



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2024 – 04:53 PM JST

PDB ID : 7YGD
EMDB ID : EMD-33816
Title : Cryo-EM structure of Tetrahymena ribozyme conformation 6 undergoing the second-step self-splicing
Authors : Li, S.; Michael, Z.P.; Zhang, X.; Greg, P.; Zhang, K.
Deposited on : 2022-07-11
Resolution : 3.41 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.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

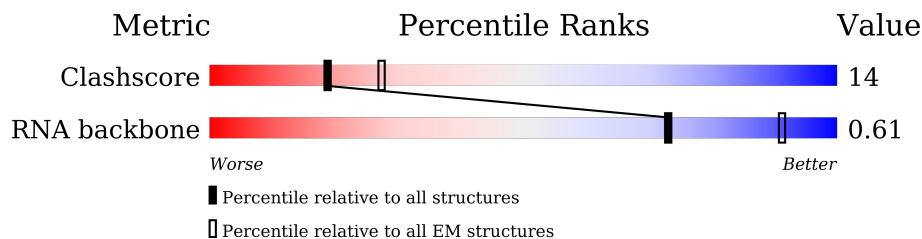
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 3.41 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
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	3	 100%
2	B	6	 33% 33% 67%
3	N	393	 36% 55% 6% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8313 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 RNA (5'-R(*UP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3	Total	C	N	O	P	0	0
			59	28	10	19	2		

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2	Total	C	N	O	P	0	0
			36	18	6	11	1		

- Molecule 3 is a RNA chain called RNA (384-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	384	Total	C	N	O	P	0	0
			8212	3671	1484	2673	384		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	17	G	-	expression tag	GB 10832
N	18	G	-	expression tag	GB 10832

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	N	6	Total	Mg	0
			6	6	

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: RNA (5'-R(*UP*CP*G)-3')

Chain A:  100%

U1
C2
G3

- Molecule 2: RNA (5'-R(*CP*C)-3')

Chain B:  33% 33% 67%

C1
C2
G
C
C
C

- Molecule 3: RNA (384-MER)

Chain N:  36% 55% 6%

G
G
U
U
U
U
G
G
A
G
G26
G27
A28
A29
A30
A31
U33
U34
A35
U36
C37
A38
A42
A46
C47
C48
U49
G50
A53
G54
A57
G58
U59
C60
U63
A64
A65
A66
C67
A70
U71
A72
G73
A74
U75
U76
G77
U78
C81
G82
G83
U84

U85
U86
A87
A88
A89
C93
A94
A95
G96
A97
U101
C102
A103
U106
U107
G108
U109
G110
G111
G112
A113
G118
G119
A123
C124
A125
G126
C127
G128
G129
U130
U131
C132
A133
G134
U135
A136
C137
G141
G148
G149
G150
A151
A152
A153
C154
U155
U156
U157
G158
A159
G160
A161

U162
G163
C164
C165
U166
U167
U168
G169
C170
A171
A172
G173
G174
G175
U179
G180
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A218
U221
C222
C223
U224
C229
A230
A231
C232
A233
G234

A235
U236
C237
U238
U239
U240
U241
G242
G245
U247
A248
U249
G250
G251
C255
A256
U259
C260
A261
C262
C266
U267
A268
A269
A270
U277
C278
G279
G280
C281
G282
A283
A284
G285
A286
U287
G288
U289
A290
U291
U292
C293
U294
U295
C296
U297
C298
A299
U300
A301
C302
G303
A304
U305

A306
U307
A308
C315
C316
U322
U323
A324
A325
U326
G327
G331
C332
U333
A334
G335
C336
G337
G338
A339
U340
G341
A342
A343
G344
G349
C350
A351
A352
C353
A354
C355
U356
G357
G358
C364
U365
G366
G367
G368
A369
A370
C371
U372
A373
A374
U375
U376
U377
G378
U379
A380
U381
G382

A385
U389
A390
U393
G395
U398
A399
G400
U401
U403
G405
G406
A407
U408
U409

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.898	Depositor
Minimum map value	-0.225	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	209.92, 209.92, 209.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/65	0.94	0/100
2	B	0.10	0/39	0.61	0/59
3	N	0.18	0/9194	0.78	1/14331 (0.0%)
All	All	0.18	0/9298	0.78	1/14490 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	315	C	N1-C2-O2	5.83	122.40	118.90

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	A	59	0	31	2	0
2	B	36	0	21	0	0
3	N	8212	0	4127	173	0
4	N	6	0	0	0	0
All	All	8313	0	4179	174	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 14.

The worst 5 of 174 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)
3:N:378:G:H1	3:N:393:U:H3	1.04	0.91
3:N:382:G:H1	3:N:389:U:H3	0.93	0.88
3:N:281:G:H1	3:N:297:U:H3	1.16	0.87
3:N:141:G:H1	3:N:162:U:H3	1.22	0.87
3:N:341:G:OP2	3:N:341:G:N2	2.20	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3/3 (100%)	2 (66%)	1 (33%)
2	B	1/6 (16%)	0	0
3	N	383/393 (97%)	56 (14%)	7 (1%)
All	All	387/402 (96%)	58 (14%)	8 (2%)

5 of 58 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	C
1	A	3	G
3	N	42	A
3	N	50	G
3	N	66	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	N	249	U
3	N	199	U
3	N	167	U
3	N	134	G
3	N	168	U

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](#)

Of 6 ligands modelled in this entry, 6 are 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

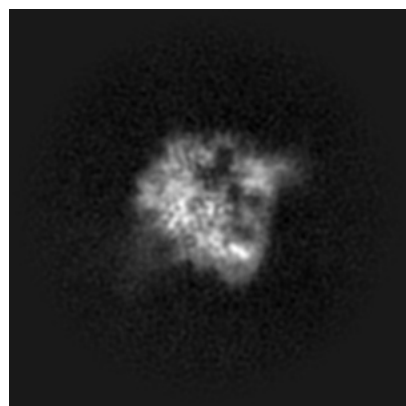
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33816. These allow visual inspection of the internal detail of the map and identification of artifacts.

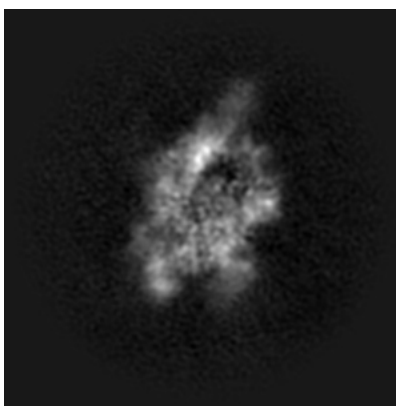
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

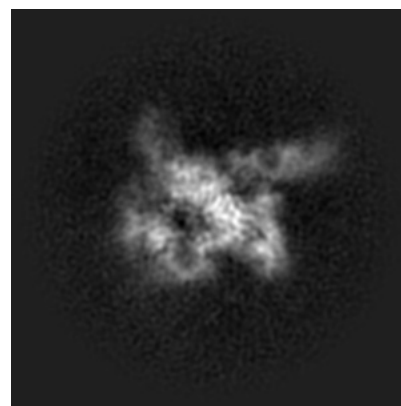
6.1.1 Primary map



X

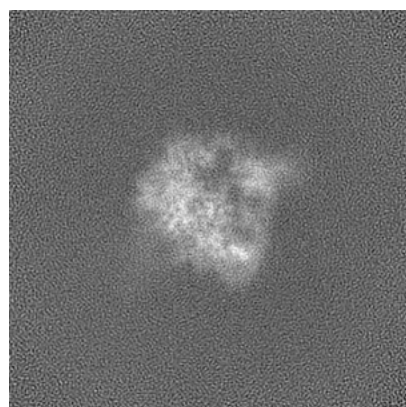


Y

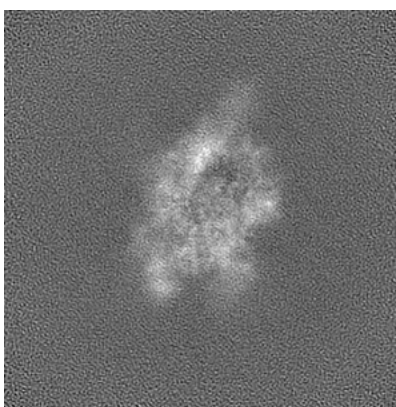


Z

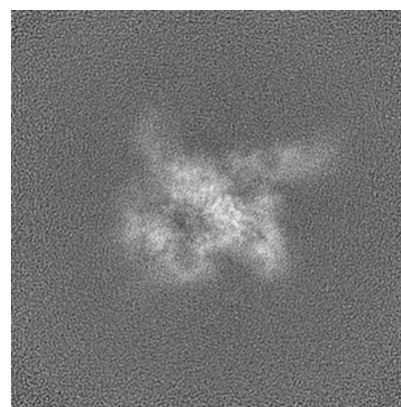
6.1.2 Raw map



X



Y

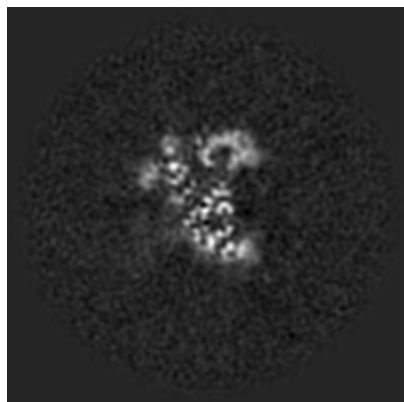


Z

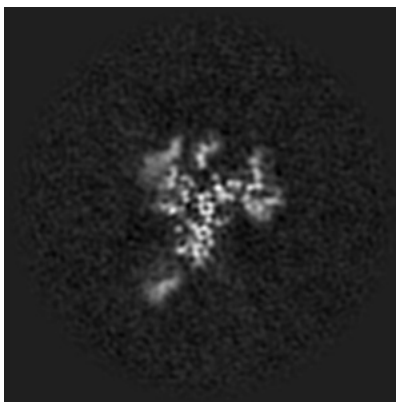
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

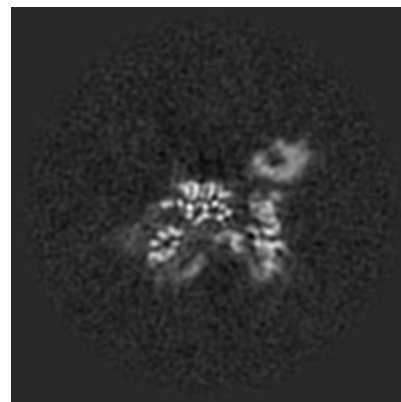
6.2.1 Primary map



X Index: 128

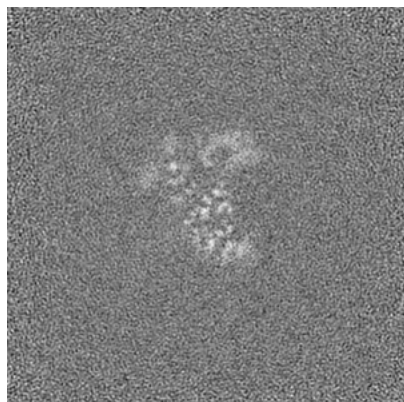


Y Index: 128

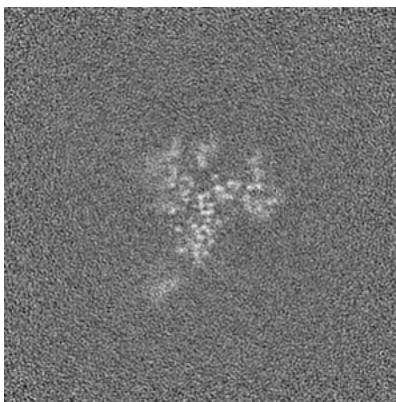


Z Index: 128

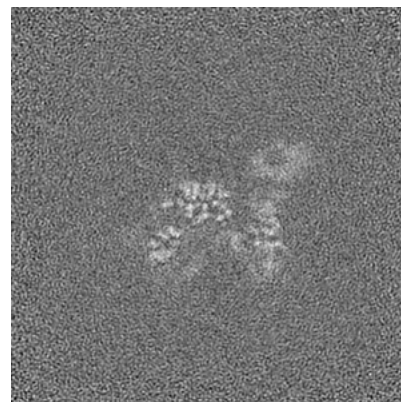
6.2.2 Raw map



X Index: 128



Y Index: 128

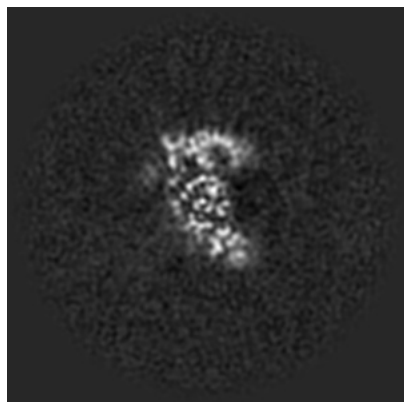


Z Index: 128

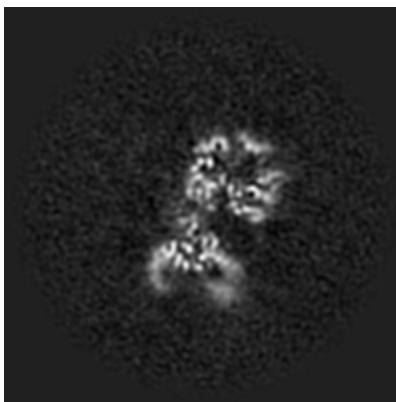
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

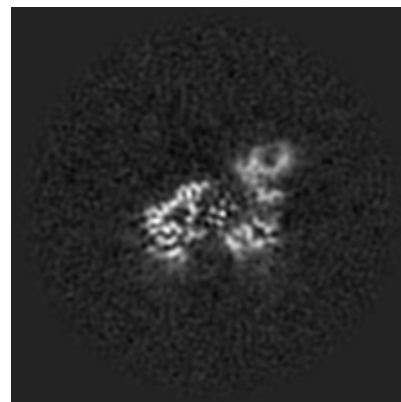
6.3.1 Primary map



X Index: 132

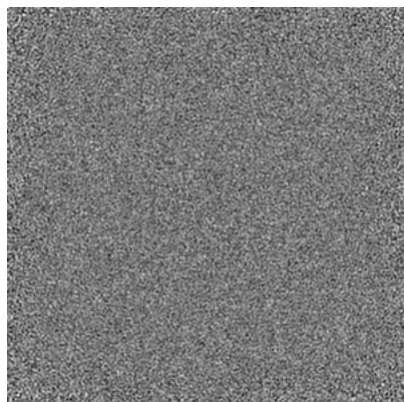


Y Index: 110

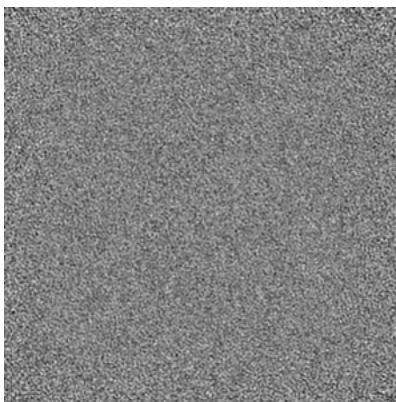


Z Index: 121

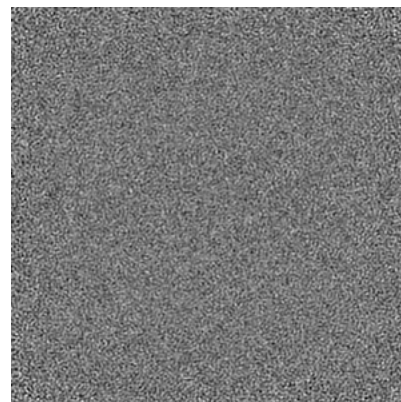
6.3.2 Raw map



X Index: 0



Y Index: 0

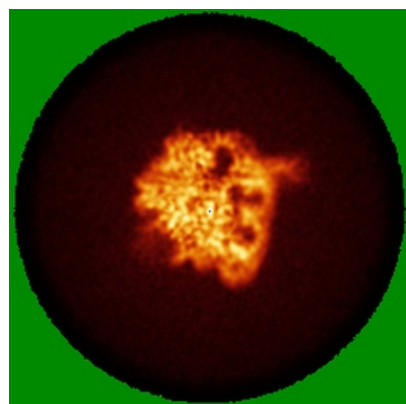


Z Index: 0

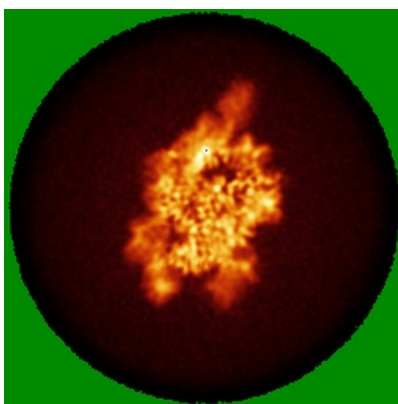
The images above show the largest variance slices of the map in three orthogonal directions.

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

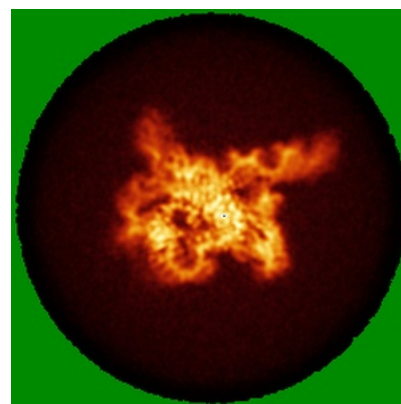
6.4.1 Primary map



X

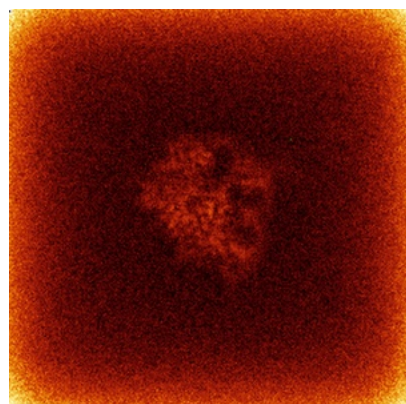


Y

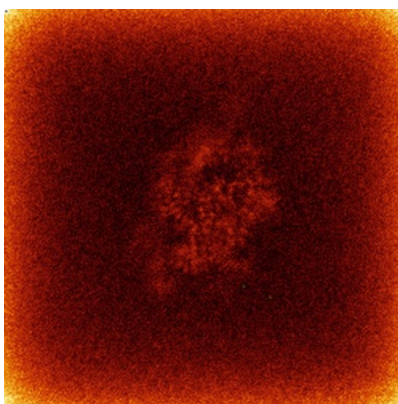


Z

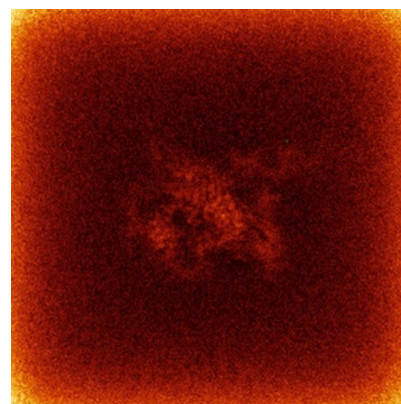
6.4.2 Raw map



X



Y

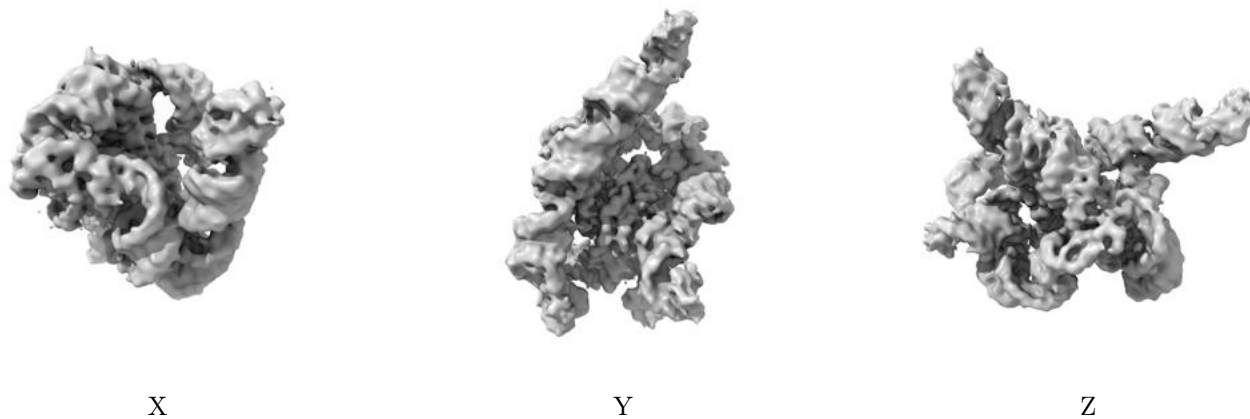


Z

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.

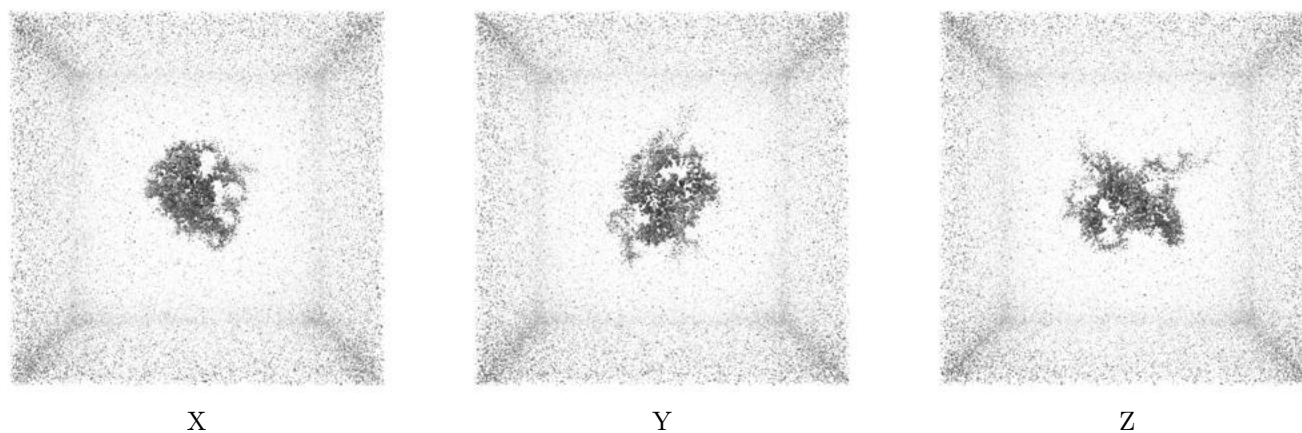
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

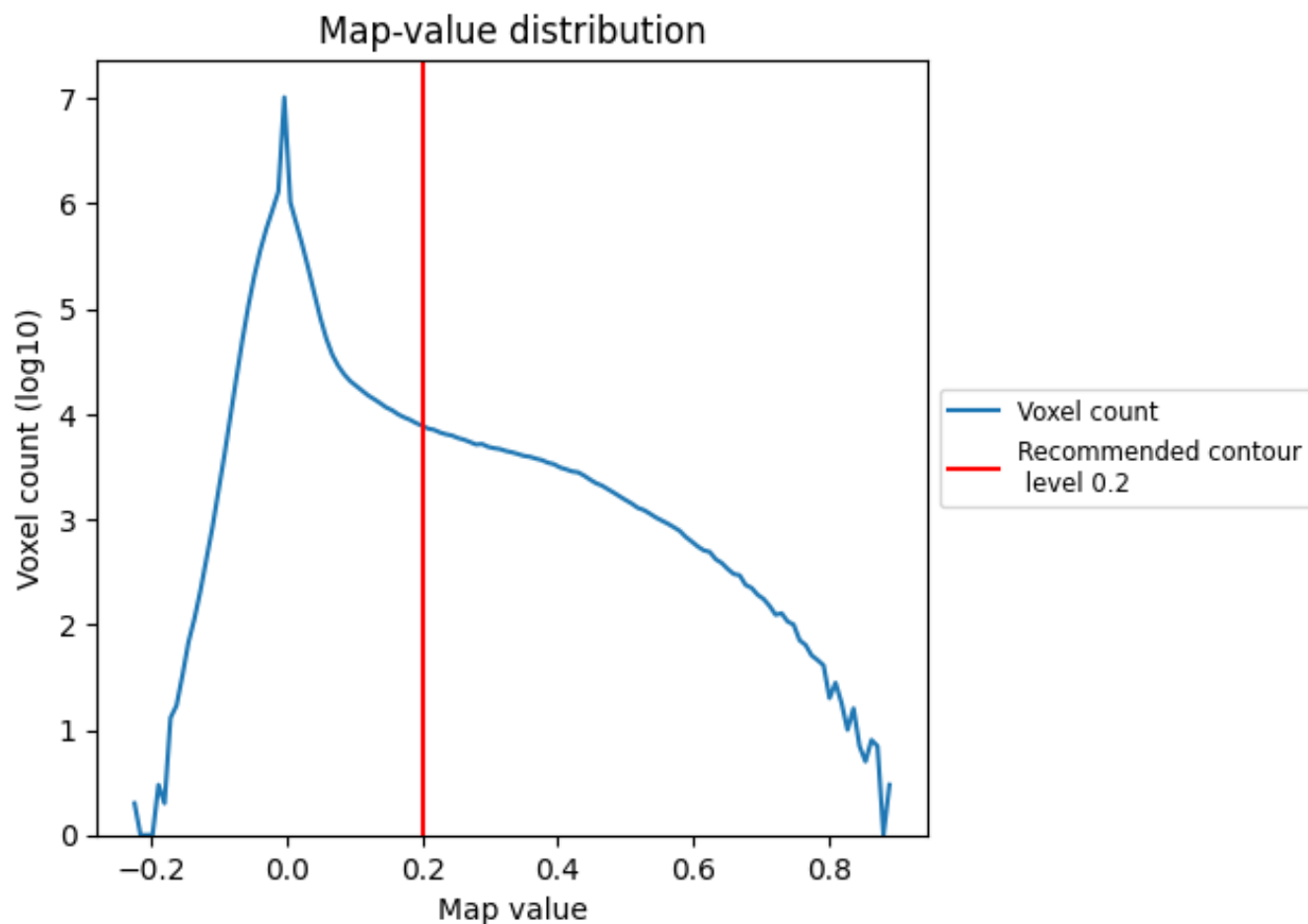
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

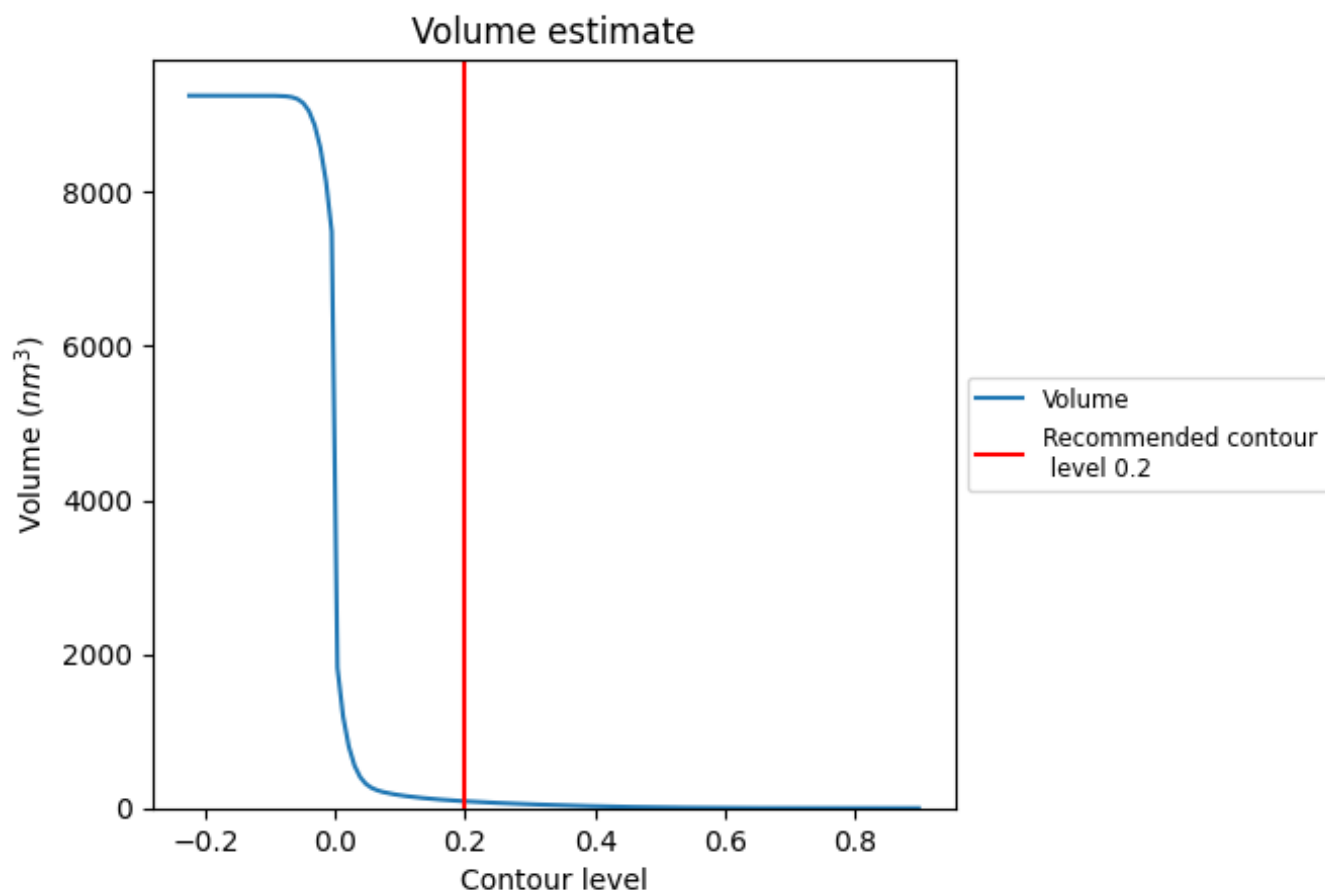
This section contains the results of statistical analysis of the map.

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.

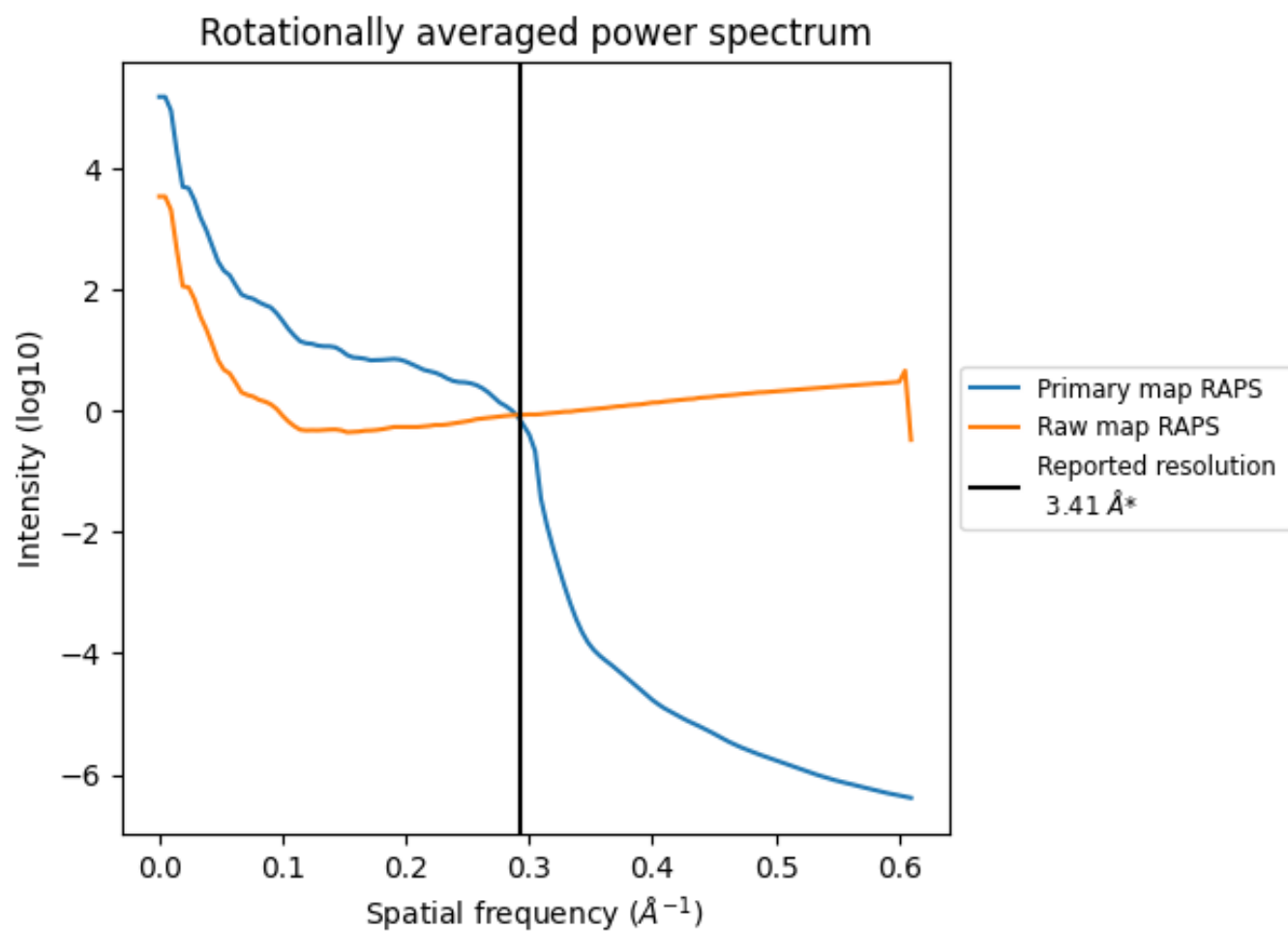
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 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 ⓘ

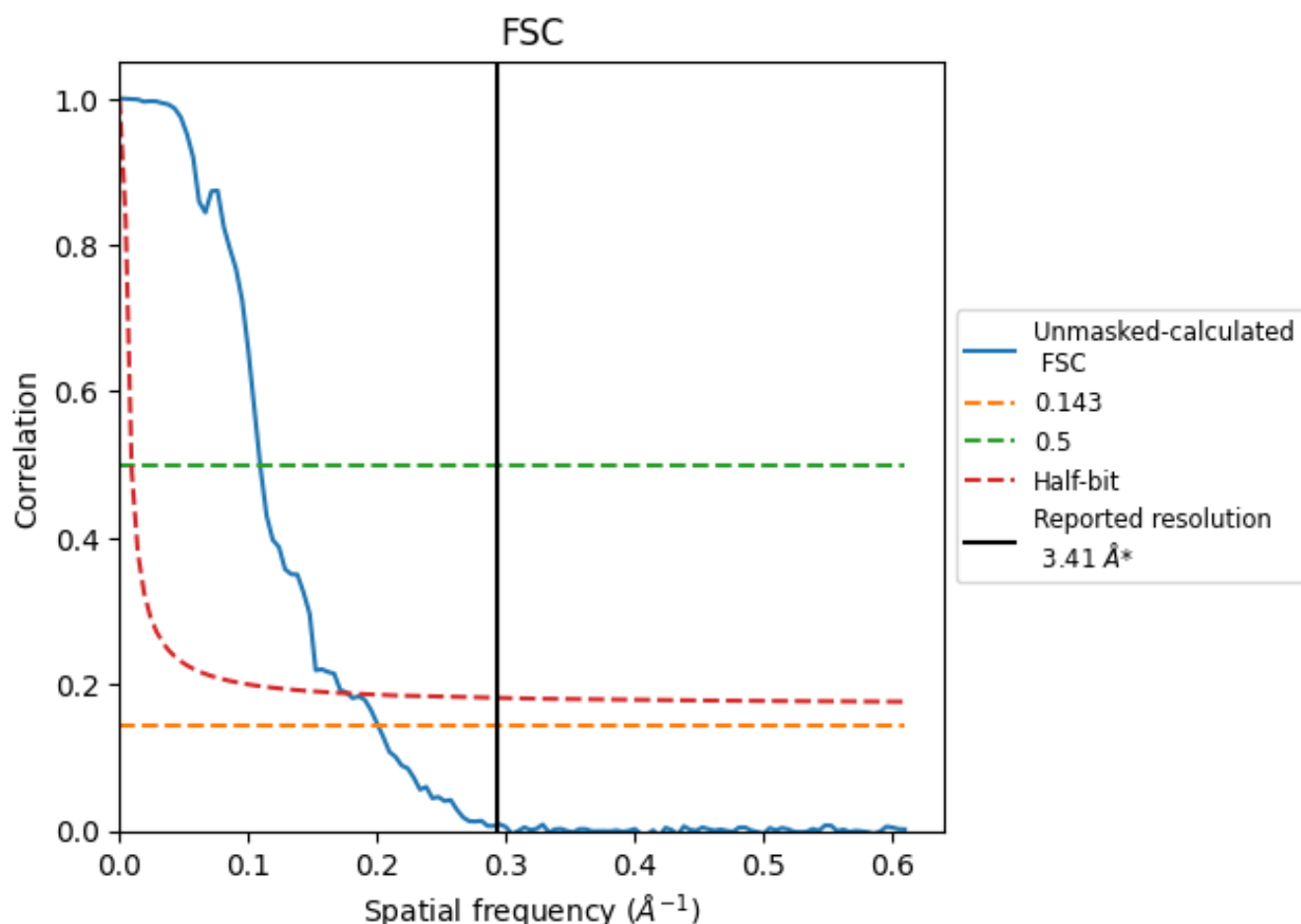


*Reported resolution corresponds to spatial frequency of 0.293 \AA^{-1}

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 0.293 Å⁻¹

8.2 Resolution estimates [i](#)

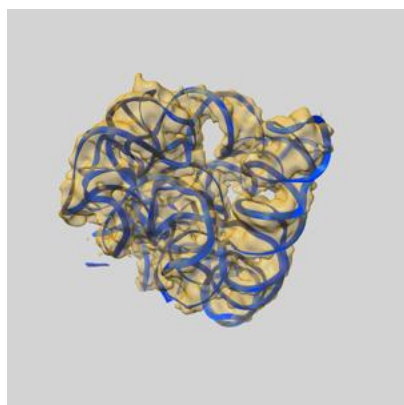
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.98	9.16	5.65

*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 4.98 differs from the reported value 3.41 by more than 10 %

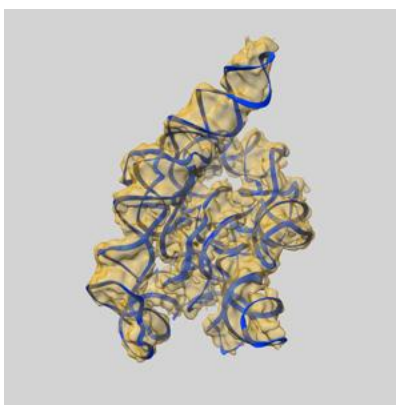
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33816 and PDB model 7YGD. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

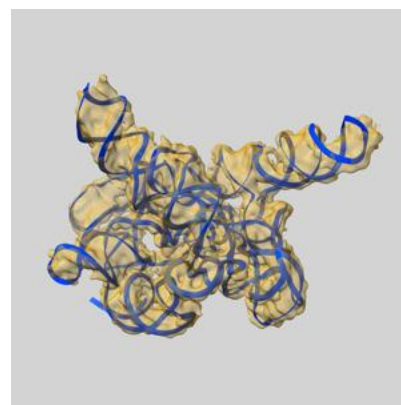
9.1 Map-model overlay [i](#)



X



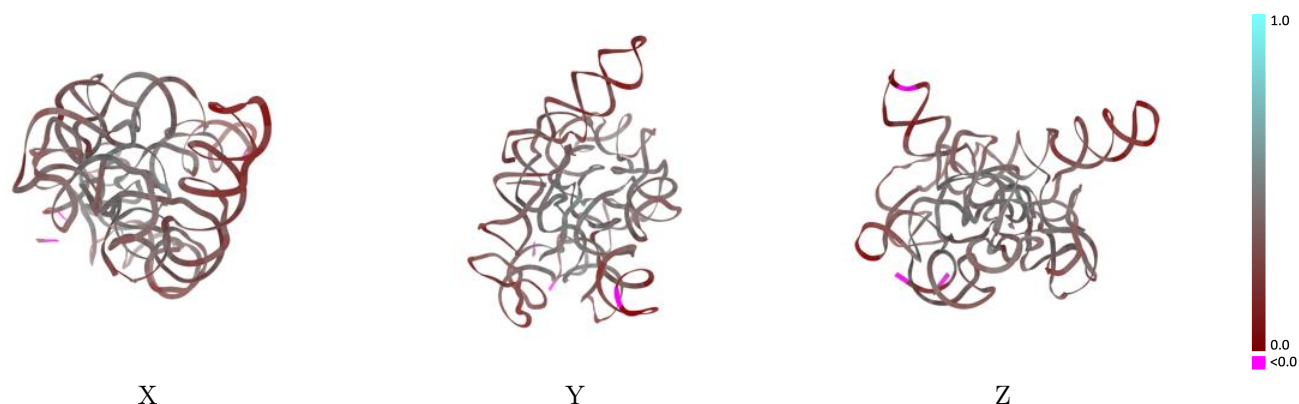
Y



Z

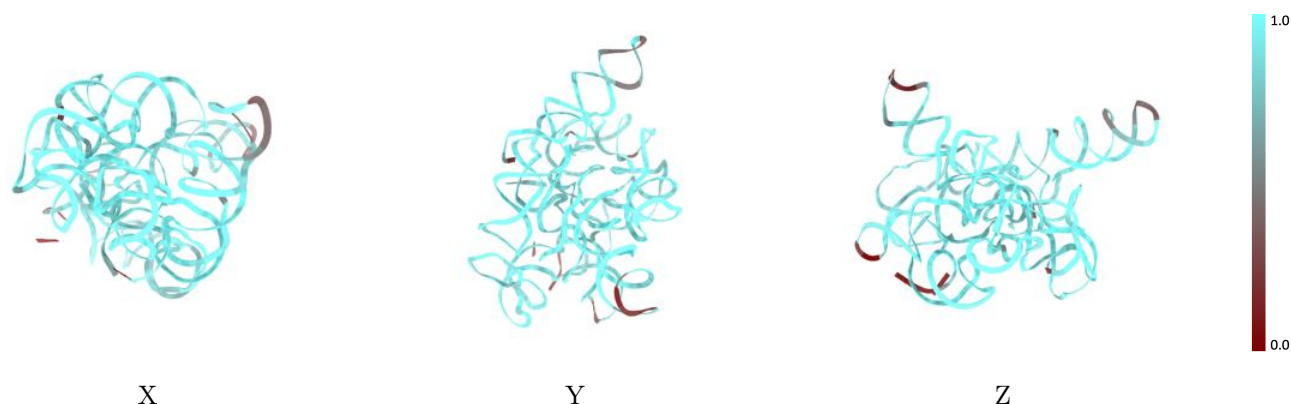
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



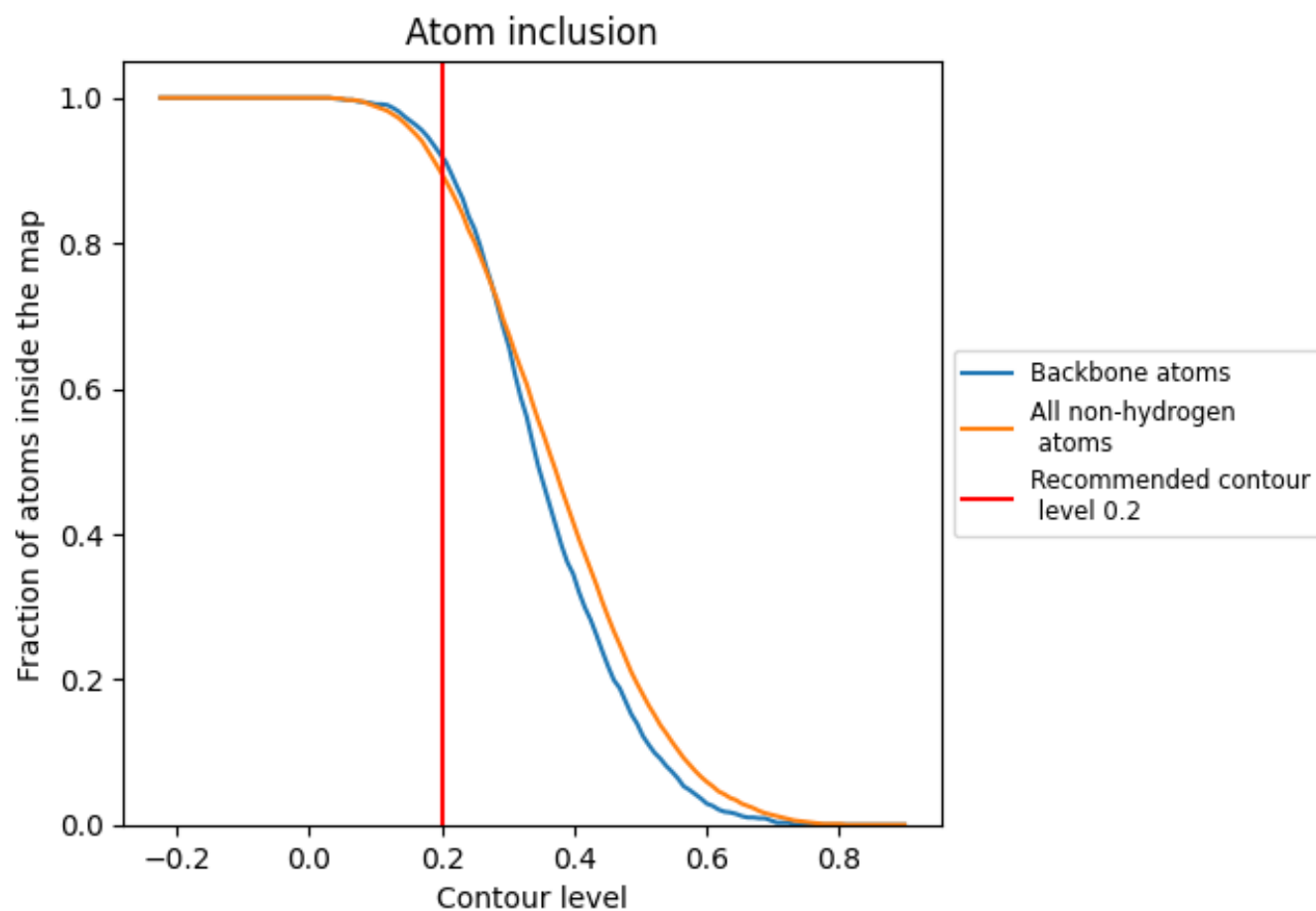
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8950	<div></div> 0.3560
A	<div></div> 0.7630	<div></div> 0.3430
B	<div></div> 0.0000	<div></div> 0.1250
N	<div></div> 0.9000	<div></div> 0.3570

