



## wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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

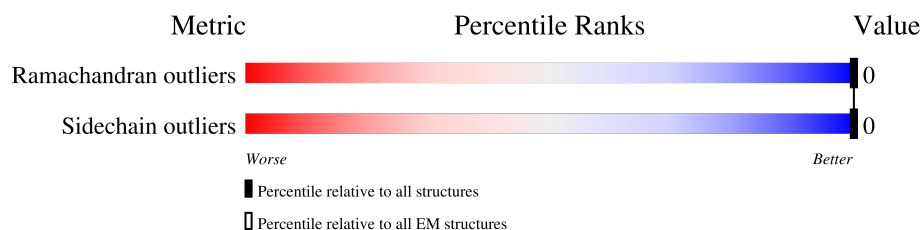
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

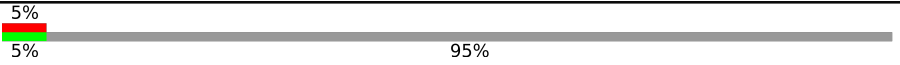
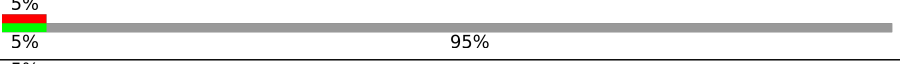
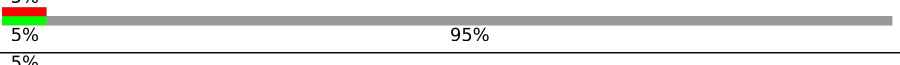
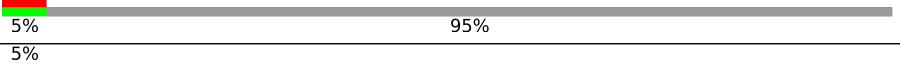
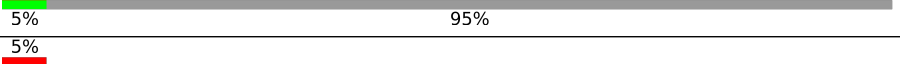
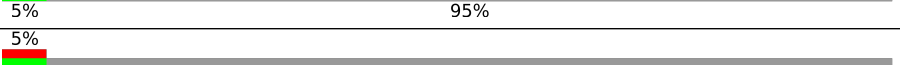
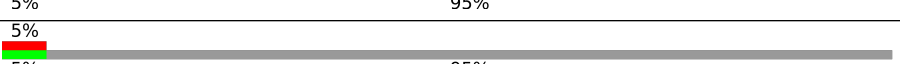
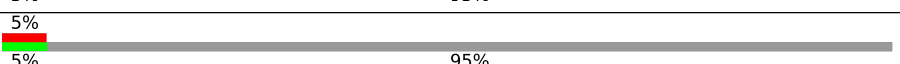

The reported resolution of this entry is 3.10 Å.

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.



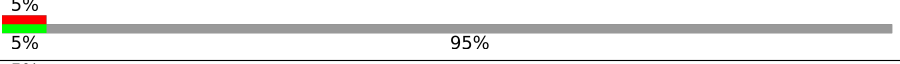
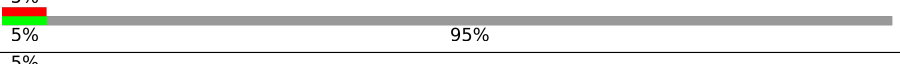
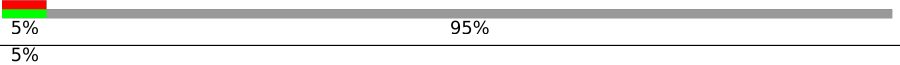
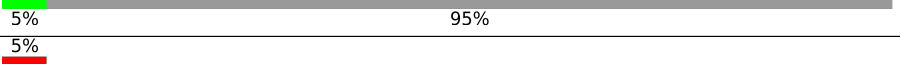
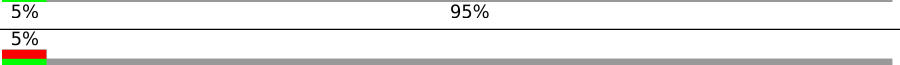
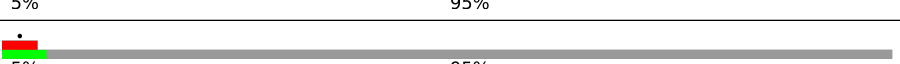
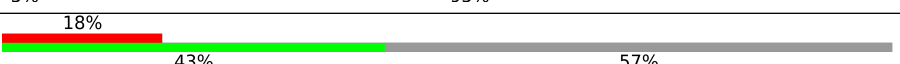


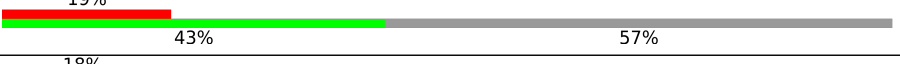
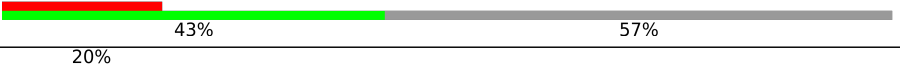



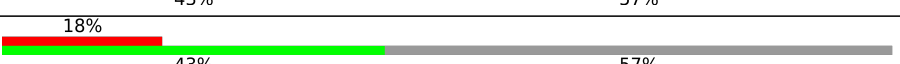
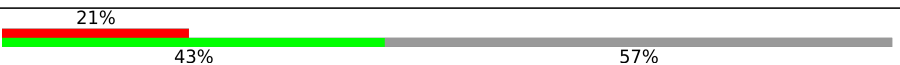







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	
1	D	395	
1	G	395	
1	J	395	
1	M	395	
1	P	395	
1	S	395	
1	V	395	
1	Y	395	

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Mol	Chain	Length	Quality of chain
1	b	395	 5% 95%
1	e	395	 5% 95%
1	h	395	 5% 95%
1	k	395	 5% 95%
1	n	395	 5% 95%
1	u	395	 5% 95%
1	y	395	 5% 95%
2	B	266	 18% 43% 57%
2	E	266	 18% 43% 57%
2	H	266	 20% 43% 57%
2	K	266	 19% 43% 57%
2	N	266	 18% 43% 57%
2	Q	266	 20% 43% 57%
2	T	266	 18% 43% 57%
2	W	266	 19% 43% 57%
2	Z	266	 17% 43% 57%
2	c	266	 18% 43% 57%
2	f	266	 21% 43% 57%
2	i	266	 18% 43% 57%
2	l	266	 17% 43% 57%
2	o	266	 18% 43% 57%
2	v	266	 20% 43% 57%
2	z	266	 20% 43% 57%

## 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 942	C 591	N 173	O 175	S 3	0	0
2	E	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	H	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	K	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	N	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	Q	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	T	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	v	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	W	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	Z	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	c	115	Total 942	C 591	N 173	O 175	S 3	0	0
2	f	115	Total 942	C 591	N 173	O 175	S 3	0	0

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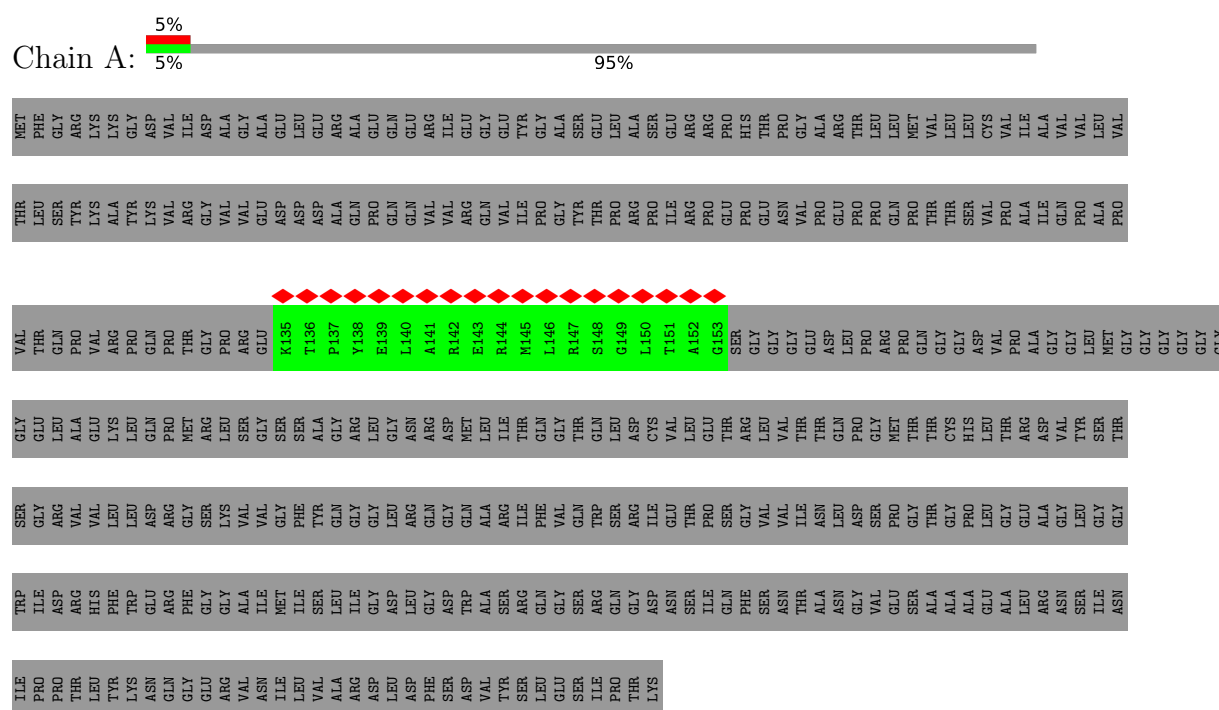
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Chain	Residue	Modelled	Actual	Comment	Reference
o	88	PRO	ARG	conflict	UNP O50336
o	89	GLN	THR	conflict	UNP O50336
z	71	ASP	ILE	conflict	UNP O50336
z	72	SER	PRO	conflict	UNP O50336
z	73	GLU	LYS	conflict	UNP O50336
z	74	ALA	PRO	conflict	UNP O50336
z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

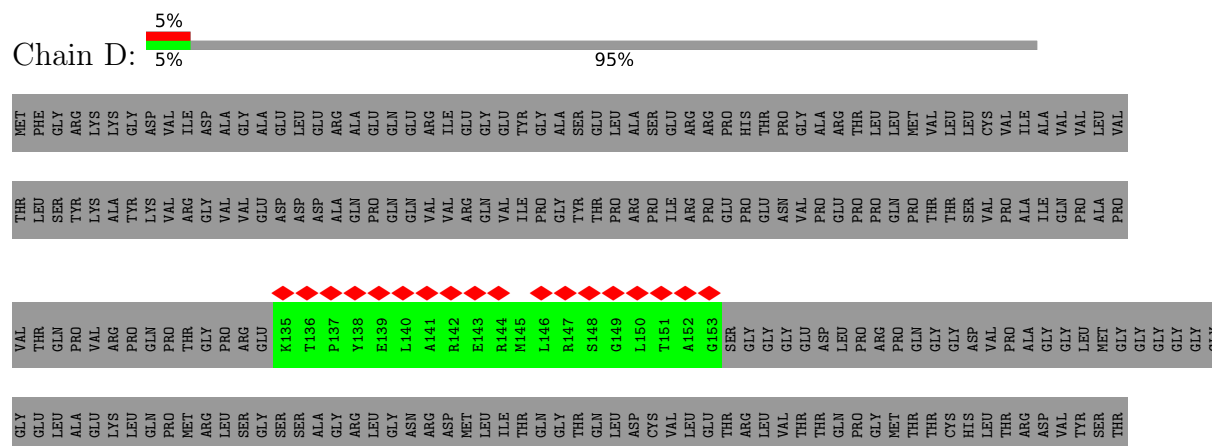
### 3 Residue-property plots

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









[illegible]

- Molecule 1: TrwE protein

[illegible]

- Molecule 1: TrwE protein

[illegible]



- Molecule 1: TrwE protein

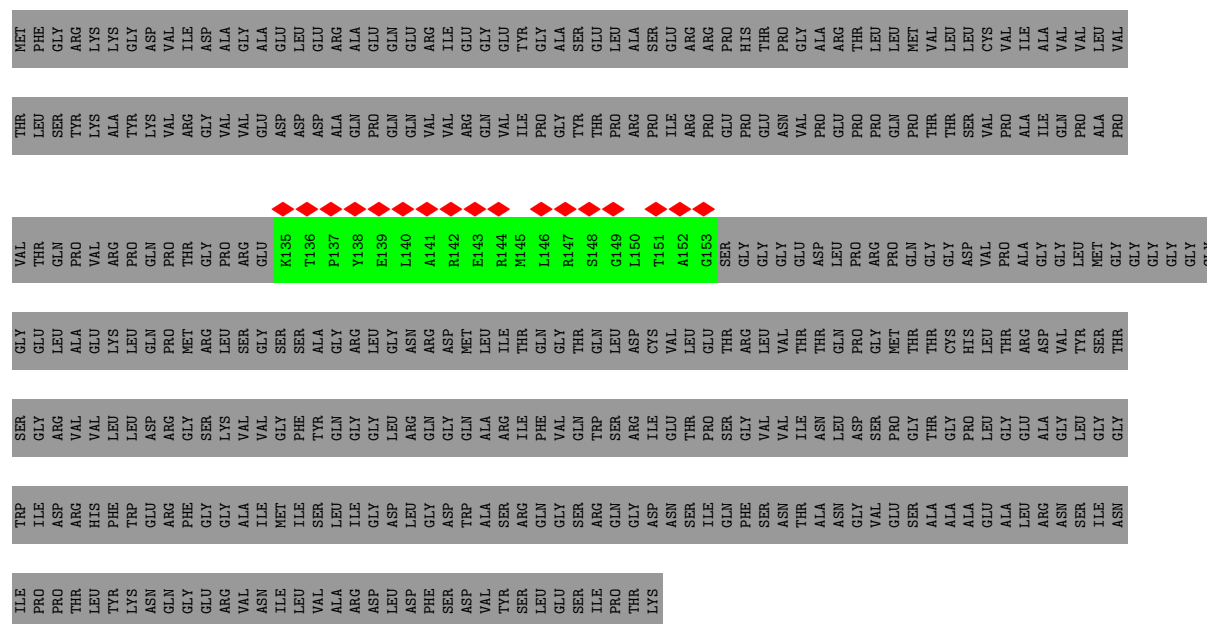
[illegible]

- Molecule 1: TrwE protein

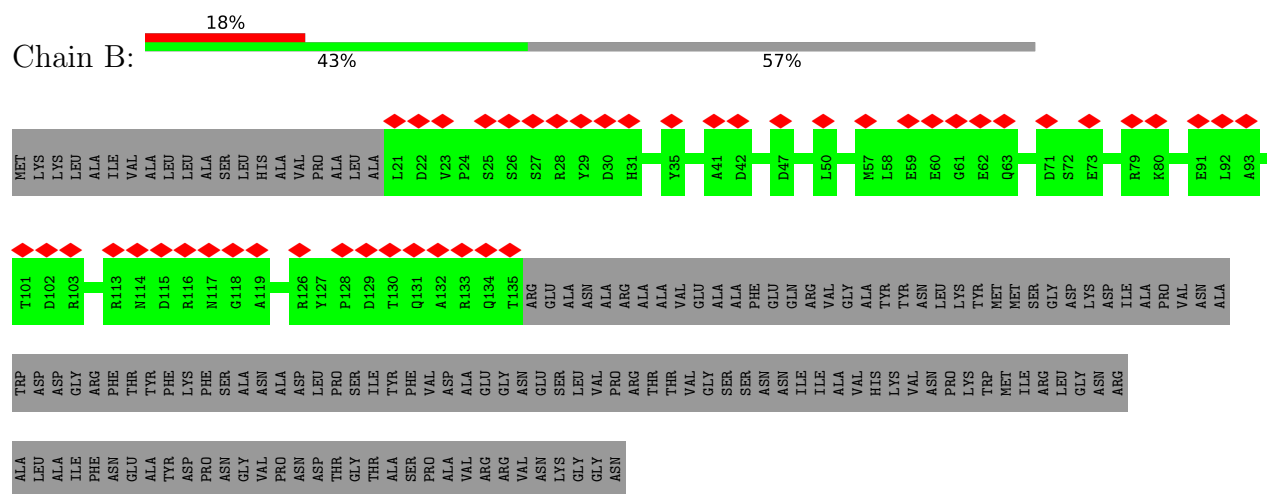


TRP	SER	GLY	THR	VAL	THR	THR	MET
ILE	GLY	LEU	GLN	THR	GLN	LEU	PHE
ASP	ARG	LEU	ALA	ARG	PRO	TYR	GLY
ARG	VAL	GLU	VAL	VAL	VAL	LYS	LYS
HIS	VAL	LEU	LYS	ARG	PRO	ALA	LYS
PHE	LEU	LEU	LEU	PRO	GLN	TYR	GLY
TRP	ASP	GLN	GLN	ARG	PRO	LYS	ASP
GLU	ARG	PRO	PRO	THR	VAL	VAL	VAL
PHE	GLY	MET	THR	THR	ARG	ILE	ILE
GLY	SER	ARG	GLY	GLY	PRO	GLY	ASP
GLY	LYS	LEU	SER	PRO	ARG	VAL	ALA
ALA	VAL	SER	ARG	ARG	VAL	GLY	GLY
ILE	VAL	GLY	GLU	THR	GLN	VAL	ALA
MET	GLY	SER	SER	K135	E136	ASP	GLU
ILE	PHE	SER	SER	T136	E137	ASP	LEU
SER	TYR	ALA	GLY	P137	E138	ALA	ARG
LEU	GLN	GLY	ARG	Y138	E139	GLN	ALA
ILE	GLY	LEU	GLY	E139	L140	GLN	GLU
ASP	LEU	ARG	ASN	L140	A141	VAL	GLN
LEU	GLY	GLN	ARG	A141	R142	ILE	ARG
GLY	GLY	ASP	ASP	R142	E143	VAL	ILE
TRP	GLN	MET	MET	E143	R144	ARG	GLU
ALA	ALA	LEU	LEU	R144	M145	GLN	GLY
SER	ARG	ILE	ILE	M145	L146	TYR	GLY
ARG	ILE	THR	GLN	L146	R147	GLY	GLY
GLN	PHE	VAL	THR	R147	S148	TYR	ALA
GLY	GLN	GLN	THR	S148	G149	THR	SER
ARG	SER	THR	GLN	G149	L150	GLU	GLU
GLY	GLY	LEU	LEU	L150	T151	ARG	LEU
ASN	ILE	CYS	CYS	T151	A152	ILE	GLY
GLU	GLU	VAL	LEU	A152	G153	ARG	ARG
THR	THR	THR	THR	G153	SER	PRO	ARG
ILE	ILE	VAL	VAL	GLY	GLY	ASN	PRO
ASN	VAL	VAL	VAL	GLY	GLY	GLY	GLY
ALA	ASN	THR	THR	GLU	ASP	VAL	ALA
ASN	LEU	GLN	GLN	ASP	LEU	GLU	THR
GLY	ASP	PRO	PRO	LEU	PRO	PRO	ARG
VAL	SER	GLY	ARG	ARG	PRO	PRO	THR
GLU	PRO	MET	MET	PRO	PRO	GLN	LEU
SER	GLY	THR	THR	GLN	THR	PRO	MET
ALA	THR	THR	THR	GLY	GLY	THR	VAL
ALA	GLY	CYS	CYS	GLY	GLY	THR	LEU
ALA	PRO	LEU	LEU	ASP	VAL	VAL	CYS
GLU	LEU	THR	THR	VAL	PRO	PRO	VAL
LEU	GLY	ARG	ARG	PRO	ALA	ALA	ILE
ALA	GLU	THR	THR	ALA	GLY	ILE	ALA
ARG	ALA	ASP	ASP	ALA	GLY	ILE	VAL
ASN	GLY	VAL	VAL	GLY	GLN	PRO	VAL
SER	LEU	TYR	TYR	LEU	LEU	PRO	VAL
ILE	GLY	SER	SER	MET	MET	ALA	LEU
ASN	GLY	THR	THR	GLY	GLY	PRO	VAL

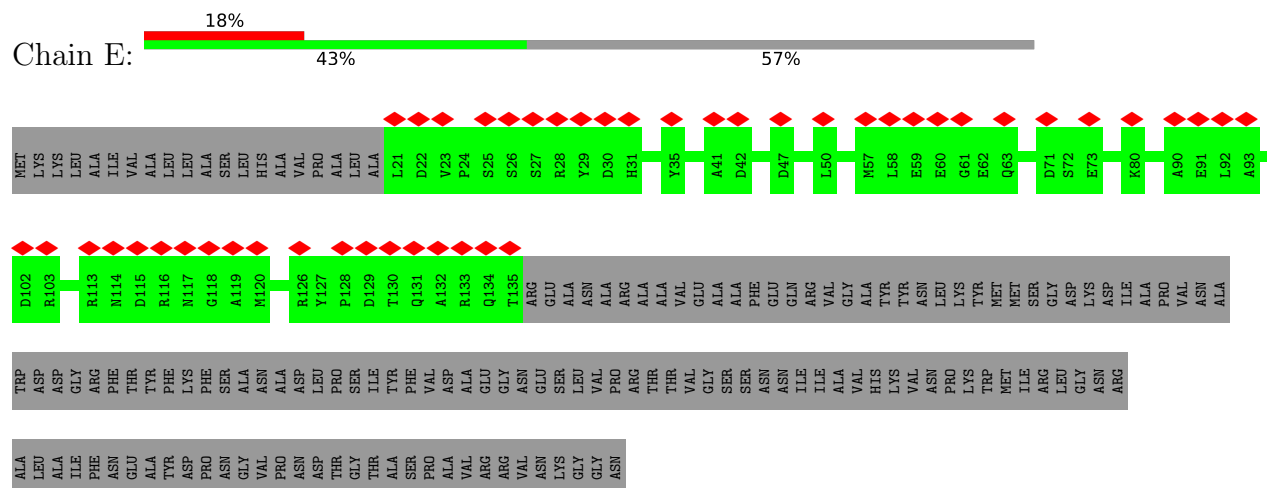




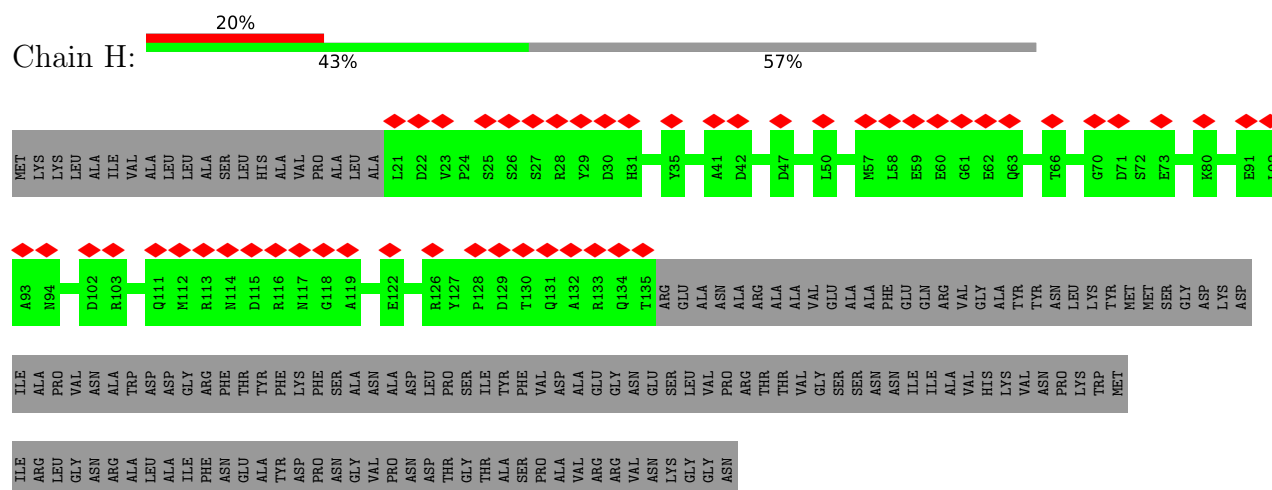
- Molecule 2: TrwF protein



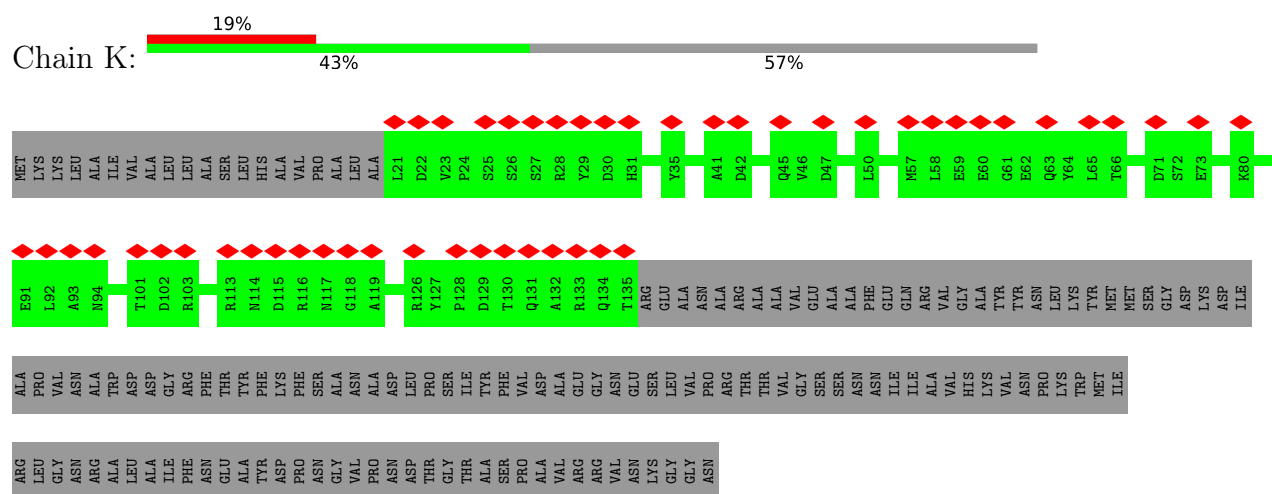
- Molecule 2: TrwF protein



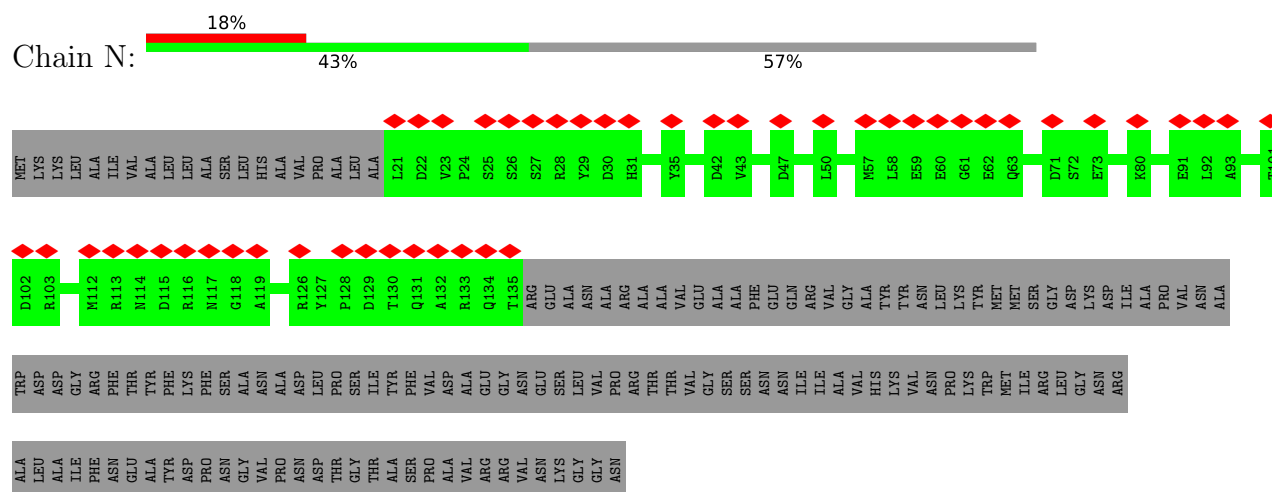
- Molecule 2: TrwF protein



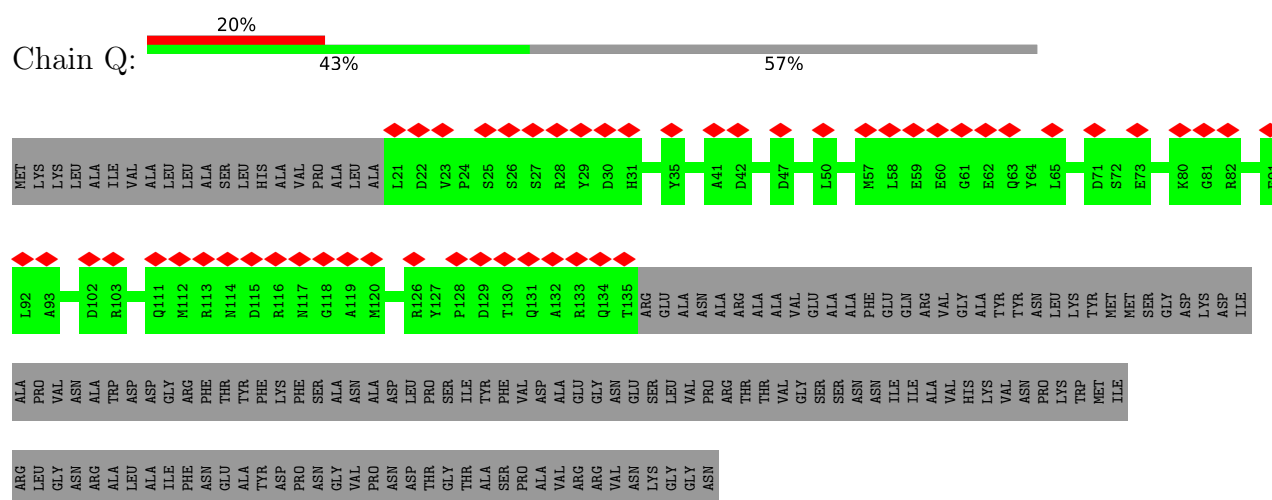
- Molecule 2: TrwF protein



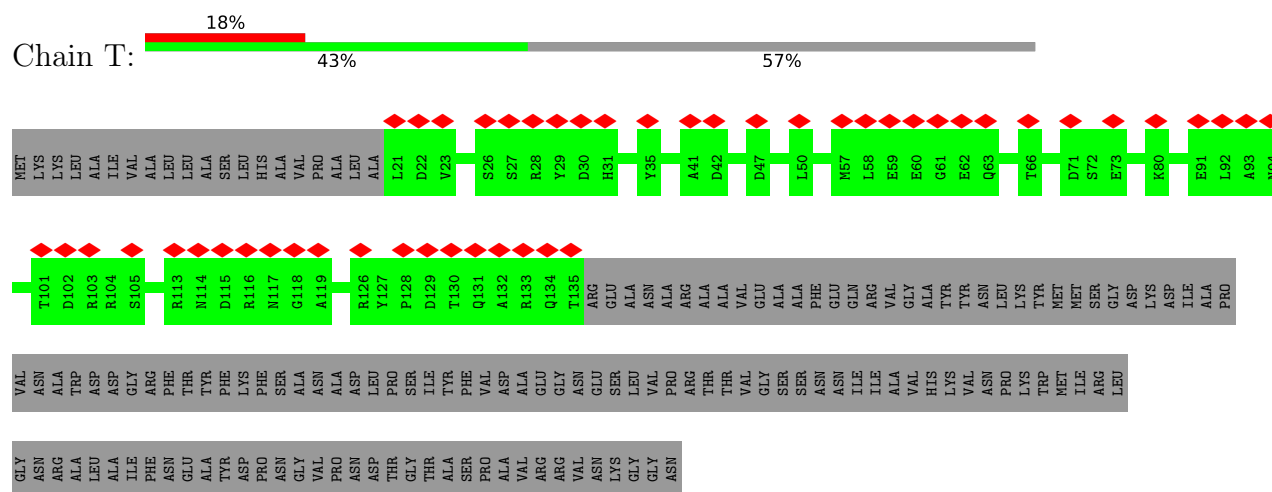
- Molecule 2: TrwF protein



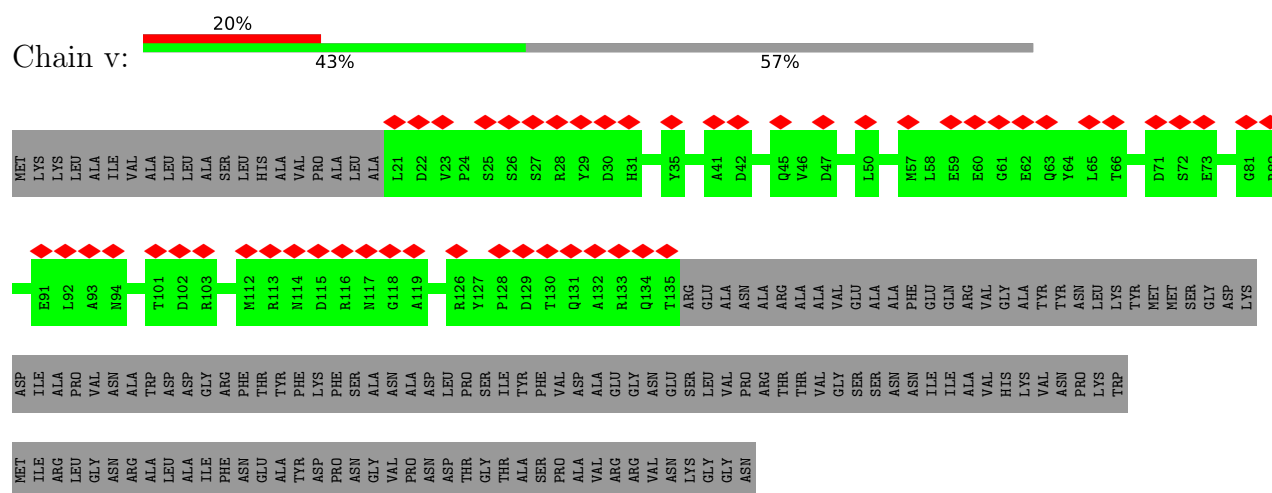
- Molecule 2: TrwF protein



- Molecule 2: TrwF protein

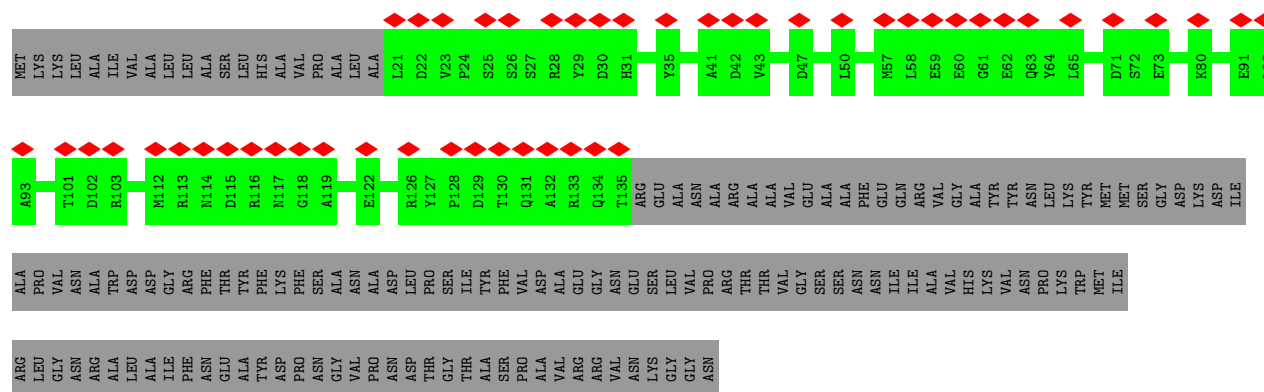


- Molecule 2: TrwF protein

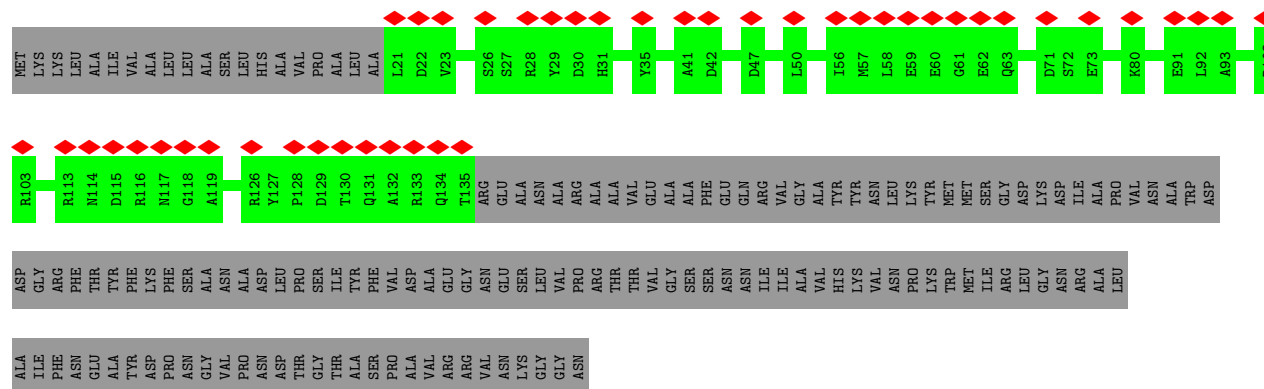


- Molecule 2: TrwF protein

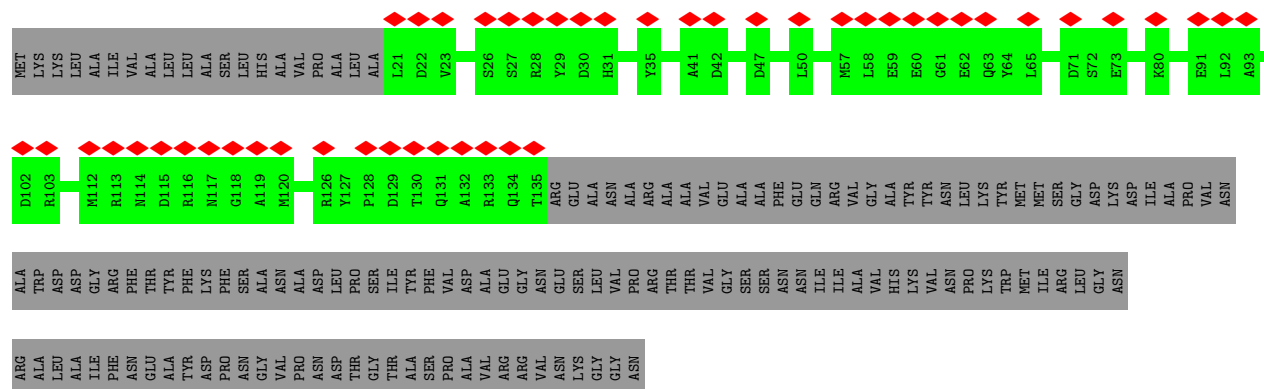




• Molecule 2: TrwF protein



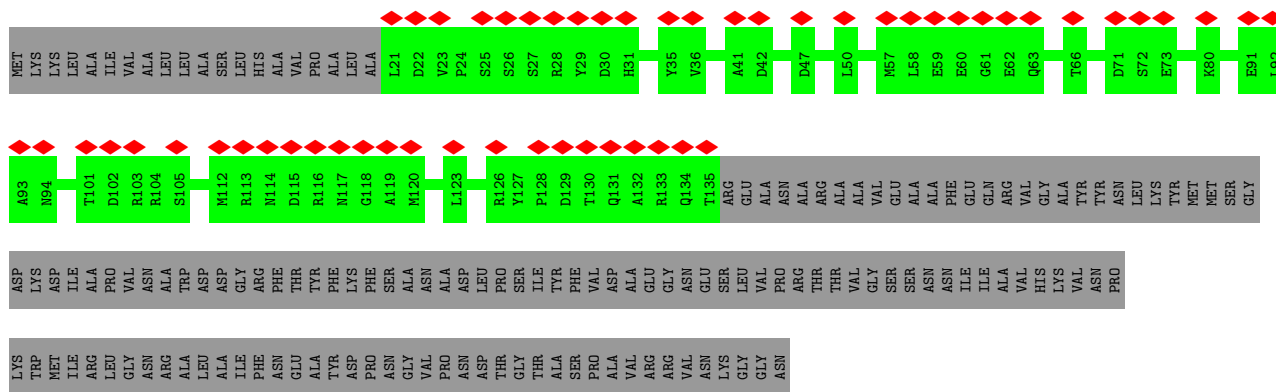
• Molecule 2: TrwF protein



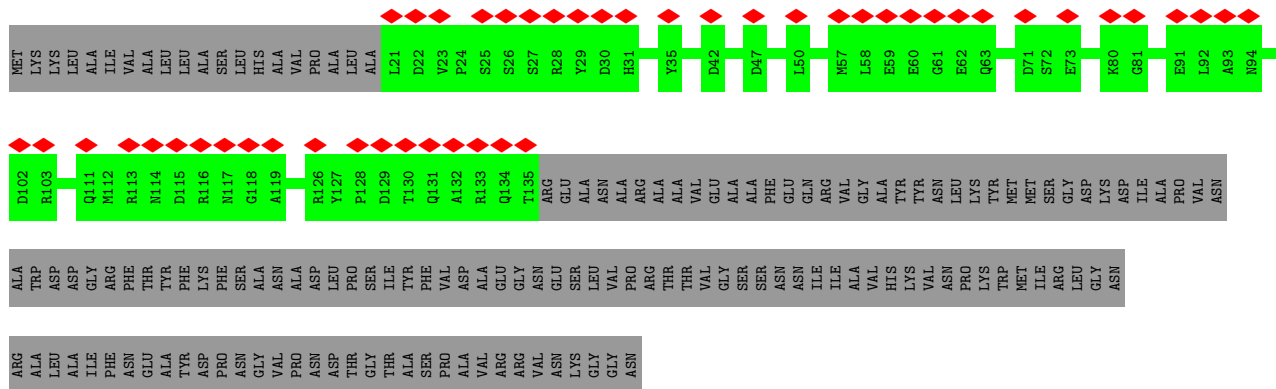
• Molecule 2: TrwF protein



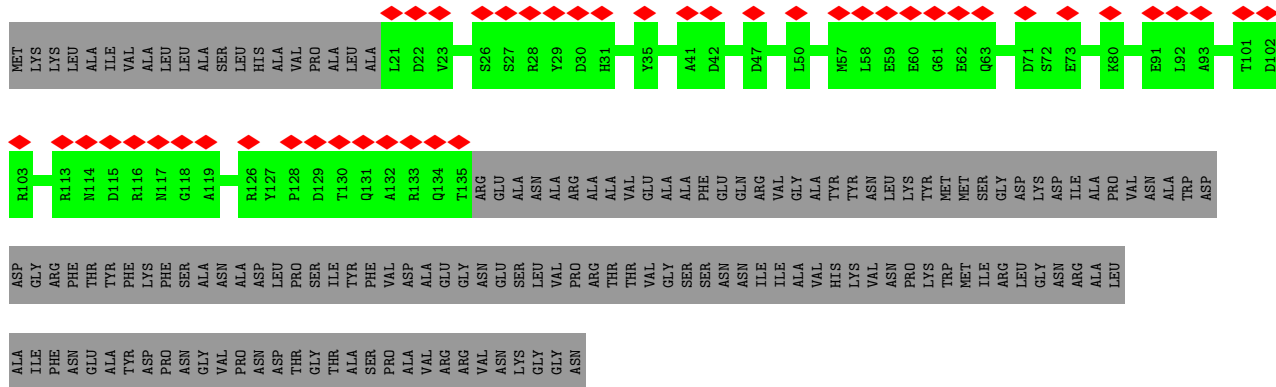




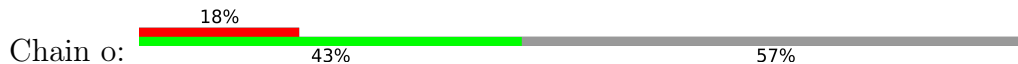
- Molecule 2: TrwF protein

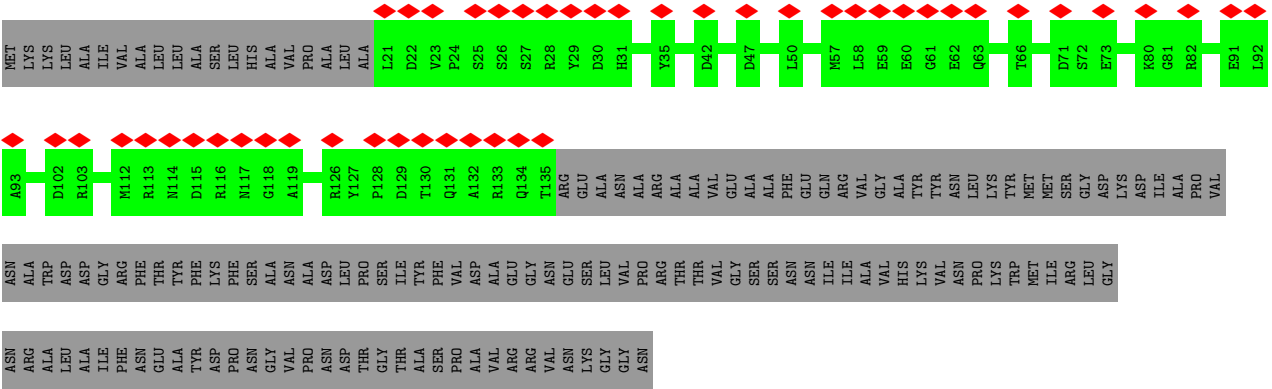


- Molecule 2: TrwF protein

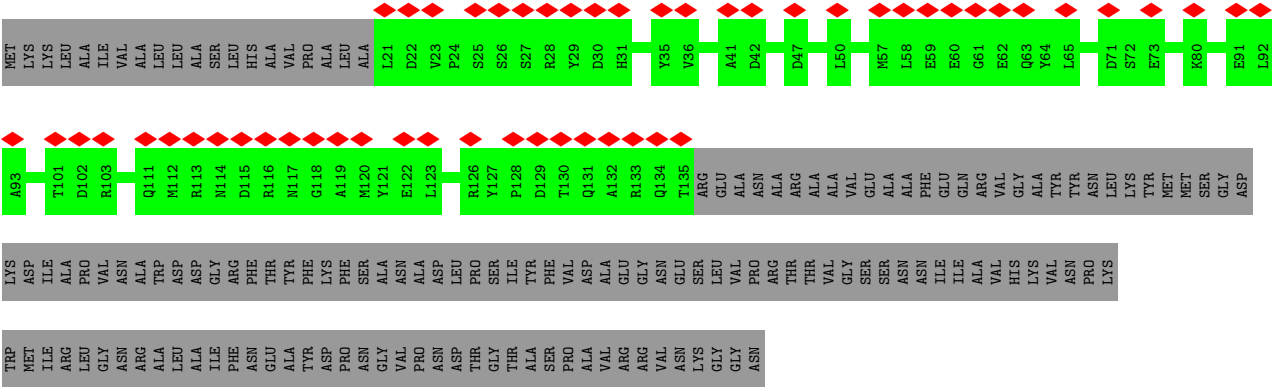


- Molecule 2: TrwF protein





• 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 (Å)	258.21402, 257.147, 85.36	wwPDB
Map dimensions	242, 241, 80	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	0.35	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. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	o	89	GLN
2	l	89	GLN
2	W	89	GLN
2	i	89	GLN
2	v	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.



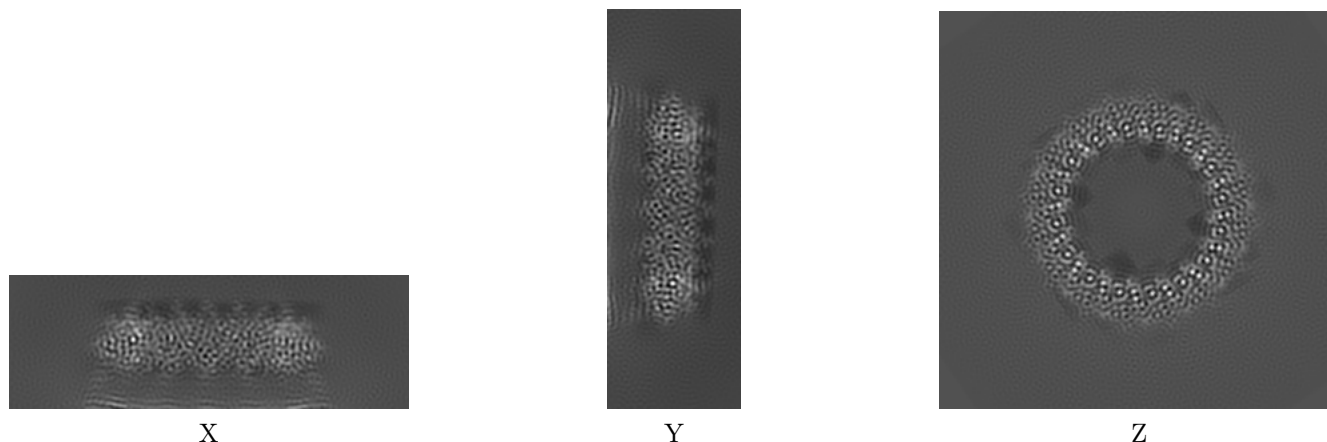
## 6 Map visualisation [i](#)

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.

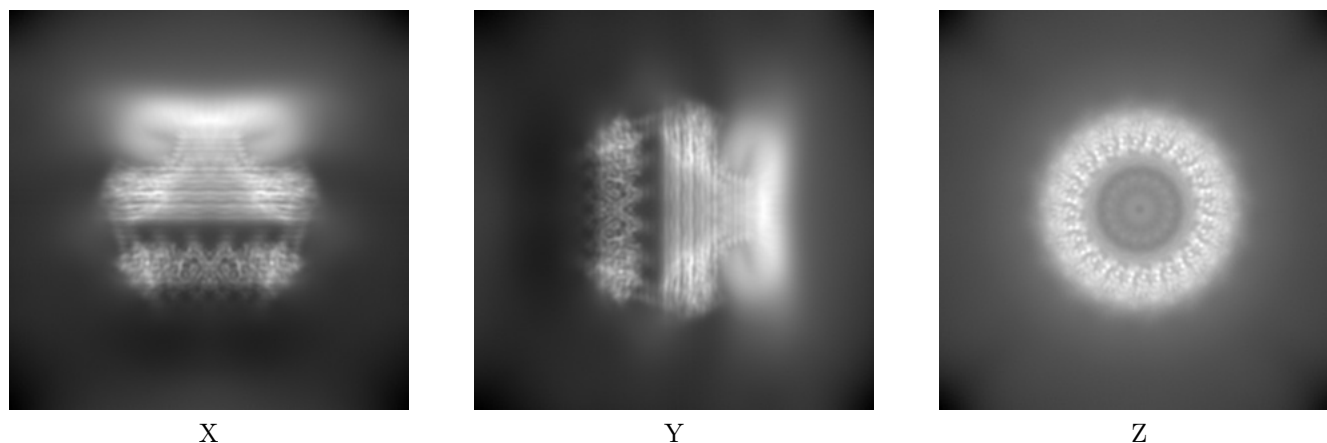
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 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](#)

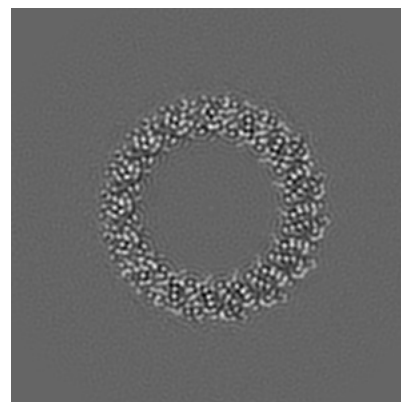
### 6.2.1 Primary map



X Index: 121

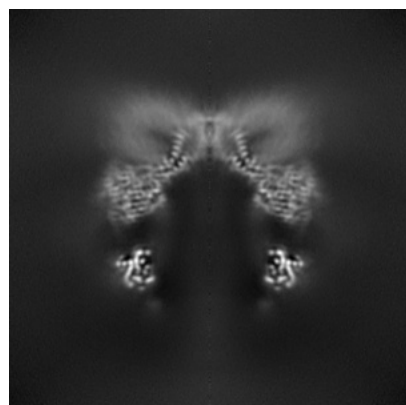


Y Index:  
120

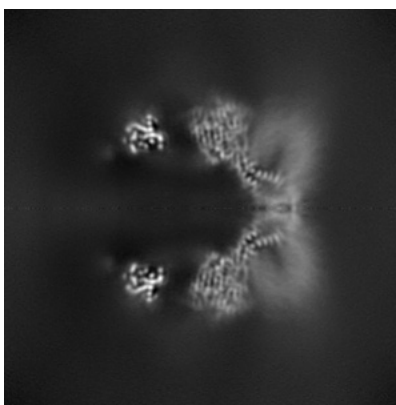


Z Index: 40

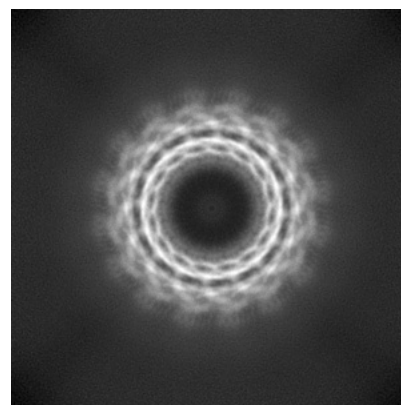
### 6.2.2 Raw map



X Index: 150



Y Index: 150

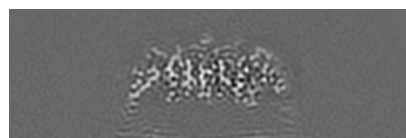


Z Index: 150

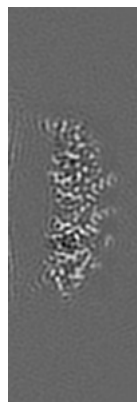
The images above show central slices of the map in three orthogonal directions.

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

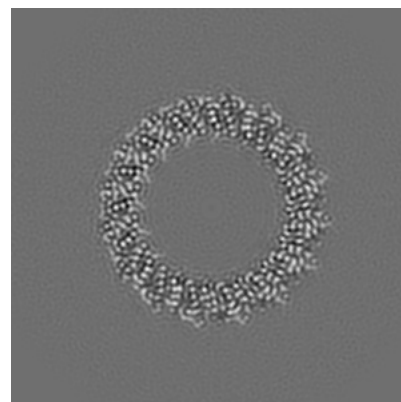
### 6.3.1 Primary map



X Index: 170

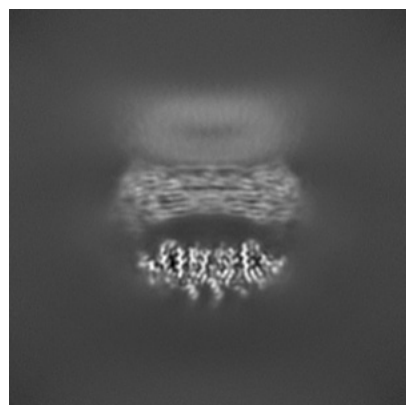


Y Index:  
74

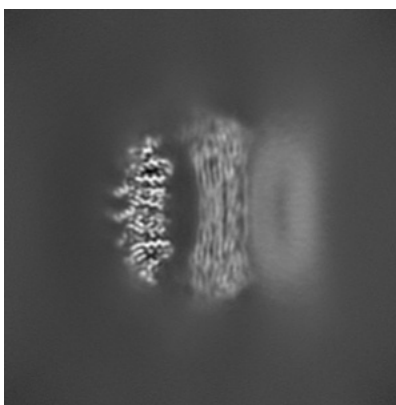


Z Index: 38

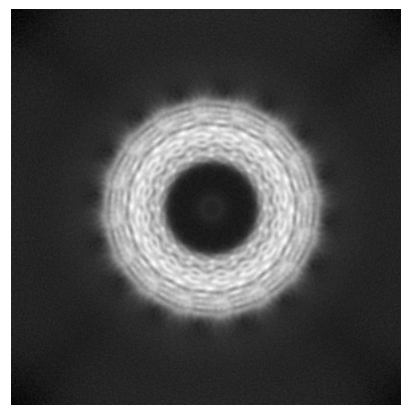
### 6.3.2 Raw map



X Index: 104



Y Index: 104

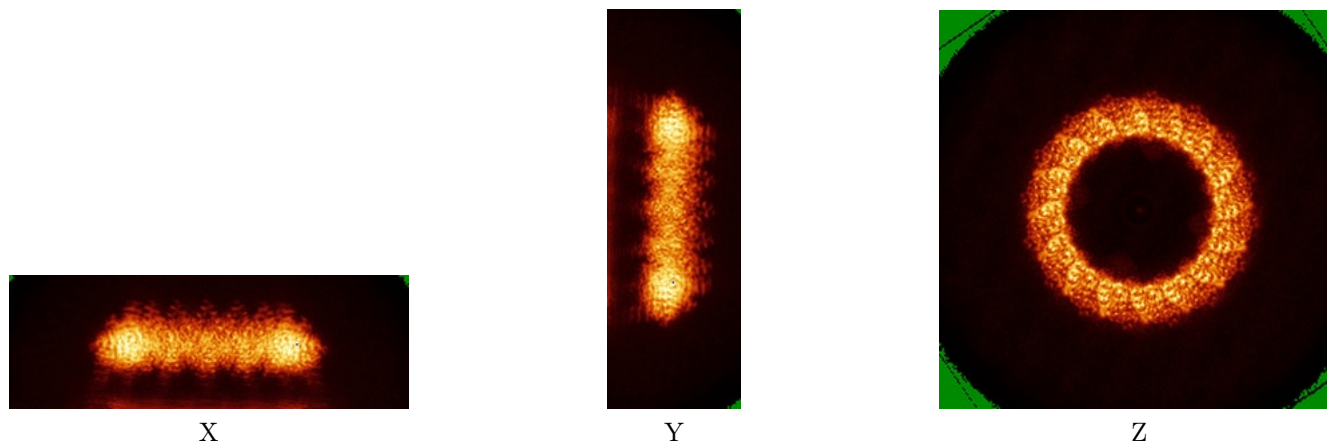


Z Index: 162

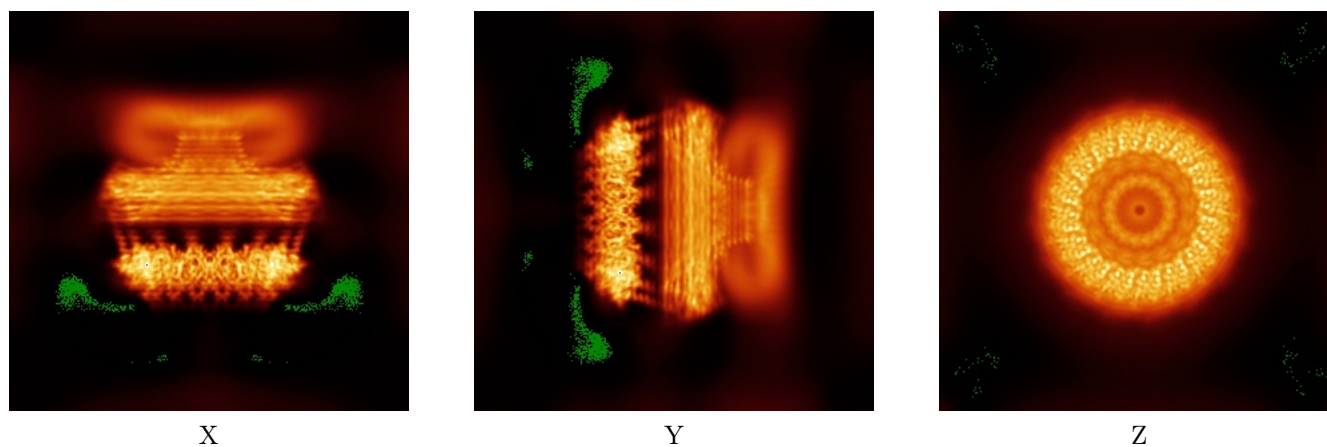
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



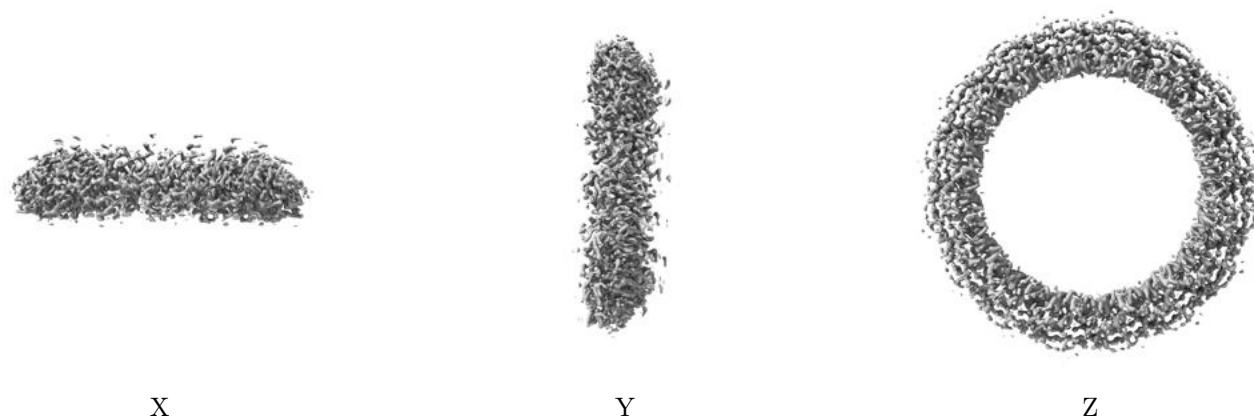
### 6.4.2 Raw map



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

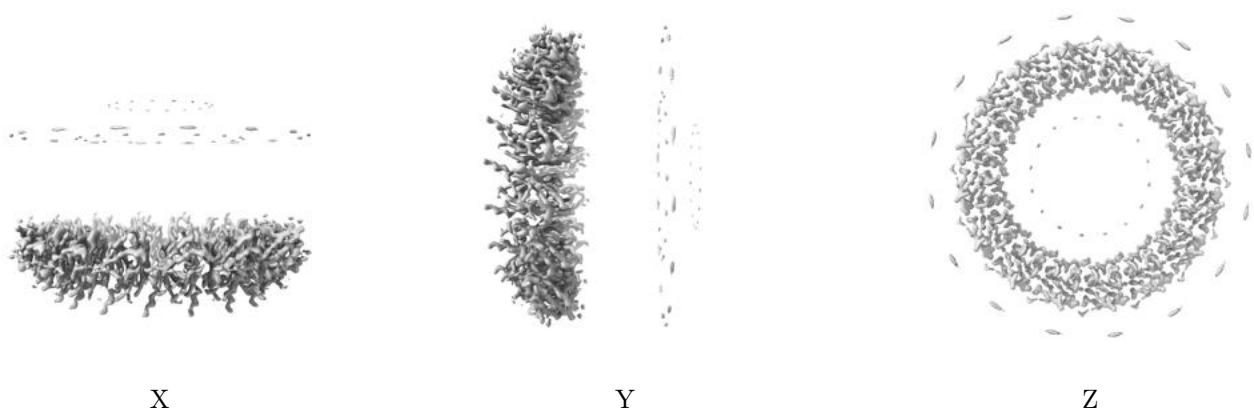
## 6.5 Orthogonal surface views [i](#)

### 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

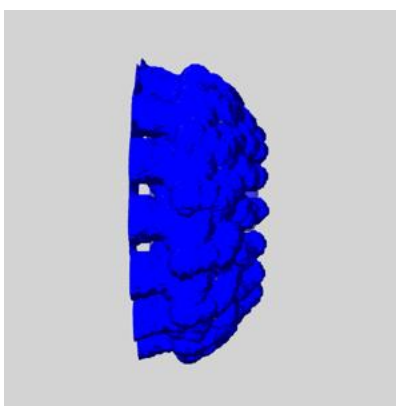
A mask typically either:

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

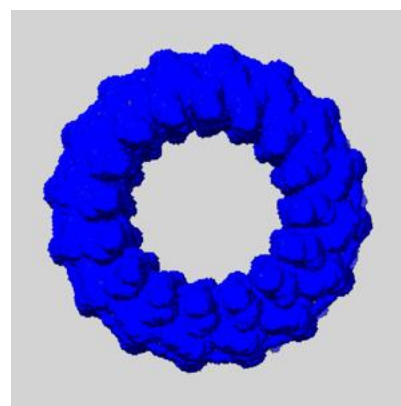
### 6.6.1 emd\_12708\_msk\_1.map [i](#)



X



Y

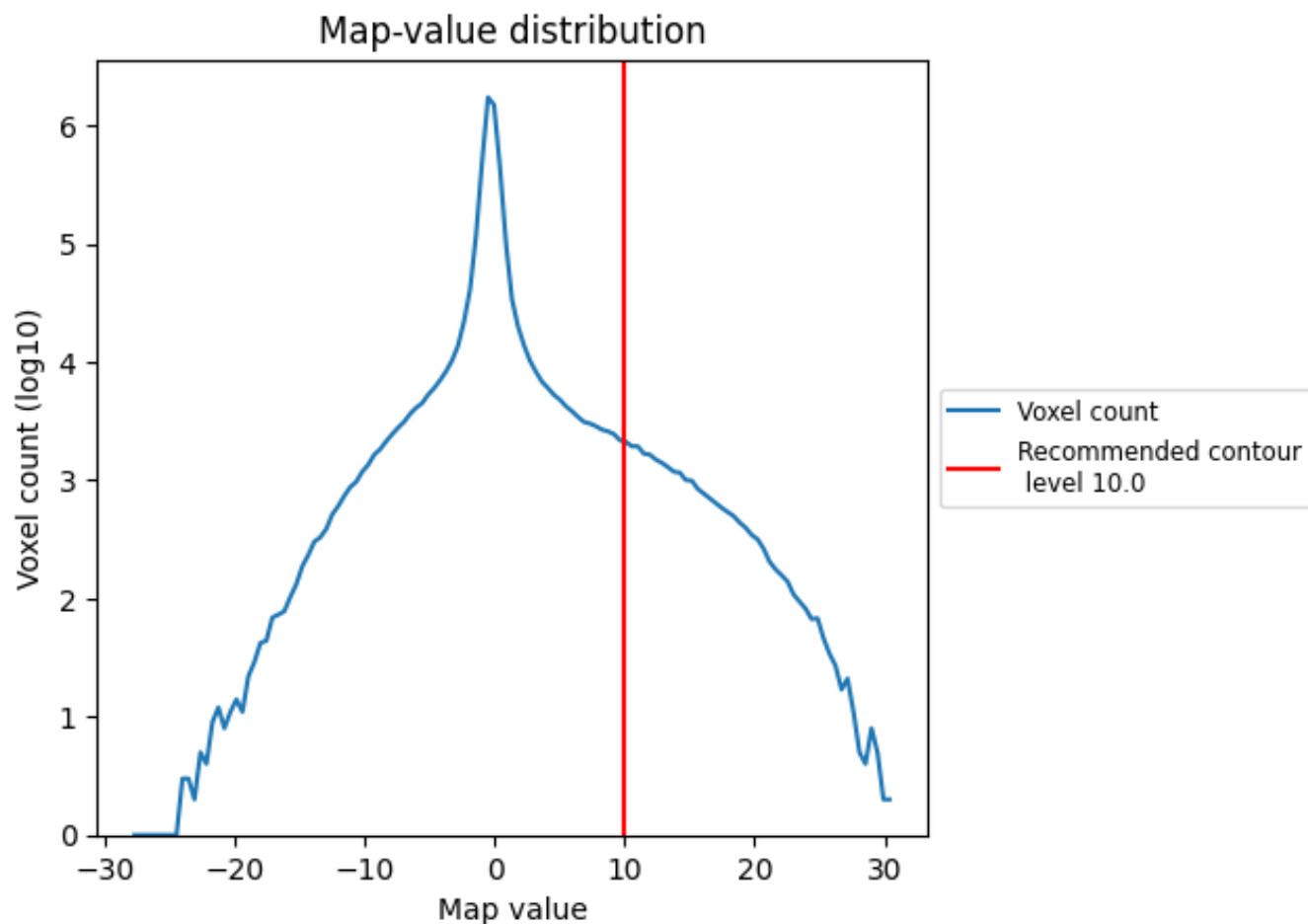


Z

## 7 Map analysis [i](#)

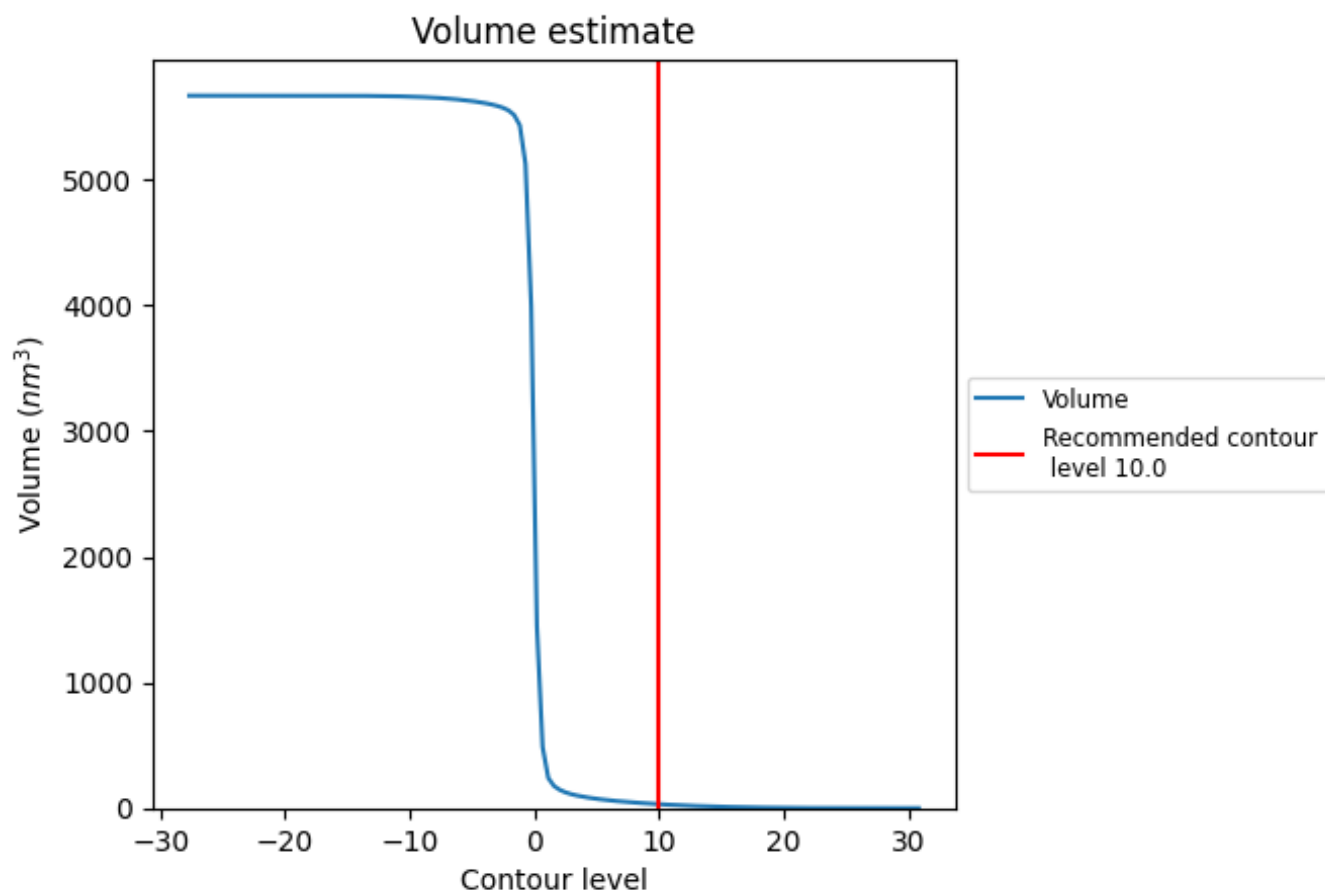
This section contains the results of statistical analysis of the map.

### 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 nm<sup>3</sup>; 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](#)

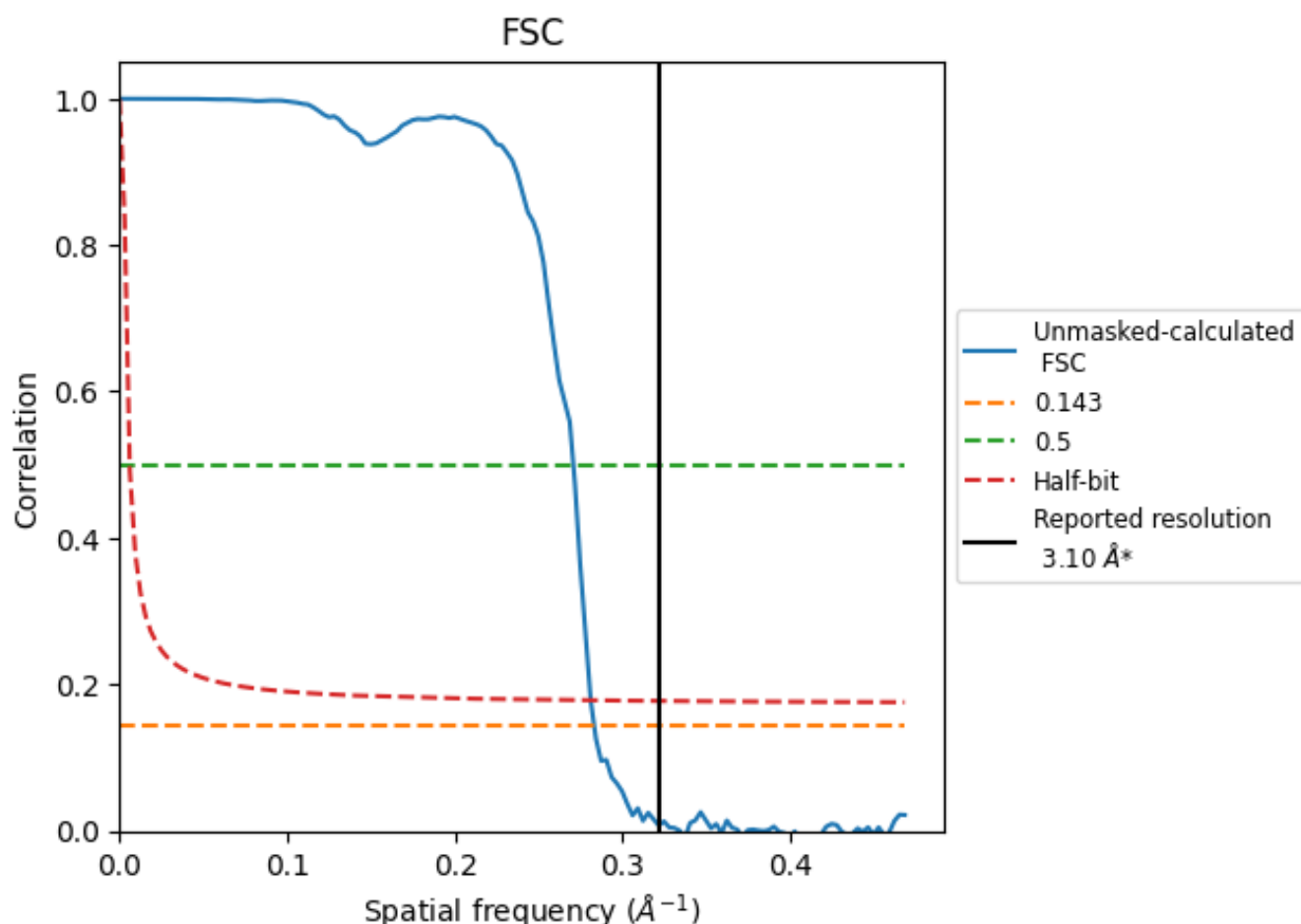
This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

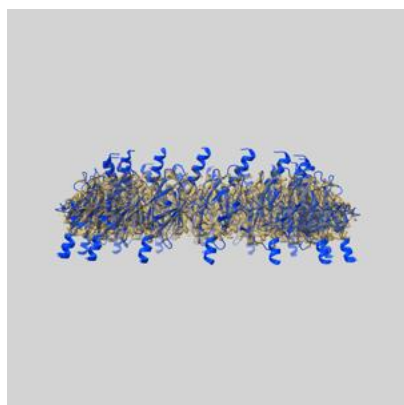
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	3.69	3.56

\*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 %

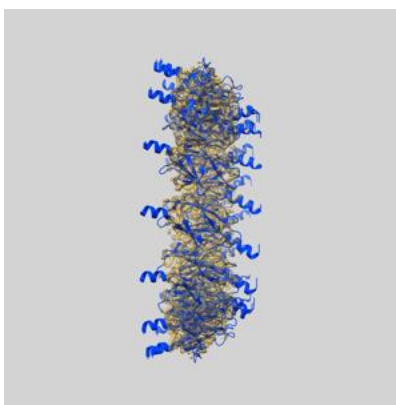
## 9 Map-model fit [i](#)

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](#).

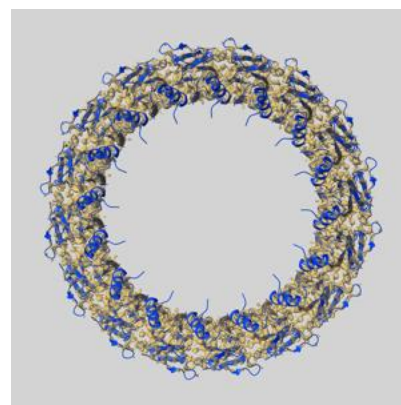
### 9.1 Map-model overlay [i](#)



X



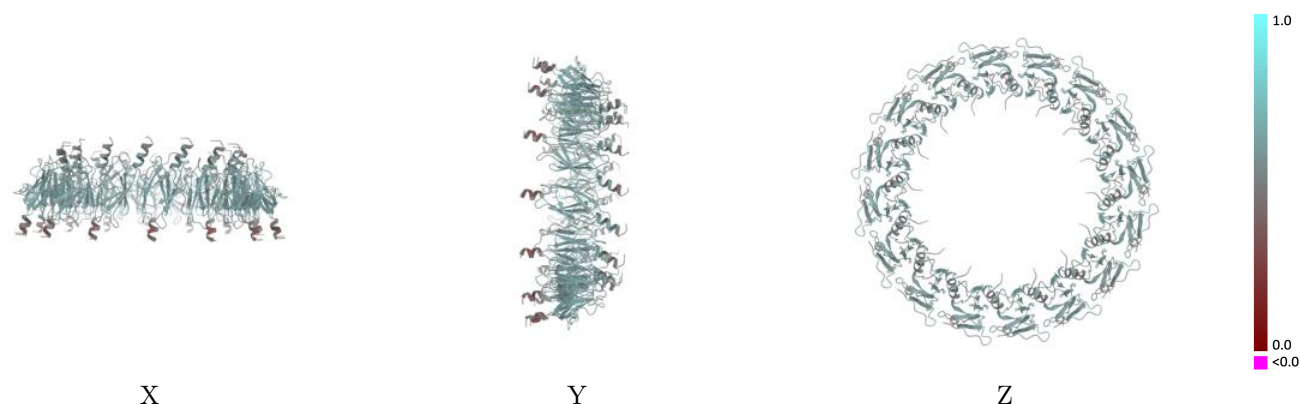
Y



Z

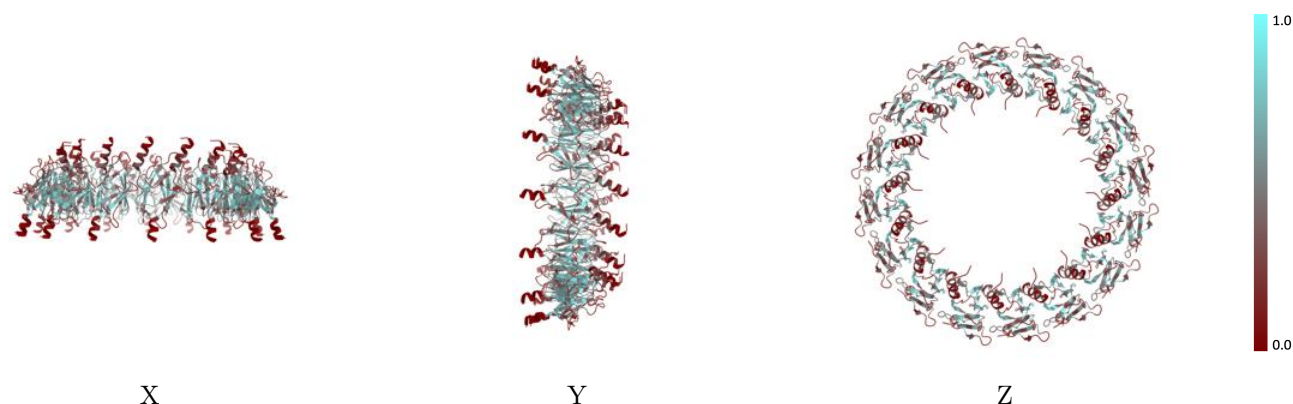
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



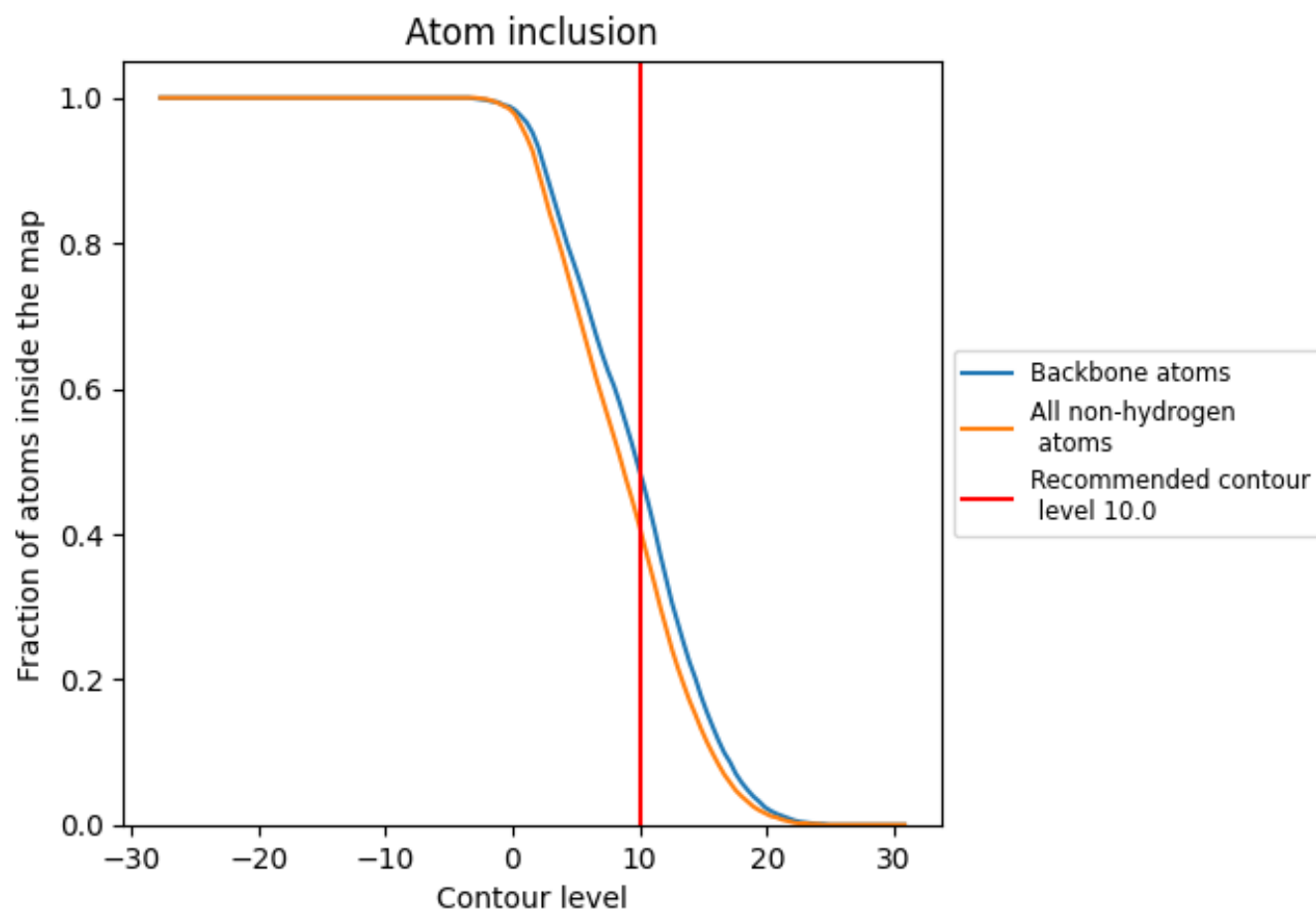
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

