



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 02:59 AM JST

PDB ID : 6AHU
EMDB ID : EMD-9627
Title : Cryo-EM structure of human Ribonuclease P with mature tRNA
Authors : Wu, J.; Niu, S.; Tan, M.; Lan, P.; Lei, M.
Deposited on : 2018-08-20
Resolution : 3.66 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

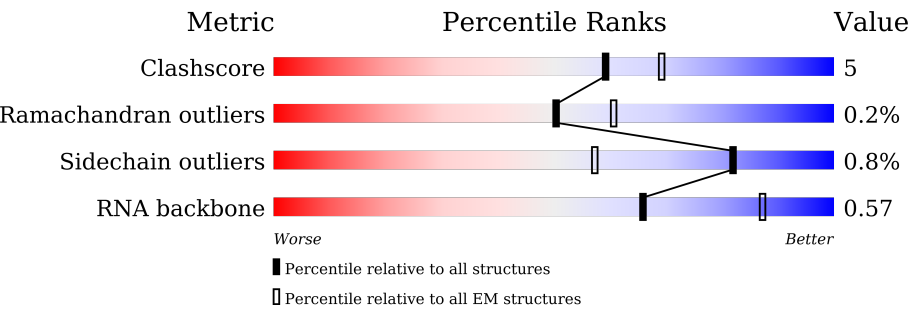
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.66 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.





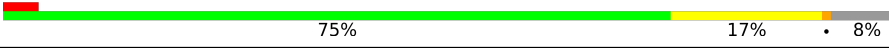



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	<div><div>65%30%.</div></div>
2	B	1024	<div><div>64%11%24%</div></div>
3	C	283	<div><div>7%57%7%36%</div></div>
4	D	220	<div><div>50%15%.34%</div></div>
5	E	163	<div><div>75%15%10%</div></div>
6	F	199	<div><div>5%57%8%35%</div></div>
7	G	140	<div><div>6%77%16%6%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	124	 77% 19% ..
9	I	268	 71% 17% 12%
9	J	268	 75% 17% • 8%
10	K	154	 6% 64% 14% 21%
11	L	363	 87% 12%
12	T	72	 11% 86% 12% •

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 29386 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 RNA chain called H1 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	341	Total	C	N	O	P	0	0
			7295	3249	1324	2381	341		

- Molecule 2 is a protein called Ribonucleases P/MRP protein subunit POP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	774	Total	C	N	O	S	0	0
			6142	3892	1121	1087	42		

- Molecule 3 is a protein called Ribonuclease P protein subunit p38.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	182	Total	C	N	O	S	0	0
			1448	918	255	270	5		

- Molecule 4 is a protein called Ribonuclease P protein subunit p29.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	145	Total	C	N	O	S	0	0
			1180	763	206	207	4		

- Molecule 5 is a protein called Ribonuclease P/MRP protein subunit POP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	147	Total	C	N	O	S	0	0
			1197	763	220	206	8		

- Molecule 6 is a protein called Ribonuclease P protein subunit p25.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	129	Total	C	N	O	S	0	0
			979	614	189	170	6		

- Molecule 7 is a protein called Ribonuclease P protein subunit p20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	131	Total	C	N	O	S	0	0
			1021	634	192	192	3		

- Molecule 8 is a protein called Ribonuclease P protein subunit p14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	121	Total	C	N	O	S	0	0
			941	611	152	173	5		

- Molecule 9 is a protein called Ribonuclease P protein subunit p30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	236	Total	C	N	O	S	0	0
			1824	1166	319	332	7		
9	J	247	Total	C	N	O	S	0	0
			1905	1221	332	345	7		

- Molecule 10 is a protein called Ribonuclease P protein subunit p21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	121	Total	C	N	O	S	0	0
			979	602	196	173	8		

- Molecule 11 is a protein called Ribonuclease P protein subunit p40.

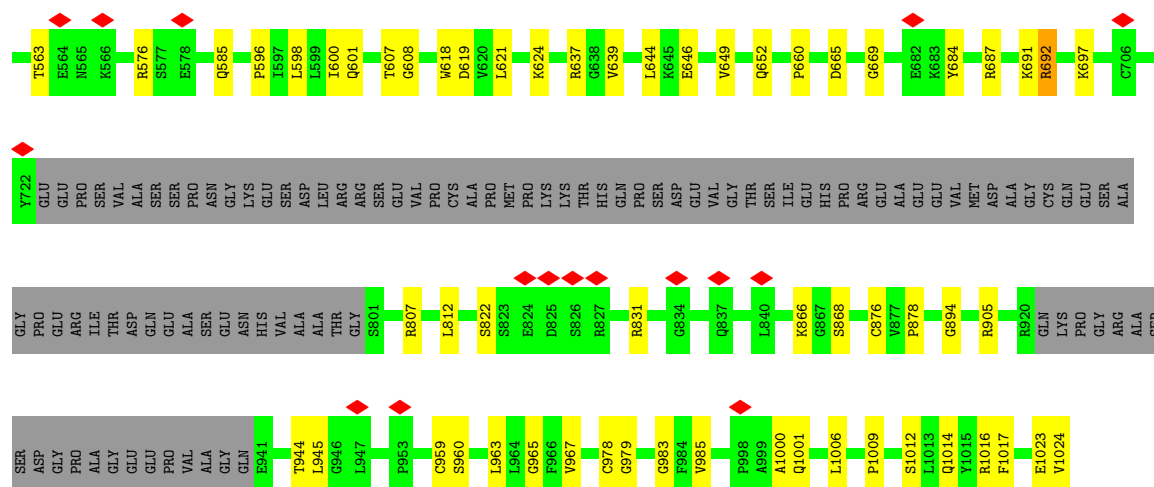
Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	362	Total	C	N	O	S	0	0
			2939	1893	489	540	17		

- Molecule 12 is a RNA chain called tRNA.

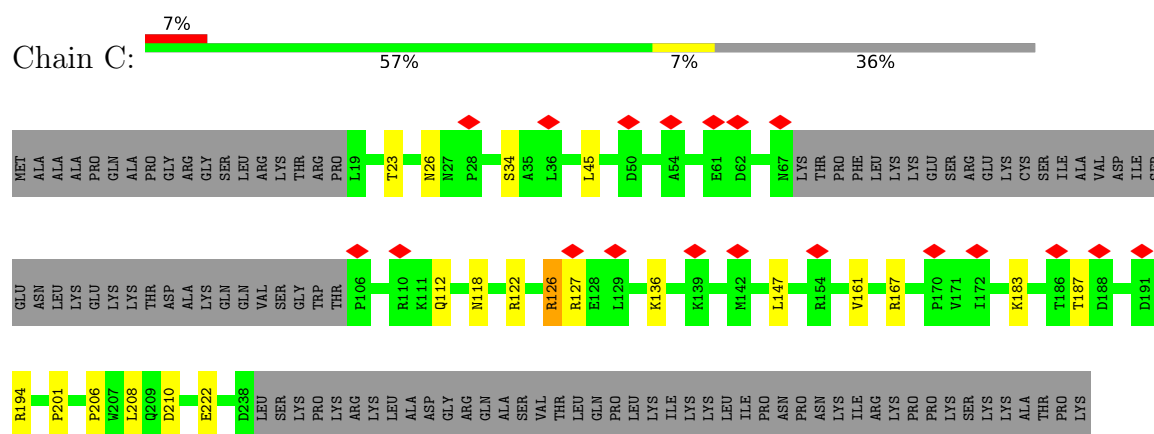
Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	72	Total	C	N	O	P	0	0
			1535	685	274	504	72		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

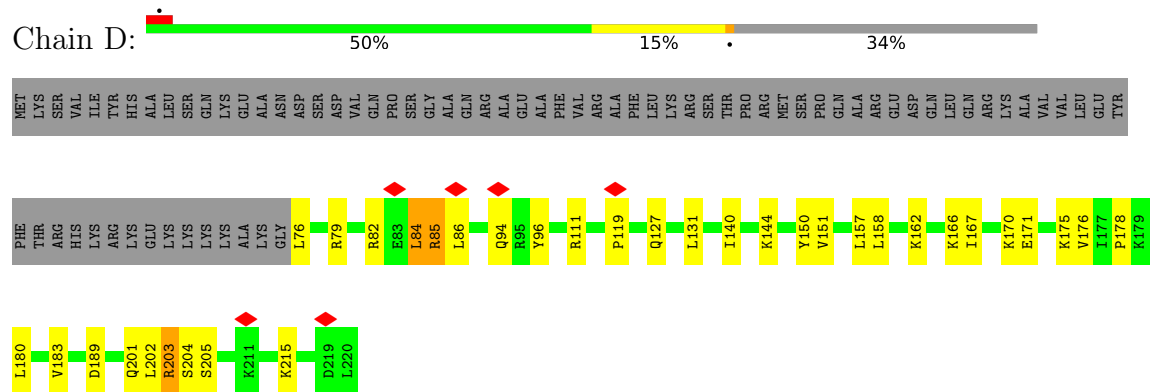
Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total	Zn	0
			1	1	



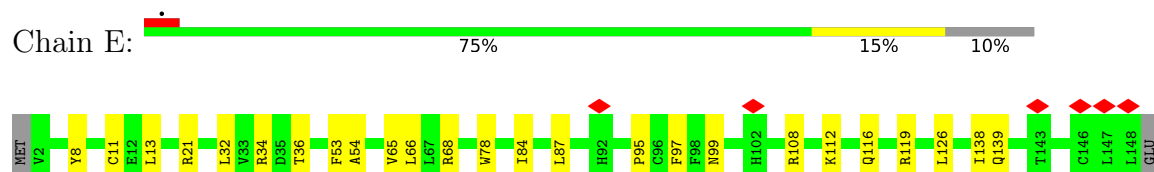
• Molecule 3: Ribonuclease P protein subunit p38



• Molecule 4: Ribonuclease P protein subunit p29

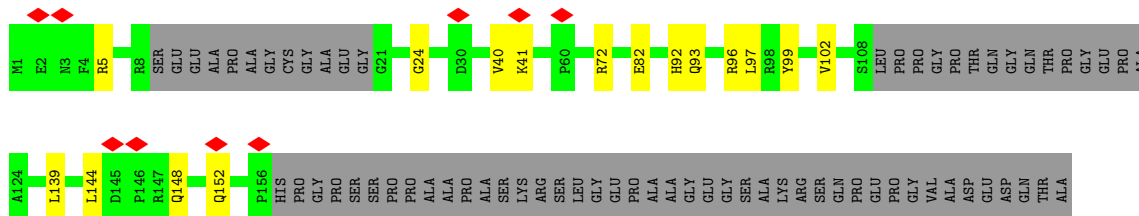


• Molecule 5: Ribonuclease P/MRP protein subunit POP5

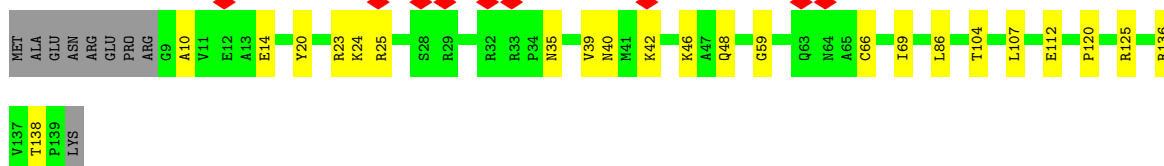
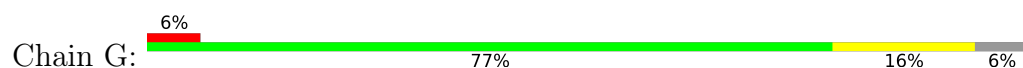


GLU
GLU
GLU
GLU
SER
GLY
GLU
GLU
ALA
ALA
GLU
MET
GLU

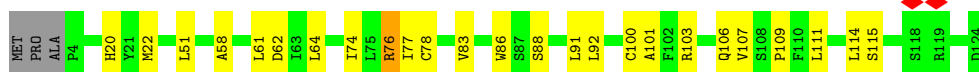
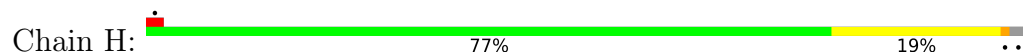
• Molecule 6: Ribonuclease P protein subunit p25



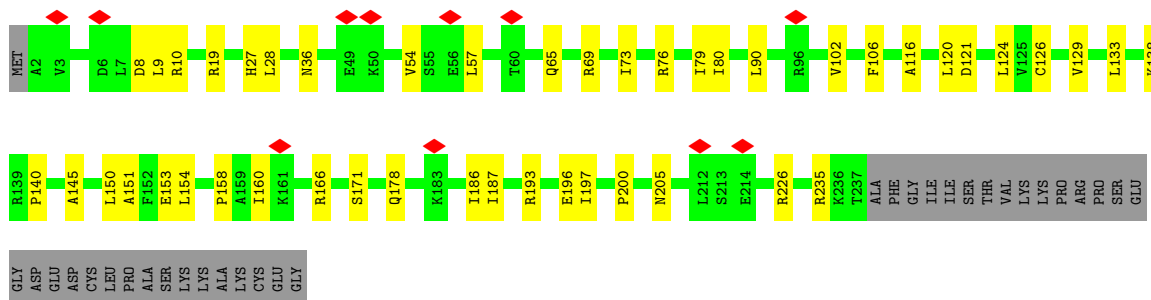
• Molecule 7: Ribonuclease P protein subunit p20



• Molecule 8: Ribonuclease P protein subunit p14

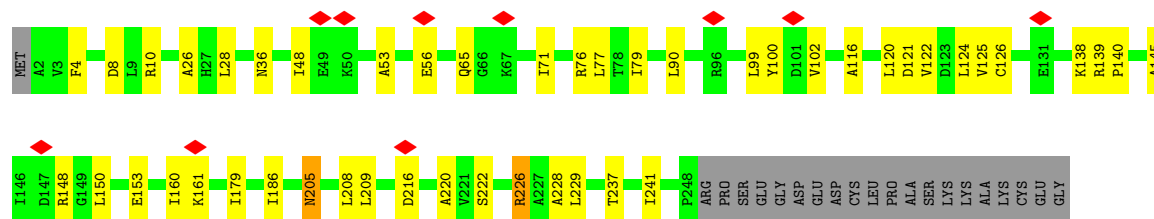


• Molecule 9: Ribonuclease P protein subunit p30

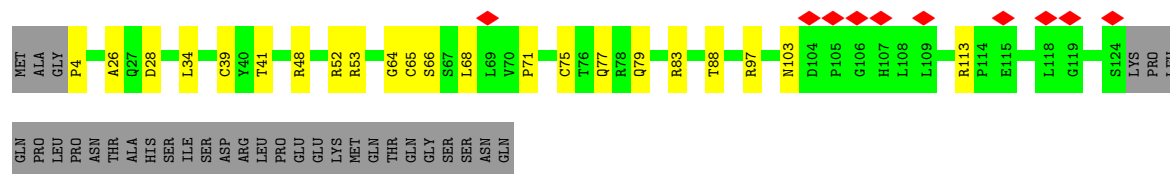


• Molecule 9: Ribonuclease P protein subunit p30

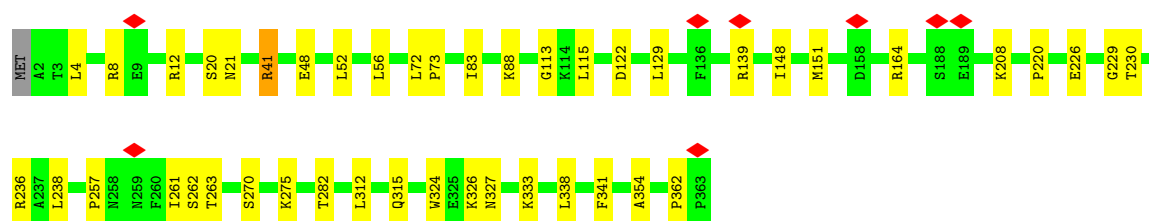
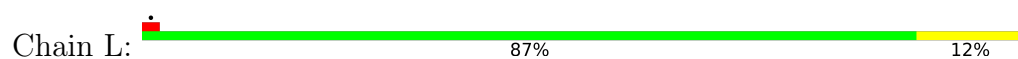




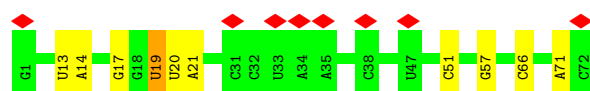
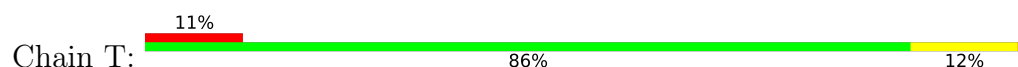
- Molecule 10: Ribonuclease P protein subunit p21



- Molecule 11: Ribonuclease P protein subunit p40



- Molecule 12: tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287700	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 ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.265	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0256	Depositor
Map size (\AA)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.17	0/8156	0.78	5/12720 (0.0%)
2	B	0.26	0/6286	0.52	0/8492
3	C	0.27	0/1468	0.51	0/1985
4	D	0.28	0/1202	0.61	0/1613
5	E	0.25	0/1220	0.49	0/1647
6	F	0.25	0/996	0.48	0/1342
7	G	0.27	0/1035	0.59	0/1402
8	H	0.26	0/958	0.61	1/1295 (0.1%)
9	I	0.26	0/1855	0.51	0/2515
9	J	0.26	0/1938	0.53	0/2627
10	K	0.25	0/997	0.53	0/1345
11	L	0.25	0/3021	0.47	0/4099
12	T	0.17	0/1715	0.76	0/2671
All	All	0.24	0/30847	0.62	6/43753 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
4	D	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	92	LEU	CA-CB-CG	7.66	132.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	A	OP1-P-O3'	5.87	118.11	105.20
1	A	126	U	P-O3'-C3'	5.71	126.55	119.70
1	A	74	G	P-O3'-C3'	5.39	126.17	119.70
1	A	326	C	P-O3'-C3'	5.15	125.88	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1000	ALA	Peptide
2	B	463	PRO	Peptide
2	B	499	ILE	Peptide
4	D	170	LYS	Peptide
4	D	171	GLU	Peptide

5.2 Too-close contacts

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	A	7295	0	3693	40	0
2	B	6142	0	6249	70	0
3	C	1448	0	1520	12	0
4	D	1180	0	1249	22	0
5	E	1197	0	1220	15	0
6	F	979	0	1022	11	0
7	G	1021	0	1041	19	0
8	H	941	0	973	18	0
9	I	1824	0	1909	25	0
9	J	1905	0	2002	30	0
10	K	979	0	979	16	0
11	L	2939	0	2884	29	0
12	T	1535	0	777	3	0
13	K	1	0	0	0	0
All	All	29386	0	25518	251	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 5.

The worst 5 of 251 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:C:H5''	2:B:866:LYS:H	1.54	0.70
5:E:119:ARG:HH22	7:G:59:GLY:HA3	1.60	0.66
2:B:493:ILE:O	7:G:25:ARG:NH2	2.29	0.66
11:L:41:ARG:HB3	11:L:315:GLN:HB3	1.78	0.65
4:D:84:LEU:HD22	4:D:86:LEU:HB2	1.79	0.64

There are no symmetry-related clashes.

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	
2	B	764/1024 (75%)	683 (89%)	79 (10%)	2 (0%)	41	74
3	C	178/283 (63%)	155 (87%)	22 (12%)	1 (1%)	25	62
4	D	143/220 (65%)	114 (80%)	26 (18%)	3 (2%)	7	38
5	E	145/163 (89%)	136 (94%)	9 (6%)	0	100	100
6	F	123/199 (62%)	112 (91%)	11 (9%)	0	100	100
7	G	129/140 (92%)	111 (86%)	18 (14%)	0	100	100
8	H	119/124 (96%)	104 (87%)	15 (13%)	0	100	100
9	I	234/268 (87%)	211 (90%)	23 (10%)	0	100	100
9	J	245/268 (91%)	224 (91%)	21 (9%)	0	100	100
10	K	119/154 (77%)	110 (92%)	9 (8%)	0	100	100
11	L	360/363 (99%)	341 (95%)	19 (5%)	0	100	100
All	All	2559/3206 (80%)	2301 (90%)	252 (10%)	6 (0%)	50	78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	204	SER
3	C	126	ARG
4	D	96	TYR
4	D	119	PRO
2	B	407	PRO

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	
2	B	671/883 (76%)	666 (99%)	5 (1%)	84	91
3	C	167/255 (66%)	166 (99%)	1 (1%)	86	93
4	D	132/196 (67%)	129 (98%)	3 (2%)	50	71
5	E	131/143 (92%)	131 (100%)	0	100	100
6	F	103/150 (69%)	103 (100%)	0	100	100
7	G	110/118 (93%)	109 (99%)	1 (1%)	78	88
8	H	104/106 (98%)	103 (99%)	1 (1%)	76	86
9	I	202/228 (89%)	200 (99%)	2 (1%)	76	86
9	J	211/228 (92%)	209 (99%)	2 (1%)	78	88
10	K	106/135 (78%)	104 (98%)	2 (2%)	57	76
11	L	331/332 (100%)	330 (100%)	1 (0%)	92	96
All	All	2268/2774 (82%)	2250 (99%)	18 (1%)	82	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	226	ARG
11	L	41	ARG
10	K	103	ASN
4	D	203	ARG
9	J	205	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	36	ASN
10	K	103	ASN
11	L	327	ASN
11	L	13	HIS
10	K	79	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	340/341 (99%)	89 (26%)	5 (1%)
12	T	71/72 (98%)	8 (11%)	0
All	All	411/413 (99%)	97 (23%)	5 (1%)

5 of 97 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	13	G
1	A	14	A
1	A	15	A
1	A	17	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	74	G
1	A	107	A
1	A	126	U
1	A	261	G
1	A	326	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

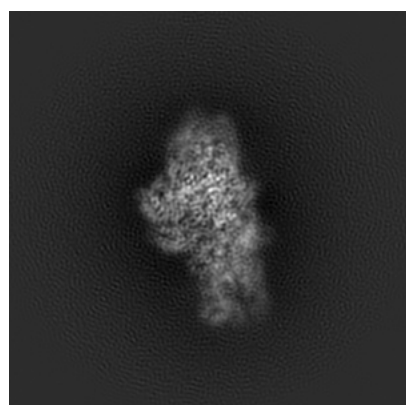
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9627. These allow visual inspection of the internal detail of the map and identification of artifacts.

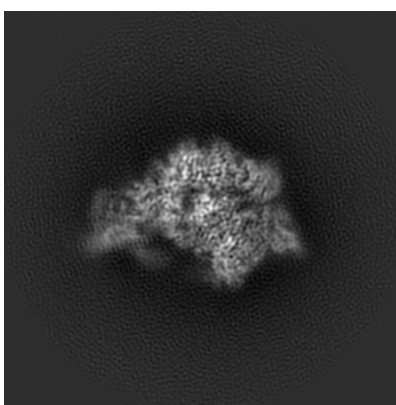
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

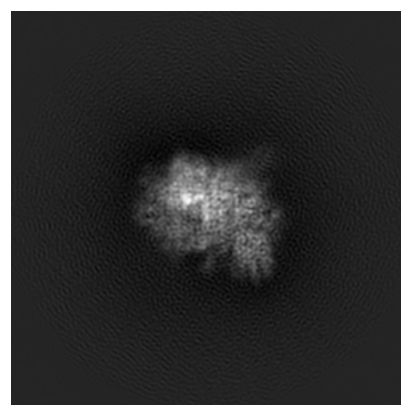
6.1.1 Primary map



X



Y

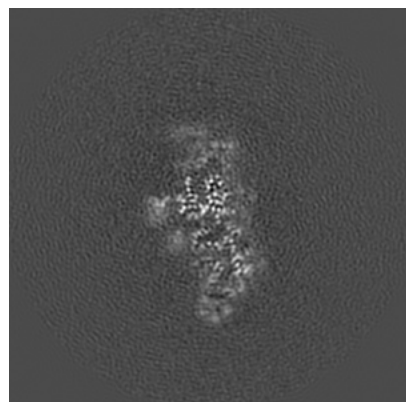


Z

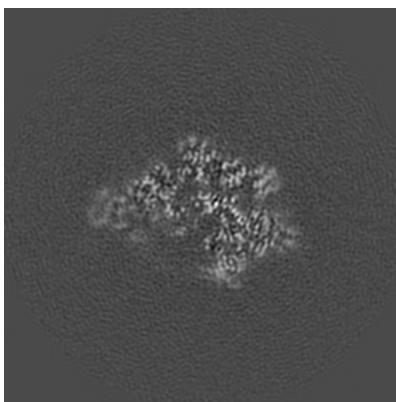
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

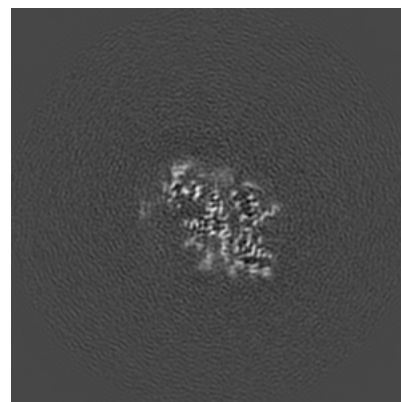
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

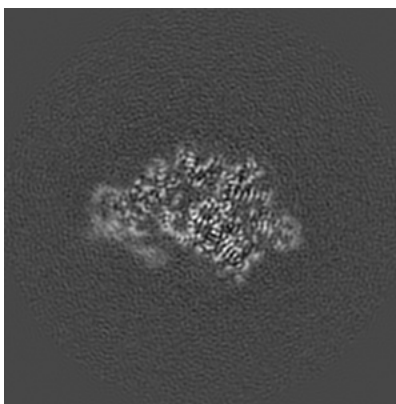
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

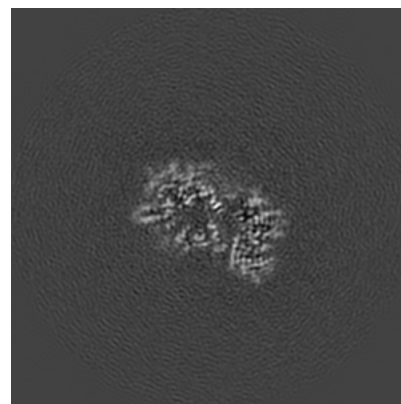
6.3.1 Primary map



X Index: 123



Y Index: 135



Z Index: 136

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

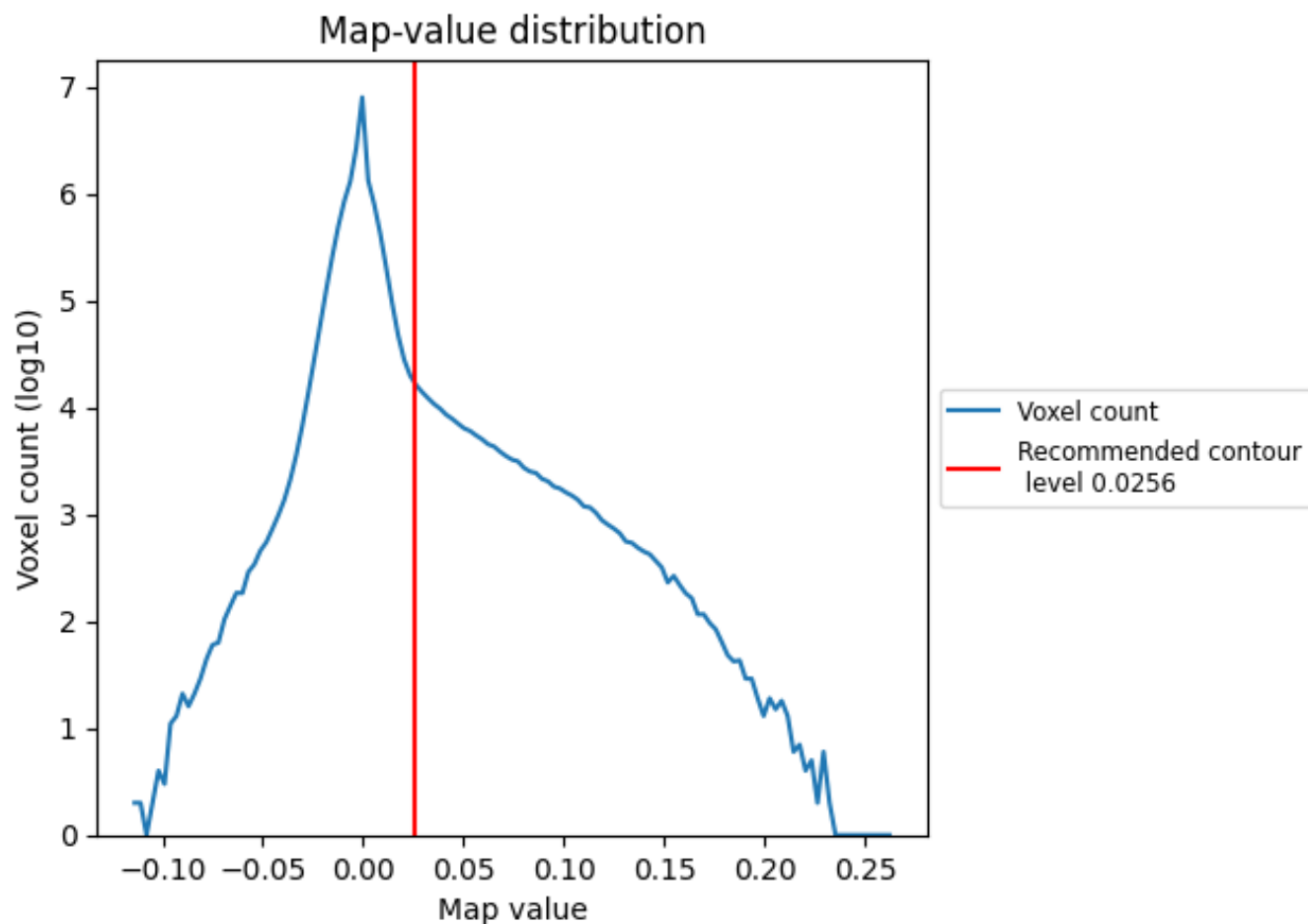
6.5 Mask visualisation

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

7 Map analysis [i](#)

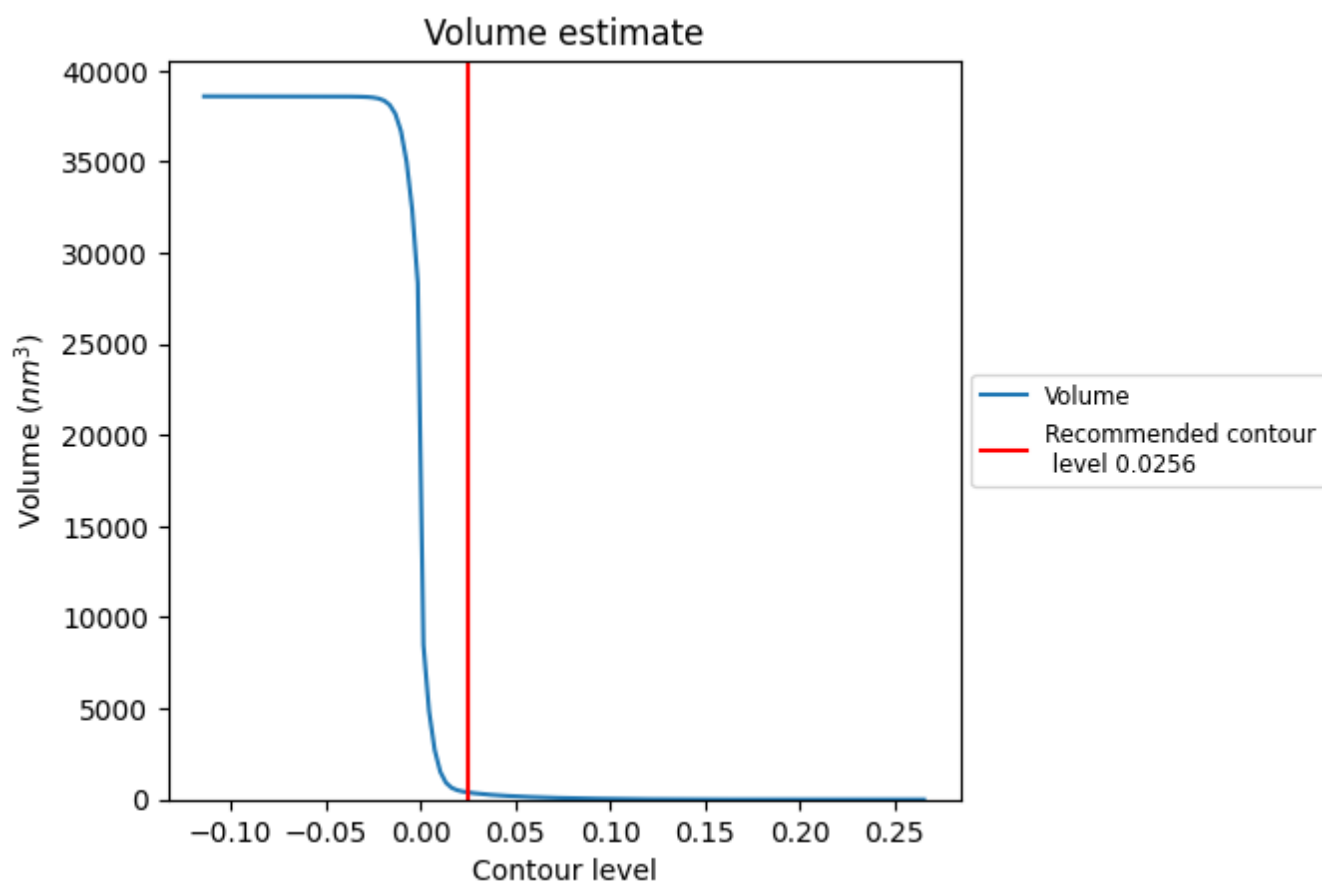
This section contains the results of statistical analysis of the map.

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.

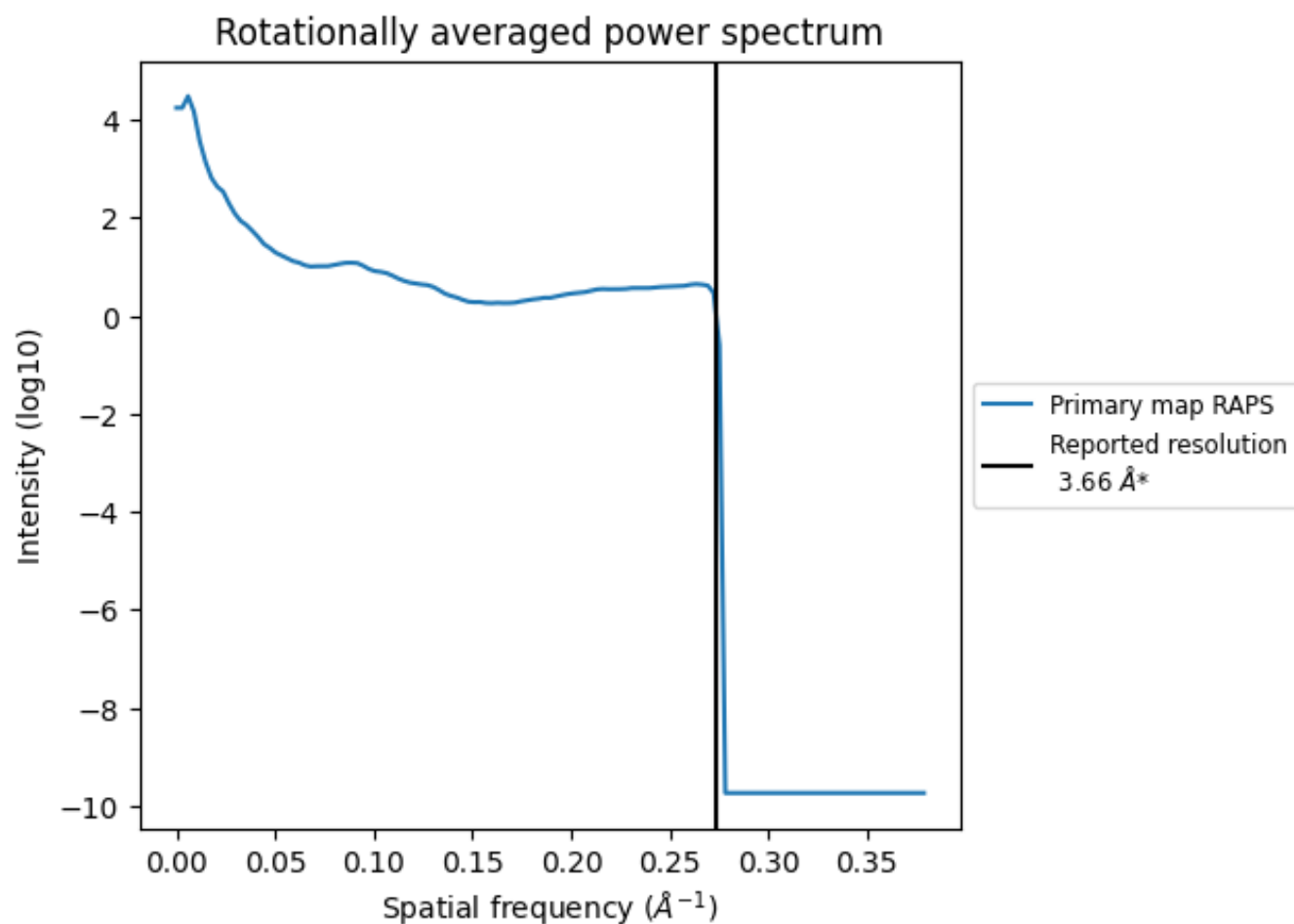
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm³; this corresponds to an approximate mass of 349 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.273 Å⁻¹

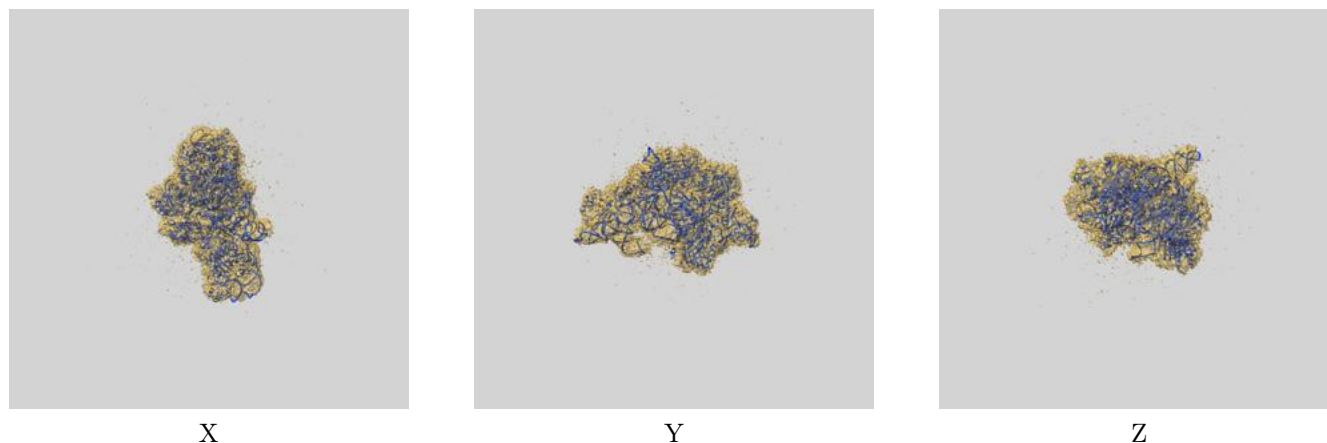
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

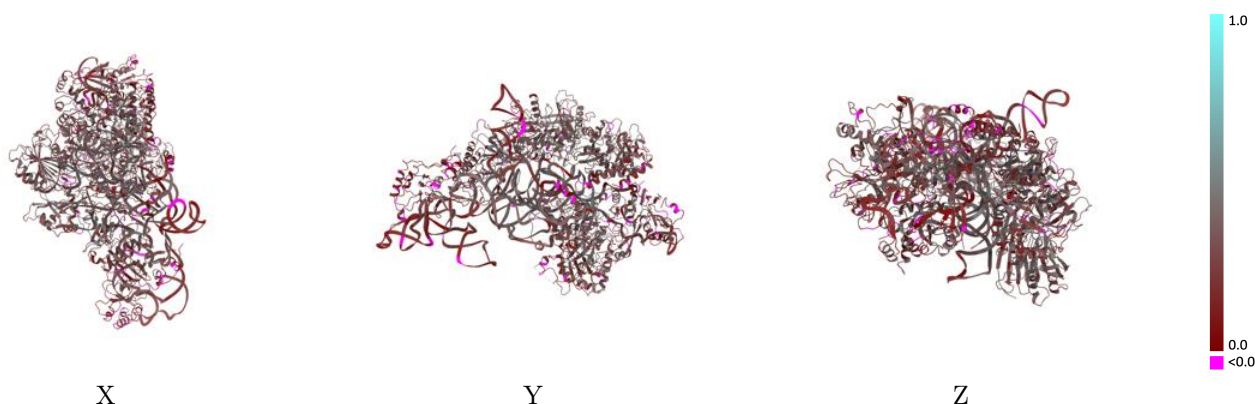
This section contains information regarding the fit between EMDB map EMD-9627 and PDB model 6AHU. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



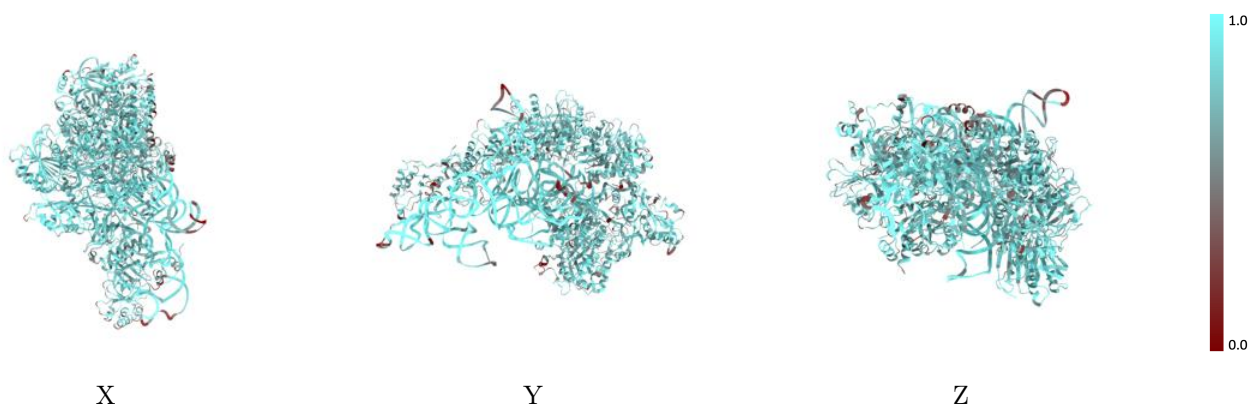
The images above show the 3D surface view of the map at the recommended contour level 0.0256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



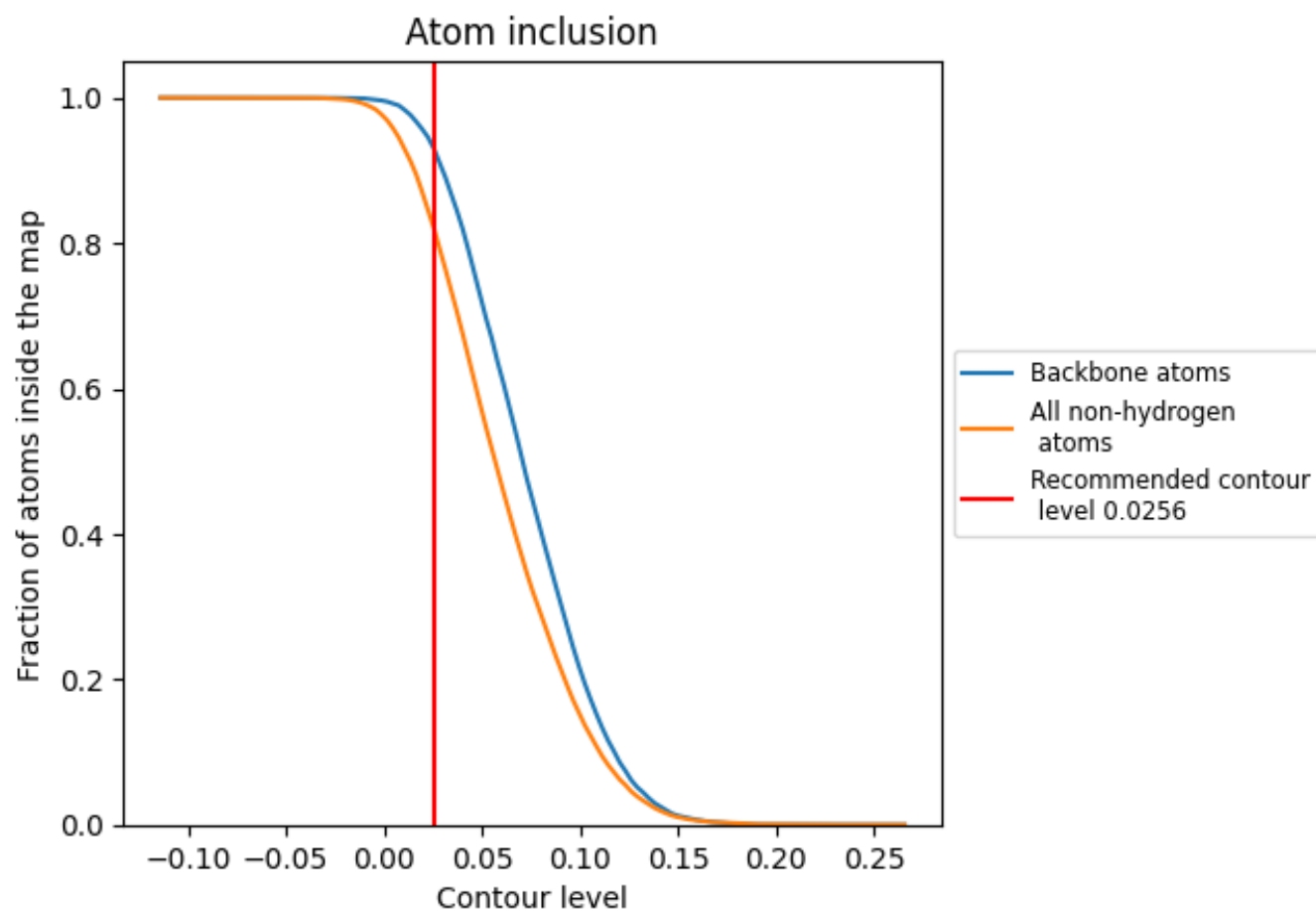
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0256).





























9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8192	 0.2880
A	 0.9197	 0.3050
B	 0.7724	 0.2870
C	 0.7252	 0.1840
D	 0.7881	 0.3030
E	 0.8003	 0.3050
F	 0.7505	 0.2010
G	 0.7732	 0.2590
H	 0.8078	 0.3370
I	 0.7701	 0.2820
J	 0.7951	 0.2960
K	 0.7800	 0.2500
L	 0.8372	 0.3450
T	 0.8039	 0.2340

