



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 02:26 AM UTC

PDB ID : 4UE4 / pdb_00004ue4
EMDB ID : EMD-2843
Title : Structural basis for targeting and elongation arrest of Bacillus signal recognition particle
Authors : Beckert, B.; Kedrov, A.; Sohmen, D.; Kempf, G.; Wild, K.; Sinning, I.; Stahlberg, H.; Wilson, D.N.; Beckmann, R.
Deposited on : 2014-12-15
Resolution : 7.00 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:

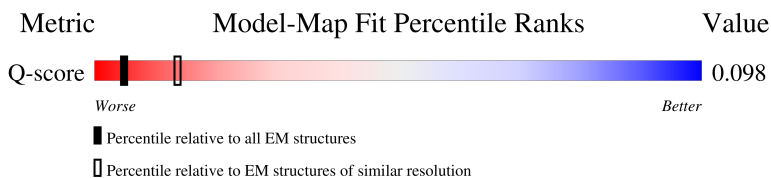
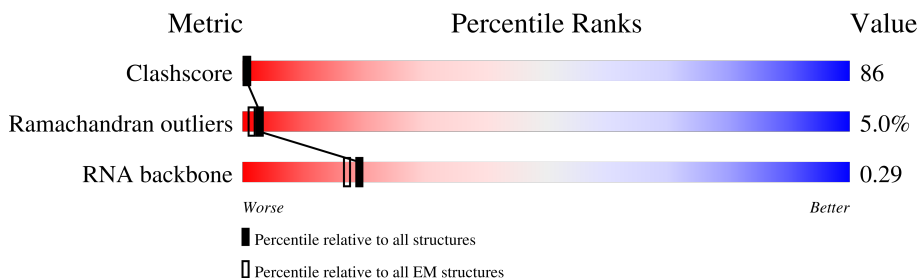
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 7.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
RNA backbone	8273	3508	-
Q-score	-	25397	483 (6.50 - 7.50)

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	266	
2	B	22	
3	C	102	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6181 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 6S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	266	Total	C	N	O	P	0	0
			5685	2535	1018	1866	266		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	deletion	GB 40130

- Molecule 2 is a protein called FTSQ SIGNAL SEQUENCE.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	22	Total	C	N	O	0	0
			88	44	22	22		

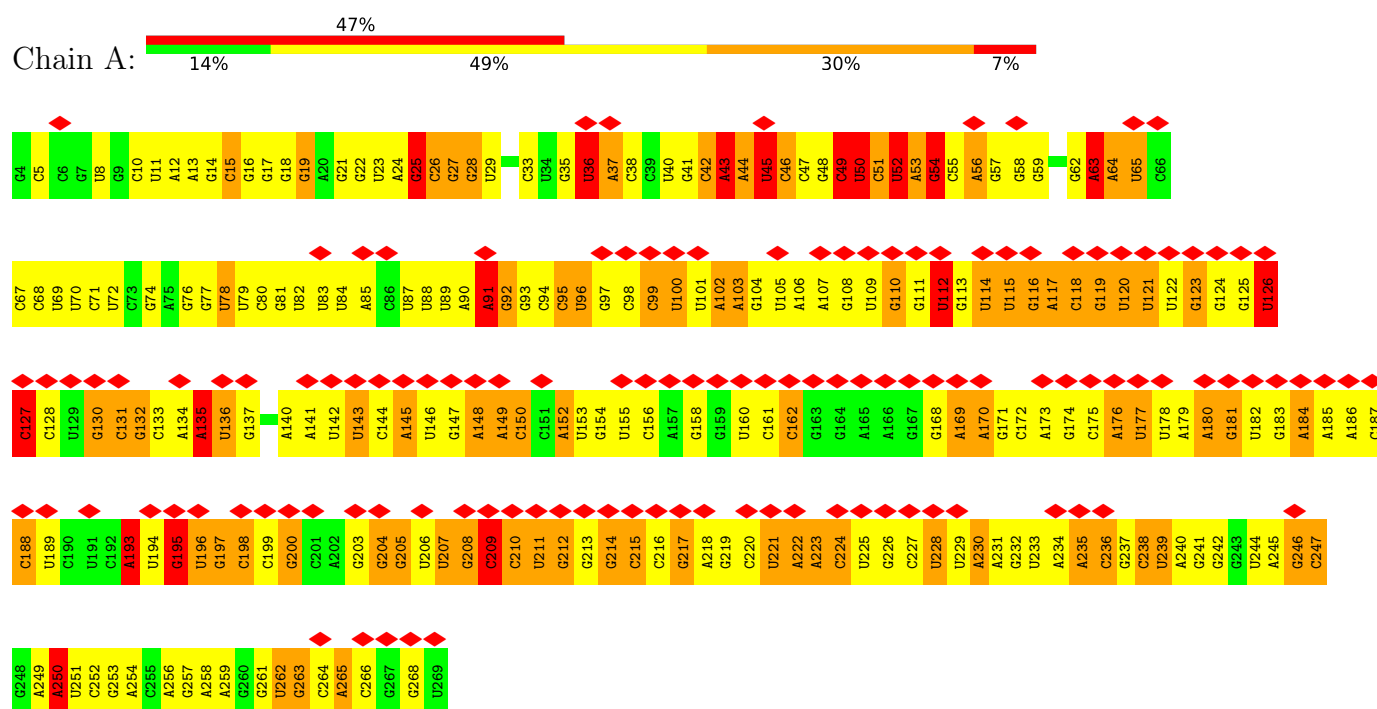
- Molecule 3 is a protein called SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	102	Total	C	N	O	0	0
			408	204	102	102		

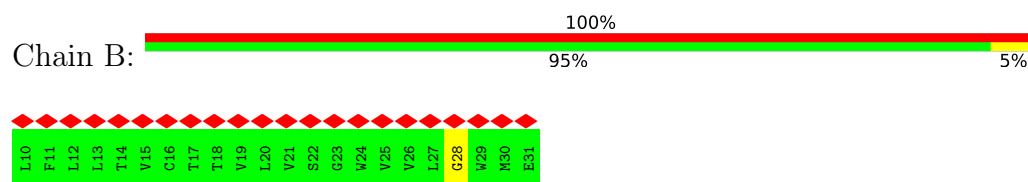
3 Residue-property plots

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.

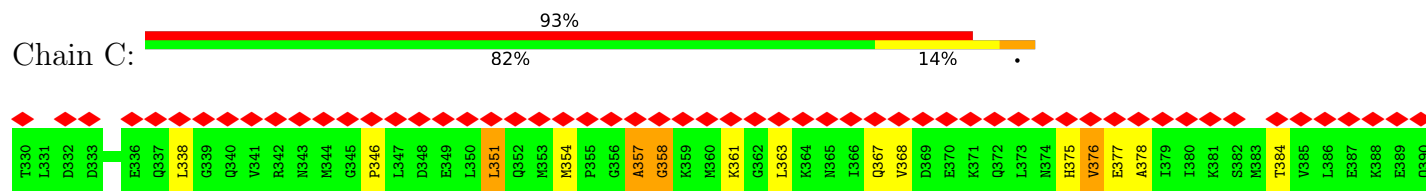
• Molecule 1: 6S RNA



• Molecule 2: FTSQ SIGNAL SEQUENCE



• Molecule 3: SIGNAL RECOGNITION PARTICLE PROTEIN



P391	D392	I393	I394	N395	A396	S397	R398	R399	K400	R401	I402	A403	K404	G405	S406	G407	T408	S409	V410	Q411	E412	R415	L416	L417	K418	Q419	F420	D421	E422	M423	K424	K425	M426	M427	K428	Q429	M430	T431
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75900	Depositor
Resolution determination method	Not provided	
CTF correction method	MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	428.250	Depositor
Minimum map value	-195.771	Depositor
Average map value	0.646	Depositor
Map value standard deviation	28.368	Depositor
Recommended contour level	100	Depositor
Map size ($\text{\AA}$)	400.26, 400.26, 400.26	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.953, 0.953, 0.953	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	4/6357 (0.1%)	1.42	66/9911 (0.7%)
2	B	0.80	0/87	1.18	1/107 (0.9%)
3	C	1.54	2/407 (0.5%)	3.11	7/507 (1.4%)
All	All	0.73	6/6851 (0.1%)	1.55	74/10525 (0.7%)

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
3	C	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	409	SER	C-N	26.23	1.69	1.33
1	A	235	A	O3'-P	-5.56	1.52	1.61
1	A	250	A	O3'-P	5.55	1.69	1.61
1	A	44	A	O3'-P	-5.48	1.52	1.61
3	C	354	MET	C-N	5.45	1.41	1.34

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	409	SER	CA-C-N	-37.79	53.94	121.97
3	C	409	SER	C-N-CA	-37.79	53.94	121.97
1	A	44	A	C4'-C3'-O3'	-23.97	77.05	113.00
3	C	409	SER	O-C-N	-22.27	92.97	122.59
1	A	54	G	C4'-C3'-O3'	-19.86	83.21	113.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	357	ALA	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	5685	0	2864	753	0
2	B	88	0	25	0	0
3	C	408	0	112	12	0
All	All	6181	0	3001	762	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 86.

The worst 5 of 762 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:135:A:C2	1:A:196:U:C2	2.29	1.20
1:A:44:A:H1'	1:A:46:C:O4'	1.47	1.14
1:A:206:U:H4'	1:A:207:U:H5'	1.30	1.12
1:A:118:C:H2'	1:A:119:G:H5'	1.27	1.08
1:A:135:A:N3	1:A:196:U:C2	2.22	1.07

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	20/22 (91%)	20 (100%)	0	0	100	100
3	C	100/102 (98%)	87 (87%)	7 (7%)	6 (6%)	1	13
All	All	120/124 (97%)	107 (89%)	7 (6%)	6 (5%)	3	16

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	351	LEU
3	C	358	GLY
3	C	363	LEU
3	C	376	VAL
3	C	346	PRO

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](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	265/266 (99%)	87 (32%)	10 (3%)

5 of 87 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	15	C
1	A	16	G
1	A	19	G
1	A	25	G
1	A	26	C

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	126	U
1	A	127	C
1	A	135	A
1	A	50	U
1	A	63	A

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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	409:SER	C	410:VAL	N	1.69

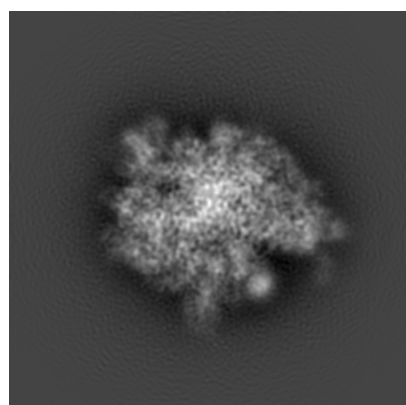
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2843. These allow visual inspection of the internal detail of the map and identification of artifacts.

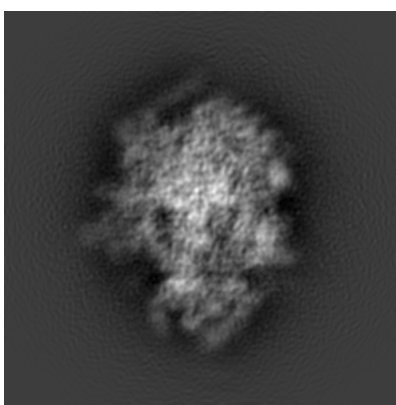
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

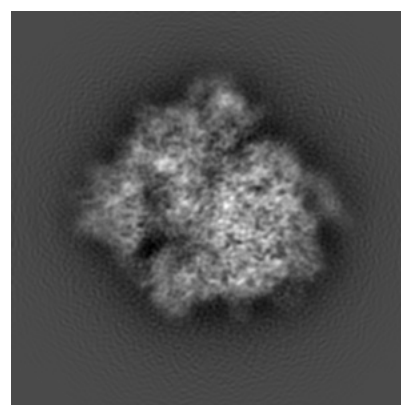
6.1.1 Primary map



X



Y

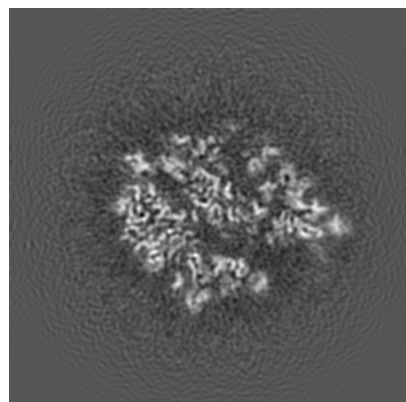


Z

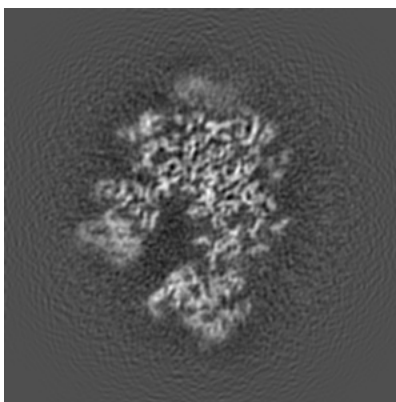
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

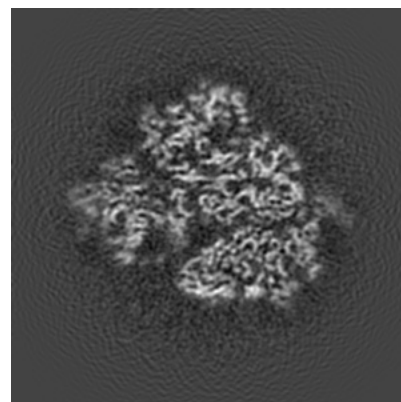
6.2.1 Primary map



X Index: 210



Y Index: 210

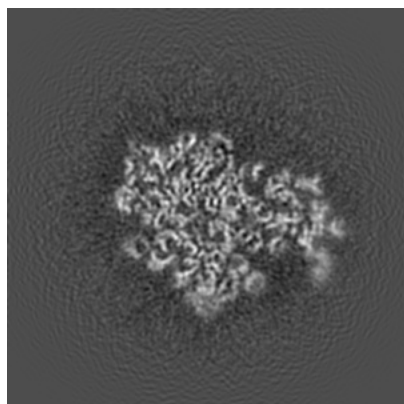


Z Index: 210

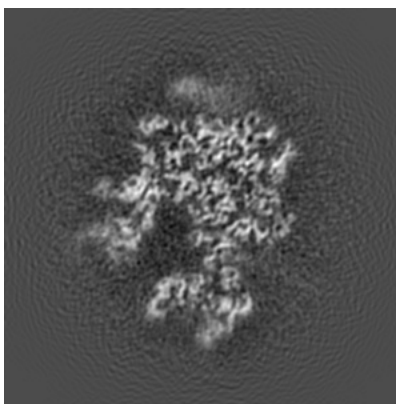
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

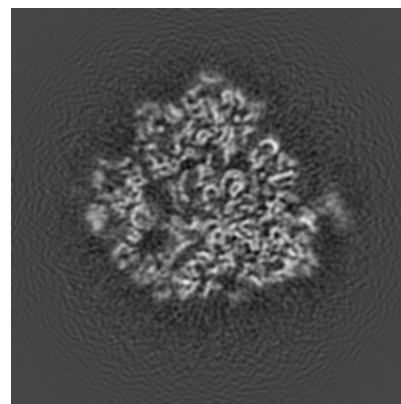
6.3.1 Primary map



X Index: 223



Y Index: 216

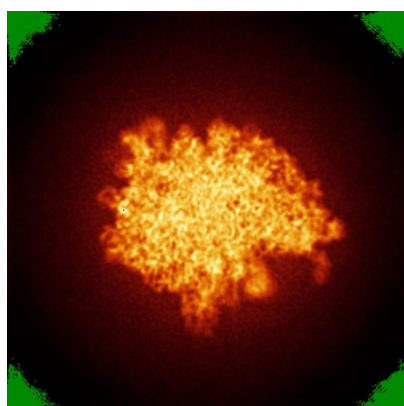


Z Index: 200

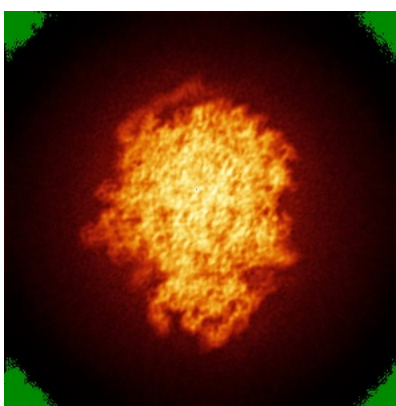
The images above show the largest variance slices of the map in three orthogonal directions.

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

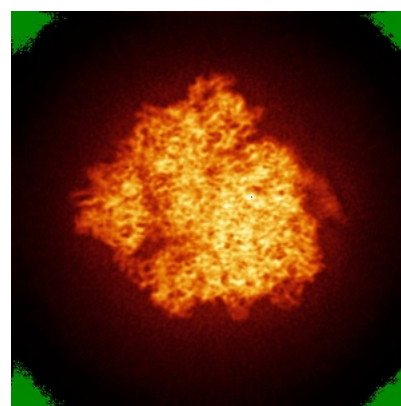
6.4.1 Primary map



X



Y



Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 100.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

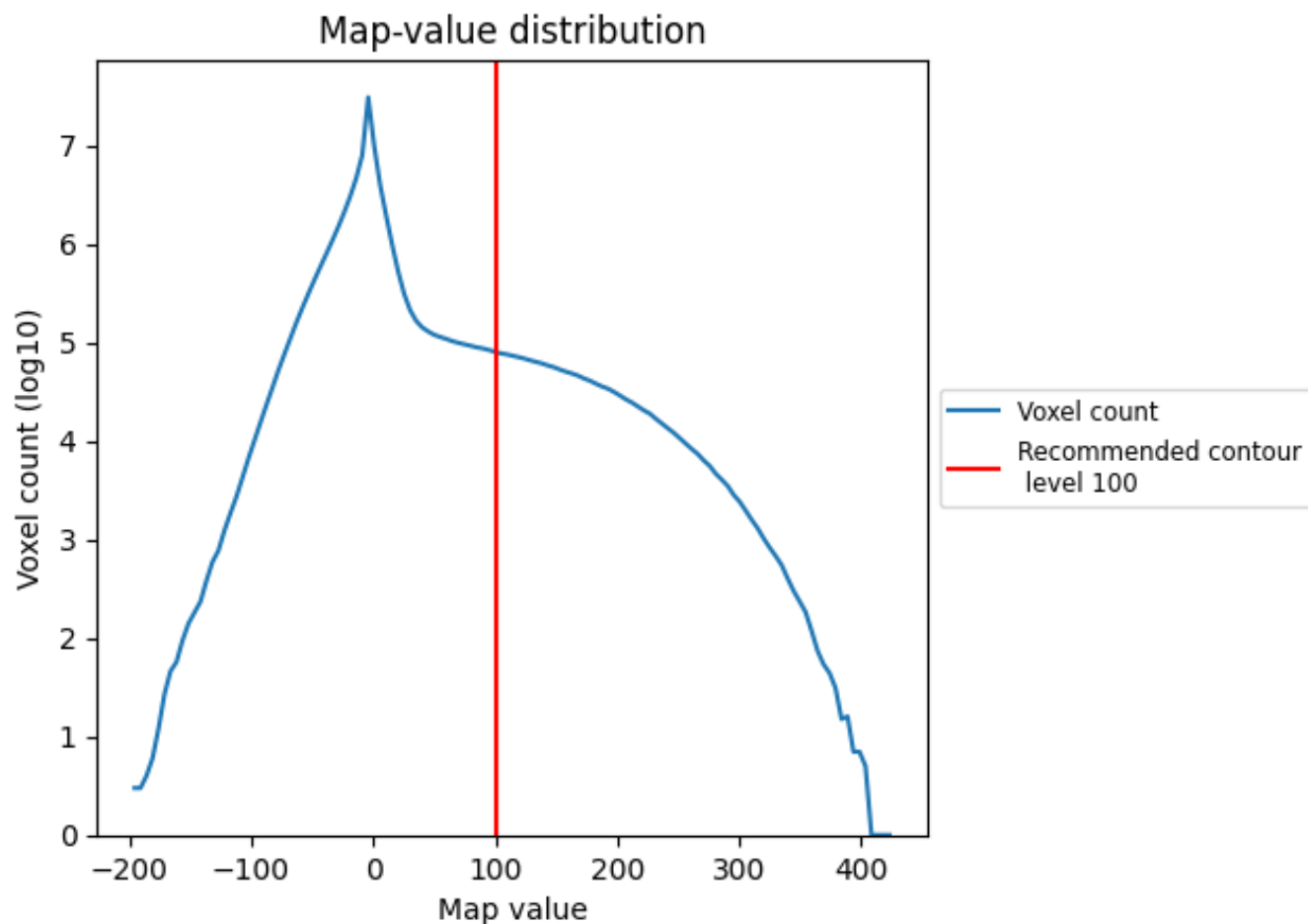
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

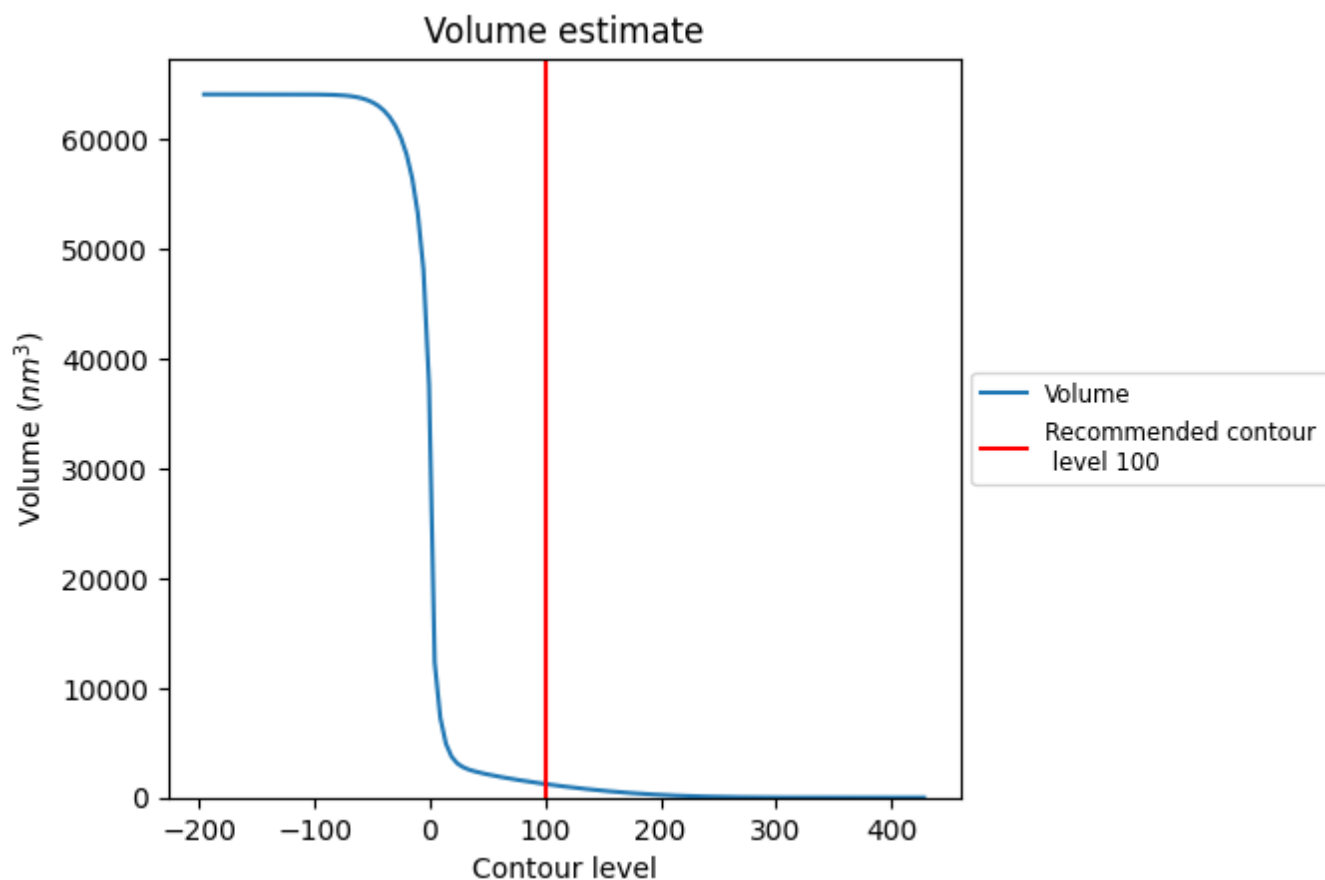
This section contains the results of statistical analysis of the map.

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.

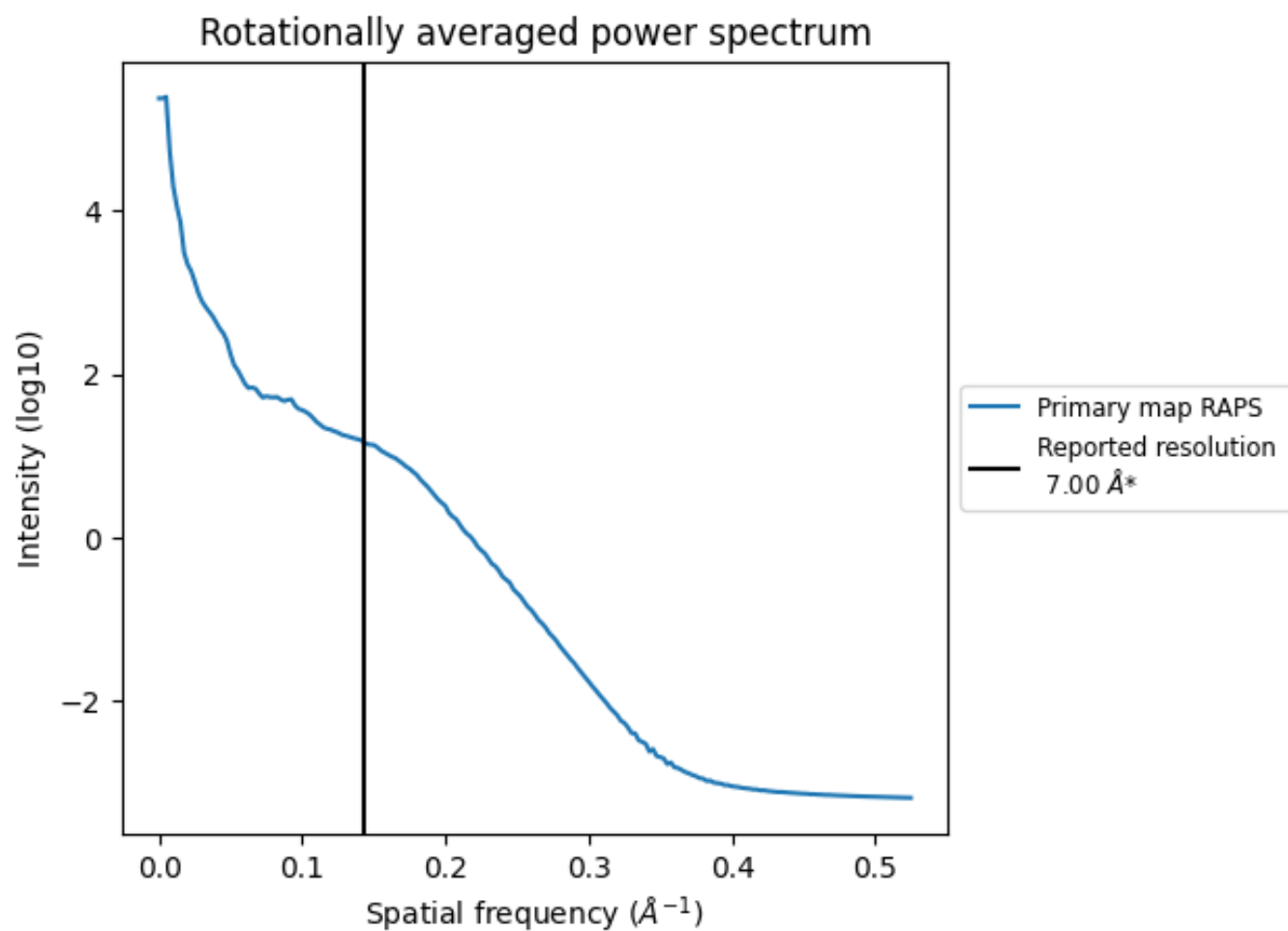
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1236 nm³; this corresponds to an approximate mass of 1116 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 0.143 Å⁻¹

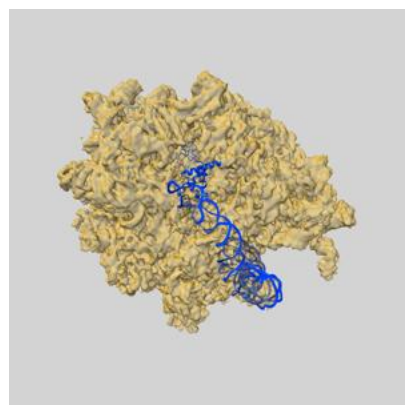
8 Fourier-Shell correlation

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

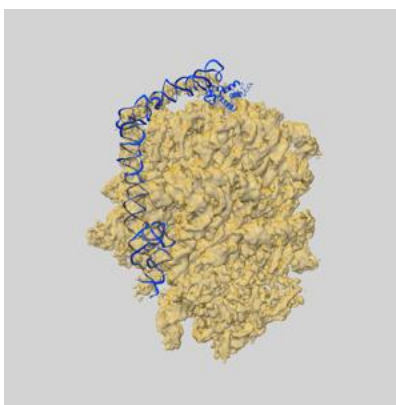
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2843 and PDB model 4UE4. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

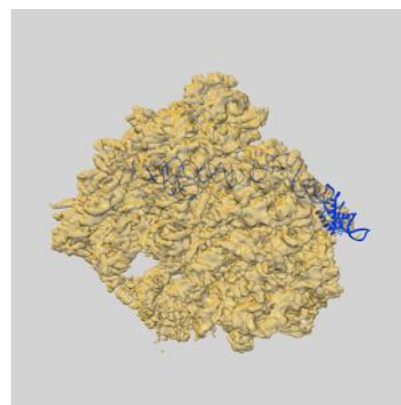
9.1 Map-model overlay [i](#)



X



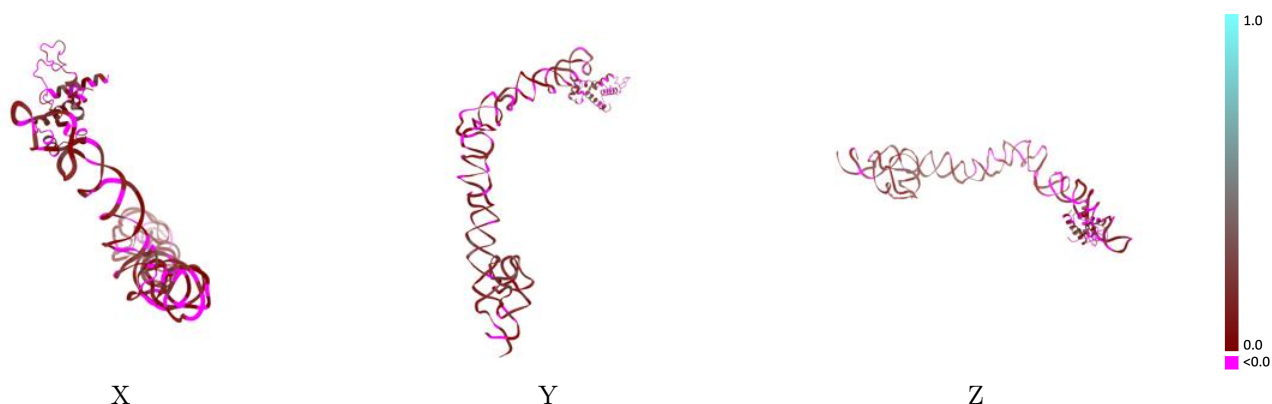
Y



Z

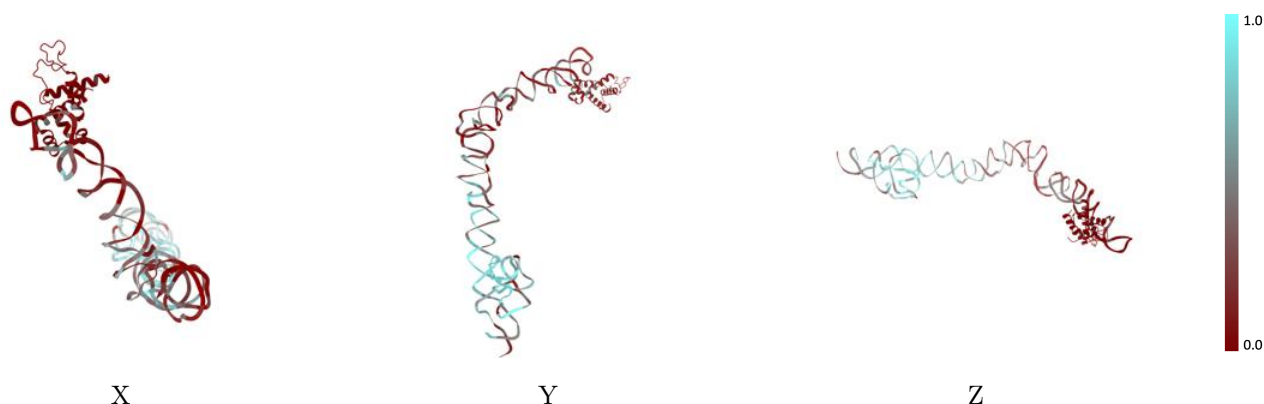
The images above show the 3D surface view of the map at the recommended contour level 100.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



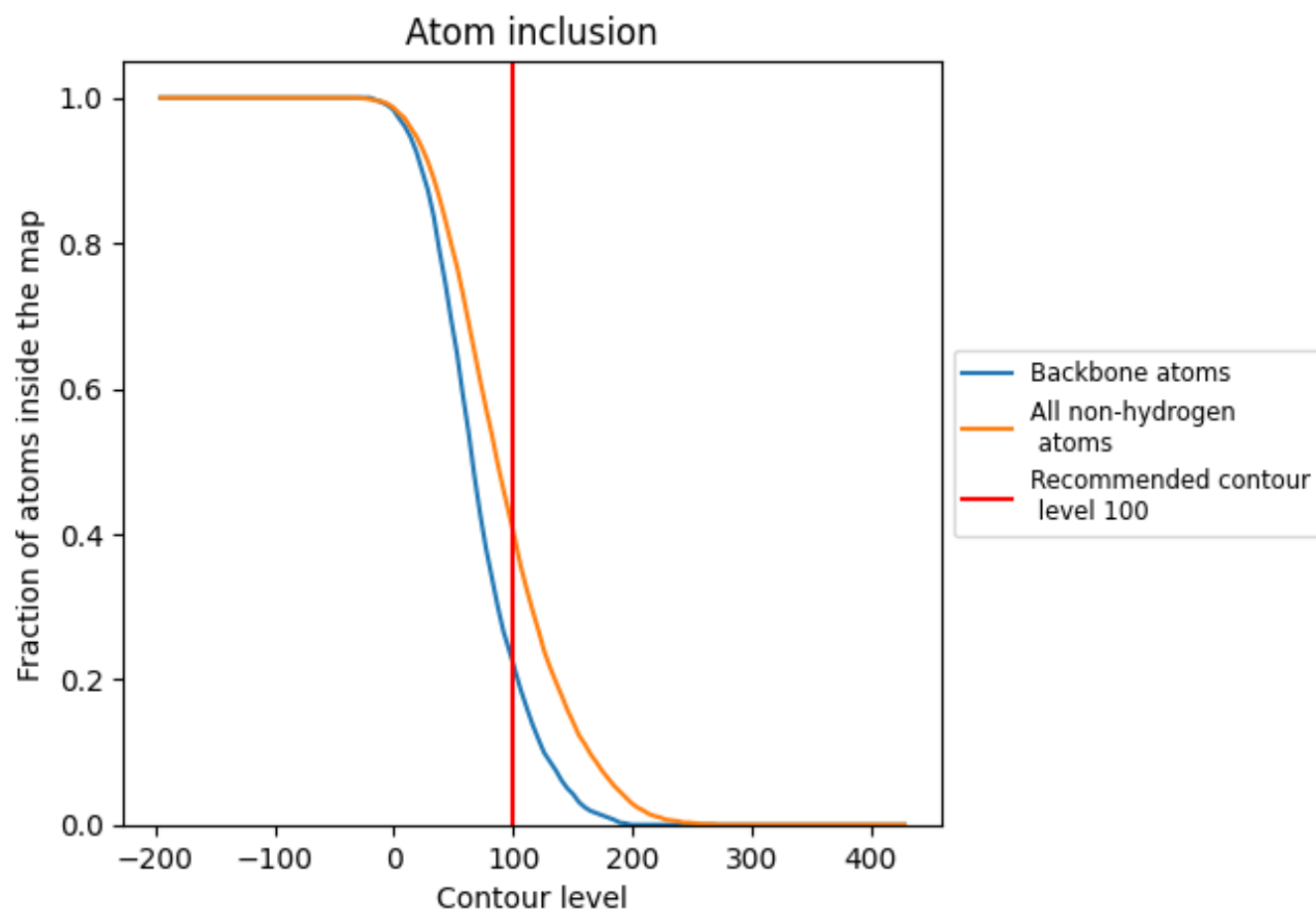
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (100).

9.4 Atom inclusion [i](#)



At the recommended contour level, 22% of all backbone atoms, 40% 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 (100) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4040	0.0980
A	0.4350	0.1010
B	0.0230	0.0490
C	0.0510	0.0540

