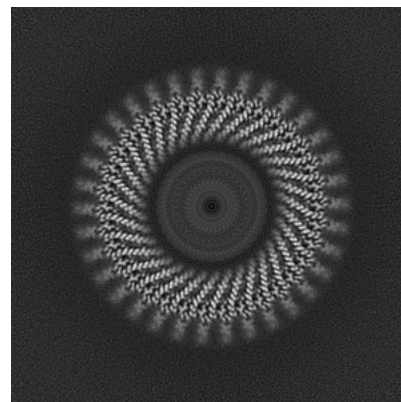
### 6.3.2 Raw map



X Index: 117



Y Index: 118



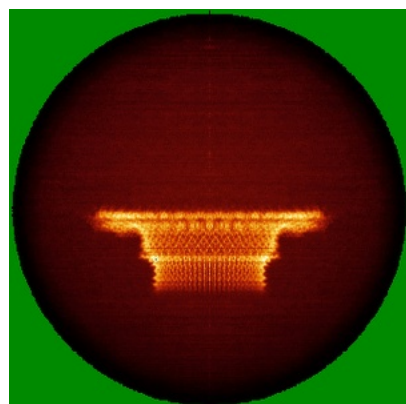
Z Index: 154

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

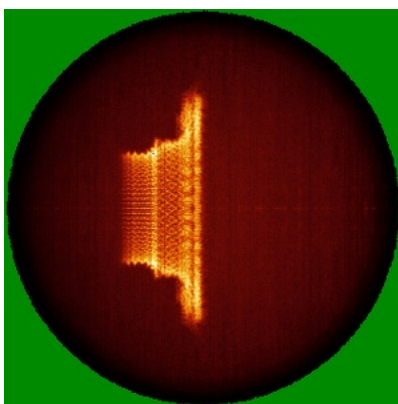


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X

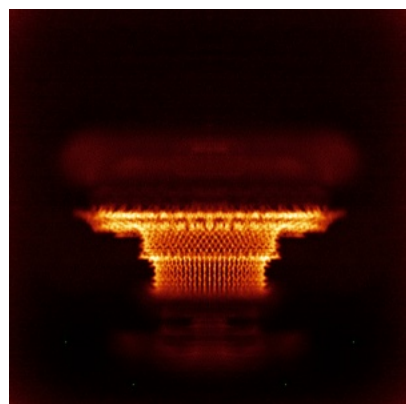


Y

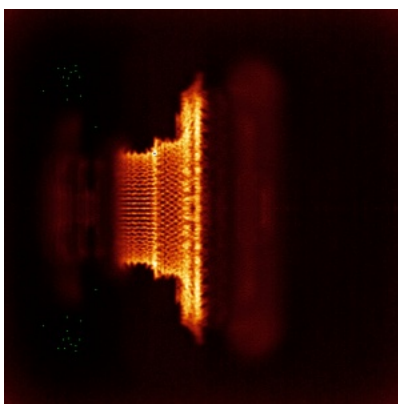


Z

### 6.4.2 Raw map



X



Y

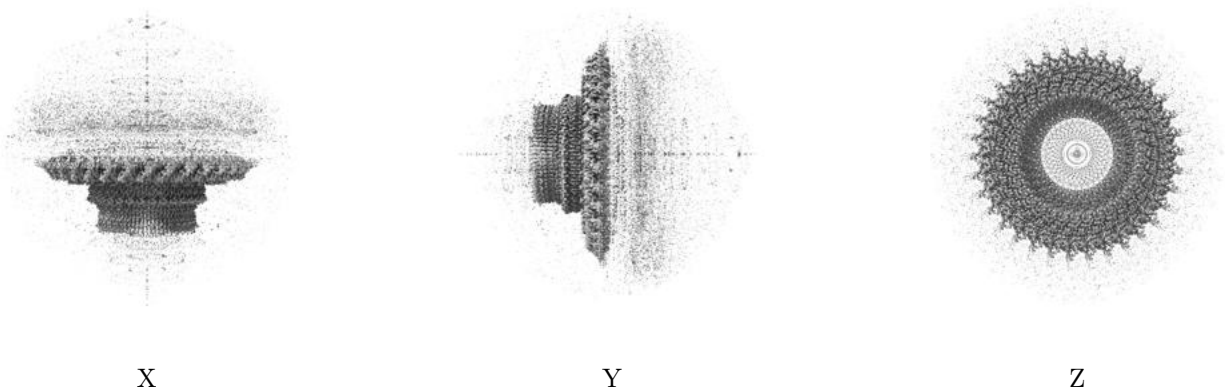


Z

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

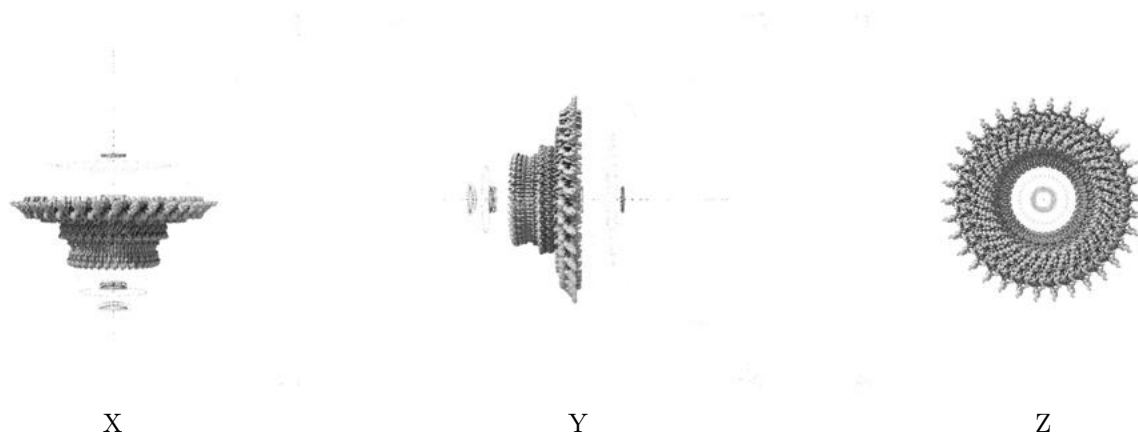
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

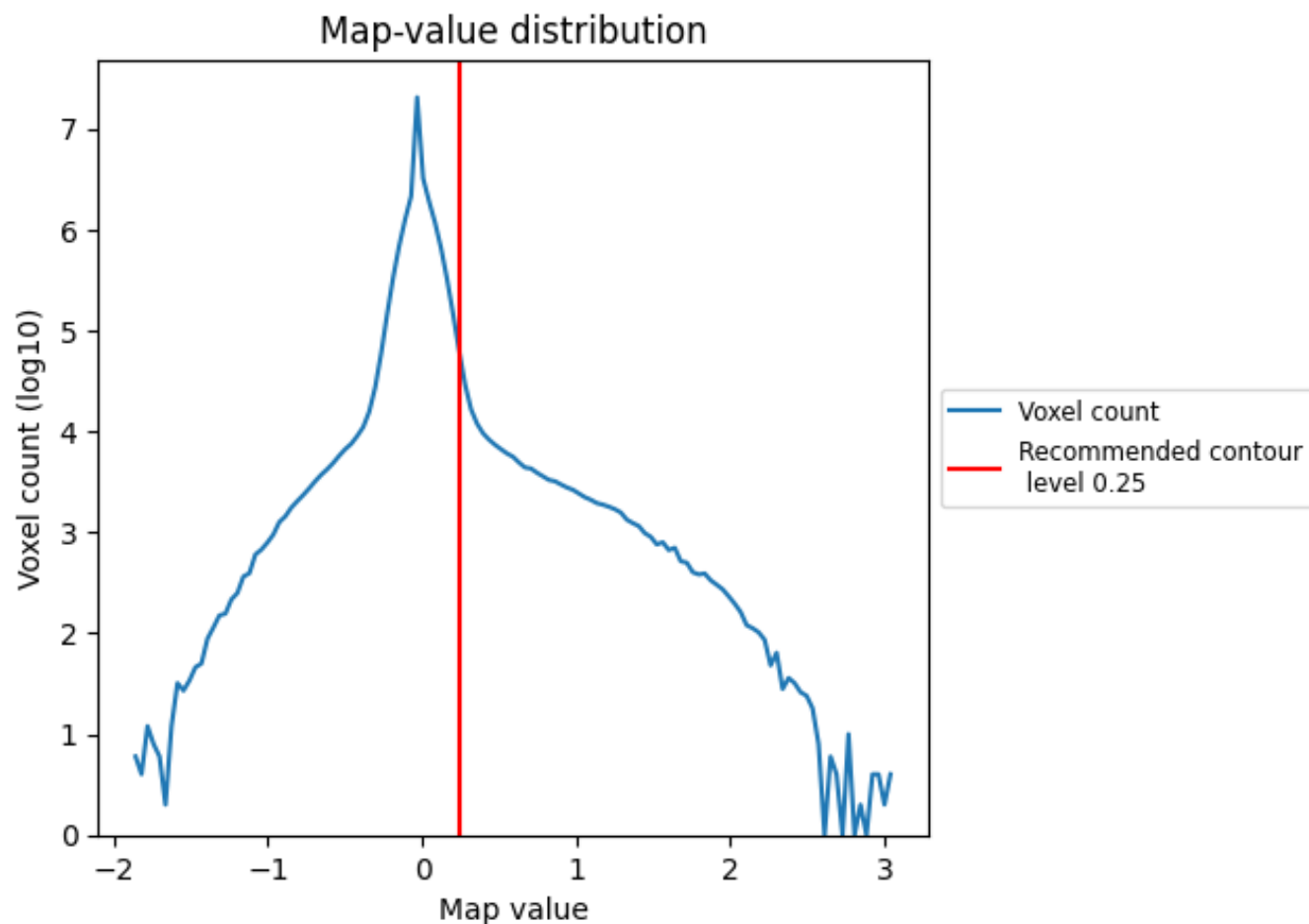
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

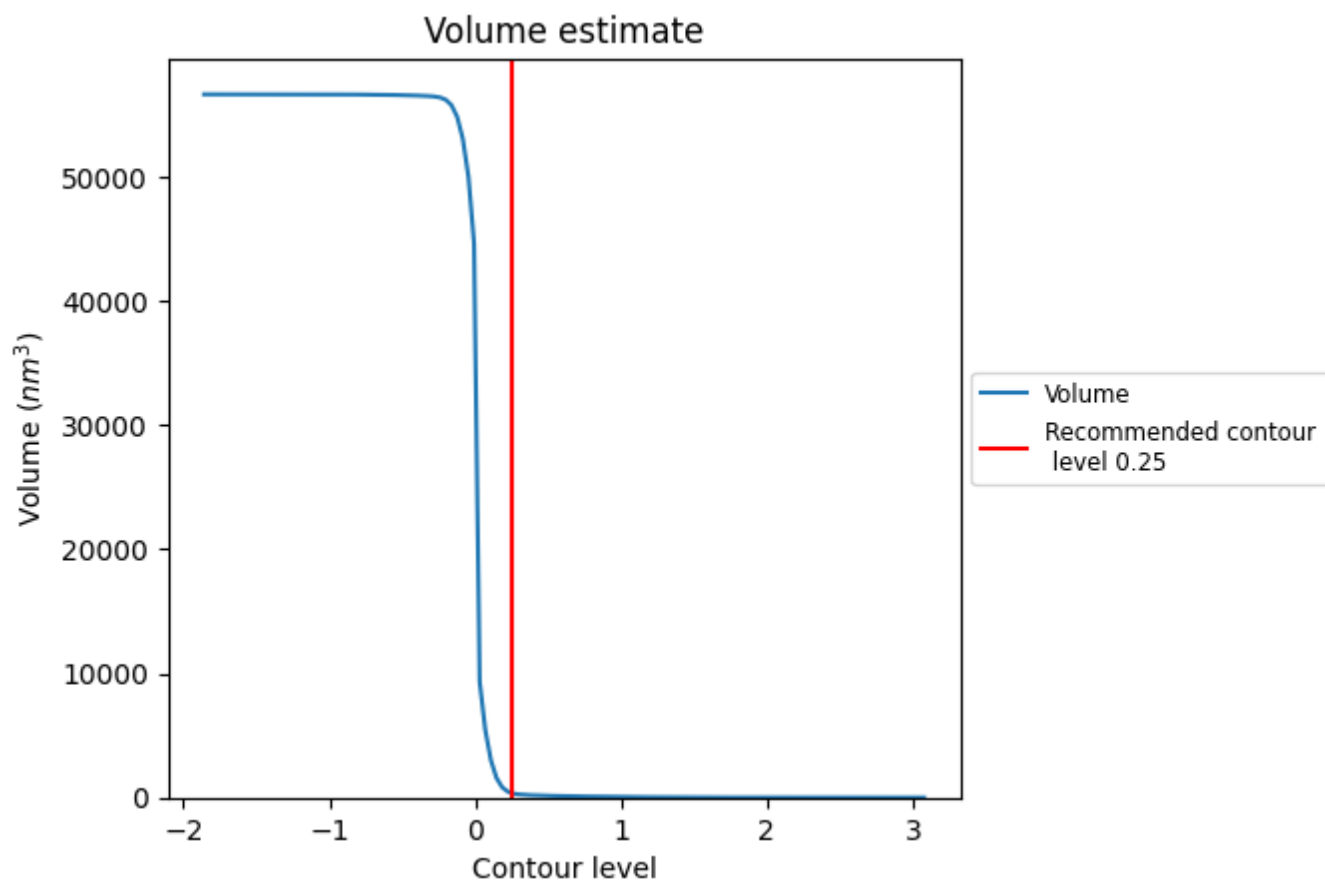
### 7.1 Map-value distribution [i](#)



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.



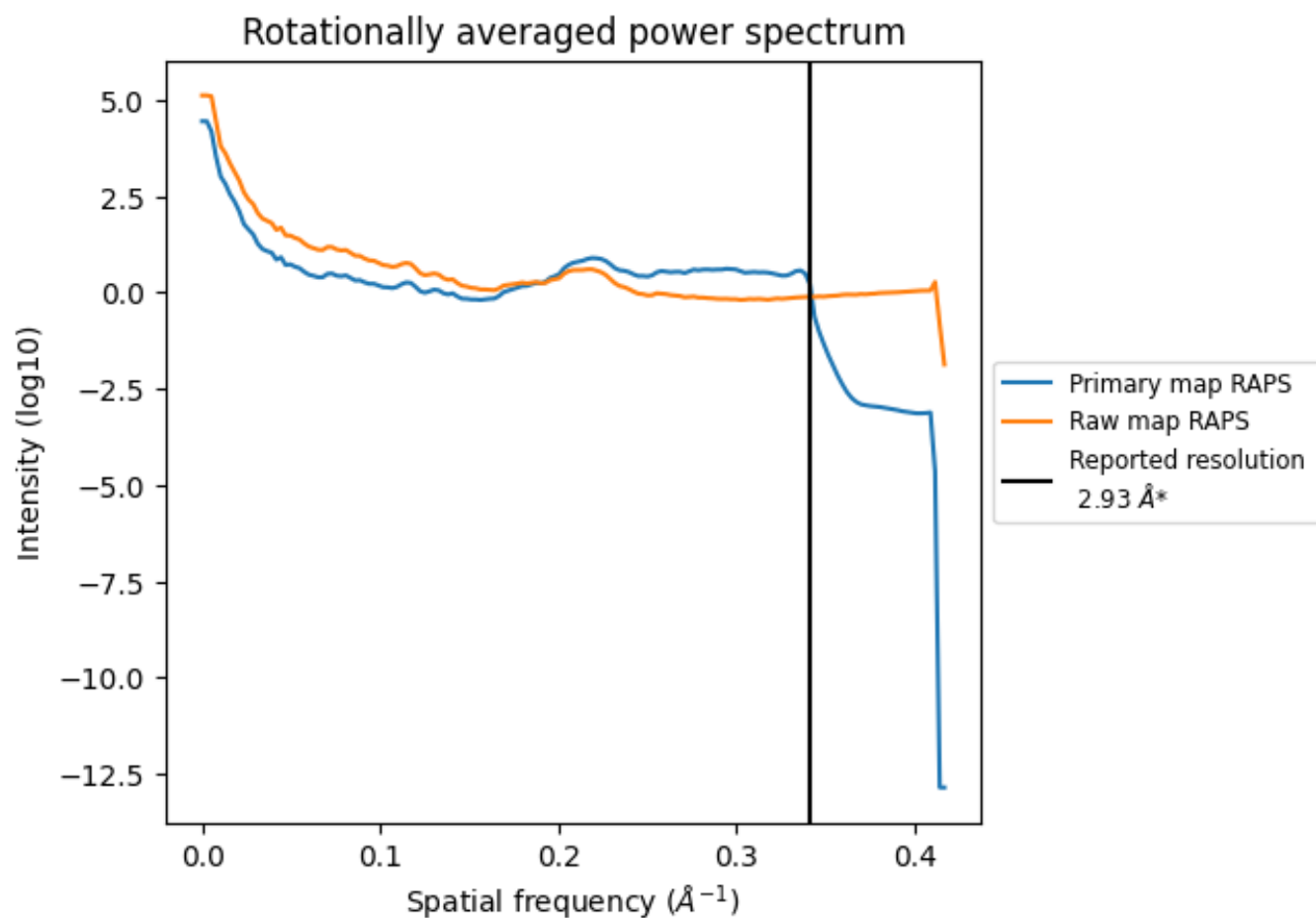
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 373 nm<sup>3</sup>; this corresponds to an approximate mass of 337 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

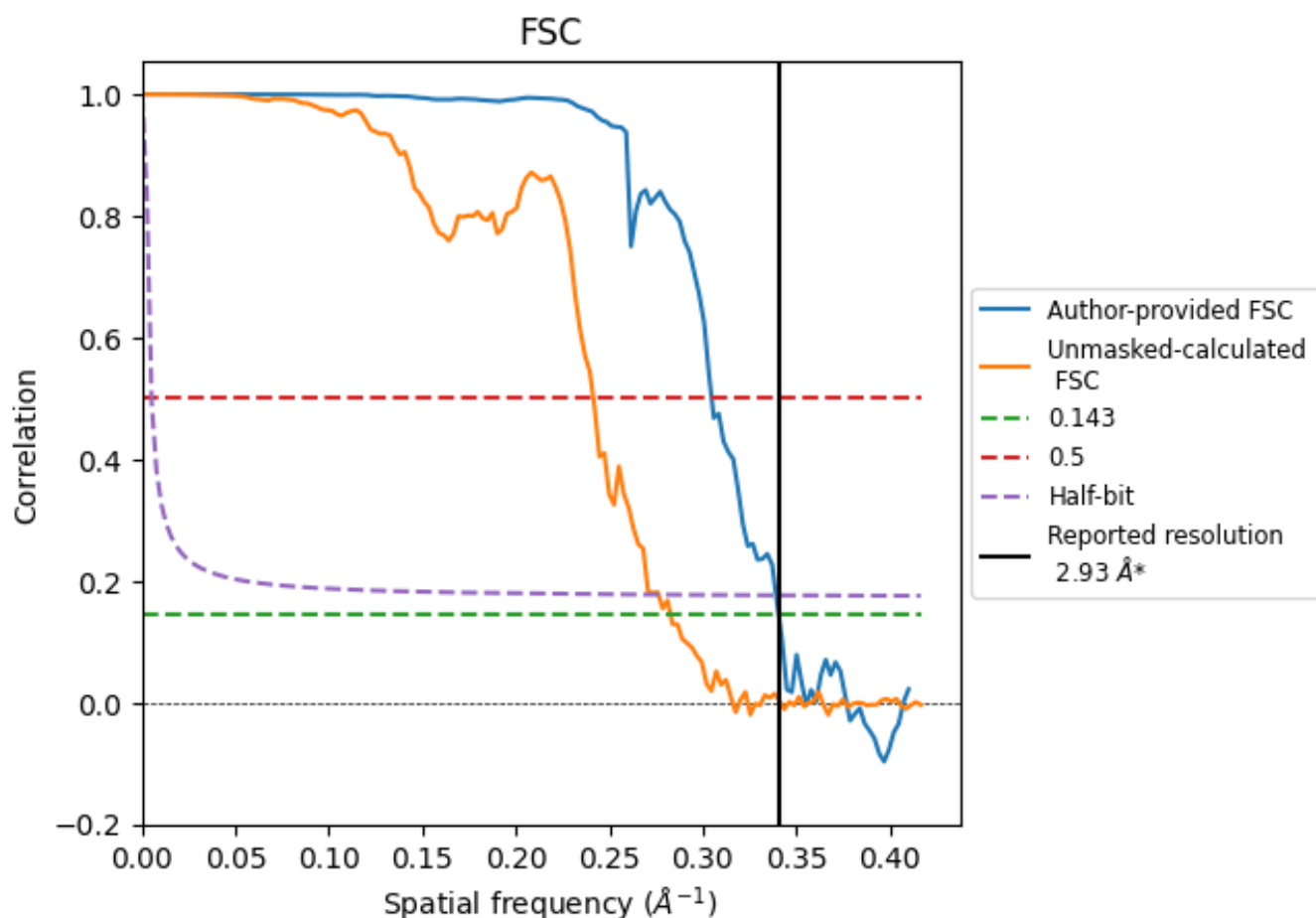


\*Reported resolution corresponds to spatial frequency of  $0.341 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.341 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

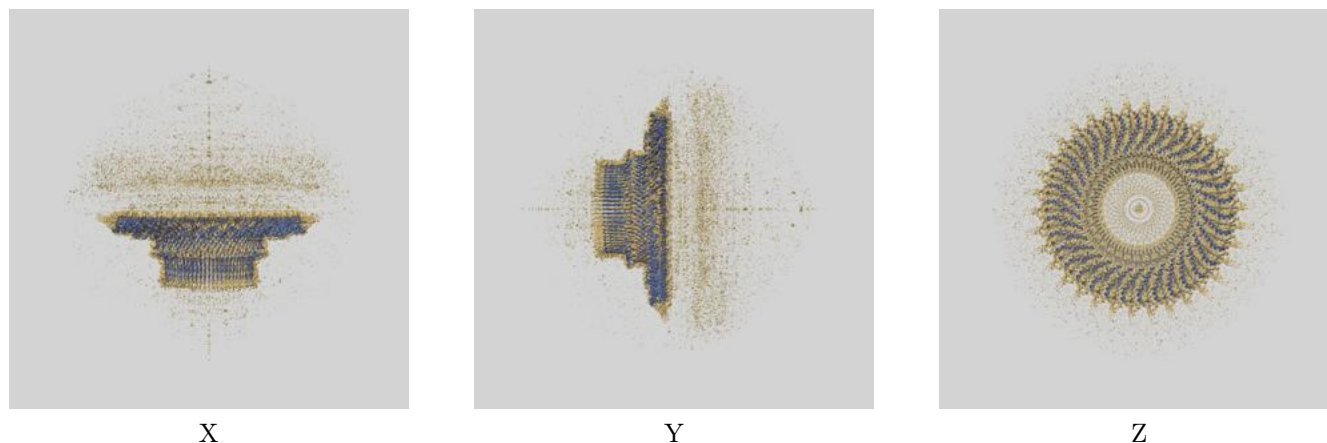
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.93	3.28	2.95
Unmasked-calculated*	3.53	4.14	3.62

\*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 3.53 differs from the reported value 2.93 by more than 10 %

## 9 Map-model fit [i](#)

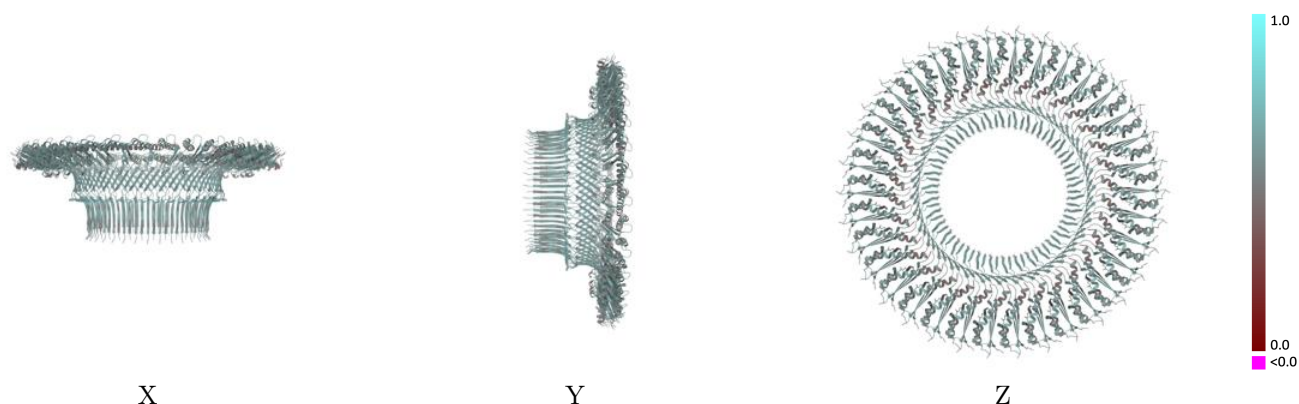
This section contains information regarding the fit between EMDB map EMD-39783 and PDB model 8Z5V. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



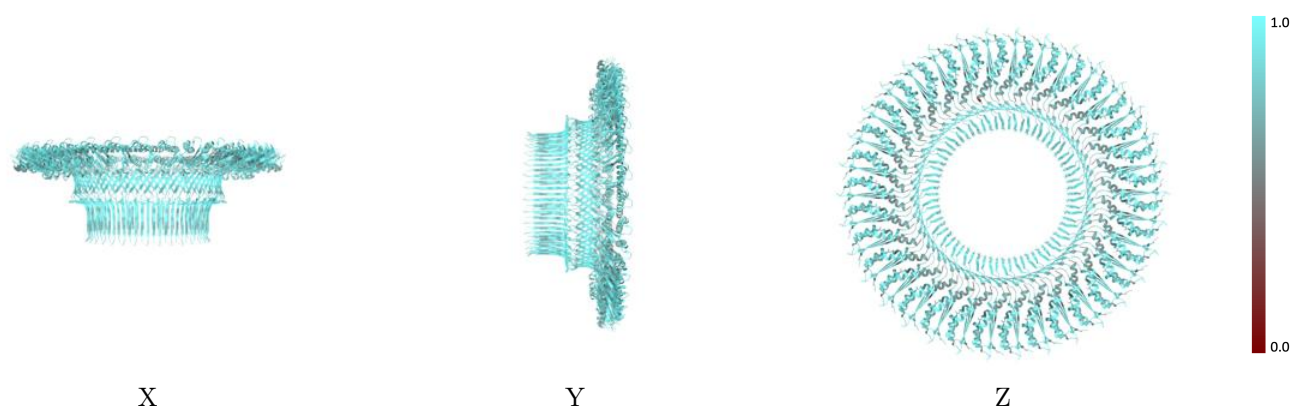
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



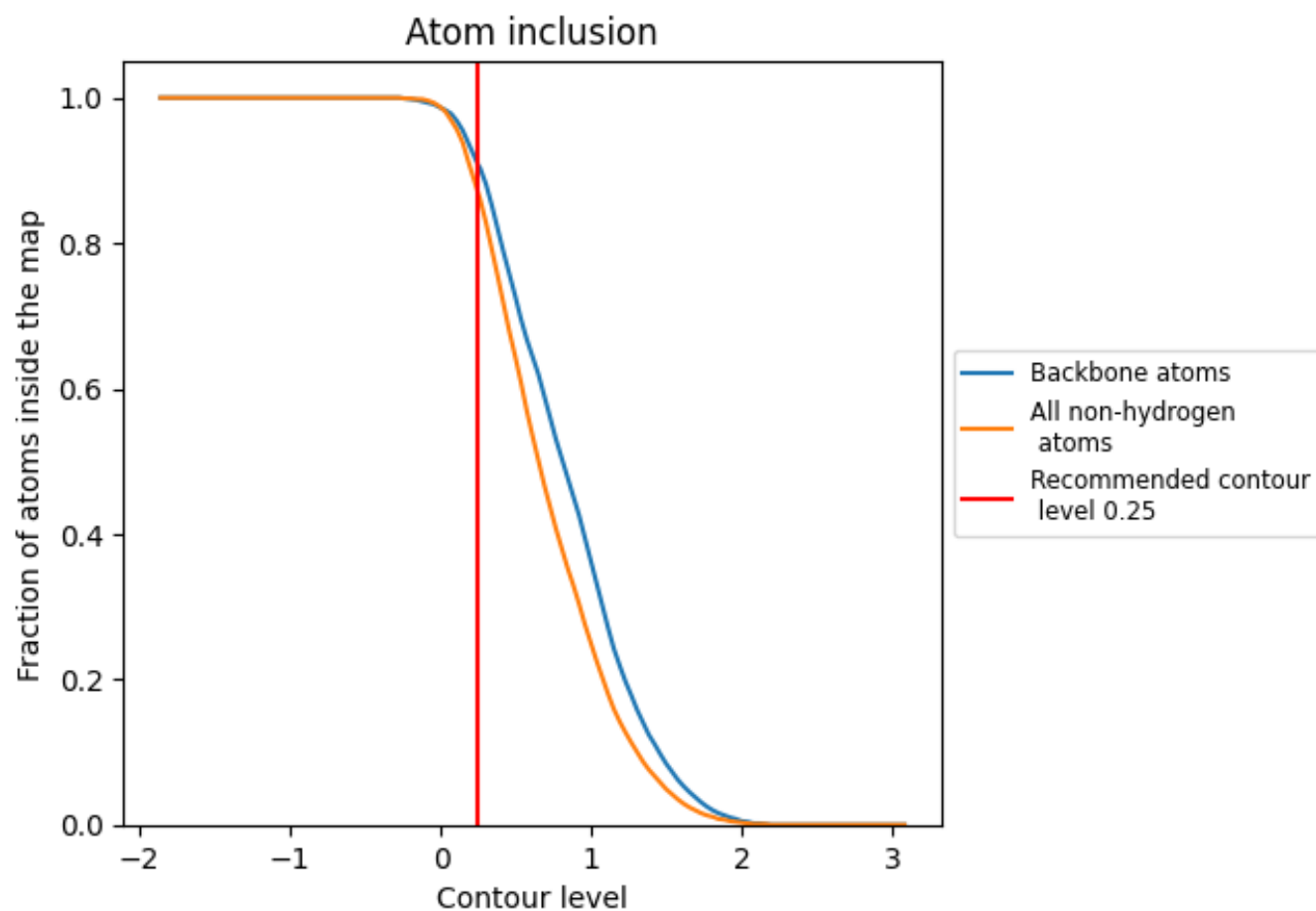
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.5590
A	 0.8670	 0.5570
B	 0.8750	 0.5590
C	 0.8720	 0.5590
D	 0.8690	 0.5580
E	 0.8640	 0.5580
F	 0.8720	 0.5570
G	 0.8610	 0.5570
H	 0.8670	 0.5570
I	 0.8700	 0.5600
J	 0.8710	 0.5590
K	 0.8660	 0.5580
L	 0.8670	 0.5580
M	 0.8630	 0.5590
N	 0.8670	 0.5590
O	 0.8630	 0.5580
P	 0.8670	 0.5570
Q	 0.8700	 0.5630
R	 0.8650	 0.5600
S	 0.8690	 0.5600
T	 0.8700	 0.5600
U	 0.8690	 0.5610
V	 0.8650	 0.5600
W	 0.8670	 0.5600
X	 0.8670	 0.5590
Y	 0.8670	 0.5590
Z	 0.8700	 0.5600
a	 0.8720	 0.5590
b	 0.8640	 0.5590
c	 0.8680	 0.5570
d	 0.8670	 0.5590
e	 0.8670	 0.5600
f	 0.8660	 0.5590
g	 0.8660	 0.5560
h	 0.8700	 0.5600

