



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:45 PM EST

PDB ID : 7S9U  
EMDB ID : EMD-24937  
Title : 44SR3C ribosomal particle  
Authors : Ortega, J.; Seffouh, A.  
Deposited on : 2021-09-21  
Resolution : 3.20 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>.

---

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

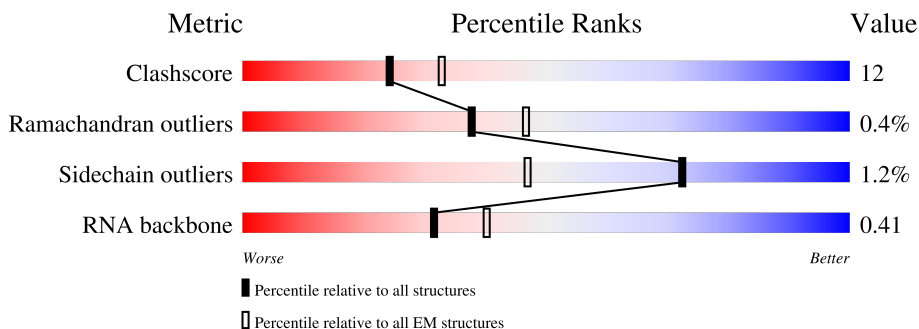
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.20 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.






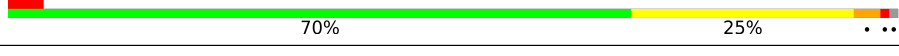

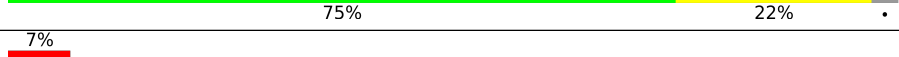

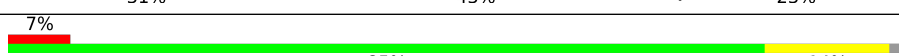
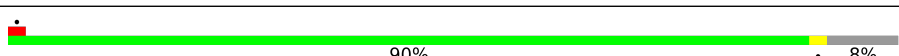

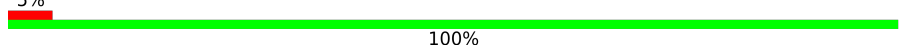

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	A	2928	8% (poor fit), 42% (0 outliers), 29% (1 outlier), 12% (2 outliers), 17% (3+ outliers)
2	C	277	22% (poor fit), 70% (0 outliers), 26% (1 outlier), 2% (2 outliers), 2% (3+ outliers)
3	D	209	5% (poor fit), 73% (0 outliers), 13% (1 outlier), 14% (2 outliers), 1% (3+ outliers)
4	E	207	8% (poor fit), 77% (0 outliers), 22% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
5	J	145	0% (poor fit), 72% (0 outliers), 25% (1 outlier), 3% (2 outliers), 0% (3+ outliers)
6	K	122	16% (poor fit), 80% (0 outliers), 20% (1 outlier), 4% (2 outliers), 0% (3+ outliers)
7	L	146	23% (poor fit), 65% (0 outliers), 23% (1 outlier), 9% (2 outliers), 0% (3+ outliers)

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
8	N	120	 80% 19%
9	P	115	 19% 75% 24%
10	Q	119	 67% 27%
11	R	102	 70% 25%
12	S	113	 76% 19%
13	T	95	 75% 22%
14	U	103	 7% 75% 22%
15	V	94	 63% 31% 43% 23%
16	Z	59	 7% 85% 14%
17	b	59	 90% 8%
18	Y	66	 6% 74% 24%
19	d	44	 5% 100%

## 2 Entry composition i

There are 19 unique types of molecules in this entry. The entry contains 68620 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 (2436-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2436	52346	23355	9704	16851	2436	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1558	C	G	conflict	GB 1864548803

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	267	2052	1277	402	367	6	0	0

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	179	1354	854	241	256	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	205	1561	980	289	290	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	142	1123	710	206	202	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 7 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	130	Total	C	N	O	S	0	0
			973	608	183	180	2		

- Molecule 8 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 9 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	114	Total	C	N	O	0	0
			936	595	184	157		

- Molecule 10 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 11 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	101	Total	C	N	O	0	0
			786	501	139	146		

- Molecule 12 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 13 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	92	Total	C	N	O	S	0	0
			741	463	136	138	4		

- Molecule 14 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	100	Total	C	N	O	S	0	0
			754	473	141	137	3		

- Molecule 15 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	72	Total	C	N	O	0	0
			561	349	109	103		

- Molecule 16 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 17 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

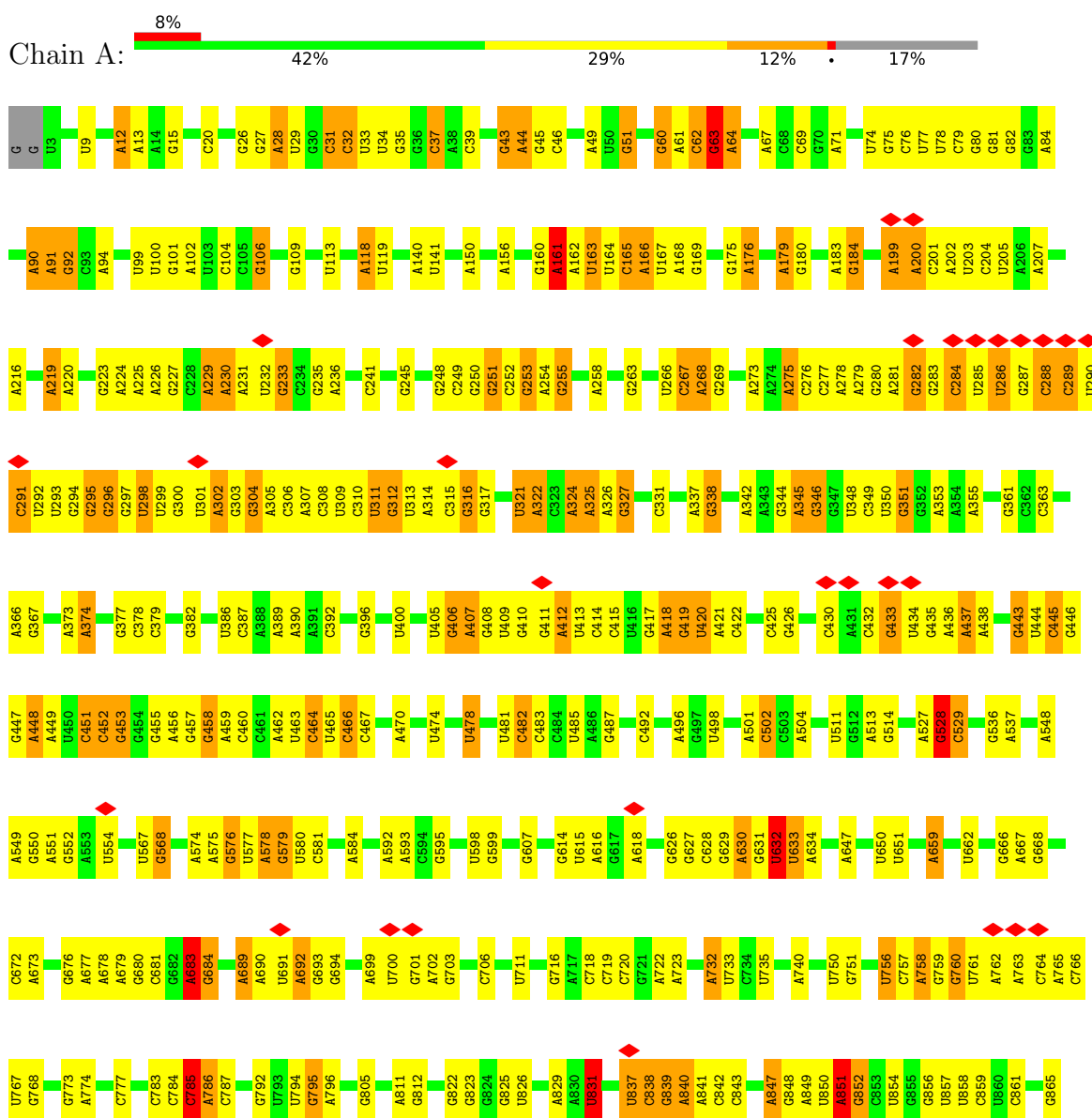
- Molecule 19 is a protein called 50S ribosomal protein L34.

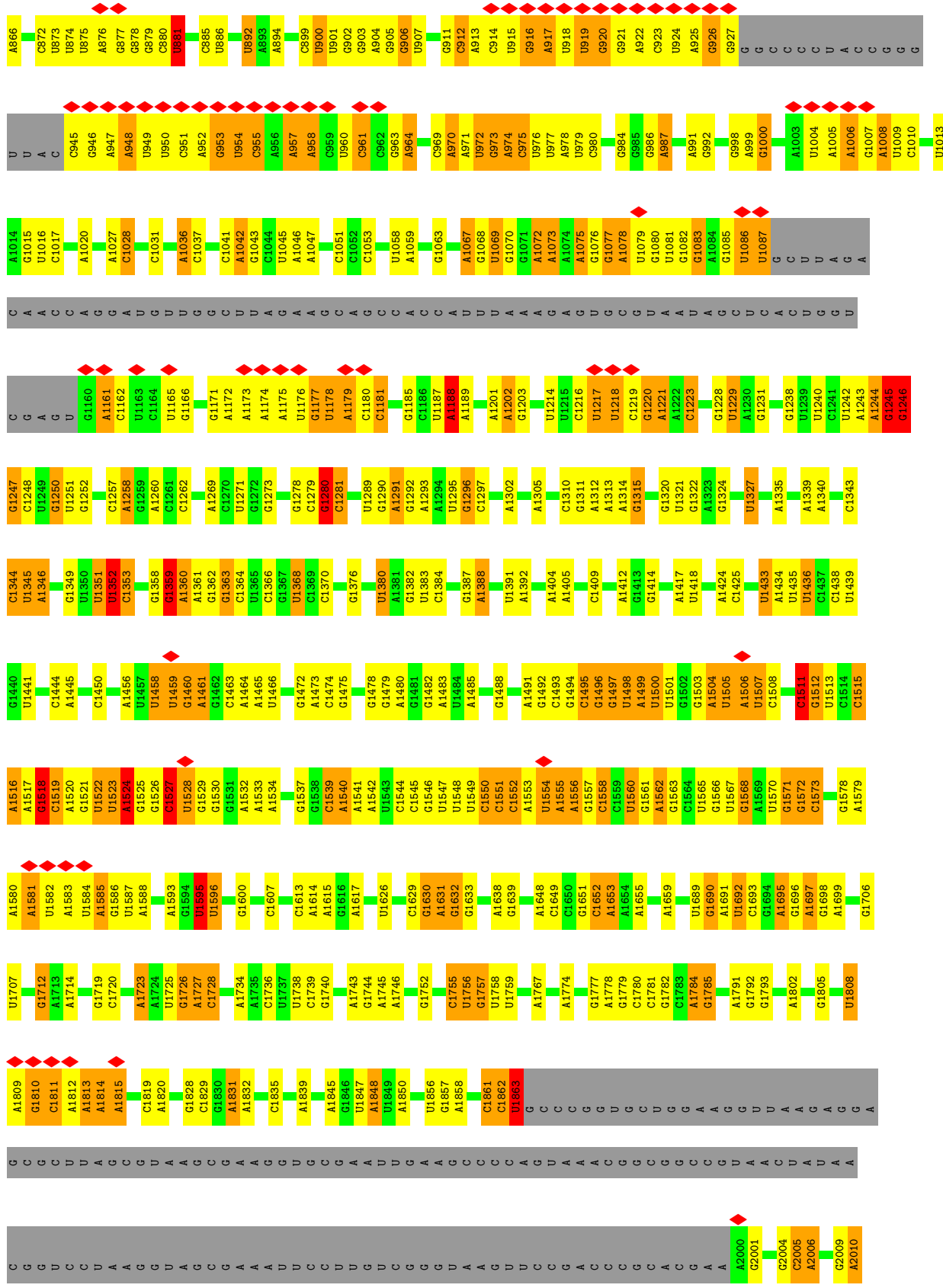
Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

### 3 Residue-property plots

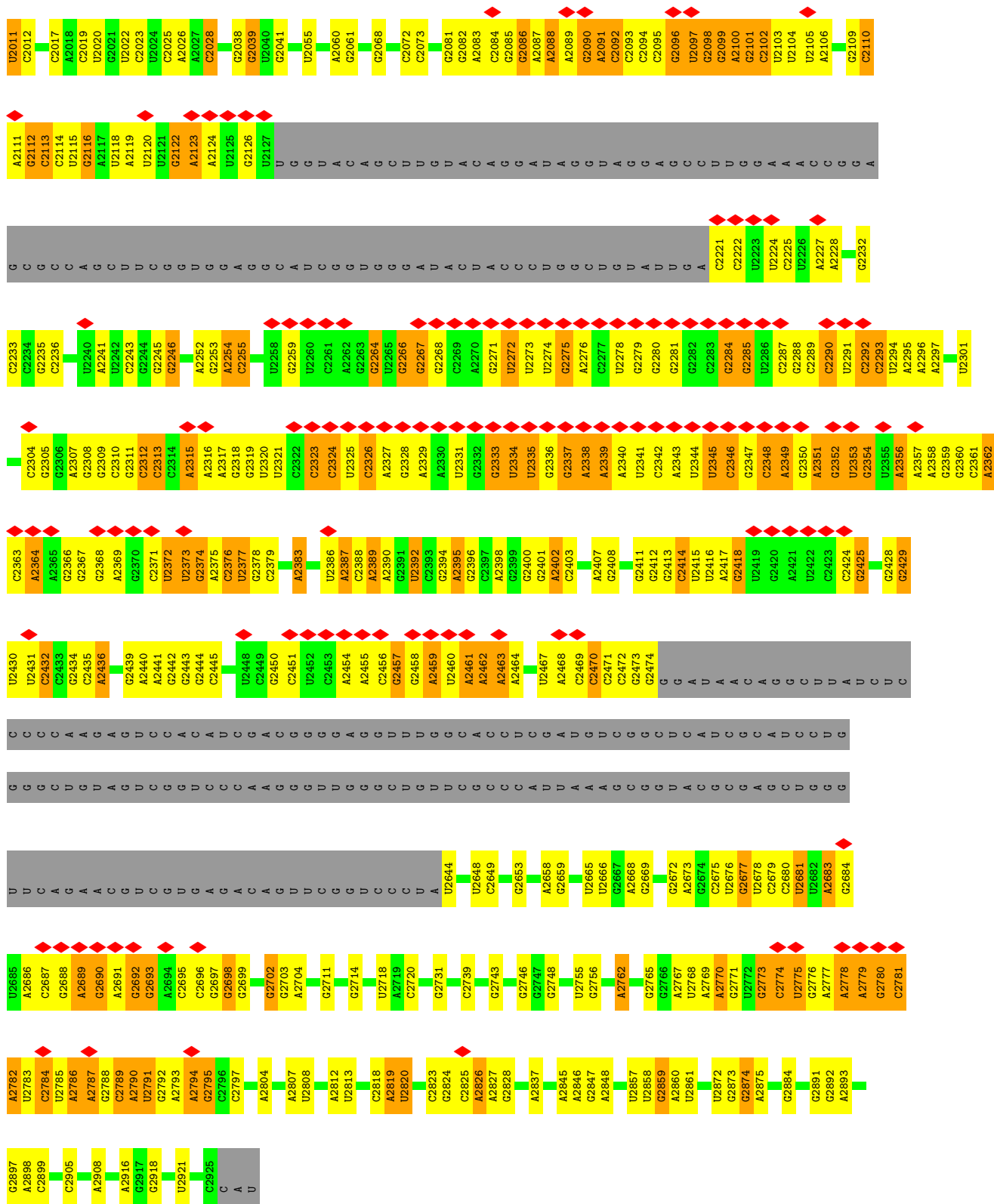
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 (2436-MER)



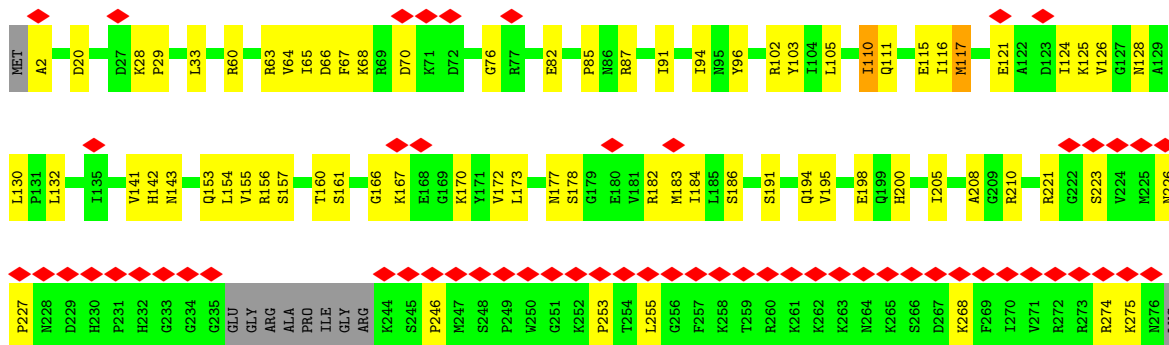




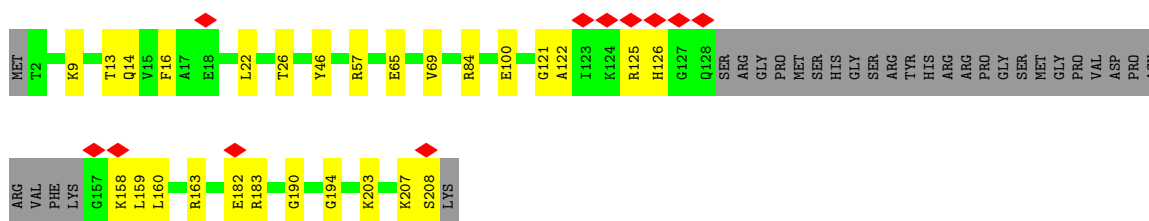


• Molecule 2: 50S ribosomal protein L2

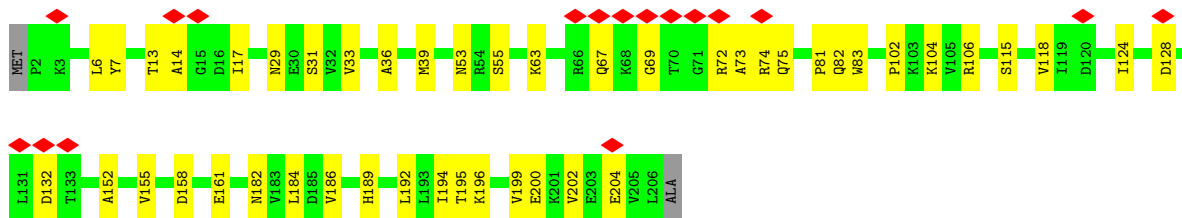
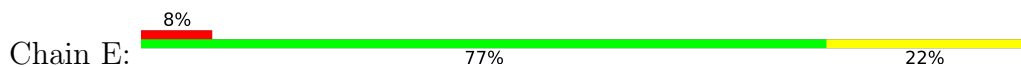




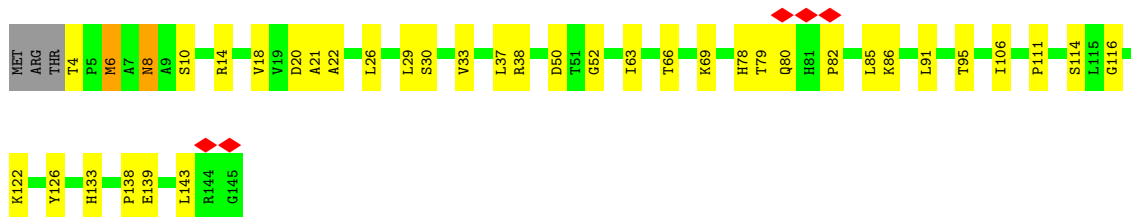
• Molecule 3: 50S ribosomal protein L3



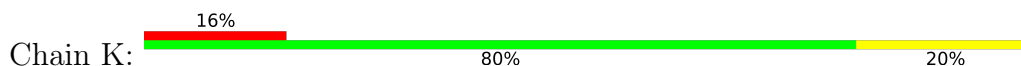
• Molecule 4: 50S ribosomal protein L4

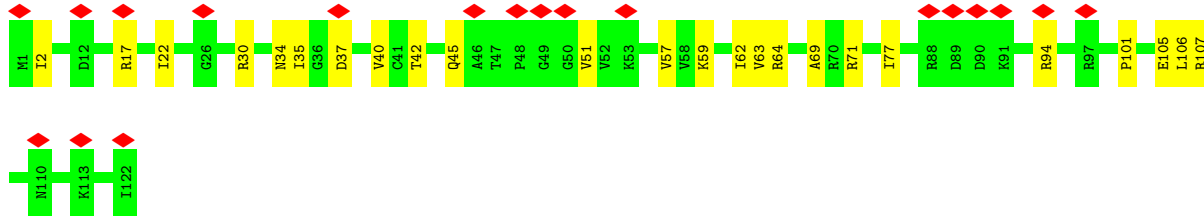


• Molecule 5: 50S ribosomal protein L13

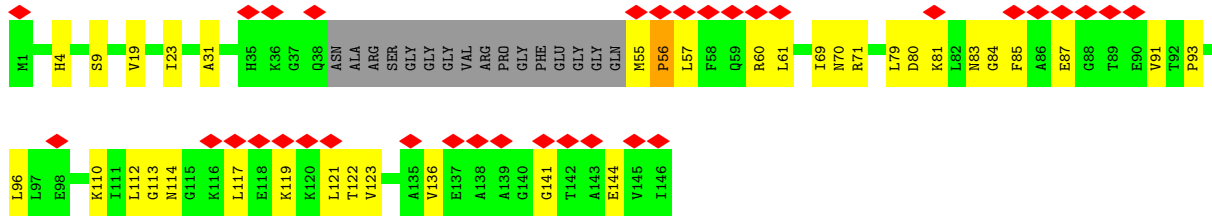


• Molecule 6: 50S ribosomal protein L14

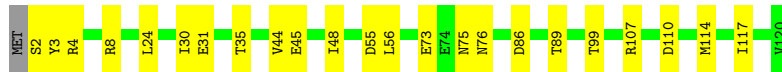
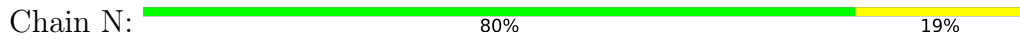




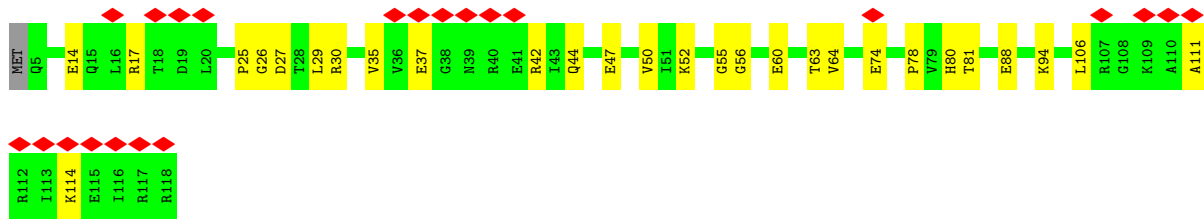
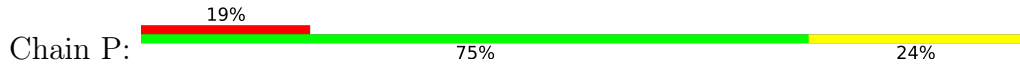
• Molecule 7: 50S ribosomal protein L15



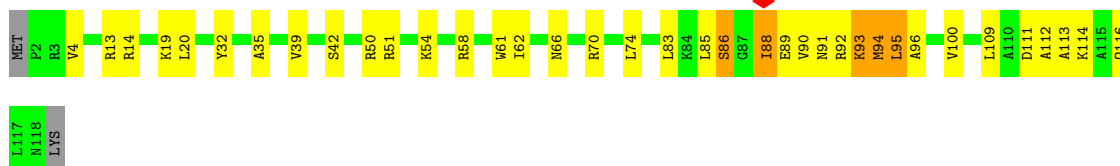
• Molecule 8: 50S ribosomal protein L17



• Molecule 9: 50S ribosomal protein L19

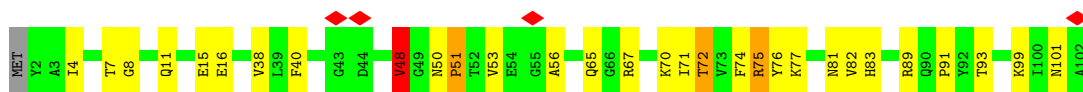


• Molecule 10: 50S ribosomal protein L20

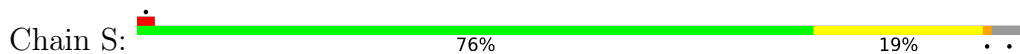


• Molecule 11: 50S ribosomal protein L21

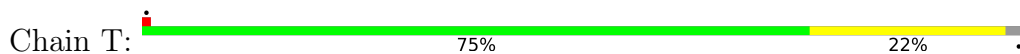




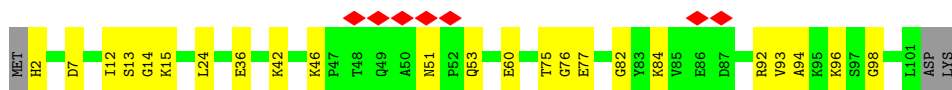
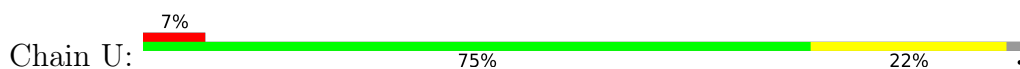
• Molecule 12: 50S ribosomal protein L22



• Molecule 13: 50S ribosomal protein L23



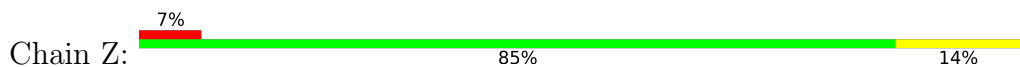
• Molecule 14: 50S ribosomal protein L24



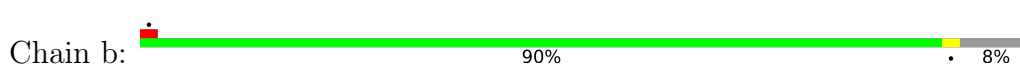
• Molecule 15: 50S ribosomal protein L27

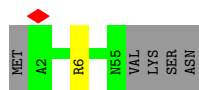


• Molecule 16: 50S ribosomal protein L30

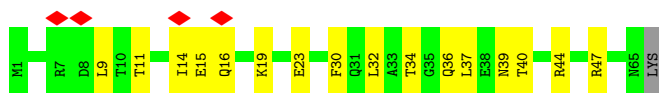
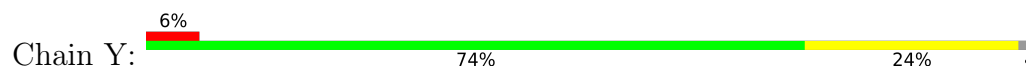


• Molecule 17: 50S ribosomal protein L32





- Molecule 18: 50S ribosomal protein L29



- Molecule 19: 50S ribosomal protein L34



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121252	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00983	Depositor
Map size (Å)	287.28, 287.28, 287.28	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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	1.20	40/58643 (0.1%)	1.05	141/91483 (0.2%)
2	C	0.44	0/2087	0.50	0/2798
3	D	0.60	0/1367	0.55	0/1830
4	E	0.66	0/1580	0.59	0/2132
5	J	0.64	0/1146	0.57	0/1542
6	K	0.47	0/927	0.54	0/1245
7	L	0.46	0/982	0.54	0/1308
8	N	0.66	0/960	0.61	0/1284
9	P	0.56	0/949	0.54	0/1269
10	Q	0.78	0/952	0.66	0/1266
11	R	0.60	0/797	0.58	0/1070
12	S	0.60	0/851	0.59	0/1146
13	T	0.62	0/747	0.56	0/995
14	U	0.58	0/764	0.54	0/1022
15	V	0.29	0/569	0.46	0/757
16	Z	0.50	0/457	0.52	0/613
17	b	0.61	0/433	0.52	0/574
18	Y	0.52	0/531	0.54	0/707
19	d	0.68	0/370	0.56	0/483
All	All	1.09	40/75112 (0.1%)	0.97	141/113524 (0.1%)

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1250	G	N9-C4	-7.41	1.32	1.38
1	A	1291	A	N9-C4	-6.89	1.33	1.37
1	A	1291	A	N7-C5	-6.45	1.35	1.39
1	A	1291	A	C5-C6	-6.07	1.35	1.41
1	A	719	C	N1-C6	-6.05	1.33	1.37

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	A	O5'-P-OP2	-19.58	87.21	110.70
1	A	1511	C	P-O3'-C3'	13.47	135.86	119.70
1	A	160	G	P-O3'-C3'	11.29	133.25	119.70
1	A	1250	G	N3-C4-C5	11.28	134.24	128.60
1	A	161	A	O5'-P-OP1	10.05	122.76	110.70

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	52346	0	26332	882	0
2	C	2052	0	2138	75	0
3	D	1354	0	1425	21	0
4	E	1561	0	1647	35	0
5	J	1123	0	1162	28	0
6	K	920	0	977	13	0
7	L	973	0	1032	31	0
8	N	953	0	983	14	0
9	P	936	0	1008	20	0
10	Q	940	0	1005	50	0
11	R	786	0	826	40	0
12	S	842	0	899	17	0
13	T	741	0	793	17	0
14	U	754	0	809	16	0
15	V	561	0	567	90	0
16	Z	455	0	491	5	0
17	b	426	0	443	0	0
18	Y	530	0	568	12	0
19	d	367	0	410	0	0
All	All	68620	0	43515	1280	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 12.

The worst 5 of 1280 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:2351:A:N6	1:A:2362:A:N6	1.62	1.42
1:A:2434:G:N2	1:A:2442:G:C6	1.94	1.35
1:A:2292:C:N4	1:A:2307:A:C6	1.96	1.34
1:A:1525:G:C2	1:A:1560:U:O2	1.81	1.33
1:A:2328:G:O6	1:A:2347:G:N2	1.63	1.32

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	C	263/277 (95%)	219 (83%)	44 (17%)	0	100	100
3	D	175/209 (84%)	155 (89%)	20 (11%)	0	100	100
4	E	203/207 (98%)	165 (81%)	38 (19%)	0	100	100
5	J	140/145 (97%)	124 (89%)	16 (11%)	0	100	100
6	K	120/122 (98%)	101 (84%)	19 (16%)	0	100	100
7	L	126/146 (86%)	107 (85%)	18 (14%)	1 (1%)	19	58
8	N	117/120 (98%)	101 (86%)	16 (14%)	0	100	100
9	P	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
10	Q	115/119 (97%)	94 (82%)	18 (16%)	3 (3%)	5	31
11	R	99/102 (97%)	81 (82%)	16 (16%)	2 (2%)	7	38
12	S	107/113 (95%)	97 (91%)	9 (8%)	1 (1%)	17	56
13	T	90/95 (95%)	74 (82%)	16 (18%)	0	100	100
14	U	98/103 (95%)	75 (76%)	23 (24%)	0	100	100
15	V	70/94 (74%)	48 (69%)	21 (30%)	1 (1%)	11	46
16	Z	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
17	b	52/59 (88%)	45 (86%)	7 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Y	63/66 (96%)	52 (82%)	10 (16%)	1 (2%)	9	43
19	d	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
All	All	2048/2195 (93%)	1727 (84%)	312 (15%)	9 (0%)	38	69

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	L	56	PRO
10	Q	86	SER
11	R	51	PRO
10	Q	88	ILE
12	S	11	ARG

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	218/225 (97%)	212 (97%)	6 (3%)	43	74
3	D	144/170 (85%)	144 (100%)	0	100	100
4	E	169/170 (99%)	168 (99%)	1 (1%)	86	94
5	J	120/123 (98%)	117 (98%)	3 (2%)	47	77
6	K	101/101 (100%)	101 (100%)	0	100	100
7	L	101/110 (92%)	100 (99%)	1 (1%)	76	90
8	N	99/100 (99%)	99 (100%)	0	100	100
9	P	99/100 (99%)	99 (100%)	0	100	100
10	Q	96/98 (98%)	93 (97%)	3 (3%)	40	72
11	R	83/84 (99%)	80 (96%)	3 (4%)	35	69
12	S	90/93 (97%)	90 (100%)	0	100	100
13	T	83/85 (98%)	83 (100%)	0	100	100
14	U	84/87 (97%)	84 (100%)	0	100	100
15	V	56/74 (76%)	54 (96%)	2 (4%)	35	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Z	52/53 (98%)	52 (100%)	0	100	100
17	b	48/53 (91%)	47 (98%)	1 (2%)	53	79
18	Y	56/57 (98%)	56 (100%)	0	100	100
19	d	39/39 (100%)	39 (100%)	0	100	100
All	All	1738/1822 (95%)	1718 (99%)	20 (1%)	72	88

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	R	48	VAL
15	V	28	ARG
17	b	6	ARG
15	V	80	PHE
4	E	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
11	R	65	GLN
11	R	83	HIS
17	b	40	HIS
12	S	37	ASN
14	U	53	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2430/2928 (82%)	729 (30%)	47 (1%)

5 of 729 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	12	A
1	A	13	A
1	A	15	G
1	A	28	A

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1595	U
1	A	1861	C
1	A	1630	G
1	A	1755	C
1	A	2099	G

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

#### 5.7 Other polymers [i](#)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

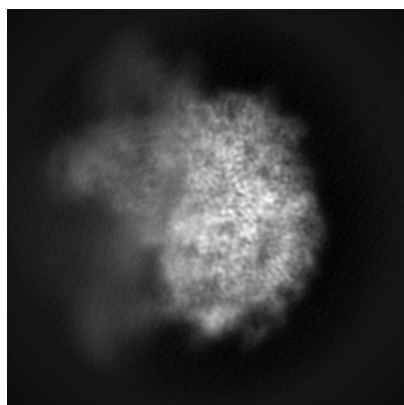
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24937. These allow visual inspection of the internal detail of the map and identification of artifacts.

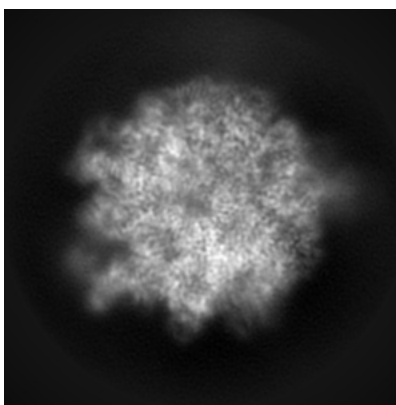
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

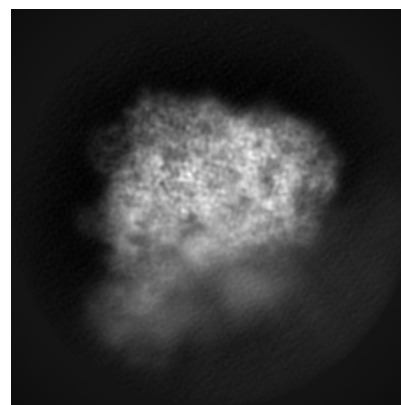
#### 6.1.1 Primary map



X



Y

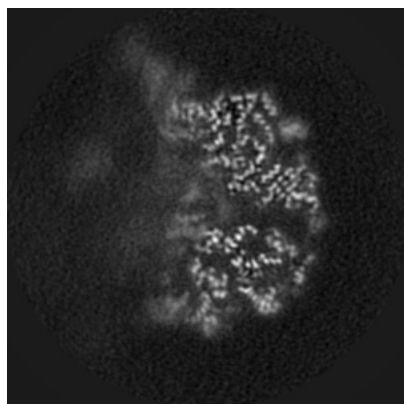


Z

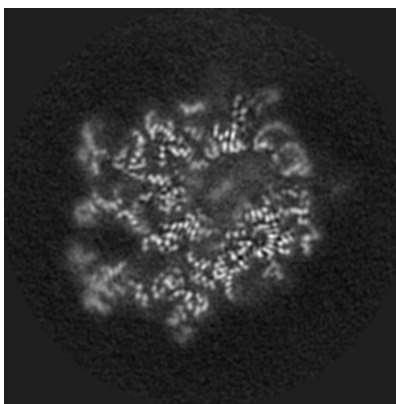
The images above show the map projected in three orthogonal directions.

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

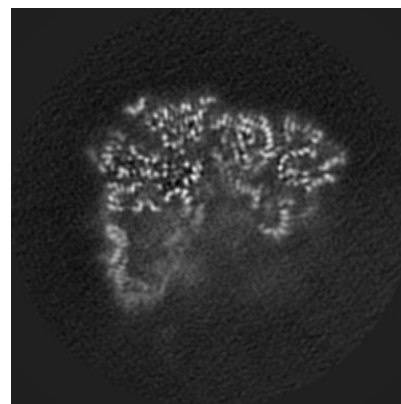
#### 6.2.1 Primary map



X Index: 168



Y Index: 168

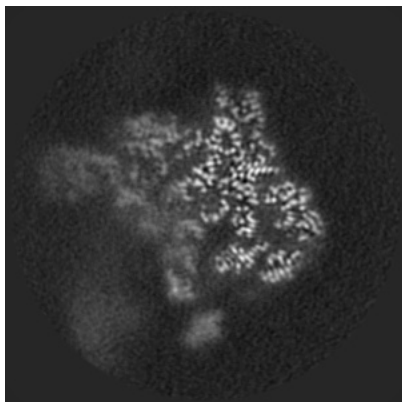


Z Index: 168

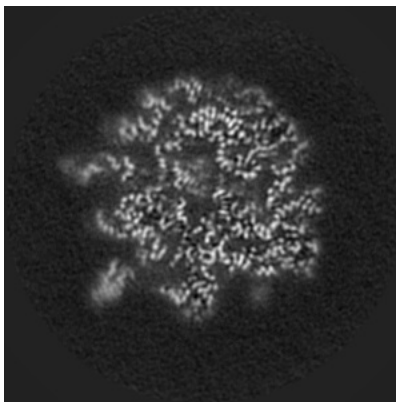
The images above show central slices of the map in three orthogonal directions.

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

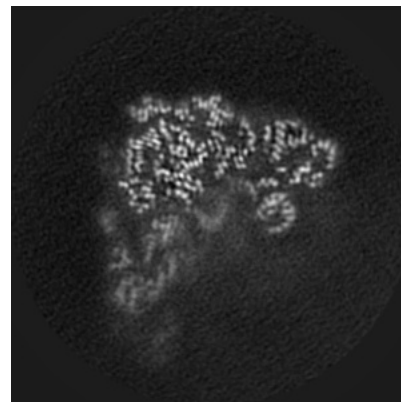
### 6.3.1 Primary map



X Index: 125



Y Index: 197



Z Index: 176

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 0.00983. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

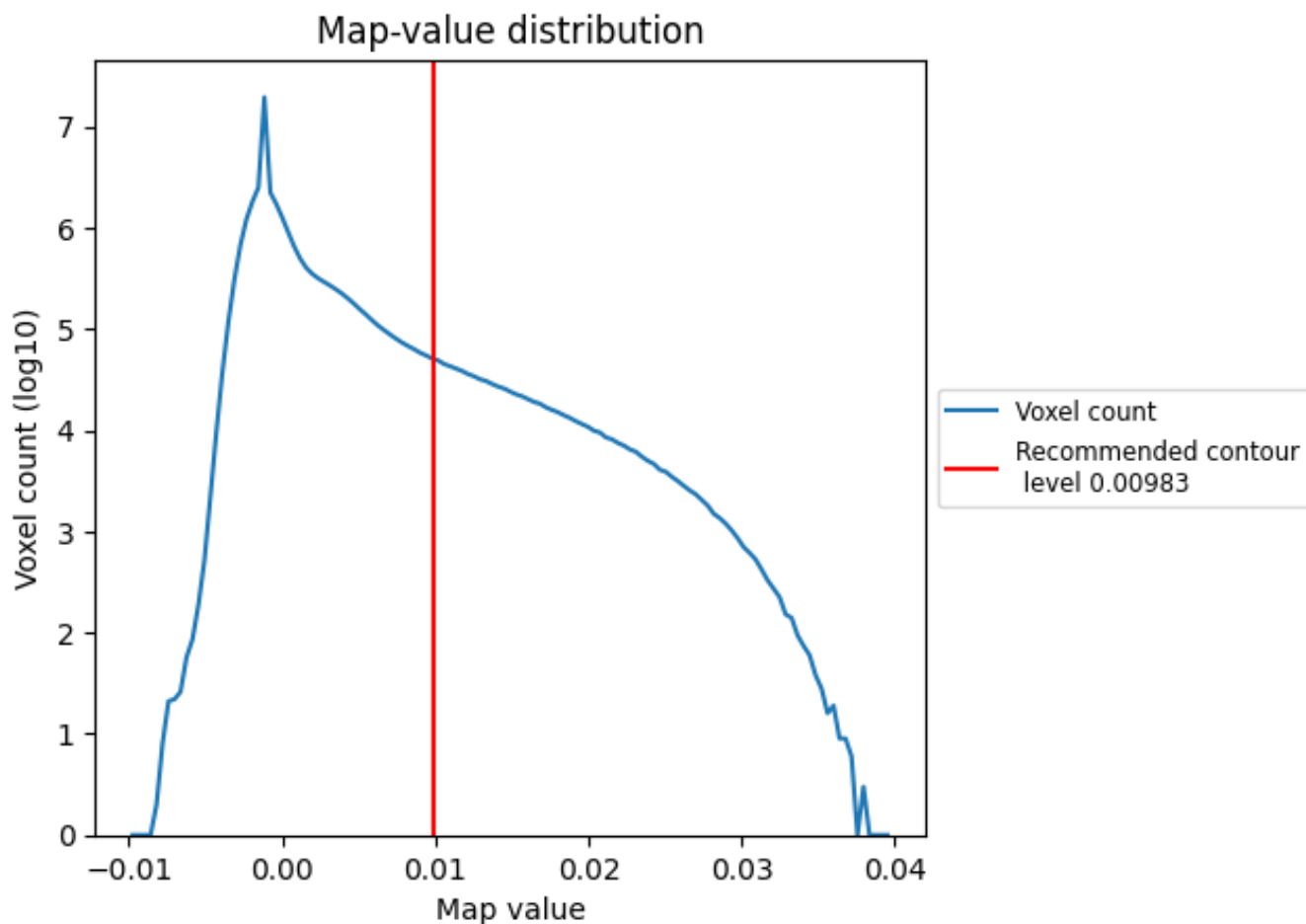
## 6.5 Mask visualisation

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.

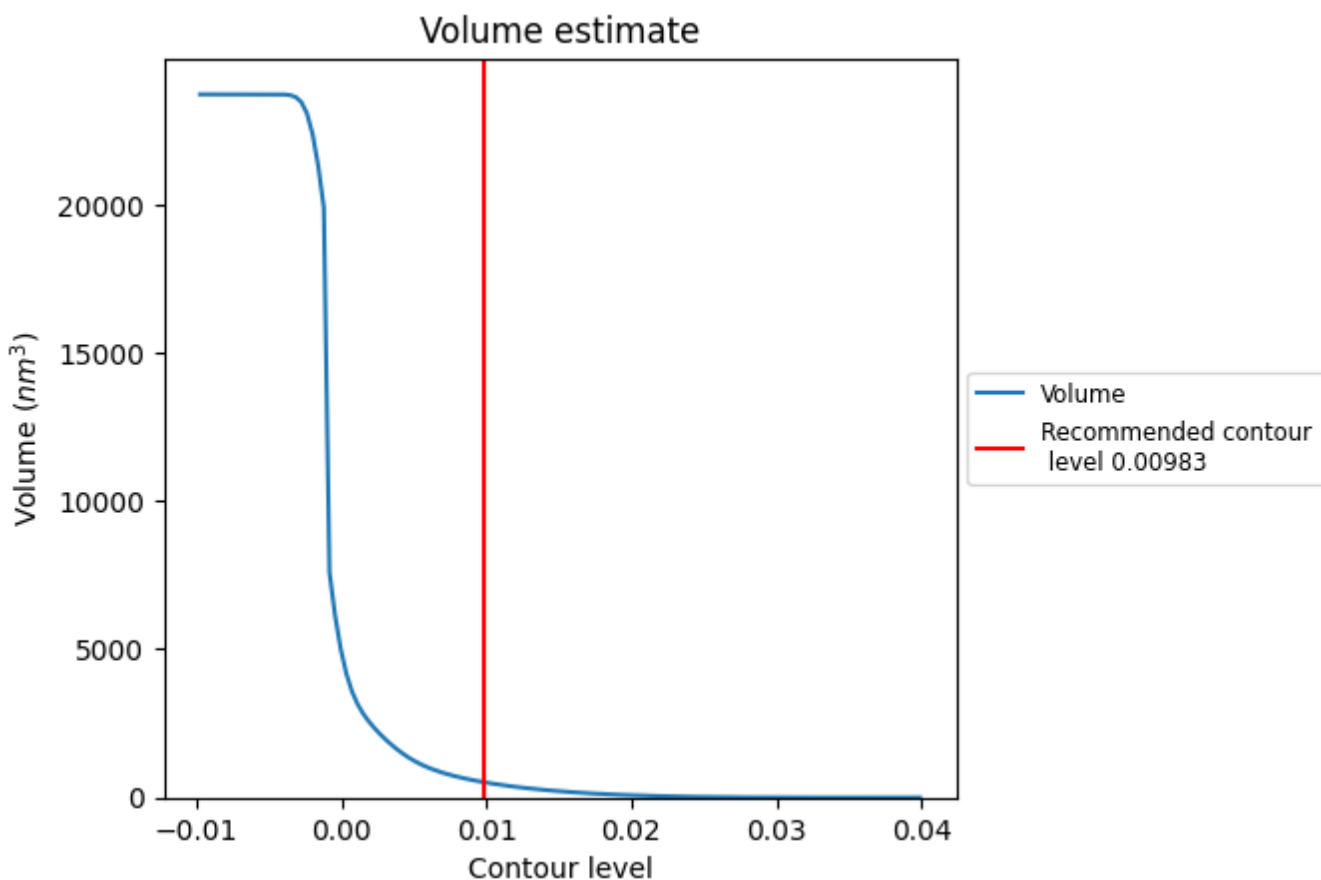
### 7.1 Map-value distribution [i](#)



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.



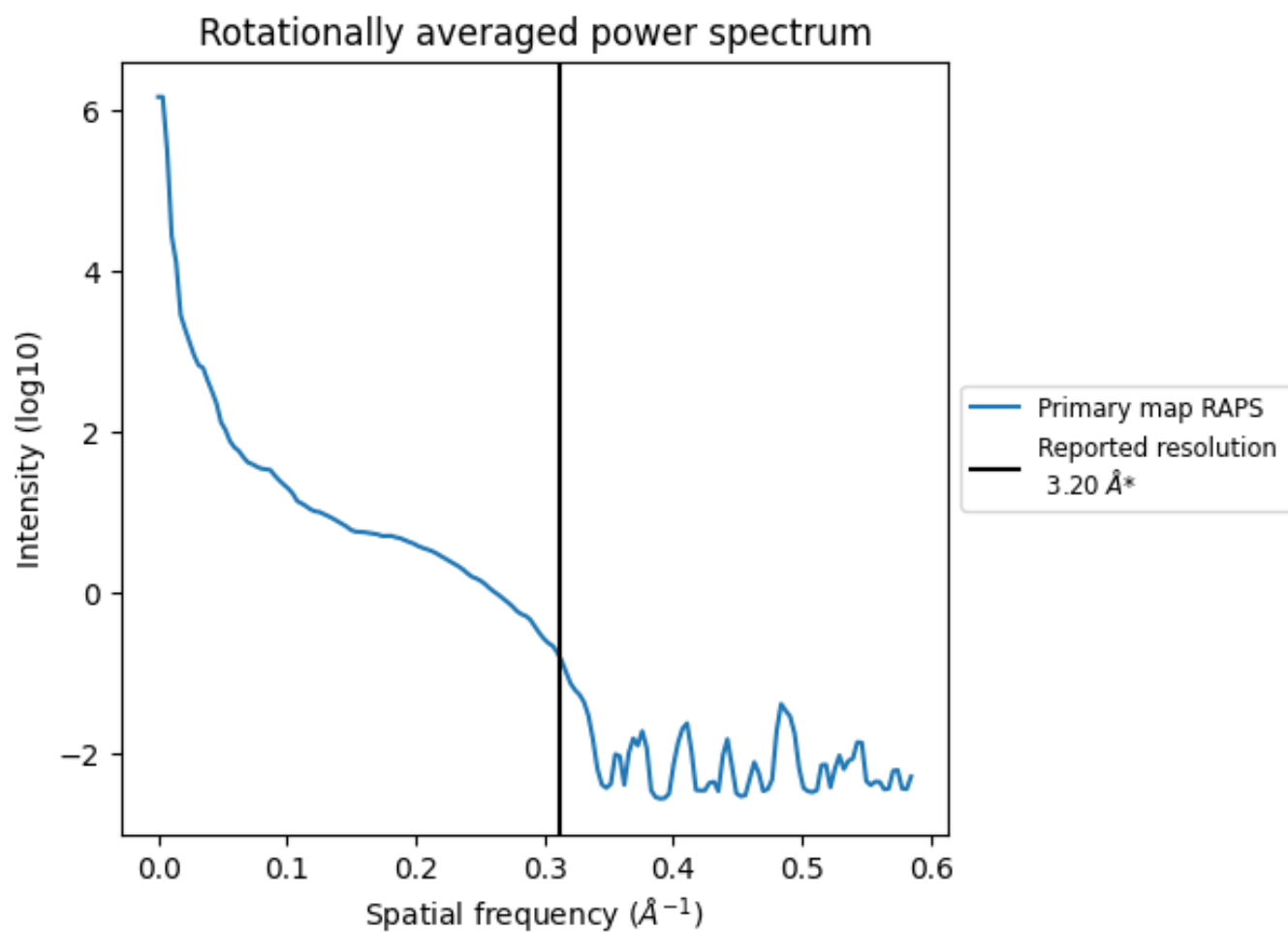
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm<sup>3</sup>; this corresponds to an approximate mass of 468 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

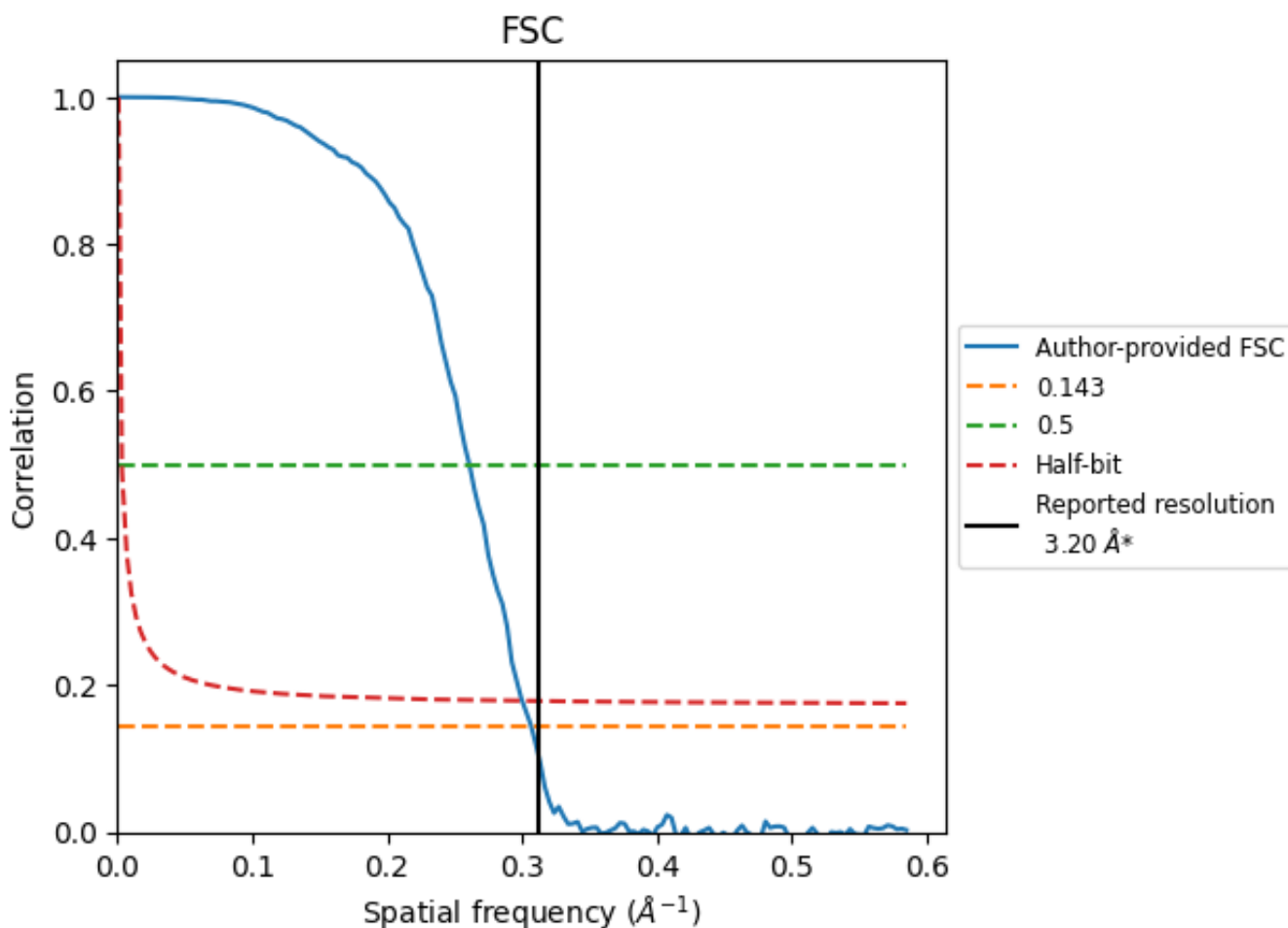


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{\AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

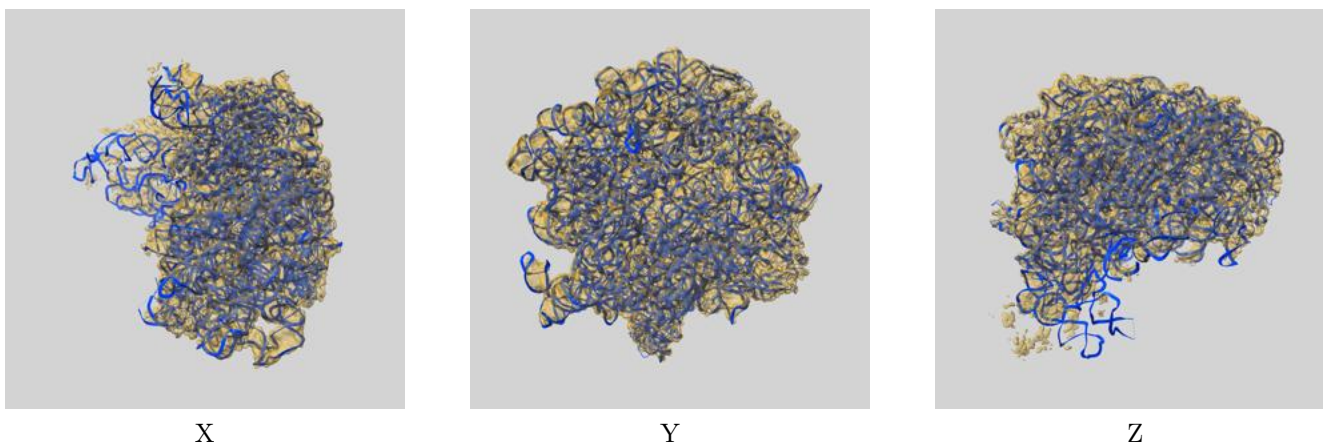
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.26	3.83	3.33
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

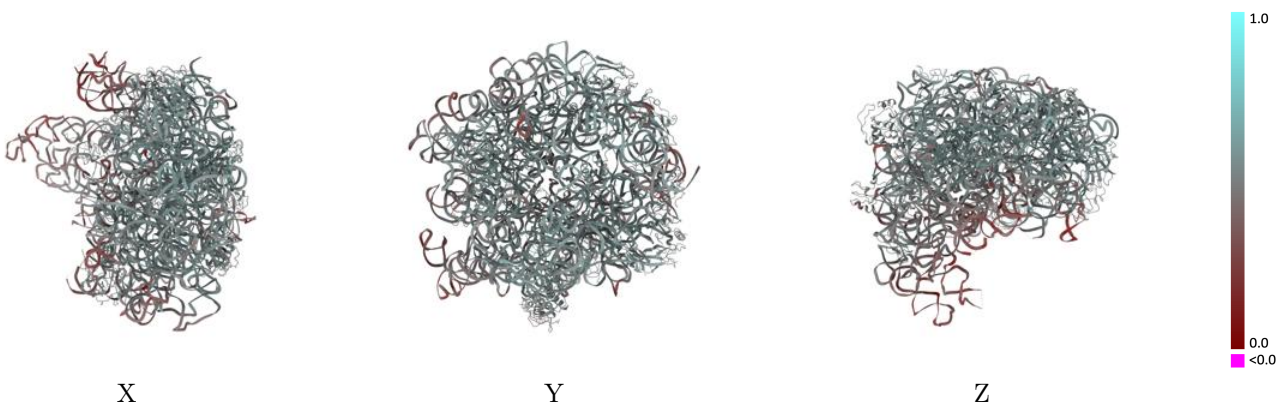
This section contains information regarding the fit between EMDB map EMD-24937 and PDB model 7S9U. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



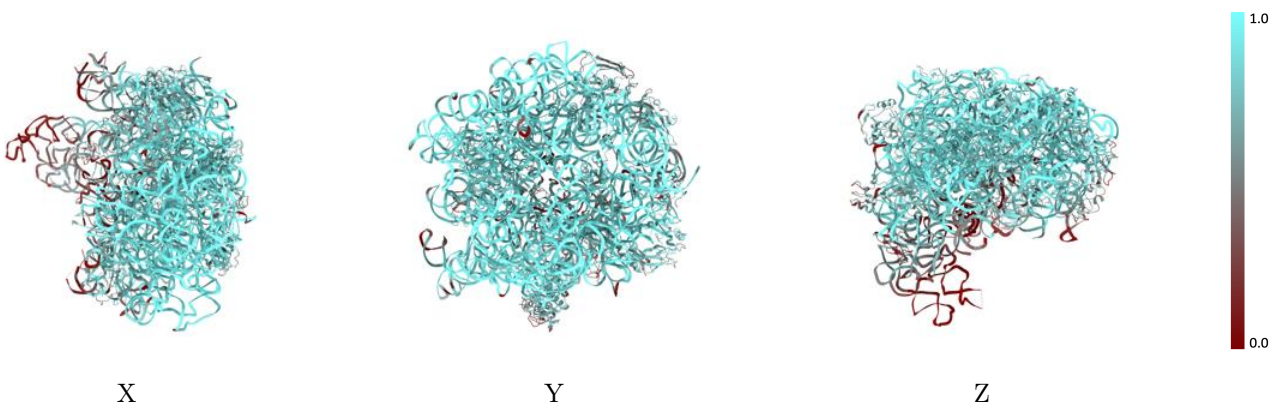
The images above show the 3D surface view of the map at the recommended contour level 0.00983 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



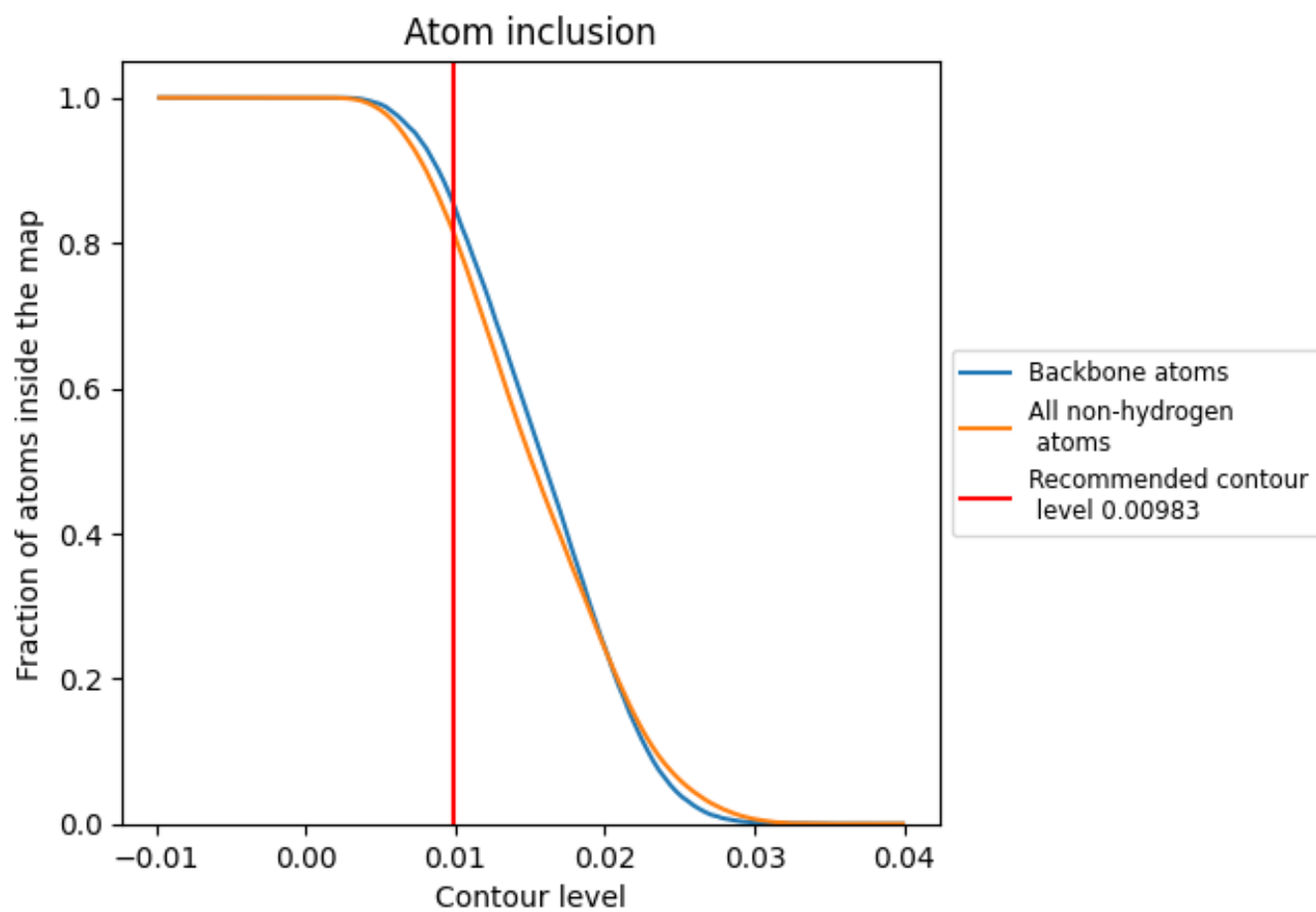
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00983).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.00983) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8176	 0.4950
A	 0.8498	 0.4870
C	 0.5970	 0.5060
D	 0.7444	 0.5350
E	 0.7533	 0.5240
J	 0.8087	 0.5250
K	 0.5741	 0.5140
L	 0.5866	 0.4750
N	 0.8593	 0.5480
P	 0.6080	 0.5190
Q	 0.8614	 0.5380
R	 0.7796	 0.5400
S	 0.8217	 0.5440
T	 0.7972	 0.5300
U	 0.7390	 0.5360
V	 0.2444	 0.4800
Y	 0.7335	 0.4860
Z	 0.6989	 0.5280
b	 0.8329	 0.5480
d	 0.8580	 0.5580

