



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2024 – 08:56 am BST

PDB ID : 8RT5  
EMDB ID : EMD-19479  
Title : I-layer structure (TrwF/VirB9CTD, TrwE/VirB10CTD) of the outer membrane core complex from the fully-assembled R388 type IV secretion system determined by cryo-EM.  
Authors : Mace, K.; Waksman, G.  
Deposited on : 2024-01-25  
Resolution : 2.69 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](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.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

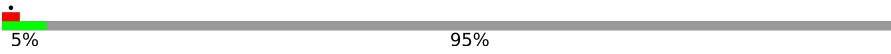
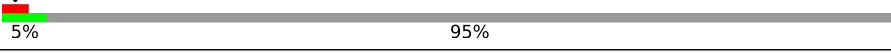
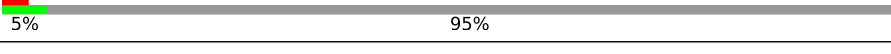
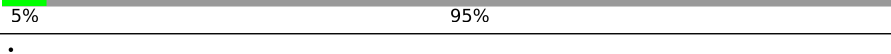
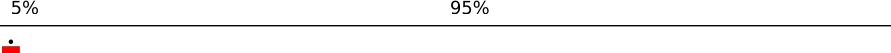
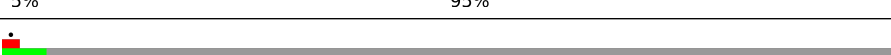
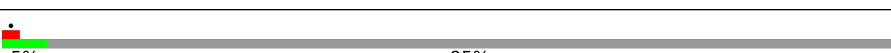
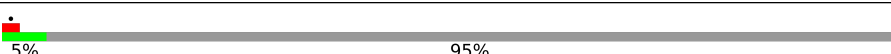

The reported resolution of this entry is 2.69 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	395	 5% 95%
1	D	395	 5% 95%
1	G	395	 5% 95%
1	J	395	 5% 95%
1	M	395	 5% 95%
1	P	395	 5% 95%
1	S	395	 5% 95%
1	V	395	 5% 95%
1	Y	395	 5% 95%

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Mol	Chain	Length	Quality of chain	
1	b	395		95%
1	e	395		95%
1	h	395		95%
1	k	395		95%
1	n	395		95%
1	u	395		95%
1	y	395		95%
2	B	266		57%
2	E	266		57%
2	H	266		57%
2	K	266		57%
2	N	266		57%
2	Q	266		57%
2	T	266		57%
2	W	266		57%
2	Z	266		57%
2	c	266		57%
2	f	266		57%
2	i	266		57%
2	l	266		57%
2	o	266		57%
2	v	266		57%
2	z	266		57%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17456 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 TrwE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	D	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	G	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	J	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	M	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	P	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	S	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	u	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	V	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	Y	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	b	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	e	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	h	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	k	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	n	19	Total 149	C 92	N 29	O 27	S 1	0	0
1	y	19	Total 149	C 92	N 29	O 27	S 1	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ASP	ASN	conflict	UNP O50337
D	335	ASP	ASN	conflict	UNP O50337
G	335	ASP	ASN	conflict	UNP O50337
J	335	ASP	ASN	conflict	UNP O50337
M	335	ASP	ASN	conflict	UNP O50337
P	335	ASP	ASN	conflict	UNP O50337
S	335	ASP	ASN	conflict	UNP O50337
u	335	ASP	ASN	conflict	UNP O50337
V	335	ASP	ASN	conflict	UNP O50337
Y	335	ASP	ASN	conflict	UNP O50337
b	335	ASP	ASN	conflict	UNP O50337
e	335	ASP	ASN	conflict	UNP O50337
h	335	ASP	ASN	conflict	UNP O50337
k	335	ASP	ASN	conflict	UNP O50337
n	335	ASP	ASN	conflict	UNP O50337
y	335	ASP	ASN	conflict	UNP O50337

- Molecule 2 is a protein called TrwF protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	E	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	H	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	K	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	N	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	Q	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	T	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	v	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	W	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	Z	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	c	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	f	115	Total	C	N	O	S	0	0
			942	591	173	175	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	i	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	l	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	o	115	Total	C	N	O	S	0	0
			942	591	173	175	3		
2	z	115	Total	C	N	O	S	0	0
			942	591	173	175	3		

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	ASP	ILE	conflict	UNP O50336
B	72	SER	PRO	conflict	UNP O50336
B	73	GLU	LYS	conflict	UNP O50336
B	74	ALA	PRO	conflict	UNP O50336
B	75	TYR	MET	conflict	UNP O50336
B	76	ALA	PRO	conflict	UNP O50336
B	77	PHE	LEU	conflict	UNP O50336
B	78	ALA	PRO	conflict	UNP O50336
B	79	ARG	GLY	conflict	UNP O50336
B	80	LYS	ARG	conflict	UNP O50336
B	81	GLY	ALA	conflict	UNP O50336
B	82	ARG	GLY	conflict	UNP O50336
B	83	HIS	ILE	conflict	UNP O50336
B	84	ILE	PHE	conflict	UNP O50336
B	85	PHE	LEU	conflict	UNP O50336
B	86	ILE	SER	conflict	UNP O50336
B	87	LYS	SER	conflict	UNP O50336
B	88	PRO	ARG	conflict	UNP O50336
B	89	GLN	THR	conflict	UNP O50336
E	71	ASP	ILE	conflict	UNP O50336
E	72	SER	PRO	conflict	UNP O50336
E	73	GLU	LYS	conflict	UNP O50336
E	74	ALA	PRO	conflict	UNP O50336
E	75	TYR	MET	conflict	UNP O50336
E	76	ALA	PRO	conflict	UNP O50336
E	77	PHE	LEU	conflict	UNP O50336
E	78	ALA	PRO	conflict	UNP O50336
E	79	ARG	GLY	conflict	UNP O50336
E	80	LYS	ARG	conflict	UNP O50336
E	81	GLY	ALA	conflict	UNP O50336
E	82	ARG	GLY	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
E	83	HIS	ILE	conflict	UNP O50336
E	84	ILE	PHE	conflict	UNP O50336
E	85	PHE	LEU	conflict	UNP O50336
E	86	ILE	SER	conflict	UNP O50336
E	87	LYS	SER	conflict	UNP O50336
E	88	PRO	ARG	conflict	UNP O50336
E	89	GLN	THR	conflict	UNP O50336
H	71	ASP	ILE	conflict	UNP O50336
H	72	SER	PRO	conflict	UNP O50336
H	73	GLU	LYS	conflict	UNP O50336
H	74	ALA	PRO	conflict	UNP O50336
H	75	TYR	MET	conflict	UNP O50336
H	76	ALA	PRO	conflict	UNP O50336
H	77	PHE	LEU	conflict	UNP O50336
H	78	ALA	PRO	conflict	UNP O50336
H	79	ARG	GLY	conflict	UNP O50336
H	80	LYS	ARG	conflict	UNP O50336
H	81	GLY	ALA	conflict	UNP O50336
H	82	ARG	GLY	conflict	UNP O50336
H	83	HIS	ILE	conflict	UNP O50336
H	84	ILE	PHE	conflict	UNP O50336
H	85	PHE	LEU	conflict	UNP O50336
H	86	ILE	SER	conflict	UNP O50336
H	87	LYS	SER	conflict	UNP O50336
H	88	PRO	ARG	conflict	UNP O50336
H	89	GLN	THR	conflict	UNP O50336
K	71	ASP	ILE	conflict	UNP O50336
K	72	SER	PRO	conflict	UNP O50336
K	73	GLU	LYS	conflict	UNP O50336
K	74	ALA	PRO	conflict	UNP O50336
K	75	TYR	MET	conflict	UNP O50336
K	76	ALA	PRO	conflict	UNP O50336
K	77	PHE	LEU	conflict	UNP O50336
K	78	ALA	PRO	conflict	UNP O50336
K	79	ARG	GLY	conflict	UNP O50336
K	80	LYS	ARG	conflict	UNP O50336
K	81	GLY	ALA	conflict	UNP O50336
K	82	ARG	GLY	conflict	UNP O50336
K	83	HIS	ILE	conflict	UNP O50336
K	84	ILE	PHE	conflict	UNP O50336
K	85	PHE	LEU	conflict	UNP O50336
K	86	ILE	SER	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
K	87	LYS	SER	conflict	UNP O50336
K	88	PRO	ARG	conflict	UNP O50336
K	89	GLN	THR	conflict	UNP O50336
N	71	ASP	ILE	conflict	UNP O50336
N	72	SER	PRO	conflict	UNP O50336
N	73	GLU	LYS	conflict	UNP O50336
N	74	ALA	PRO	conflict	UNP O50336
N	75	TYR	MET	conflict	UNP O50336
N	76	ALA	PRO	conflict	UNP O50336
N	77	PHE	LEU	conflict	UNP O50336
N	78	ALA	PRO	conflict	UNP O50336
N	79	ARG	GLY	conflict	UNP O50336
N	80	LYS	ARG	conflict	UNP O50336
N	81	GLY	ALA	conflict	UNP O50336
N	82	ARG	GLY	conflict	UNP O50336
N	83	HIS	ILE	conflict	UNP O50336
N	84	ILE	PHE	conflict	UNP O50336
N	85	PHE	LEU	conflict	UNP O50336
N	86	ILE	SER	conflict	UNP O50336
N	87	LYS	SER	conflict	UNP O50336
N	88	PRO	ARG	conflict	UNP O50336
N	89	GLN	THR	conflict	UNP O50336
Q	71	ASP	ILE	conflict	UNP O50336
Q	72	SER	PRO	conflict	UNP O50336
Q	73	GLU	LYS	conflict	UNP O50336
Q	74	ALA	PRO	conflict	UNP O50336
Q	75	TYR	MET	conflict	UNP O50336
Q	76	ALA	PRO	conflict	UNP O50336
Q	77	PHE	LEU	conflict	UNP O50336
Q	78	ALA	PRO	conflict	UNP O50336
Q	79	ARG	GLY	conflict	UNP O50336
Q	80	LYS	ARG	conflict	UNP O50336
Q	81	GLY	ALA	conflict	UNP O50336
Q	82	ARG	GLY	conflict	UNP O50336
Q	83	HIS	ILE	conflict	UNP O50336
Q	84	ILE	PHE	conflict	UNP O50336
Q	85	PHE	LEU	conflict	UNP O50336
Q	86	ILE	SER	conflict	UNP O50336
Q	87	LYS	SER	conflict	UNP O50336
Q	88	PRO	ARG	conflict	UNP O50336
Q	89	GLN	THR	conflict	UNP O50336
T	71	ASP	ILE	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
T	72	SER	PRO	conflict	UNP O50336
T	73	GLU	LYS	conflict	UNP O50336
T	74	ALA	PRO	conflict	UNP O50336
T	75	TYR	MET	conflict	UNP O50336
T	76	ALA	PRO	conflict	UNP O50336
T	77	PHE	LEU	conflict	UNP O50336
T	78	ALA	PRO	conflict	UNP O50336
T	79	ARG	GLY	conflict	UNP O50336
T	80	LYS	ARG	conflict	UNP O50336
T	81	GLY	ALA	conflict	UNP O50336
T	82	ARG	GLY	conflict	UNP O50336
T	83	HIS	ILE	conflict	UNP O50336
T	84	ILE	PHE	conflict	UNP O50336
T	85	PHE	LEU	conflict	UNP O50336
T	86	ILE	SER	conflict	UNP O50336
T	87	LYS	SER	conflict	UNP O50336
T	88	PRO	ARG	conflict	UNP O50336
T	89	GLN	THR	conflict	UNP O50336
v	71	ASP	ILE	conflict	UNP O50336
v	72	SER	PRO	conflict	UNP O50336
v	73	GLU	LYS	conflict	UNP O50336
v	74	ALA	PRO	conflict	UNP O50336
v	75	TYR	MET	conflict	UNP O50336
v	76	ALA	PRO	conflict	UNP O50336
v	77	PHE	LEU	conflict	UNP O50336
v	78	ALA	PRO	conflict	UNP O50336
v	79	ARG	GLY	conflict	UNP O50336
v	80	LYS	ARG	conflict	UNP O50336
v	81	GLY	ALA	conflict	UNP O50336
v	82	ARG	GLY	conflict	UNP O50336
v	83	HIS	ILE	conflict	UNP O50336
v	84	ILE	PHE	conflict	UNP O50336
v	85	PHE	LEU	conflict	UNP O50336
v	86	ILE	SER	conflict	UNP O50336
v	87	LYS	SER	conflict	UNP O50336
v	88	PRO	ARG	conflict	UNP O50336
v	89	GLN	THR	conflict	UNP O50336
W	71	ASP	ILE	conflict	UNP O50336
W	72	SER	PRO	conflict	UNP O50336
W	73	GLU	LYS	conflict	UNP O50336
W	74	ALA	PRO	conflict	UNP O50336
W	75	TYR	MET	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
W	76	ALA	PRO	conflict	UNP O50336
W	77	PHE	LEU	conflict	UNP O50336
W	78	ALA	PRO	conflict	UNP O50336
W	79	ARG	GLY	conflict	UNP O50336
W	80	LYS	ARG	conflict	UNP O50336
W	81	GLY	ALA	conflict	UNP O50336
W	82	ARG	GLY	conflict	UNP O50336
W	83	HIS	ILE	conflict	UNP O50336
W	84	ILE	PHE	conflict	UNP O50336
W	85	PHE	LEU	conflict	UNP O50336
W	86	ILE	SER	conflict	UNP O50336
W	87	LYS	SER	conflict	UNP O50336
W	88	PRO	ARG	conflict	UNP O50336
W	89	GLN	THR	conflict	UNP O50336
Z	71	ASP	ILE	conflict	UNP O50336
Z	72	SER	PRO	conflict	UNP O50336
Z	73	GLU	LYS	conflict	UNP O50336
Z	74	ALA	PRO	conflict	UNP O50336
Z	75	TYR	MET	conflict	UNP O50336
Z	76	ALA	PRO	conflict	UNP O50336
Z	77	PHE	LEU	conflict	UNP O50336
Z	78	ALA	PRO	conflict	UNP O50336
Z	79	ARG	GLY	conflict	UNP O50336
Z	80	LYS	ARG	conflict	UNP O50336
Z	81	GLY	ALA	conflict	UNP O50336
Z	82	ARG	GLY	conflict	UNP O50336
Z	83	HIS	ILE	conflict	UNP O50336
Z	84	ILE	PHE	conflict	UNP O50336
Z	85	PHE	LEU	conflict	UNP O50336
Z	86	ILE	SER	conflict	UNP O50336
Z	87	LYS	SER	conflict	UNP O50336
Z	88	PRO	ARG	conflict	UNP O50336
Z	89	GLN	THR	conflict	UNP O50336
c	71	ASP	ILE	conflict	UNP O50336
c	72	SER	PRO	conflict	UNP O50336
c	73	GLU	LYS	conflict	UNP O50336
c	74	ALA	PRO	conflict	UNP O50336
c	75	TYR	MET	conflict	UNP O50336
c	76	ALA	PRO	conflict	UNP O50336
c	77	PHE	LEU	conflict	UNP O50336
c	78	ALA	PRO	conflict	UNP O50336
c	79	ARG	GLY	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
c	80	LYS	ARG	conflict	UNP O50336
c	81	GLY	ALA	conflict	UNP O50336
c	82	ARG	GLY	conflict	UNP O50336
c	83	HIS	ILE	conflict	UNP O50336
c	84	ILE	PHE	conflict	UNP O50336
c	85	PHE	LEU	conflict	UNP O50336
c	86	ILE	SER	conflict	UNP O50336
c	87	LYS	SER	conflict	UNP O50336
c	88	PRO	ARG	conflict	UNP O50336
c	89	GLN	THR	conflict	UNP O50336
f	71	ASP	ILE	conflict	UNP O50336
f	72	SER	PRO	conflict	UNP O50336
f	73	GLU	LYS	conflict	UNP O50336
f	74	ALA	PRO	conflict	UNP O50336
f	75	TYR	MET	conflict	UNP O50336
f	76	ALA	PRO	conflict	UNP O50336
f	77	PHE	LEU	conflict	UNP O50336
f	78	ALA	PRO	conflict	UNP O50336
f	79	ARG	GLY	conflict	UNP O50336
f	80	LYS	ARG	conflict	UNP O50336
f	81	GLY	ALA	conflict	UNP O50336
f	82	ARG	GLY	conflict	UNP O50336
f	83	HIS	ILE	conflict	UNP O50336
f	84	ILE	PHE	conflict	UNP O50336
f	85	PHE	LEU	conflict	UNP O50336
f	86	ILE	SER	conflict	UNP O50336
f	87	LYS	SER	conflict	UNP O50336
f	88	PRO	ARG	conflict	UNP O50336
f	89	GLN	THR	conflict	UNP O50336
i	71	ASP	ILE	conflict	UNP O50336
i	72	SER	PRO	conflict	UNP O50336
i	73	GLU	LYS	conflict	UNP O50336
i	74	ALA	PRO	conflict	UNP O50336
i	75	TYR	MET	conflict	UNP O50336
i	76	ALA	PRO	conflict	UNP O50336
i	77	PHE	LEU	conflict	UNP O50336
i	78	ALA	PRO	conflict	UNP O50336
i	79	ARG	GLY	conflict	UNP O50336
i	80	LYS	ARG	conflict	UNP O50336
i	81	GLY	ALA	conflict	UNP O50336
i	82	ARG	GLY	conflict	UNP O50336
i	83	HIS	ILE	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
i	84	ILE	PHE	conflict	UNP O50336
i	85	PHE	LEU	conflict	UNP O50336
i	86	ILE	SER	conflict	UNP O50336
i	87	LYS	SER	conflict	UNP O50336
i	88	PRO	ARG	conflict	UNP O50336
i	89	GLN	THR	conflict	UNP O50336
l	71	ASP	ILE	conflict	UNP O50336
l	72	SER	PRO	conflict	UNP O50336
l	73	GLU	LYS	conflict	UNP O50336
l	74	ALA	PRO	conflict	UNP O50336
l	75	TYR	MET	conflict	UNP O50336
l	76	ALA	PRO	conflict	UNP O50336
l	77	PHE	LEU	conflict	UNP O50336
l	78	ALA	PRO	conflict	UNP O50336
l	79	ARG	GLY	conflict	UNP O50336
l	80	LYS	ARG	conflict	UNP O50336
l	81	GLY	ALA	conflict	UNP O50336
l	82	ARG	GLY	conflict	UNP O50336
l	83	HIS	ILE	conflict	UNP O50336
l	84	ILE	PHE	conflict	UNP O50336
l	85	PHE	LEU	conflict	UNP O50336
l	86	ILE	SER	conflict	UNP O50336
l	87	LYS	SER	conflict	UNP O50336
l	88	PRO	ARG	conflict	UNP O50336
l	89	GLN	THR	conflict	UNP O50336
o	71	ASP	ILE	conflict	UNP O50336
o	72	SER	PRO	conflict	UNP O50336
o	73	GLU	LYS	conflict	UNP O50336
o	74	ALA	PRO	conflict	UNP O50336
o	75	TYR	MET	conflict	UNP O50336
o	76	ALA	PRO	conflict	UNP O50336
o	77	PHE	LEU	conflict	UNP O50336
o	78	ALA	PRO	conflict	UNP O50336
o	79	ARG	GLY	conflict	UNP O50336
o	80	LYS	ARG	conflict	UNP O50336
o	81	GLY	ALA	conflict	UNP O50336
o	82	ARG	GLY	conflict	UNP O50336
o	83	HIS	ILE	conflict	UNP O50336
o	84	ILE	PHE	conflict	UNP O50336
o	85	PHE	LEU	conflict	UNP O50336
o	86	ILE	SER	conflict	UNP O50336
o	87	LYS	SER	conflict	UNP O50336

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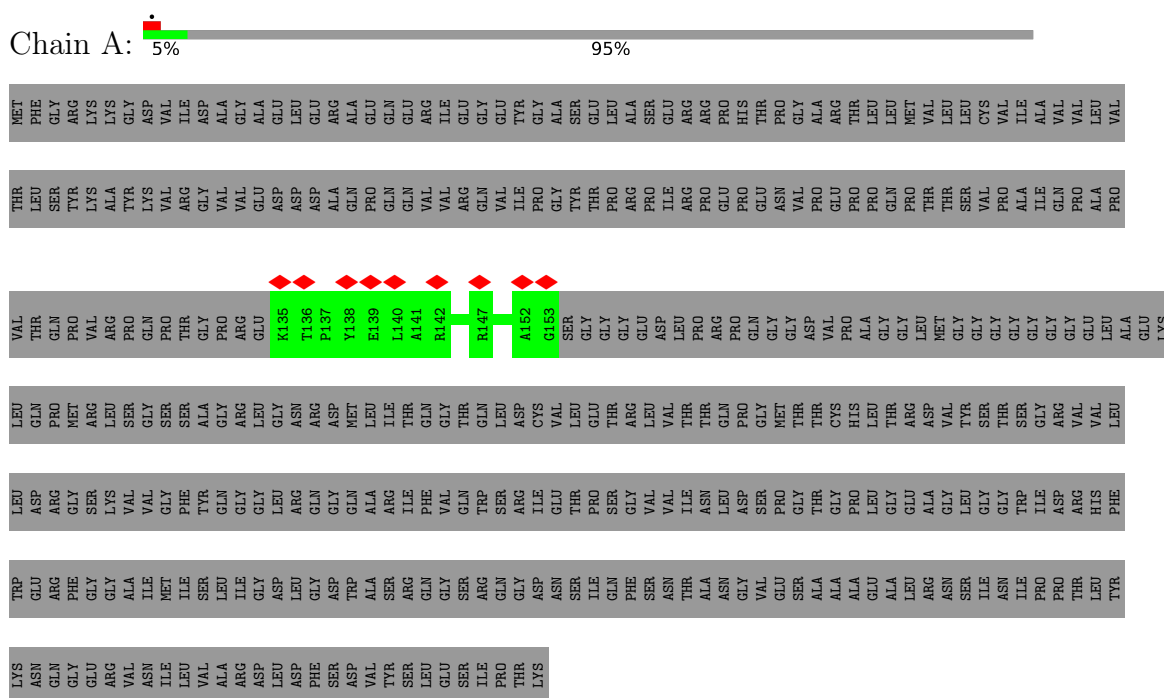
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Chain	Residue	Modelled	Actual	Comment	Reference
o	88	PRO	ARG	conflict	UNP O50336
o	89	GLN	THR	conflict	UNP O50336
z	71	ASP	ILE	conflict	UNP O50336
z	72	SER	PRO	conflict	UNP O50336
z	73	GLU	LYS	conflict	UNP O50336
z	74	ALA	PRO	conflict	UNP O50336
z	75	TYR	MET	conflict	UNP O50336
z	76	ALA	PRO	conflict	UNP O50336
z	77	PHE	LEU	conflict	UNP O50336
z	78	ALA	PRO	conflict	UNP O50336
z	79	ARG	GLY	conflict	UNP O50336
z	80	LYS	ARG	conflict	UNP O50336
z	81	GLY	ALA	conflict	UNP O50336
z	82	ARG	GLY	conflict	UNP O50336
z	83	HIS	ILE	conflict	UNP O50336
z	84	ILE	PHE	conflict	UNP O50336
z	85	PHE	LEU	conflict	UNP O50336
z	86	ILE	SER	conflict	UNP O50336
z	87	LYS	SER	conflict	UNP O50336
z	88	PRO	ARG	conflict	UNP O50336
z	89	GLN	THR	conflict	UNP O50336

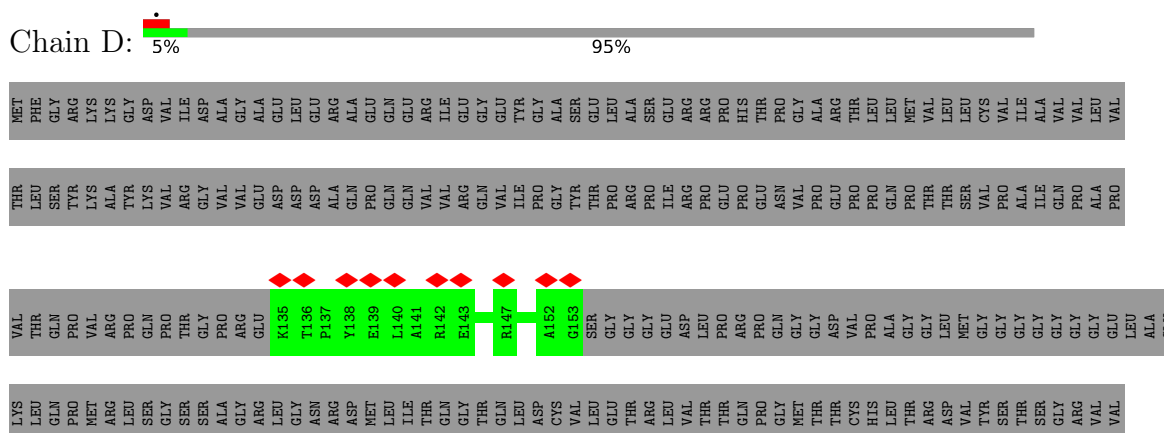
### 3 Residue-property plots

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: TrwE protein



#### • Molecule 1: TrwE protein







WORLDWIDE  
PDB  
PROTEIN DATA BANK



[illegible]

- Molecule 1: TrwE protein

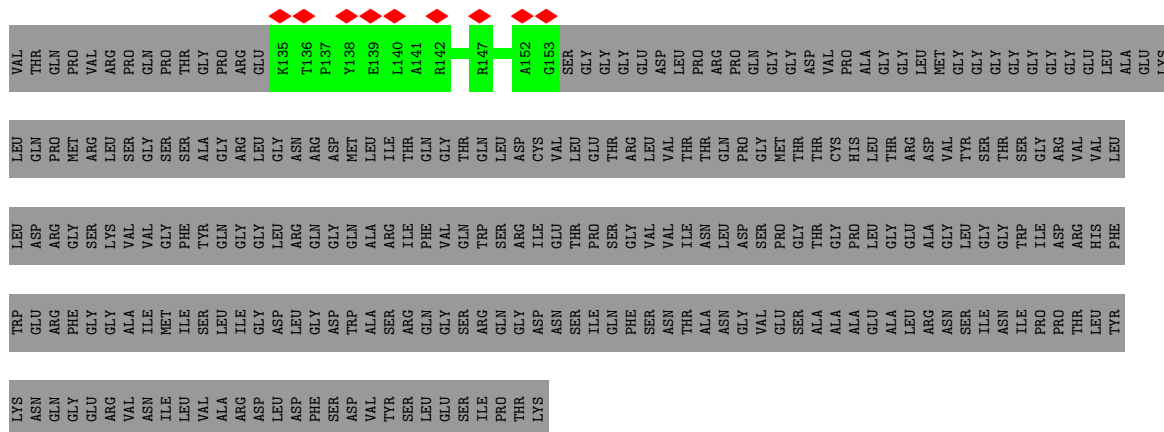
Chain u:  5% 95%

THR	LYS	LEU	LYS	VAL	THR	MET
LYS	LEU	GLN	THR	THR	LEU	PHE
GLN	GLN	PRO	PRO	GLN	SER	GLY
ARG	ARG	MET	VAL	ARG	LYS	LYS
GLY	SER	ARG	PRO	GLN	THR	LYS
LYS	LEU	LEU	PRO	ARG	LYS	ASP
VAL	SER	SER	GLN	GLY	VAL	ILE
VAL	GLY	SER	THR	THR	VAL	VAL
THR	SER	ALA	PRO	ALA	VAL	ASP
VAL	GLY	ARG	ARG	GLY	VAL	ALA
ARG	LEU	LEU	GLY	GLU	GLU	ALA
ASP	GLY	LEU	GLY	K135	ASP	GLU
ASP	GLY	ASN	GLY	T136	ASP	GLU
PHE	GLY	ARG	ARG	E139	ALA	GLU
SER	GLY	ASP	MET	L140	GLN	ALA
ASP	GLN	LEU	ILE	R141	GLN	GLU
VAL	ALA	ALA	ILE	R142	GLN	GLU
TYR	SER	ARG	ILE	E143	VAL	ARG
LEU	ARG	PHE	THR	R144	VAL	ILE
LEU	VAL	VAL	GLY	THR	ARG	GLY
ALA	SER	GLN	THR	GLN	VAL	GLY
ARG	ILE	TRP	LEU	R147	ILE	GLU
ASP	GLY	SER	LEU	A152	PRO	TYR
ASP	ASP	ARG	ASP	G153	PRO	GLY
ASP	ILE	ILE	CYS	THR	GLY	ALA
GLY	GLU	THR	VAL	SER	GLY	SER
ASN	GLY	LEU	GLY	GLY	ILE	ALA
ASN	GLY	THR	VAL	LEU	GLU	ALA
ASN	VAL	ARG	VAL	ASP	ARG	SER
ALA	VAL	THR	THR	LEU	PRO	ARG
ASN	ALA	THR	ASN	ARG	GLU	ARG
ASN	LEU	ASN	GLN	PRO	PRO	THR
GLY	ASP	ASP	PRO	ARG	GLU	THR
VAL	SER	SER	GLY	GLN	VAL	LEU
LEU	LEU	PRO	MET	GLY	VAL	LEU
LEU	GLY	THR	THR	GLY	ALA	LEU
ALA	GLY	GLY	CYS	VAL	PRO	CYS
ALA	PRO	LEU	HIS	PRO	PRO	VAL
GLU	LEU	THR	LEU	ALA	GLN	VAL
ALA	GLY	GLU	THR	GLY	PRO	VAL
ARG	GLU	ARG	LEU	GLY	THR	VAL
ASN	ALA	ASP	VAL	MET	THR	LEU
ASN	GLY	GLY	VAL	GLY	SER	LEU
SER	LEU	THR	THR	GLY	VAL	LEU
ILE	GLY	SER	SER	GLY	PRO	CYS
ASN	GLY	THR	THR	GLY	ALA	ILE
ASN	GLY	THR	SER	GLY	ILE	ALA
ILE	THR	THR	SER	GLY	GLN	ALA
PRO	ILE	ASP	GLY	GLY	ILE	VAL
THR	ASP	ARG	THR	GLY	PRO	VAL
LYS	LYS	HIS	VAL	LEU	PRO	VAL
				ALA	ALA	VAL

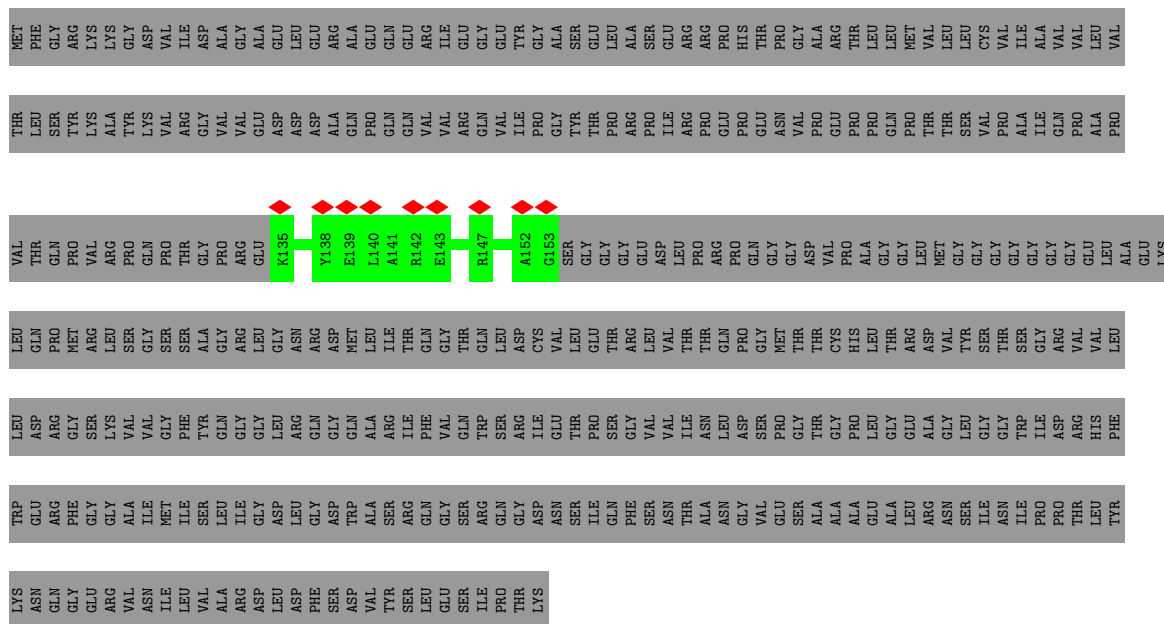
- Molecule 1: TrwE protein

Chain V:  5% 95%

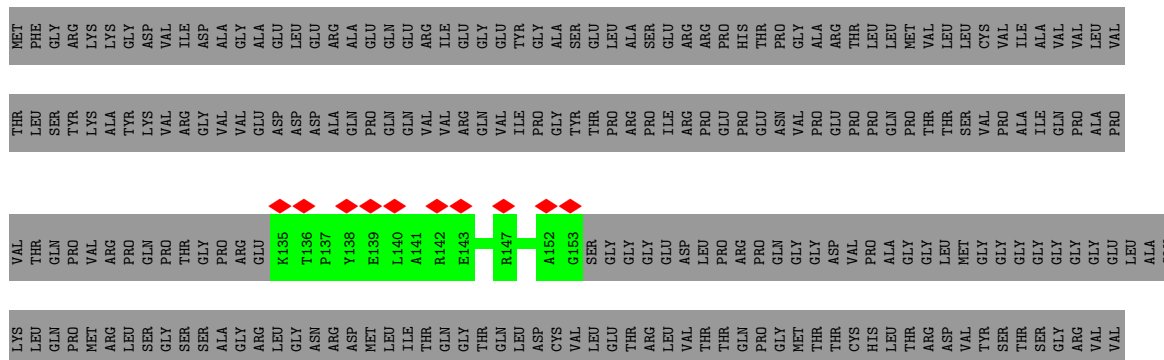
[illegible]

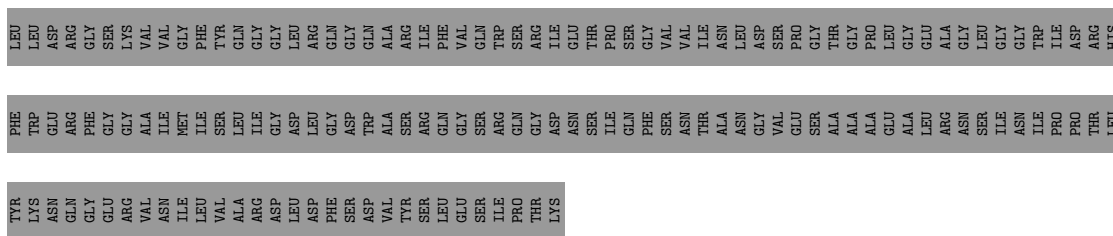


- Molecule 1: TrwE protein

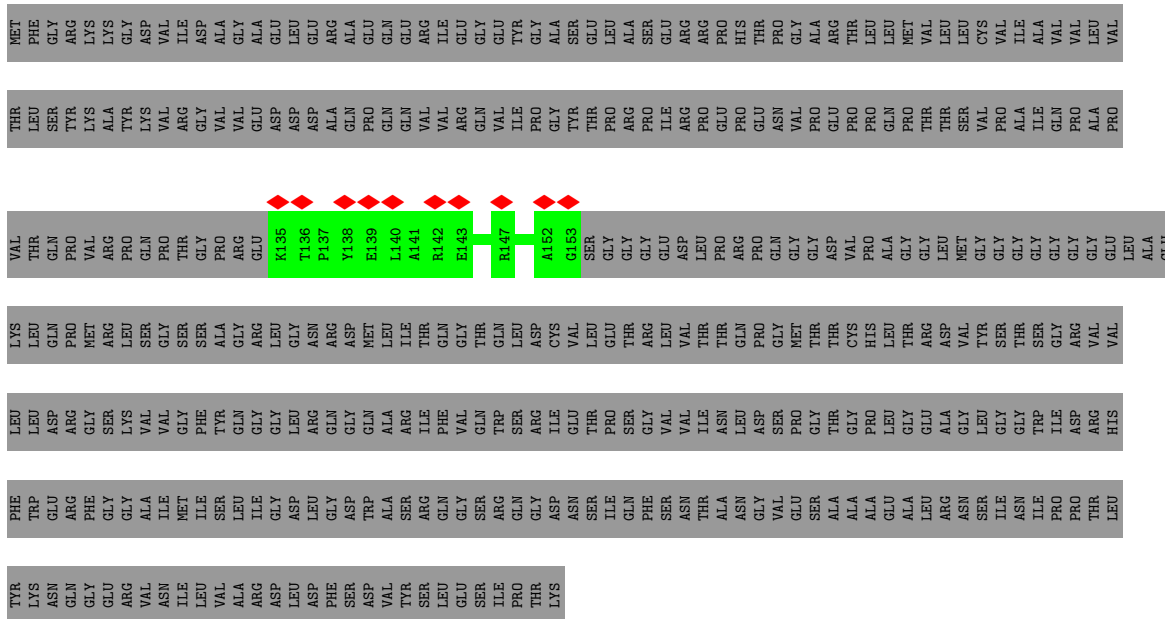


- Molecule 1: TrwE protein

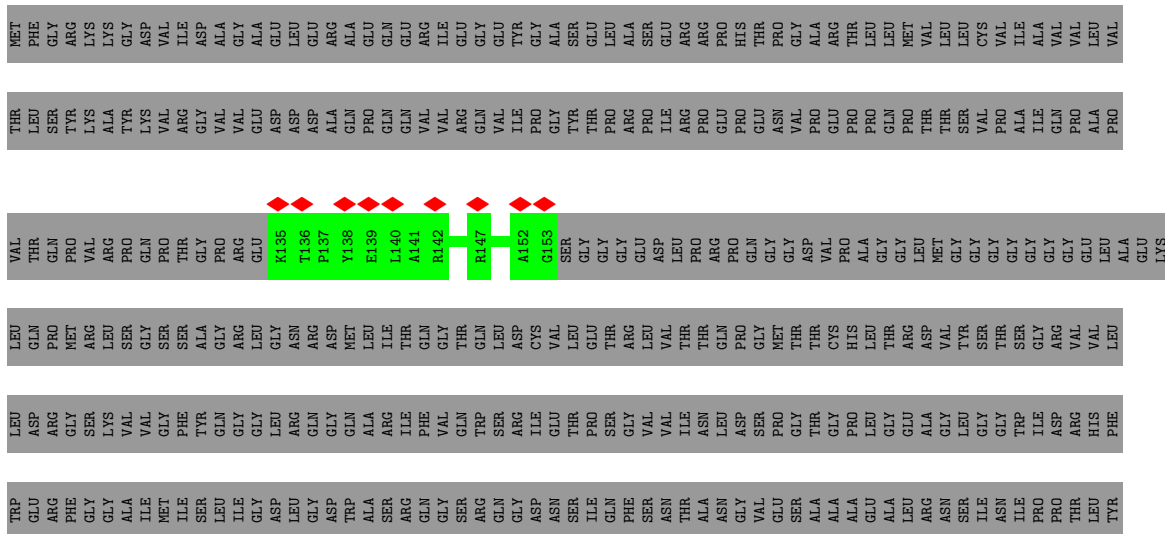




- Molecule 1: TrwE protein

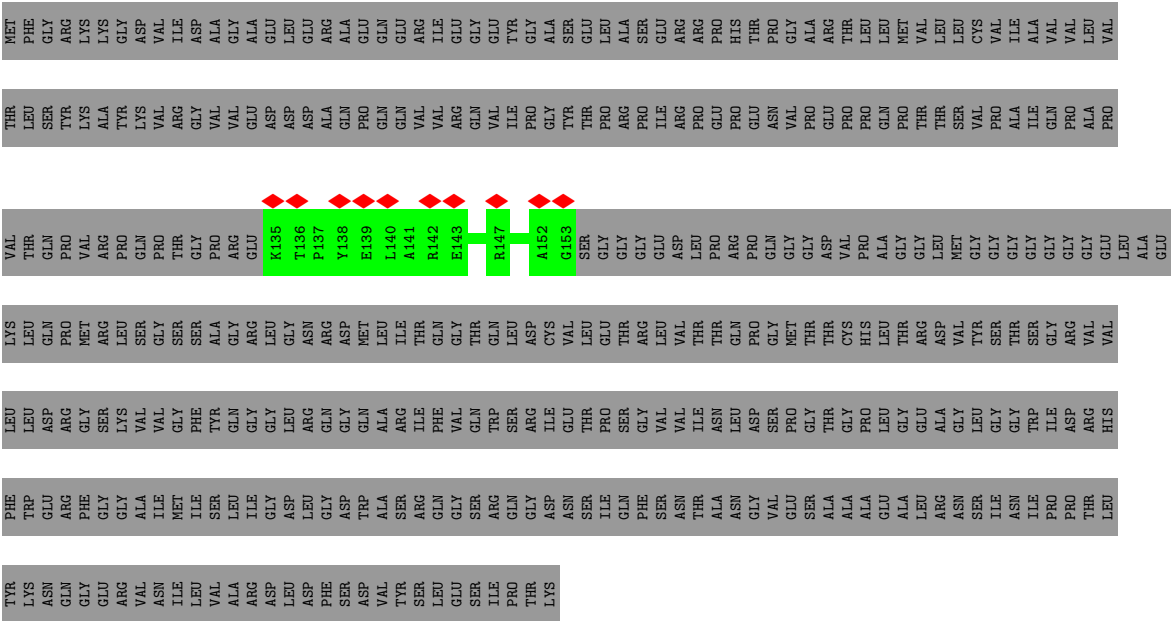


- Molecule 1: TrwE protein

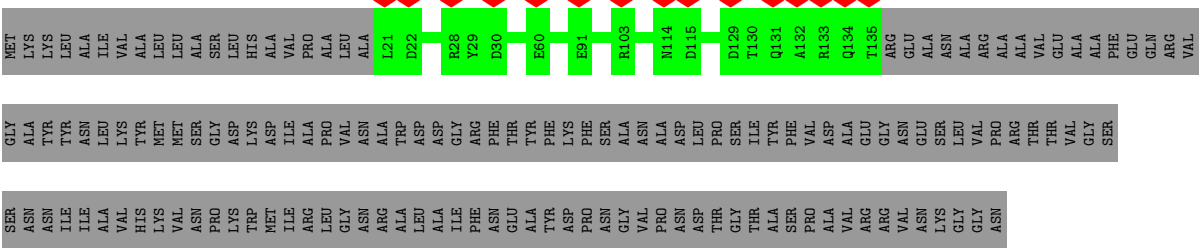




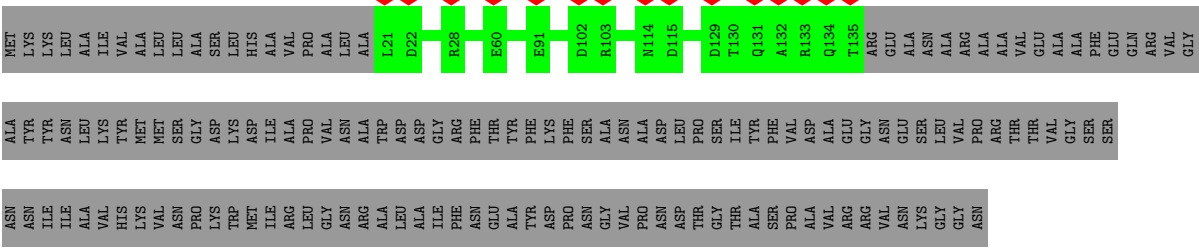
WORLD WIDE  
**PDB**  
PROTEIN DATA BANK



• Molecule 2: TrwF protein



• Molecule 2: TrwF protein



• Molecule 2: TrwF protein



- Molecule 2: TrwF protein



Position	Residue	Conservation	Phylogenetic Information	Biological Information
1	ALA	0.00	None	None
2	TYR	0.00	None	None
3	ASN	0.00	None	None
4	ILE	0.00	None	None
5	ALA	0.00	None	None
6	VAL	0.00	None	None
7	HIS	0.00	None	None
8	LYS	0.00	None	None
9	VAL	0.00	None	None
10	VAL	0.00	None	None
11	VAL	0.00	None	None
12	ASN	0.00	None	None
13	PRO	0.00	None	None
14	GLY	0.00	None	None
15	ASP	0.00	None	None
16	LYS	0.00	None	None
17	TRP	0.00	None	None
18	MET	0.00	None	None
19	ILE	0.00	None	None
20	ARG	0.00	None	None
21	LEU	0.00	None	None
22	GLY	0.00	None	None
23	ASN	0.00	None	None
24	ARG	0.00	None	None
25	ALA	0.00	None	None
26	LEU	0.00	None	None
27	ASP	0.00	None	None
28	GLY	0.00	None	None
29	ARG	0.00	None	None
30	ASP	0.00	None	None
31	THR	0.00	None	None
32	GLY	0.00	None	None
33	THR	0.00	None	None
34	ALA	0.00	None	None
35	SER	0.00	None	None
36	PRO	0.00	None	None
37	GLY	0.00	None	None
38	GLY	0.00	None	None
39	ASN	0.00	None	None
40	ASN	0.00	None	None
41	ASN	0.00	None	None
42	ILE	0.00	None	None
43	ALA	0.00	None	None
44	VAL	0.00	None	None
45	VAL	0.00	None	None
46	ARG	0.00	None	None
47	ARG	0.00	None	None
48	VAL	0.00	None	None
49	ASN	0.00	None	None
50	GLU	0.00	None	None
51	ASN	0.00	None	None
52	GLU	0.00	None	None
53	SER	0.00	None	None
54	LEU	0.00	None	None
55	VAL	0.00	None	None
56	PRO	0.00	None	None
57	ALA	0.00	None	None
58	THR	0.00	None	None
59	ARG	0.00	None	None
60	ALA	0.00	None	None
61	GLU	0.00	None	None
62	VAL	0.00	None	None
63	ALA	0.00	None	None
64	ALA	0.00	None	None
65	GLN	0.00	None	None
66	ARG	0.00	None	None
67	GLN	0.00	None	None
68	VAL	0.00	None	None
69	VAL	0.00	None	None
70	THR	0.00	None	None
71	THR	0.00	None	None
72	VAL	0.00	None	None
73	GLY	0.00	None	None
74	SER	0.00	None	None
75	SER	0.00	None	None
76	ALA	0.00	None	None
77	THR	0.00	None	None
78	THR	0.00	None	None
79	THR	0.00	None	None
80	THR	0.00	None	None
81	THR	0.00	None	None
82	THR	0.00	None	None
83	THR	0.00	None	None
84	THR	0.00	None	None
85	THR	0.00	None	None
86	THR	0.00	None	None
87	THR	0.00	None	None
88	THR			

- Molecule 2: TrwF protein

[illegible]

- Molecule 2: TrwF protein

[illegible]

- Molecule 2: TrwF protein



MET LYS LYS LEU LEU ALA ILE VAL ALA ALA LEU LEU LEU ALA SER LEU LEU HIS ALA VAL PRO PRO LEU LEU ALA L21 L22 R23 E60 E91 R103 D115 D129 T130 Q131 A132 R133 Q134 T135 ARG GLU GLU ASN ALA ALA ARG ARG ALA ALA VAL VAL ALA ALA PHE GLU GLN ARG ARG VAL VAL GLY ALA



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

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

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



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

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

● Molecule 2: TrwF protein



MET  
LYS  
LYS  
LEU  
ALA  
ILE  
VAL  
VAL  
ALA  
LEU  
SER  
LEU  
HIS  
VAL  
PRO  
ALA  
LEU  
ALA  
T21  
D22  
R28  
Y29  
D30  
E60  
E91  
R103  
D115  
D129  
T130  
Q131  
A132  
R133  
Q134  
T135  
ARG  
GLU  
ALA  
ASN  
ALA  
SER  
ALA  
ARG  
ALA  
PRO  
VAL  
THR  
GLU  
ALA  
PHE  
GLY  
GLN  
ARG  
VAL  
GLY

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

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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	784923	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	57.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.950	Depositor
Minimum map value	-0.337	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	320.1, 320.1, 320.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	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	0.32	0/150	0.67	0/199
1	D	0.33	0/150	0.67	0/199
1	G	0.33	0/150	0.67	0/199
1	J	0.32	0/150	0.67	0/199
1	M	0.33	0/150	0.67	0/199
1	P	0.32	0/150	0.67	0/199
1	S	0.33	0/150	0.67	0/199
1	V	0.32	0/150	0.67	0/199
1	Y	0.33	0/150	0.67	0/199
1	b	0.32	0/150	0.67	0/199
1	e	0.33	0/150	0.67	0/199
1	h	0.33	0/150	0.67	0/199
1	k	0.33	0/150	0.67	0/199
1	n	0.33	0/150	0.67	0/199
1	u	0.33	0/150	0.67	0/199
1	y	0.33	0/150	0.67	0/199
2	B	0.39	0/962	0.50	0/1302
2	E	0.39	0/962	0.50	0/1302
2	H	0.39	0/962	0.50	0/1302
2	K	0.39	0/962	0.50	0/1302
2	N	0.39	0/962	0.50	0/1302
2	Q	0.39	0/962	0.50	0/1302
2	T	0.39	0/962	0.50	0/1302
2	W	0.39	0/962	0.50	0/1302
2	Z	0.39	0/962	0.50	0/1302
2	c	0.39	0/962	0.50	0/1302
2	f	0.39	0/962	0.50	0/1302
2	i	0.39	0/962	0.50	0/1302
2	l	0.39	0/962	0.50	0/1302
2	o	0.39	0/962	0.50	0/1302
2	v	0.39	0/962	0.50	0/1302
2	z	0.39	0/962	0.50	0/1302
All	All	0.38	0/17792	0.53	0/24016

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	17/395 (4%)	17 (100%)	0	0	100	100
1	D	17/395 (4%)	17 (100%)	0	0	100	100
1	G	17/395 (4%)	17 (100%)	0	0	100	100
1	J	17/395 (4%)	17 (100%)	0	0	100	100
1	M	17/395 (4%)	17 (100%)	0	0	100	100
1	P	17/395 (4%)	17 (100%)	0	0	100	100
1	S	17/395 (4%)	17 (100%)	0	0	100	100
1	V	17/395 (4%)	17 (100%)	0	0	100	100
1	Y	17/395 (4%)	17 (100%)	0	0	100	100
1	b	17/395 (4%)	17 (100%)	0	0	100	100
1	e	17/395 (4%)	17 (100%)	0	0	100	100
1	h	17/395 (4%)	17 (100%)	0	0	100	100
1	k	17/395 (4%)	17 (100%)	0	0	100	100
1	n	17/395 (4%)	17 (100%)	0	0	100	100
1	u	17/395 (4%)	17 (100%)	0	0	100	100
1	y	17/395 (4%)	17 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	E	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	H	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	K	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	N	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	Q	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	T	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	W	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	Z	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	c	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	f	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	i	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	l	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	o	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	v	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
2	z	113/266 (42%)	111 (98%)	2 (2%)	0	100	100
All	All	2080/10576 (20%)	2048 (98%)	32 (2%)	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	15/318 (5%)	15 (100%)	0	100	100
1	D	15/318 (5%)	15 (100%)	0	100	100
1	G	15/318 (5%)	15 (100%)	0	100	100
1	J	15/318 (5%)	15 (100%)	0	100	100
1	M	15/318 (5%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	15/318 (5%)	15 (100%)	0	100	100
1	S	15/318 (5%)	15 (100%)	0	100	100
1	V	15/318 (5%)	15 (100%)	0	100	100
1	Y	15/318 (5%)	15 (100%)	0	100	100
1	b	15/318 (5%)	15 (100%)	0	100	100
1	e	15/318 (5%)	15 (100%)	0	100	100
1	h	15/318 (5%)	15 (100%)	0	100	100
1	k	15/318 (5%)	15 (100%)	0	100	100
1	n	15/318 (5%)	15 (100%)	0	100	100
1	u	15/318 (5%)	15 (100%)	0	100	100
1	y	15/318 (5%)	15 (100%)	0	100	100
2	B	99/216 (46%)	99 (100%)	0	100	100
2	E	99/216 (46%)	99 (100%)	0	100	100
2	H	99/216 (46%)	99 (100%)	0	100	100
2	K	99/216 (46%)	99 (100%)	0	100	100
2	N	99/216 (46%)	99 (100%)	0	100	100
2	Q	99/216 (46%)	99 (100%)	0	100	100
2	T	99/216 (46%)	99 (100%)	0	100	100
2	W	99/216 (46%)	99 (100%)	0	100	100
2	Z	99/216 (46%)	99 (100%)	0	100	100
2	c	99/216 (46%)	99 (100%)	0	100	100
2	f	99/216 (46%)	99 (100%)	0	100	100
2	i	99/216 (46%)	99 (100%)	0	100	100
2	l	99/216 (46%)	99 (100%)	0	100	100
2	o	99/216 (46%)	99 (100%)	0	100	100
2	v	99/216 (46%)	99 (100%)	0	100	100
2	z	99/216 (46%)	99 (100%)	0	100	100
All	All	1824/8544 (21%)	1824 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

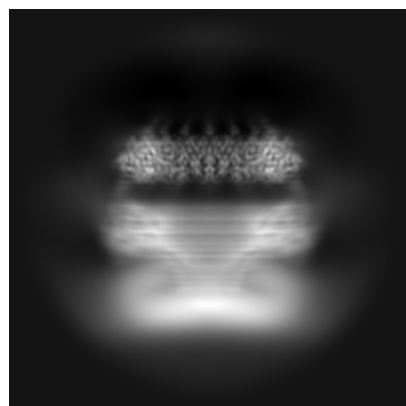
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19479. These allow visual inspection of the internal detail of the map and identification of artifacts.

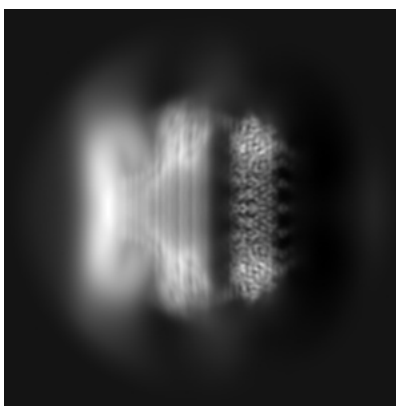
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

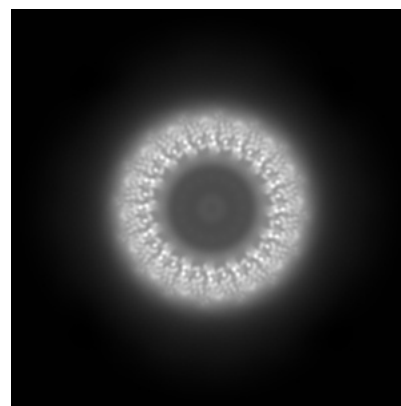
#### 6.1.1 Primary map



X

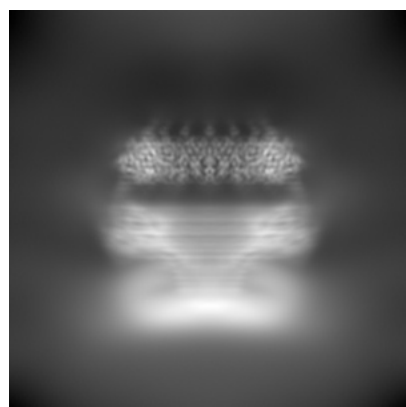


Y

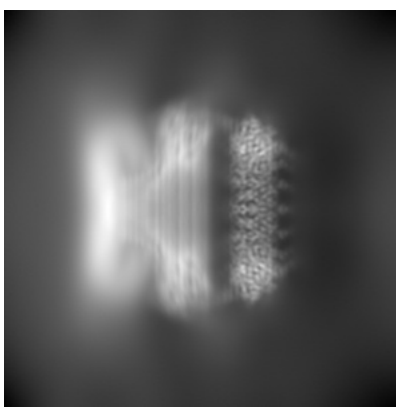


Z

#### 6.1.2 Raw map



X



Y



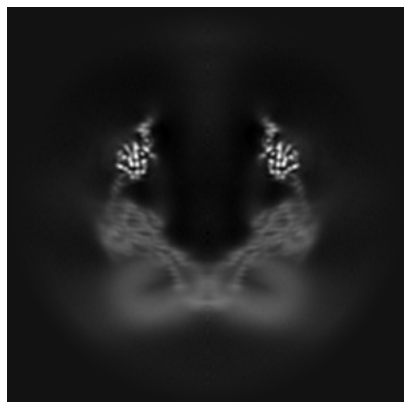
Z

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

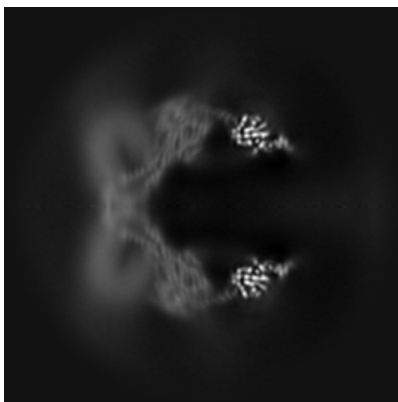


## 6.2 Central slices [i](#)

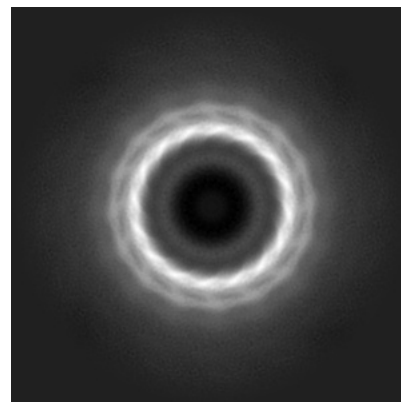
### 6.2.1 Primary map



X Index: 150

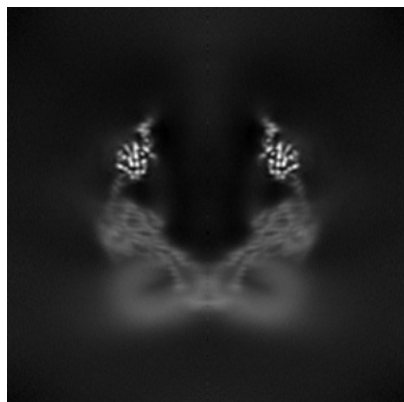


Y Index: 150

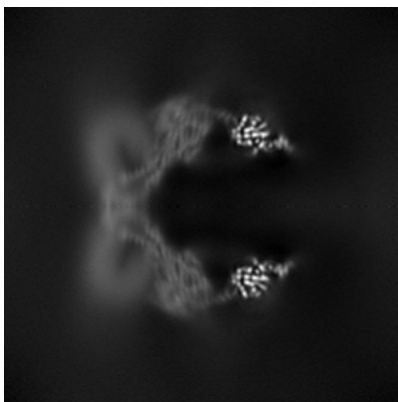


Z Index: 150

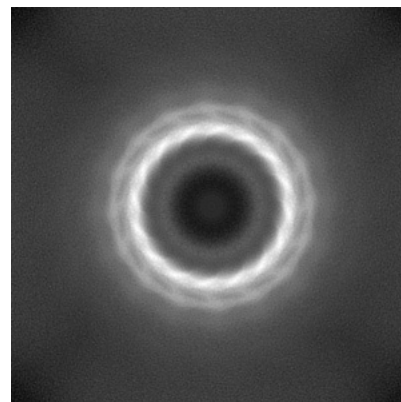
### 6.2.2 Raw map



X Index: 150



Y Index: 150

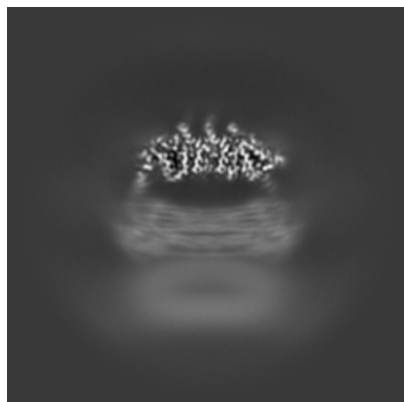


Z Index: 150

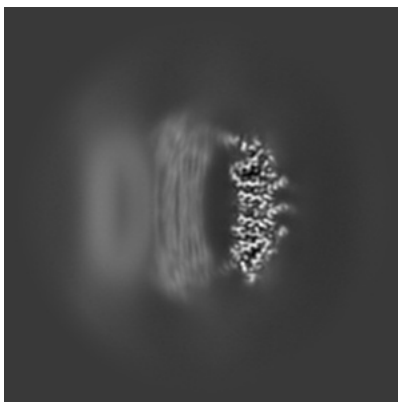
The images above show central slices of the map in three orthogonal directions.

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

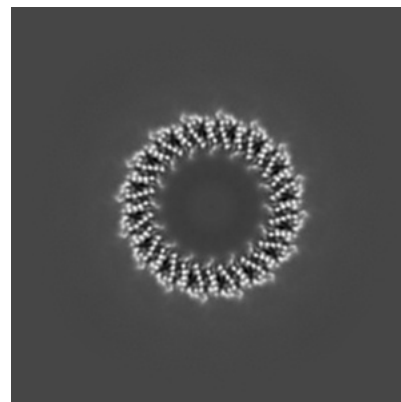
### 6.3.1 Primary map



X Index: 104

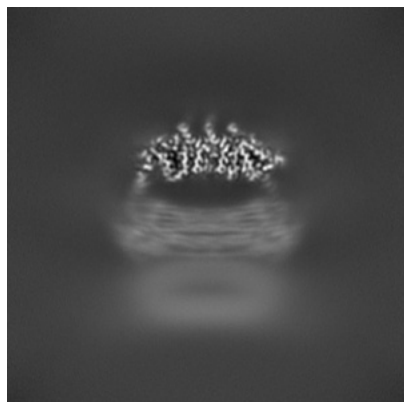


Y Index: 104

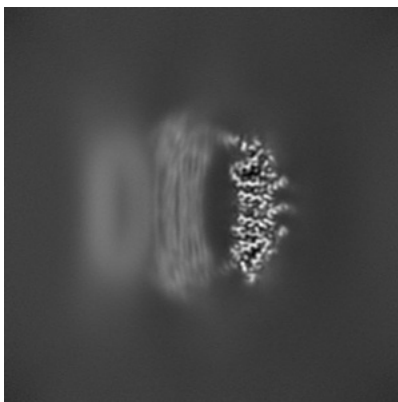


Z Index: 187

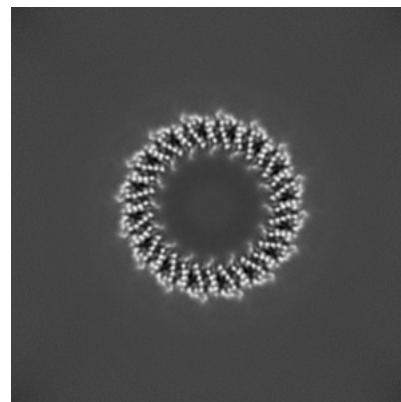
### 6.3.2 Raw map



X Index: 104



Y Index: 104

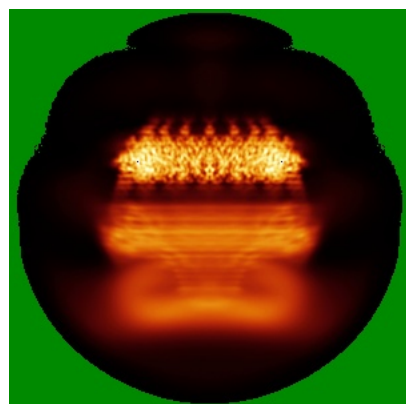


Z Index: 187

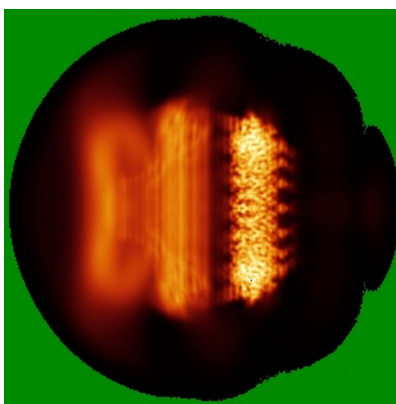
The images above show the largest variance slices of the map in three orthogonal directions.

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

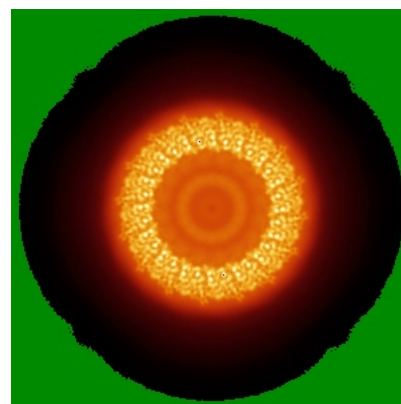
### 6.4.1 Primary map



X

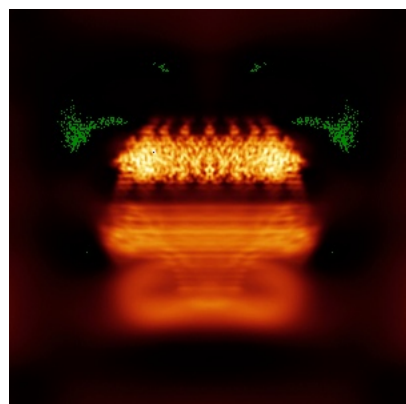


Y

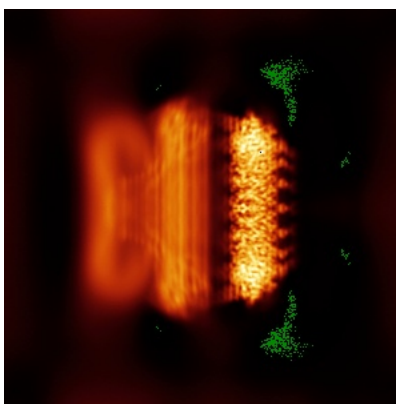


Z

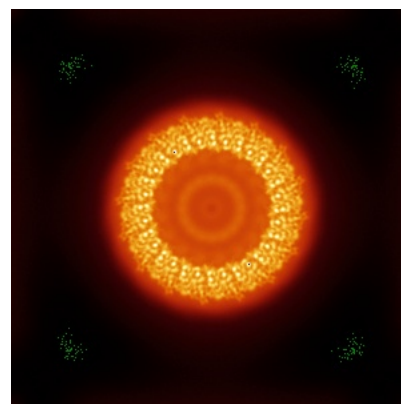
### 6.4.2 Raw map



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 0.4. 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.

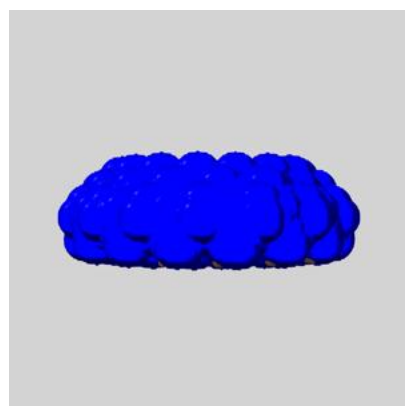
## 6.6 Mask visualisation [i](#)

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

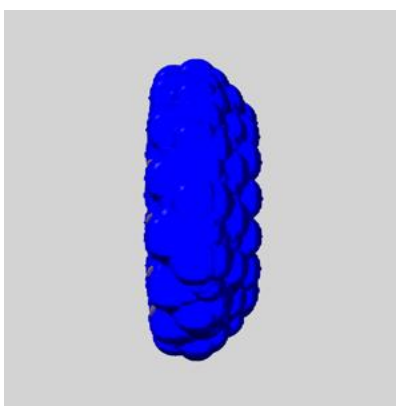
A mask typically either:

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

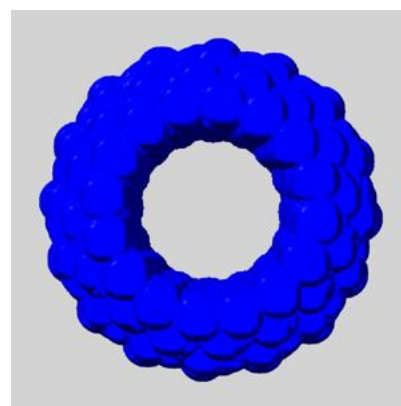
### 6.6.1 emd\_19479\_msk\_1.map [i](#)



X



Y

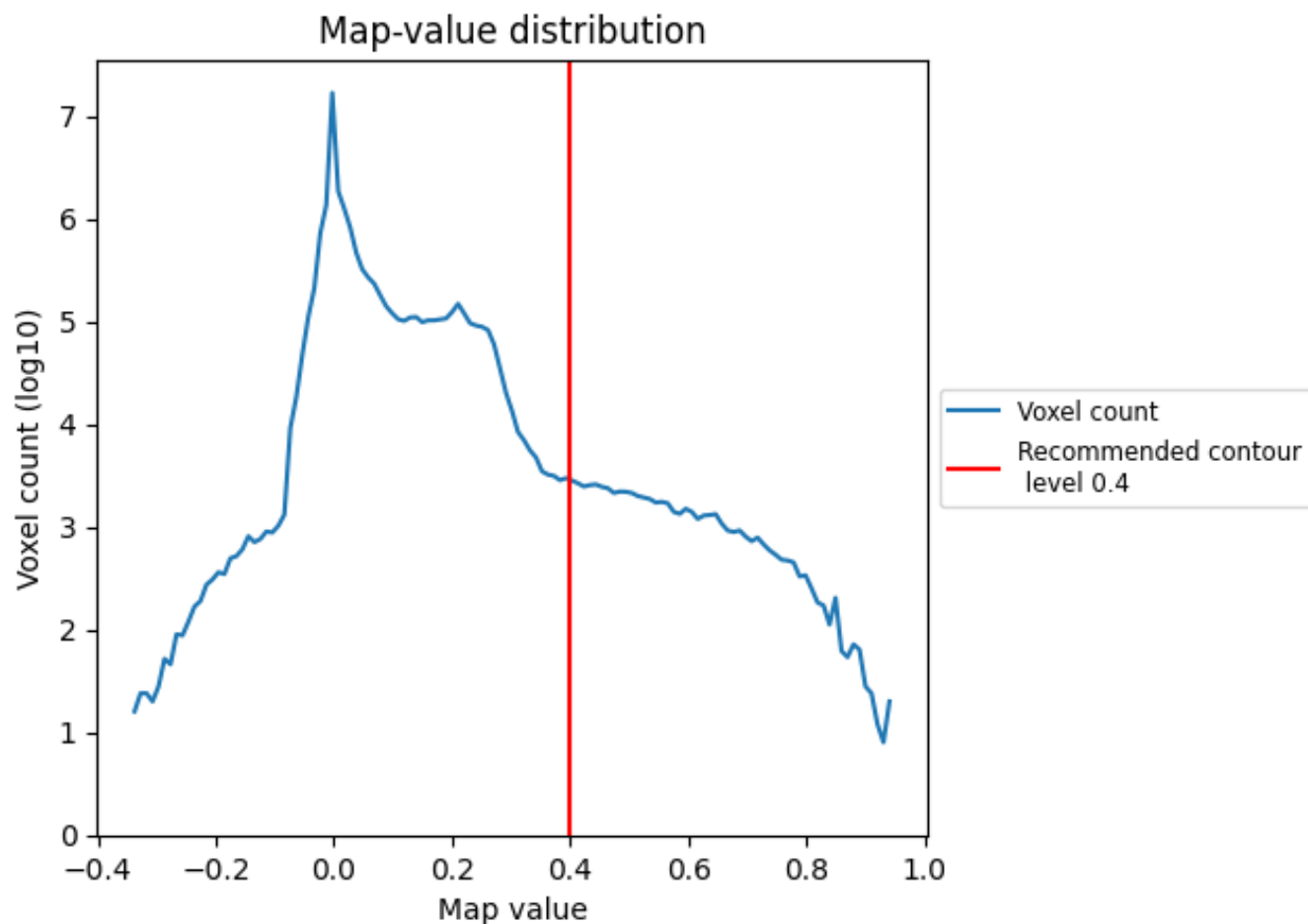


Z

## 7 Map analysis [i](#)

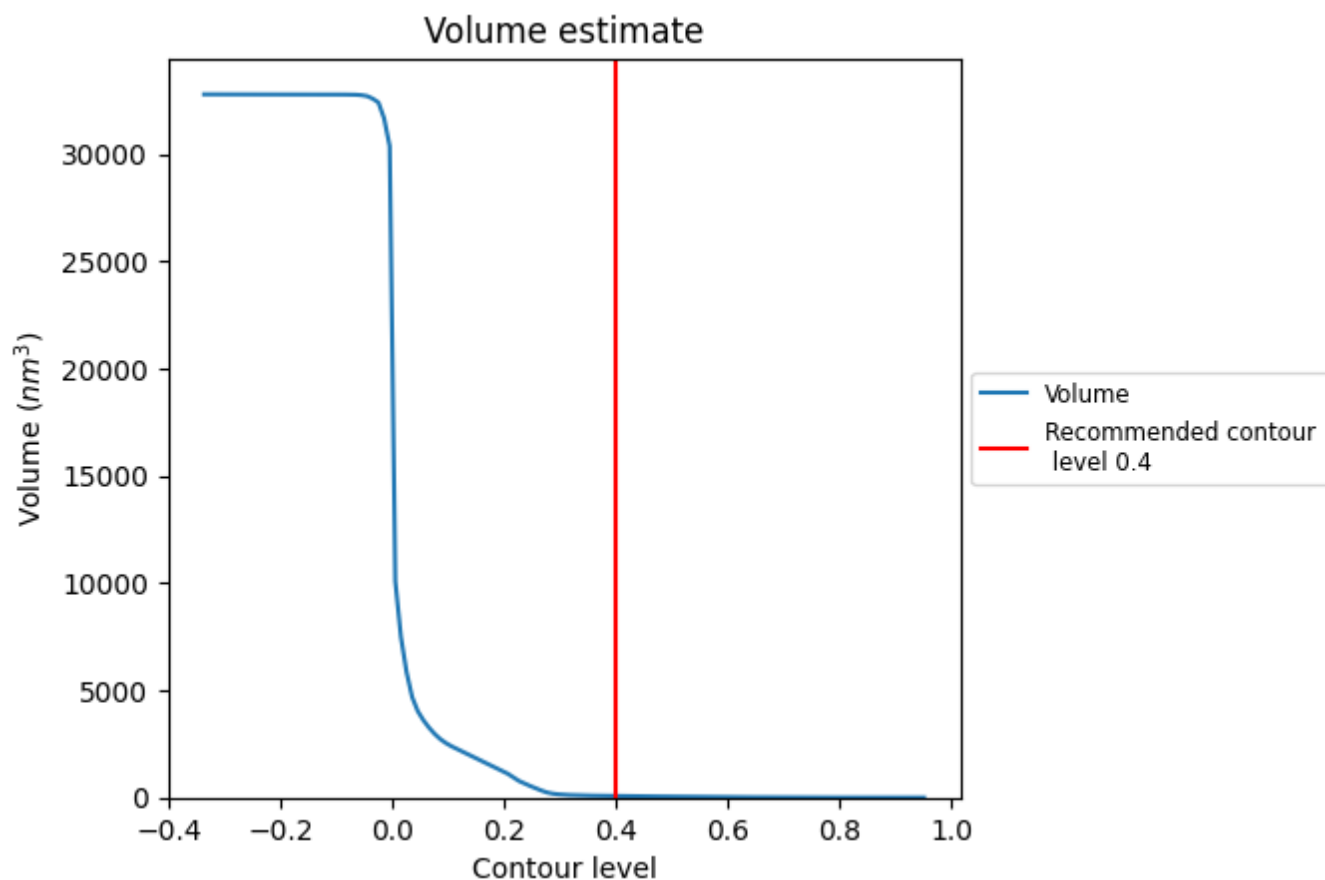
This section contains the results of statistical analysis of the map.

### 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.

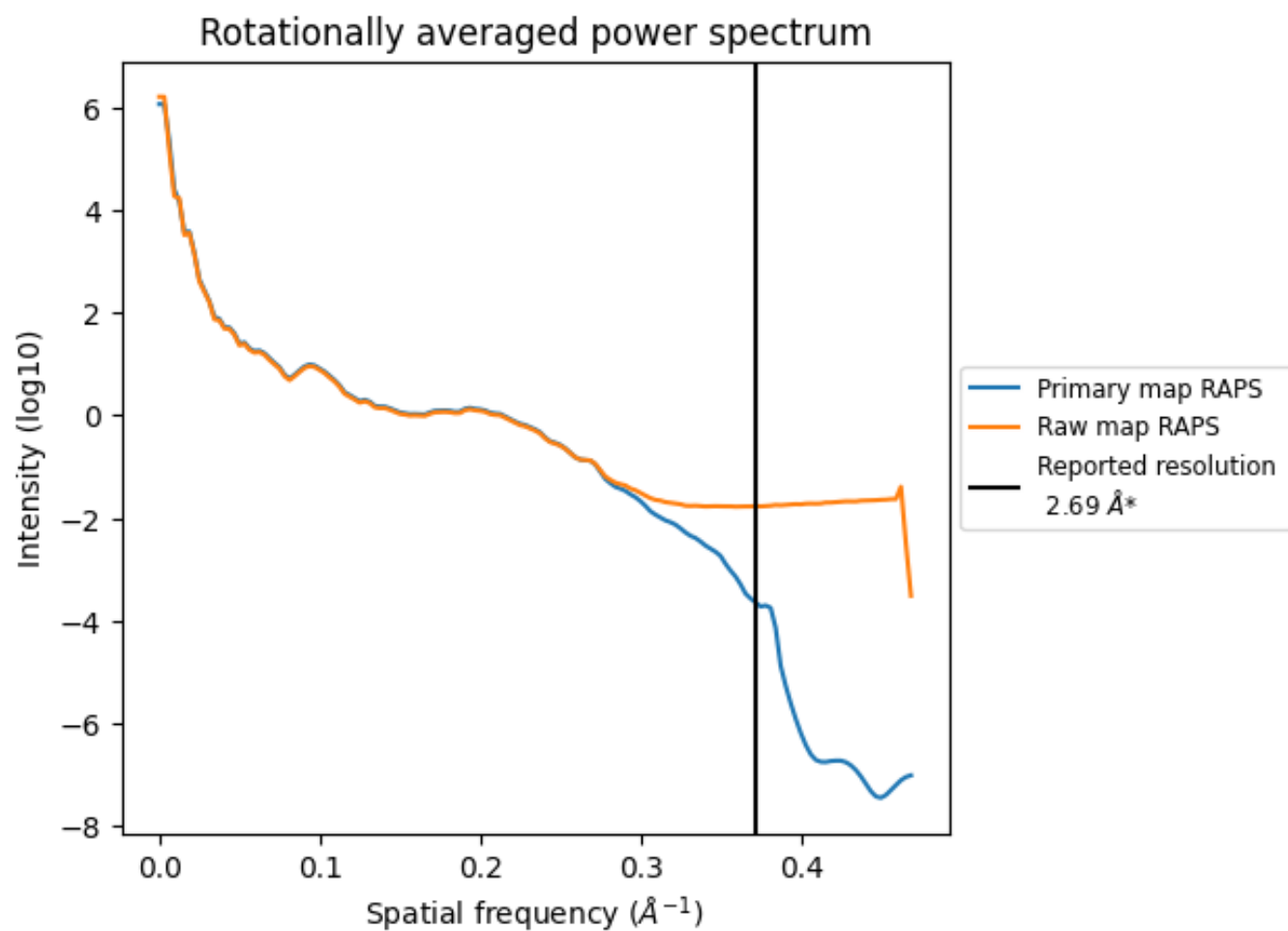
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm<sup>3</sup>; this corresponds to an approximate mass of 67 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 ⓘ



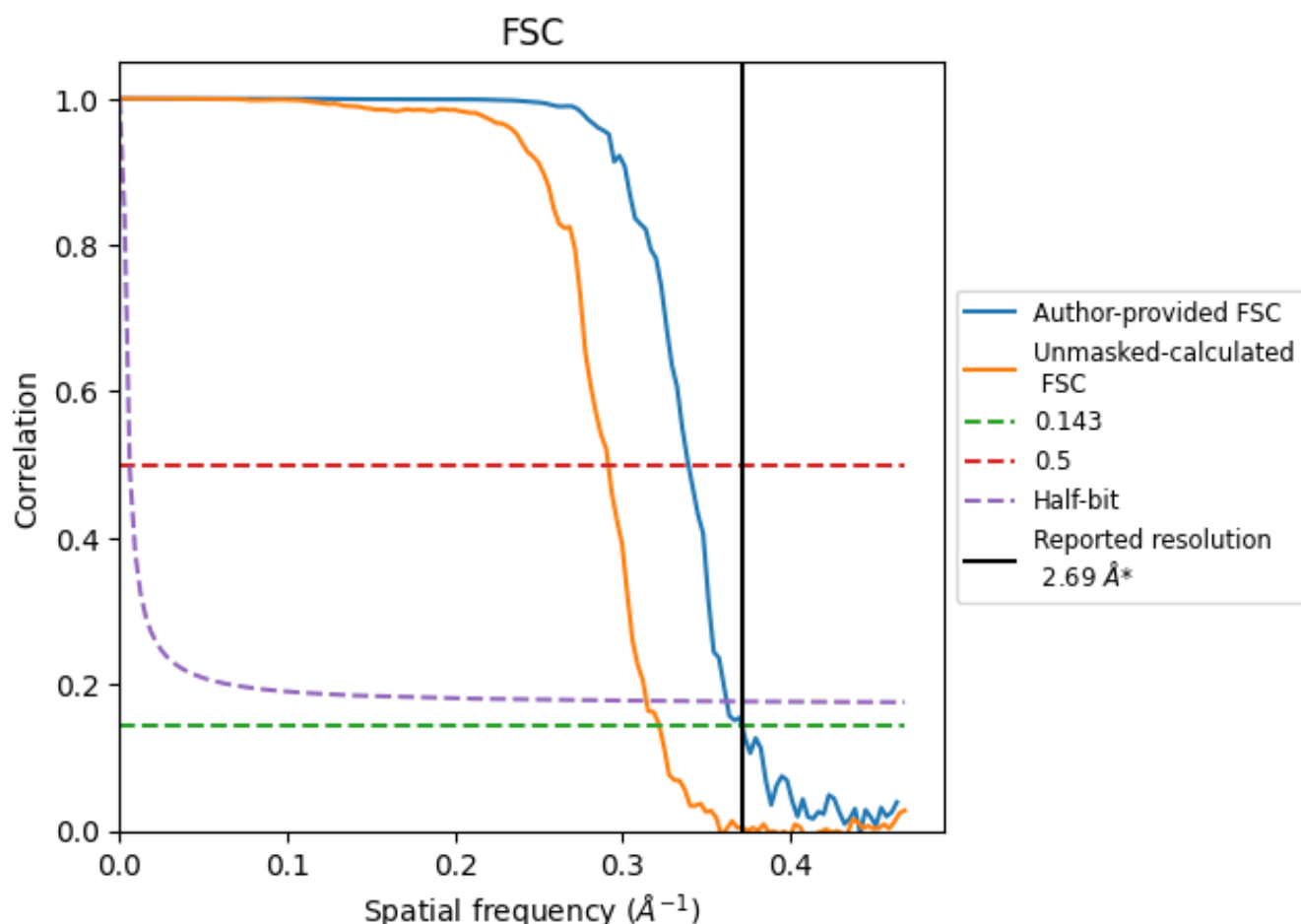
\*Reported resolution corresponds to spatial frequency of 0.372 Å<sup>-1</sup>



## 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 0.372  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

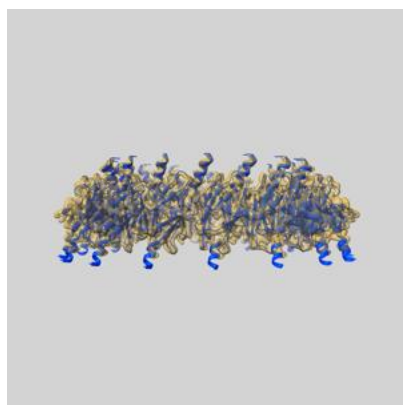
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	2.95	2.76
Unmasked-calculated*	3.10	3.43	3.18

\*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 3.10 differs from the reported value 2.69 by more than 10 %

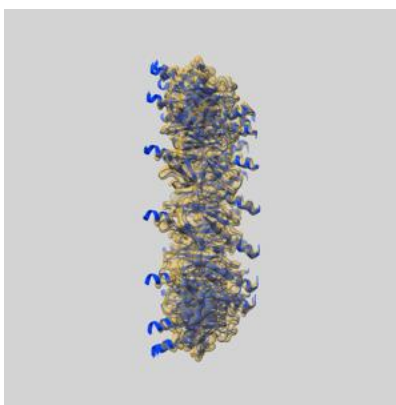
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19479 and PDB model 8RT5. Per-residue inclusion information can be found in section [3](#) on page [14](#).

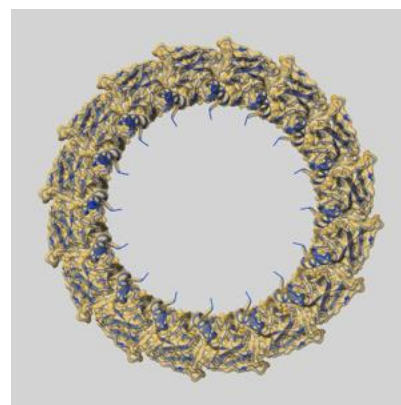
### 9.1 Map-model overlay [i](#)



X



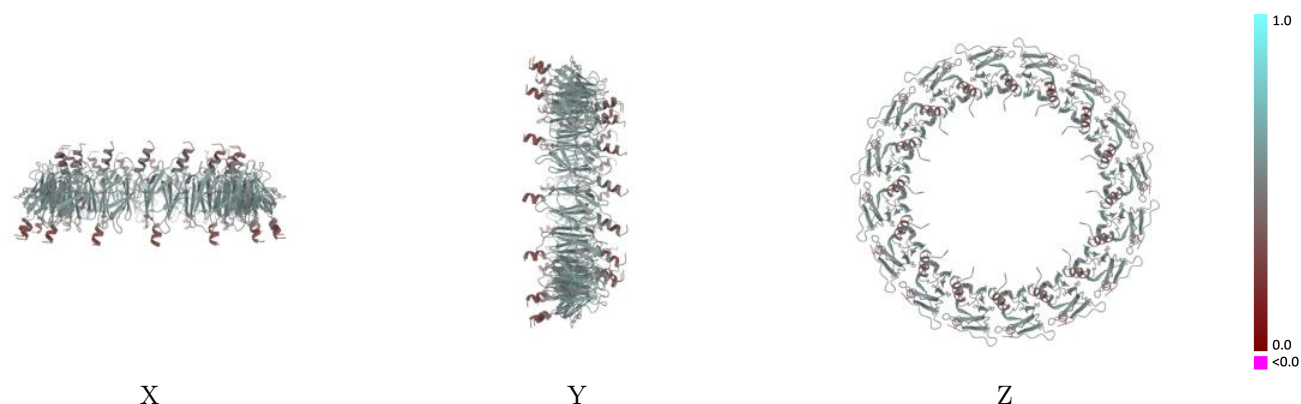
Y



Z

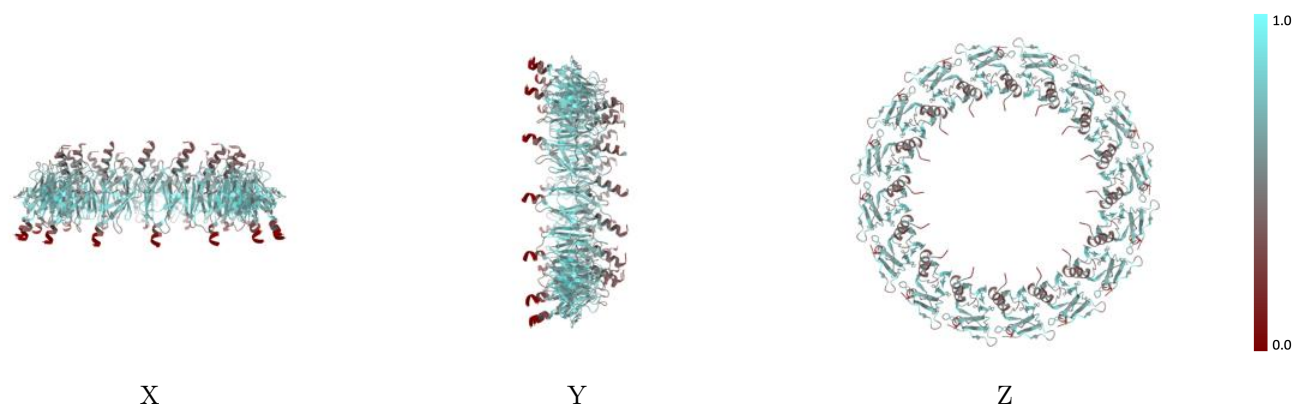
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



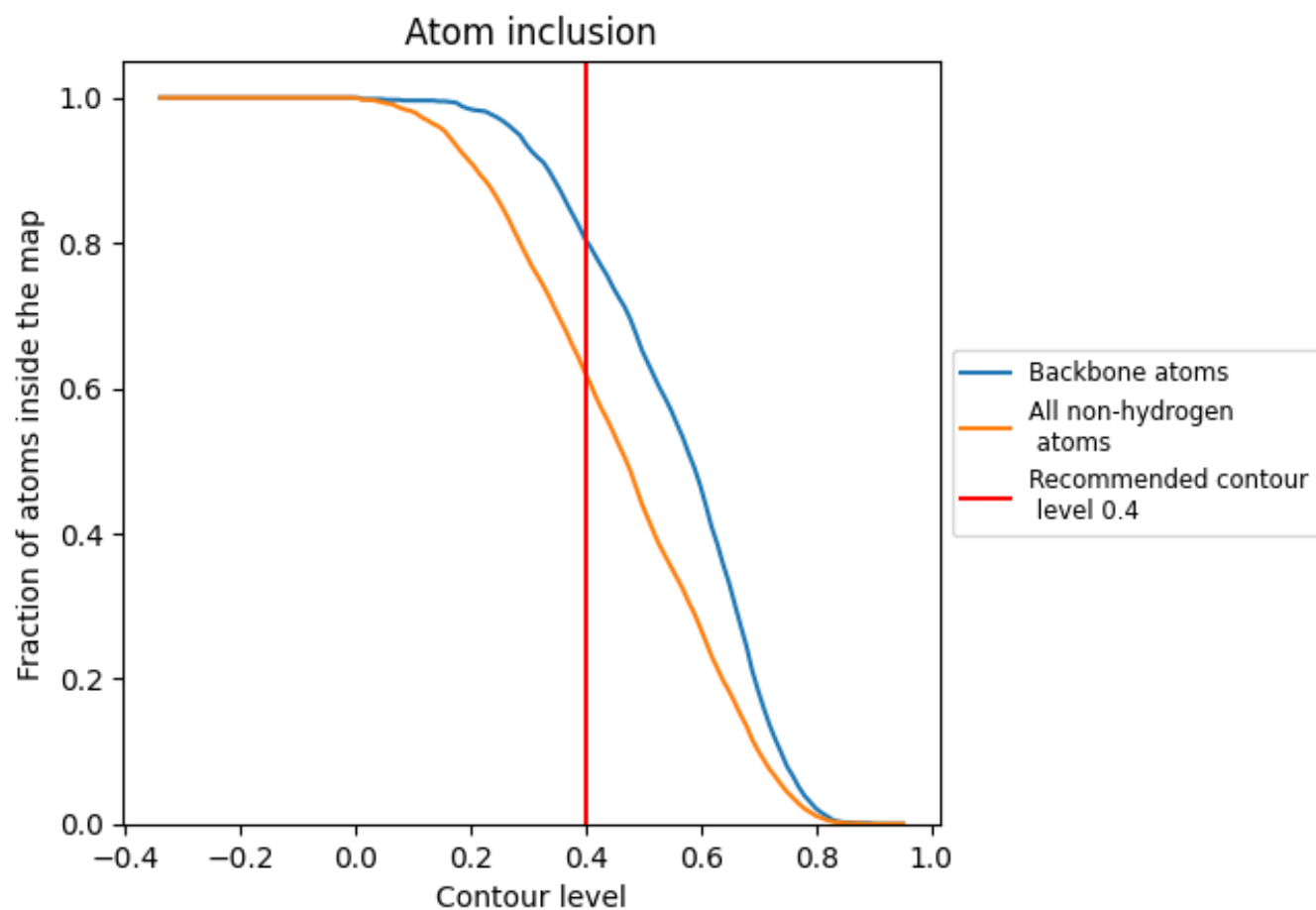
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 62% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6190	 0.5050
A	 0.4150	 0.4560
B	 0.6500	 0.5150
D	 0.4220	 0.4570
E	 0.6490	 0.5140
G	 0.4150	 0.4530
H	 0.6490	 0.5160
J	 0.3940	 0.4470
K	 0.6560	 0.5150
M	 0.4010	 0.4380
N	 0.6500	 0.5140
P	 0.4080	 0.4520
Q	 0.6540	 0.5130
S	 0.4150	 0.4350
T	 0.6560	 0.5150
V	 0.4010	 0.4520
W	 0.6530	 0.5120
Y	 0.4010	 0.4540
Z	 0.6540	 0.5120
b	 0.4010	 0.4530
c	 0.6500	 0.5130
e	 0.4150	 0.4630
f	 0.6550	 0.5150
h	 0.3940	 0.4520
i	 0.6450	 0.5140
k	 0.4080	 0.4330
l	 0.6520	 0.5110
n	 0.4010	 0.4330
o	 0.6560	 0.5130
u	 0.3940	 0.4360
v	 0.6500	 0.5150
y	 0.4150	 0.4590
z	 0.6560	 0.5160

