

Full wwPDB EM Validation Report (i)

Jun 28, 2023 – 12:28 pm BST

PDB ID : 7ZN2

EMDB ID : EMD-14799

Title: Tail tip of siphophage T5: full complex after interaction with its bacterial

receptor FhuA

Authors: Linares, R.; Arnaud, C.A.; Effantin, G.; Darnault, C.; Epalle, N.; Boeri Erba,

E.; Schoehn, G.; Breyton, C.

Deposited on : 2022-04-20

Resolution : 4.29 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 (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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ: 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

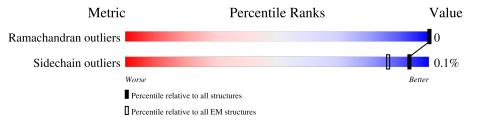
Validation Pipeline (wwPDB-VP) : 2.33

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 4.29 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
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 <=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	b	949	100%	
1	С	949	100%	
1	d	949	17%	
2	h	1219	• 96%	
2	i	1219	• 96%	
2	j	1219	• 96%	
3	e	688	98%	•
3	f	688	48% 97%	
3	g	688	50% 85%	14%

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Mol	Chain	$oxed{f Length}$	Quality of chain
			<u></u>
4	J	140	99%
4	K	140	99%
			8%
4	L	140	100%
4	M	140	100%
4	N	140	99%
			8%
4	О	140	99%
4	Р	140	100%
4	0		6%
4	Q	140	100% 7%
4	R	140	99%
4	S	140	99%
			9%
4	Т	140	100%
4	U	140	100%
	C	200	•
5	G	298	100%
5	Н	298	100%
5	I	298	100%
6	V	204	100%
6	W	204	100%
6	X	204	1000
0	Λ	204	100%
6	Y	204	100%
6	Z	204	100%
6	a	204	17%
7	A	464	100%
7	В	464	12%
1		404	100%
7	С	464	100%
7	D	464	100%
<u> </u>		101	Ctidt

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Mol	Chain	Length	Quality of chain
7	E	464	100%
7	F	464	100%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 89393 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 Probable baseplate hub protein.

Mol	Chain	Residues		A		AltConf	Trace		
1	d	949	Total	С	N	О	S	0	0
1	u	949	7576	4811	1274	1481	10	0	
1		949	Total	С	N	О	S	0	0
1	С	949	7576	4811	1274	1481	10	0	
1	h	949	Total	С	N	О	S	0	0
1	ט	343	7576	4811	1274	1481	10		

• Molecule 2 is a protein called Pore-forming tail tip protein pb2.

Mol	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$		AltConf	Trace	
2	j	43	Total 328	C 200		O 67	S 1	0	0
2	h	43	Total 328	C 200		O 67	S 1	0	0
2	i	43	Total 328	C 200	N 60	O 67	S 1	0	0

• Molecule 3 is a protein called Straight fiber protein pb4.

Mol	Chain	Residues		At		AltConf	Trace		
3	f	669	Total	С	N	О	S	0	0
)	1	009	5143	3274	854	1000	15	U	0
3	0	671	Total	С	N	О	S	0	0
)	е	071	5163	3285	859	1004	15	0	
3	ď	589	Total	С	N	О	S	0	0
0	g	969	4546	2897	758	877	14	U	U

• Molecule 4 is a protein called L-shaped tail fiber protein p132.

Mol	Chain	Residues		At	oms	AltConf	Trace		
1	B	139	Total	С	N	О	S	0	0
4	11	159	1048	653	175	217	3	0	U

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Mol	Chain	Residues		At	oms			AltConf	Trace
4	Q	140	Total	С	N	О	S	0	0
4	Q	140	1056	658	176	218	4	U	U
4	S	139	Total	С	N	О	S	0	0
4	b	139	1048	653	175	217	3	0	U
4	N	139	Total	С	N	О	S	0	0
4	11	139	1048	653	175	217	3	0	0
4	M	140	Total	С	N	О	S	0	0
4	IVI	140	1056	658	176	218	4	0	
4	О	139	Total	С	N	О	S	0	0
4		139	1048	653	175	217	3	U	U
4	J	139	Total	С	N	О	S	0	0
4	J	109	1048	653	175	217	3	U	U
4	L	140	Total	С	N	Ο	S	0	0
4	П	140	1056	658	176	218	4	0	U
4	U	140	Total	С	N	О	S	0	0
4	U	140	1056	658	176	218	4	0	
4	K	139	Total	С	N	О	S	0	0
4	11	109	1048	653	175	217	3	0	
4	Р	140	Total	С	N	О	S	0	0
4	1	140	1056	658	176	218	4	U	U
4	Т	140	Total	С	N	О	S	0	0
4	1	140	1056	658	176	218	4		U

• Molecule 5 is a protein called Minor tail protein.

Mol	Chain	Residues		At		AltConf	Trace		
5	Ţ	298	Total	С	N	О	S	0	0
	1	290	2423	1551	398	464	10	U	0
5	Н	298	Total	С	N	Ο	S	0	0
9	11	290	2423	1551	398	464	10	0	0
5	G	298	Total	С	N	О	S	0	0
	G	290	2423	1551	398	464	10	U	U

• Molecule 6 is a protein called Distal tail protein.

Mol	Chain	Residues		Ato		AltConf	Trace		
6	a	204	Total	С	N	О	S	0	0
	а	204	1610	1030	264	313	3	U	U
6	X	204	Total	С	N	О	S	0	0
	Λ	204	1610	1030	264	313	3	0	U
6	V	204	Total	С	N	О	S	0	0
	1	204	1610	1030	264	313	3	U	U

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Mol	Chain	Residues		Ato		AltConf	Trace		
6	W	204	Total	С	N	О	S	0	0
0	VV	204	1610	1030	264	313	3	0	U
6	V	204	Total	С	N	О	S	0	0
0	V	204	1610	1030	264	313	3	0	U
6	7	204	Total	С	N	О	S	0	0
0	L	204	1610	1030	264	313	3	0	U

• Molecule 7 is a protein called Tail tube protein.

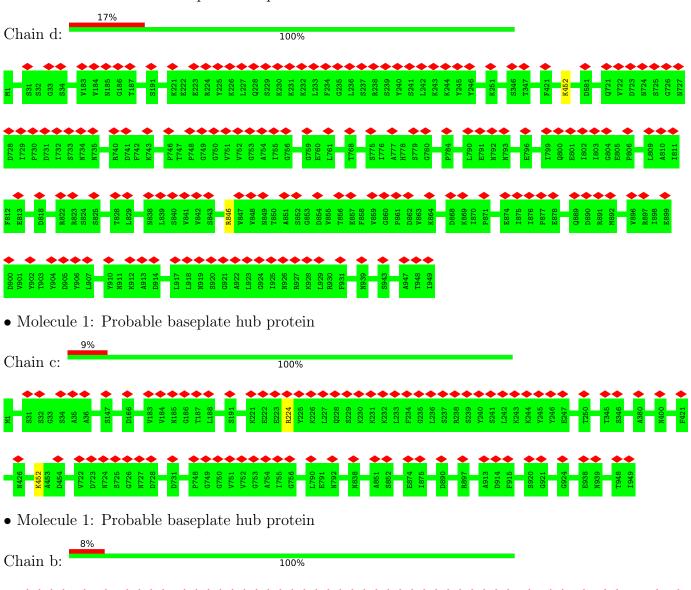
Mol	Chain	Residues		At	oms			AltConf	Trace
7	F	464	Total	С	N	О	S	0	0
'	I'	404	3546	2217	597	722	10	0	0
7	Е	464	Total	С	N	О	S	0	0
'	<u> 1</u> 2	404	3546	2217	597	722	10	0	0
7	С	464	Total	С	N	О	S	0	0
'		404	3546	2217	597	722	10	0	U
7	D	464	Total	С	N	О	S	0	0
'	ט	404	3546	2217	597	722	10	0	U
7	A	464	Total	С	N	О	S	0	0
'	A	404	3546	2217	597	722	10	0	U
7	В	464	Total	С	N	О	S	0	0
	D	404	3546	2217	597	722	10	0	U



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: Probable baseplate hub protein



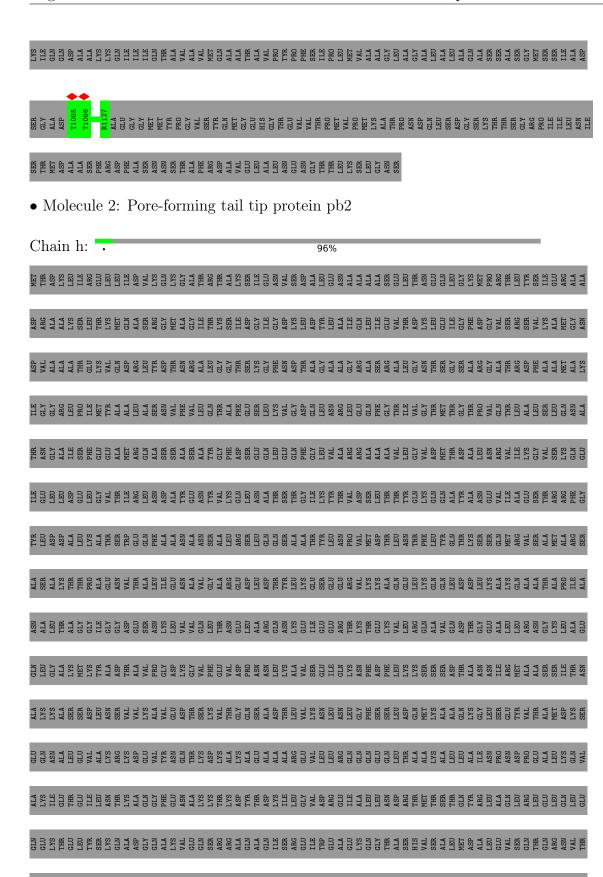




 \bullet Molecule 2: Pore-forming tail tip protein pb2

Chain j: • 96%
MET ASP ILE ASP ILE ASP ILE ASP ALA ALA ALA ALA ALA ALA ALA
ASP ARA ALA ALA ALA ALA ALA ALA ALA ALA ALA
ASP ALA ALA ALA ALA ALA ALA ASP ASP ASP ASP ASP ASP ASP ALA ALA ALA ALA ALA ALA ALA AL
11.6 0.17 0.17 0.17 0.17 0.17 0.17 0.17 0.17
THR ASN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
11.E 0.1.U 1.E.U 1
7.R ASP ASP ASP ALA ALA ALA ALA ALA ALA ALA AL
ALA SER ALA LYS LYS THR PRO ALA ALA ALA ALA ALA ALA ALA A
ASN ALA ALA ALA ALA ALA ALA ALA ASP GLU
GLN GLY ALA ALA ALA ALA ALA ALA ALA
ALA LYS ALA SER ASR SER ASR VAL VAL VAL LYS GLN VAL LYS GLN VAL GLN GLN GLN GLN GLN GLN GLN G
GLU GLU GLU GLU GLU GLU GLU GLU
ALA LIYS LILE GLU THR GLU THR GLU GLU GLU ALA ASN ALA ASN ALA ASN ALA ASN ASN
GLN GLU GLU GLU GLU GLU GLU GLU
GLV GLN GLN GLN GLN GLN GLN GLN
GLY THR
GLY SER SER MET HER







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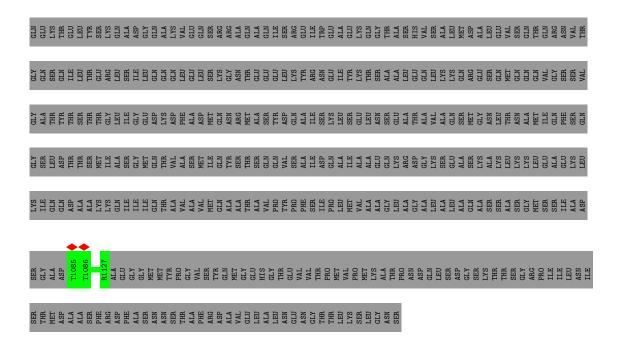




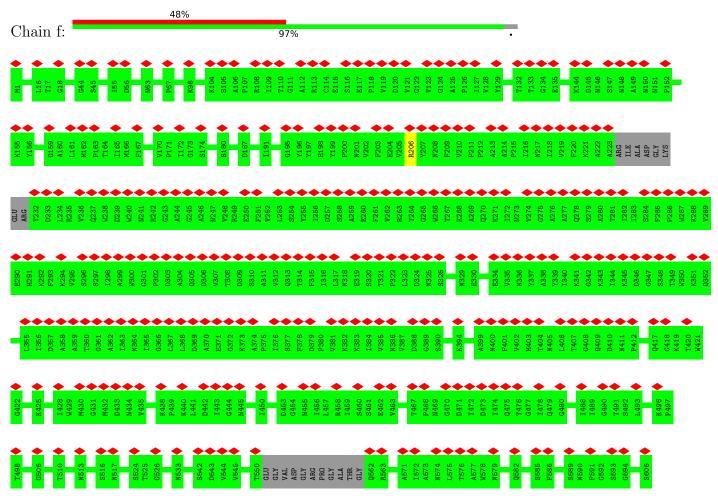
• Molecule 2: Pore-forming tail tip protein pb2

Chain i: MARCHARA MAR COUNTY OF THE PROPERTY OF THE





• Molecule 3: Straight fiber protein pb4



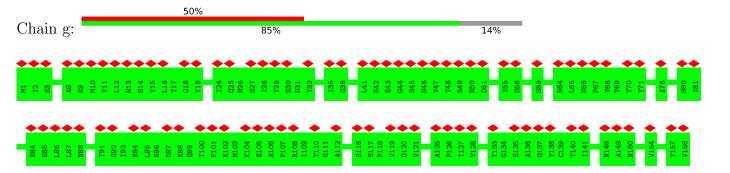




• Molecule 3: Straight fiber protein pb4



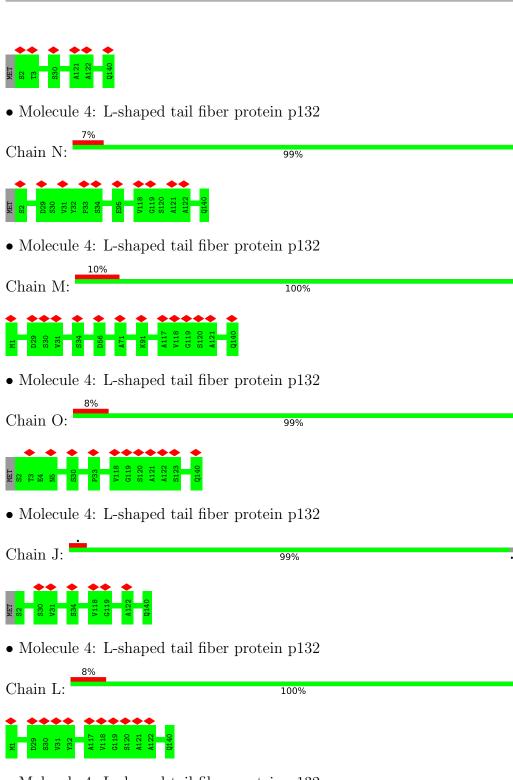
• Molecule 3: Straight fiber protein pb4











• Molecule 4: L-shaped tail fiber protein p132

Chain U: 100%



• Molecule 4: L-shaped tail fiber protein p132



5%	
Chain K: 99%	
MET	
• Molecule 4: L-shaped tail fiber protein p132	
Chain P: 100%	
830 V31 V118 G119 S120 A121 A122 Q140	
• Molecule 4: L-shaped tail fiber protein p132	
Chain T: 100%	
W1 V32 V32 V334 V32 V334 V318 V318 V318 V318 V318 V318 V318 V318	
• Molecule 5: Minor tail protein	
Chain I: 100%	_
There are no outlier residues recorded for this chain.	
• Molecule 5: Minor tail protein	
Chain H: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 5: Minor tail protein	
<u>.</u>	
Chain G: 100%	
M1	
• Molecule 6: Distal tail protein	
Chain a: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 6: Distal tail protein	
Chain X:	





• Molecule 6: Distal tail protein

Chain Y:

100%

There are no outlier residues recorded for this chain.

• Molecule 6: Distal tail protein

Chain W:

100%

There are no outlier residues recorded for this chain.

• Molecule 6: Distal tail protein

Chain V:

100%

There are no outlier residues recorded for this chain.

• Molecule 6: Distal tail protein

Chain Z:

100%

There are no outlier residues recorded for this chain.

• Molecule 7: Tail tube protein

Chain F:

100%



• Molecule 7: Tail tube protein

Chain E:

100%



• Molecule 7: Tail tube protein

149

Chain C:

100%









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0214	Depositor
Map size (Å)	459.34, 459.34, 459.34	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.351, 1.351, 1.351	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).

Mal	Mol Chain		Bond lengths		Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	b	0.27	0/7740	0.49	0/10500		
1	С	0.27	0/7740	0.49	0/10500		
1	d	0.27	0/7740	0.49	0/10500		
2	h	0.26	0/331	0.54	0/444		
2	i	0.25	0/331	0.54	0/444		
2	j	0.26	0/331	0.53	0/444		
3	е	0.26	0/5285	0.47	0/7208		
3	f	0.26	0/5265	0.47	0/7182		
3	g	0.26	0/4650	0.48	0/6332		
4	J	0.26	0/1062	0.54	0/1443		
4	K	0.26	0/1062	0.54	0/1443		
4	L	0.30	0/1070	0.55	0/1453		
4	M	0.26	0/1070	0.54	0/1453		
4	N	0.26	0/1062	0.54	0/1443		
4	О	0.27	0/1062	0.54	0/1443		
4	Р	0.30	0/1070	0.55	0/1453		
4	Q	0.26	0/1070	0.54	0/1453		
4	R	0.26	0/1062	0.54	0/1443		
4	S	0.26	0/1062	0.54	0/1443		
4	Т	0.30	0/1070	0.55	0/1453		
4	U	0.26	0/1070	0.53	0/1453		
5	G	0.28	0/2483	0.50	0/3370		
5	Н	0.28	0/2483	0.50	0/3370		
5	I	0.28	0/2483	0.50	0/3370		
6	V	0.28	0/1649	0.48	0/2239		
6	W	0.27	0/1649	0.47	0/2239		
6	X	0.28	0/1649	0.48	0/2239		
6	Y	0.27	0/1649	0.47	0/2239		
6	Z	0.28	0/1649	0.48	0/2239		
6	a	0.27	0/1649	0.47	0/2239		
7	A	0.27	0/3604	0.50	0/4904		
7	В	0.26	0/3604	0.50	0/4904		
7	С	0.26	0/3604	0.50	0/4904		
7	D	0.26	0/3604	0.50	0/4904		



Mol	Chain	Bond lengths		Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
7	Е	0.26	0/3604	0.50	0/4904	
7	F	0.26	0/3604	0.50	0/4904	
All	All	0.27	0/91172	0.50	0/123898	

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	b	947/949~(100%)	903 (95%)	44 (5%)	0	100 100
1	c	947/949~(100%)	918 (97%)	29 (3%)	0	100 100
1	d	$947/949\ (100\%)$	898 (95%)	49 (5%)	0	100 100
2	h	41/1219~(3%)	41 (100%)	0	0	100 100
2	i	41/1219~(3%)	40 (98%)	1 (2%)	0	100 100
2	j	$41/1219 \ (3\%)$	41 (100%)	0	0	100 100
3	e	$665/688\ (97\%)$	636 (96%)	29 (4%)	0	100 100
3	f	663/688~(96%)	648 (98%)	15 (2%)	0	100 100
3	g	583/688~(85%)	568 (97%)	15 (3%)	0	100 100
4	J	$137/140\ (98\%)$	133 (97%)	4 (3%)	0	100 100
4	K	$137/140\ (98\%)$	133 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
4	L	138/140~(99%)	133 (96%)	5 (4%)	0	100	100
4	M	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
4	N	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	О	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	Р	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
4	Q	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
4	R	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	S	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
4	Т	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
4	U	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
5	G	296/298 (99%)	286 (97%)	10 (3%)	0	100	100
5	Н	296/298 (99%)	286 (97%)	10 (3%)	0	100	100
5	I	296/298 (99%)	287 (97%)	9 (3%)	0	100	100
6	V	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
6	W	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
6	X	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
6	Y	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
6	Z	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
6	a	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
7	A	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
7	В	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
7	С	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
7	D	462/464 (100%)	446 (96%)	16 (4%)	0	100	100
7	Е	462/464 (100%)	444 (96%)	18 (4%)	0	100	100
7	F	462/464 (100%)	446 (96%)	16 (4%)	0	100	100
All	All	11397/15150 (75%)	10997 (96%)	400 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	Perce	ntiles
1	b	834/834 (100%)	832 (100%)	2 (0%)	93	96
1	c	834/834 (100%)	832 (100%)	2 (0%)	93	96
1	d	834/834 (100%)	832 (100%)	2 (0%)	93	96
2	h	36/980 (4%)	36 (100%)	0	100	100
2	i	36/980 (4%)	36 (100%)	0	100	100
2	j	36/980~(4%)	36 (100%)	0	100	100
3	е	562/572~(98%)	562 (100%)	0	100	100
3	f	560/572~(98%)	559 (100%)	1 (0%)	93	96
3	g	490/572~(86%)	489 (100%)	1 (0%)	93	96
4	J	118/119 (99%)	118 (100%)	0	100	100
4	K	118/119 (99%)	118 (100%)	0	100	100
4	L	$119/119\ (100\%)$	119 (100%)	0	100	100
4	M	119/119 (100%)	119 (100%)	0	100	100
4	N	118/119 (99%)	118 (100%)	0	100	100
4	О	118/119 (99%)	118 (100%)	0	100	100
4	Р	$119/119\ (100\%)$	119 (100%)	0	100	100
4	Q	$119/119\ (100\%)$	119 (100%)	0	100	100
4	R	$118/119\ (99\%)$	118 (100%)	0	100	100
4	S	$118/119\ (99\%)$	118 (100%)	0	100	100
4	Т	$119/119\ (100\%)$	119 (100%)	0	100	100
4	U	119/119 (100%)	119 (100%)	0	100	100
5	G	273/273 (100%)	273 (100%)	0	100	100
5	Н	273/273 (100%)	273 (100%)	0	100	100
5	I	273/273 (100%)	273 (100%)	0	100	100
6	V	181/181 (100%)	181 (100%)	0	100	100
6	W	181/181 (100%)	181 (100%)	0	100	100
6	X	181/181 (100%)	181 (100%)	0	100	100
6	Y	181/181 (100%)	181 (100%)	0	100	100
6	Z	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
6	a	181/181 (100%)	181 (100%)	0	100	100
7	A	394/394 (100%)	394 (100%)	0	100	100
7	В	394/394 (100%)	394 (100%)	0	100	100
7	C	394/394 (100%)	394 (100%)	0	100	100
7	D	$394/394\ (100\%)$	394 (100%)	0	100	100
7	E	394/394 (100%)	394 (100%)	0	100	100
7	F	394/394 (100%)	394 (100%)	0	100	100
All	All	9913/12855 (77%)	9905 (100%)	8 (0%)	93	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	d	452	LYS
1	d	846	ARG
1	c	224	ARG
1	С	452	LYS
3	f	206	ARG
3	g	206	ARG
1	b	452	LYS
1	b	846	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	911	ASN
3	f	386	ASN
3	g	13	ASN
3	g	25	GLN
7	F	31	GLN
5	Н	216	ASN
7	С	151	GLN
7	A	151	GLN
7	В	151	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-14799. These allow visual inspection of the internal detail of the map and identification of artifacts.

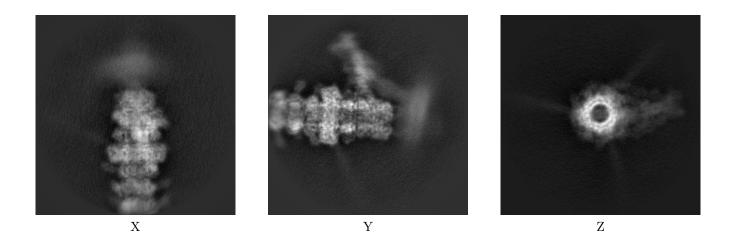
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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.

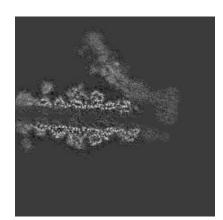


6.2 Central slices (i)

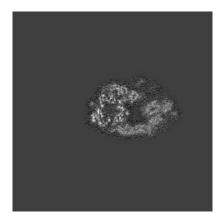
6.2.1 Primary map







Y Index: 170

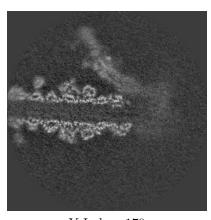


Z Index: 170

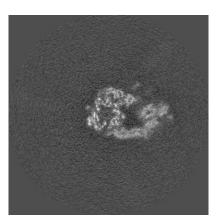
6.2.2 Raw map



X Index: 170



Y Index: 170



Z Index: 170

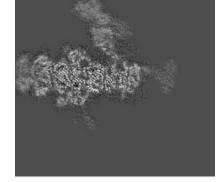
The images above show central slices of the map in three orthogonal directions.

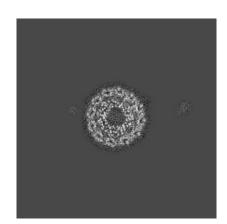


6.3 Largest variance slices (i)

6.3.1 Primary map





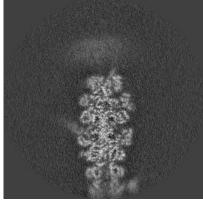


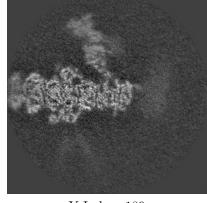
X Index: 186

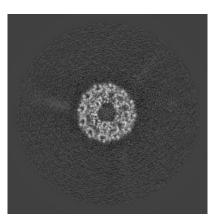
Y Index: 189

Z Index: 99

6.3.2 Raw map







X Index: 186

Y Index: 189

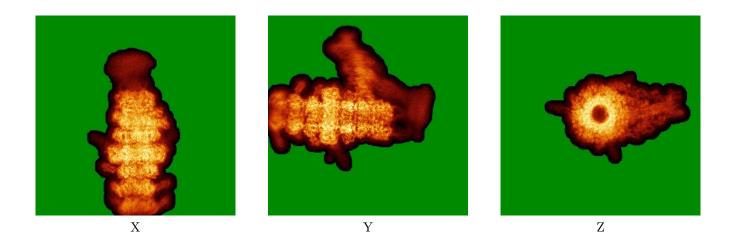
Z Index: 97

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

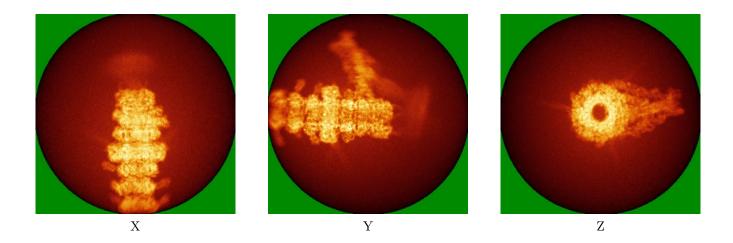


6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map

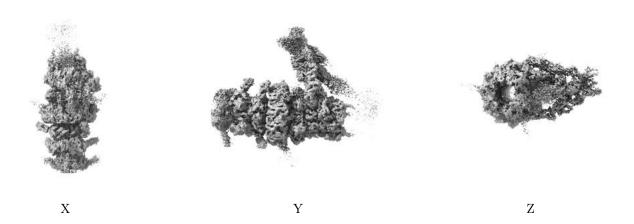


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



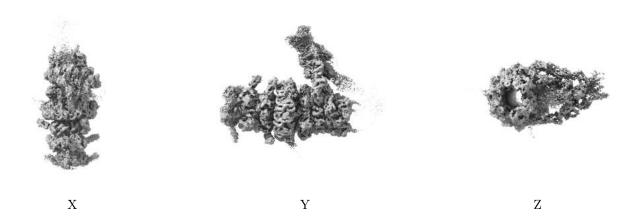
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0214. 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)

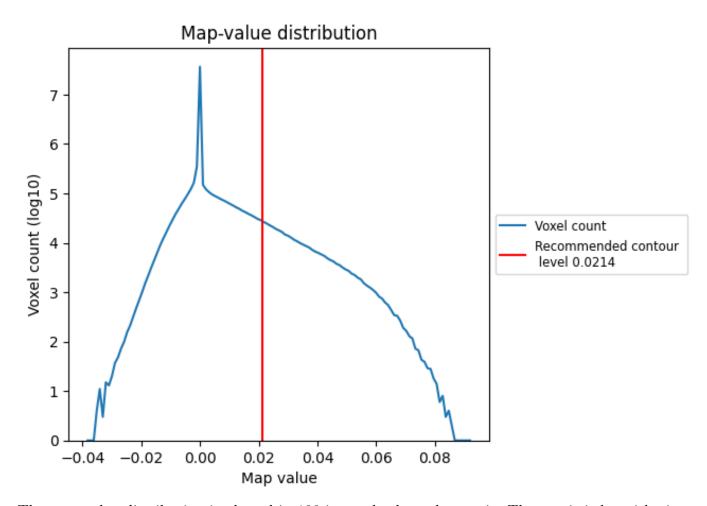
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

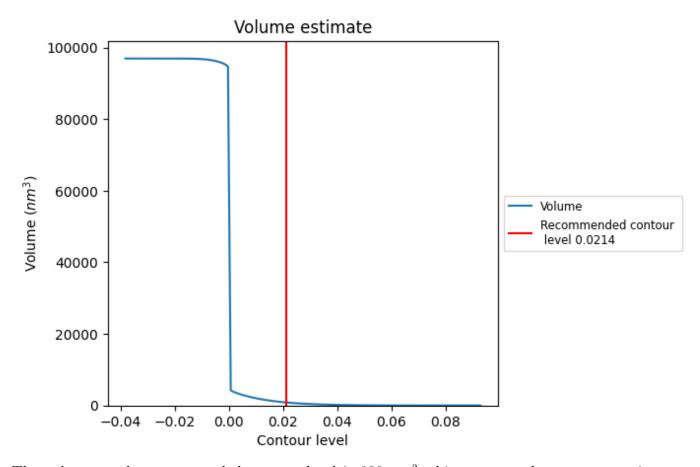
7.1 Map-value distribution (i)



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)

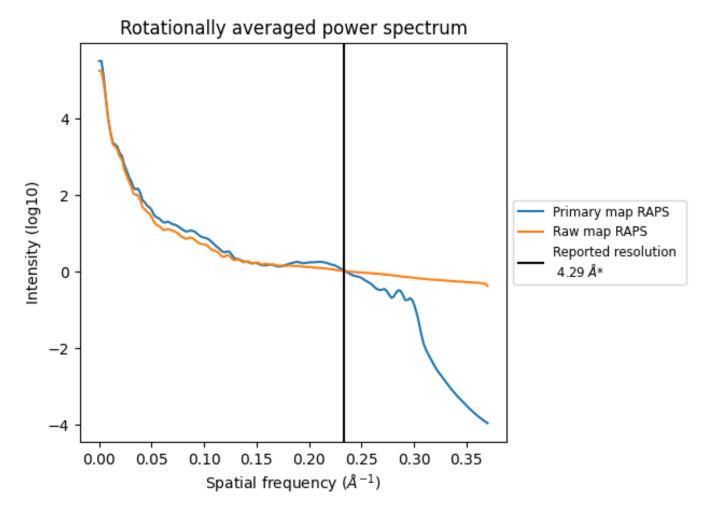


The volume at the recommended contour level is $830~\mathrm{nm^3}$; this corresponds to an approximate mass of $750~\mathrm{kDa}$.

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)



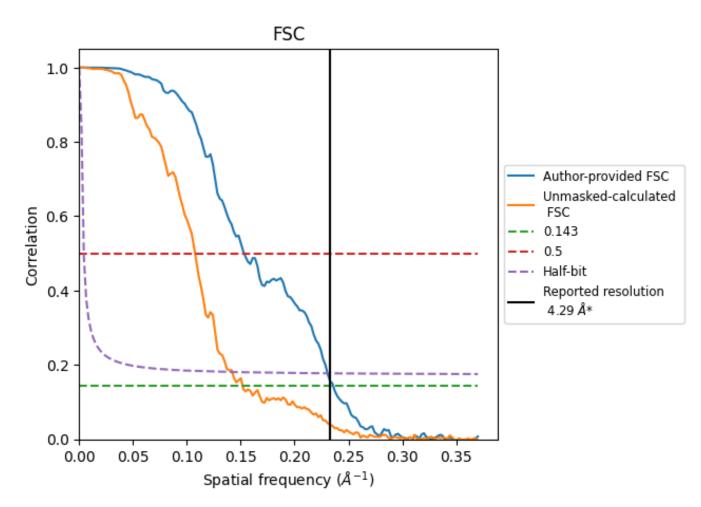
^{*}Reported resolution corresponds to spatial frequency of 0.233 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 $\rm \mathring{A}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	4.29	-	-
Author-provided FSC curve	4.24	6.53	4.34
Unmasked-calculated*	6.59	9.30	7.04

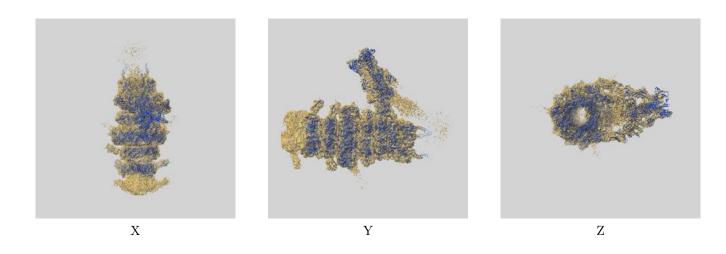
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.59 differs from the reported value 4.29 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14799 and PDB model 7ZN2. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)

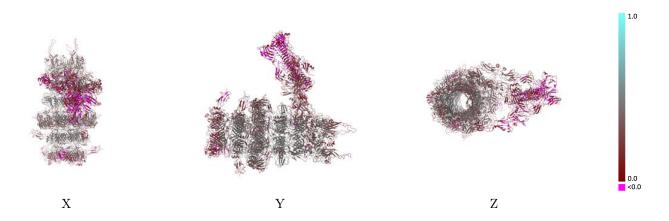


The images above show the 3D surface view of the map at the recommended contour level 0.0214 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



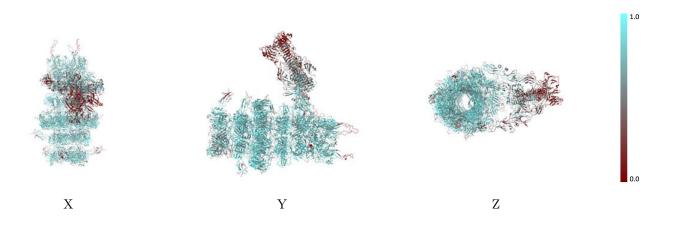
EMD-14799, 7ZN2

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.

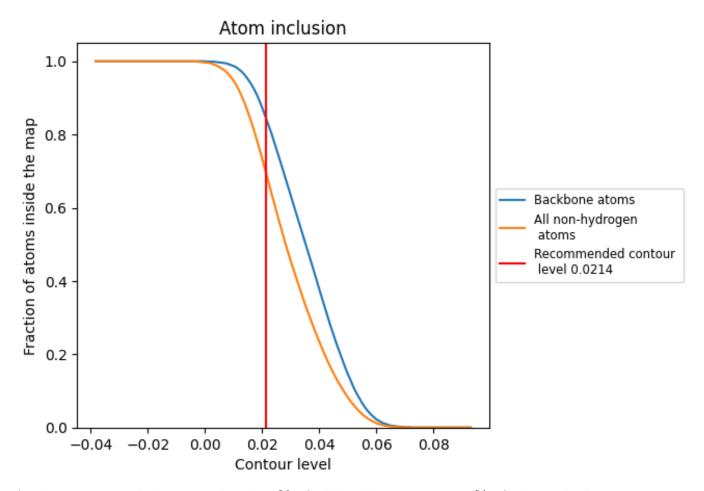
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0214).



9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0214) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.3200
A	0.6820	0.2530
В	0.6860	0.2560
С	0.6750	0.2500
D	0.7840	0.3770
E	0.7730	0.3780
F	0.7840	0.3810
G	0.8300	0.4530
Н	0.8350	0.4410
I	0.8350	0.4490
J	0.7690	0.3530
K	0.7490	0.3230
L	0.7280	0.3410
M	0.7480	0.3490
N	0.7560	0.3210
О	0.7480	0.3280
Р	0.7500	0.3500
Q	0.7700	0.3660
R	0.7640	0.3370
S	0.7720	0.3530
T	0.7520	0.3560
U	0.7780	0.3700
V	0.8250	0.4360
W	0.8300	0.4350
X	0.8290	0.4220
Y	0.8430	0.4390
Z	0.8580	0.4340
a	0.8640	0.4430
b	0.7250	0.3550
С	0.7280	0.3500
d	0.6870	0.3150
e	0.4020	0.1680
f	0.4090	0.1340
g	0.3460	0.1050
h	0.7280	0.3450



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Chain	Atom inclusion	Q-score
i	0.6690	0.3230
j	0.7590	0.3630

