

Feb 4, 2024 – 08:08 AM EST

PDB ID	:	1PDI
EMDB ID	:	EMD-1048
Title	:	Fitting of the C-terminal part of the short tail fibers into the cryo-EM recon-
		struction of T4 baseplate
Authors	:	Kostyuchenko, V.A.; Leiman, P.G.; Chipman, P.R.; Kanamaru, S.; van Raaij,
		M.J.; Arisaka, F.; Mesyanzhinov, V.V.; Rossmann, M.G.
Deposited on	:	2003-05-19
Resolution	:	12.00 Å(reported)
Based on initial model	:	10CY

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 (i) 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 (i)) were used in the production of this report:

:	0.0.1. dev 70
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.36
	::

Clashscore

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 12.00 Å.

158937

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.

Metri	2	Percen	Percentile Ranks		
Clashscore				0	
	Worse			Better	
	Percentile relativ	ve to all structures			
	Percentile relativ	ve to all EM structures			
Metri	c Wh	ole archive	EM structures	7	
INIGUI I	℃ (≠	$\neq \mathbf{Entries}$)	(#Entries)		

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.

4297

Mol	Chain	Length	Quality of chain
1	А	278	100%
1	В	278	100%
1	С	278	100%
1	D	278	• 100%
1	Е	278	100%
1	F	278	100%
1	G	278	100%
1	Н	278	100%
1	Ι	278	100%
1	J	278	



Mol	Chain	Length	Quality of chain
1	Κ	278	100%
1	L	278	100%
1	М	278	100%
1	Ν	278	100%
1	0	278	100%
1	Р	278	100%
1	Q	278	100%
1	R	278	• 100%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5004 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.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	А	278	Total C 278 278	0	278
1	В	278	Total C 278 278	0	278
1	С	278	Total C 278 278	0	278
1	D	278	Total C 278 278	0	278
1	Е	278	Total C 278 278	0	278
1	F	278	Total C 278 278	0	278
1	G	278	Total C 278 278	0	278
1	Н	278	Total C 278 278	0	278
1	Ι	278	Total C 278 278	0	278
1	J	278	Total C 278 278	0	278
1	K	278	Total C 278 278	0	278
1	L	278	Total C 278 278	0	278
1	М	278	Total C 278 278	0	278
1	Ν	278	Total C 278 278	0	278
1	О	278	Total C 278 278	0	278
1	Р	278	Total C 278 278	0	278
1	Q	278	Total C 278 278	0	278

• Molecule 1 is a protein called Short tail fiber protein.



Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf	Trace
1	R	278	Total 278	C 278	0	278

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	289	HIS	GLN	SEE REMARK 999	UNP P10930
А	295	THR	ILE	SEE REMARK 999	UNP P10930
А	297	ASN	TYR	SEE REMARK 999	UNP P10930
А	303	ASN	GLU	SEE REMARK 999	UNP P10930
А	304	ASN	ASP	SEE REMARK 999	UNP P10930
А	306	LEU	PHE	SEE REMARK 999	UNP P10930
А	310	SER	ASN	SEE REMARK 999	UNP P10930
А	320	ASN	ARG	SEE REMARK 999	UNP P10930
А	329	LYS	ASN	SEE REMARK 999	UNP P10930
А	331	VAL	ILE	SEE REMARK 999	UNP P10930
А	386	SER	ASN	SEE REMARK 999	UNP P10930
А	387	SER	PRO	SEE REMARK 999	UNP P10930
В	289	HIS	GLN	SEE REMARK 999	UNP P10930
В	295	THR	ILE	SEE REMARK 999	UNP P10930
В	297	ASN	TYR	SEE REMARK 999	UNP P10930
В	303	ASN	GLU	SEE REMARK 999	UNP P10930
В	304	ASN	ASP	SEE REMARK 999	UNP P10930
В	306	LEU	PHE	SEE REMARK 999	UNP P10930
В	310	SER	ASN	SEE REMARK 999	UNP P10930
В	320	ASN	ARG	SEE REMARK 999	UNP P10930
В	329	LYS	ASN	SEE REMARK 999	UNP P10930
В	331	VAL	ILE	SEE REMARK 999	UNP P10930
В	386	SER	ASN	SEE REMARK 999	UNP P10930
В	387	SER	PRO	SEE REMARK 999	UNP P10930
С	289	HIS	GLN	SEE REMARK 999	UNP P10930
С	295	THR	ILE	SEE REMARK 999	UNP P10930
С	297	ASN	TYR	SEE REMARK 999	UNP P10930
С	303	ASN	GLU	SEE REMARK 999	UNP P10930
С	304	ASN	ASP	SEE REMARK 999	UNP P10930
С	306	LEU	PHE	SEE REMARK 999	UNP P10930
С	310	SER	ASN	SEE REMARK 999	UNP P10930
С	320	ASN	ARG	SEE REMARK 999	UNP P10930
С	329	LYS	ASN	SEE REMARK 999	UNP P10930
С	331	VAL	ILE	SEE REMARK 999	UNP P10930
С	386	SER	ASN	SEE REMARK 999	UNP P10930
С	387	SER	PRO	SEE REMARK 999	UNP P10930



Chain	Residue	Modelled	Actual	Comment	Reference
D	289	HIS	GLN	SEE REMARK 999	UNP P10930
D	295	THR	ILE	SEE REMARK 999	UNP P10930
D	297	ASN	TYR	SEE REMARK 999	UNP P10930
D	303	ASN	GLU	SEE REMARK 999	UNP P10930
D	304	ASN	ASP	SEE REMARK 999	UNP P10930
D	306	LEU	PHE	SEE REMARK 999	UNP P10930
D	310	SER	ASN	SEE REMARK 999	UNP P10930
D	320	ASN	ARG	SEE REMARK 999	UNP P10930
D	329	LYS	ASN	SEE REMARK 999	UNP P10930
D	331	VAL	ILE	SEE REMARK 999	UNP P10930
D	386	SER	ASN	SEE REMARK 999	UNP P10930
D	387	SER	PRO	SEE REMARK 999	UNP P10930
Е	289	HIS	GLN	SEE REMARK 999	UNP P10930
Е	295	THR	ILE	SEE REMARK 999	UNP P10930
Ε	297	ASN	TYR	SEE REMARK 999	UNP P10930
E	303	ASN	GLU	SEE REMARK 999	UNP P10930
E	304	ASN	ASP	SEE REMARK 999	UNP P10930
E	306	LEU	PHE	SEE REMARK 999	UNP P10930
E	310	SER	ASN	SEE REMARK 999	UNP P10930
E	320	ASN	ARG	SEE REMARK 999	UNP P10930
E	329	LYS	ASN	SEE REMARK 999	UNP P10930
E	331	VAL	ILE	SEE REMARK 999	UNP P10930
E	386	SER	ASN	SEE REMARK 999	UNP P10930
E	387	SER	PRO	SEE REMARK 999	UNP P10930
F	289	HIS	GLN	SEE REMARK 999	UNP P10930
F	295	THR	ILE	SEE REMARK 999	UNP P10930
F	297	ASN	TYR	SEE REMARK 999	UNP P10930
F	303	ASN	GLU	SEE REMARK 999	UNP P10930
F	304	ASN	ASP	SEE REMARK 999	UNP P10930
F	306	LEU	PHE	SEE REMARK 999	UNP P10930
F	310	SER	ASN	SEE REMARK 999	UNP P10930
F	320	ASN	ARG	SEE REMARK 999	UNP P10930
F	329	LYS	ASN	SEE REMARK 999	UNP P10930
F	331	VAL	ILE	SEE REMARK 999	UNP P10930
F	386	SER	ASN	SEE REMARK 999	UNP P10930
F	387	SER	PRO	SEE REMARK 999	UNP P10930
G	289	HIS	GLN	SEE REMARK 999	UNP P10930
G	295	THR	ILE	SEE REMARK 999	UNP P10930
G	297	ASN	TYR	SEE REMARK 999	UNP P10930
G	303	ASN	GLU	SEE REMARK 999	UNP P10930
G	304	ASN	ASP	SEE REMARK 999	UNP P10930
G	306	LEU	PHE	SEE REMARK 999	UNP P10930



Chain	Residue	Modelled	Actual	Comment	Reference
G	310	SER	ASN	SEE REMARK 999	UNP P10930
G	320	ASN	ARG	SEE REMARK 999	UNP P10930
G	329	LYS	ASN	SEE REMARK 999	UNP P10930
G	331	VAL	ILE	SEE REMARK 999	UNP P10930
G	386	SER	ASN	SEE REMARK 999	UNP P10930
G	387	SER	PRO	SEE REMARK 999	UNP P10930
Н	289	HIS	GLN	SEE REMARK 999	UNP P10930
Н	295	THR	ILE	SEE REMARK 999	UNP P10930
Н	297	ASN	TYR	SEE REMARK 999	UNP P10930
Н	303	ASN	GLU	SEE REMARK 999	UNP P10930
Н	304	ASN	ASP	SEE REMARK 999	UNP P10930
Н	306	LEU	PHE	SEE REMARK 999	UNP P10930
Н	310	SER	ASN	SEE REMARK 999	UNP P10930
Н	320	ASN	ARG	SEE REMARK 999	UNP P10930
Н	329	LYS	ASN	SEE REMARK 999	UNP P10930
Н	331	VAL	ILE	SEE REMARK 999	UNP P10930
Н	386	SER	ASN	SEE REMARK 999	UNP P10930
Н	387	SER	PRO	SEE REMARK 999	UNP P10930
Ι	289	HIS	GLN	SEE REMARK 999	UNP P10930
Ι	295	THR	ILE	SEE REMARK 999	UNP P10930
Ι	297	ASN	TYR	SEE REMARK 999	UNP P10930
Ι	303	ASN	GLU	SEE REMARK 999	UNP P10930
Ι	304	ASN	ASP	SEE REMARK 999	UNP P10930
Ι	306	LEU	PHE	SEE REMARK 999	UNP P10930
I	310	SER	ASN	SEE REMARK 999	UNP P10930
Ι	320	ASN	ARG	SEE REMARK 999	UNP P10930
I	329	LYS	ASN	SEE REMARK 999	UNP P10930
I	331	VAL	ILE	SEE REMARK 999	UNP P10930
I	386	SER	ASN	SEE REMARK 999	UNP P10930
I	387	SER	PRO	SEE REMARK 999	UNP P10930
J	289	HIS	GLN	SEE REMARK 999	UNP P10930
J	295	THR	ILE	SEE REMARK 999	UNP P10930
J	297	ASN	TYR	SEE REMARK 999	UNP P10930
J	303	ASN	GLU	SEE REMARK 999	UNP P10930
J	304	ASN	ASP	SEE REMARK 999	UNP P10930
J	306	LEU	PHE	SEE REMARK 999	UNP P10930
J	310	SER	ASN	SEE REMARK 999	UNP P10930
J	320	ASN	ARG	SEE REMARK 999	UNP P10930
J	329	LYS	ASN	SEE REMARK 999	UNP P10930
J	331	VAL	ILE	SEE REMARK 999	UNP P10930
J	386	SER	ASN	SEE REMARK 999	UNP P10930
J	387	SER	PRO	SEE REMARK 999	UNP P10930



Chain		Modelled	Actual	Comment	Reference
K	289	HIS	GLN	SEE REMARK 999	UNP P10930
K	295	THR	ILE	SEE REMARK 999	UNP P10930
K	297	ASN	TYR	SEE REMARK 999	UNP P10930
K	303	ASN	GLU	SEE REMARK 999	UNP P10930
К	304	ASN	ASP	SEE REMARK 999	UNP P10930
K	306	LEU	PHE	SEE REMARK 999	UNP P10930
K	310	SER	ASN	SEE REMARK 999	UNP P10930
K	320	ASN	ARG	SEE REMARK 999	UNP P10930
K	329	LYS	ASN	SEE REMARK 999	UNP P10930
K	331	VAL	ILE	SEE REMARK 999	UNP P10930
K	386	SER	ASN	SEE REMARK 999	UNP P10930
K	387	SER	PRO	SEE REMARK 999	UNP P10930
L	289	HIS	GLN	SEE REMARK 999	UNP P10930
L	295	THR	ILE	SEE REMARK 999	UNP P10930
L	297	ASN	TYR	SEE REMARK 999	UNP P10930
L	303	ASN	GLU	SEE REMARK 999	UNP P10930
L	304	ASN	ASP	SEE REMARK 999	UNP P10930
L	306	LEU	PHE	SEE REMARK 999	UNP P10930
L	310	SER	ASN	SEE REMARK 999	UNP P10930
L	320	ASN	ARG	SEE REMARK 999	UNP P10930
L	329	LYS	ASN	SEE REMARK 999	UNP P10930
L	331	VAL	ILE	SEE REMARK 999	UNP P10930
L	386	SER	ASN	SEE REMARK 999	UNP P10930
L	387	SER	PRO	SEE REMARK 999	UNP P10930
M	289	HIS	GLN	SEE REMARK 999	UNP P10930
M	295	THR	ILE	SEE REMARK 999	UNP P10930
M	297	ASN	TYR	SEE REMARK 999	UNP P10930
M	303	ASN	GLU	SEE REMARK 999	UNP P10930
M	304	ASN	ASP	SEE REMARK 999	UNP P10930
M	306	LEU	PHE	SEE REMARK 999	UNP P10930
M M	310	SER ASN	ASN	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
	320	ASN LYS	ARG ASN	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
M M	329 331	VAL	ILE	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
M	386	SER SER	ASN	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
M	387	SER	PRO	SEE REMARK 999	UNP P10930
N N	289	HIS	GLN	SEE REMARK 999	UNP P10930
N N	289	THR	ILE	SEE REMARK 999	UNP P10930
N	295	ASN	TYR	SEE REMARK 999	UNP P10930
N	303	ASN	GLU	SEE REMARK 999	UNP P10930
N	304	ASN	ASP	SEE REMARK 999	UNP P10930
N	306	LEU	PHE	SEE REMARK 999	UNP P10930
	000				0111 1 10000



Chain	Residue	Modelled	Actual	Comment	Reference
N	310	SER	ASN	SEE REMARK 999	UNP P10930
N	320	ASN	ARG	SEE REMARK 999	UNP P10930
N	329	LYS	ASN	SEE REMARK 999	UNP P10930
N	331	VAL	ILE	SEE REMARK 999	UNP P10930
N	386	SER	ASN	SEE REMARK 999	UNP P10930
N	387	SER	PRO	SEE REMARK 999	UNP P10930
0	289	HIS	GLN	SEE REMARK 999	UNP P10930
0	295	THR	ILE	SEE REMARK 999	UNP P10930
0	297	ASN	TYR	SEE REMARK 999	UNP P10930
0	303	ASN	GLU	SEE REMARK 999	UNP P10930
0	304	ASN	ASP	SEE REMARK 999	UNP P10930
0	306	LEU	PHE	SEE REMARK 999	UNP P10930
0	310	SER	ASN	SEE REMARK 999	UNP P10930
0	320	ASN	ARG	SEE REMARK 999	UNP P10930
0	329	LYS	ASN	SEE REMARK 999	UNP P10930
0	331	VAL	ILE	SEE REMARK 999	UNP P10930
0	386	SER	ASN	SEE REMARK 999	UNP P10930
0	387	SER	PRO	SEE REMARK 999	UNP P10930
Р	289	HIS	GLN	SEE REMARK 999	UNP P10930
Р	295	THR	ILE	SEE REMARK 999	UNP P10930
Р	297	ASN	TYR	SEE REMARK 999	UNP P10930
Р	303	ASN	GLU	SEE REMARK 999	UNP P10930
P	304	ASN	ASP	SEE REMARK 999	UNP P10930
Р	306	LEU	PHE	SEE REMARK 999	UNP P10930
P	310	SER	ASN	SEE REMARK 999	UNP P10930
P	320	ASN	ARG	SEE REMARK 999	UNP P10930
P	329	LYS	ASN	SEE REMARK 999	UNP P10930
P	331	VAL	ILE	SEE REMARK 999	UNP P10930
P	386	SER	ASN	SEE REMARK 999	
P	387	SER	PRO	SEE REMARK 999	UNP P10930
Q	289	HIS	GLN	SEE REMARK 999	UNP P10930
Q	295	THR	ILE	SEE REMARK 999	UNP P10930
Q	297	ASN	TYR	SEE REMARK 999	UNP P10930
Q	303	ASN	GLU	SEE REMARK 999	UNP P10930
Q	304	ASN LEU	ASP PHE	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
Q	306 310	SER	ASN	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
Q	320	ASN	ARG	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
Q Q	320	LYS	ARG	SEE REMARK 999 SEE REMARK 999	UNP P10930 UNP P10930
Q	331	VAL	ILE	SEE REMARK 999	UNP P10930
Q	386	SER	ASN	SEE REMARK 999	UNP P10930
Q	387	SER	PRO	SEE REMARK 999	UNP P10930
L V	301	J JUN	INU	SEE REMARK 999	0101 E 10990



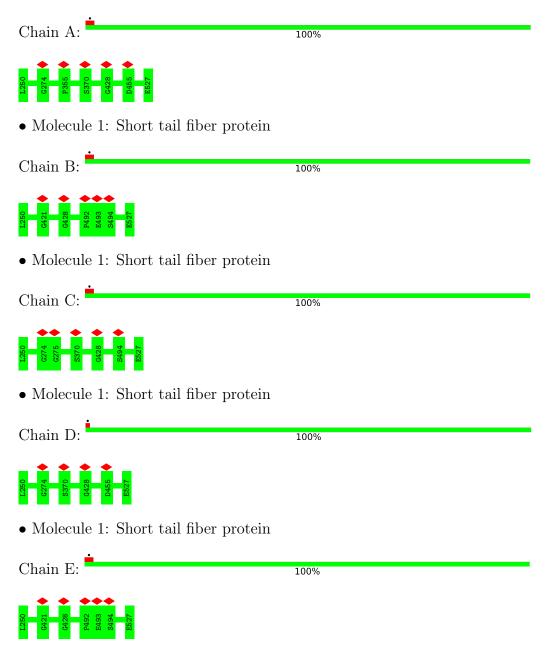
Chain	Residue	Modelled	Actual	Comment	Reference
R	289	HIS	GLN	SEE REMARK 999	UNP P10930
R	295	THR	ILE	SEE REMARK 999	UNP P10930
R	297	ASN	TYR	SEE REMARK 999	UNP P10930
R	303	ASN	GLU	SEE REMARK 999	UNP P10930
R	304	ASN	ASP	SEE REMARK 999	UNP P10930
R	306	LEU	PHE	SEE REMARK 999	UNP P10930
R	310	SER	ASN	SEE REMARK 999	UNP P10930
R	320	ASN	ARG	SEE REMARK 999	UNP P10930
R	329	LYS	ASN	SEE REMARK 999	UNP P10930
R	331	VAL	ILE	SEE REMARK 999	UNP P10930
R	386	SER	ASN	SEE REMARK 999	UNP P10930
R	387	SER	PRO	SEE REMARK 999	UNP P10930



3 Residue-property plots (i)

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.

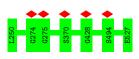
• Molecule 1: Short tail fiber protein





• Molecule 1: Short tail fiber protein	
Chain F:	100%
L250 C2714 C2775 C2775 <t< td=""><td></td></t<>	
• Molecule 1: Short tail fiber protein	
Chain G:	100%
L250 G274 G428 D455 E527	
• Molecule 1: Short tail fiber protein	
Chain H:	100%
1250 7422 1492 1492 1493 1493 1493 1493 1494 1493 1494	
• Molecule 1: Short tail fiber protein	
Chain I:	100%
L250 C274 C275 G275 G275 <	
• Molecule 1: Short tail fiber protein	
Chain J:	100%
L250 2370 8370 6428 €428	
• Molecule 1: Short tail fiber protein	
Chain K:	100%
1250 7421 7492 5494 5494 5527	
• Molecule 1: Short tail fiber protein	
Chain L:	100%





• Molecule 1: Short tail fiber protein

Chain M:	100%
1250 12750 127555 12755 12755 12755 12755 127555 12755 12755 12755 12755 1275	
• Molecule 1: Short tail fiber protein	
Chain N:	100%
L250 G421 P402 E403 E403 E403 E403 E403 E403	
• Molecule 1: Short tail fiber protein	
Chain O:	100%
L250 C274 C275 C275 S370 S428 C428 E527	
• Molecule 1: Short tail fiber protein	
Chain P:	100%
L250 C27 C370 C428 D455 E527	
• Molecule 1: Short tail fiber protein	
Chain Q:	100%
1250 6421 6428 8494 8494 8527	
• Molecule 1: Short tail fiber protein	
Chain R:	100%
L250 G27 4 S370 G228 S370 €282 E527	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	945	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF correction of individual particles with Wiener filtering	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	10.345	Depositor
Minimum map value	-7.648	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.45	Depositor
Map size (Å)	583.8291, 583.8291, 583.8291	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles ($^{\circ}$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.97872, 2.97872, 2.97872	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	278	0	0	0	0
1	В	278	0	0	0	0
1	С	278	0	0	0	0
1	D	278	0	0	0	0
1	Е	278	0	0	0	0
1	F	278	0	0	0	0
1	G	278	0	0	0	0
1	Н	278	0	0	0	0
1	Ι	278	0	0	0	0
1	J	278	0	0	0	0
1	Κ	278	0	0	0	0
1	L	278	0	0	0	0
1	М	278	0	0	0	0
1	Ν	278	0	0	0	0
1	0	278	0	0	0	0
1	Р	278	0	0	0	0
1	Q	278	0	0	0	0
1	R	278	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5004	0	0	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

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.



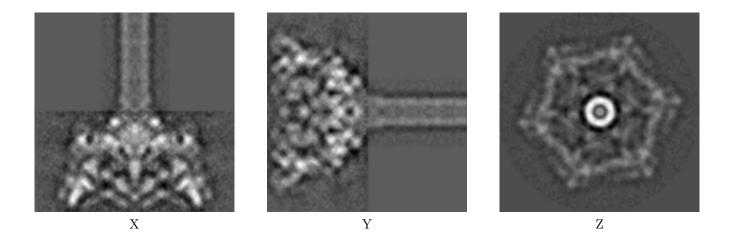
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1048. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

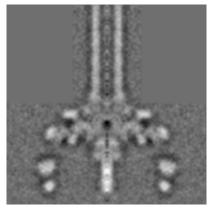
6.1.1 Primary map



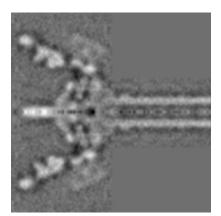
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

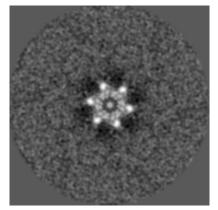
6.2.1 Primary map



X Index: 98



Y Index: 98



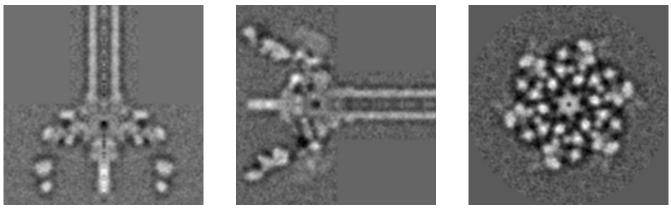
Z Index: 98



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: 98

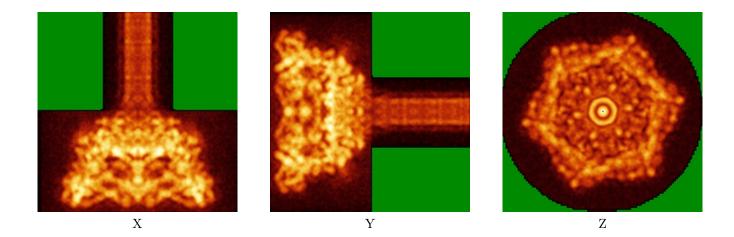
Y Index: 100

Z Index: 60

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

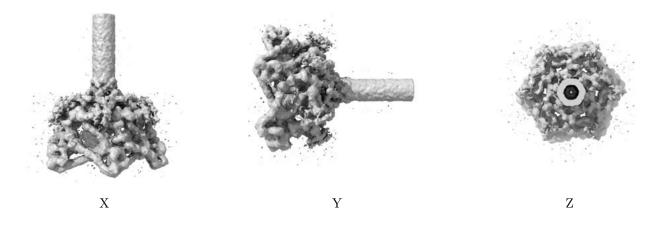


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 1.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

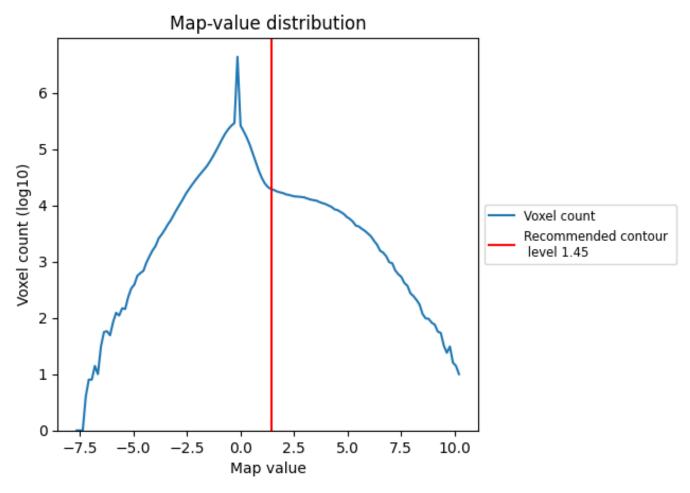
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

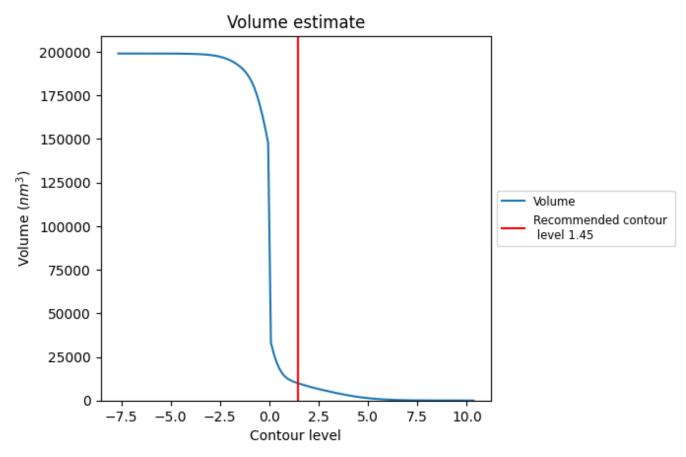
7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)

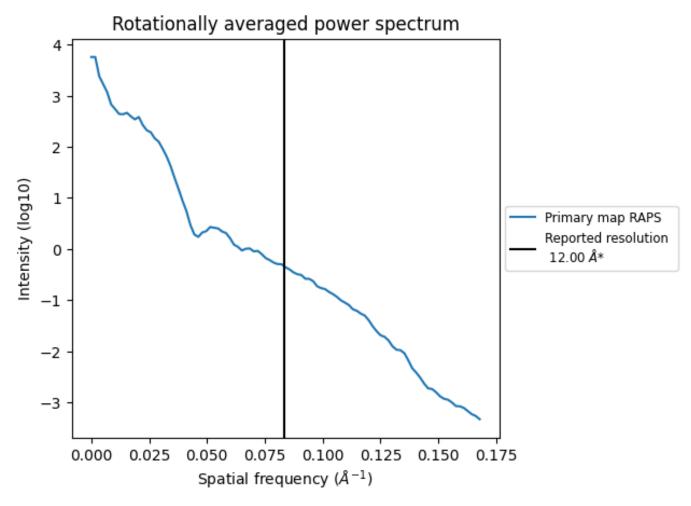


The volume at the recommended contour level is $9896~{\rm nm^3};$ this corresponds to an approximate mass of $8939~{\rm kDa}.$

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)



*Reported resolution corresponds to spatial frequency of 0.083 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

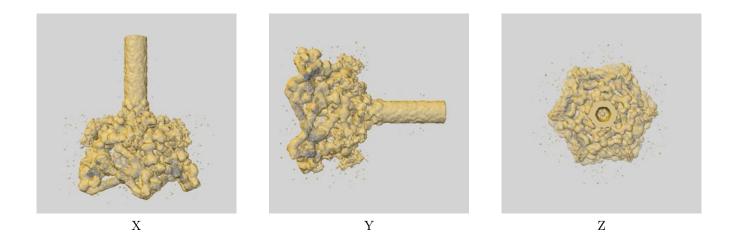
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1048 and PDB model 1PDI. Per-residue inclusion information can be found in section 3 on page 11.

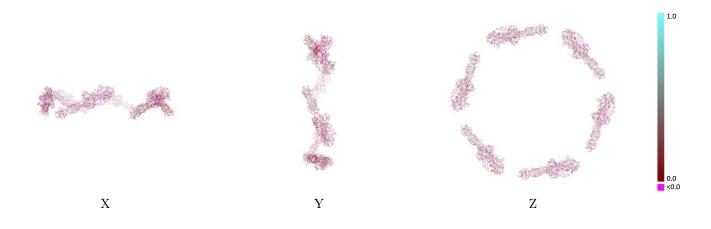
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 1.45 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.

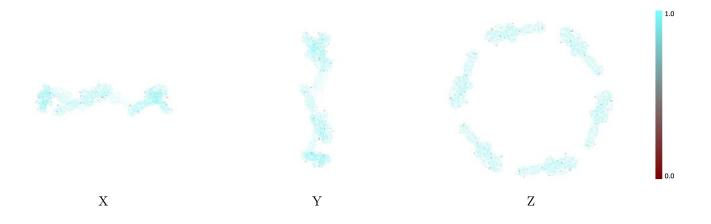


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

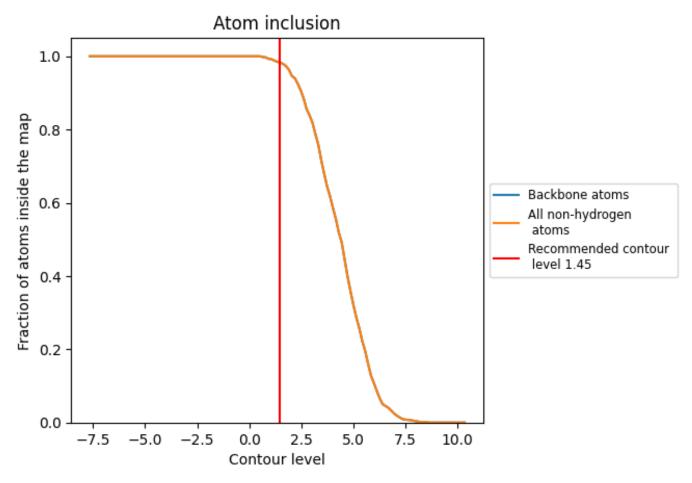
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.45).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9830	0.0670
А	0.9820	0.0840
В	0.9820	0.0630
С	0.9820	0.0590
D	0.9860	0.0750
Е	0.9820	0.0630
F	0.9820	0.0540
G	0.9860	0.0660
Н	0.9820	0.0700
Ι	0.9820	0.0570
J	0.9820	0.0620
K	0.9820	0.0800
L	0.9820	0.0560
М	0.9860	0.0720
Ν	0.9820	0.0800
О	0.9820	0.0520
Р	0.9860	0.0840
Q	0.9820	0.0690
R	0.9820	0.0560

