



Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 02:39 am BST

PDB ID : 7O3T
EMDB ID : EMD-12708
Title : I-layer structure (TrwF/VirB9NTD, TrwE/VirB10NTD) of the outer membrane core complex from the fully-assembled R388 type IV secretion system determined by cryo-EM.
Authors : Mace, K.; Vadakkepat, A.K.; Lukyanova, N.; Waksman, G.
Deposited on : 2021-04-03
Resolution : 3.10 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.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 3.10 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.



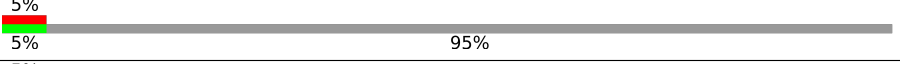
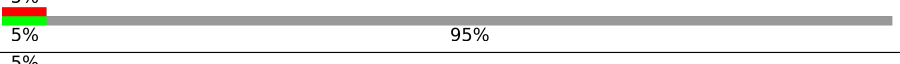
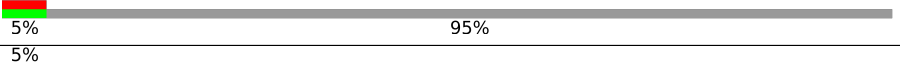
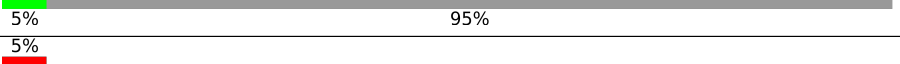
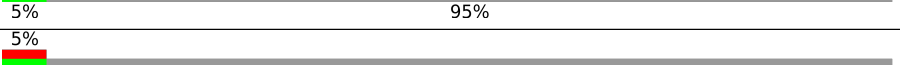
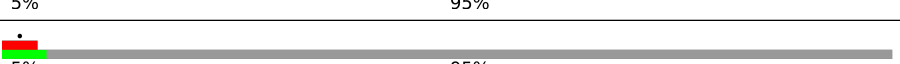
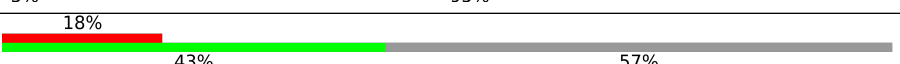


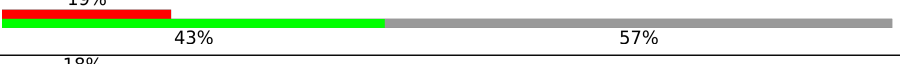
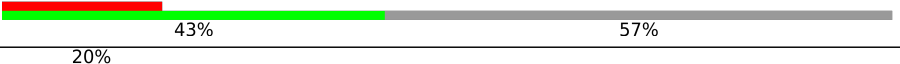



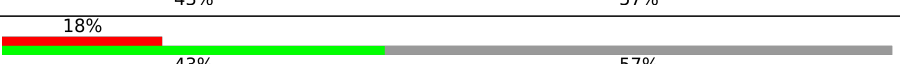
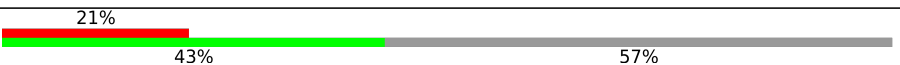







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 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	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	D	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	G	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	J	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	M	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	P	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	S	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	V	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>
1	Y	395	<div> <div>5%</div> <div>5%</div> <div>95%</div> </div>

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

2 Entry composition

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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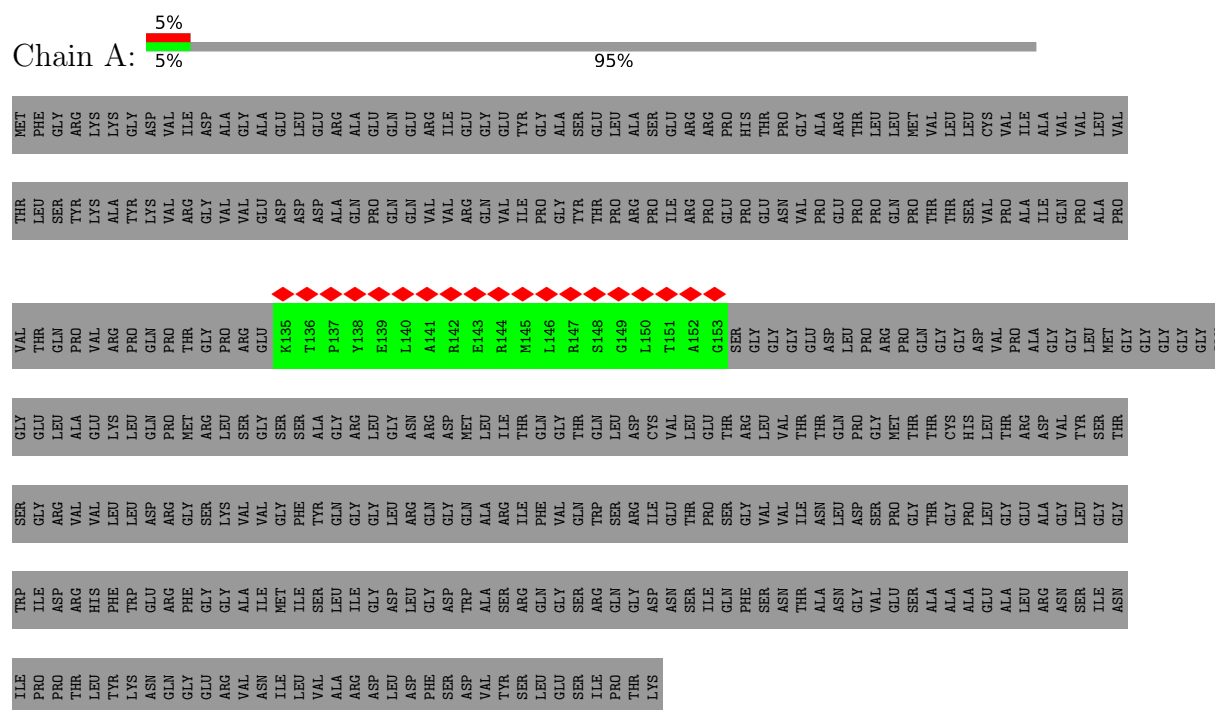
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Chain	Residue	Modelled	Actual	Comment	Reference
o	88	PRO	ARG	conflict	UNP O50336
o	89	GLN	THR	conflict	UNP O50336
z	71	ASP	ILE	conflict	UNP O50336
z	72	SER	PRO	conflict	UNP O50336
z	73	GLU	LYS	conflict	UNP O50336
z	74	ALA	PRO	conflict	UNP O50336
z	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

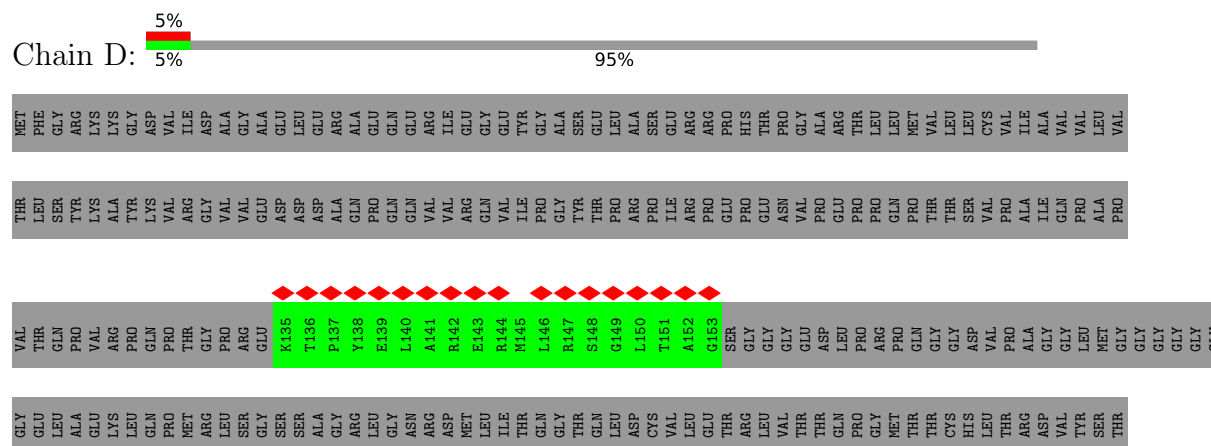
3 Residue-property plots

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



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

- Molecule 1: TrwE protein

[illegible]

- Molecule 1: TrwE protein

[illegible]



ILE	TRP	SER	GLY	VAL	THR	MET
PRO	ILE	GLY	LEU	GLN	LEU	PHE
PRO	ASP	ARG	LEU	GLN	TYR	ARG
THR	ARG	VAL	ALA	VAL	LYS	ARG
LEU	HIS	VAL	GLU	VAL	ALA	LYS
TYR	PHE	LEU	LYS	ARG	TYR	GLY
LYS	TRP	LEU	LEU	PRO	VAL	ASP
ASN	GLU	ASP	GLN	GLN	LYS	ASP
GLY	ARG	ARG	PRO	THR	VAL	ILE
GLY	PHE	GLY	MET	THR	GLY	ASP
GLY	GLY	SER	ARG	GLY	VAL	ALA
ARG	GLY	LYS	LEU	PRO	GLY	ALA
VAL	ALA	VAL	SER	ARG	VAL	GLY
ASN	ILE	VAL	GLY	GLU	GLU	ALA
ILE	MET	GLY	SER	K135	ASP	GLU
LEU	ILE	PHE	SER	T136	ASP	LEU
VAL	SER	TYR	ALA	P137	ALA	GLY
ALA	LEU	GLN	GLY	Y138	GLN	ARG
ARG	ILE	GLY	LEU	E139	GLN	ASP
ASP	ASP	GLY	GLY	L140	GLN	GLN
LEU	LEU	ARG	ASN	A141	VAL	GLN
PHE	GLY	GLN	ARG	A142	VAL	VAL
SER	ASP	GLY	ASP	R143	ILE	ILE
ASP	TRP	GLN	MET	E143	ARG	GLU
VAL	VAL	ALA	LEU	R144	GLN	GLY
TYR	SER	ARG	ILE	M145	VAL	GLU
SER	ARG	ILE	THR	L146	ILE	GLY
LEU	GLY	PHE	GLN	R147	PRO	GLY
GLY	GLY	VAL	GLY	S148	TYR	ALA
SER	ARG	GLN	THR	G149	THR	SER
PRO	GLN	TRP	GLN	L150	THR	GLU
THR	GLY	SER	LEU	T151	PRO	GLU
LYS	ASN	ILE	VAL	A152	ARG	ARG
ASN	ASN	THR	GLU	G153	PRO	ARG
ILE	ILE	PRO	THR	SER	GLU	PRO
GLN	GLN	SER	THR	GLY	PRO	HIS
PHE	PHE	GLY	ARG	GLY	THR	THR
SER	SER	VAL	LEU	GLY	ASN	PRO
ASN	ASN	VAL	VAL	GLY	VAL	GLY
THR	THR	ILE	THR	GLY	PRO	GLY
ALA	ALA	ASN	THR	ASP	PRO	SER
ASN	ASN	LEU	GLN	LEU	GLN	LEU
GLY	GLY	ASP	PRO	PRO	THR	VAL
VAL	VAL	SER	GLY	ARG	GLY	ARG
LEU	GLU	PRO	MET	PRO	VAL	ALA
SER	SER	GLY	THR	GLN	ALA	ILE
ALA	ALA	GLY	THR	GLY	THR	ALA
ALA	ALA	GLY	CYS	GLY	THR	ILE
GLU	GLU	LEU	HIS	ASP	SER	ALA
LEU	GLY	LEU	LEU	VAL	VAL	ALA
LEU	GLY	GLY	THR	PRO	PRO	ALA
ARG	ALA	ARG	THR	VAL	ALA	ILE
ALA	ARG	ALA	ASP	GLY	ILE	ALA
ASN	ASN	GLY	VAL	GLY	GLN	ALA
SER	SER	LEU	TYR	GLY	PRO	VAL
ILE	ILE	SER	THR	LEU	ALA	VAL
ASN	ASN	GLY	THR	MET	PRO	LEU
				GLY	GLY	VAL
				GLY	GLY	VAL
				GLY	GLY	VAL
				GLY	GLY	VAL
				GLY	GLY	VAL

- Molecule 1: TrwE protein

[illegible]

- Molecule 1: TrwE protein

[illegible]

- Molecule 1: TrwE protein



ILE	TRP	SER	GLY	VAL	THR	MET
PRO	ILE	GLY	LEU	GLN	LEU	PHE
PRO	ASP	ARG	LEU	GLN	SER	ARG
THR	ARG	VAL	ALA	PRO	TYR	LYS
LEU	HIS	VAL	GLU	VAL	ALA	LYS
TYR	PHE	LEU	LYS	ARG	TYR	ASP
TRP	LEU	LEU	LEU	PRO	GLN	GLY
ASN	ASP	ASP	GLN	GLN	LYS	ASP
GLN	ARG	ARG	PRO	THR	VAL	ILE
GLY	PHE	GLY	MET	THR	ARG	ASP
GLU	GLY	SER	ARG	GLY	VAL	GLY
ARG	GLY	LYS	LEU	PRO	VAL	ALA
VAL	ALA	VAL	SER	ARG	VAL	GLY
ASN	ILE	VAL	GLY	ARG	GLU	ASP
ILE	MET	GLY	SER	R135	ASP	ALA
LEU	ILE	PHE	SER	T136	ASP	GLN
VAL	SER	TYR	ALA	Y137	ALA	ALA
ALA	LEU	GLN	GLY	Y138	GLN	GLN
ARG	ILE	GLY	ARG	E139	VAL	GLN
ASP	GLY	GLY	LEU	L140	GLN	GLY
ASP	ASP	ARG	ASN	A141	VAL	ILE
PER	GLY	GLN	ARG	R142	VAL	ILE
SER	ASP	GLY	ASP	E143	ARG	GLU
ASP	TRP	GLN	MET	R144	GLN	GLY
VAL	ALA	ALA	LEU	M145	VAL	GLY
ARG	SER	ARG	ILE	L146	GLN	TYR
GLN	SER	ILE	THR	R147	GLY	GLY
LEU	GLY	VAL	GLY	S148	THR	SER
GLY	GLY	GLN	THR	G149	PRO	GLU
SER	ARG	SER	LEU	L150	ARG	ALA
ASN	ILE	ILE	CYS	T151	PRO	GLU
ASN	GLU	GLU	VAL	A152	ILE	GLU
SER	THR	THR	LEU	G153	ARG	ARG
ILE	PRO	PRO	GLU	SER	PRO	ARG
GLN	GLN	SER	THR	GLY	GLU	HIS
PHE	SER	GLY	ARG	GLY	THR	THR
PER	VAL	VAL	VAL	GLY	VAL	PRO
ASN	THR	ILE	THR	ASP	GLY	LEU
ALA	ALA	ASN	THR	GLU	PRO	LEU
ASN	ASN	LEU	GLN	LEU	ARG	GLN
GLY	GLY	ASP	PRO	PRO	GLN	PRO
VAL	VAL	SER	GLY	ARG	THR	MET
GLU	GLU	PRO	MET	THR	GLN	VAL
SER	SER	GLY	THR	THR	GLY	THR
ALA	ALA	GLY	CYS	GLY	THR	LEU
ALA	ALA	GLY	HIS	ASP	SER	VAL
GLU	GLU	LEU	LEU	VAL	VAL	CYS
ALA	ALA	GLY	THR	PRO	PRO	ILE
LEU	LEU	GLY	ARG	ALA	ALA	ALA
ARG	ARG	ALA	ASP	ALA	ILE	VAL
ASN	ASN	GLY	VAL	GLY	GLN	VAL
SER	SER	LEU	TYR	ILE	PRO	VAL
ILE	ILE	GLY	SER	GLY	ALA	LEU
ASN	ASN	GLY	THR	MET	PRO	VAL
THR	THR	GLY	THR	GLY	GLY	VAL
LYS	LYS	GLY	THR	GLY	GLY	VAL

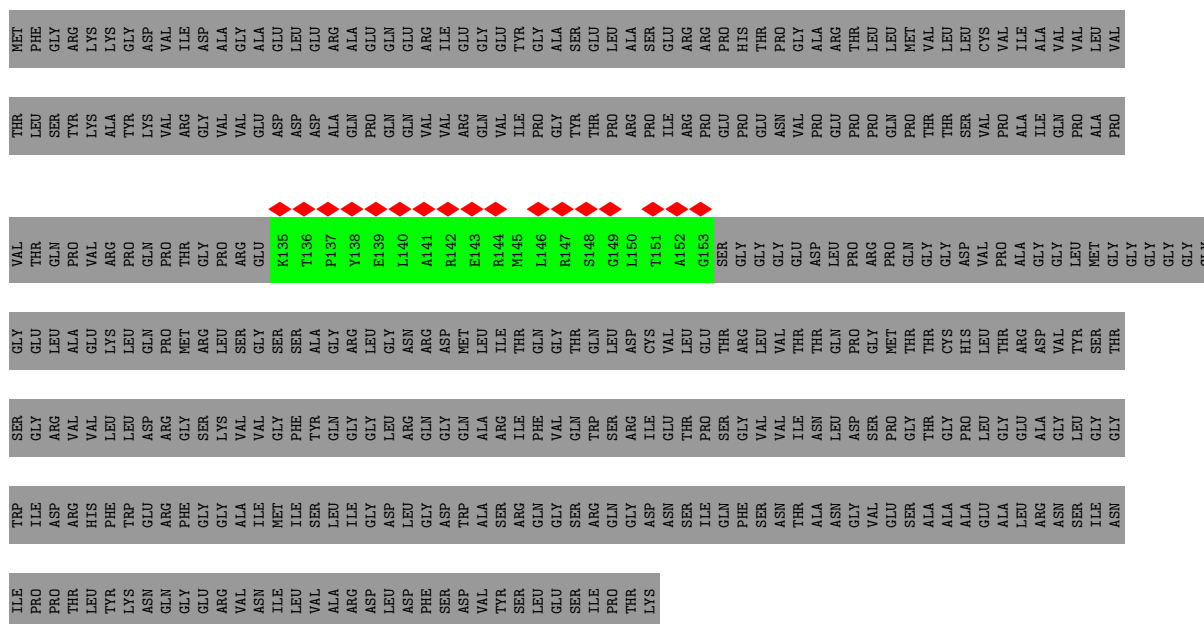
- Molecule 1: TrwE protein



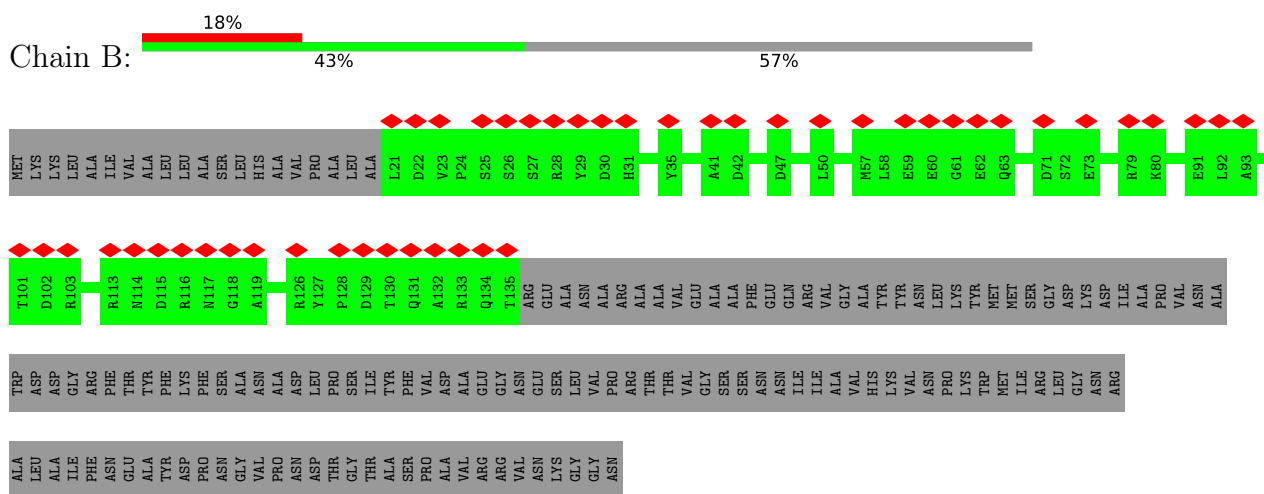
TRP	ILE	GLY	SER	GLY	VAL	THR	THR	MET
ASP	ASP	ARG	GLY	LEU	GLN	LEU	SER	PHE
ARG	VAL	VAL	ALA	PRO	THR	PRO	TYR	ARG
PHE	LEU	LEU	LYS	ARG	VAL	ALA	LYS	LYS
TRP	LEU	LEU	LEU	PRO	GLN	TYR	GLY	ASP
GLU	ASP	GLN	GLN	ARG	GLN	LYS	VAL	GLY
ARG	ARG	PRO	PRO	THR	THR	VAL	VAL	ILE
PHE	GLY	MET	GLY	ARG	GLY	ARG	GLY	ASP
GLY	GLY	SER	LYS	LEU	PRO	VAL	VAL	ALA
ALA	VAL	SER	VAL	SER	ARG	VAL	VAL	GLY
ILE	VAL	GLY	VAL	GLY	K135	GLU	GLU	ALA
MET	GLY	SER	GLY	SER	T136	ASP	ASP	GLU
ILE	PHE	TYR	ALA	ALA	P137	ASP	ASP	LEU
LEU	GLN	GLY	ARG	GLY	Y138	ALA	ALA	ARG
ILE	GLY	GLY	ARG	LEU	E139	GLN	GLN	ALA
ASP	LEU	LEU	ASN	GLY	L140	VAL	VAL	GLU
LEU	ASP	ARG	ARG	ARG	A141	ARG	ARG	GLN
GLY	GLN	GLY	GLY	ASP	R142	VAL	VAL	ARG
ASP	ASP	GLY	GLN	MET	E143	ARG	ARG	ILE
TRP	GLN	GLN	GLN	LEU	R144	GLN	GLY	GLU
ALA	ALA	ARG	ILE	ILE	M145	VAL	ILE	GLY
SER	ARG	ILE	ILE	THR	L146	PRO	PRO	TYR
GLN	ARG	PHE	VAL	GLY	R147	GLY	GLY	GLY
GLY	SER	GLY	VAL	THR	S148	THR	THR	SER
ARG	ARG	TRP	GLN	GLN	G149	PRO	THR	GLU
GLN	GLN	SER	SER	LEU	L150	ARG	ARG	LEU
GLY	GLY	ARG	VAL	LEU	T151	GLY	GLY	ALA
PHE	SER	GLY	VAL	VAL	A152	ASN	PRO	ALA
ASN	ASN	GLU	ILE	THR	SER	GLY	VAL	GLY
ASN	THR	THR	THR	LEU	G153	GLU	PRO	ALA
ILE	PRO	PRO	GLU	GLU	THR	ASP	PRO	ALA
GLN	SER	SER	GLN	THR	ARG	LEU	GLU	ALA
ASN	GLY	GLY	VAL	ARG	GLY	LEU	ARG	THR
PHE	SER	VAL	VAL	LEU	GLY	PRO	PRO	THR
ASN	ASN	VAL	ILE	VAL	THR	ARG	PRO	THR
THR	THR	ILE	THR	THR	THR	GLN	PRO	THR
ALA	ALA	ASN	ASN	THR	THR	GLN	GLN	LEU
ASN	ASN	LEU	LEU	GLN	GLN	LEU	GLN	LEU
GLY	GLY	ASP	ASP	PRO	PRO	PRO	PRO	LEU
VAL	VAL	SER	SER	MET	MET	ARG	GLN	LEU
GLU	GLU	PRO	GLY	GLY	THR	THR	THR	MET
SER	SER	THR	THR	THR	CYS	CYS	THR	VAL
ALA	ALA	GLY	THR	GLY	GLY	GLY	THR	VAL
ALA	ALA	PRO	PRO	HIS	ASP	ASP	SER	CYS
GLU	GLU	LEU	LEU	LEU	VAL	VAL	VAL	VAL
LEU	LEU	GLY	GLY	THR	PRO	PRO	PRO	ALA
LEU	LEU	ALA	GLU	THR	ALA	ALA	ALA	ILE
ARG	ARG	ALA	ASP	ASP	GLY	GLY	ILE	ALA
ASN	ASN	GLY	VAL	VAL	GLY	GLY	GLN	ALA
SER	SER	LEU	GLY	TYR	LEU	LEU	PRO	VAL
ILE	ILE	GLY	SER	SER	MET	MET	ALA	LEU
ASN	ASN	GLY	GLY	THR	THR	GLY	PRO	VAL



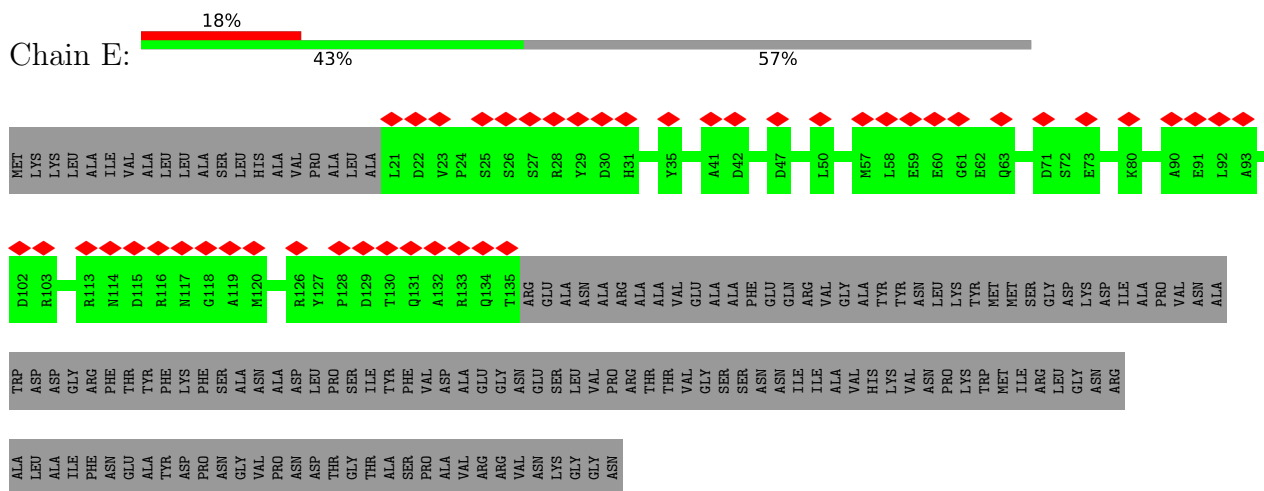
WORLDWIDE
PDB
PROTEIN DATA BANK



- Molecule 2: TrwF protein



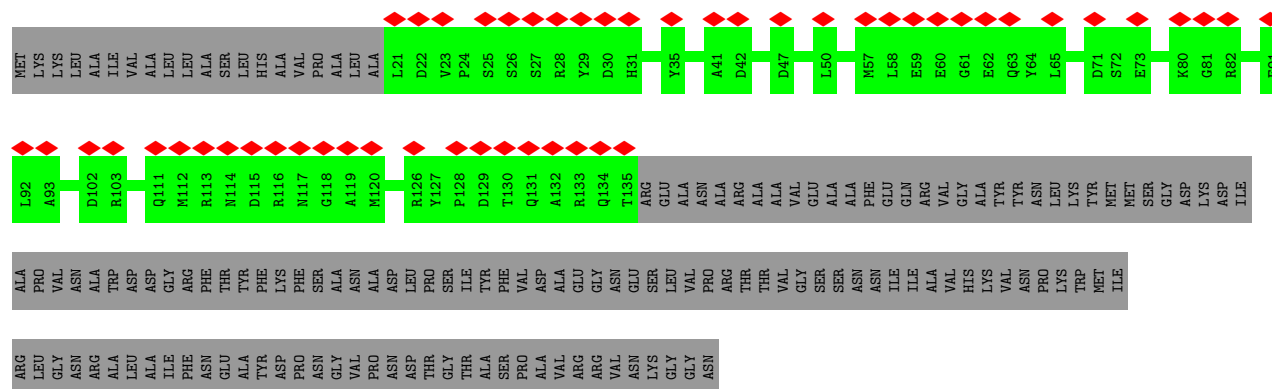
- Molecule 2: TrwF protein



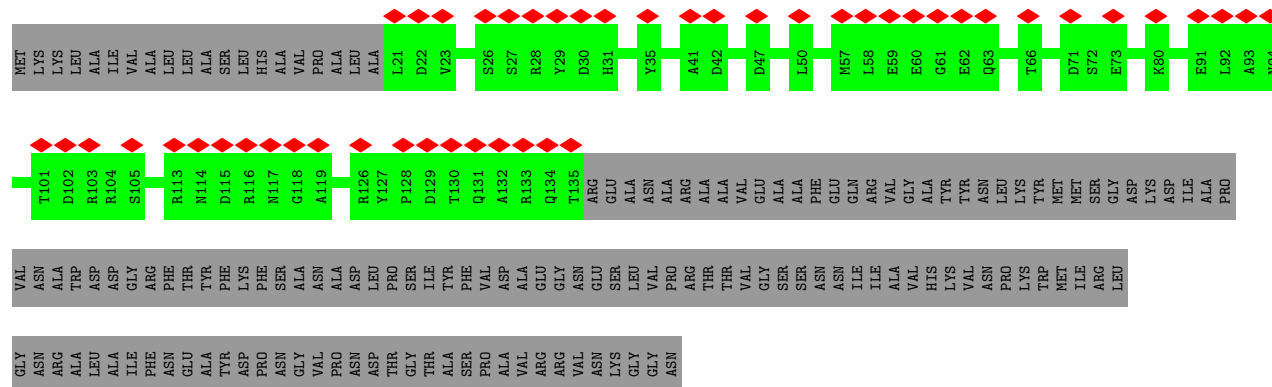
Chain H: 

Chain K:  19% 43% 57%

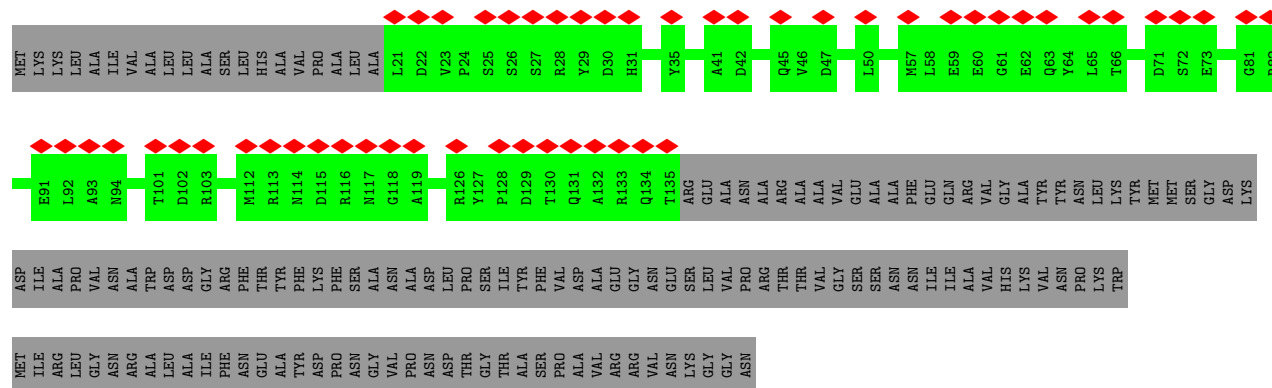
Chain N:  18% 43% 57%



• Molecule 2: TrwF protein

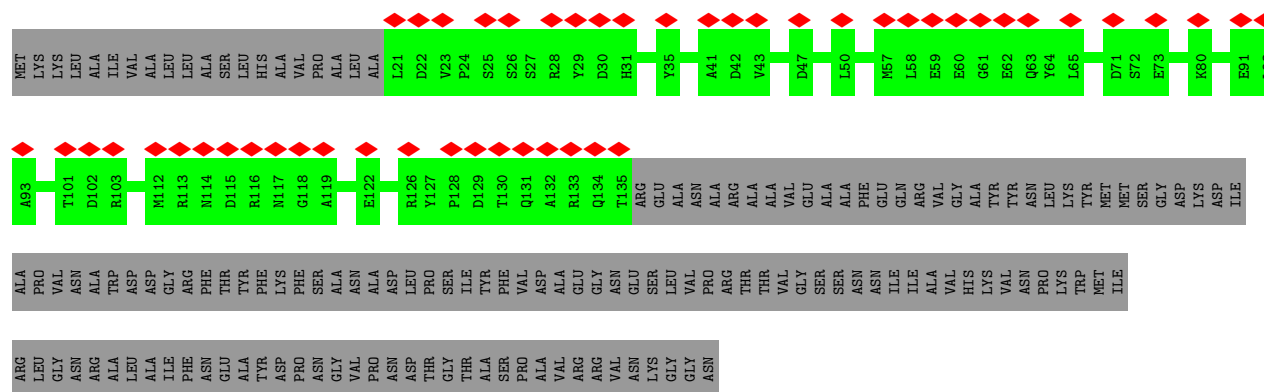


• Molecule 2: TrwF protein

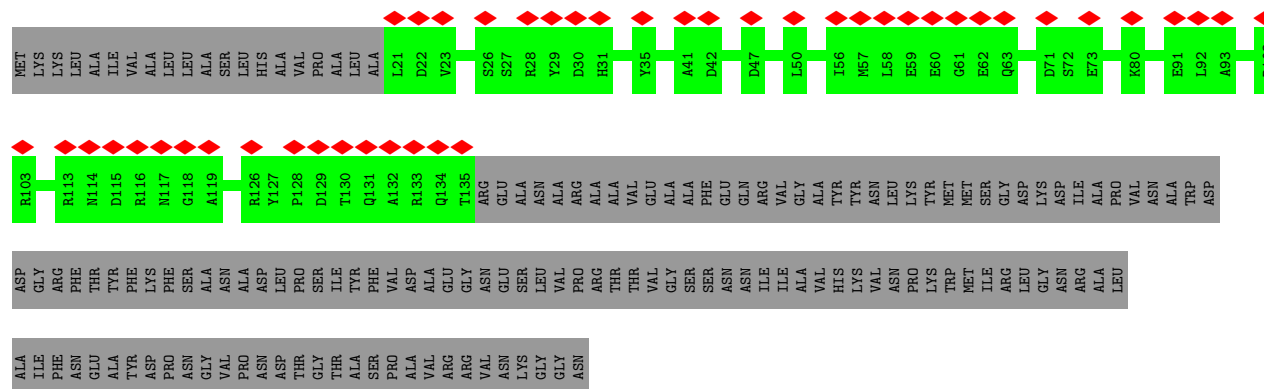


• Molecule 2: TrwF protein

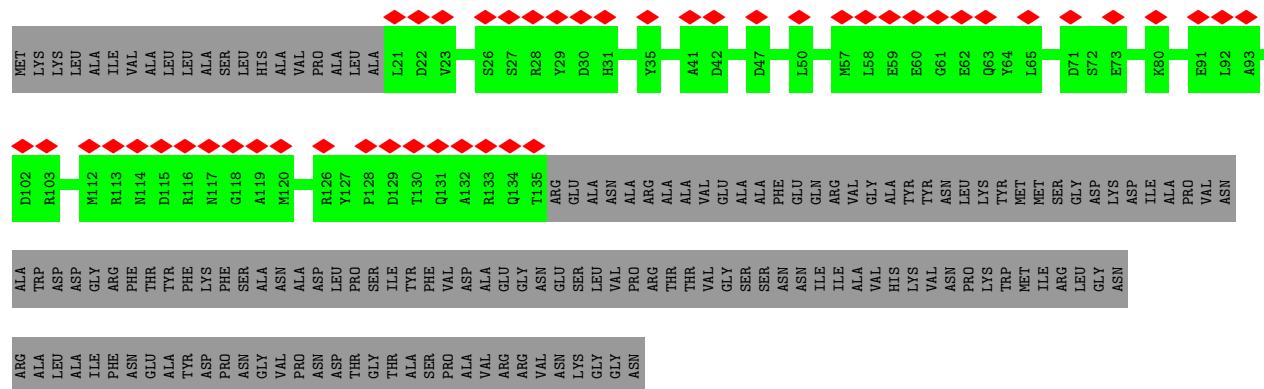




• Molecule 2: TrwF protein

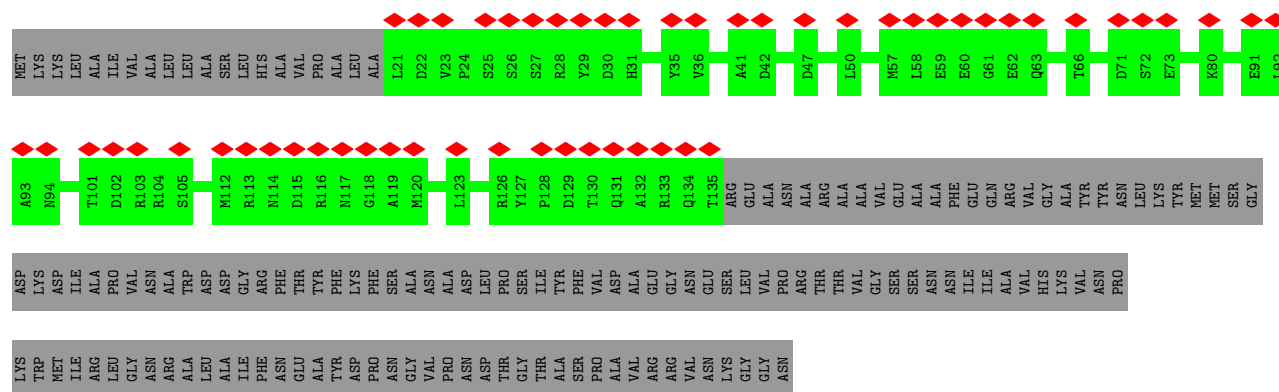


• Molecule 2: TrwF protein

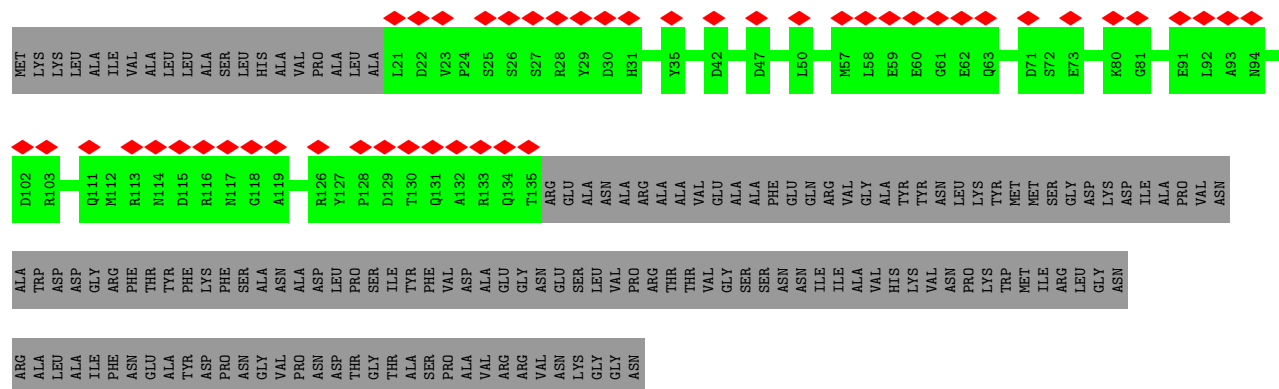


• Molecule 2: TrwF protein

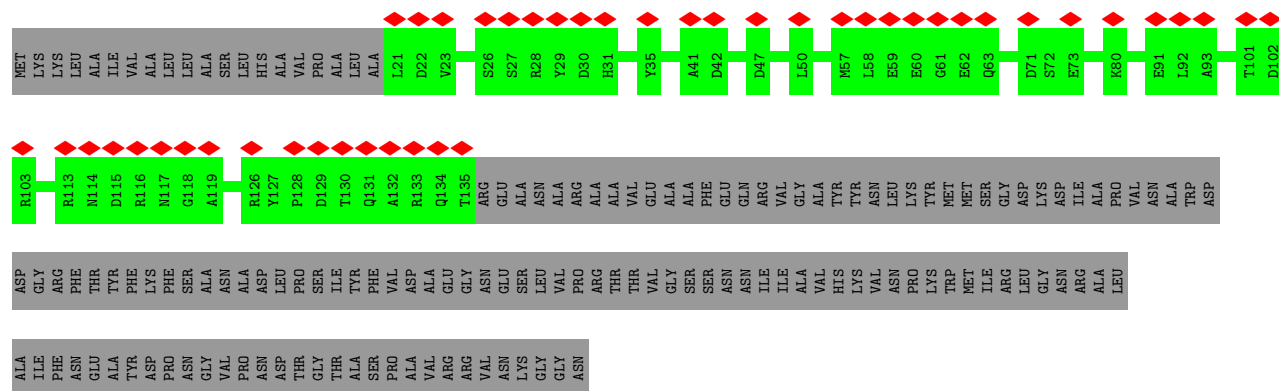




• Molecule 2: TrwF protein

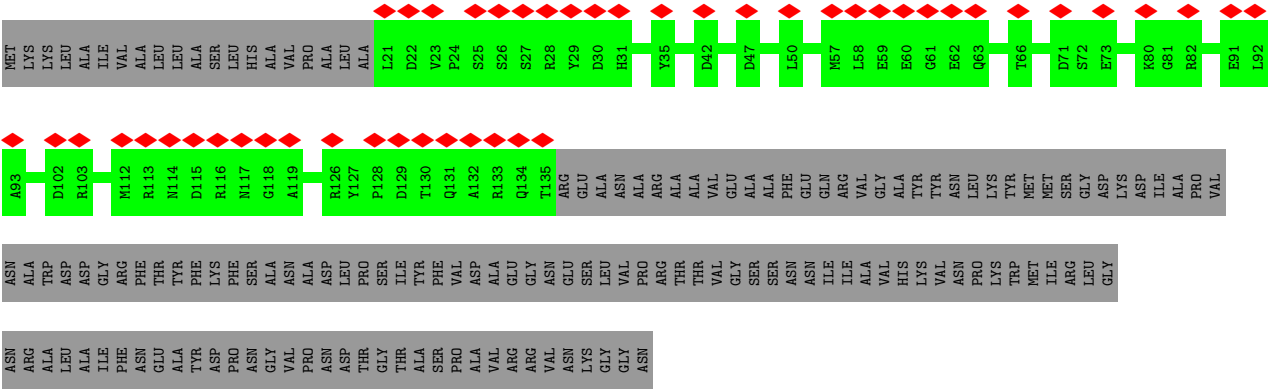


• Molecule 2: TrwF protein

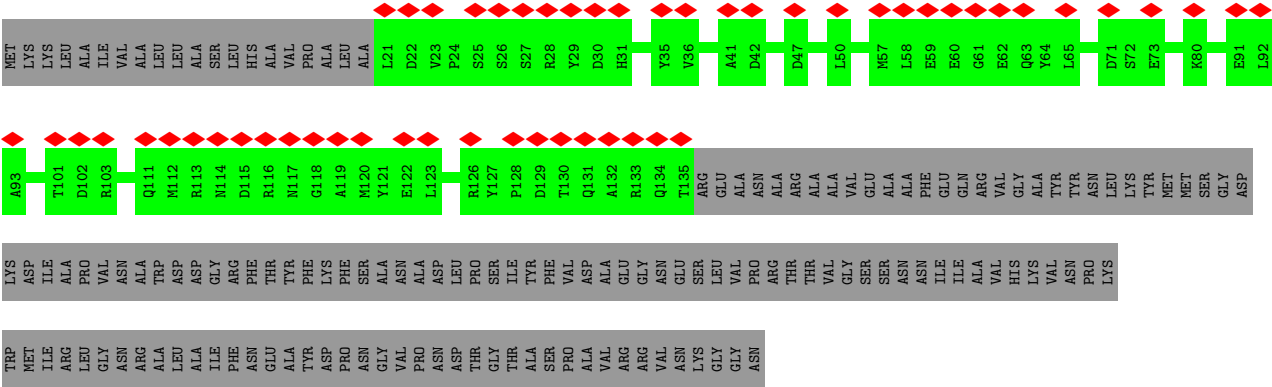


• Molecule 2: TrwF protein





• Molecule 2: TrwF protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C16	Depositor
Number of particles used	1280606	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 ($e^-/\text{\AA}^2$)	57.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.829	Depositor
Minimum map value	-27.674	Depositor
Average map value	0.018	Depositor
Map value standard deviation	1.623	Depositor
Recommended contour level	10.0	Depositor
Map size (\AA)	258.21402, 257.147, 85.36	wwPDB
Map dimensions	242, 241, 80	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.35	0/150	0.55	0/199
1	D	0.35	0/150	0.55	0/199
1	G	0.34	0/150	0.55	0/199
1	J	0.34	0/150	0.55	0/199
1	M	0.35	0/150	0.55	0/199
1	P	0.35	0/150	0.55	0/199
1	S	0.34	0/150	0.55	0/199
1	V	0.35	0/150	0.55	0/199
1	Y	0.35	0/150	0.55	0/199
1	b	0.35	0/150	0.55	0/199
1	e	0.35	0/150	0.55	0/199
1	h	0.35	0/150	0.55	0/199
1	k	0.35	0/150	0.55	0/199
1	n	0.35	0/150	0.55	0/199
1	u	0.35	0/150	0.54	0/199
1	y	0.34	0/150	0.55	0/199
2	B	0.60	0/962	0.52	0/1302
2	E	0.60	0/962	0.52	0/1302
2	H	0.60	0/962	0.52	0/1302
2	K	0.60	0/962	0.52	0/1302
2	N	0.60	0/962	0.52	0/1302
2	Q	0.60	0/962	0.52	0/1302
2	T	0.60	0/962	0.52	0/1302
2	W	0.60	0/962	0.52	0/1302
2	Z	0.60	0/962	0.52	0/1302
2	c	0.60	0/962	0.52	0/1302
2	f	0.60	0/962	0.53	0/1302
2	i	0.60	0/962	0.52	0/1302
2	l	0.60	0/962	0.52	0/1302
2	o	0.60	0/962	0.53	0/1302
2	v	0.60	0/962	0.52	0/1302
2	z	0.60	0/962	0.53	0/1302
All	All	0.58	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%)	110 (97%)	3 (3%)	0	100	100
2	E	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	H	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	K	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	N	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	Q	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	T	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	W	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	Z	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	c	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	f	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	i	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	l	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	o	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	v	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
2	z	113/266 (42%)	110 (97%)	3 (3%)	0	100	100
All	All	2080/10576 (20%)	2032 (98%)	48 (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. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	89	GLN
2	E	89	GLN
2	H	89	GLN
2	K	89	GLN
2	N	89	GLN
2	Q	89	GLN
2	T	89	GLN
2	v	89	GLN
2	W	89	GLN
2	Z	89	GLN
2	c	89	GLN
2	f	89	GLN
2	i	89	GLN
2	l	89	GLN
2	o	89	GLN
2	z	89	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

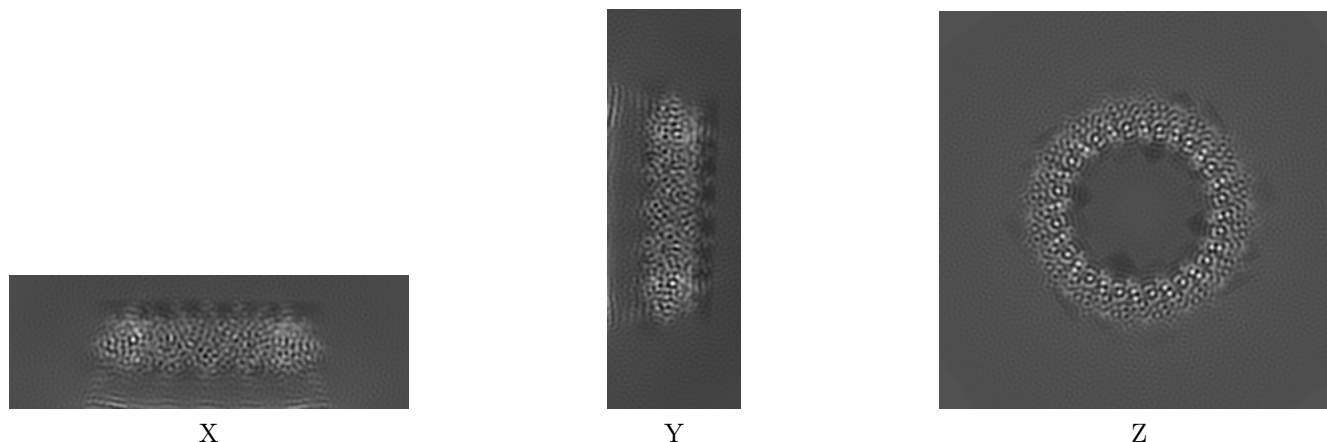
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12708. These allow visual inspection of the internal detail of the map and identification of artifacts.

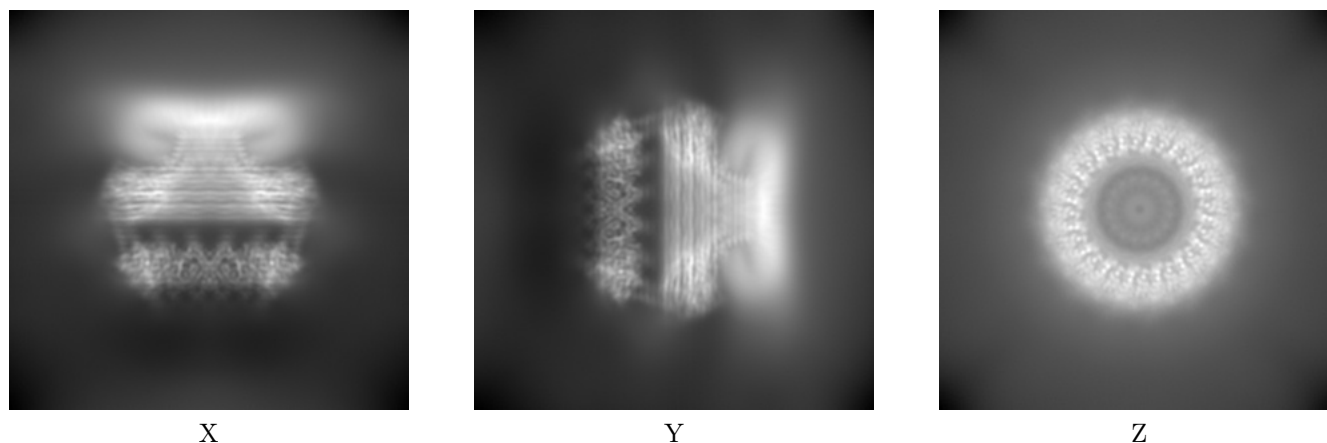
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



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

6.2 Central slices [i](#)

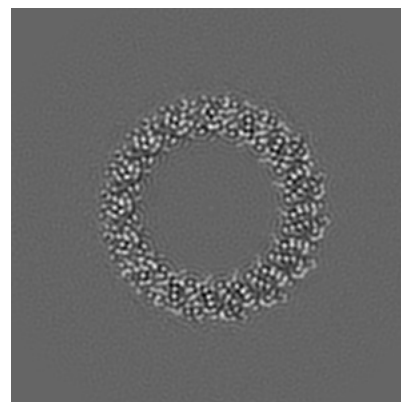
6.2.1 Primary map



X Index: 121

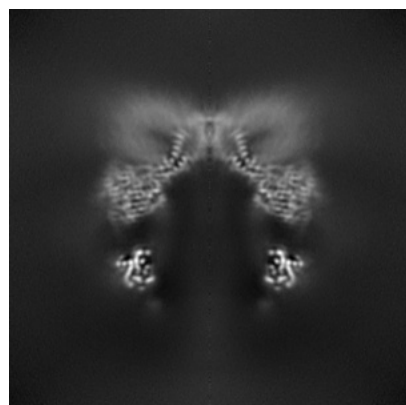


Y Index:
120

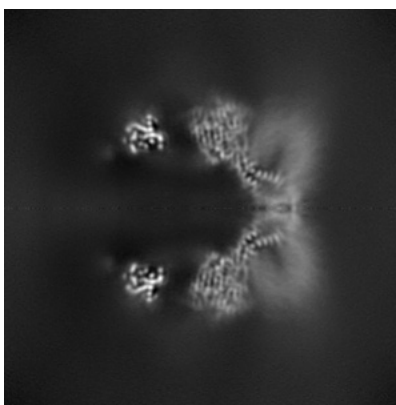


Z Index: 40

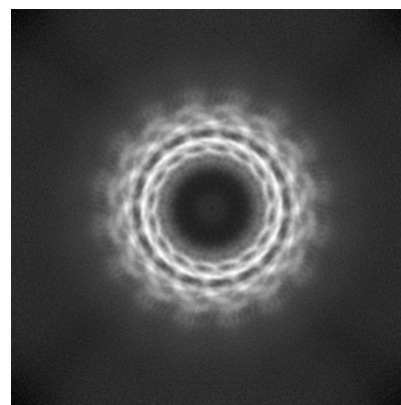
6.2.2 Raw map



X Index: 150



Y Index: 150

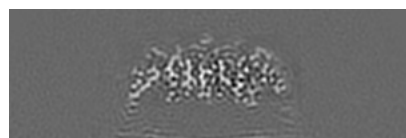


Z Index: 150

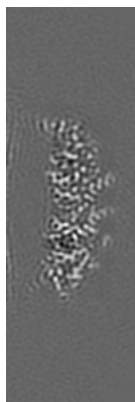
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

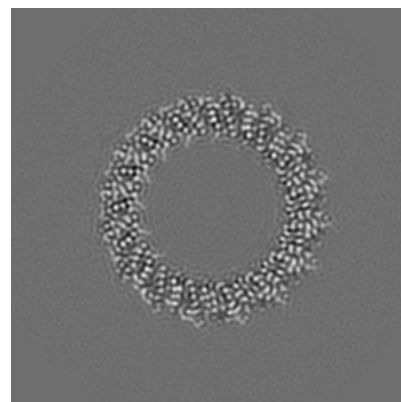
6.3.1 Primary map



X Index: 170

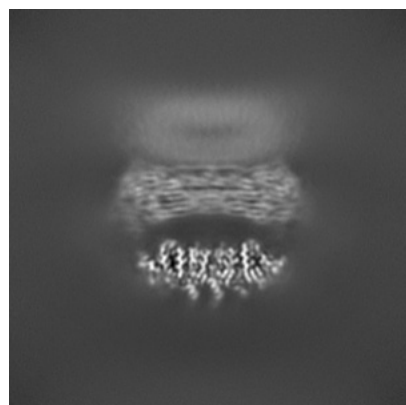


Y Index:
74

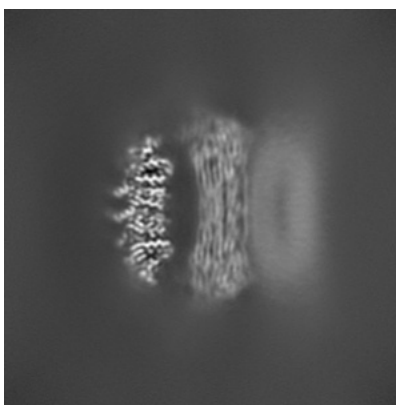


Z Index: 38

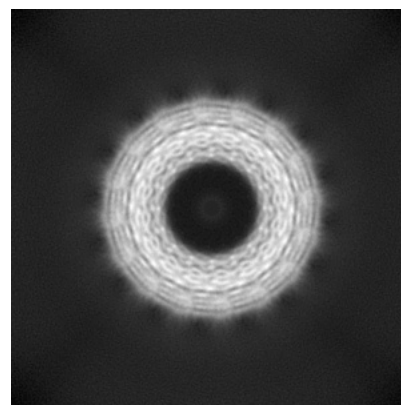
6.3.2 Raw map



X Index: 104



Y Index: 104

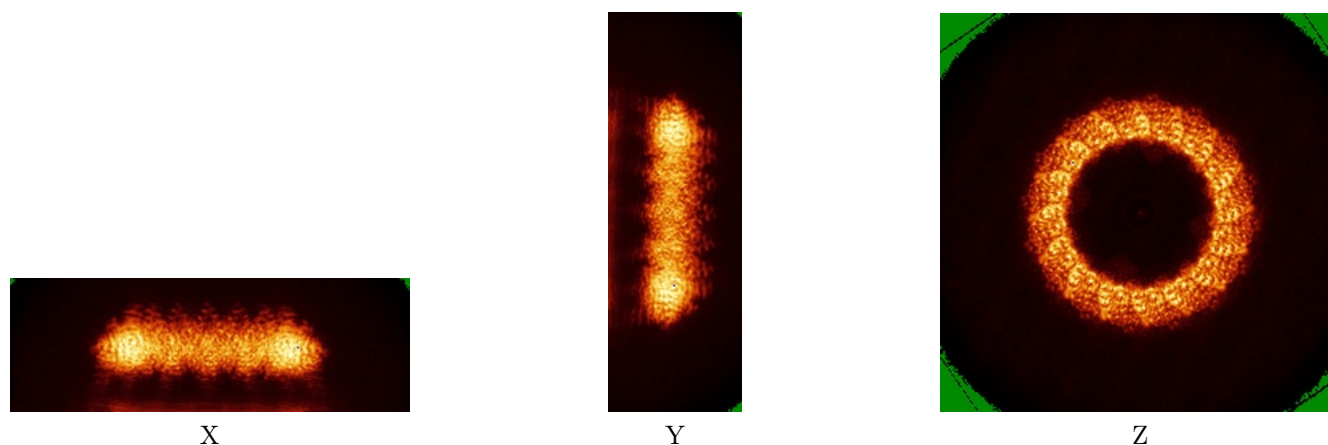


Z Index: 162

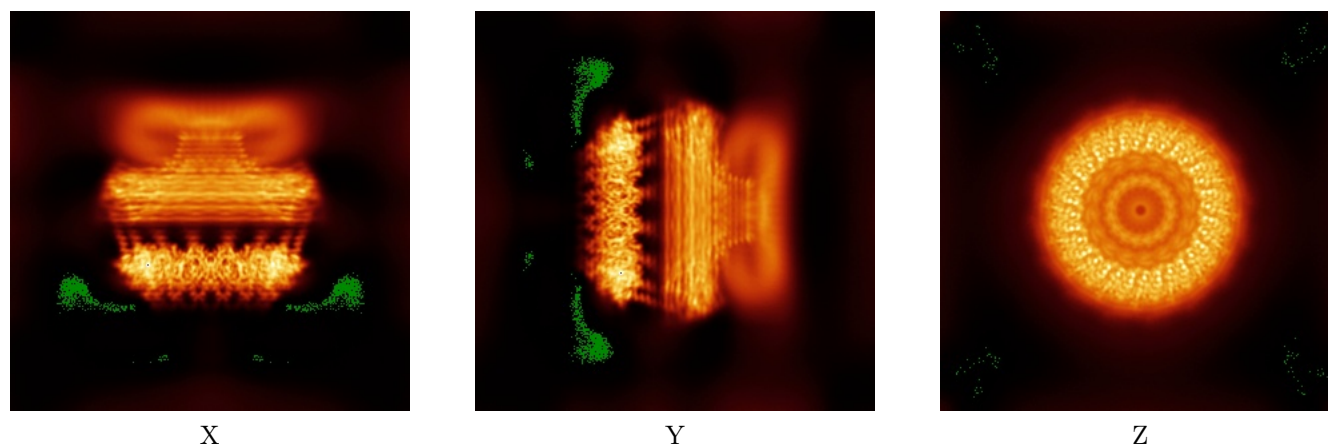
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



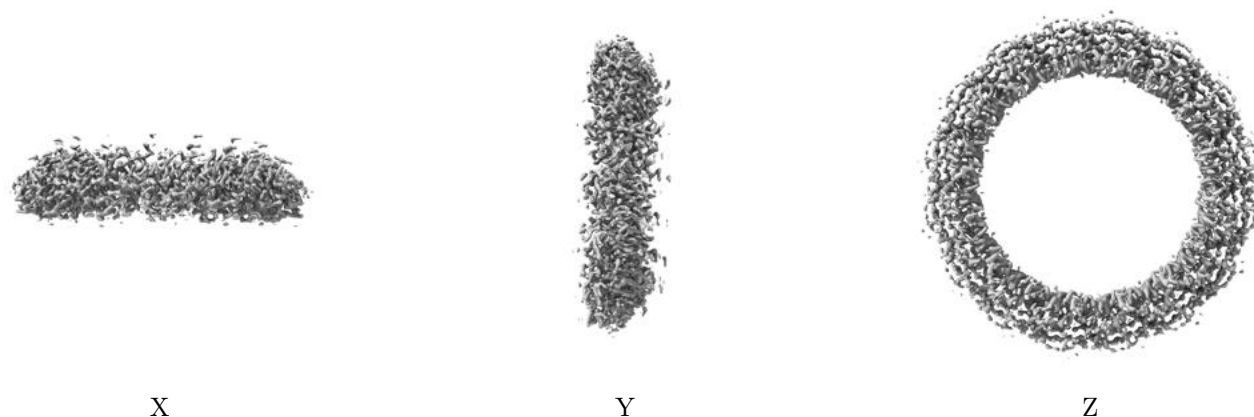
6.4.2 Raw map



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.

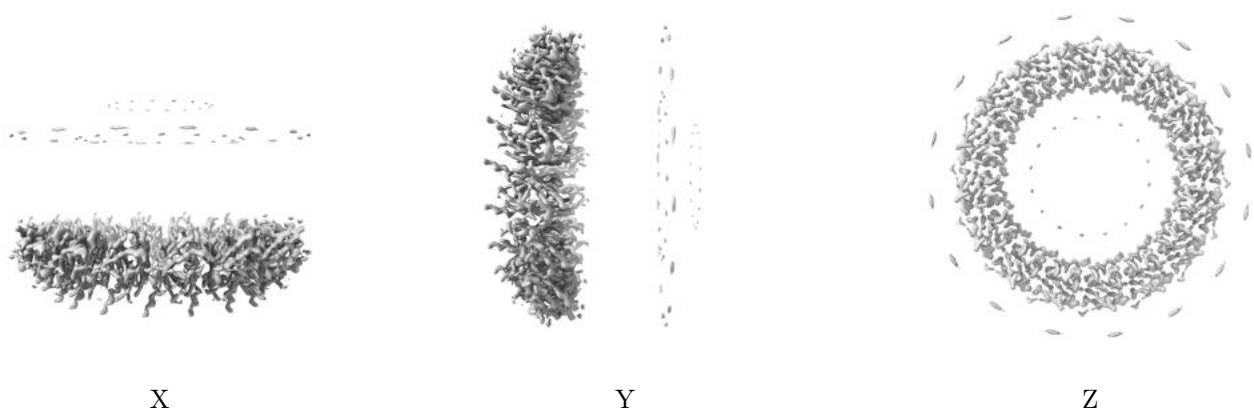
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. 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

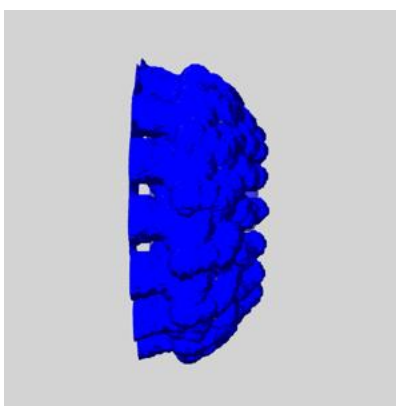
A mask typically either:

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

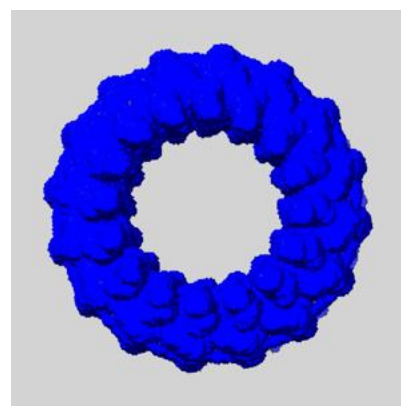
6.6.1 emd_12708_msk_1.map [i](#)



X



Y

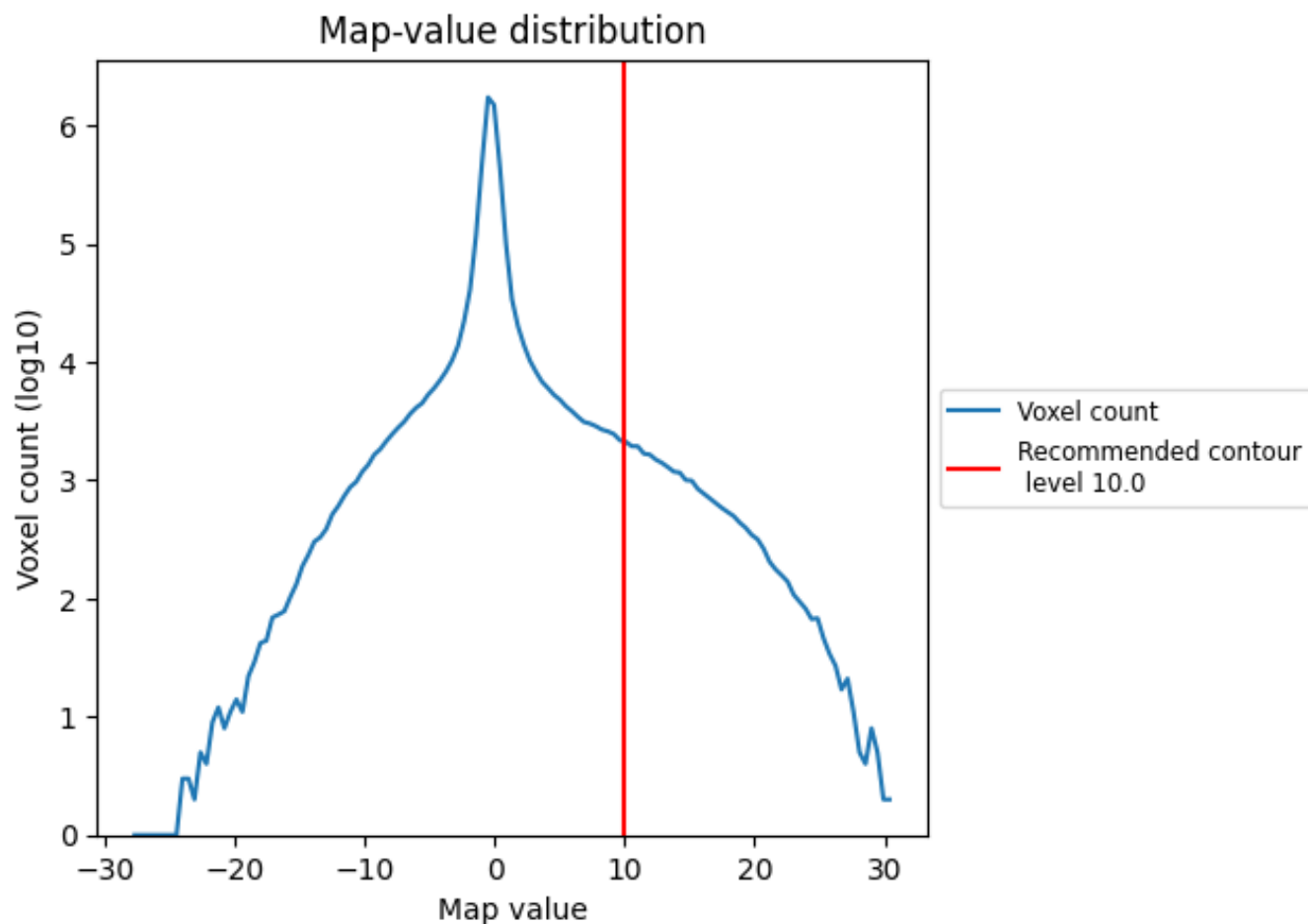


Z

7 Map analysis [i](#)

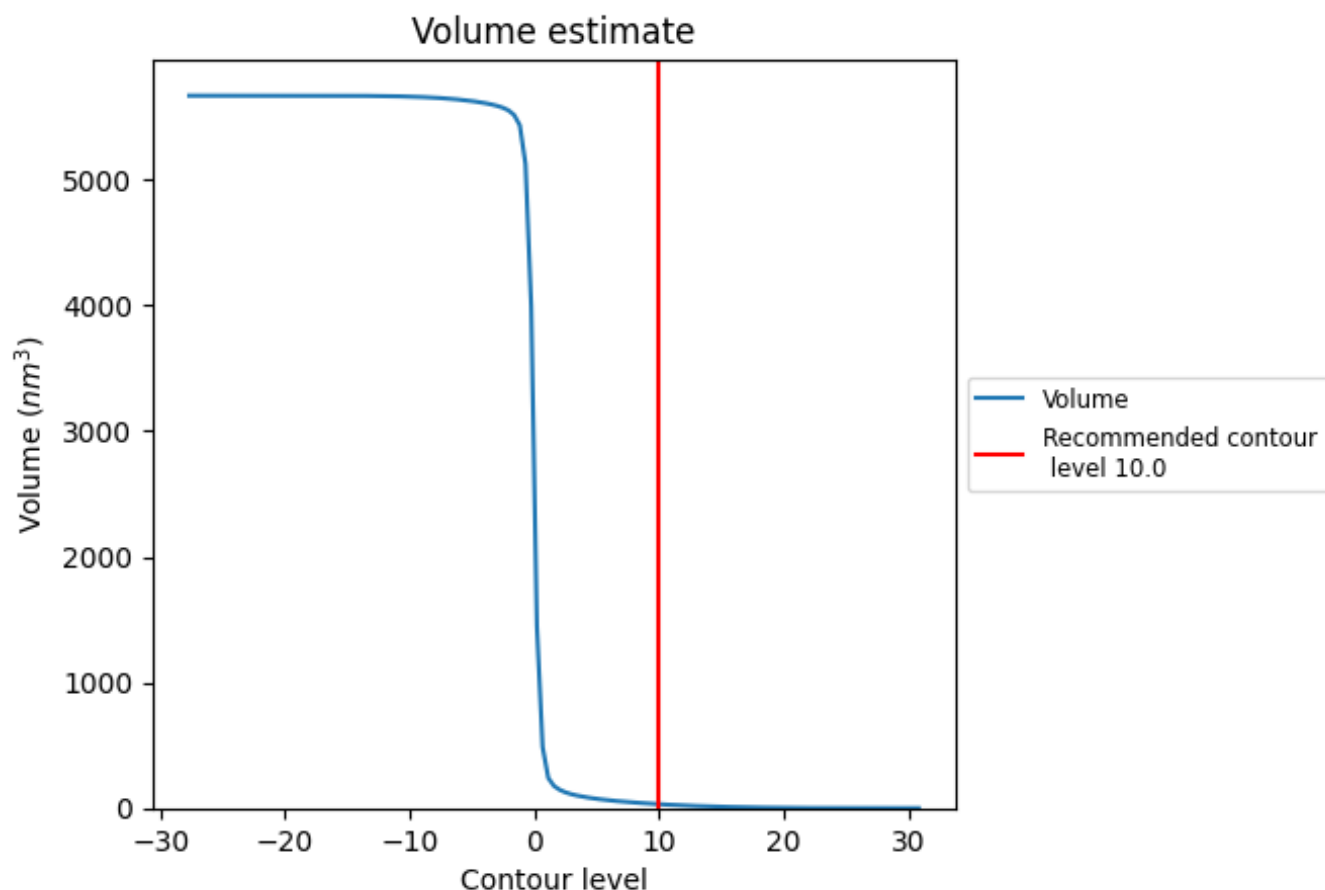
This section contains the results of statistical analysis of the map.

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 31 nm³; this corresponds to an approximate mass of 28 kDa.

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

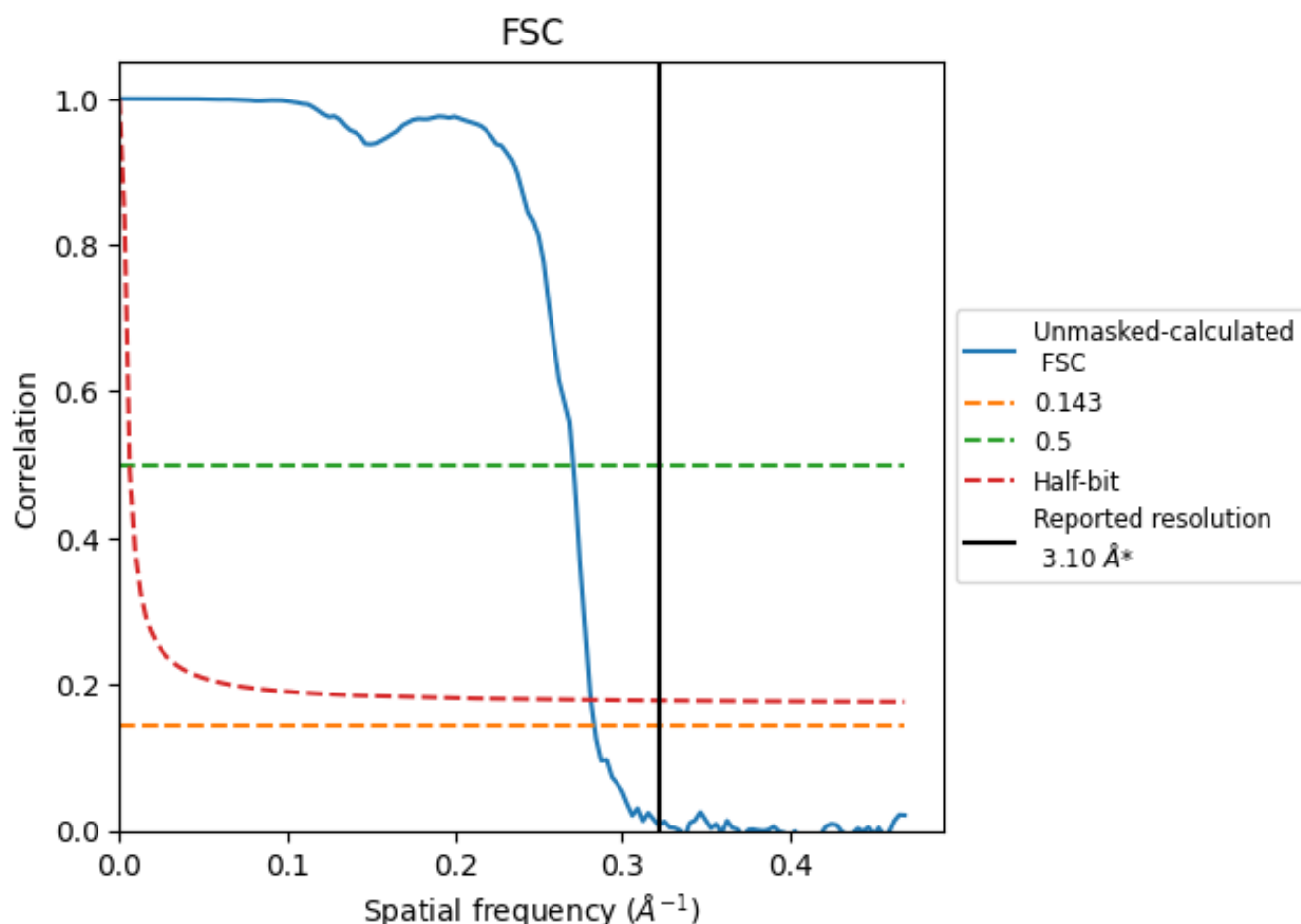
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

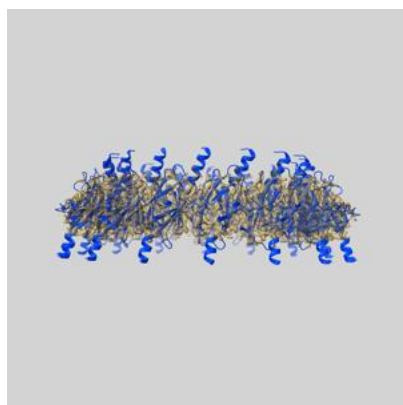
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	3.69	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.1 by more than 10 %

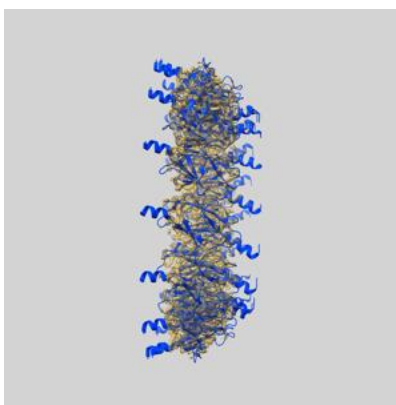
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12708 and PDB model 7O3T. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

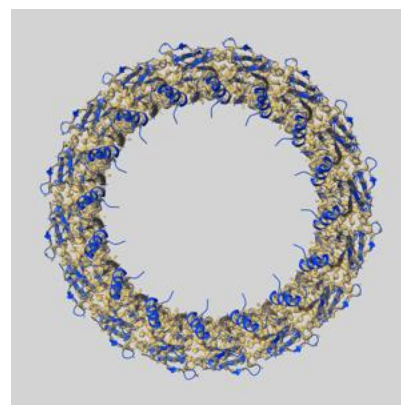
9.1 Map-model overlay [i](#)



X



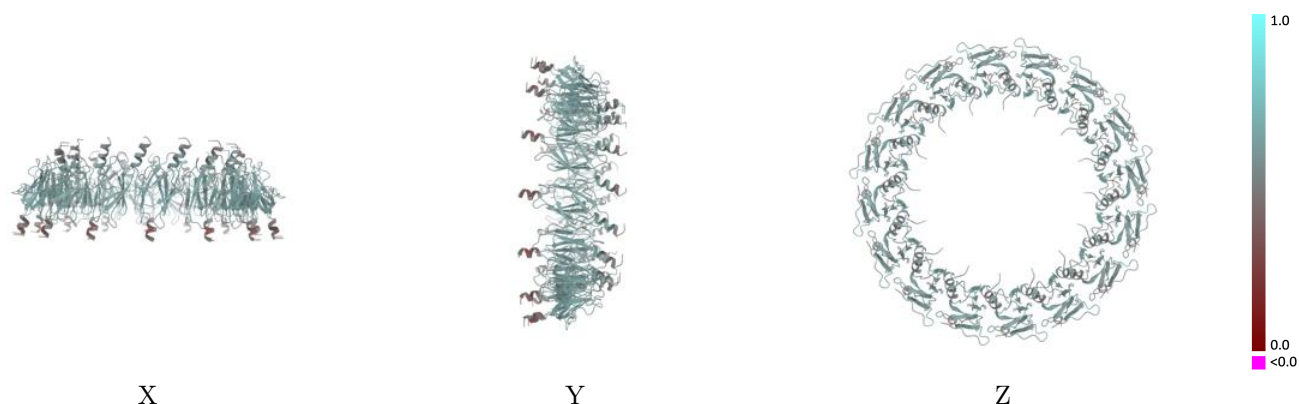
Y



Z

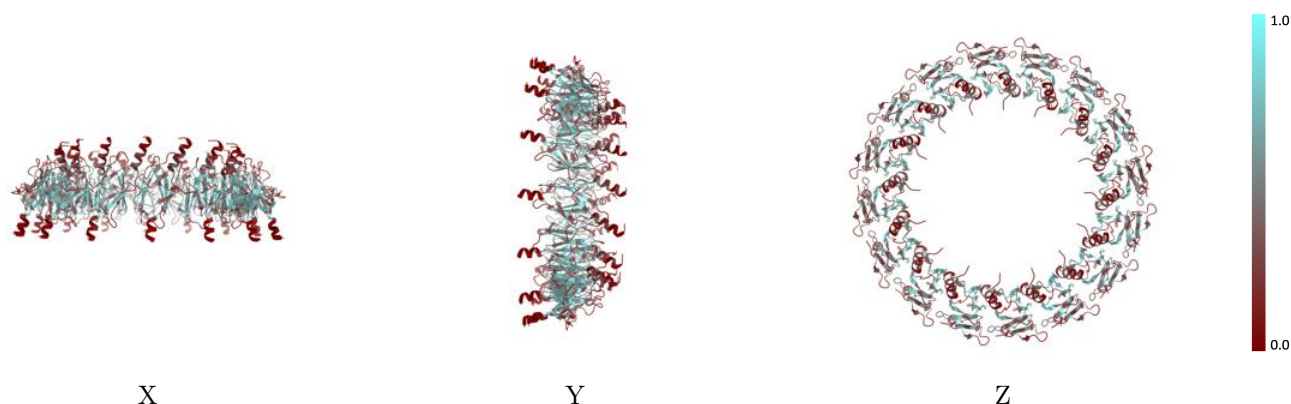
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



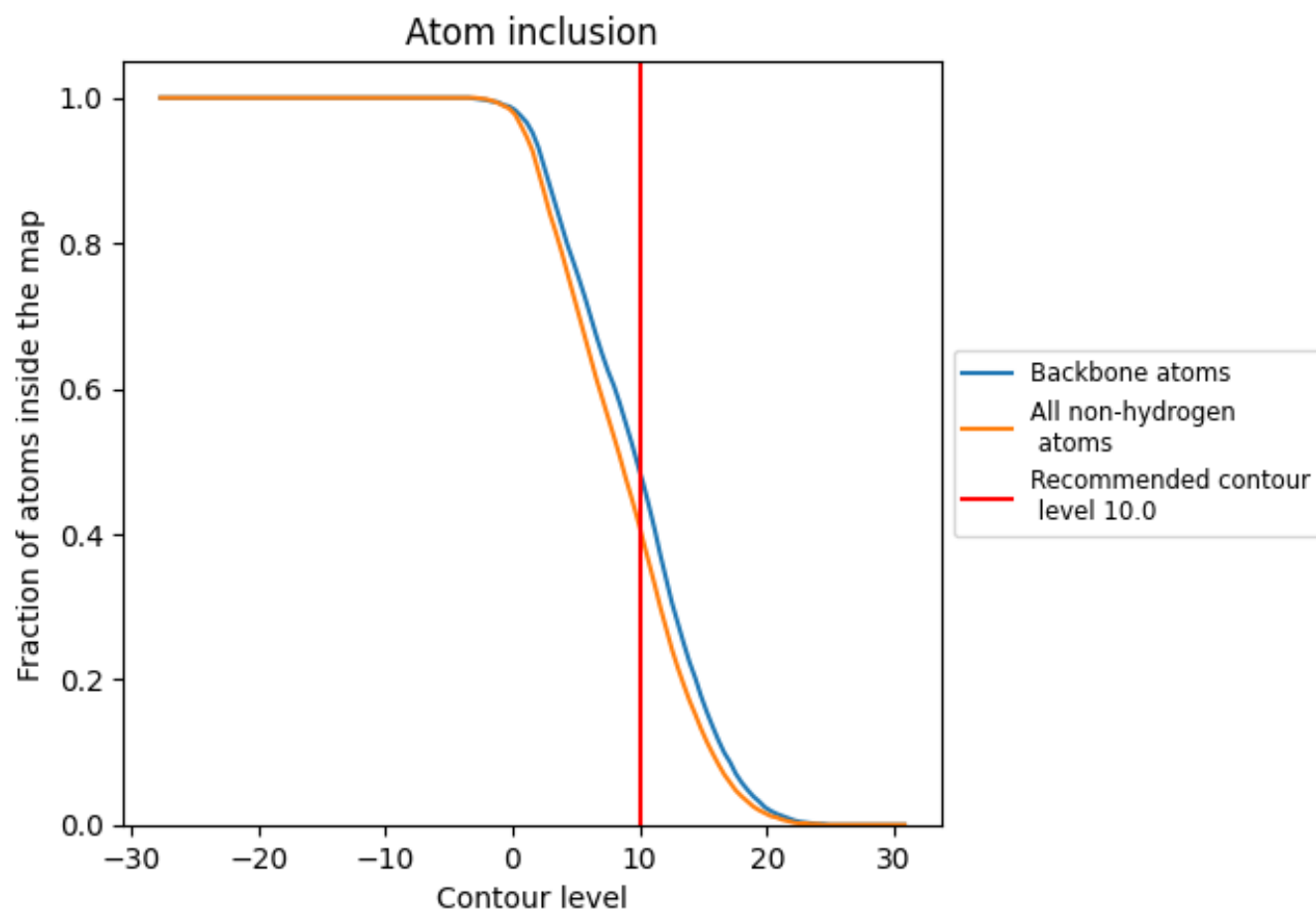
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10.0).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 41% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4100	 0.5640
A	 0.1410	 0.5480
B	 0.4520	 0.5700
D	 0.1760	 0.5250
E	 0.4590	 0.5680
G	 0.1060	 0.5450
H	 0.4370	 0.5710
J	 0.1830	 0.5230
K	 0.4480	 0.5720
M	 0.1340	 0.5380
N	 0.4430	 0.5680
P	 0.2110	 0.5250
Q	 0.4500	 0.5660
S	 0.1270	 0.5240
T	 0.4570	 0.5690
V	 0.1480	 0.5290
W	 0.4570	 0.5700
Y	 0.1760	 0.5270
Z	 0.4630	 0.5630
b	 0.1200	 0.5420
c	 0.4620	 0.5680
e	 0.1550	 0.5330
f	 0.4120	 0.5700
h	 0.1690	 0.5390
i	 0.4500	 0.5690
k	 0.1690	 0.5260
l	 0.4770	 0.5700
n	 0.1200	 0.5390
o	 0.4440	 0.5690
u	 0.1550	 0.5260
v	 0.4350	 0.5690
y	 0.2110	 0.5310
z	 0.4400	 0.5710

