



## wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 03:16 PM EST

PDB ID : 6WLR  
EMDB ID : EMD-21839  
Title : SAM-IV riboswitch with SAM models, 4.8 Angstrom resolution  
Authors : Kappel, K.; Zhang, K.; Su, Z.; Watkins, A.M.; Kladwang, W.; Li, S.; Pintilie, G.; Topkar, V.V.; Rangan, R.; Zheludev, I.N.; Yesselman, J.D.; Chiu, W.; Das, R.  
Deposited on : 2020-04-20  
Resolution : 4.80 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](mailto: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>.

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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

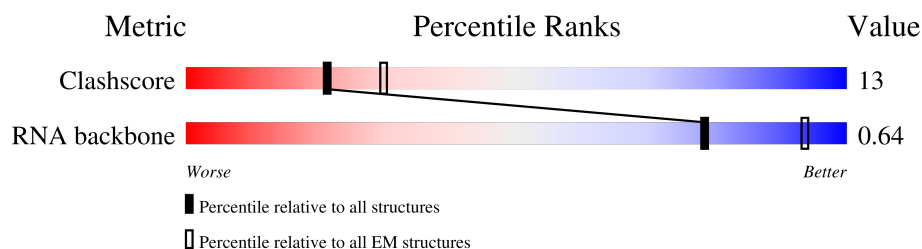
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	119	<div> <div>21%</div> <div>47%</div> <div>34%</div> <div>18%</div> <div>.</div> </div>
1	10-A	119	<div> <div>51%</div> <div>29%</div> <div>19%</div> </div>
1	11-A	119	<div> <div>50%</div> <div>36%</div> <div>13%</div> <div>.</div> </div>
1	12-A	119	<div> <div>56%</div> <div>30%</div> <div>13%</div> </div>
1	13-A	119	<div> <div>61%</div> <div>27%</div> <div>12%</div> </div>
1	14-A	119	<div> <div>54%</div> <div>30%</div> <div>16%</div> </div>
1	15-A	119	<div> <div>49%</div> <div>32%</div> <div>19%</div> </div>
1	16-A	119	<div> <div>46%</div> <div>36%</div> <div>18%</div> </div>
1	17-A	119	<div> <div>48%</div> <div>38%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	18-A	119	 49%37%14%
1	19-A	119	 45%39%14%.
1	2-A	119	 55%32%13%
1	20-A	119	 52%30%17%.
1	3-A	119	 53%32%14%.
1	4-A	119	 50%34%15%
1	5-A	119	 50%32%18%.
1	6-A	119	 56%29%14%
1	7-A	119	 57%29%13%.
1	8-A	119	 53%31%16%
1	9-A	119	 59%27%14%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 76720 atoms, of which 25780 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 (119-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	2-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	3-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	4-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	5-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	6-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	7-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	8-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	9-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	10-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	11-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	12-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	13-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	14-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	15-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	16-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0
1	17-A	119	Total 3836	C 1134	H 1289	N 465	O 830	P 118	0	0

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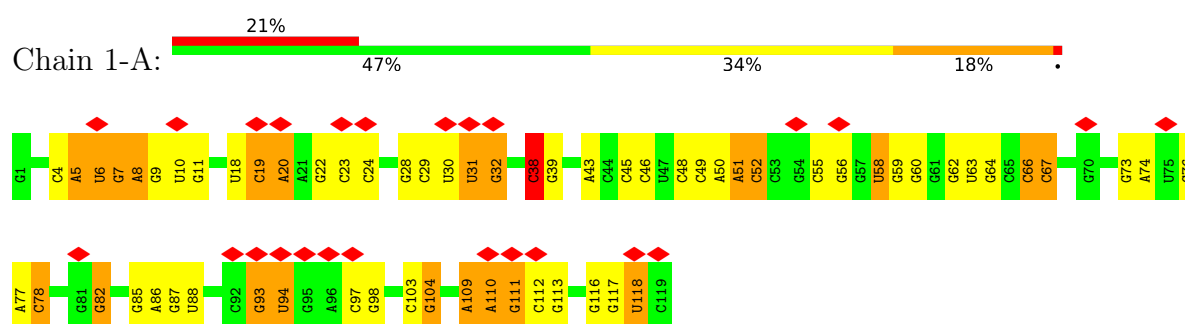
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Mol	Chain	Residues	Atoms						AltConf	Trace
1	18-A	119	Total	C	H	N	O	P	0	0
			3836	1134	1289	465	830	118		
1	19-A	119	Total	C	H	N	O	P	0	0
			3836	1134	1289	465	830	118		
1	20-A	119	Total	C	H	N	O	P	0	0
			3836	1134	1289	465	830	118		

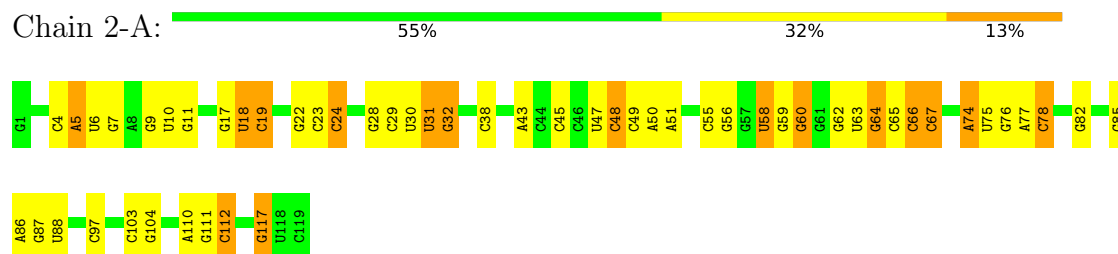
### 3 Residue-property plots

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.

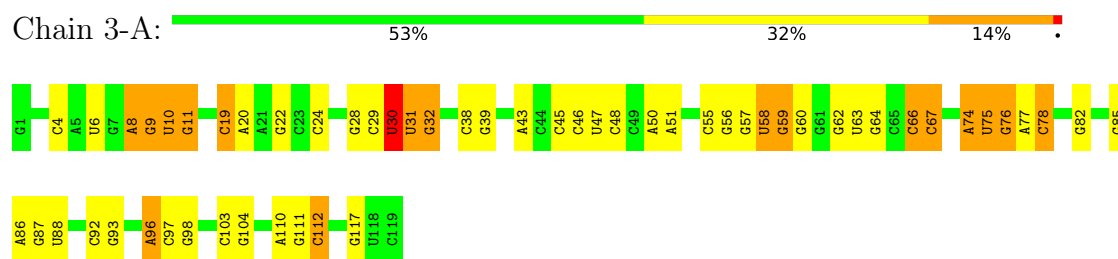
- Molecule 1: RNA (119-MER)



- Molecule 1: RNA (119-MER)

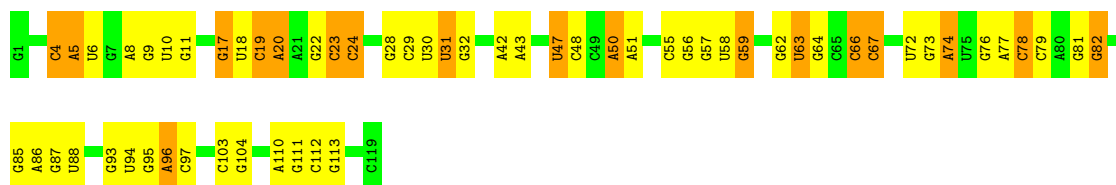


- Molecule 1: RNA (119-MER)



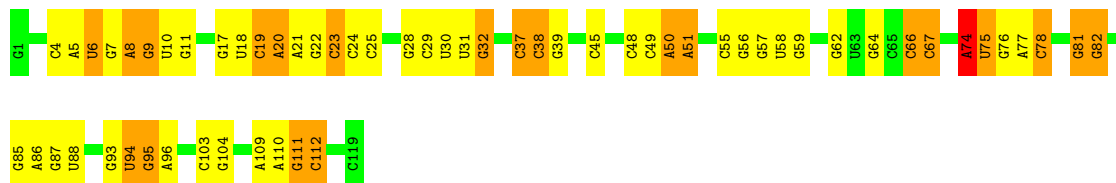
- Molecule 1: RNA (119-MER)





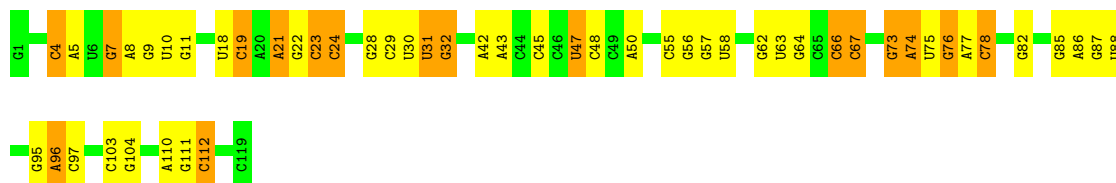
- Molecule 1: RNA (119-MER)

Chain 5-A: 50% 32% 18%



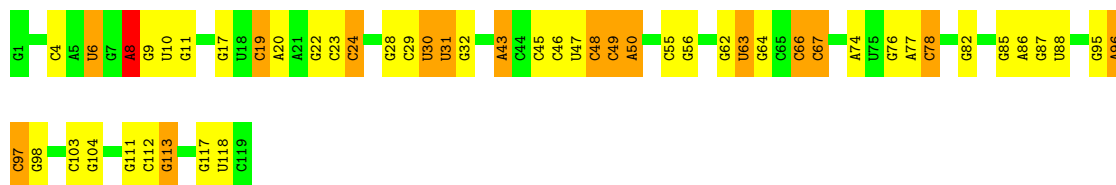
- Molecule 1: RNA (119-MER)

Chain 6-A: 56% 29% 14%



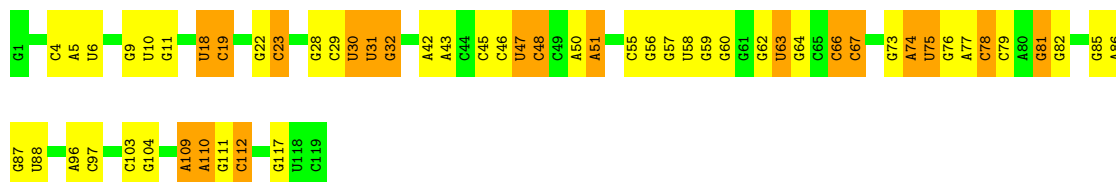
- Molecule 1: RNA (119-MER)

Chain 7-A: 57% 29% 13%



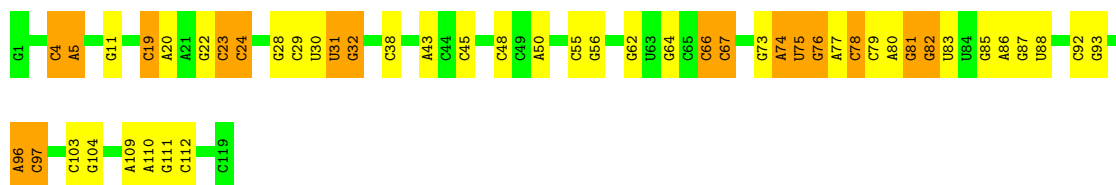
- Molecule 1: RNA (119-MER)

Chain 8-A: 53% 31% 16%

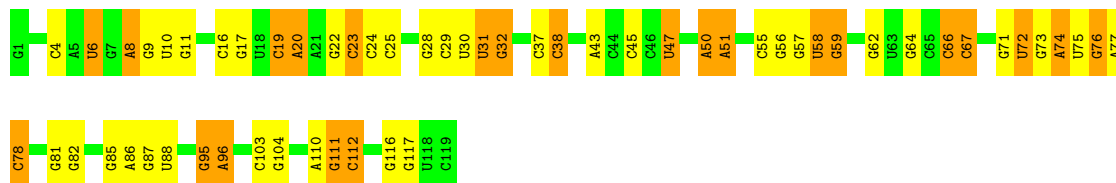


- Molecule 1: RNA (119-MER)

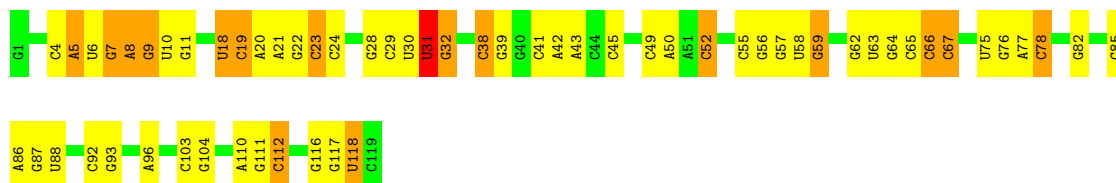
Chain 9-A: 59% 27% 14%



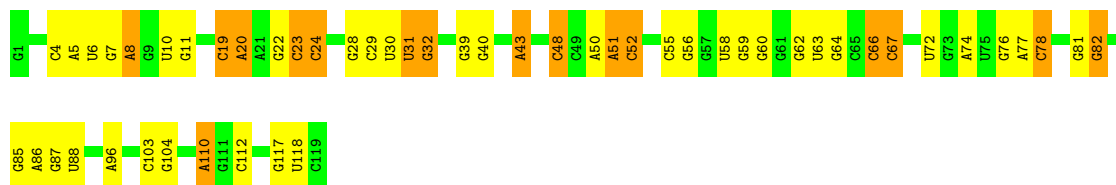
- Molecule 1: RNA (119-MER)



- Molecule 1: RNA (119-MER)



- Molecule 1: RNA (119-MER)



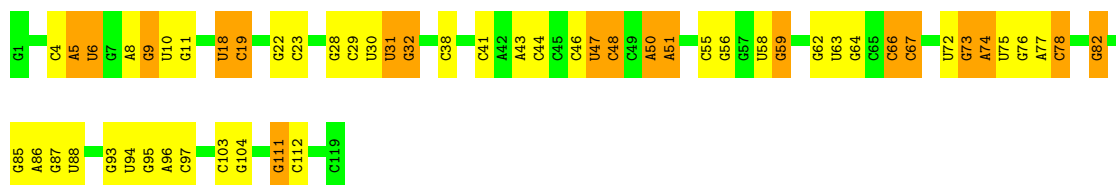
- Molecule 1: RNA (119-MER)



- Molecule 1: RNA (119-MER)

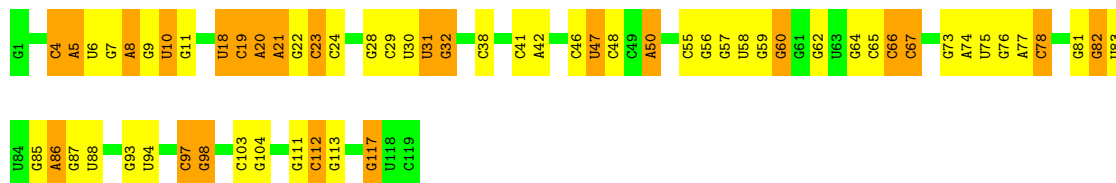






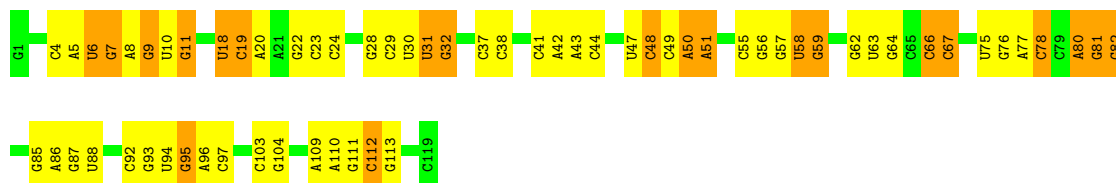
- Molecule 1: RNA (119-MER)

Chain 15-A:



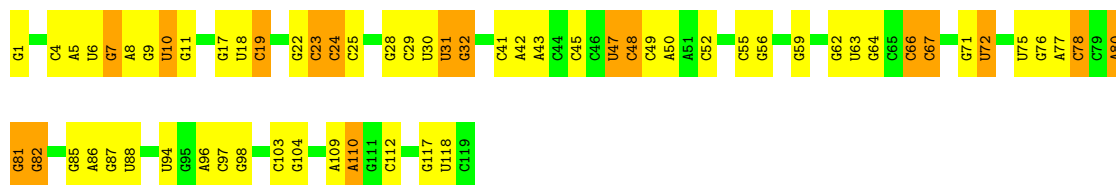
- Molecule 1: RNA (119-MER)

Chain 16-A:



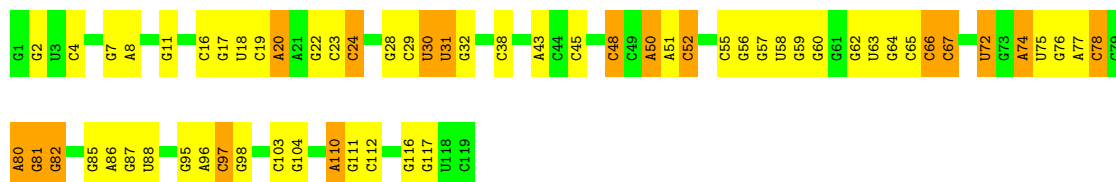
- Molecule 1: RNA (119-MER)

Chain 17-A:



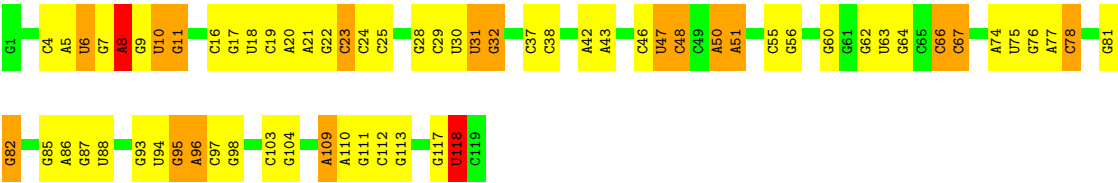
- Molecule 1: RNA (119-MER)

Chain 18-A:

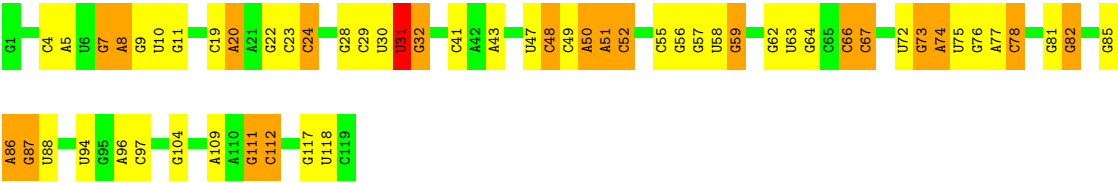


- Molecule 1: RNA (119-MER)

Chain 19-A:



● Molecule 1: RNA (119-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225303	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45.6	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	3.698	Depositor
Minimum map value	-2.322	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.287	Depositor
Recommended contour level	1.2	Depositor
Map size ( $\text{\AA}$ )	178.07999, 178.07999, 178.07999	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	1-A	0.37	0/2847	0.87	1/4442 (0.0%)
1	2-A	0.38	0/2847	0.89	2/4442 (0.0%)
1	3-A	0.40	0/2847	0.90	3/4442 (0.1%)
1	4-A	0.38	0/2847	0.89	1/4442 (0.0%)
1	5-A	0.39	0/2847	0.89	1/4442 (0.0%)
1	6-A	0.37	0/2847	0.87	0/4442
1	7-A	0.41	1/2847 (0.0%)	0.88	1/4442 (0.0%)
1	8-A	0.38	0/2847	0.88	0/4442
1	9-A	0.37	0/2847	0.87	0/4442
1	10-A	0.39	0/2847	0.88	0/4442
1	11-A	0.38	0/2847	0.88	1/4442 (0.0%)
1	12-A	0.38	0/2847	0.88	0/4442
1	13-A	0.39	0/2847	0.89	0/4442
1	14-A	0.39	1/2847 (0.0%)	0.86	0/4442
1	15-A	0.38	0/2847	0.87	0/4442
1	16-A	0.38	0/2847	0.87	1/4442 (0.0%)
1	17-A	0.38	0/2847	0.87	0/4442
1	18-A	0.39	0/2847	0.89	0/4442
1	19-A	0.39	0/2847	0.93	4/4442 (0.1%)
1	20-A	0.40	1/2847 (0.0%)	0.91	5/4442 (0.1%)
All	All	0.39	3/56940 (0.0%)	0.88	20/88840 (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
1	19-A	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	49	C	O3'-P	-9.10	1.50	1.61
1	14-A	59	G	C3'-C2'	-6.55	1.45	1.52
1	20-A	94	U	C4'-O4'	-5.12	1.38	1.45

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	19-A	8	A	C2'-C3'-O3'	13.92	140.13	109.50
1	7-A	8	A	C5'-C4'-O4'	9.13	120.06	109.10
1	19-A	118	U	C5'-C4'-O4'	8.73	119.58	109.10
1	3-A	38	C	O4'-C1'-N1	8.53	115.03	108.20
1	2-A	112	C	O4'-C1'-N1	7.43	114.14	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	19-A	8	A	C3'

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	1-A	2547	1289	1290	47	0
1	2-A	2547	1289	1290	55	0
1	3-A	2547	1289	1290	50	0
1	4-A	2547	1289	1290	44	0
1	5-A	2547	1289	1290	65	0
1	6-A	2547	1289	1290	49	0
1	7-A	2547	1289	1290	36	0
1	8-A	2547	1289	1290	57	0
1	9-A	2547	1289	1290	48	0
1	10-A	2547	1289	1290	61	0
1	11-A	2547	1289	1290	52	0
1	12-A	2547	1289	1290	47	0
1	13-A	2547	1289	1290	33	0
1	14-A	2547	1289	1290	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	15-A	2547	1289	1290	53	0
1	16-A	2547	1289	1290	54	0
1	17-A	2547	1289	1290	59	0
1	18-A	2547	1289	1290	45	0
1	19-A	2547	1289	1290	48	0
1	20-A	2547	1289	1290	51	0
All	All	50940	25780	25800	1007	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 13.

The worst 5 of 1007 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:32:G:C8	1:A:32:G:OP2	1.77	1.36
1:A:20:A:H8	1:A:20:A:OP2	1.09	1.35
1:A:32:G:OP1	1:A:32:G:C8	1.84	1.31
1:A:32:G:OP2	1:A:32:G:O4'	1.53	1.25
1:A:32:G:OP1	1:A:32:G:C8	1.90	1.24

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	1-A	118/119 (99%)	29 (24%)	5 (4%)
1	10-A	118/119 (99%)	27 (22%)	6 (5%)
1	11-A	118/119 (99%)	24 (20%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	12-A	118/119 (99%)	24 (20%)	3 (2%)
1	13-A	118/119 (99%)	22 (18%)	1 (0%)
1	14-A	118/119 (99%)	22 (18%)	4 (3%)
1	15-A	118/119 (99%)	28 (23%)	3 (2%)
1	16-A	118/119 (99%)	27 (22%)	4 (3%)
1	17-A	118/119 (99%)	23 (19%)	1 (0%)
1	18-A	118/119 (99%)	21 (17%)	3 (2%)
1	19-A	118/119 (99%)	28 (23%)	3 (2%)
1	2-A	118/119 (99%)	23 (19%)	4 (3%)
1	20-A	118/119 (99%)	29 (24%)	3 (2%)
1	3-A	118/119 (99%)	23 (19%)	5 (4%)
1	4-A	118/119 (99%)	24 (20%)	2 (1%)
1	5-A	118/119 (99%)	26 (22%)	3 (2%)
1	6-A	118/119 (99%)	23 (19%)	1 (0%)
1	7-A	118/119 (99%)	21 (17%)	4 (3%)
1	8-A	118/119 (99%)	24 (20%)	4 (3%)
1	9-A	118/119 (99%)	23 (19%)	3 (2%)
All	All	2360/2380 (99%)	491 (20%)	64 (2%)

5 of 491 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1-A	4	C
1	1-A	5	A
1	1-A	6	U
1	1-A	7	G
1	1-A	9	G

5 of 64 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	18-A	80	A
1	19-A	10	U
1	8-A	18	U
1	7-A	96	A
1	19-A	66	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 [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.



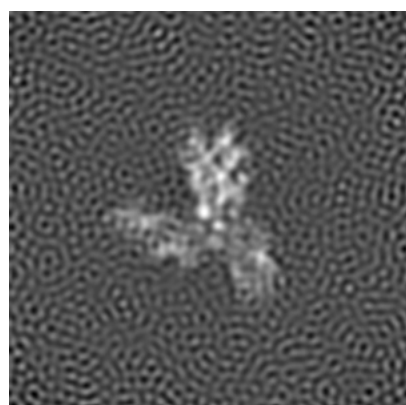
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21839. These allow visual inspection of the internal detail of the map and identification of artifacts.

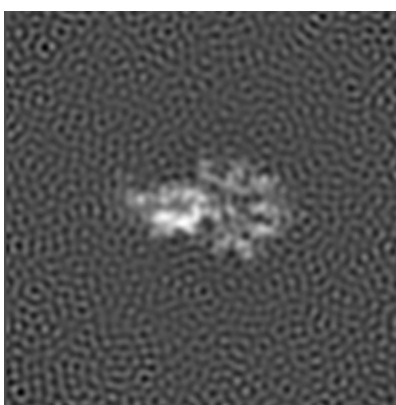
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

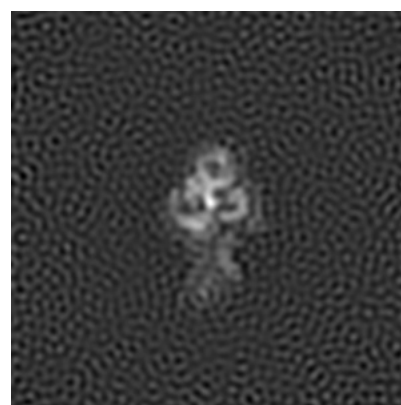
#### 6.1.1 Primary map



X



Y

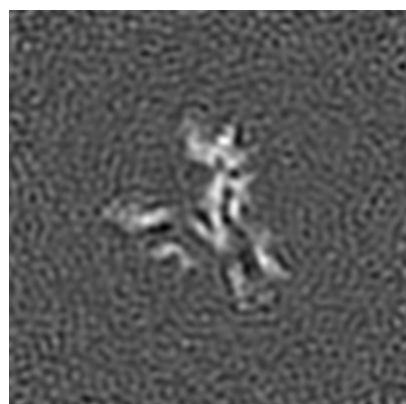


Z

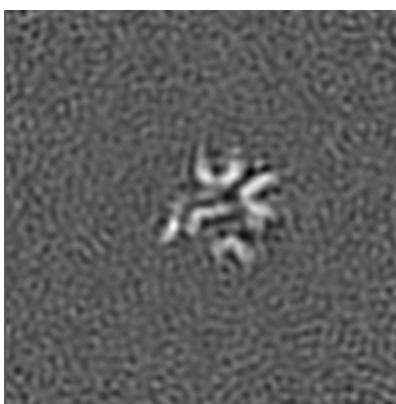
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 84



Y Index: 84

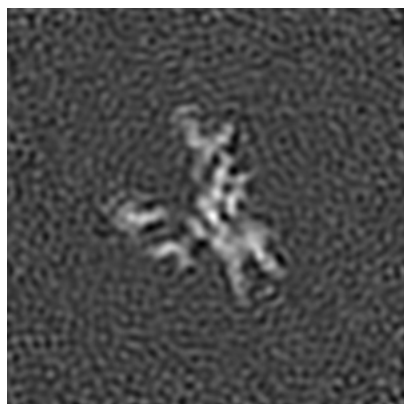


Z Index: 84

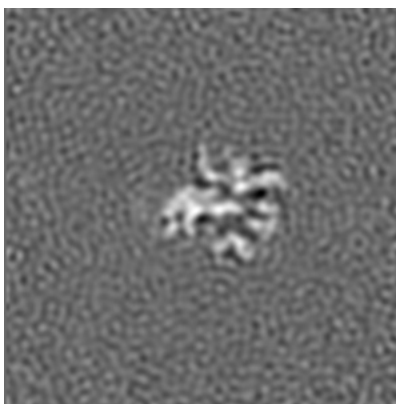
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

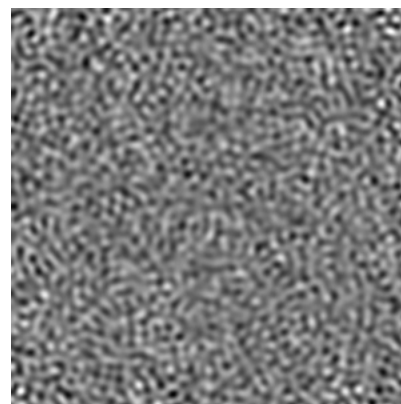
### 6.3.1 Primary map



X Index: 82



Y Index: 87



Z Index: 167

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

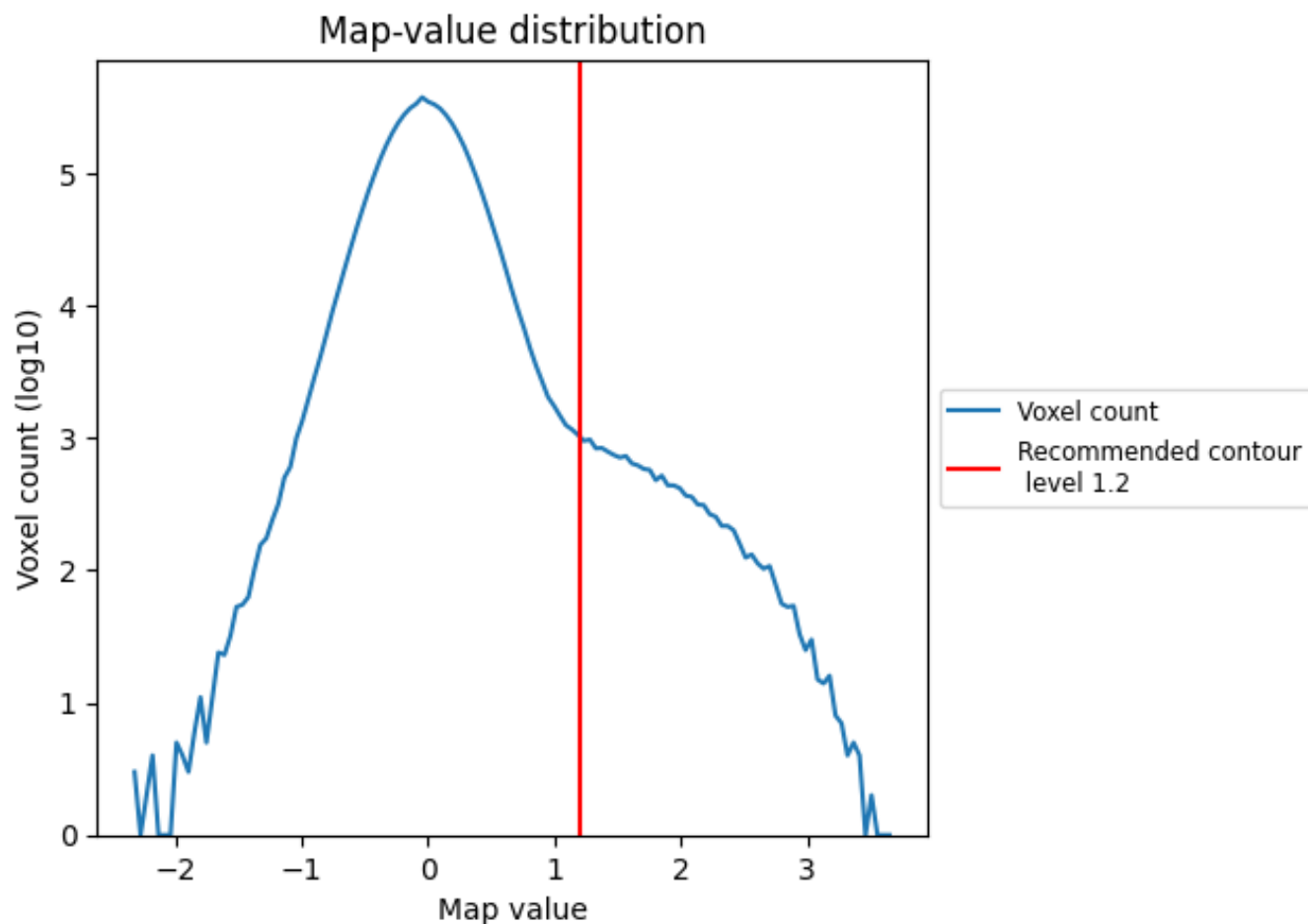
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

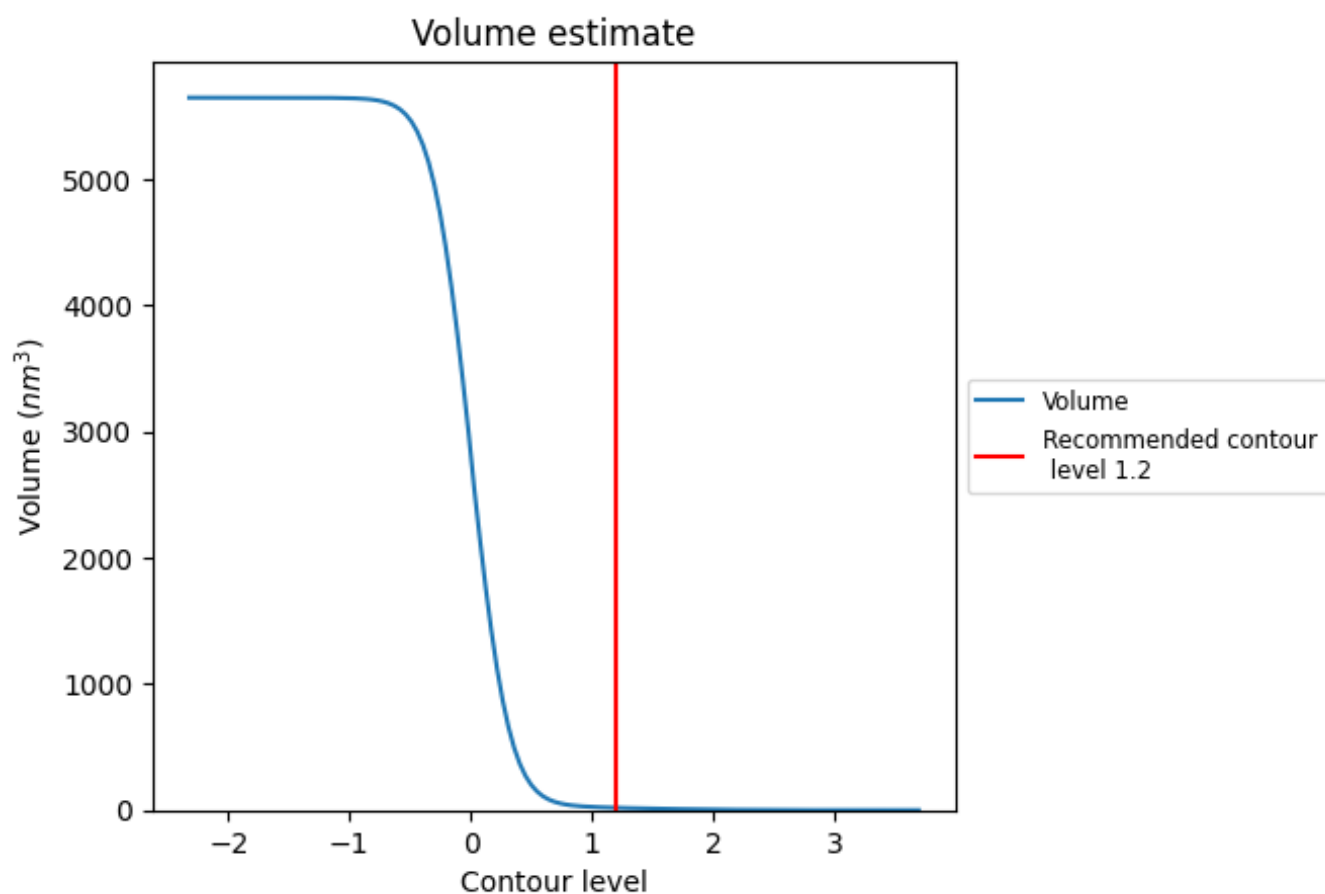
This section contains the results of statistical analysis of the map.

### 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.

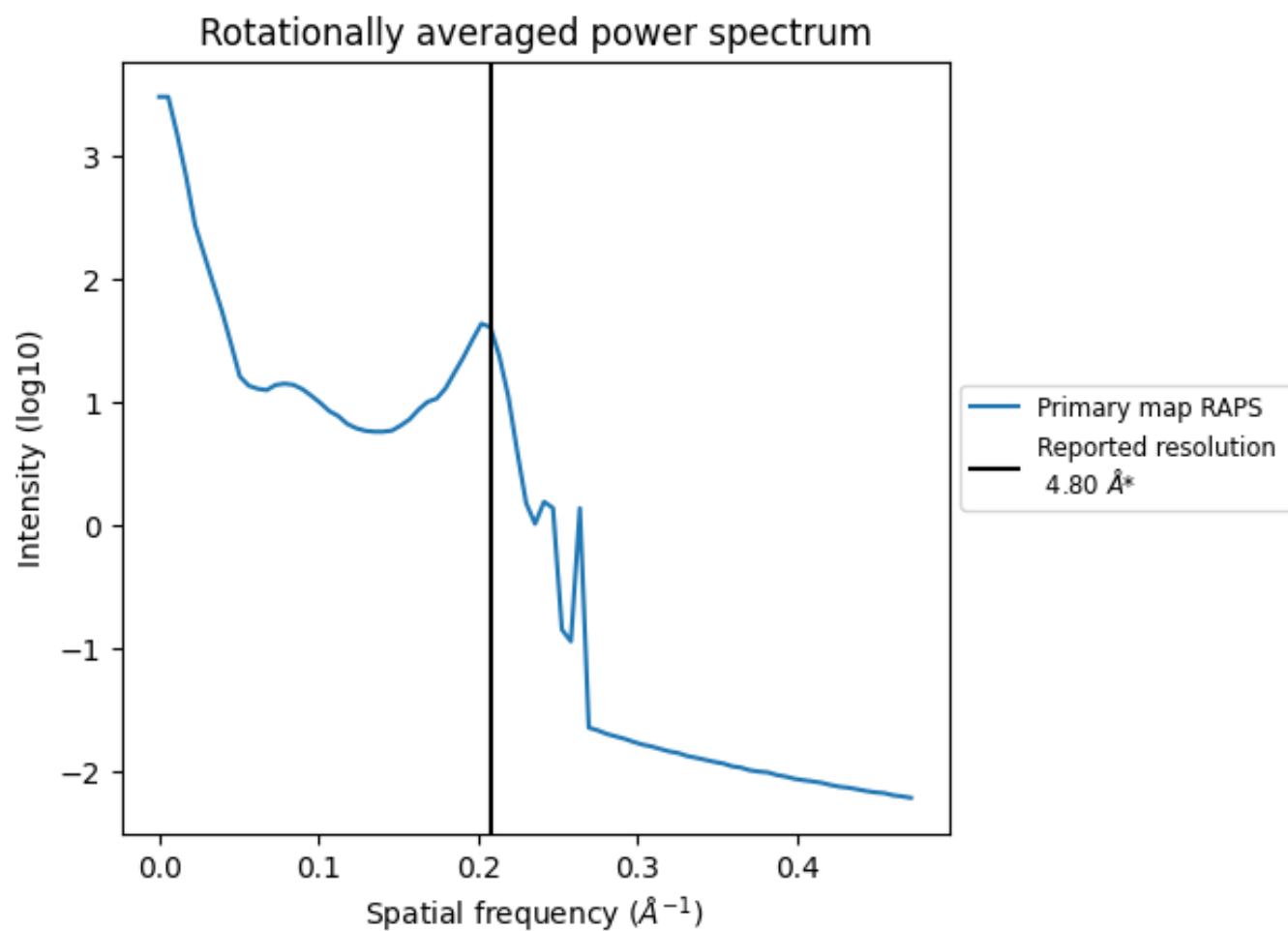
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 19 nm<sup>3</sup>; this corresponds to an approximate mass of 17 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 0.208 Å<sup>-1</sup>

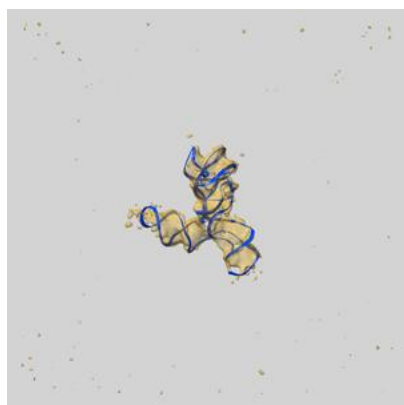
## 8 Fourier-Shell correlation

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

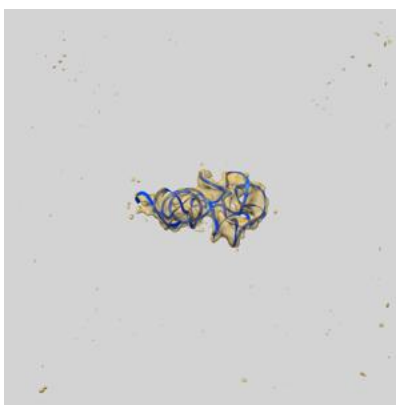
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21839 and PDB model 6WLR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

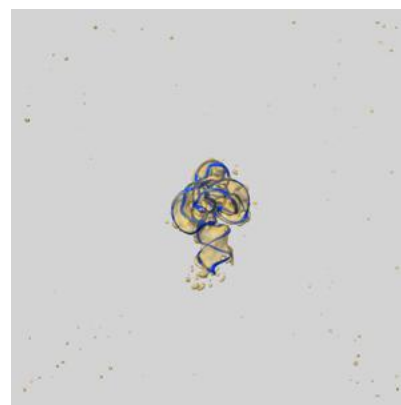
### 9.1 Map-model overlay [i](#)



X



Y



Z

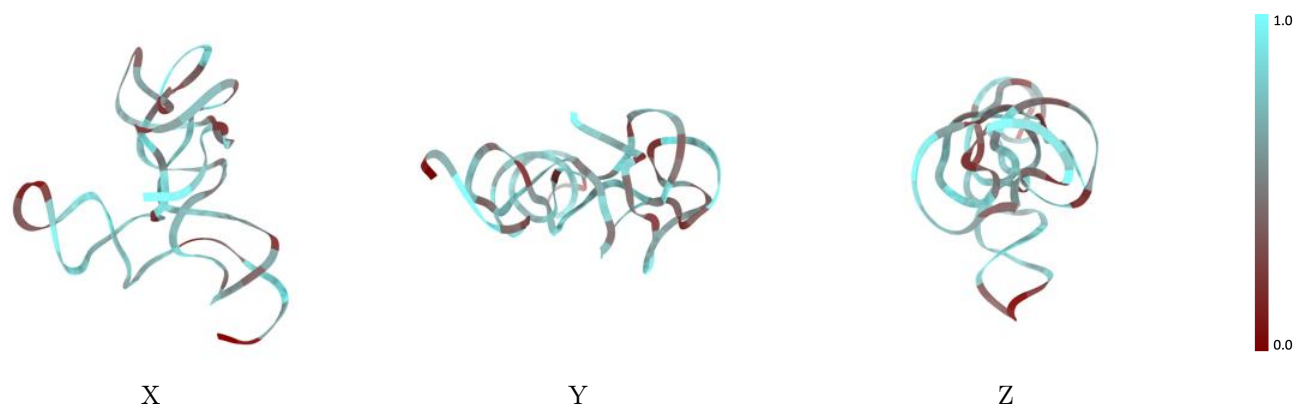
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



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

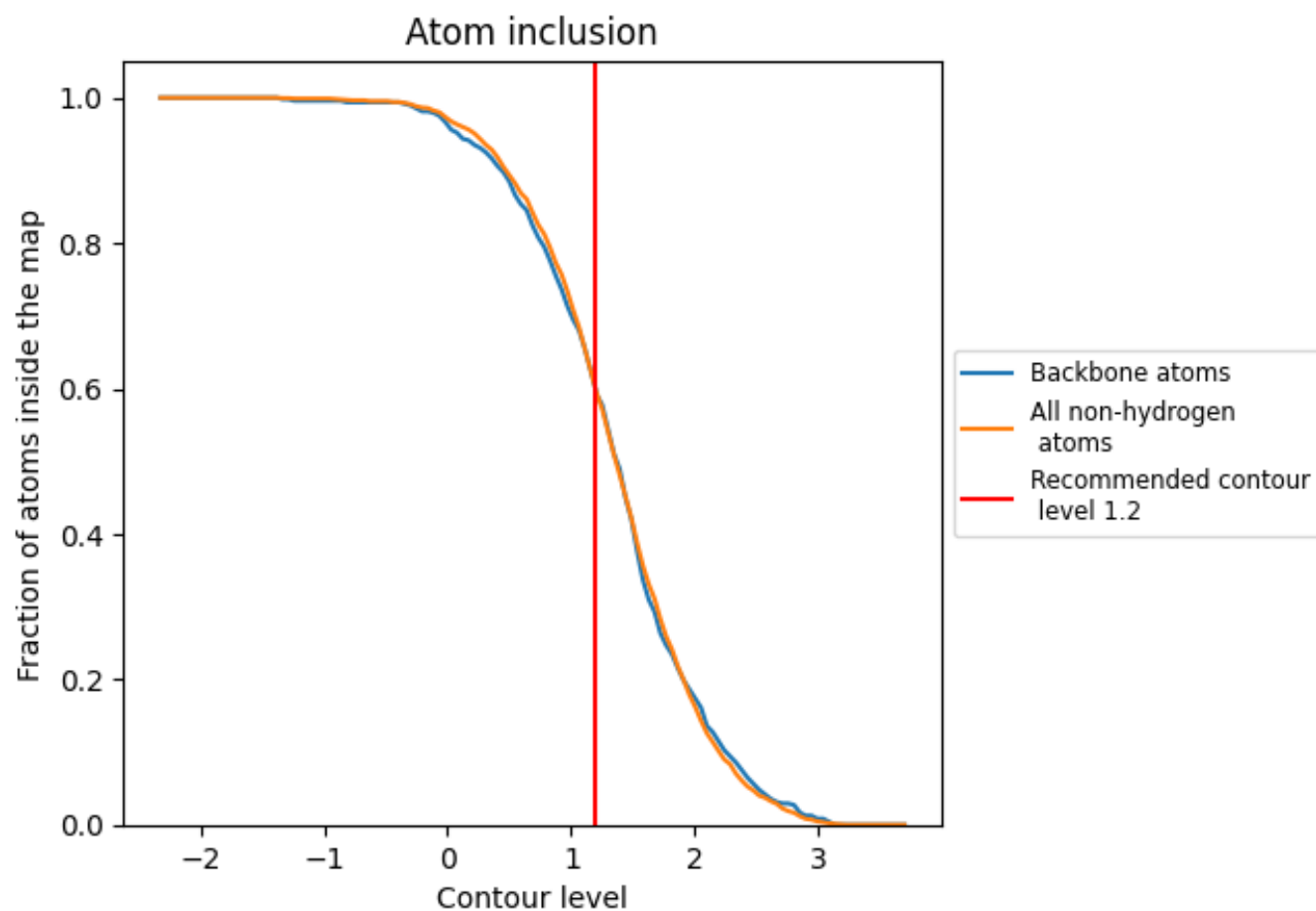
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 60% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	<div></div> 0.5969
A	<div></div> 0.5991

