



## wwPDB EM Validation Summary Report

Nov 20, 2022 – 04:58 pm GMT


PDB ID : 4ADX  
EMDB ID : EMD-2012  
Title : The Cryo-EM Structure of the Archaeal 50S Ribosomal Subunit in Complex with Initiation Factor 6  
Authors : Greber, B.J.; Boehringer, D.; Godinic-Mikulcic, V.; Crnkovic, A.; Ibba, M.; Weygand-Durasevic, I.; Ban, N.  
Deposited on : 2012-01-04  
Resolution : 6.60 Å (reported)  
Based on initial models : 3O58, 4A17, 3CC2, 4A19

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:

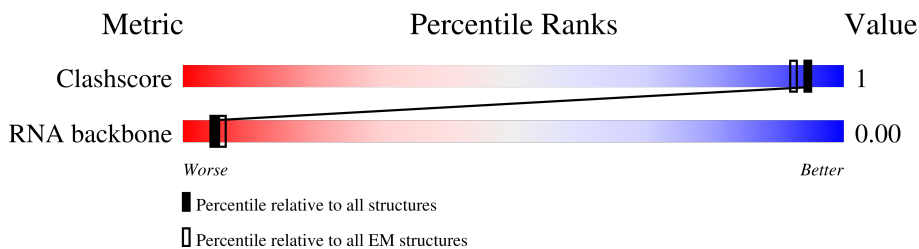
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.60 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)
Clashescore	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	0	2923	
2	1	57	
3	2	50	
4	3	92	
5	4	123	
6	5	129	
7	6	104	
8	7	126	
9	8	133	

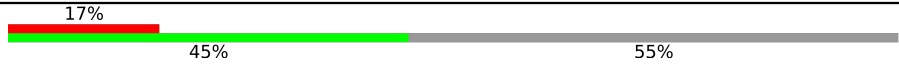

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Mol	Chain	Length	Quality of chain
10	9	122	31% 99%
11	A	240	43% 99%
12	B	338	34% 99%
13	C	246	32% 99%
14	D	177	15% 79% 21%
15	E	178	31% 97%
16	F	120	14% 98%
17	G	78	32% 100%
18	H	177	32% 88% 12%
19	I	222	26% 99%
20	J	145	29% 96%
21	K	132	39% 100%
22	L	165	35% 85% 15%
23	M	196	42% 92% 7%
24	N	187	32% 99%
25	O	116	27% 99%
26	P	149	23% 95% 5%
27	Q	96	36% 99%
28	R	155	33% 97%
29	S	85	21% 95% 5%
30	T	120	21% 98%
31	U	67	13% 78% 22%
32	V	71	15% 90% 10%
33	W	154	39% 100%
34	X	92	29% 89% 11%

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Mol	Chain	Length	Quality of chain
35	Y	241	
36	Z	92	

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 7164 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	0	2688	Total P 2688 2688	0	2688

- Molecule 2 is a protein called RPL37E.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	1	56	Total C 56 56	0	56

- Molecule 3 is a protein called RPL39E.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	2	46	Total C 46 46	0	46

- Molecule 4 is a protein called RPL44E.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	3	92	Total C 92 92	0	92

- Molecule 5 is a protein called RPL34E.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	4	90	Total C 90 90	0	90

- Molecule 6 is a protein called RPL40E.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	5	50	Total C 50 50	0	50

- Molecule 7 is a protein called RPL30E.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	6	96	Total C 96 96	0	96

- Molecule 8 is a protein called RPL14E.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	7	77	Total C 77 77	0	77

- Molecule 9 is a RNA chain called 23S Ribosomal RNA EXPANSION SEGMENTS.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	8	133	Total P 133 133	0	133

- Molecule 10 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	9	121	Total P 121 121	0	121

- Molecule 11 is a protein called RPL2.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	A	237	Total C 237 237	0	237

- Molecule 12 is a protein called RPL3.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	B	337	Total C 337 337	0	337

- Molecule 13 is a protein called RPL4.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	C	246	Total C 246 246	0	246

- Molecule 14 is a protein called RPL5.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	D	139	Total C 139 139	0	139

- Molecule 15 is a protein called RPL6.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	E	172	Total C 172 172	0	172

- Molecule 16 is a protein called RPL7AE.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	F	119	Total C 119 119	0	119

- Molecule 17 is a protein called RPLX.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	G	78	Total C 78 78	0	78

- Molecule 18 is a protein called RPL10E.

Mol	Chain	Residues	Atoms	AltConf	Trace
18	H	156	Total C 156 156	0	156

- Molecule 19 is a protein called AIF6.

Mol	Chain	Residues	Atoms	AltConf	Trace
19	I	220	Total C 220 220	0	220

- Molecule 20 is a protein called RPL13.

Mol	Chain	Residues	Atoms	AltConf	Trace
20	J	139	Total C 139 139	0	139

- Molecule 21 is a protein called RPL14.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	K	132	Total C 132 132	0	132

- Molecule 22 is a protein called RPL15.

Mol	Chain	Residues	Atoms	AltConf	Trace
22	L	140	Total C 140 140	0	140

- Molecule 23 is a protein called RPL15E.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	M	182	Total C 182 182	0	182

- Molecule 24 is a protein called RPL18.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	N	185	Total C 185 185	0	185

- Molecule 25 is a protein called RPL18E.

Mol	Chain	Residues	Atoms	AltConf	Trace
25	O	115	Total C 115 115	0	115

- Molecule 26 is a protein called RPL19E.

Mol	Chain	Residues	Atoms	AltConf	Trace
26	P	142	Total C 142 142	0	142

- Molecule 27 is a protein called RPL21E.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	Q	95	Total C 95 95	0	95

- Molecule 28 is a protein called RPL22.



Mol	Chain	Residues	Atoms	AltConf	Trace
28	R	150	Total C 150 150	0	150

- Molecule 29 is a protein called RPL23.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	S	81	Total C 81 81	0	81

- Molecule 30 is a protein called RPL24.

Mol	Chain	Residues	Atoms	AltConf	Trace
30	T	117	Total C 117 117	0	117

- Molecule 31 is a protein called RPL24E.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	U	52	Total C 52 52	0	52

- Molecule 32 is a protein called RPL29.

Mol	Chain	Residues	Atoms	AltConf	Trace
32	V	64	Total C 64 64	0	64

- Molecule 33 is a protein called RPL30.

Mol	Chain	Residues	Atoms	AltConf	Trace
33	W	154	Total C 154 154	0	154

- Molecule 34 is a protein called RPL31E.

Mol	Chain	Residues	Atoms	AltConf	Trace
34	X	82	Total C 82 82	0	82

- Molecule 35 is a protein called RPL32E.

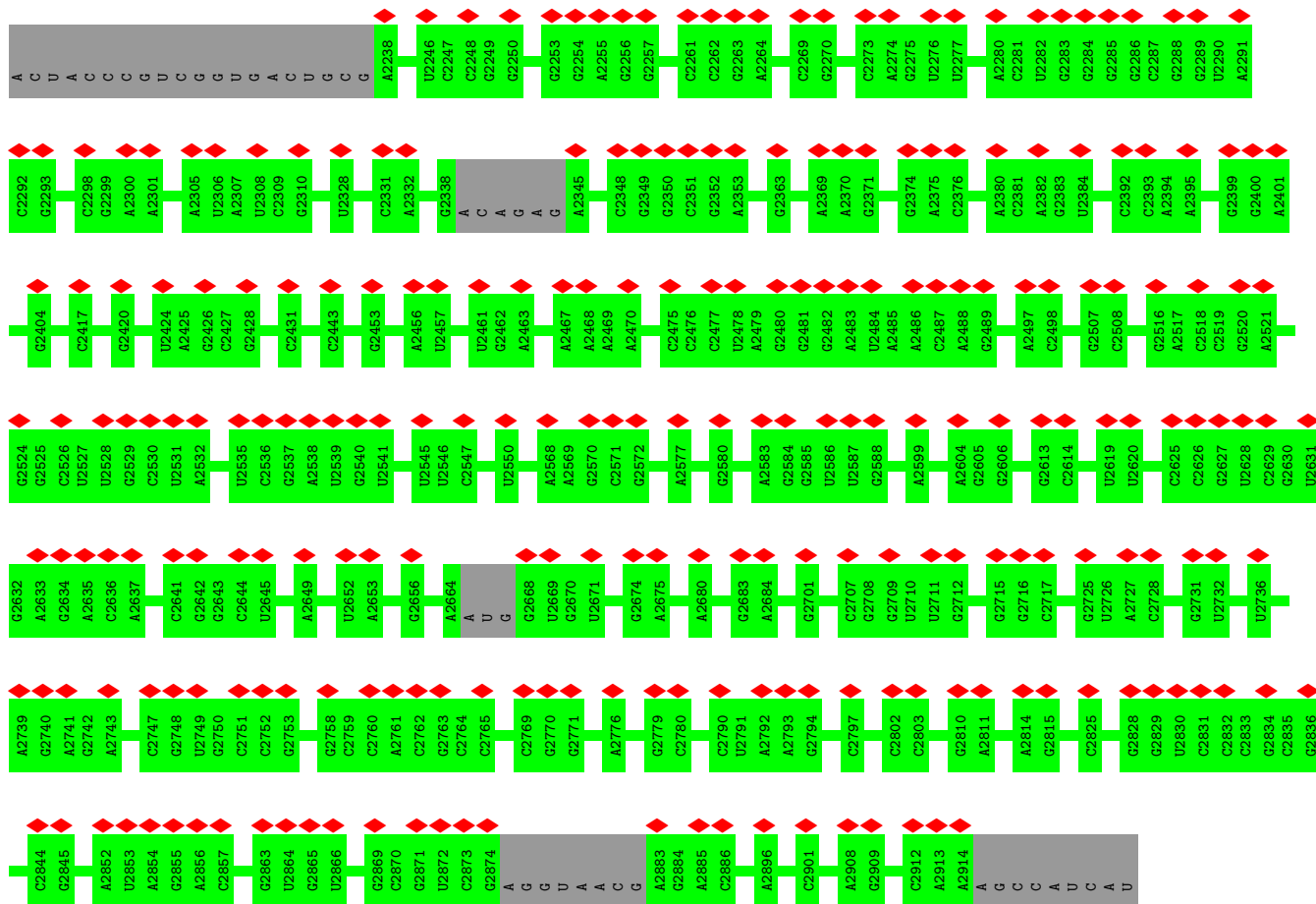
Mol	Chain	Residues	Atoms		AltConf	Trace
35	Y	108	Total 108	C 108	0	108

- Molecule 36 is a protein called RPL37AE.

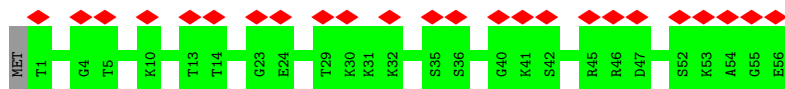
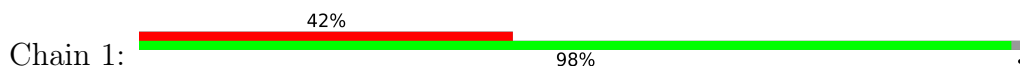
Mol	Chain	Residues	Atoms		AltConf	Trace
36	Z	73	Total 73	C 73	0	73



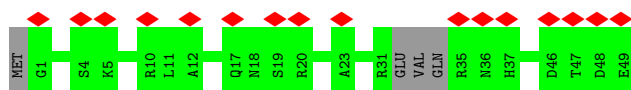
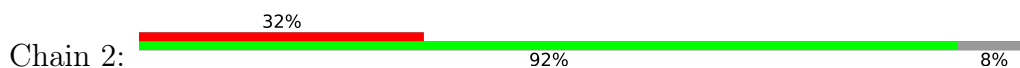




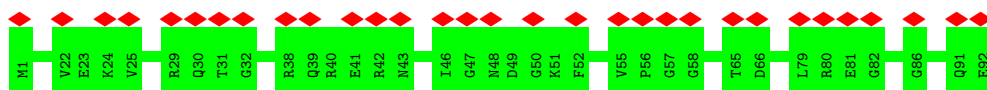
• Molecule 2: RPL37E



• Molecule 3: RPL39E

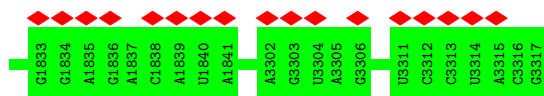


• Molecule 4: RPL44E

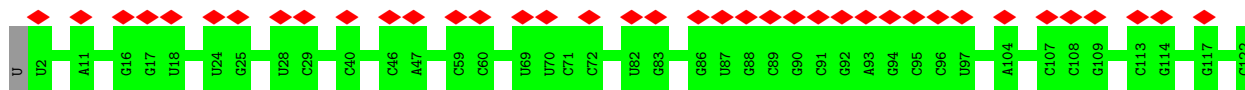


• Molecule 5: RPL34E

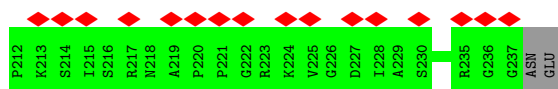
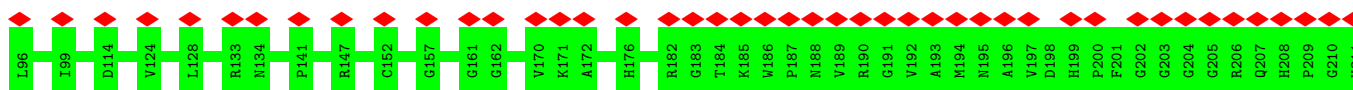
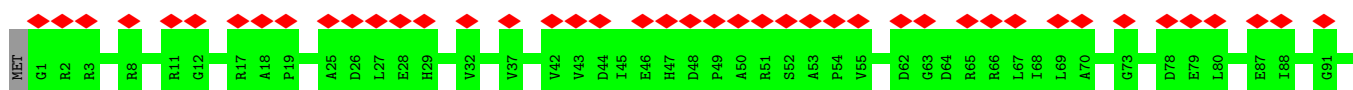
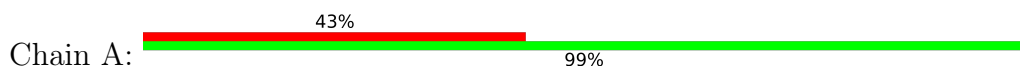




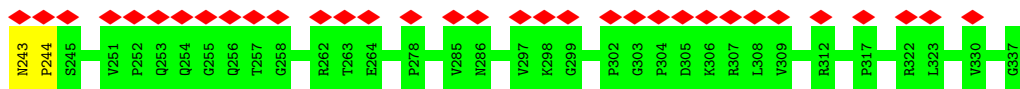
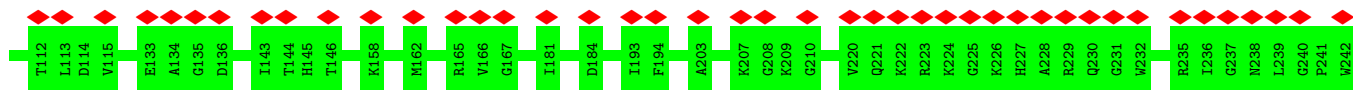
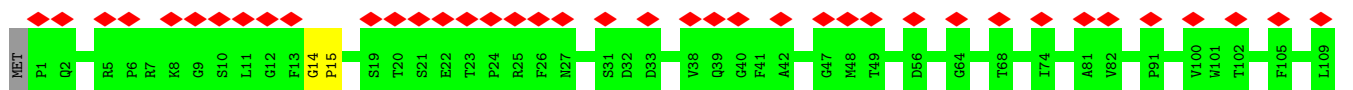
- Molecule 10: 5S Ribosomal RNA



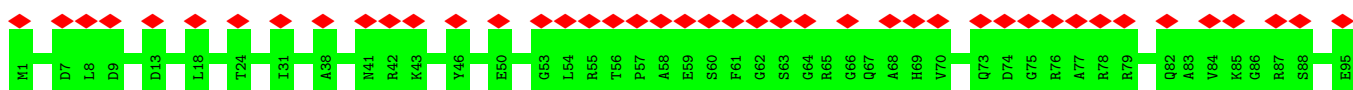
- Molecule 11: RPL2

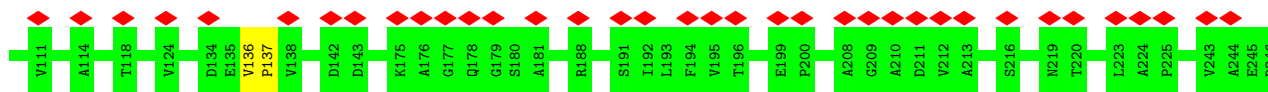


- Molecule 12: RPL3

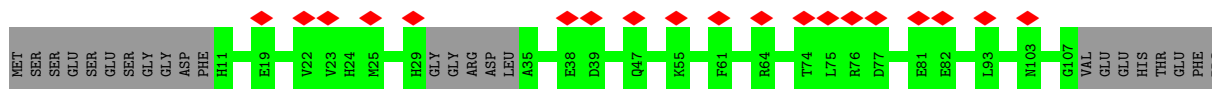
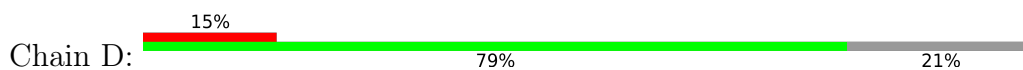


- Molecule 13: RPL4

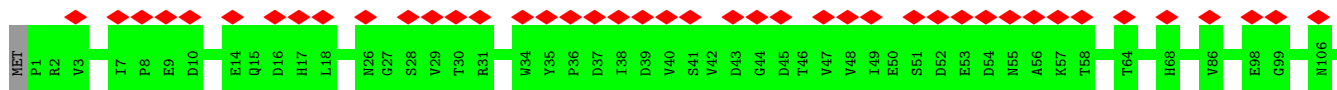




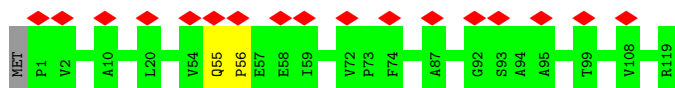
- Molecule 14: RPL5



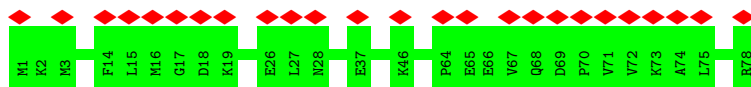
- Molecule 15: RPL6



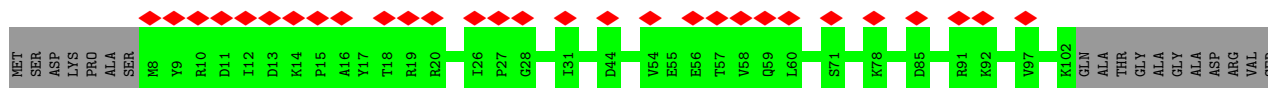
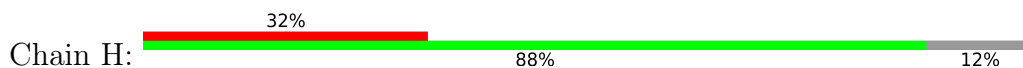
- Molecule 16: RPL7AE



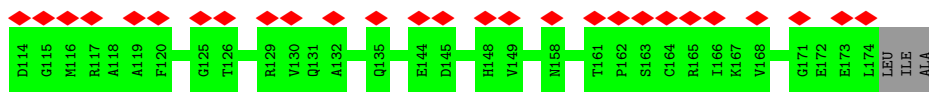
- Molecule 17: RPLX



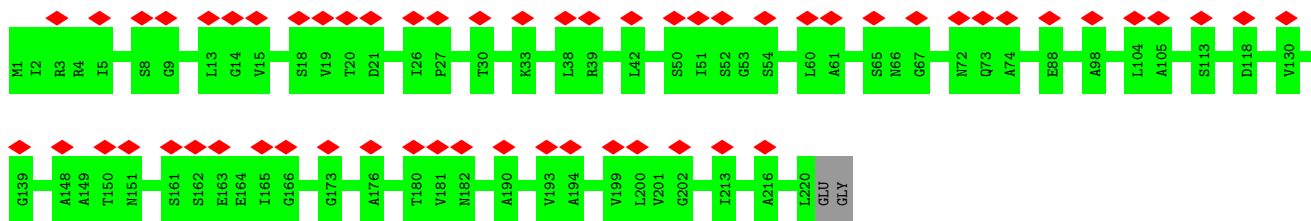
- Molecule 18: RPL10E



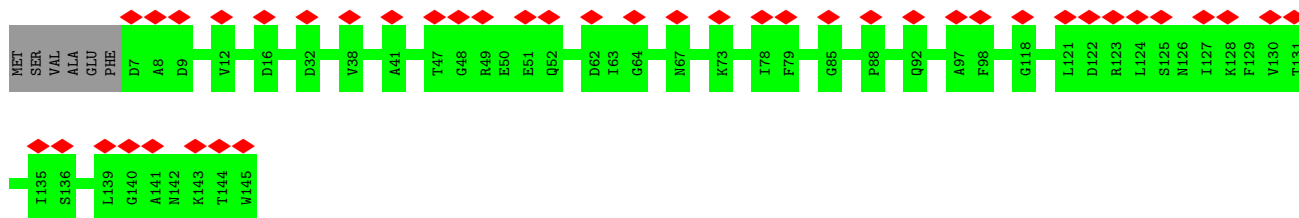




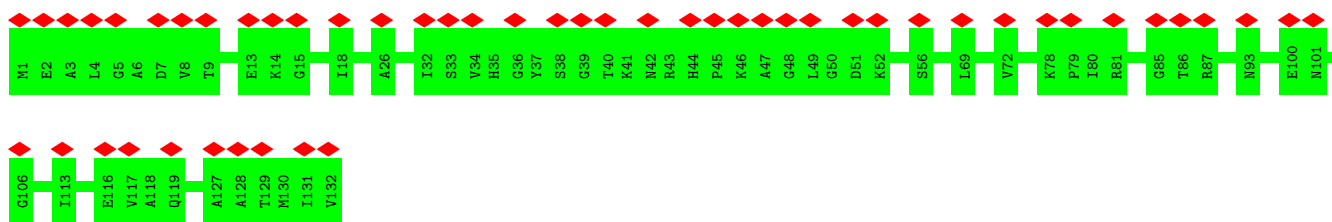
• Molecule 19: AIF6



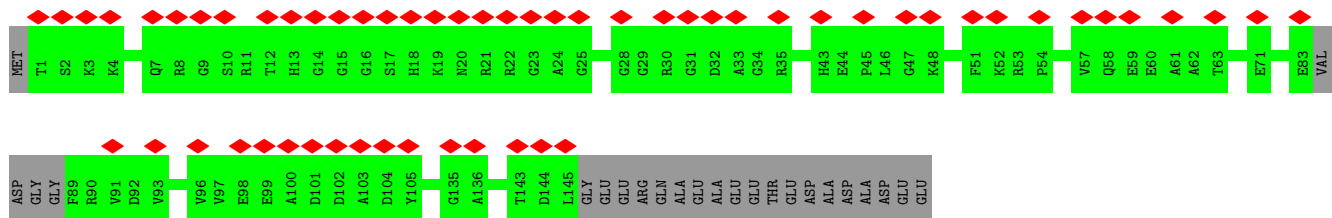
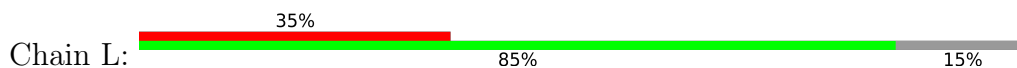
• Molecule 20: RPL13



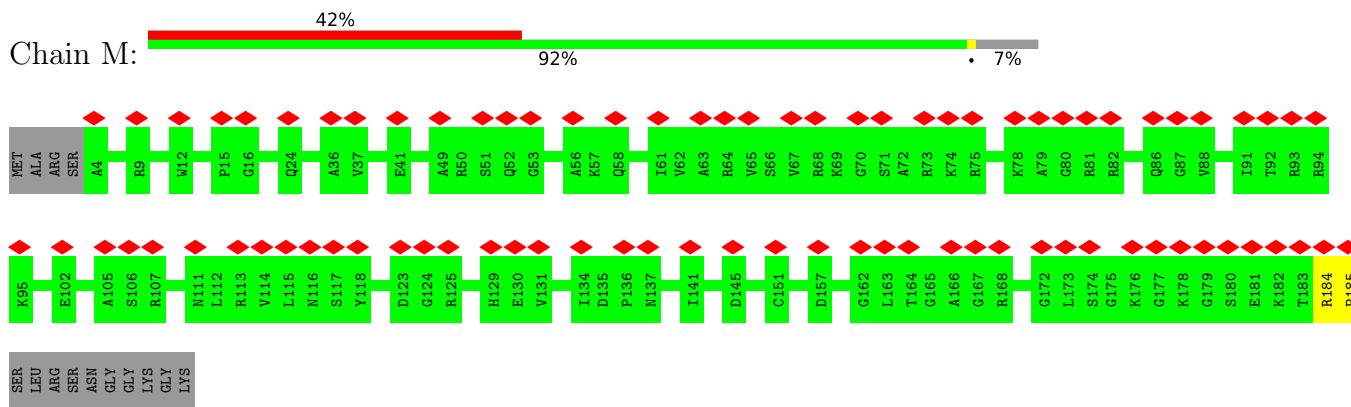
• Molecule 21: RPL14



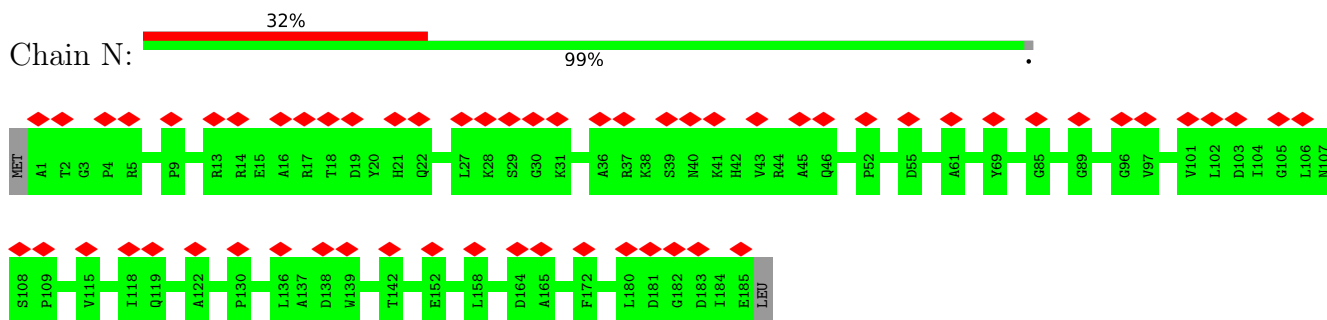
• Molecule 22: RPL15



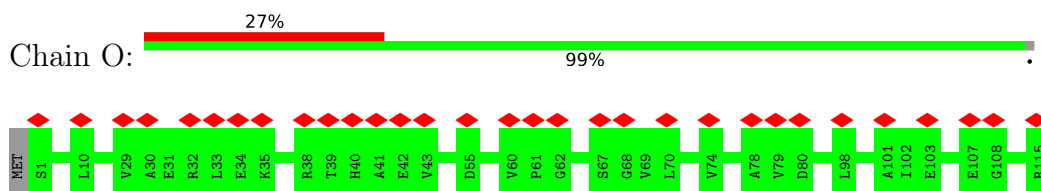
• Molecule 23: RPL15E



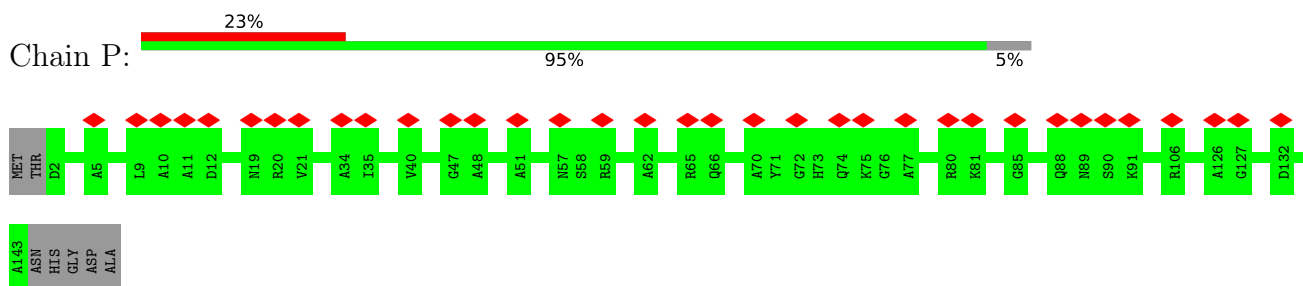
• Molecule 24: RPL18



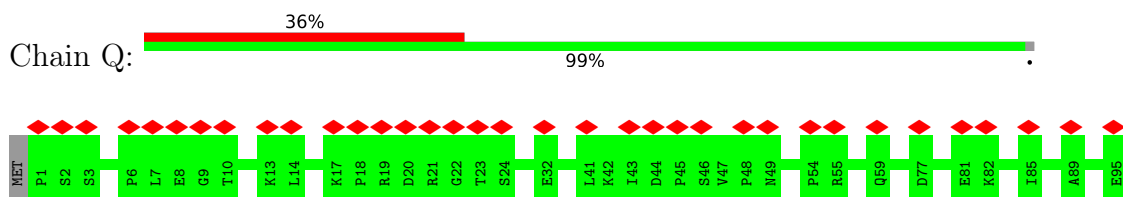
• Molecule 25: RPL18E



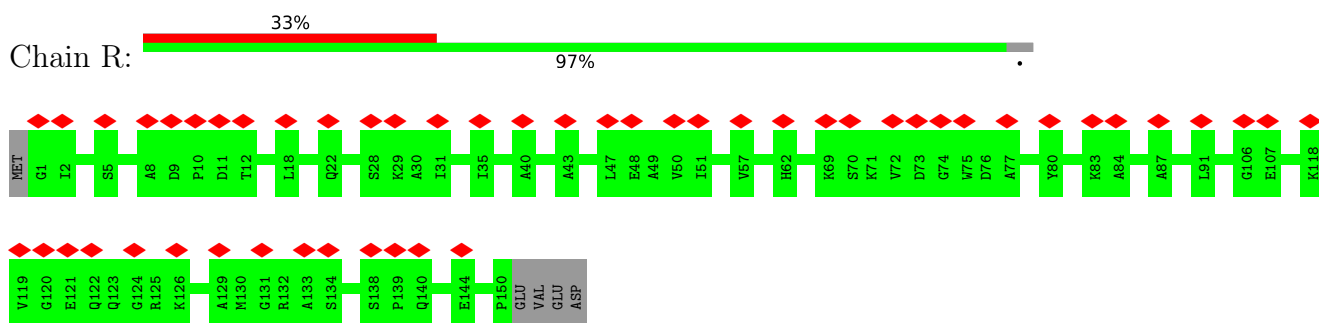
• Molecule 26: RPL19E



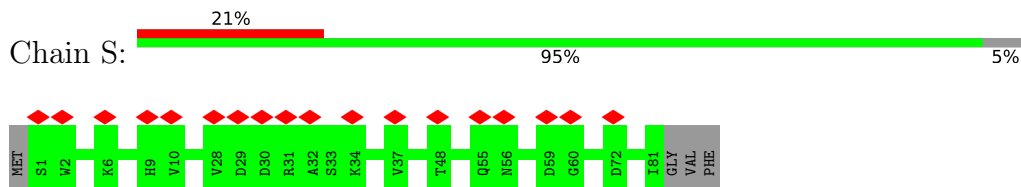
• Molecule 27: RPL21E



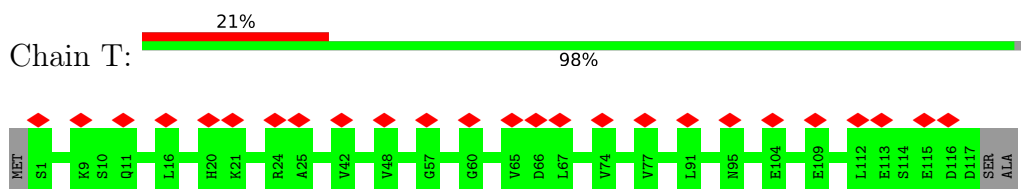
• Molecule 28: RPL22



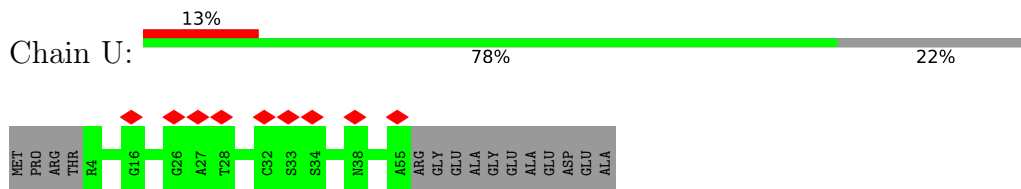
- Molecule 29: RPL23



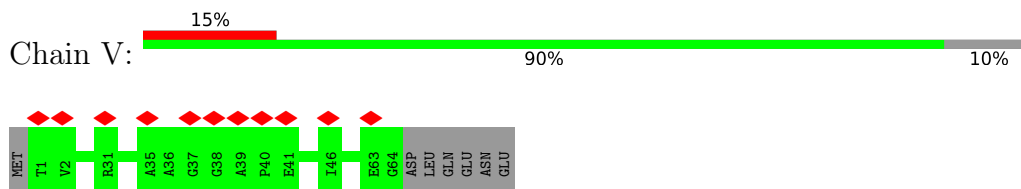
- Molecule 30: RPL24



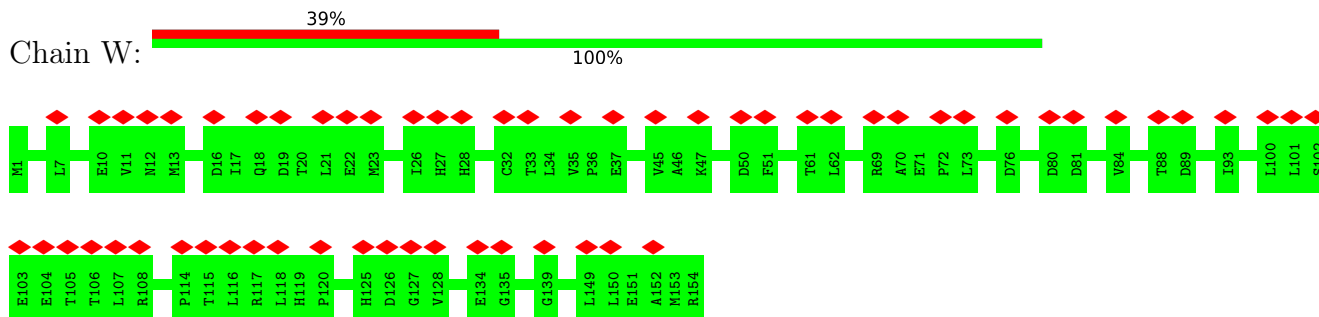
- Molecule 31: RPL24E



- Molecule 32: RPL29



- Molecule 33: RPL30





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70364	Depositor
Resolution determination method	Not provided	
CTF correction method	BY CCD FRAME	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	83000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	276.055	Depositor
Minimum map value	-201.716	Depositor
Average map value	-10.795	Depositor
Map value standard deviation	22.579	Depositor
Recommended contour level	30.0	Depositor
Map size ( $\text{\AA}$ )	325.8, 325.8, 325.8	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.81, 1.81, 1.81	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	0	2688	0	0	3	0
2	1	56	0	0	0	0
3	2	46	0	0	0	0
4	3	92	0	0	0	0
5	4	90	0	0	2	0
6	5	50	0	0	0	0
7	6	96	0	0	1	0
8	7	77	0	0	0	0
9	8	133	0	0	0	0
10	9	121	0	0	0	0
11	A	237	0	0	0	0
12	B	337	0	0	2	0
13	C	246	0	0	1	0
14	D	139	0	0	0	0
15	E	172	0	0	0	0
16	F	119	0	0	1	0
17	G	78	0	0	0	0
18	H	156	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	I	220	0	0	0	0
20	J	139	0	0	0	0
21	K	132	0	0	0	0
22	L	140	0	0	0	0
23	M	182	0	0	1	0
24	N	185	0	0	0	0
25	O	115	0	0	0	0
26	P	142	0	0	0	0
27	Q	95	0	0	0	0
28	R	150	0	0	0	0
29	S	81	0	0	0	0
30	T	117	0	0	0	0
31	U	52	0	0	0	0
32	V	64	0	0	0	0
33	W	154	0	0	0	0
34	X	82	0	0	0	0
35	Y	108	0	0	0	0
36	Z	73	0	0	0	0
All	All	7164	0	0	8	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 1.

The worst 5 of 8 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)
1:0:1488:U:P	5:4:11:CYS:CA	2.82	0.67
1:0:1614:G:P	5:4:55:GLY:CA	2.88	0.61
12:B:14:GLY:CA	12:B:15:PRO:CA	2.80	0.59
1:0:1604:G:P	7:6:87:CYS:CA	2.92	0.58
12:B:243:ASN:CA	12:B:244:PRO:CA	2.93	0.47

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 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	0	0/2923	-	-
10	9	0/122	-	-
9	8	0/133	-	-
All	All	0/3178	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

### 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.



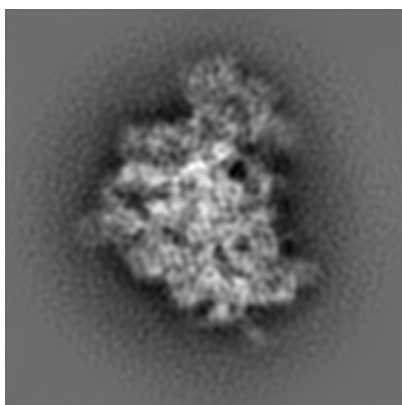
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2012. These allow visual inspection of the internal detail of the map and identification of artifacts.

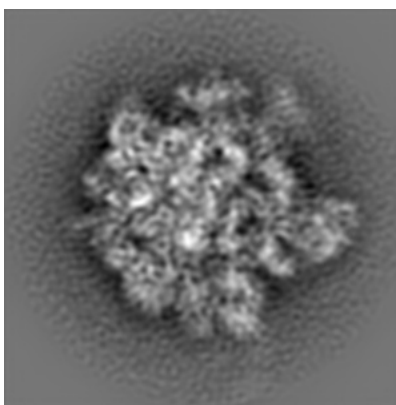
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

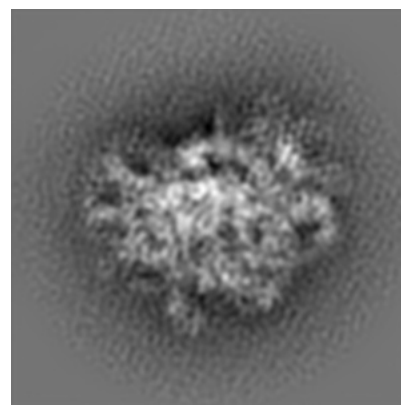
#### 6.1.1 Primary map



X



Y

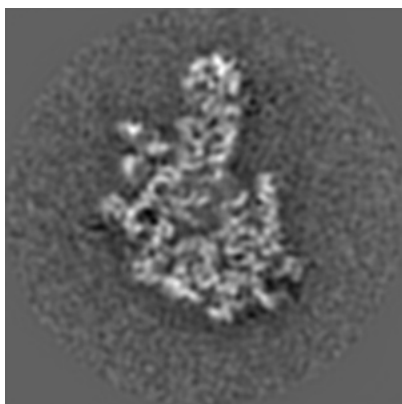


Z

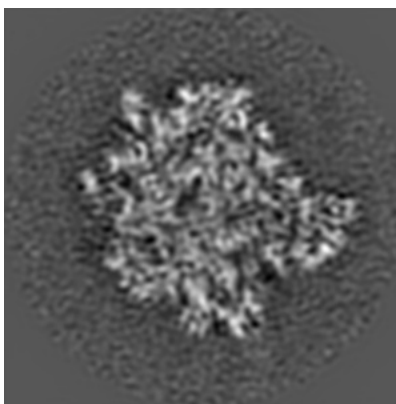
The images above show the map projected in three orthogonal directions.

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

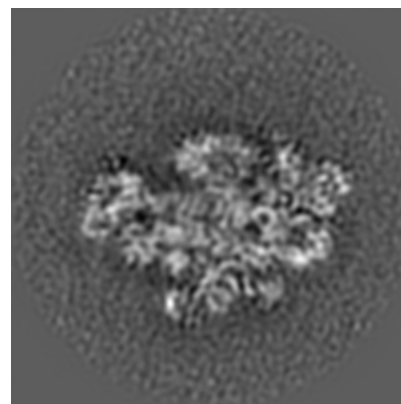
#### 6.2.1 Primary map



X Index: 90



Y Index: 90

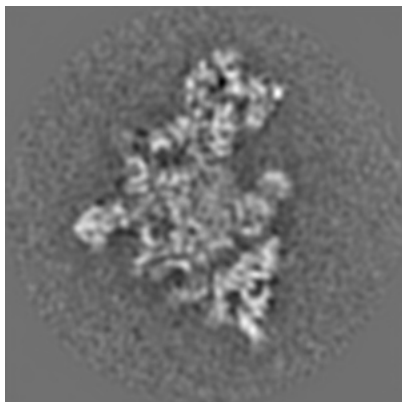


Z Index: 90

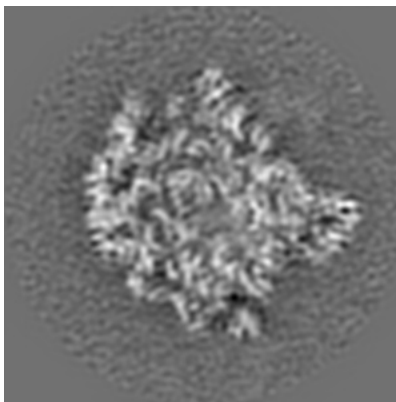
The images above show central slices of the map in three orthogonal directions.

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

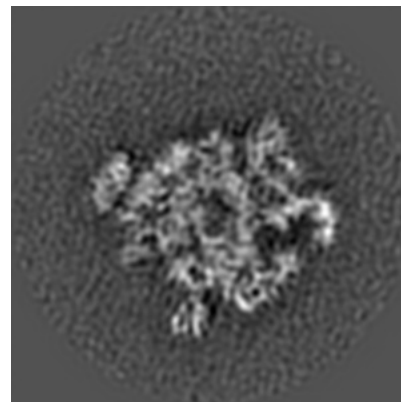
### 6.3.1 Primary map



X Index: 83



Y Index: 96



Z Index: 81

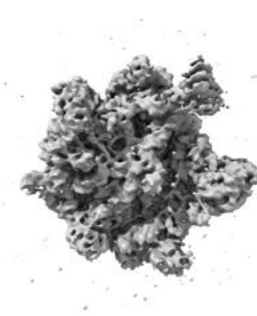
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

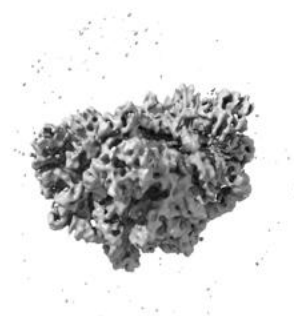
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 30.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

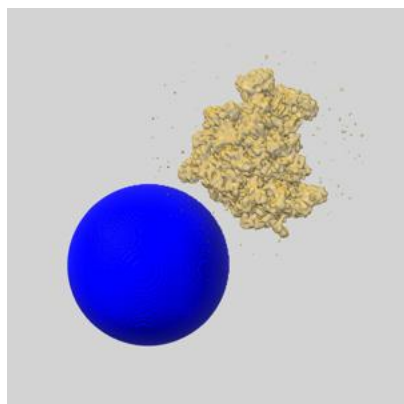
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

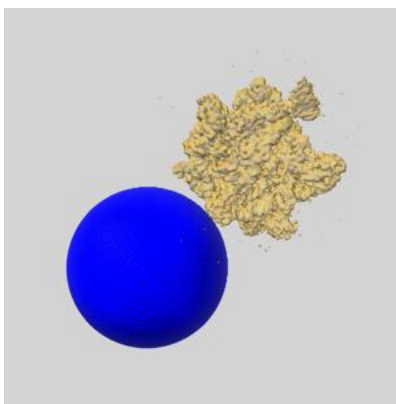
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

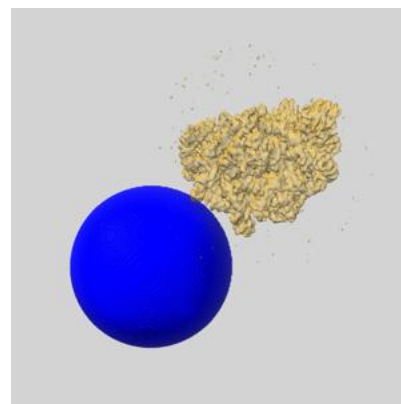
### 6.5.1 emd\_2012\_msk.map [i](#)



X



Y

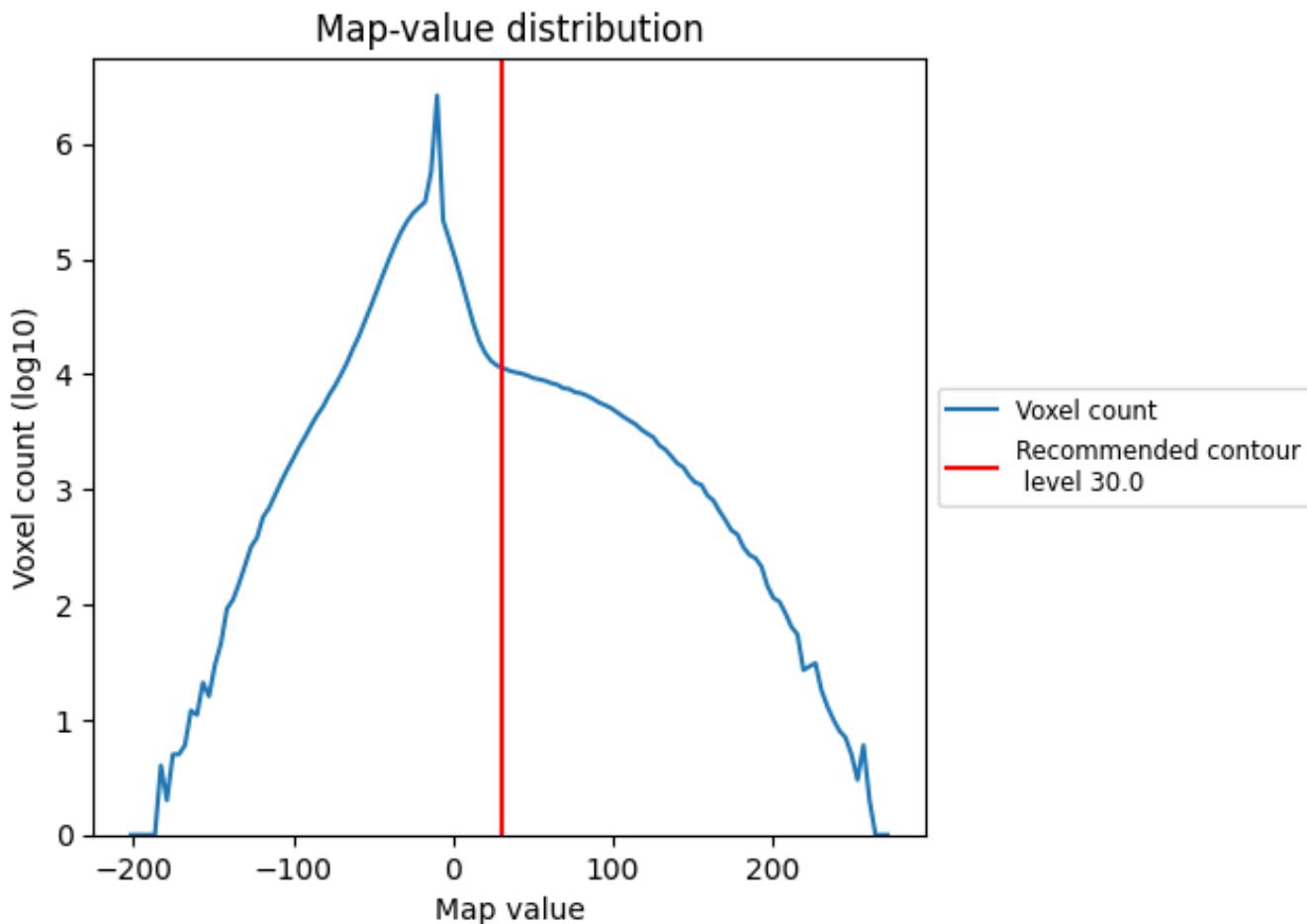


Z

## 7 Map analysis [i](#)

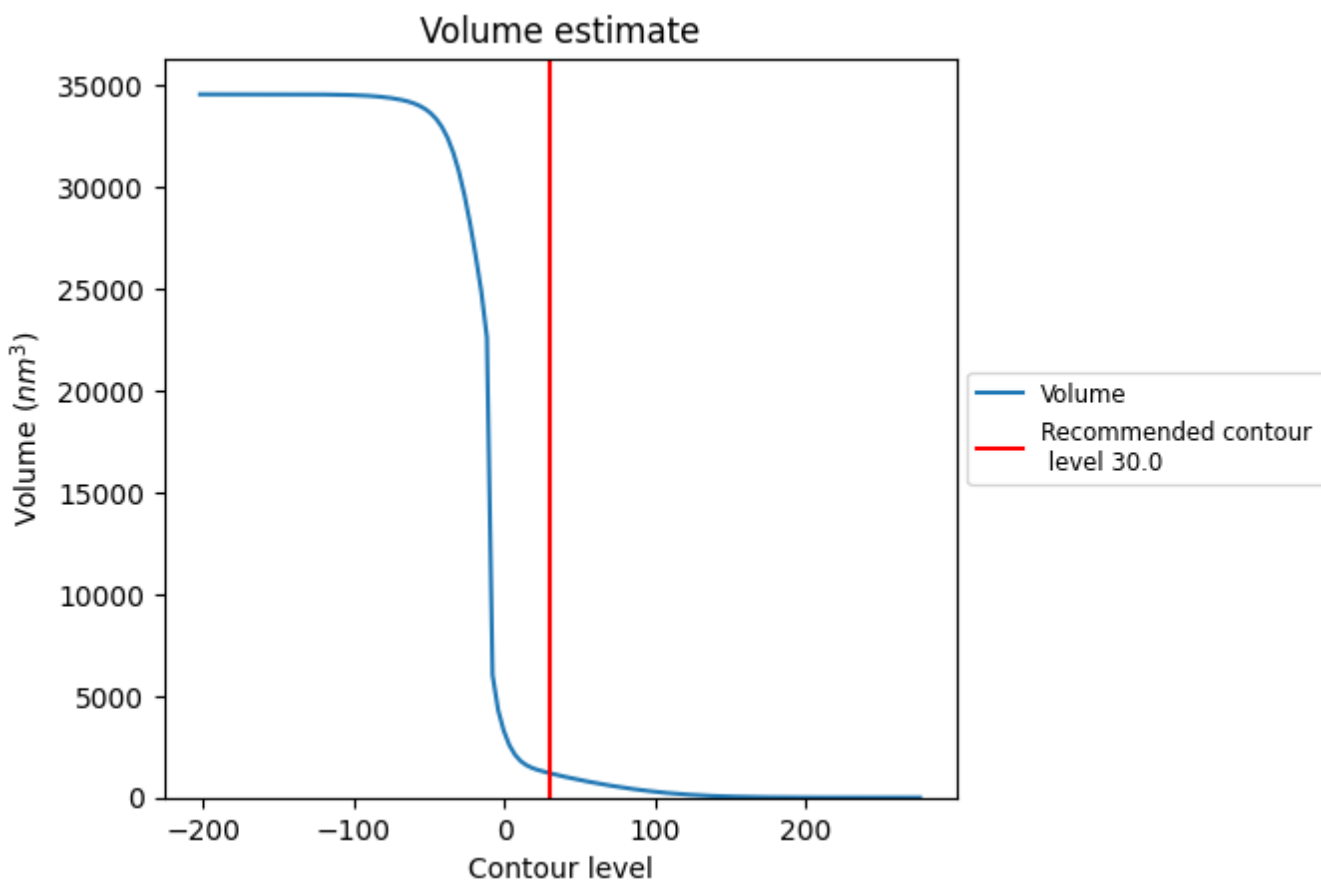
This section contains the results of statistical analysis of the map.

### 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.

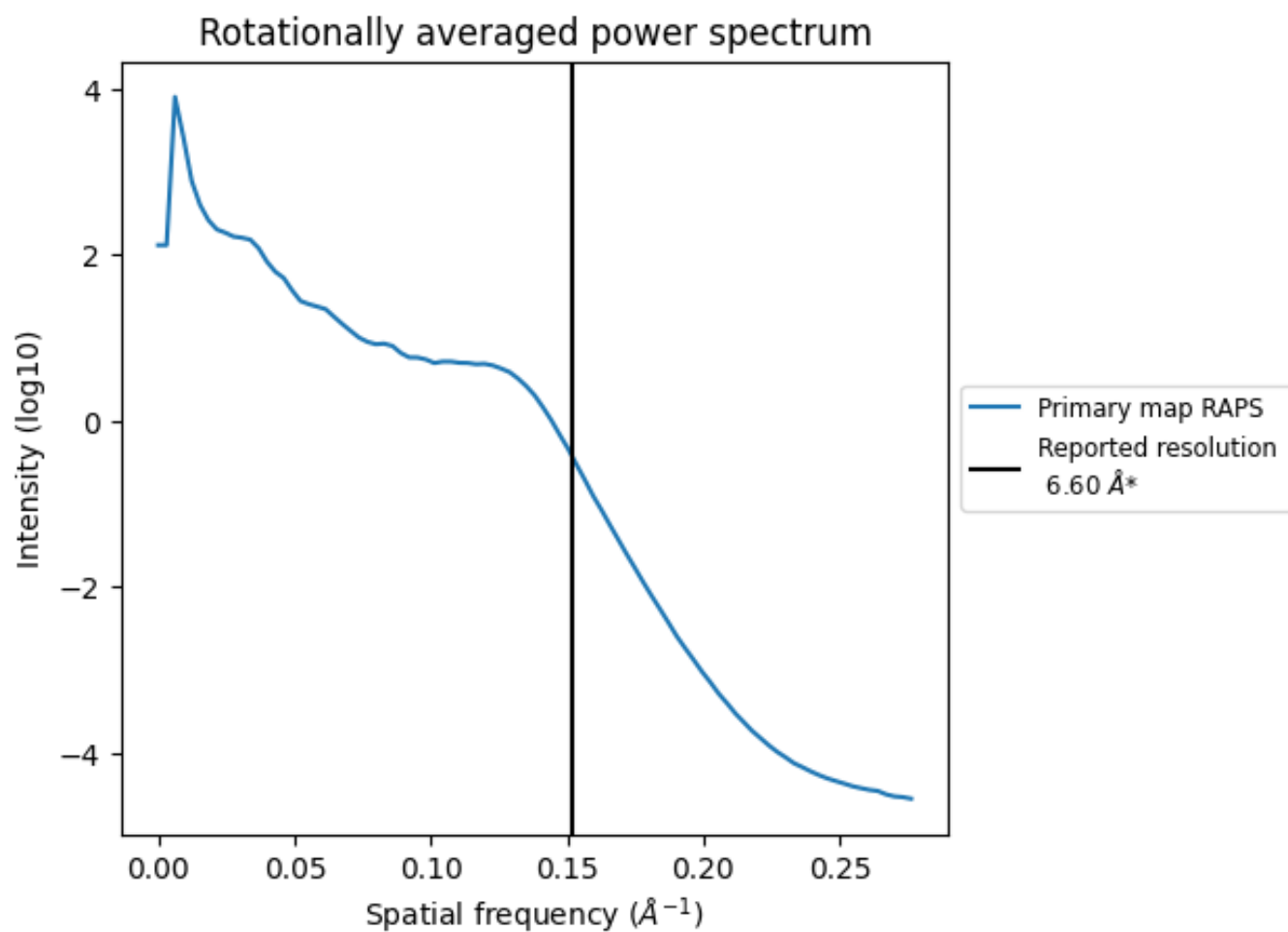
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1203  $\text{nm}^3$ ; this corresponds to an approximate mass of 1087 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 0.152 Å<sup>-1</sup>

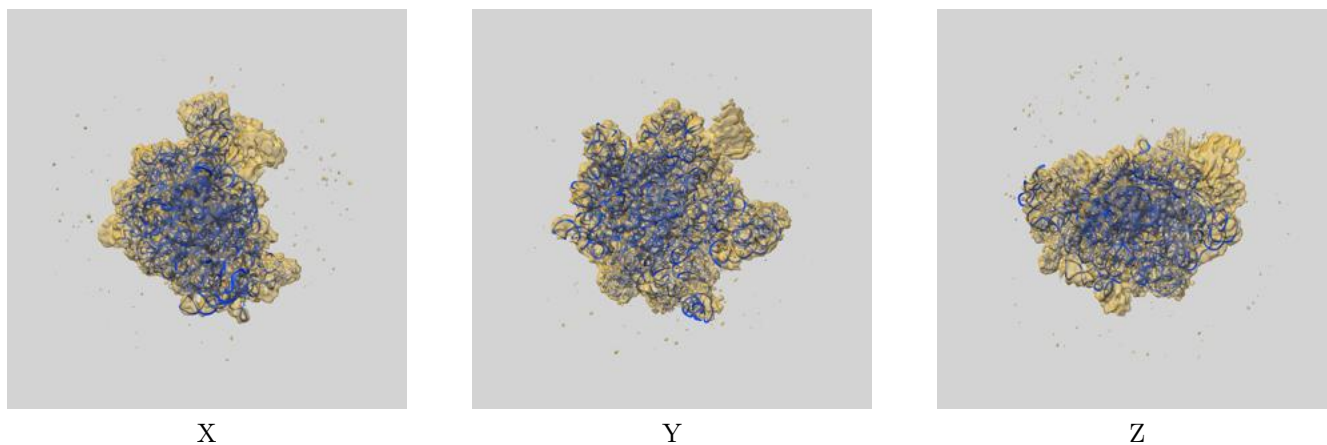
## 8 Fourier-Shell correlation

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-2012 and PDB model 4ADX. Per-residue inclusion information can be found in section 3 on page 11.

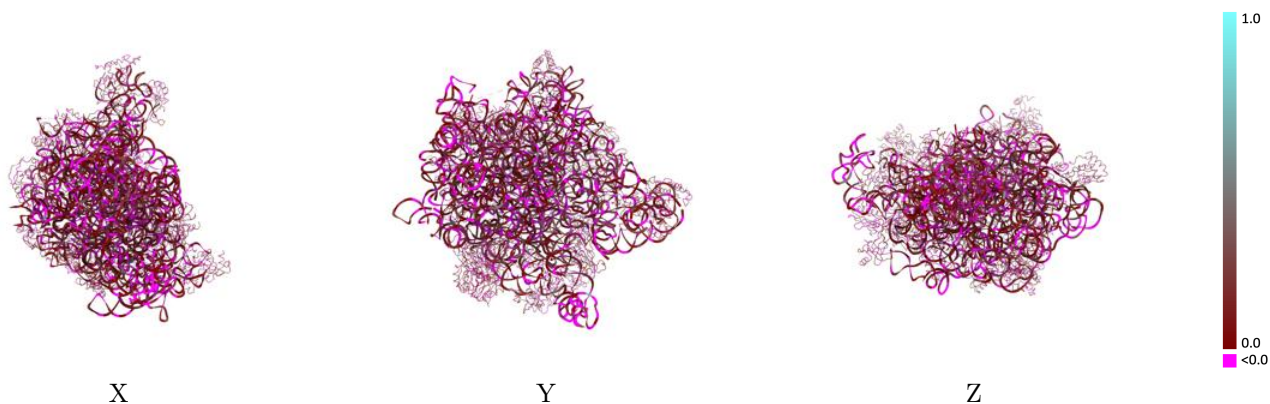
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 30.0 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.

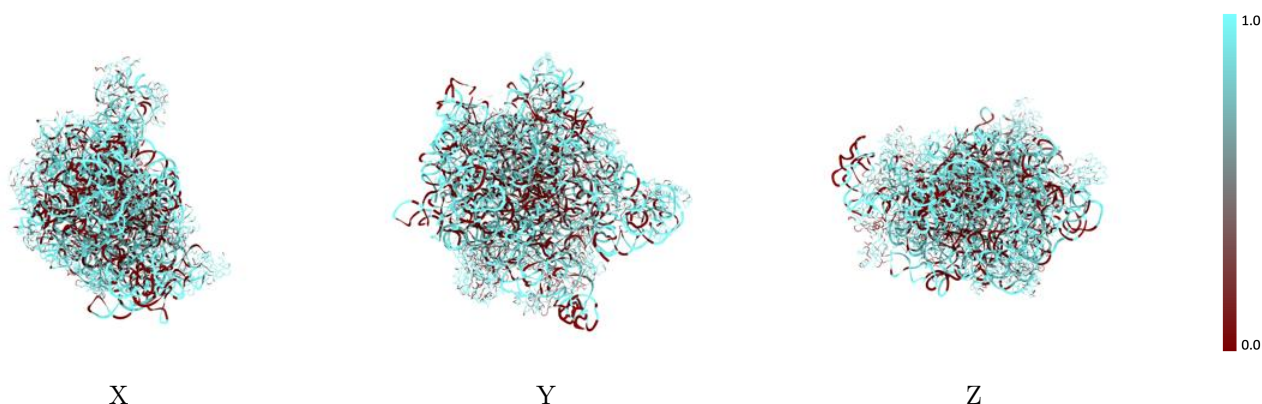


## 9.2 Q-score mapped to coordinate model [i](#)



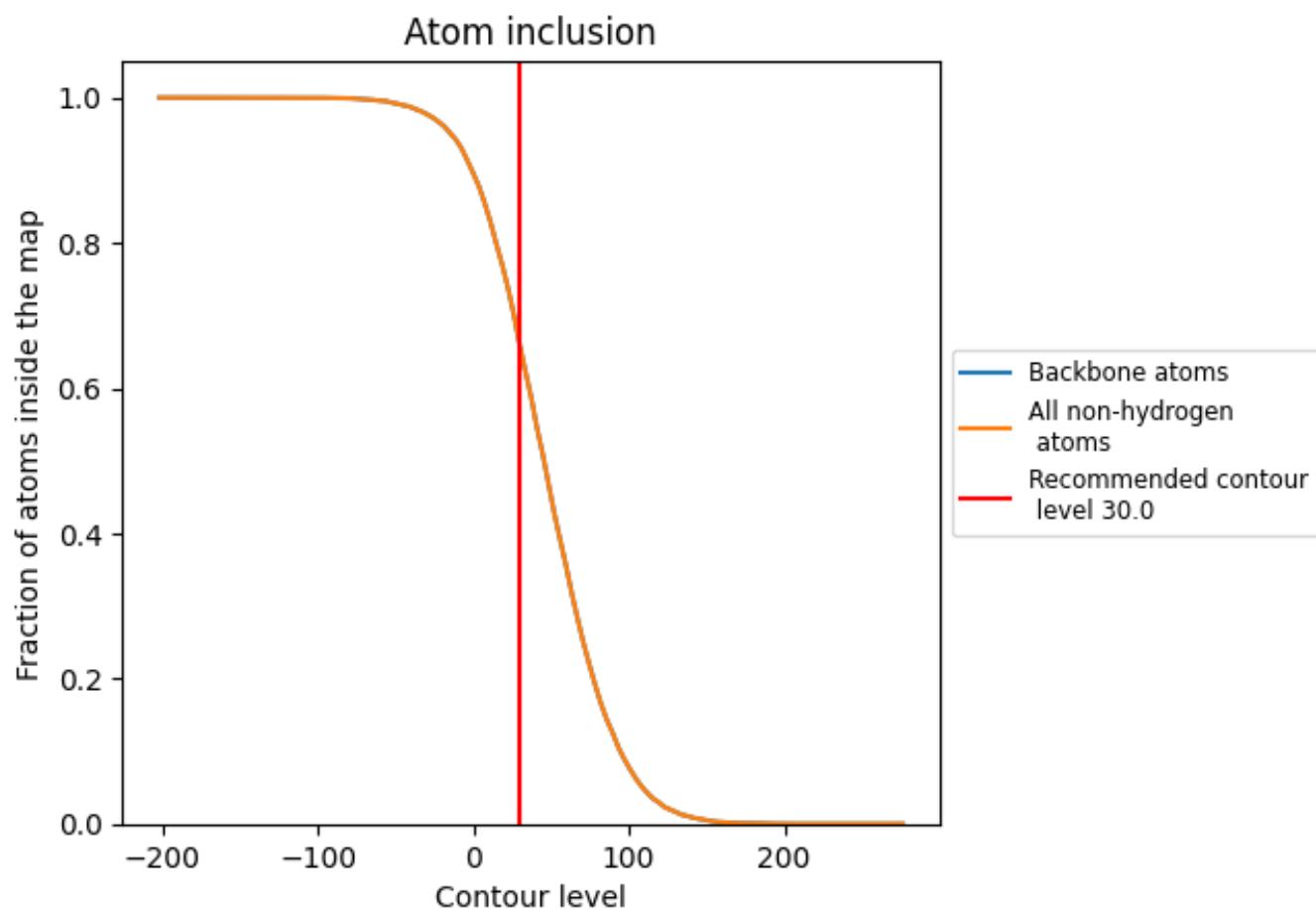
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (30.0).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (30.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6575	 0.0950
0	 0.6317	 0.0820
1	 0.5714	 0.0930
2	 0.6522	 0.1330
3	 0.6630	 0.1020
4	 0.6000	 0.1000
5	 0.3400	 0.0530
6	 0.8750	 0.1210
7	 0.7273	 0.0840
8	 0.5188	 0.0250
9	 0.6860	 0.0800
A	 0.5612	 0.1080
B	 0.6588	 0.0970
C	 0.6789	 0.1090
D	 0.8129	 0.0850
E	 0.6802	 0.1050
F	 0.8571	 0.1210
G	 0.6795	 0.0710
H	 0.6410	 0.1070
I	 0.7364	 0.1100
J	 0.6978	 0.1100
K	 0.6136	 0.1120
L	 0.5857	 0.0990
M	 0.5495	 0.1180
N	 0.6757	 0.0940
O	 0.7304	 0.1160
P	 0.7535	 0.1080
Q	 0.6316	 0.1260
R	 0.6600	 0.1160
S	 0.7778	 0.1240
T	 0.7863	 0.1240
U	 0.8269	 0.1310
V	 0.8281	 0.1100
W	 0.6104	 0.0800
X	 0.6707	 0.0980



*Continued on next page...*

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Chain	Atom inclusion	Q-score
Y	 0.6111	 0.1050
Z	 0.7671	 0.1120