



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:37 PM UTC

PDB ID : 8FTE / pdb_00008fte
EMDB ID : EMD-29424
Title : CryoEM strucutre of 22-mer RBM2 of the Salmonella MS-ring
Authors : Singh, P.S.; Nakagawa, T.; Cecchini, G.; Iverson, T.M.
Deposited on : 2023-01-12
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

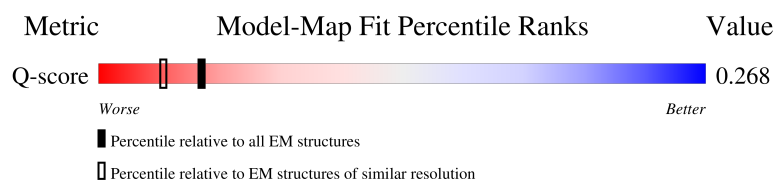
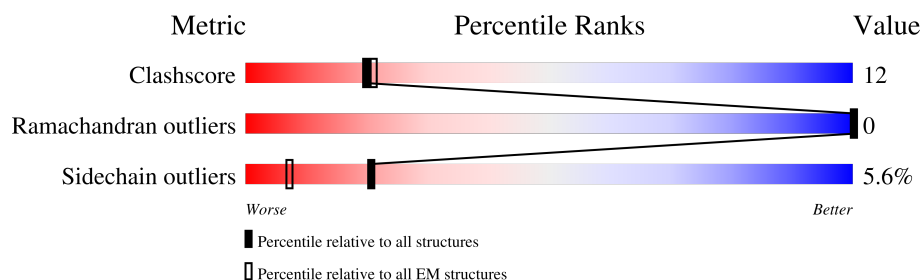
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



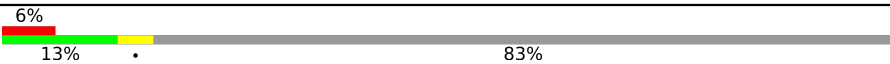
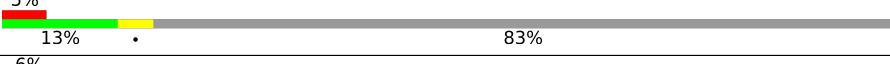
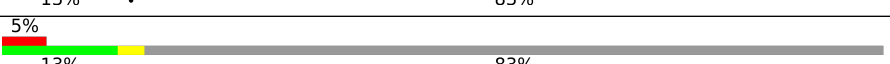
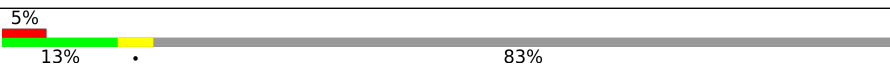
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	
1	C	560	
1	D	560	

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Mol	Chain	Length	Quality of chain
1	E	560	
1	F	560	
1	G	560	
1	H	560	
1	I	560	
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	V	560	
1	W	560	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 14564 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.

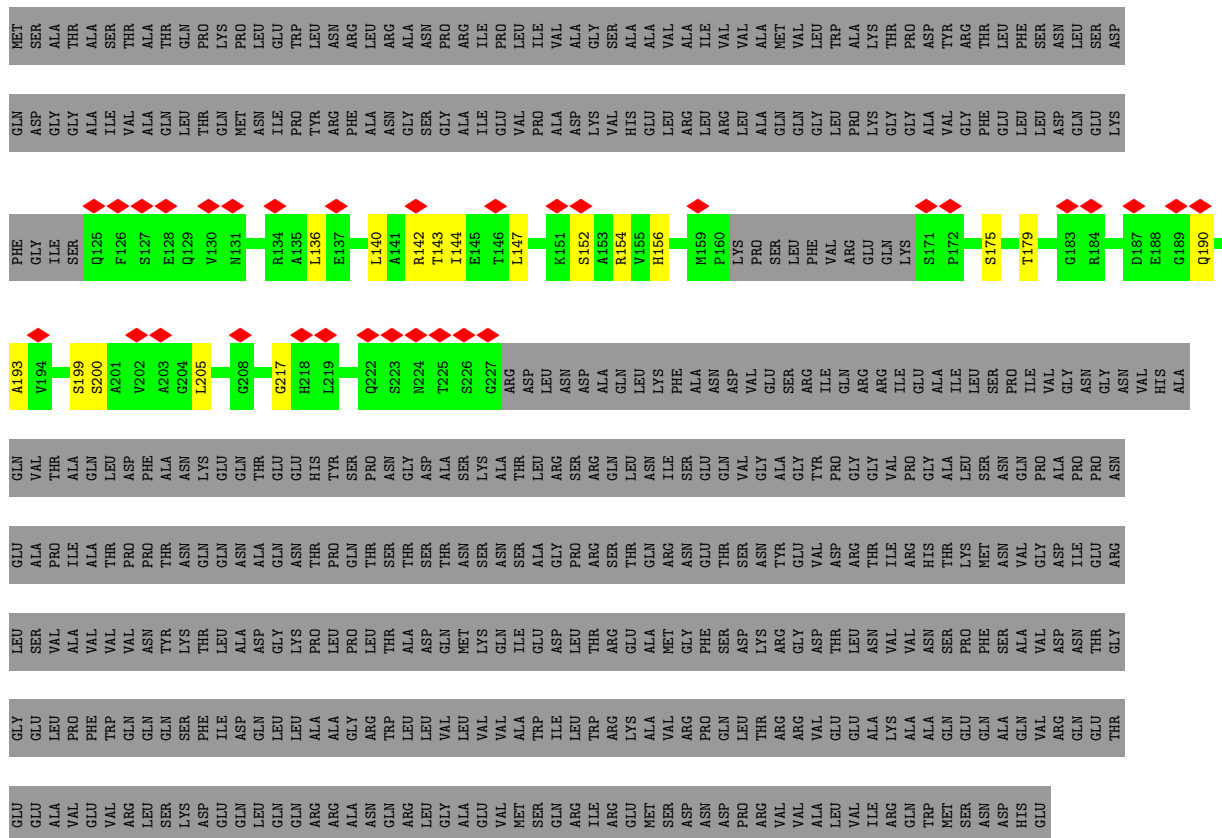
- Molecule 1 is a protein called Flagellar M-ring protein.

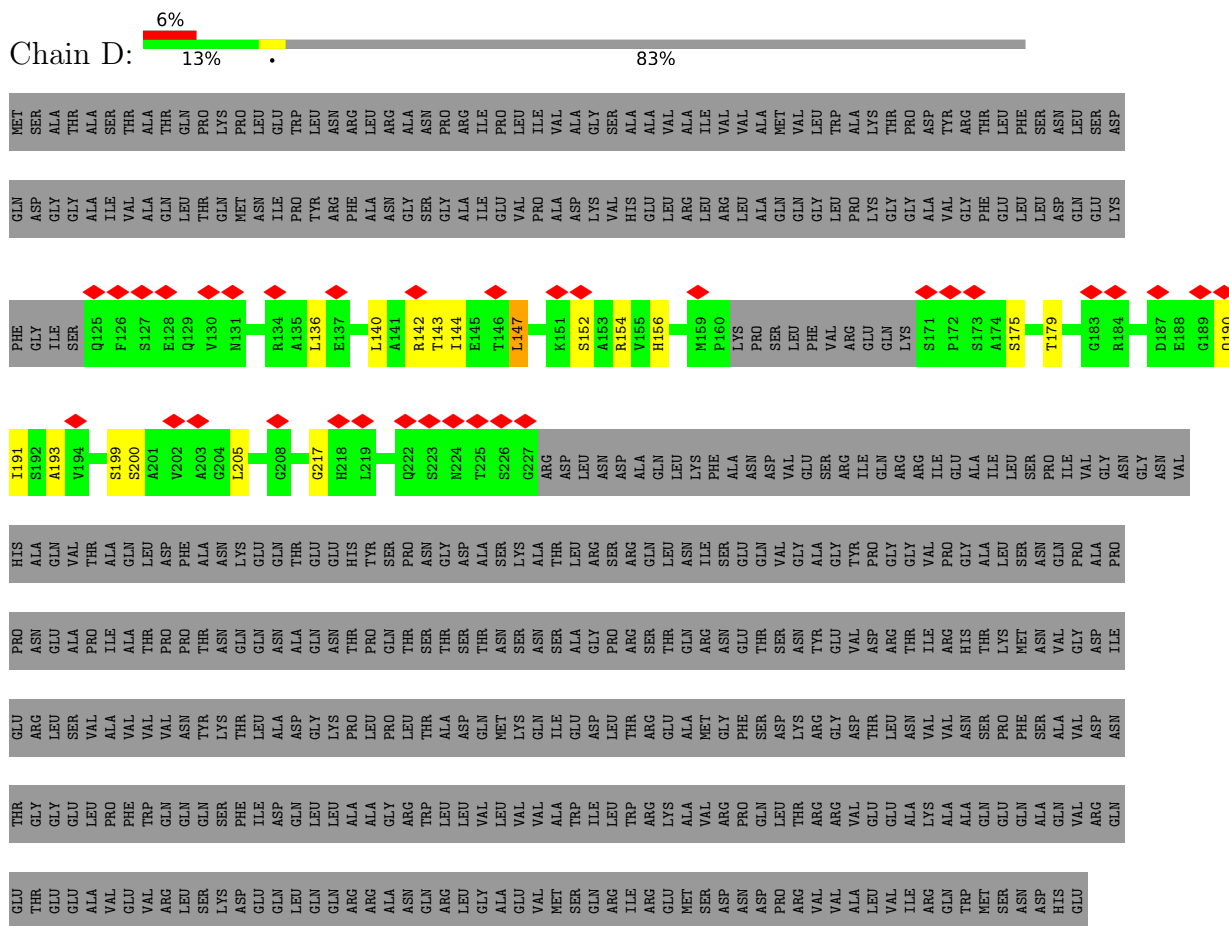
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	B	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	C	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	D	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	E	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	F	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	G	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	H	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	I	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	J	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	K	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	L	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	M	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	N	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	O	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	P	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	Q	93	Total 662	C 409	N 119	O 133	S 1	0	0

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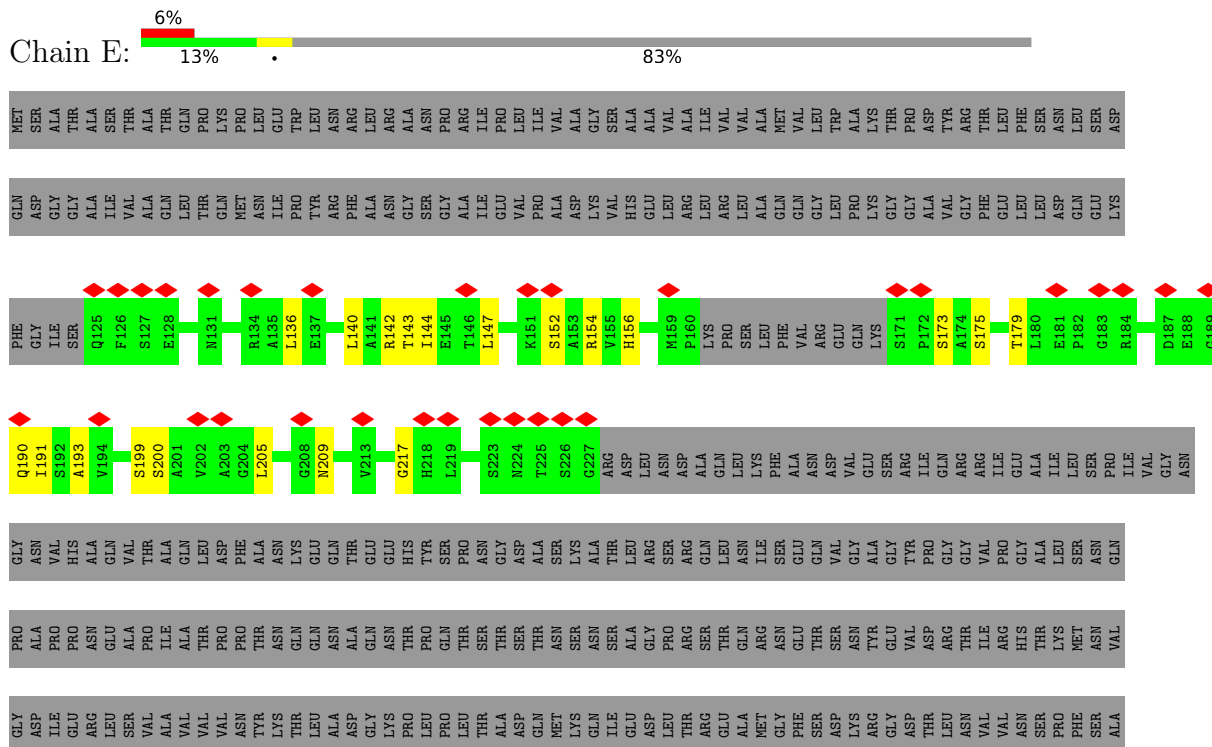
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	S	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	T	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	V	93	Total 662	C 409	N 119	O 133	S 1	0	0
1	W	93	Total 662	C 409	N 119	O 133	S 1	0	0





- Molecule 1: Flagellar M-ring protein

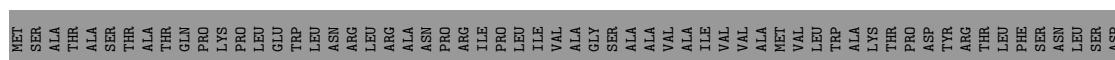


GLU

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



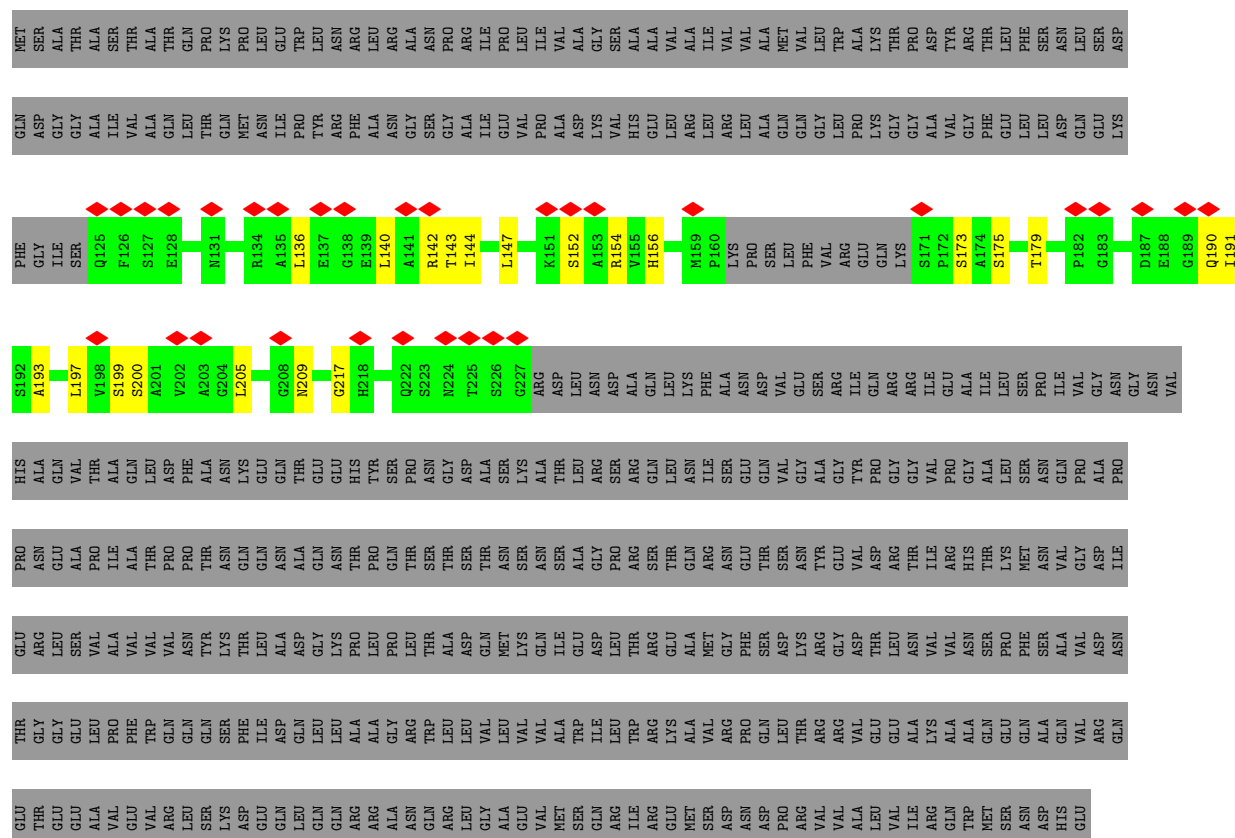
Sequence logo for the 1000bp upstream region of the human POU3F1 gene. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows amino acid positions from -1000 to +1000. Red diamonds indicate positions with significant enrichment of a specific amino acid. The legend shows the amino acids: PHE, GLY, ILE, SER, Q125, F126, S127, E128, M131, R134, A135, L136, L140, T142, I144, E145, T146, L147, K151, S152, A153, R154, V155, H156, M159, P160, LYS, PRO, SER, LEU, PHE, VAL, ARG, GLU, GLN, LYS, S171, P172, S173, A174, S175, T179, G183, D187, Q190, I191, S192, A193, V194.

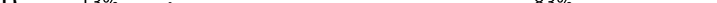


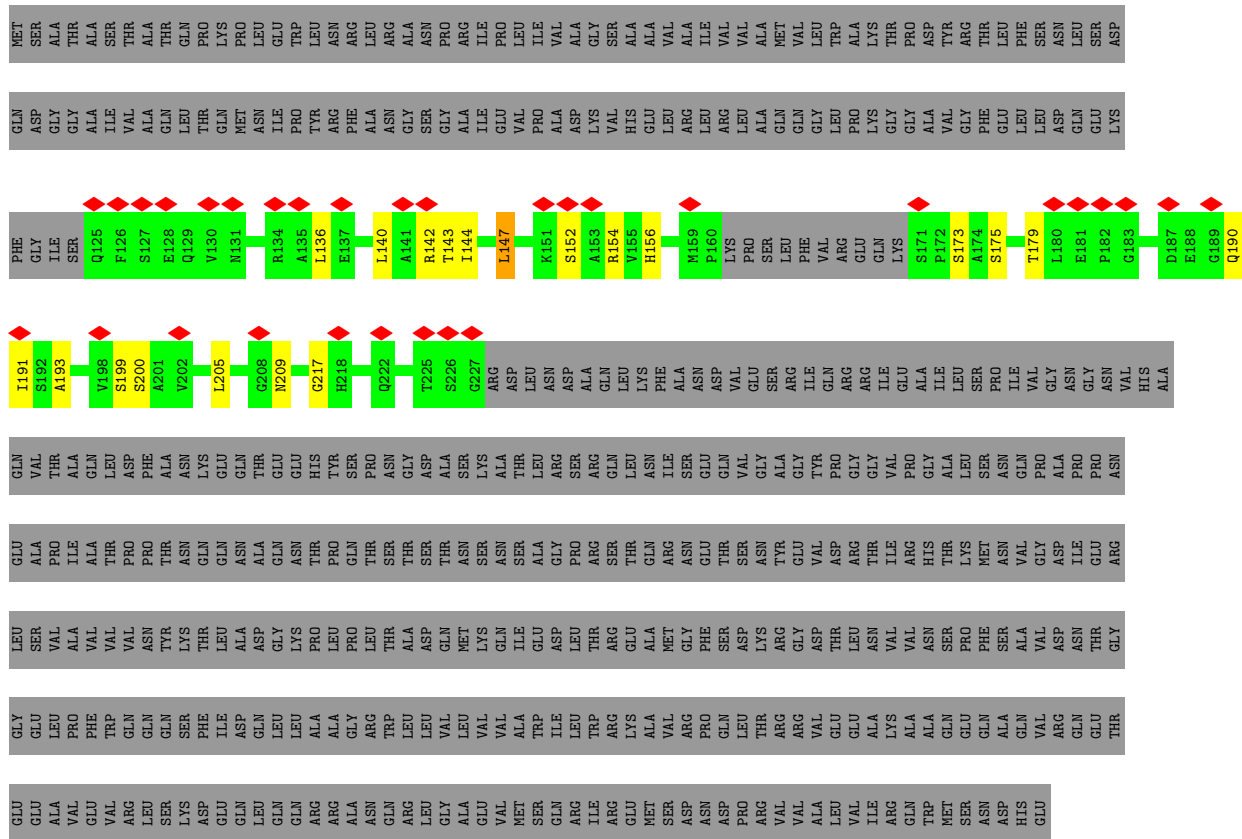


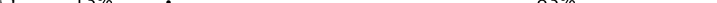
Chain K: 6% 13% . 83%

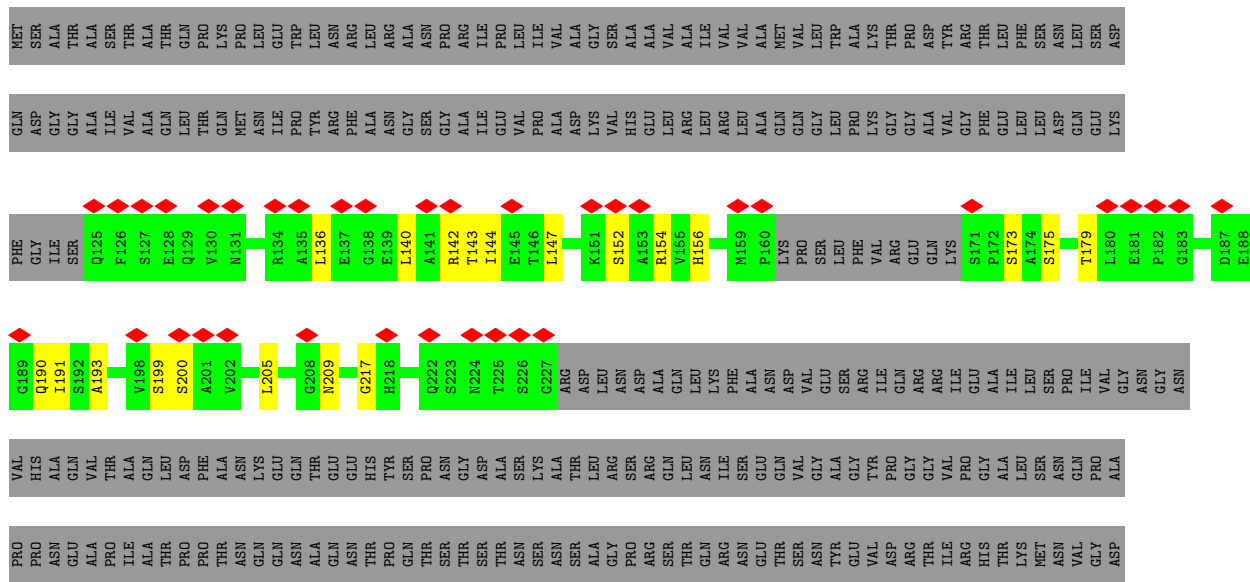




Chain R:  6% 13% 83%



Chain S:  6% 13% 83%

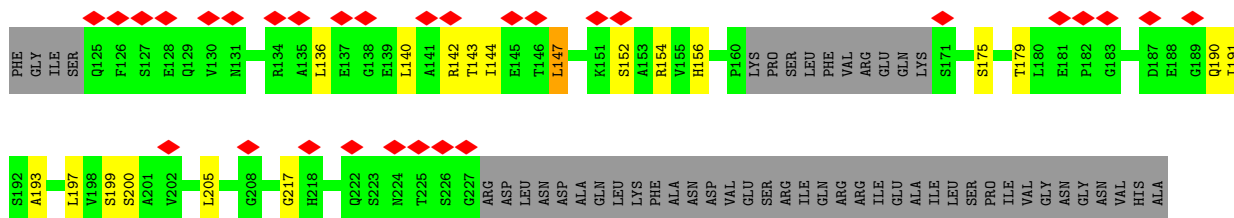


GLN
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THR
GLU
GLU
GLU
ALA
VAL
GLU
VAL
ARG
LEU
SER
LYS
ASP
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GLN
LEU
GLN
GLN
ARG
ARG
ALA
ASN
GLN
ARG
MET
SER
GLN
ARG
ILE
GLU
MET
SER
ASP
ASN
ASP
PRO
ARG
VAL
VAL
ALA
LEU
ILE
ILE
GLN
GLN
TRP
MET
SER
ASN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

- Molecule 1: Flagellar M-ring protein



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



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

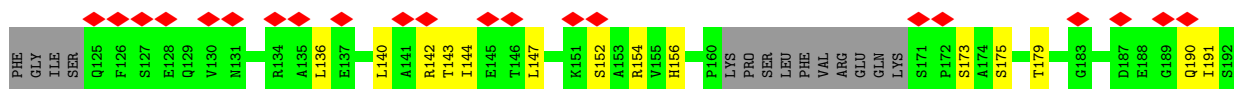
GLU GLU ALA ALA VAL VAL VAL LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ARG ALA ALA ASN ARG LEU GLY GLU VAL MET SER GLN ARG ARG ILE ARG GLU MET SER ASP ASN ASP PRO ARG VAL VAL ALA LEU LEU ILE ARG GLN TRP MET SER ASN ASP HIS GLU

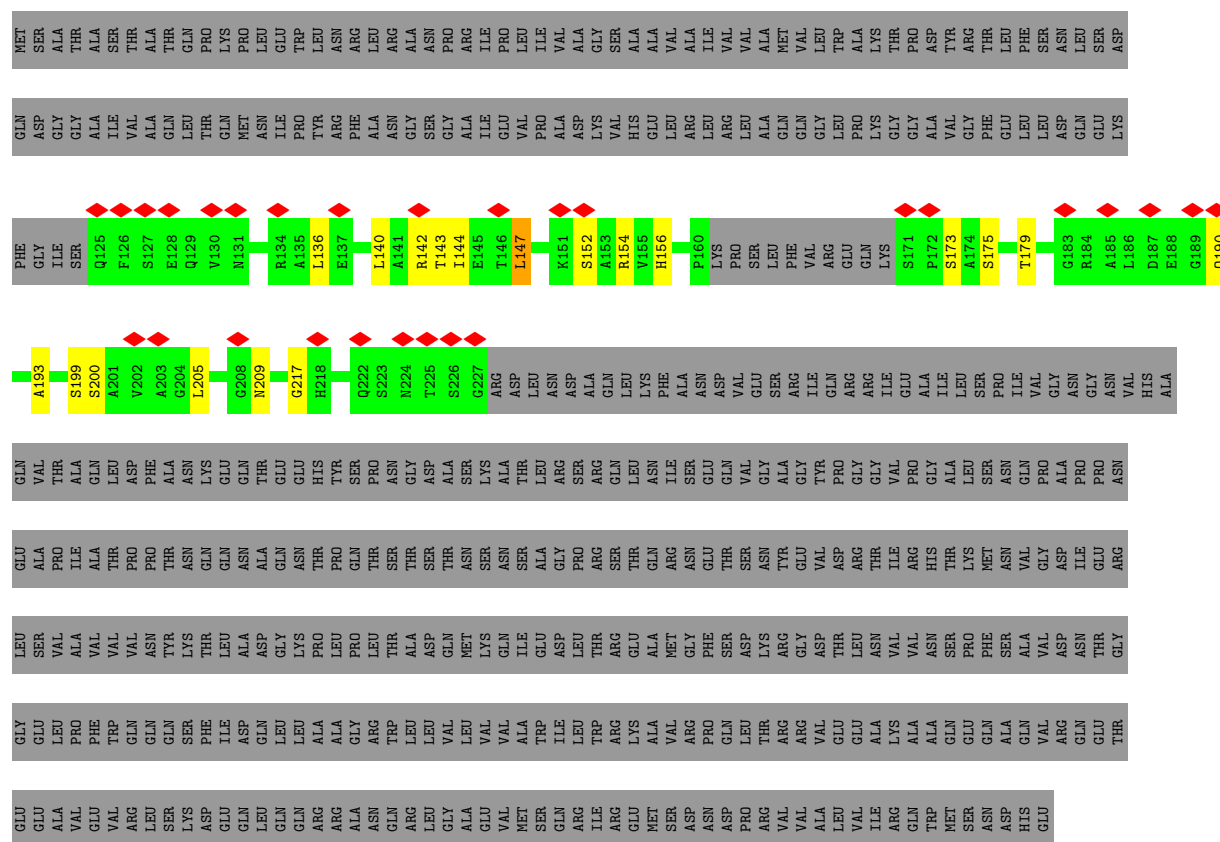
- Molecule 1: Flagellar M-ring protein



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C22	Depositor
Number of particles used	100096	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)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	60.906	Depositor
Minimum map value	-47.601	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	11.9	Depositor
Map size (Å)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.15	0/671	0.37	0/916
1	B	0.15	0/671	0.37	0/916
1	C	0.19	0/671	0.38	0/916
1	D	0.15	0/671	0.37	0/916
1	E	0.15	0/671	0.37	0/916
1	F	0.16	0/671	0.37	0/916
1	G	0.15	0/671	0.37	0/916
1	H	0.15	0/671	0.37	0/916
1	I	0.15	0/671	0.37	0/916
1	J	0.15	0/671	0.37	0/916
1	K	0.15	0/671	0.37	0/916
1	L	0.15	0/671	0.37	0/916
1	M	0.15	0/671	0.37	0/916
1	N	0.15	0/671	0.37	0/916
1	O	0.15	0/671	0.37	0/916
1	P	0.15	0/671	0.37	0/916
1	Q	0.15	0/671	0.37	0/916
1	R	0.15	0/671	0.37	0/916
1	S	0.15	0/671	0.37	0/916
1	T	0.16	0/671	0.37	0/916
1	V	0.15	0/671	0.37	0/916
1	W	0.15	0/671	0.37	0/916
All	All	0.16	0/14762	0.37	0/20152

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	662	0	653	30	0
1	B	662	0	653	28	0
1	C	662	0	653	25	0
1	D	662	0	653	27	0
1	E	662	0	653	27	0
1	F	662	0	653	28	0
1	G	662	0	653	29	0
1	H	662	0	653	27	0
1	I	662	0	653	26	0
1	J	662	0	653	29	0
1	K	662	0	653	27	0
1	L	662	0	653	27	0
1	M	662	0	653	27	0
1	N	662	0	653	27	0
1	O	662	0	653	28	0
1	P	662	0	653	29	0
1	Q	662	0	653	28	0
1	R	662	0	653	28	0
1	S	662	0	653	28	0
1	T	662	0	653	28	0
1	V	662	0	653	28	0
1	W	662	0	653	28	0
All	All	14564	0	14366	358	0

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

All (358) 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:S:217:GLY:HA2	1:T:190:GLN:CB	2.00	0.92
1:I:217:GLY:CA	1:J:190:GLN:CB	2.49	0.91
1:S:217:GLY:CA	1:T:190:GLN:CB	2.48	0.91
1:B:217:GLY:HA2	1:C:190:GLN:CB	2.02	0.90
1:I:217:GLY:HA2	1:J:190:GLN:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:CB	1:W:217:GLY:CA	2.50	0.89
1:A:217:GLY:HA2	1:B:190:GLN:CB	2.02	0.89
1:F:217:GLY:CA	1:G:190:GLN:CB	2.51	0.89
1:A:217:GLY:CA	1:B:190:GLN:CB	2.50	0.89
1:O:217:GLY:HA2	1:P:190:GLN:CB	2.02	0.89
1:C:217:GLY:CA	1:D:190:GLN:CB	2.50	0.89
1:A:190:GLN:CB	1:W:217:GLY:HA2	2.02	0.89
1:C:217:GLY:HA2	1:D:190:GLN:CB	2.03	0.89
1:G:217:GLY:CA	1:H:190:GLN:CB	2.51	0.88
1:V:217:GLY:CA	1:W:190:GLN:CB	2.50	0.88
1:D:154:ARG:NH1	1:E:142:ARG:NH2	2.20	0.88
1:K:217:GLY:CA	1:L:190:GLN:CB	2.52	0.88
1:M:217:GLY:CA	1:N:190:GLN:CB	2.51	0.88
1:P:217:GLY:CA	1:Q:190:GLN:CB	2.50	0.88
1:P:217:GLY:HA2	1:Q:190:GLN:CB	2.03	0.88
1:V:217:GLY:HA2	1:W:190:GLN:CB	2.03	0.88
1:H:154:ARG:NH1	1:I:142:ARG:NH2	2.21	0.88
1:R:217:GLY:HA2	1:S:190:GLN:CB	2.04	0.88
1:J:217:GLY:CA	1:K:190:GLN:CB	2.51	0.88
1:Q:217:GLY:HA2	1:R:190:GLN:CB	2.04	0.88
1:B:217:GLY:CA	1:C:190:GLN:CB	2.50	0.88
1:J:217:GLY:HA2	1:K:190:GLN:CB	2.03	0.88
1:N:217:GLY:CA	1:O:190:GLN:CB	2.52	0.88
1:D:154:ARG:NH1	1:E:142:ARG:CZ	2.36	0.88
1:M:154:ARG:NH1	1:N:142:ARG:NH2	2.22	0.88
1:E:217:GLY:CA	1:F:190:GLN:CB	2.51	0.88
1:E:217:GLY:HA2	1:F:190:GLN:CB	2.04	0.87
1:F:217:GLY:HA2	1:G:190:GLN:CB	2.03	0.87
1:G:217:GLY:HA2	1:H:190:GLN:CB	2.03	0.87
1:Q:154:ARG:NH1	1:R:142:ARG:NH2	2.22	0.87
1:Q:154:ARG:NH1	1:R:142:ARG:CZ	2.37	0.87
1:Q:217:GLY:CA	1:R:190:GLN:CB	2.51	0.87
1:R:217:GLY:CA	1:S:190:GLN:CB	2.51	0.87
1:L:154:ARG:NH1	1:M:142:ARG:NH2	2.23	0.87
1:O:217:GLY:CA	1:P:190:GLN:CB	2.51	0.87
1:L:217:GLY:CA	1:M:190:GLN:CB	2.52	0.87
1:D:217:GLY:CA	1:E:190:GLN:CB	2.52	0.87
1:K:154:ARG:NH1	1:L:142:ARG:NH2	2.23	0.87
1:C:154:ARG:NH1	1:D:142:ARG:CZ	2.37	0.87
1:K:217:GLY:HA2	1:L:190:GLN:CB	2.04	0.87
1:T:154:ARG:NH1	1:V:142:ARG:NH2	2.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:154:ARG:NH1	1:W:142:ARG:CZ	2.37	0.87
1:G:154:ARG:NH1	1:H:142:ARG:CZ	2.38	0.86
1:N:154:ARG:NH1	1:O:142:ARG:NH2	2.23	0.86
1:L:217:GLY:HA2	1:M:190:GLN:CB	2.04	0.86
1:A:154:ARG:NH1	1:B:142:ARG:CZ	2.38	0.86
1:C:154:ARG:NH1	1:D:142:ARG:NH2	2.22	0.86
1:M:154:ARG:NH1	1:N:142:ARG:CZ	2.38	0.86
1:M:217:GLY:HA2	1:N:190:GLN:CB	2.04	0.86
1:P:154:ARG:NH1	1:Q:142:ARG:NH2	2.23	0.86
1:A:142:ARG:CZ	1:W:154:ARG:NH1	2.38	0.86
1:D:217:GLY:HA2	1:E:190:GLN:CB	2.06	0.86
1:E:154:ARG:NH1	1:F:142:ARG:CZ	2.38	0.86
1:H:217:GLY:CA	1:I:190:GLN:CB	2.54	0.86
1:I:154:ARG:NH1	1:J:142:ARG:NH2	2.23	0.86
1:P:154:ARG:NH1	1:Q:142:ARG:CZ	2.39	0.86
1:R:154:ARG:NH1	1:S:142:ARG:NH2	2.23	0.86
1:I:154:ARG:NH1	1:J:142:ARG:CZ	2.37	0.86
1:N:217:GLY:HA2	1:O:190:GLN:CB	2.04	0.86
1:H:154:ARG:NH1	1:I:142:ARG:CZ	2.38	0.86
1:F:154:ARG:NH1	1:G:142:ARG:CZ	2.39	0.86
1:G:154:ARG:NH1	1:H:142:ARG:NH2	2.23	0.86
1:J:154:ARG:NH1	1:K:142:ARG:NH2	2.24	0.86
1:K:154:ARG:NH1	1:L:142:ARG:CZ	2.39	0.86
1:N:154:ARG:NH1	1:O:142:ARG:CZ	2.39	0.86
1:V:154:ARG:NH1	1:W:142:ARG:NH2	2.22	0.86
1:R:154:ARG:NH1	1:S:142:ARG:CZ	2.39	0.85
1:A:154:ARG:NH1	1:B:142:ARG:NH2	2.24	0.85
1:L:154:ARG:NH1	1:M:142:ARG:CZ	2.39	0.85
1:E:154:ARG:NH1	1:F:142:ARG:NH2	2.23	0.85
1:B:154:ARG:NH1	1:C:142:ARG:CZ	2.39	0.85
1:T:154:ARG:NH1	1:V:142:ARG:CZ	2.39	0.85
1:T:217:GLY:CA	1:V:190:GLN:CB	2.54	0.85
1:T:217:GLY:HA2	1:V:190:GLN:CB	2.06	0.85
1:A:142:ARG:NH2	1:W:154:ARG:NH1	2.23	0.85
1:F:154:ARG:NH1	1:G:142:ARG:NH2	2.24	0.84
1:H:217:GLY:HA2	1:I:190:GLN:CB	2.07	0.84
1:O:154:ARG:NH1	1:P:142:ARG:NH2	2.25	0.84
1:J:154:ARG:NH1	1:K:142:ARG:CZ	2.39	0.84
1:O:154:ARG:NH1	1:P:142:ARG:CZ	2.41	0.84
1:S:154:ARG:NH1	1:T:142:ARG:CZ	2.40	0.84
1:B:154:ARG:NH1	1:C:142:ARG:NH2	2.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:154:ARG:NH1	1:T:142:ARG:NH2	2.26	0.83
1:S:175:SER:HB2	1:T:200:SER:OG	1.79	0.82
1:I:175:SER:HB2	1:J:200:SER:OG	1.80	0.82
1:A:175:SER:HB2	1:B:200:SER:OG	1.81	0.81
1:F:175:SER:HB2	1:G:200:SER:OG	1.82	0.80
1:G:175:SER:HB2	1:H:200:SER:OG	1.82	0.80
1:A:200:SER:OG	1:W:175:SER:HB2	1.81	0.80
1:O:175:SER:HB2	1:P:200:SER:OG	1.81	0.80
1:I:217:GLY:HA3	1:J:190:GLN:CB	2.11	0.80
1:B:175:SER:HB2	1:C:200:SER:OG	1.81	0.80
1:P:175:SER:HB2	1:Q:200:SER:OG	1.82	0.80
1:J:175:SER:HB2	1:K:200:SER:OG	1.82	0.80
1:C:175:SER:HB2	1:D:200:SER:OG	1.82	0.80
1:E:175:SER:HB2	1:F:200:SER:OG	1.82	0.80
1:M:175:SER:HB2	1:N:200:SER:OG	1.82	0.80
1:N:175:SER:HB2	1:O:200:SER:OG	1.82	0.80
1:K:175:SER:HB2	1:L:200:SER:OG	1.83	0.79
1:L:175:SER:HB2	1:M:200:SER:OG	1.83	0.79
1:Q:175:SER:HB2	1:R:200:SER:OG	1.82	0.79
1:A:190:GLN:CB	1:W:217:GLY:HA3	2.12	0.79
1:G:217:GLY:HA3	1:H:190:GLN:CB	2.13	0.79
1:R:175:SER:HB2	1:S:200:SER:OG	1.82	0.79
1:V:217:GLY:HA3	1:W:190:GLN:CB	2.12	0.79
1:C:217:GLY:HA3	1:D:190:GLN:CB	2.12	0.79
1:D:175:SER:HB2	1:E:200:SER:OG	1.83	0.79
1:F:217:GLY:HA3	1:G:190:GLN:CB	2.13	0.79
1:A:217:GLY:HA3	1:B:190:GLN:CB	2.12	0.79
1:V:175:SER:HB2	1:W:200:SER:OG	1.82	0.79
1:B:217:GLY:HA3	1:C:190:GLN:CB	2.13	0.78
1:E:217:GLY:HA3	1:F:190:GLN:CB	2.14	0.78
1:J:217:GLY:HA3	1:K:190:GLN:CB	2.14	0.78
1:S:217:GLY:HA3	1:T:190:GLN:CB	2.11	0.78
1:M:217:GLY:HA3	1:N:190:GLN:CB	2.13	0.78
1:D:217:GLY:HA3	1:E:190:GLN:CB	2.13	0.78
1:P:217:GLY:HA3	1:Q:190:GLN:CB	2.13	0.78
1:L:217:GLY:HA3	1:M:190:GLN:CB	2.14	0.78
1:H:175:SER:HB2	1:I:200:SER:OG	1.84	0.78
1:O:217:GLY:HA3	1:P:190:GLN:CB	2.14	0.78
1:Q:217:GLY:HA3	1:R:190:GLN:CB	2.13	0.77
1:K:217:GLY:HA3	1:L:190:GLN:CB	2.14	0.76
1:T:175:SER:HB2	1:V:200:SER:OG	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:GLY:HA3	1:I:190:GLN:CB	2.16	0.76
1:R:217:GLY:HA3	1:S:190:GLN:CB	2.14	0.76
1:N:217:GLY:HA3	1:O:190:GLN:CB	2.14	0.75
1:T:217:GLY:HA3	1:V:190:GLN:CB	2.16	0.73
1:D:154:ARG:CZ	1:E:142:ARG:NH2	2.52	0.72
1:Q:154:ARG:CZ	1:R:142:ARG:NH2	2.54	0.71
1:M:154:ARG:CZ	1:N:142:ARG:NH2	2.54	0.71
1:C:154:ARG:CZ	1:D:142:ARG:NH2	2.53	0.70
1:G:154:ARG:CZ	1:H:142:ARG:NH2	2.54	0.70
1:I:154:ARG:CZ	1:J:142:ARG:NH2	2.53	0.70
1:V:154:ARG:CZ	1:W:142:ARG:NH2	2.53	0.70
1:A:154:ARG:CZ	1:B:142:ARG:NH2	2.54	0.70
1:H:154:ARG:CZ	1:I:142:ARG:NH2	2.54	0.70
1:A:142:ARG:NH2	1:W:154:ARG:CZ	2.54	0.70
1:P:154:ARG:CZ	1:Q:142:ARG:NH2	2.55	0.70
1:E:154:ARG:CZ	1:F:142:ARG:NH2	2.55	0.70
1:N:154:ARG:CZ	1:O:142:ARG:NH2	2.55	0.69
1:K:154:ARG:CZ	1:L:142:ARG:NH2	2.55	0.69
1:B:154:ARG:CZ	1:C:142:ARG:NH2	2.56	0.69
1:R:154:ARG:CZ	1:S:142:ARG:NH2	2.55	0.69
1:T:154:ARG:CZ	1:V:142:ARG:NH2	2.55	0.68
1:F:154:ARG:CZ	1:G:142:ARG:NH2	2.56	0.68
1:L:154:ARG:CZ	1:M:142:ARG:NH2	2.55	0.68
1:J:154:ARG:CZ	1:K:142:ARG:NH2	2.56	0.68
1:O:154:ARG:CZ	1:P:142:ARG:NH2	2.57	0.68
1:S:154:ARG:CZ	1:T:142:ARG:NH2	2.56	0.67
1:D:154:ARG:CZ	1:E:142:ARG:HH21	2.10	0.64
1:M:154:ARG:CZ	1:N:142:ARG:HH21	2.11	0.63
1:C:154:ARG:CZ	1:D:142:ARG:HH21	2.11	0.63
1:A:154:ARG:CZ	1:B:142:ARG:HH21	2.12	0.63
1:D:154:ARG:HH12	1:E:142:ARG:NE	1.97	0.62
1:Q:154:ARG:CZ	1:R:142:ARG:HH21	2.11	0.62
1:I:154:ARG:HH12	1:J:142:ARG:NE	1.97	0.62
1:V:154:ARG:CZ	1:W:142:ARG:HH21	2.11	0.62
1:C:154:ARG:HH12	1:D:142:ARG:NE	1.98	0.62
1:H:154:ARG:CZ	1:I:142:ARG:HH21	2.11	0.62
1:V:154:ARG:HH12	1:W:142:ARG:NE	1.97	0.62
1:A:142:ARG:NE	1:W:154:ARG:HH12	1.98	0.62
1:M:154:ARG:HH12	1:N:142:ARG:NE	1.98	0.62
1:N:154:ARG:CZ	1:O:142:ARG:HH21	2.13	0.62
1:R:154:ARG:CZ	1:S:142:ARG:HH21	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:ARG:HH12	1:H:142:ARG:NE	1.98	0.62
1:I:154:ARG:CZ	1:J:142:ARG:HH21	2.11	0.62
1:A:154:ARG:HH12	1:B:142:ARG:NE	1.98	0.61
1:L:154:ARG:CZ	1:M:142:ARG:HH21	2.12	0.61
1:E:154:ARG:CZ	1:F:142:ARG:HH21	2.12	0.61
1:Q:154:ARG:HH12	1:R:142:ARG:NE	1.98	0.61
1:A:142:ARG:HH21	1:W:154:ARG:CZ	2.12	0.61
1:B:154:ARG:CZ	1:C:142:ARG:HH21	2.13	0.61
1:L:154:ARG:HH12	1:M:142:ARG:NE	1.99	0.61
1:E:154:ARG:HH12	1:F:142:ARG:NE	1.99	0.61
1:G:154:ARG:CZ	1:H:142:ARG:HH21	2.12	0.61
1:K:154:ARG:HH12	1:L:142:ARG:NE	1.99	0.61
1:P:154:ARG:HH12	1:Q:142:ARG:NE	1.99	0.61
1:N:154:ARG:HH12	1:O:142:ARG:NE	2.00	0.60
1:B:154:ARG:HH12	1:C:142:ARG:NE	2.00	0.60
1:P:154:ARG:CZ	1:Q:142:ARG:HH21	2.12	0.60
1:J:154:ARG:HH12	1:K:142:ARG:NE	2.00	0.60
1:J:154:ARG:CZ	1:K:142:ARG:HH21	2.13	0.60
1:K:154:ARG:CZ	1:L:142:ARG:HH21	2.12	0.60
1:O:154:ARG:CZ	1:P:142:ARG:HH21	2.14	0.60
1:R:154:ARG:HH12	1:S:142:ARG:NE	1.99	0.60
1:S:154:ARG:CZ	1:T:142:ARG:HH21	2.14	0.60
1:H:154:ARG:HH12	1:I:142:ARG:NE	1.99	0.59
1:T:154:ARG:CZ	1:V:142:ARG:HH21	2.12	0.59
1:F:154:ARG:CZ	1:G:142:ARG:HH21	2.13	0.59
1:S:154:ARG:HH12	1:T:142:ARG:NE	2.00	0.59
1:T:154:ARG:HH12	1:V:142:ARG:NE	2.00	0.59
1:F:154:ARG:HH12	1:G:142:ARG:NE	1.99	0.59
1:O:154:ARG:HH12	1:P:142:ARG:NE	2.01	0.59
1:L:152:SER:O	1:L:179:THR:OG1	2.23	0.57
1:J:152:SER:O	1:J:179:THR:OG1	2.23	0.57
1:N:152:SER:O	1:N:179:THR:OG1	2.23	0.57
1:Q:152:SER:O	1:Q:179:THR:OG1	2.23	0.57
1:H:152:SER:O	1:H:179:THR:OG1	2.23	0.56
1:O:156:HIS:CE1	1:P:143:THR:HG21	2.41	0.56
1:P:152:SER:O	1:P:179:THR:OG1	2.23	0.56
1:S:156:HIS:CE1	1:T:143:THR:HG21	2.41	0.56
1:I:154:ARG:NH1	1:J:142:ARG:NE	2.54	0.56
1:S:152:SER:O	1:S:179:THR:OG1	2.23	0.56
1:F:152:SER:O	1:F:179:THR:OG1	2.23	0.56
1:N:199:SER:HA	1:N:205:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:199:SER:HA	1:Q:205:LEU:HD23	1.88	0.56
1:W:199:SER:HA	1:W:205:LEU:HD23	1.88	0.56
1:O:199:SER:HA	1:O:205:LEU:HD23	1.88	0.55
1:S:199:SER:HA	1:S:205:LEU:HD23	1.88	0.55
1:T:199:SER:HA	1:T:205:LEU:HD23	1.89	0.55
1:A:199:SER:HA	1:A:205:LEU:HD23	1.88	0.55
1:I:152:SER:O	1:I:179:THR:OG1	2.23	0.55
1:R:199:SER:HA	1:R:205:LEU:HD23	1.88	0.55
1:V:152:SER:O	1:V:179:THR:OG1	2.23	0.55
1:B:156:HIS:CE1	1:C:143:THR:HG21	2.41	0.55
1:D:154:ARG:NH1	1:E:142:ARG:NE	2.54	0.55
1:F:156:HIS:CE1	1:G:143:THR:HG21	2.42	0.55
1:J:156:HIS:CE1	1:K:143:THR:HG21	2.42	0.55
1:P:199:SER:HA	1:P:205:LEU:HD23	1.88	0.55
1:R:152:SER:O	1:R:179:THR:OG1	2.23	0.55
1:B:199:SER:HA	1:B:205:LEU:HD23	1.88	0.55
1:C:199:SER:HA	1:C:205:LEU:HD23	1.88	0.55
1:G:152:SER:O	1:G:179:THR:OG1	2.23	0.55
1:L:199:SER:HA	1:L:205:LEU:HD23	1.88	0.55
1:N:156:HIS:CE1	1:O:143:THR:HG21	2.42	0.55
1:V:199:SER:HA	1:V:205:LEU:HD23	1.88	0.55
1:V:154:ARG:NH1	1:W:142:ARG:NE	2.54	0.55
1:K:152:SER:O	1:K:179:THR:OG1	2.23	0.55
1:K:199:SER:HA	1:K:205:LEU:HD23	1.89	0.55
1:M:199:SER:HA	1:M:205:LEU:HD23	1.88	0.55
1:P:156:HIS:CE1	1:Q:143:THR:HG21	2.42	0.55
1:D:152:SER:O	1:D:179:THR:OG1	2.23	0.55
1:E:152:SER:O	1:E:179:THR:OG1	2.23	0.55
1:A:152:SER:O	1:A:179:THR:OG1	2.23	0.55
1:E:199:SER:HA	1:E:205:LEU:HD23	1.88	0.55
1:G:154:ARG:NH1	1:H:142:ARG:NE	2.55	0.55
1:K:156:HIS:CE1	1:L:143:THR:HG21	2.42	0.55
1:R:156:HIS:CE1	1:S:143:THR:HG21	2.42	0.55
1:C:152:SER:O	1:C:179:THR:OG1	2.23	0.55
1:D:199:SER:HA	1:D:205:LEU:HD23	1.89	0.55
1:F:199:SER:HA	1:F:205:LEU:HD23	1.88	0.55
1:I:199:SER:HA	1:I:205:LEU:HD23	1.88	0.55
1:L:156:HIS:CE1	1:M:143:THR:HG21	2.42	0.55
1:H:199:SER:HA	1:H:205:LEU:HD23	1.89	0.54
1:A:143:THR:HG21	1:W:156:HIS:CE1	2.43	0.54
1:T:152:SER:O	1:T:179:THR:OG1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NH1	1:B:142:ARG:NE	2.55	0.54
1:B:152:SER:O	1:B:179:THR:OG1	2.23	0.54
1:J:199:SER:HA	1:J:205:LEU:HD23	1.89	0.54
1:M:152:SER:O	1:M:179:THR:OG1	2.23	0.54
1:B:154:ARG:NH1	1:C:142:ARG:NE	2.56	0.54
1:G:199:SER:HA	1:G:205:LEU:HD23	1.88	0.54
1:T:156:HIS:CE1	1:V:143:THR:HG21	2.42	0.54
1:W:152:SER:O	1:W:179:THR:OG1	2.23	0.54
1:M:154:ARG:NH1	1:N:142:ARG:NE	2.55	0.54
1:M:156:HIS:CE1	1:N:143:THR:HG21	2.43	0.54
1:I:156:HIS:CE1	1:J:143:THR:HG21	2.43	0.54
1:K:154:ARG:NH1	1:L:142:ARG:NE	2.56	0.54
1:Q:156:HIS:CE1	1:R:143:THR:HG21	2.43	0.54
1:A:156:HIS:CE1	1:B:143:THR:HG21	2.42	0.54
1:H:156:HIS:CE1	1:I:143:THR:HG21	2.43	0.54
1:E:156:HIS:CE1	1:F:143:THR:HG21	2.43	0.54
1:F:154:ARG:NH1	1:G:142:ARG:NE	2.56	0.54
1:G:156:HIS:CE1	1:H:143:THR:HG21	2.43	0.54
1:P:154:ARG:NH1	1:Q:142:ARG:NE	2.56	0.54
1:C:154:ARG:NH1	1:D:142:ARG:NE	2.54	0.53
1:O:152:SER:O	1:O:179:THR:OG1	2.23	0.53
1:V:156:HIS:CE1	1:W:143:THR:HG21	2.43	0.53
1:Q:154:ARG:NH1	1:R:142:ARG:NE	2.55	0.53
1:C:156:HIS:CE1	1:D:143:THR:HG21	2.43	0.53
1:H:154:ARG:NH1	1:I:142:ARG:NE	2.56	0.52
1:D:156:HIS:CE1	1:E:143:THR:HG21	2.44	0.52
1:J:154:ARG:NH1	1:K:142:ARG:NE	2.56	0.52
1:R:154:ARG:NH1	1:S:142:ARG:NE	2.56	0.52
1:S:154:ARG:NH1	1:T:142:ARG:NE	2.56	0.52
1:A:142:ARG:NE	1:W:154:ARG:NH1	2.55	0.51
1:O:154:ARG:NH1	1:P:142:ARG:NE	2.57	0.51
1:L:154:ARG:NH1	1:M:142:ARG:NE	2.56	0.51
1:N:154:ARG:NH1	1:O:142:ARG:NE	2.56	0.50
1:J:173:SER:OG	1:J:209:ASN:OD1	2.29	0.50
1:M:173:SER:OG	1:M:209:ASN:OD1	2.29	0.50
1:T:154:ARG:NH1	1:V:142:ARG:NE	2.57	0.49
1:N:173:SER:OG	1:N:209:ASN:OD1	2.29	0.49
1:E:154:ARG:NH1	1:F:142:ARG:NE	2.56	0.48
1:F:190:GLN:O	1:F:193:ALA:HB3	2.14	0.48
1:O:190:GLN:O	1:O:193:ALA:HB3	2.14	0.48
1:E:190:GLN:O	1:E:193:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:GLN:O	1:I:193:ALA:HB3	2.14	0.48
1:L:190:GLN:O	1:L:193:ALA:HB3	2.14	0.48
1:N:190:GLN:O	1:N:193:ALA:HB3	2.14	0.48
1:R:190:GLN:O	1:R:193:ALA:HB3	2.14	0.48
1:C:190:GLN:O	1:C:193:ALA:HB3	2.14	0.48
1:P:190:GLN:O	1:P:193:ALA:HB3	2.14	0.48
1:G:190:GLN:O	1:G:193:ALA:HB3	2.14	0.48
1:A:190:GLN:O	1:A:193:ALA:HB3	2.14	0.48
1:S:190:GLN:O	1:S:193:ALA:HB3	2.14	0.48
1:H:190:GLN:O	1:H:193:ALA:HB3	2.14	0.48
1:J:190:GLN:O	1:J:193:ALA:HB3	2.14	0.48
1:K:173:SER:OG	1:K:209:ASN:OD1	2.32	0.48
1:B:190:GLN:O	1:B:193:ALA:HB3	2.14	0.47
1:Q:190:GLN:O	1:Q:193:ALA:HB3	2.14	0.47
1:V:190:GLN:O	1:V:193:ALA:HB3	2.14	0.47
1:W:190:GLN:O	1:W:193:ALA:HB3	2.14	0.47
1:M:190:GLN:O	1:M:193:ALA:HB3	2.14	0.47
1:K:190:GLN:O	1:K:193:ALA:HB3	2.14	0.47
1:T:190:GLN:O	1:T:193:ALA:HB3	2.14	0.47
1:D:190:GLN:O	1:D:193:ALA:HB3	2.14	0.47
1:L:173:SER:OG	1:L:209:ASN:OD1	2.33	0.47
1:E:173:SER:OG	1:E:209:ASN:OD1	2.34	0.46
1:P:147:LEU:HD22	1:P:147:LEU:HA	1.83	0.46
1:M:147:LEU:HD22	1:M:147:LEU:HA	1.83	0.46
1:O:173:SER:OG	1:O:209:ASN:OD1	2.33	0.46
1:A:147:LEU:HD22	1:A:147:LEU:HA	1.83	0.45
1:R:173:SER:OG	1:R:209:ASN:OD1	2.35	0.44
1:J:147:LEU:HD22	1:J:147:LEU:HA	1.83	0.44
1:F:147:LEU:HD22	1:F:147:LEU:HA	1.83	0.43
1:D:191:ILE:HD13	1:D:191:ILE:HA	1.90	0.43
1:R:147:LEU:HD22	1:R:147:LEU:HA	1.83	0.43
1:Q:173:SER:OG	1:Q:209:ASN:OD1	2.36	0.42
1:S:175:SER:OG	1:T:197:LEU:CD2	2.67	0.42
1:R:191:ILE:HD13	1:R:191:ILE:HA	1.90	0.42
1:P:191:ILE:HD13	1:P:191:ILE:HA	1.90	0.42
1:Q:191:ILE:HD13	1:Q:191:ILE:HA	1.90	0.42
1:S:191:ILE:HD13	1:S:191:ILE:HA	1.90	0.42
1:I:175:SER:OG	1:J:197:LEU:CD2	2.68	0.42
1:A:175:SER:HB2	1:B:200:SER:HG	1.82	0.41
1:D:147:LEU:HD22	1:D:147:LEU:HA	1.83	0.41
1:G:173:SER:OG	1:G:209:ASN:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:173:SER:OG	1:S:209:ASN:OD1	2.37	0.41
1:T:147:LEU:HD22	1:T:147:LEU:HA	1.83	0.41
1:A:173:SER:OG	1:A:209:ASN:OD1	2.37	0.41
1:E:191:ILE:HD13	1:E:191:ILE:HA	1.90	0.41
1:T:191:ILE:HD13	1:T:191:ILE:HA	1.90	0.41
1:O:191:ILE:HD13	1:O:191:ILE:HA	1.90	0.41
1:B:147:LEU:HD22	1:B:147:LEU:HA	1.83	0.41
1:G:191:ILE:HD13	1:G:191:ILE:HA	1.90	0.41
1:W:173:SER:OG	1:W:209:ASN:OD1	2.38	0.41
1:A:197:LEU:CD2	1:W:175:SER:OG	2.69	0.41
1:F:154:ARG:HA	1:F:154:ARG:HD3	1.95	0.41
1:L:147:LEU:HA	1:L:147:LEU:HD22	1.83	0.41
1:N:191:ILE:HD13	1:N:191:ILE:HA	1.90	0.41
1:O:175:SER:OG	1:P:197:LEU:CD2	2.69	0.41
1:V:191:ILE:HD13	1:V:191:ILE:HA	1.90	0.41
1:W:147:LEU:HD22	1:W:147:LEU:HA	1.83	0.41
1:P:175:SER:OG	1:Q:197:LEU:CD2	2.69	0.41
1:A:175:SER:OG	1:B:197:LEU:CD2	2.69	0.40
1:H:147:LEU:HD22	1:H:147:LEU:HA	1.83	0.40
1:F:175:SER:OG	1:G:197:LEU:CD2	2.69	0.40
1:J:175:SER:OG	1:K:197:LEU:CD2	2.70	0.40
1:V:154:ARG:HA	1:V:154:ARG:HD3	1.95	0.40
1:G:147:LEU:HA	1:G:147:LEU:HD22	1.83	0.40
1:H:191:ILE:HD13	1:H:191:ILE:HA	1.91	0.40
1:V:173:SER:OG	1:V:209:ASN:OD1	2.39	0.40

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	89/560 (16%)	86 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	C	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	D	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	E	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	F	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	G	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	H	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	I	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	J	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	K	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	L	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	M	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	N	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	O	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	P	89/560 (16%)	85 (96%)	4 (4%)	0	100	100
1	Q	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	R	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	S	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	T	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	V	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
1	W	89/560 (16%)	86 (97%)	3 (3%)	0	100	100
All	All	1958/12320 (16%)	1891 (97%)	67 (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	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	B	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	C	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	D	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	E	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	F	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	G	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	H	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	I	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	J	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	K	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	L	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	M	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	N	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	O	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	P	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	Q	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	R	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	S	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	T	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	V	72/467 (15%)	68 (94%)	4 (6%)	19	45
1	W	72/467 (15%)	68 (94%)	4 (6%)	19	45
All	All	1584/10274 (15%)	1496 (94%)	88 (6%)	21	45

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	140	LEU
1	A	144	ILE
1	A	147	LEU
1	B	136	LEU
1	B	140	LEU
1	B	144	ILE
1	B	147	LEU

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Mol	Chain	Res	Type
1	C	136	LEU
1	C	140	LEU
1	C	144	ILE
1	C	147	LEU
1	D	136	LEU
1	D	140	LEU
1	D	144	ILE
1	D	147	LEU
1	E	136	LEU
1	E	140	LEU
1	E	144	ILE
1	E	147	LEU
1	F	136	LEU
1	F	140	LEU
1	F	144	ILE
1	F	147	LEU
1	G	136	LEU
1	G	140	LEU
1	G	144	ILE
1	G	147	LEU
1	H	136	LEU
1	H	140	LEU
1	H	144	ILE
1	H	147	LEU
1	I	136	LEU
1	I	140	LEU
1	I	144	ILE
1	I	147	LEU
1	J	136	LEU
1	J	140	LEU
1	J	144	ILE
1	J	147	LEU
1	K	136	LEU
1	K	140	LEU
1	K	144	ILE
1	K	147	LEU
1	L	136	LEU
1	L	140	LEU
1	L	144	ILE
1	L	147	LEU
1	M	136	LEU
1	M	140	LEU

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Mol	Chain	Res	Type
1	M	144	ILE
1	M	147	LEU
1	N	136	LEU
1	N	140	LEU
1	N	144	ILE
1	N	147	LEU
1	O	136	LEU
1	O	140	LEU
1	O	144	ILE
1	O	147	LEU
1	P	136	LEU
1	P	140	LEU
1	P	144	ILE
1	P	147	LEU
1	Q	136	LEU
1	Q	140	LEU
1	Q	144	ILE
1	Q	147	LEU
1	R	136	LEU
1	R	140	LEU
1	R	144	ILE
1	R	147	LEU
1	S	136	LEU
1	S	140	LEU
1	S	144	ILE
1	S	147	LEU
1	T	136	LEU
1	T	140	LEU
1	T	144	ILE
1	T	147	LEU
1	V	136	LEU
1	V	140	LEU
1	V	144	ILE
1	V	147	LEU
1	W	136	LEU
1	W	140	LEU
1	W	144	ILE
1	W	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	196	HIS
1	A	209	ASN
1	A	222	GLN
1	B	156	HIS
1	B	209	ASN
1	B	222	GLN
1	C	156	HIS
1	C	196	HIS
1	C	209	ASN
1	C	222	GLN
1	D	156	HIS
1	D	209	ASN
1	D	222	GLN
1	E	156	HIS
1	E	209	ASN
1	E	222	GLN
1	F	156	HIS
1	F	222	GLN
1	G	156	HIS
1	G	196	HIS
1	G	209	ASN
1	G	222	GLN
1	H	156	HIS
1	H	209	ASN
1	H	222	GLN
1	I	156	HIS
1	I	209	ASN
1	I	222	GLN
1	J	156	HIS
1	J	209	ASN
1	J	222	GLN
1	K	156	HIS
1	K	196	HIS
1	K	209	ASN
1	K	222	GLN
1	L	156	HIS
1	L	196	HIS
1	L	222	GLN
1	M	156	HIS
1	M	196	HIS
1	M	209	ASN
1	M	222	GLN

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Mol	Chain	Res	Type
1	N	156	HIS
1	N	209	ASN
1	N	222	GLN
1	O	156	HIS
1	O	209	ASN
1	O	222	GLN
1	P	156	HIS
1	P	196	HIS
1	P	209	ASN
1	P	222	GLN
1	Q	156	HIS
1	Q	196	HIS
1	Q	222	GLN
1	R	156	HIS
1	R	196	HIS
1	R	209	ASN
1	R	222	GLN
1	S	156	HIS
1	S	196	HIS
1	S	209	ASN
1	S	222	GLN
1	T	156	HIS
1	T	209	ASN
1	T	222	GLN
1	V	156	HIS
1	V	209	ASN
1	V	222	GLN
1	W	156	HIS
1	W	209	ASN
1	W	222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

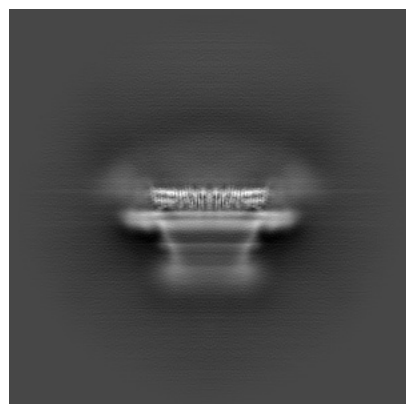
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29424. These allow visual inspection of the internal detail of the map and identification of artifacts.

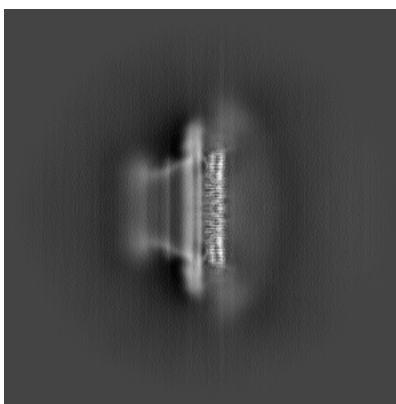
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

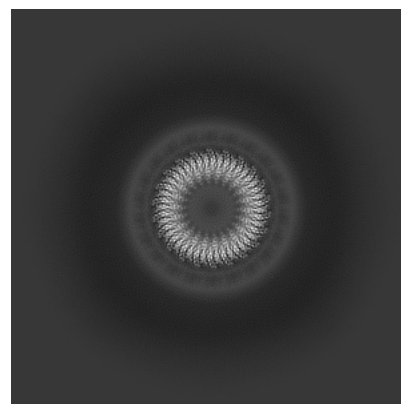
6.1.1 Primary map



X

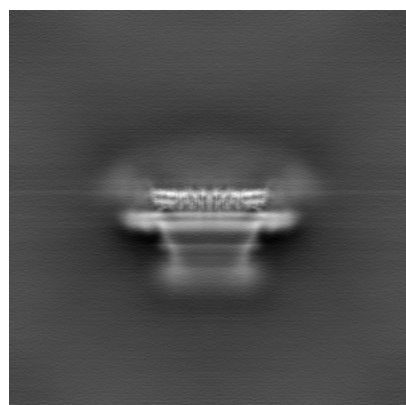


Y

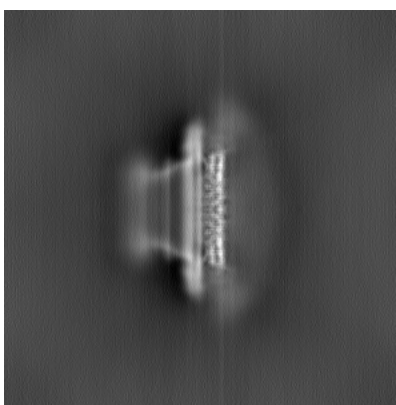


Z

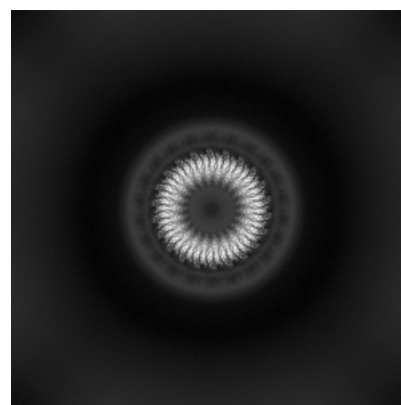
6.1.2 Raw map



X



Y

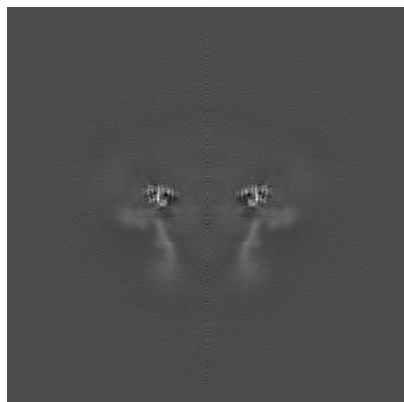


Z

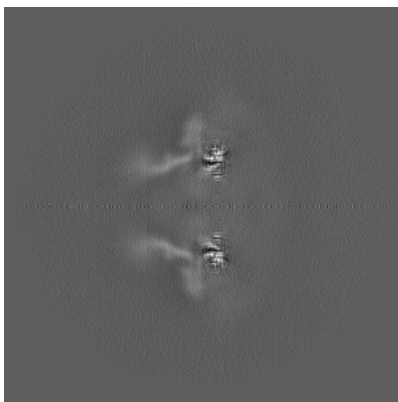
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

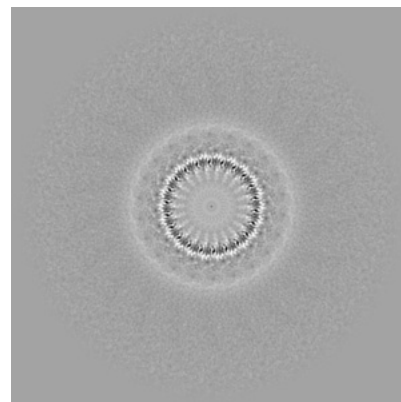
6.2.1 Primary map



X Index: 200

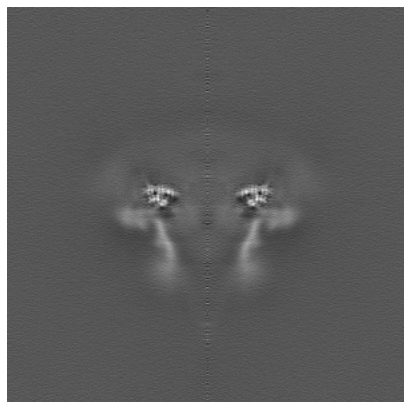


Y Index: 200

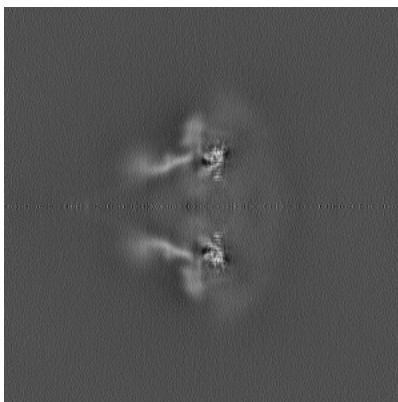


Z Index: 200

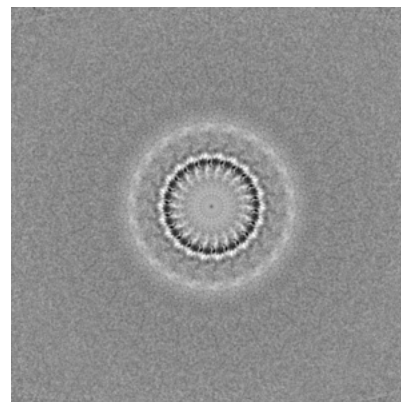
6.2.2 Raw map



X Index: 200



Y Index: 200

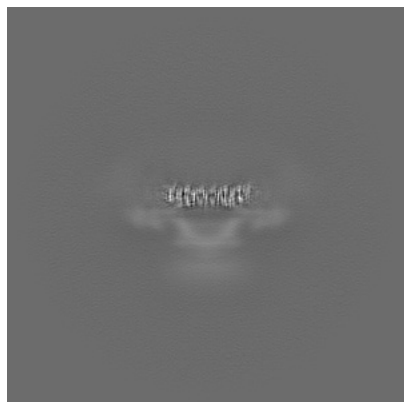


Z Index: 200

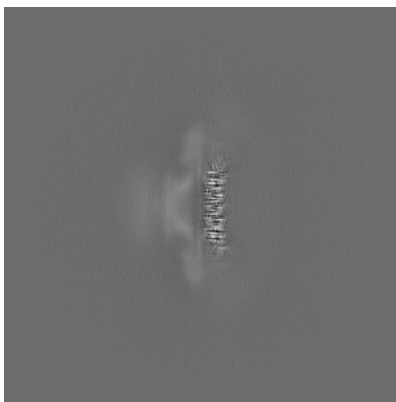
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

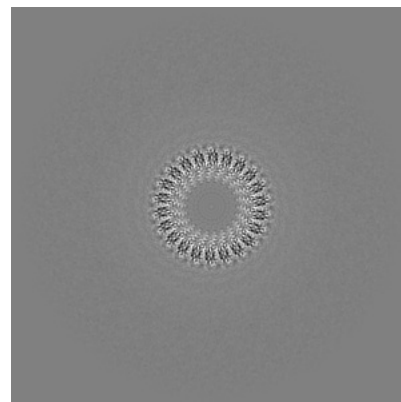
6.3.1 Primary map



X Index: 241

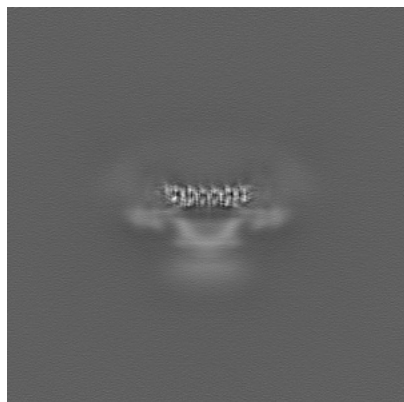


Y Index: 158

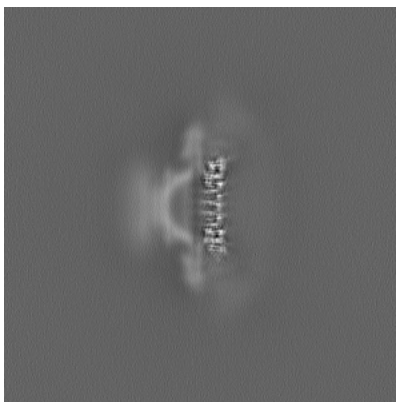


Z Index: 213

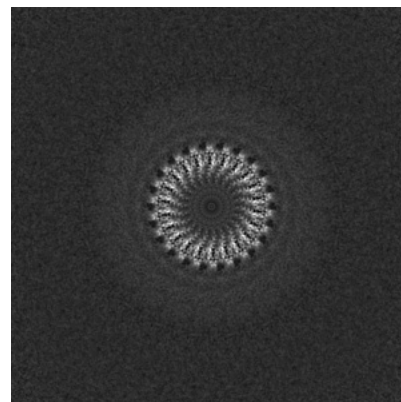
6.3.2 Raw map



X Index: 159



Y Index: 163

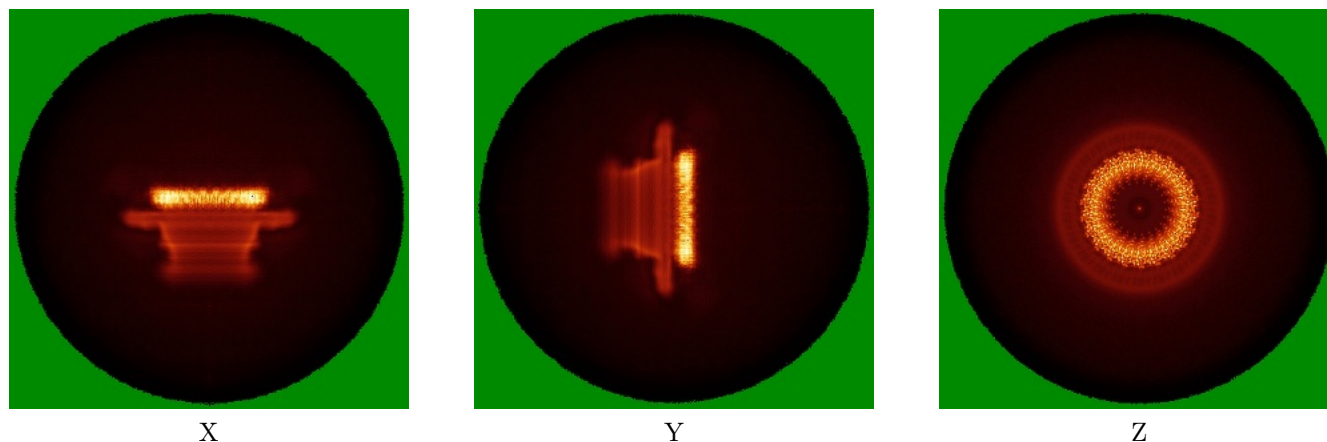


Z Index: 216

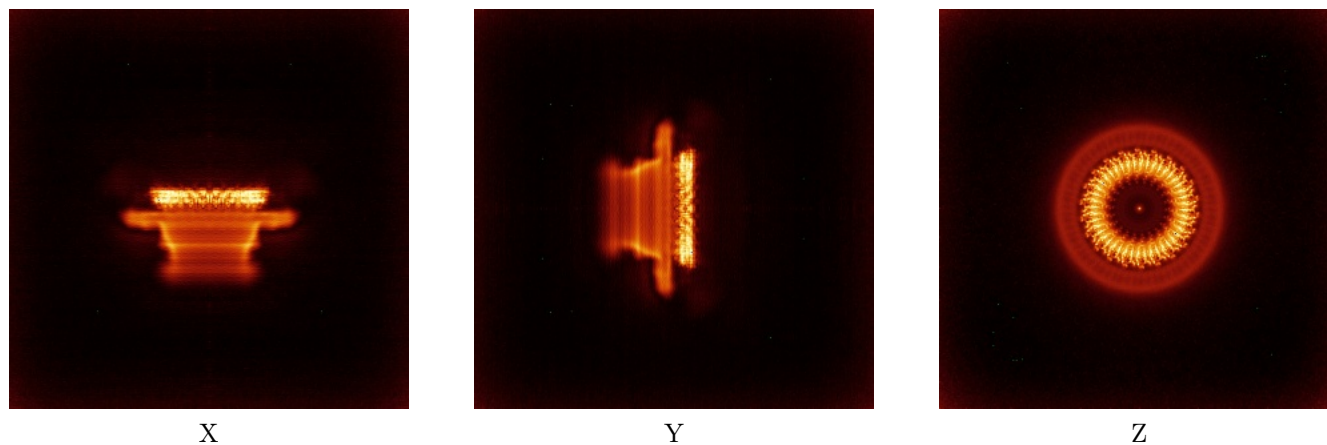
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

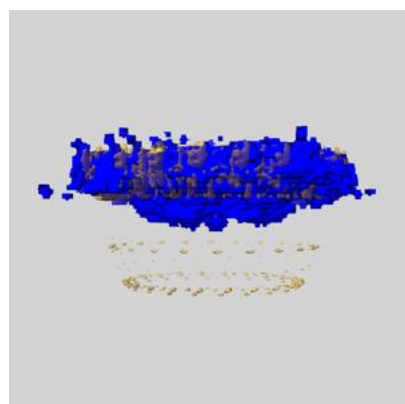
6.6 Mask visualisation [i](#)

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

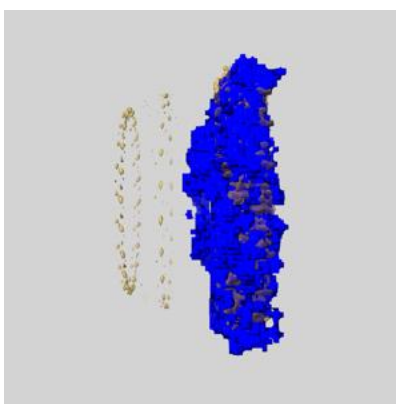
A mask typically either:

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

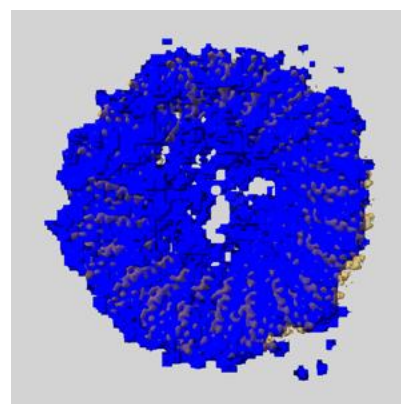
6.6.1 emd_29424_msk_1.map [i](#)



X



Y

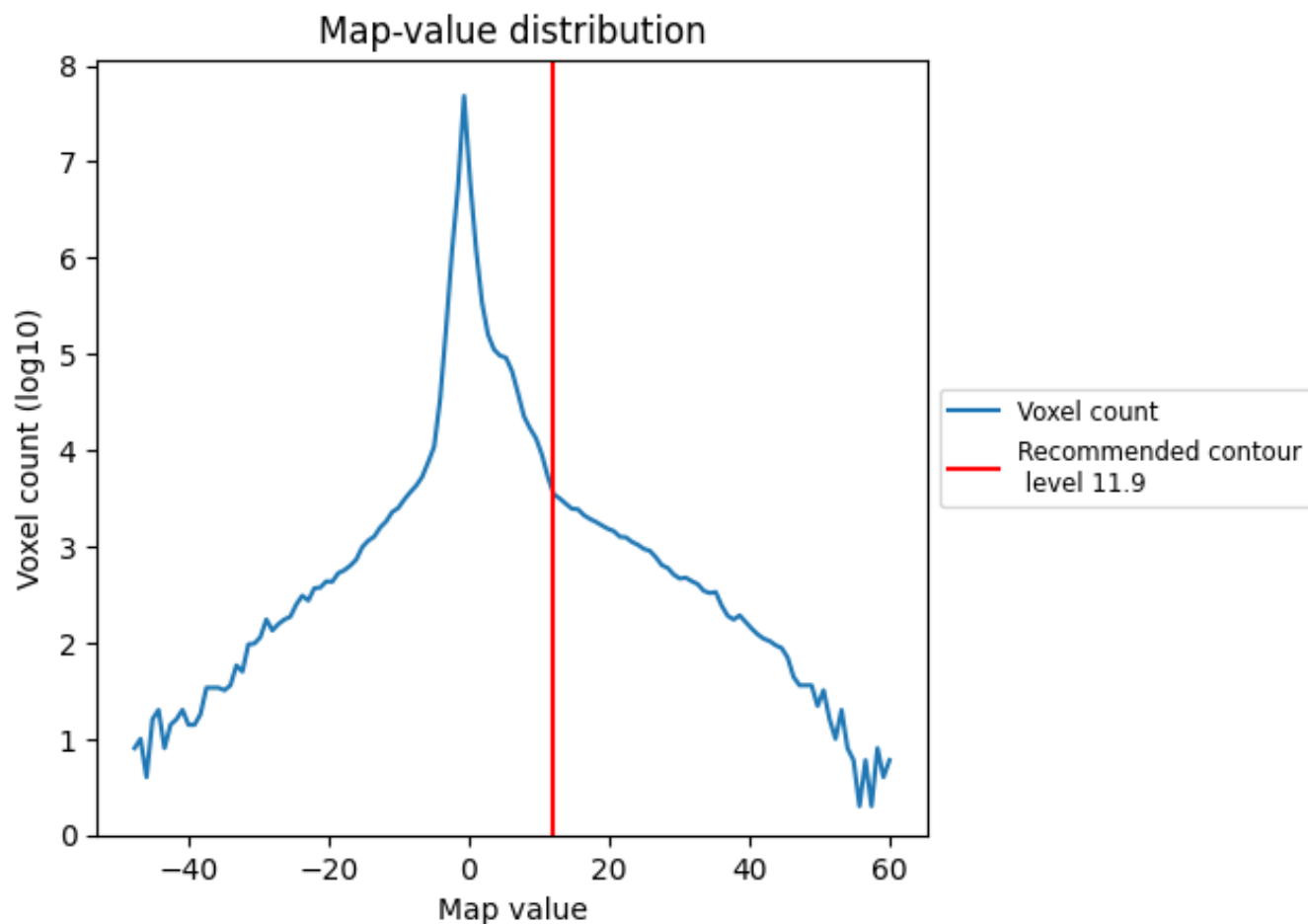


Z

7 Map analysis [i](#)

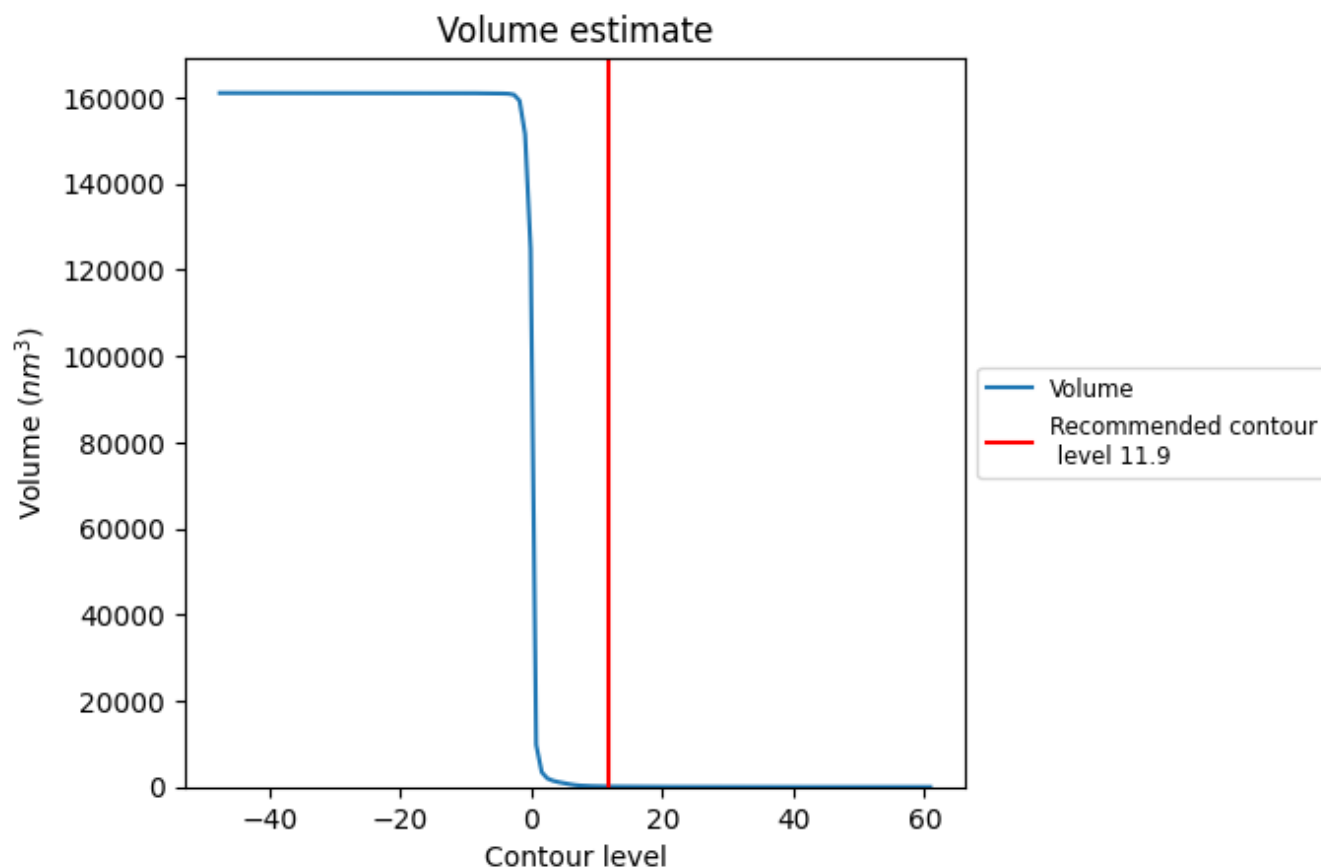
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

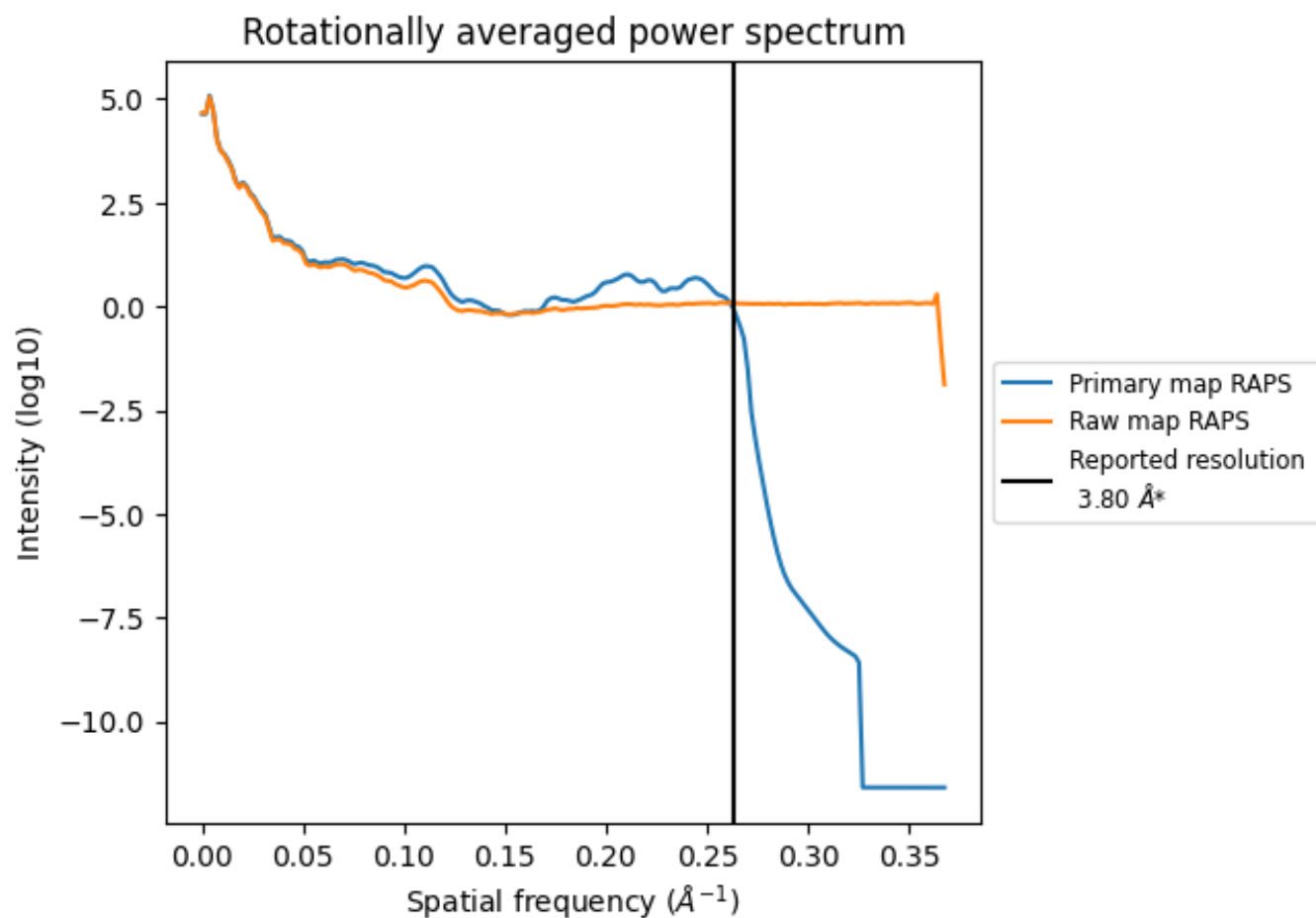
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 92 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

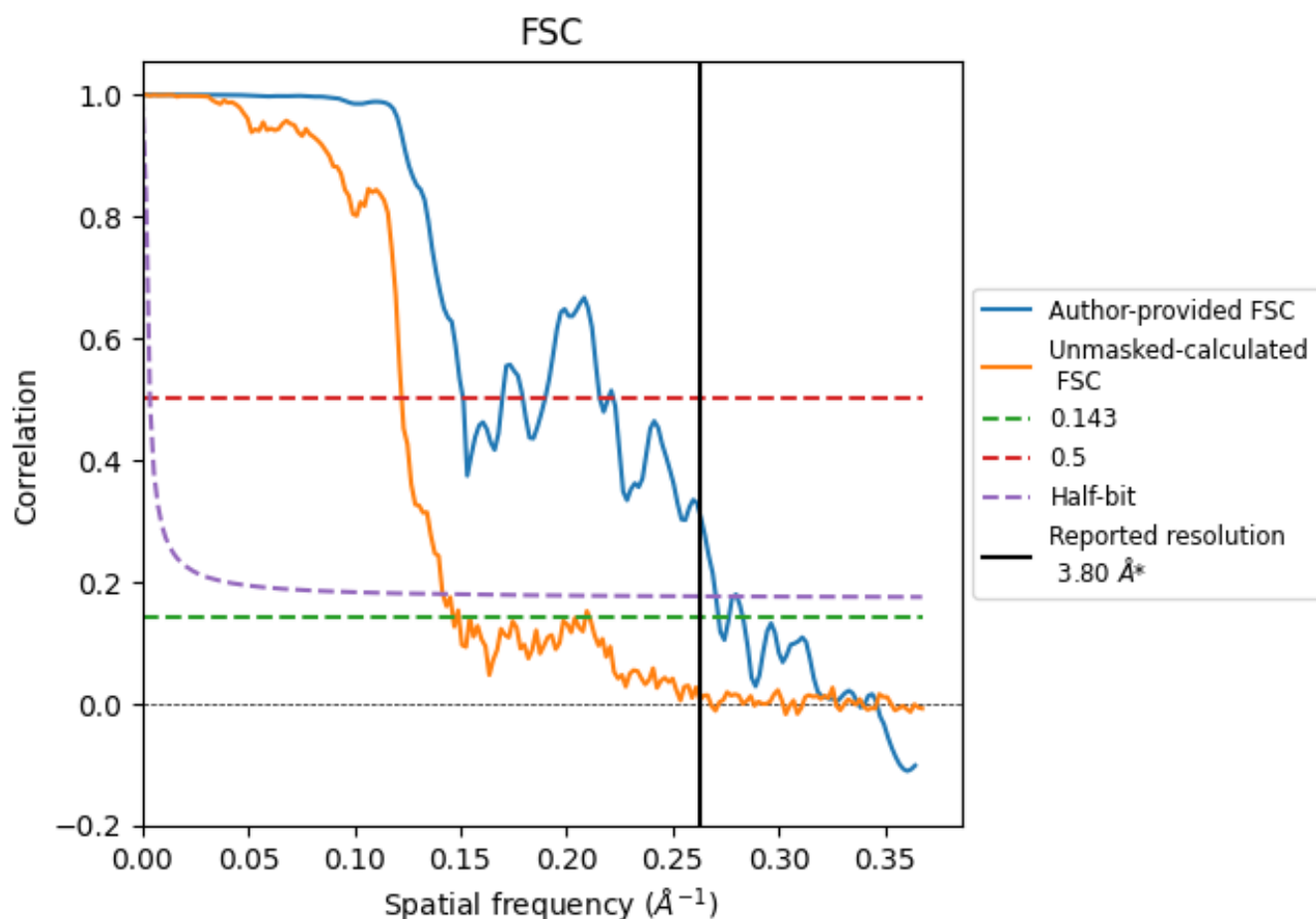


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

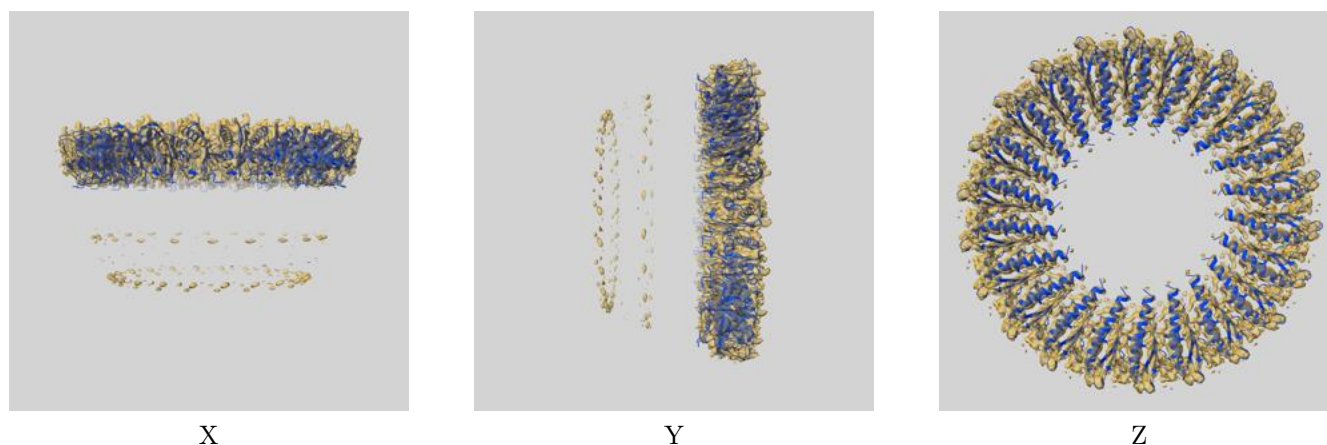
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.68	6.61	3.70
Unmasked-calculated*	6.83	8.18	7.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.83 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29424 and PDB model 8FTE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



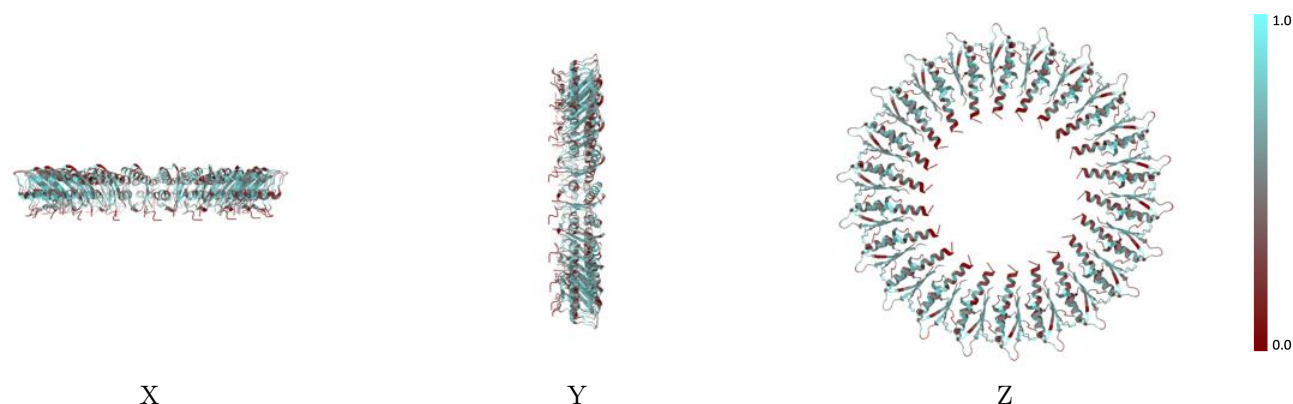
The images above show the 3D surface view of the map at the recommended contour level 11.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



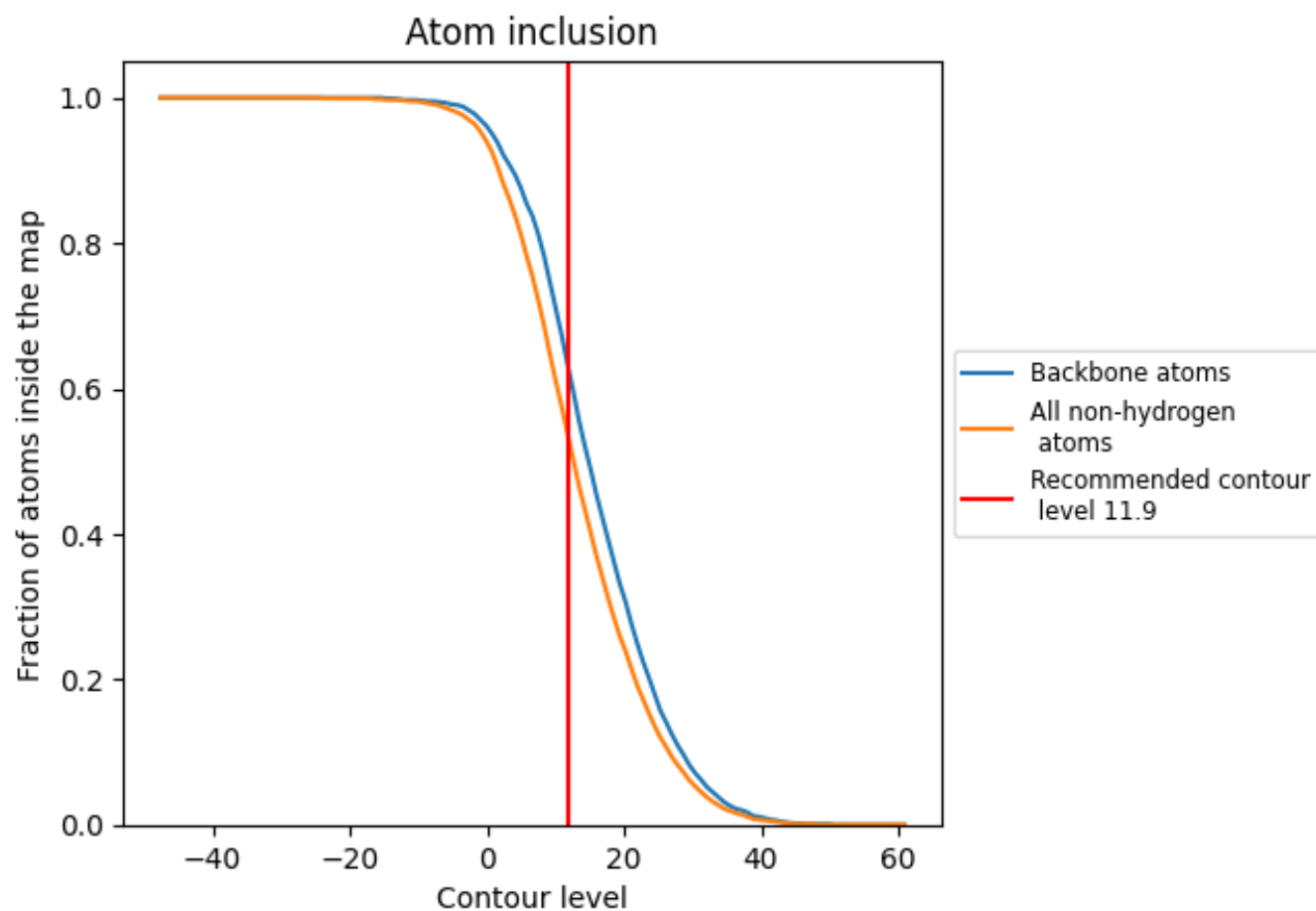
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (11.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 53% 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 (11.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5320	 0.2680
A	 0.5190	 0.2540
B	 0.5210	 0.2490
C	 0.5140	 0.2490
D	 0.5160	 0.2420
E	 0.5180	 0.2420
F	 0.5250	 0.2450
G	 0.5270	 0.2500
H	 0.5190	 0.2530
I	 0.5220	 0.2720
J	 0.5390	 0.2800
K	 0.5310	 0.2830
L	 0.5530	 0.2930
M	 0.5620	 0.2980
N	 0.5500	 0.2940
O	 0.5560	 0.2880
P	 0.5410	 0.2820
Q	 0.5370	 0.2740
R	 0.5370	 0.2690
S	 0.5300	 0.2690
T	 0.5330	 0.2740
V	 0.5240	 0.2640
W	 0.5370	 0.2630

