



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 02:09 PM UTC

PDB ID : 9HUS / pdb\_00009hus  
EMDB ID : EMD-52418  
Title : Structure of WT E.coli ribosome with complexed filament nascent chain at length 31, with P-site tRNAs  
Authors : Mitropoulou, A.; Wlodarski, T.; Plessa, E.; Cabrita, L.D.; Christodoulou, J.  
Deposited on : 2024-12-23  
Resolution : 2.40 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:

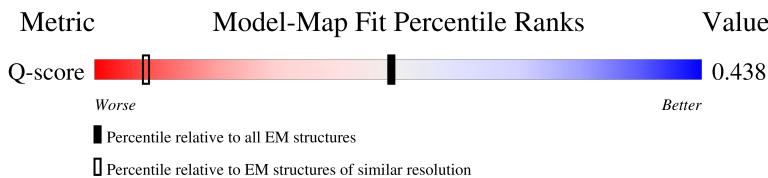
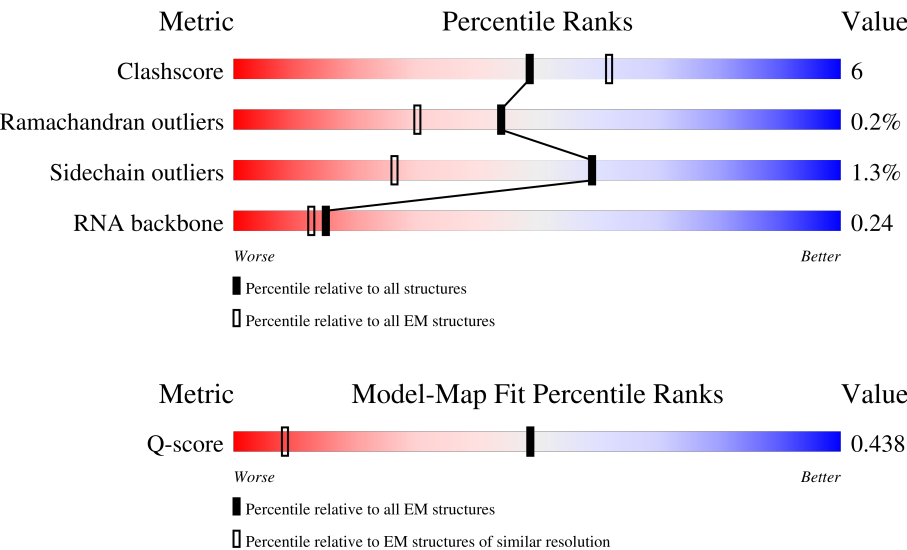
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





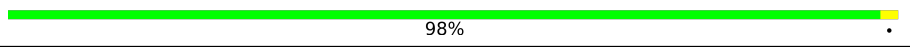
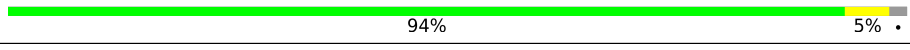



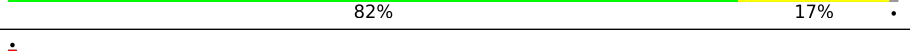
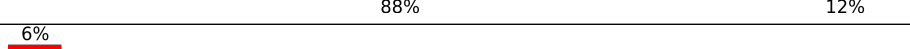
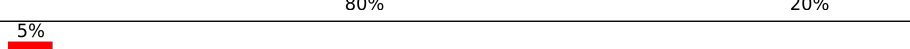
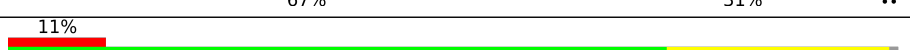

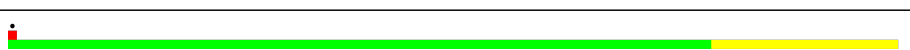

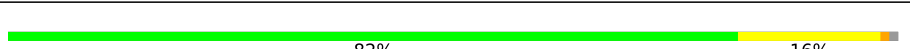





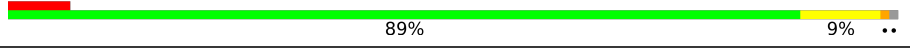
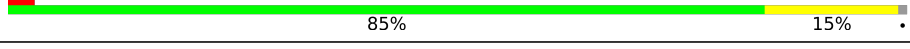



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 ( 1.90 - 2.90 )

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	78	<div><div></div><div>85%</div><div>14%</div><div></div></div>
2	1	63	<div><div>13%</div><div>70%</div><div>27%</div><div></div></div>
3	2	59	<div><div></div><div>80%</div><div>17%</div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	57	
5	4	55	
6	6	46	
7	7	65	
8	8	50	
9	a	120	
10	b	2904	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	j	142	
18	k	123	
19	l	144	
20	m	136	
21	n	127	
22	o	117	
23	p	115	
24	q	118	
25	r	103	
26	s	110	
27	t	100	
28	u	104	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	w	94	<div><div></div><div>5%</div><div>94%</div><div>6%</div></div>
30	y	85	<div><div></div><div>71%</div><div>19%</div><div>5%</div><div></div></div>
31	v	77	<div><div></div><div>31%</div><div>55%</div><div>14%</div></div>
32	z	148	<div><div></div><div>7%</div><div></div><div>86%</div></div>

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90875 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 protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2901	Total	C	N	O	P	0	0
			62281	27784	11464	20132	2901		

- Molecule 11 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 15 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 21 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 23 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 25 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 27 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called Large ribosomal subunit protein uL24.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	u	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 29 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 30 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	y	82	Total	C	N	O	S	0	0
			619	383	127	108	1		

- Molecule 31 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 32 is a protein called Gelation factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	z	20	Total	C	N	O	0	0
			181	126	30	25		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	1	MET	-	initiating methionine	UNP P13466
z	2	HIS	-	expression tag	UNP P13466
z	3	HIS	-	expression tag	UNP P13466
z	4	HIS	-	expression tag	UNP P13466
z	5	HIS	-	expression tag	UNP P13466
z	6	HIS	-	expression tag	UNP P13466
z	7	HIS	-	expression tag	UNP P13466
z	8	ALA	-	expression tag	UNP P13466
z	9	SER	-	expression tag	UNP P13466
z	130	GLU	-	expression tag	UNP P13466
z	131	LEU	-	expression tag	UNP P13466
z	132	PHE	-	expression tag	UNP P13466
z	133	SER	-	expression tag	UNP P13466

*Continued on next page...*


*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
z	134	THR	-	expression tag	UNP P13466
z	135	PRO	-	expression tag	UNP P13466
z	136	VAL	-	expression tag	UNP P13466
z	137	TRP	-	expression tag	UNP P13466
z	138	ILE	-	expression tag	UNP P13466
z	139	TRP	-	expression tag	UNP P13466
z	140	TRP	-	expression tag	UNP P13466
z	141	TRP	-	expression tag	UNP P13466
z	142	PRO	-	expression tag	UNP P13466
z	143	ARG	-	expression tag	UNP P13466
z	144	ILE	-	expression tag	UNP P13466
z	145	ARG	-	expression tag	UNP P13466
z	146	GLY	-	expression tag	UNP P13466
z	147	PRO	-	expression tag	UNP P13466
z	148	PRO	-	expression tag	UNP P13466

### 3 Residue-property plots [i](#)

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.

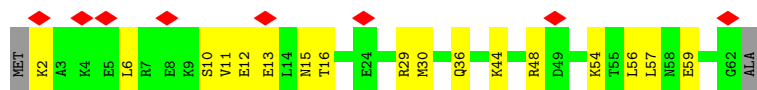
- Molecule 1: Large ribosomal subunit protein bL28

Chain 0: 




- Molecule 2: Large ribosomal subunit protein uL29

Chain 1: 



- Molecule 3: Large ribosomal subunit protein uL30

Chain 2: 



- Molecule 4: Large ribosomal subunit protein bL32

Chain 3: 



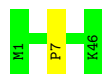
- Molecule 5: Large ribosomal subunit protein bL33

Chain 4: 



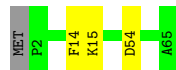
- Molecule 6: Large ribosomal subunit protein bL34

Chain 6:  98%



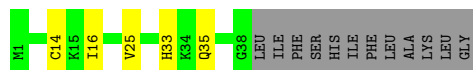
- Molecule 7: Large ribosomal subunit protein bL35

Chain 7:  94%



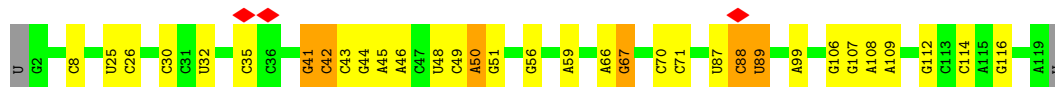
- Molecule 8: 50S ribosomal protein L36

Chain 8:  66% 10% 24%



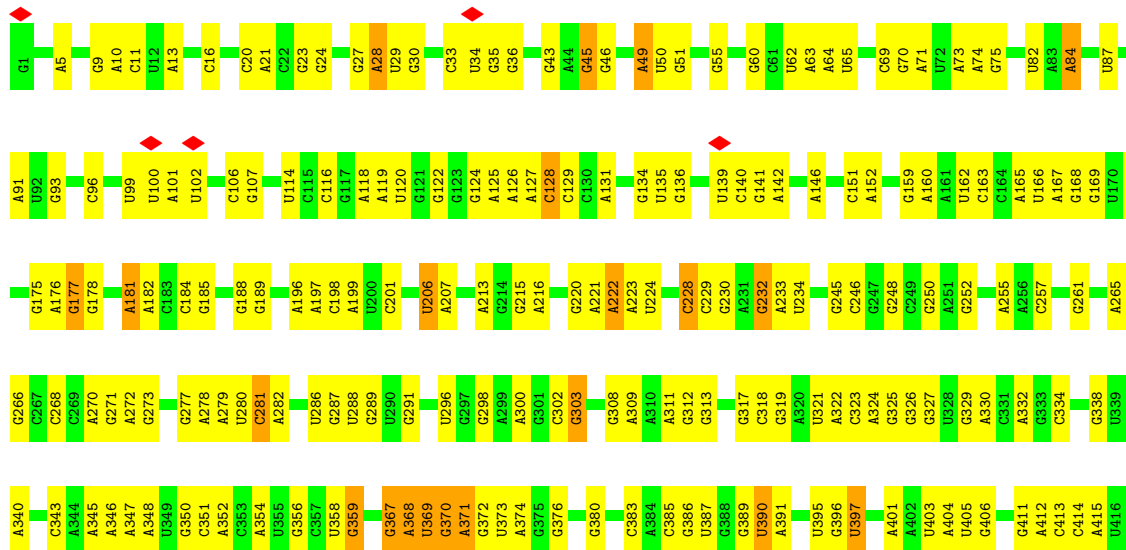
- Molecule 9: 5S rRNA

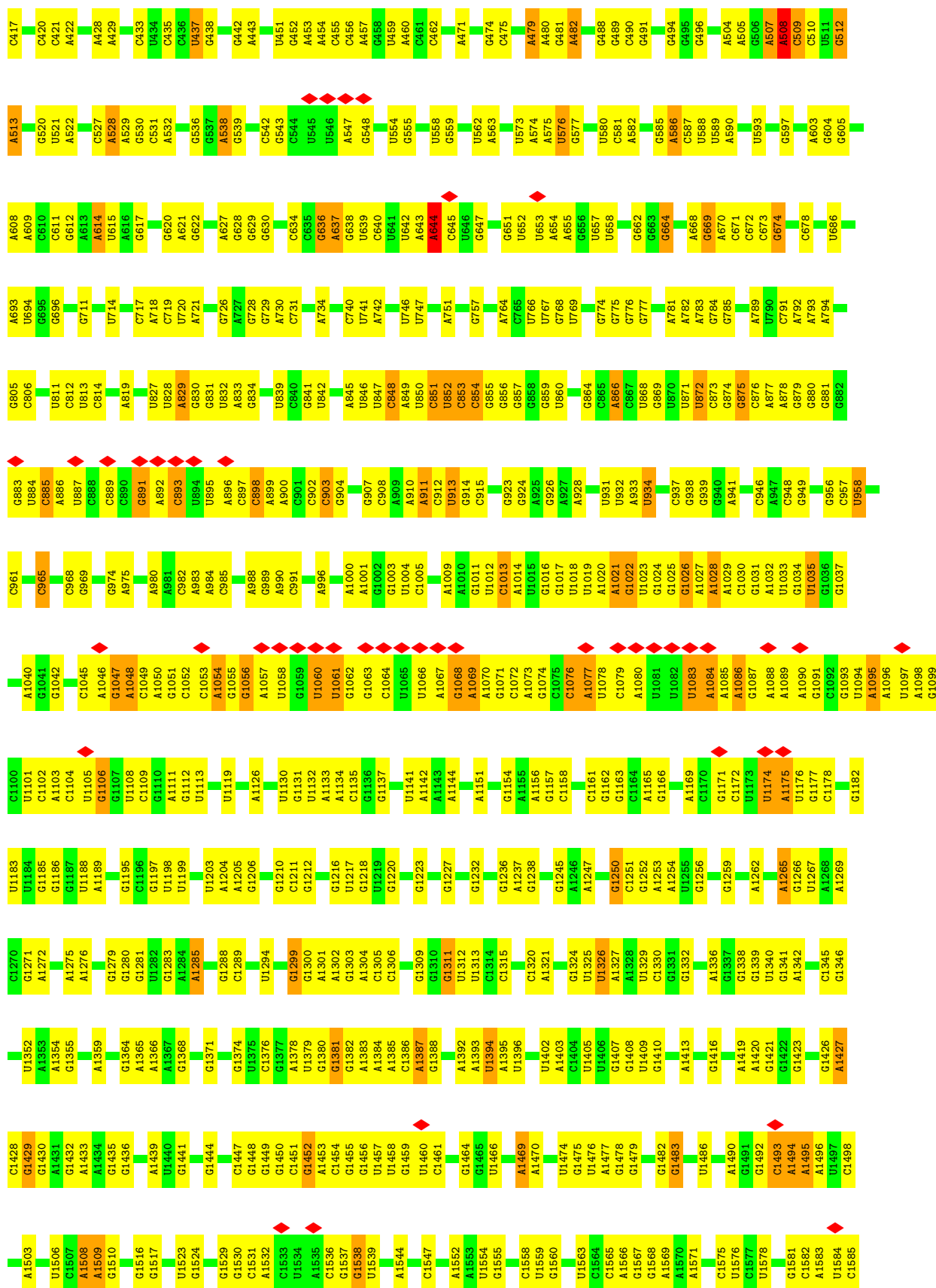
Chain a:  71% 22% 5%



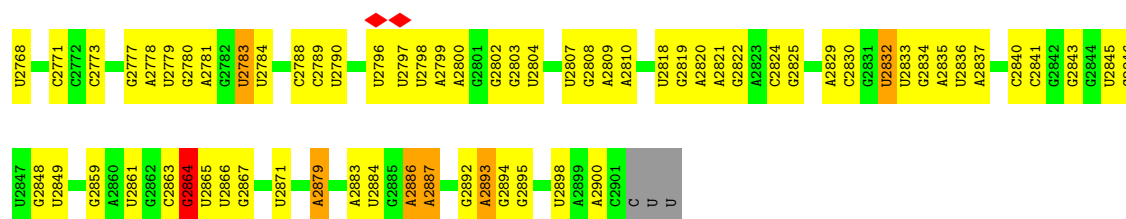
- Molecule 10: 23S rRNA

Chain b:  49% 43% 7%



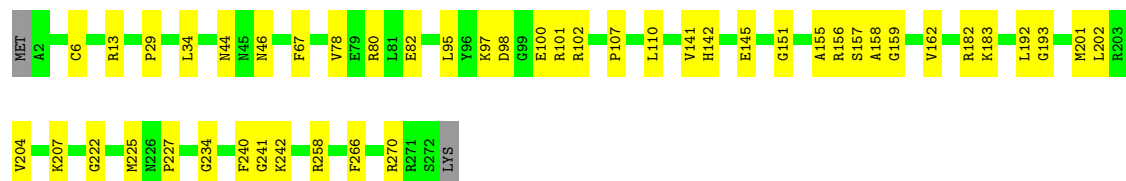






- Molecule 11: Large ribosomal subunit protein uL2

Chain c: 82% 17%



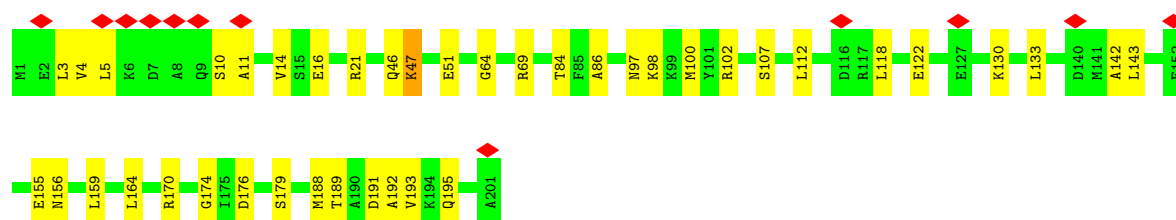
- Molecule 12: 50S ribosomal protein L3

Chain d: 88% 12%



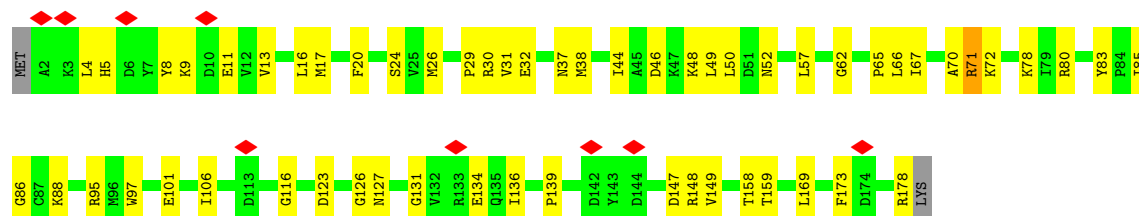
- Molecule 13: Large ribosomal subunit protein uL4

Chain e: 6% 80% 20%

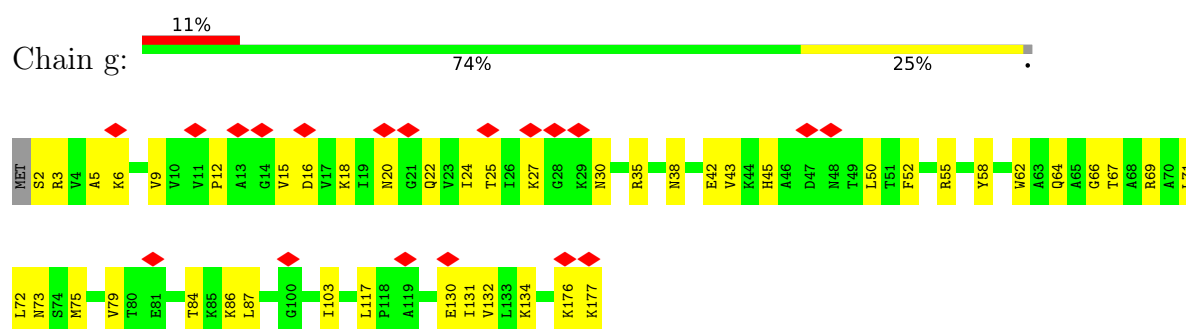


- Molecule 14: Large ribosomal subunit protein uL5

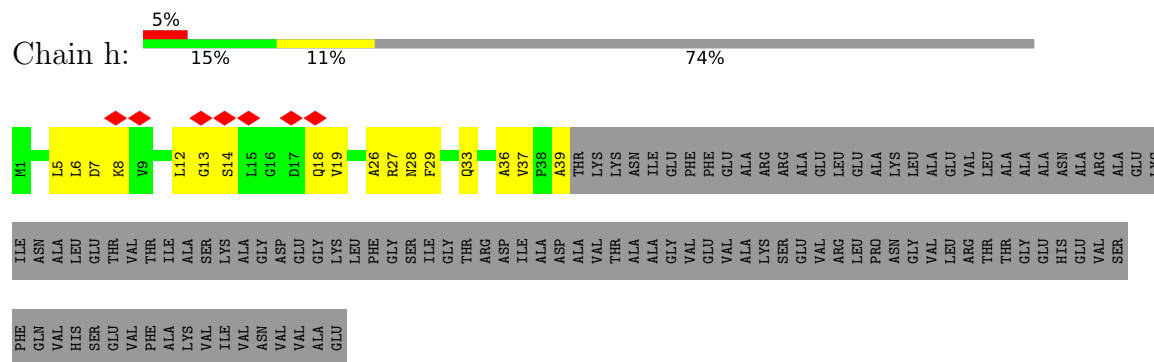
Chain f: 5% 67% 31%



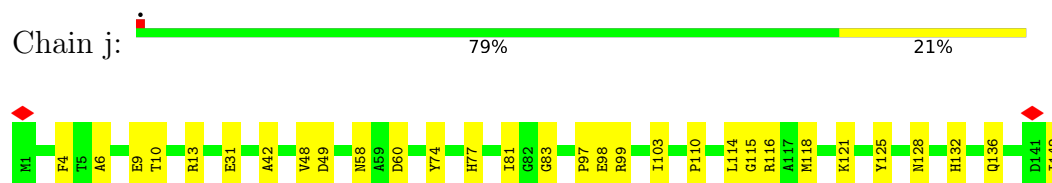
- Molecule 15: Large ribosomal subunit protein uL6



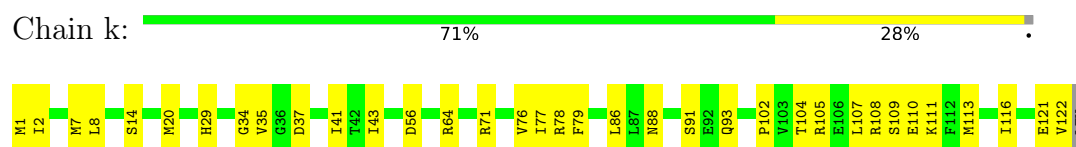
- Molecule 16: Large ribosomal subunit protein bL9



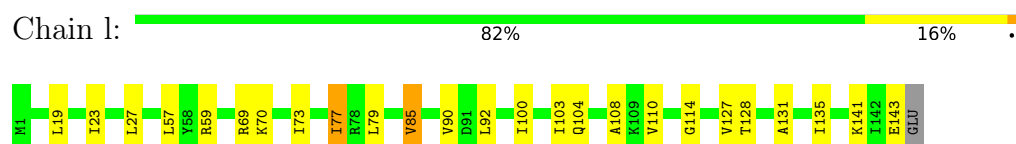
- Molecule 17: Large ribosomal subunit protein uL13



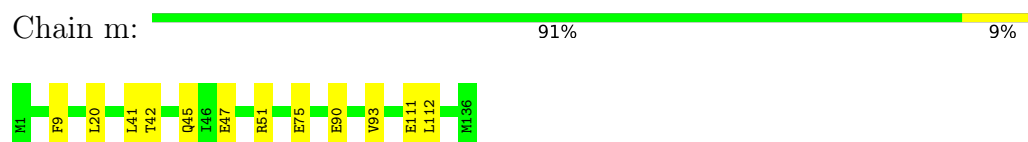
- Molecule 18: Large ribosomal subunit protein uL14



- Molecule 19: Large ribosomal subunit protein uL15



- Molecule 20: 50S ribosomal protein L16






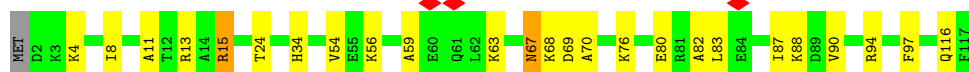
- Molecule 21: Large ribosomal subunit protein bL17

Chain n:  73% 21% 6%




- Molecule 22: Large ribosomal subunit protein uL18

Chain o:  78% 20% ..




- Molecule 23: Large ribosomal subunit protein bL19

Chain p:  77% 21% .




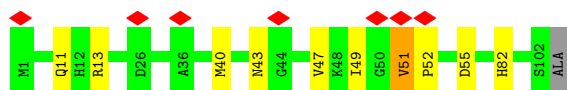
- Molecule 24: Large ribosomal subunit protein bL20

Chain q:  86% 13% .




- Molecule 25: Large ribosomal subunit protein bL21

Chain r:  7% 89% 9% ..




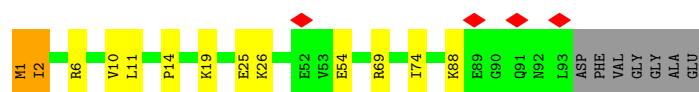
- Molecule 26: Large ribosomal subunit protein uL22

Chain s:  85% 15% .

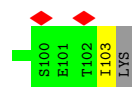
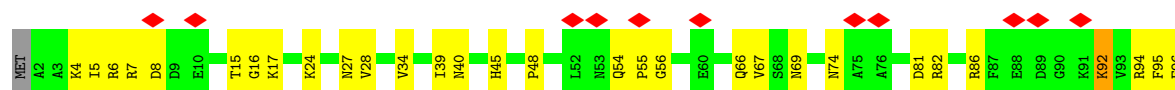


- Molecule 27: Large ribosomal subunit protein uL23

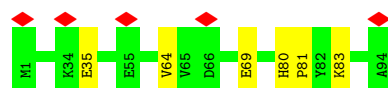
Chain t:  80% 11% • 7%



- Molecule 28: Large ribosomal subunit protein uL24



- Molecule 29: Large ribosomal subunit protein bL25



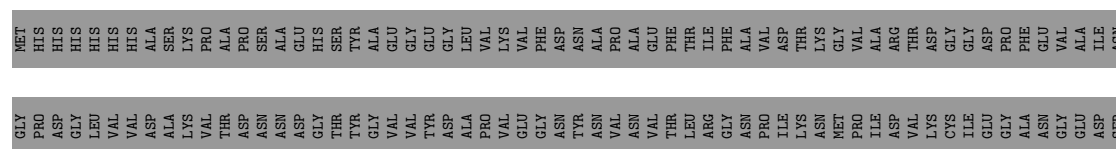
- Molecule 30: Large ribosomal subunit protein bL27



- Molecule 31: P-site tRNA



- Molecule 32: Gelation factor





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	14.45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0077	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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	0	0.39	0/635	0.52	0/848
2	1	0.31	0/496	0.46	0/660
3	2	0.35	0/443	0.40	0/593
4	3	0.47	0/440	0.72	0/588
5	4	0.48	0/416	0.66	0/554
6	6	0.39	0/380	0.48	0/498
7	7	0.46	0/513	0.57	0/676
8	8	0.39	0/302	0.48	0/397
9	a	0.38	0/2828	0.36	0/4410
10	b	0.54	4/69757 (0.0%)	0.74	32/108827 (0.0%)
11	c	0.37	0/2121	0.48	0/2852
12	d	0.40	0/1586	0.48	0/2134
13	e	0.33	0/1571	0.43	1/2113 (0.0%)
14	f	0.40	0/1434	0.62	0/1926
15	g	0.35	0/1343	0.52	0/1816
16	h	0.28	0/290	0.63	0/392
17	j	0.42	0/1152	0.47	1/1551 (0.1%)
18	k	0.40	0/947	0.47	0/1268
19	l	0.63	0/1052	0.82	1/1401 (0.1%)
20	m	0.36	0/1093	0.50	0/1460
21	n	0.40	0/973	0.52	0/1301
22	o	0.42	0/902	0.60	0/1209
23	p	0.38	0/920	0.43	0/1231
24	q	0.42	0/960	0.47	0/1278
25	r	0.53	0/823	0.65	0/1100
26	s	0.37	0/852	0.41	0/1142
27	t	0.39	0/744	0.53	0/994
28	u	0.39	0/787	0.57	0/1051
29	w	0.34	0/766	0.43	0/1025
30	y	0.99	6/626 (1.0%)	1.14	10/826 (1.2%)
31	v	0.44	0/1839	0.48	0/2866
32	z	0.95	0/192	1.22	1/267 (0.4%)
All	All	0.51	10/99183 (0.0%)	0.69	46/149254 (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
30	y	0	4
32	z	0	2
All	All	0	6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	507	A	O3'-P	28.41	2.03	1.61
10	b	2059	A	O3'-P	25.67	1.99	1.61
10	b	2058	A	O3'-P	20.95	1.92	1.61
10	b	509	C	O3'-P	-20.51	1.30	1.61
30	y	6	ALA	C-O	-13.78	1.06	1.24

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	509	C	O3'-P-O5'	27.47	145.21	104.00
10	b	507	A	O3'-P-O5'	23.79	139.69	104.00
10	b	2059	A	P-O3'-C3'	-23.47	84.99	120.20
10	b	2058	A	O3'-P-O5'	21.50	136.25	104.00
10	b	507	A	P-O3'-C3'	16.97	145.66	120.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	y	3	HIS	Mainchain
30	y	5	LYS	Mainchain
30	y	6	ALA	Mainchain
30	y	7	GLY	Mainchain
32	z	143	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	625	0	652	7	0
2	1	495	0	526	13	0
3	2	439	0	482	6	0
4	3	434	0	445	11	0
5	4	409	0	440	8	0
6	6	377	0	418	1	0
7	7	504	0	572	2	0
8	8	301	0	341	3	0
9	a	2529	0	1281	14	0
10	b	62281	0	31323	440	0
11	c	2082	0	2154	30	0
12	d	1565	0	1616	24	0
13	e	1552	0	1619	27	0
14	f	1410	0	1444	51	0
15	g	1323	0	1371	27	0
16	h	287	0	307	13	0
17	j	1129	0	1162	21	0
18	k	938	0	1012	25	0
19	l	1043	0	1123	11	0
20	m	1074	0	1157	9	0
21	n	960	0	1000	18	0
22	o	892	0	923	17	0
23	p	908	0	956	22	0
24	q	947	0	1019	16	0
25	r	810	0	834	5	0
26	s	845	0	909	14	0
27	t	738	0	807	9	0
28	u	779	0	831	23	0
29	w	753	0	780	4	0
30	y	619	0	641	22	0
31	v	1646	0	828	86	0
32	z	181	0	174	14	0
All	All	90875	0	59147	862	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 6.

The worst 5 of 862 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)
10:b:1924:C:C3'	31:v:14:A:C8	1.78	1.55
10:b:892:A:H8	10:b:893:C:C6	1.26	1.52
10:b:892:A:C8	10:b:893:C:C6	1.96	1.49
10:b:1924:C:C1'	31:v:14:A:C8	1.95	1.47
10:b:1924:C:C1'	31:v:14:A:H8	1.22	1.47

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	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
3	2	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	3	53/57 (93%)	49 (92%)	4 (8%)	0	100	100
5	4	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
6	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
7	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
8	8	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
12	d	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
13	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
14	f	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	21	32
15	g	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
16	h	37/149 (25%)	32 (86%)	5 (14%)	0	100	100
17	j	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
18	k	120/123 (98%)	116 (97%)	4 (3%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	l	141/144 (98%)	132 (94%)	9 (6%)	0	100	100
20	m	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
21	n	118/127 (93%)	111 (94%)	7 (6%)	0	100	100
22	o	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
23	p	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
24	q	115/118 (98%)	115 (100%)	0	0	100	100
25	r	100/103 (97%)	93 (93%)	5 (5%)	2 (2%)	6	7
26	s	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
27	t	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
28	u	100/104 (96%)	83 (83%)	17 (17%)	0	100	100
29	w	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
30	y	78/85 (92%)	71 (91%)	5 (6%)	2 (3%)	4	4
32	z	18/148 (12%)	15 (83%)	2 (11%)	1 (6%)	1	1
All	All	3072/3427 (90%)	2924 (95%)	142 (5%)	6 (0%)	44	58

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	r	52	PRO
30	y	7	GLY
25	r	51	VAL
30	y	44	LYS
32	z	132	PHE

### 5.3.2 Protein sidechains ⓘ

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	
1	0	67/68 (98%)	67 (100%)	0	100	100
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	47 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	46/48 (96%)	44 (96%)	2 (4%)	26	44
5	4	45/49 (92%)	44 (98%)	1 (2%)	45	67
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	51 (100%)	0	100	100
8	8	34/44 (77%)	34 (100%)	0	100	100
11	c	216/218 (99%)	216 (100%)	0	100	100
12	d	164/164 (100%)	164 (100%)	0	100	100
13	e	165/165 (100%)	165 (100%)	0	100	100
14	f	148/150 (99%)	144 (97%)	4 (3%)	39	62
15	g	137/138 (99%)	136 (99%)	1 (1%)	76	88
16	h	30/114 (26%)	30 (100%)	0	100	100
17	j	116/116 (100%)	116 (100%)	0	100	100
18	k	103/104 (99%)	103 (100%)	0	100	100
19	l	102/103 (99%)	94 (92%)	8 (8%)	11	20
20	m	109/109 (100%)	109 (100%)	0	100	100
21	n	100/103 (97%)	100 (100%)	0	100	100
22	o	86/87 (99%)	82 (95%)	4 (5%)	23	41
23	p	98/100 (98%)	98 (100%)	0	100	100
24	q	89/90 (99%)	89 (100%)	0	100	100
25	r	84/84 (100%)	79 (94%)	5 (6%)	17	31
26	s	92/93 (99%)	92 (100%)	0	100	100
27	t	80/84 (95%)	78 (98%)	2 (2%)	42	64
28	u	83/85 (98%)	82 (99%)	1 (1%)	63	81
29	w	78/78 (100%)	78 (100%)	0	100	100
30	y	61/63 (97%)	60 (98%)	1 (2%)	55	76
32	z	19/121 (16%)	14 (74%)	5 (26%)	0	0
All	All	2542/2772 (92%)	2508 (99%)	34 (1%)	59	80

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	y	5	LYS
32	z	128	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	z	144	ILE
19	l	85	VAL
19	l	77	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
22	o	29	HIS
24	q	44	GLN
22	o	67	ASN
23	p	10	GLN
24	q	81	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2900/2904 (99%)	1198 (41%)	0
31	v	76/77 (98%)	20 (26%)	0
9	a	117/120 (97%)	21 (17%)	0
All	All	3093/3101 (99%)	1239 (40%)	0

5 of 1239 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	25	U
9	a	26	C
9	a	30	C
9	a	32	U
9	a	35	C

There are no RNA pucker outliers to report.

## 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	b	4
30	y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	8:GLY	C	9:SER	N	3.63
1	b	507:A	O3'	508:A	P	2.03
1	b	2059:A	O3'	2060:A	P	1.99
1	b	2058:A	O3'	2059:A	P	1.92
1	b	509:C	O3'	510:C	P	1.30

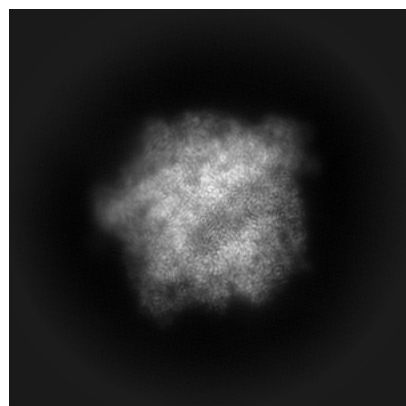
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52418. These allow visual inspection of the internal detail of the map and identification of artifacts.

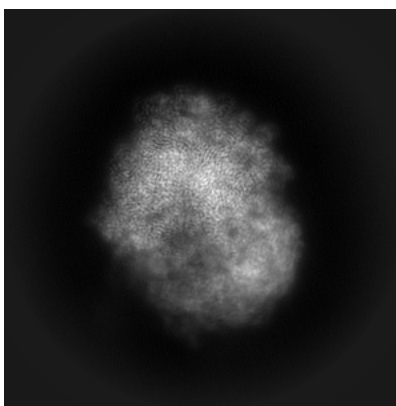
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

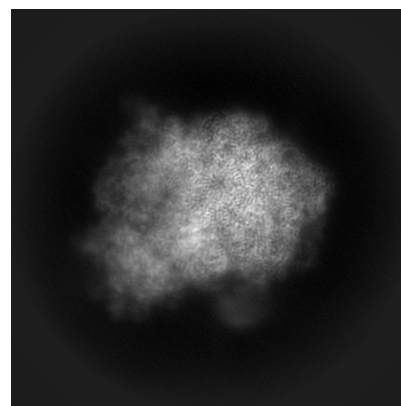
#### 6.1.1 Primary map



X

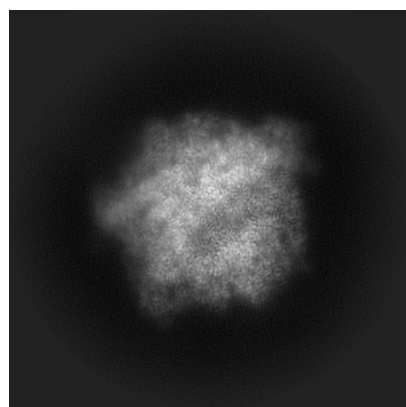


Y

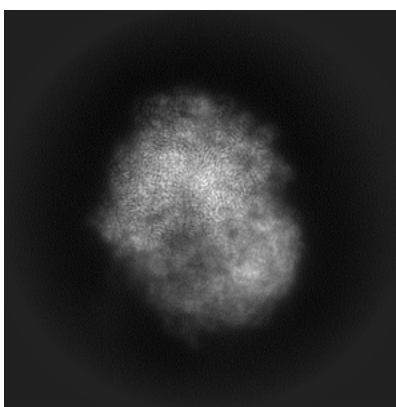


Z

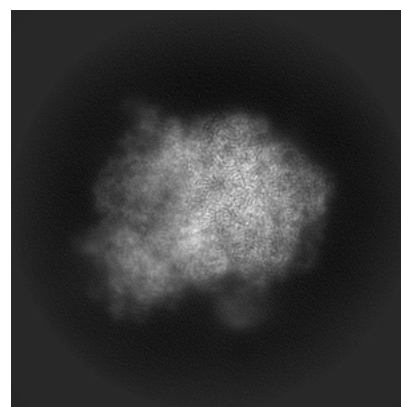
#### 6.1.2 Raw map



X



Y

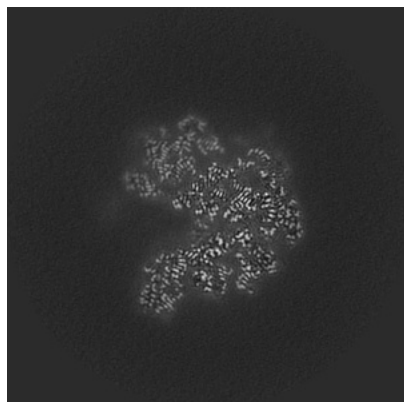


Z

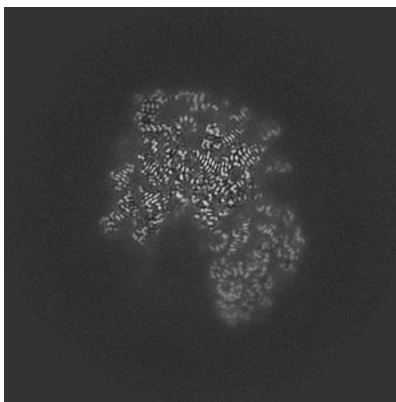
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

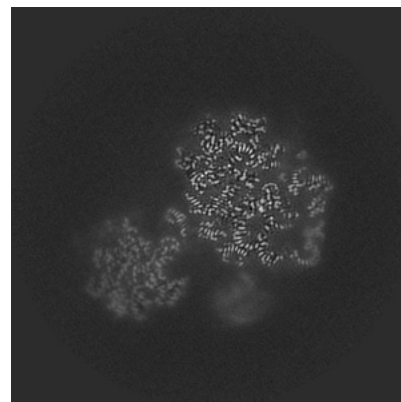
### 6.2.1 Primary map



X Index: 240

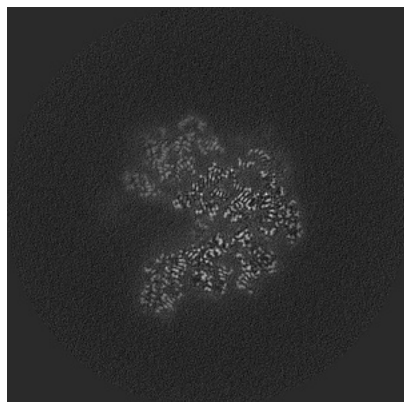


Y Index: 240

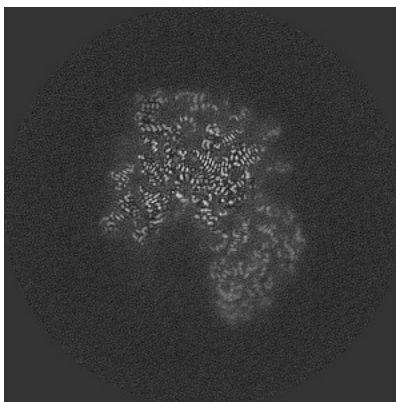


Z Index: 240

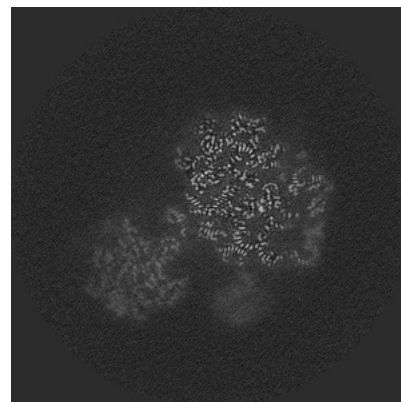
### 6.2.2 Raw map



X Index: 240



Y Index: 240

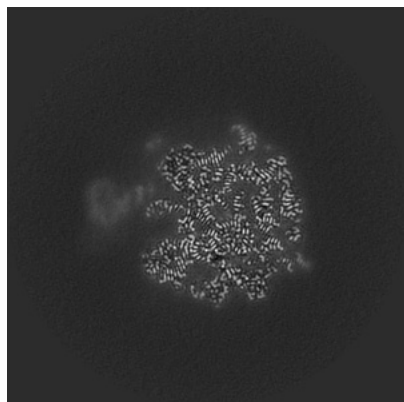


Z Index: 240

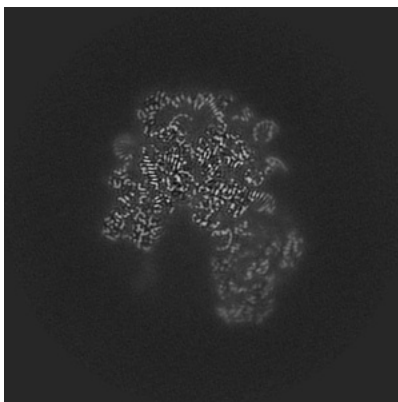
The images above show central slices of the map in three orthogonal directions.

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

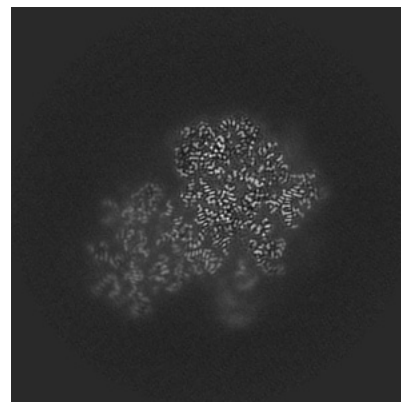
### 6.3.1 Primary map



X Index: 271

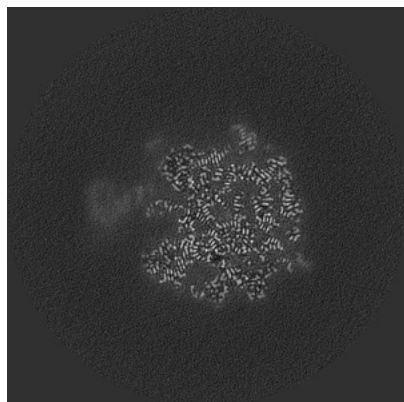


Y Index: 247

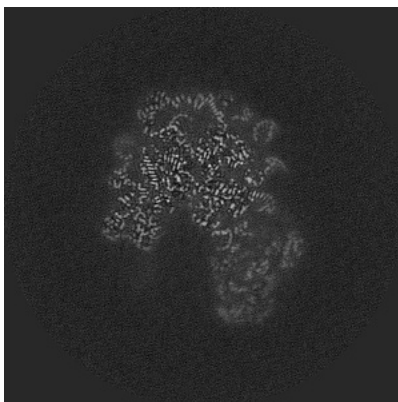


Z Index: 255

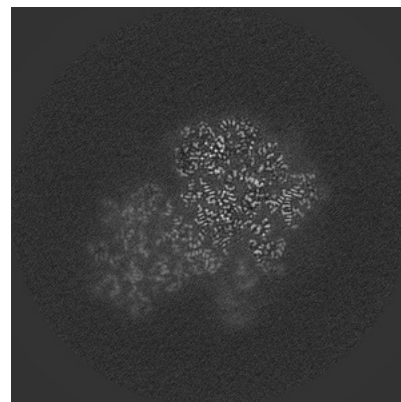
### 6.3.2 Raw map



X Index: 271



Y Index: 247



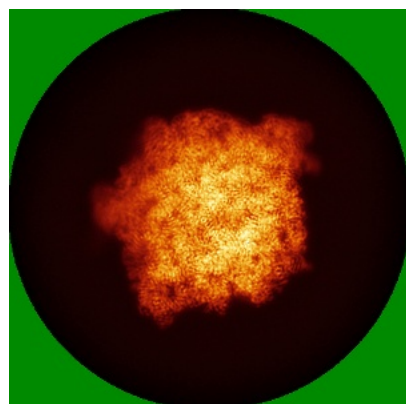
Z Index: 255

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

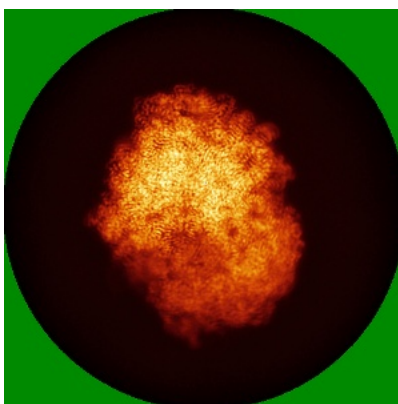


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

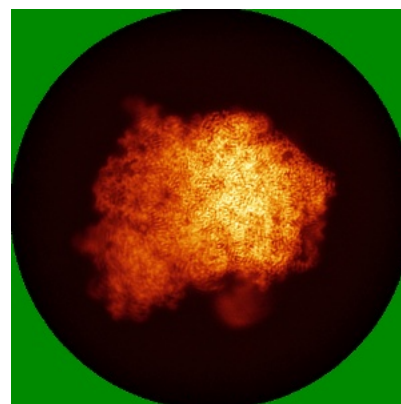
### 6.4.1 Primary map



X

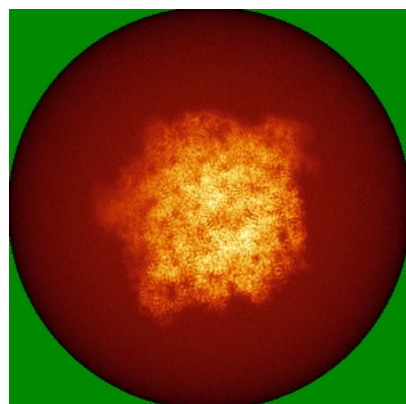


Y

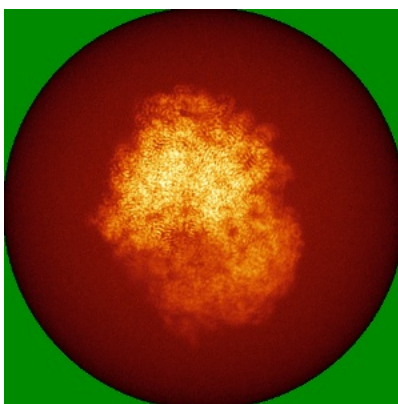


Z

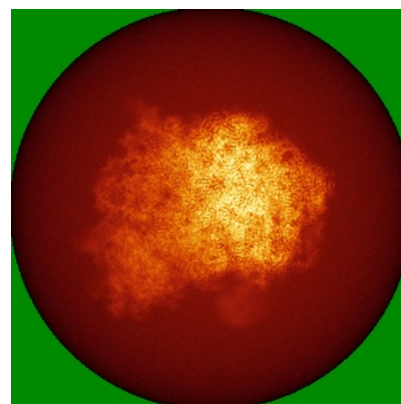
### 6.4.2 Raw map



X



Y



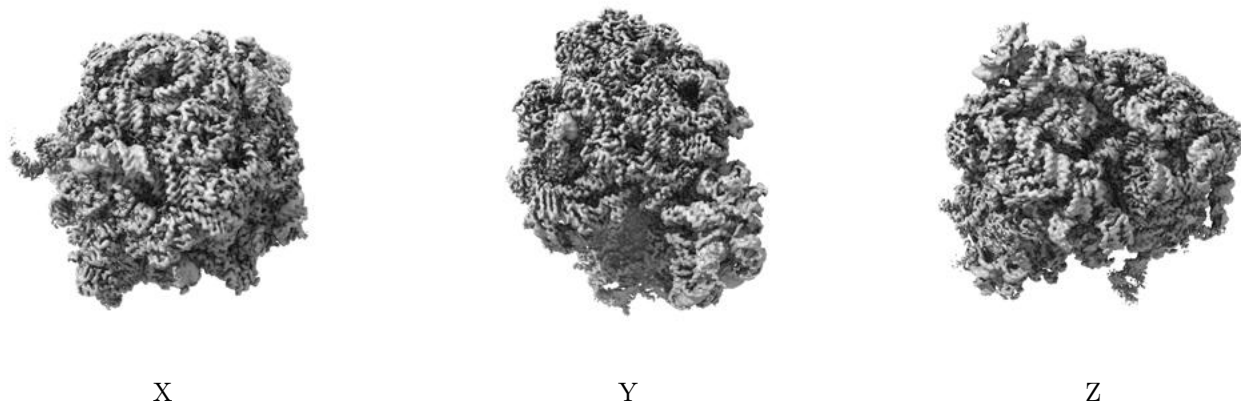
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



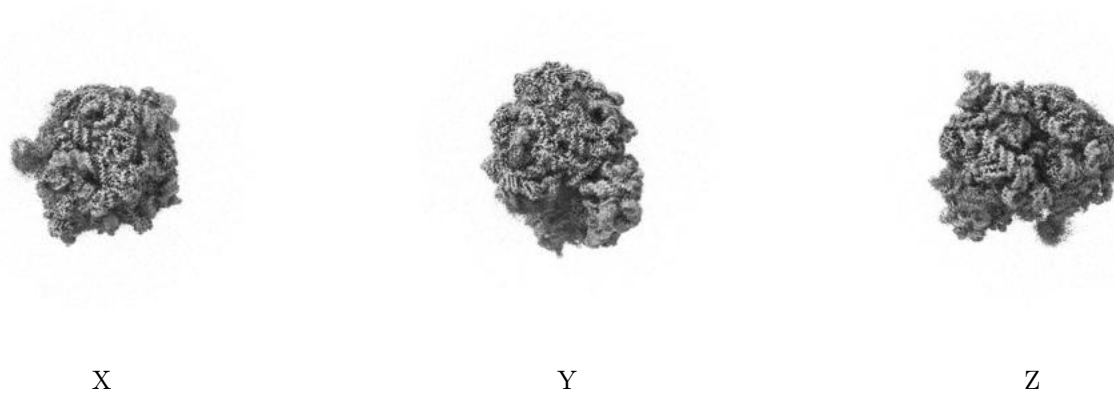
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

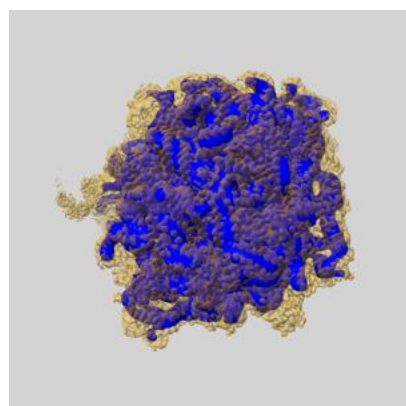
## 6.6 Mask visualisation [i](#)

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

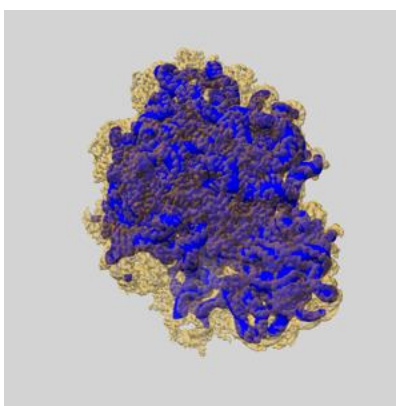
A mask typically either:

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

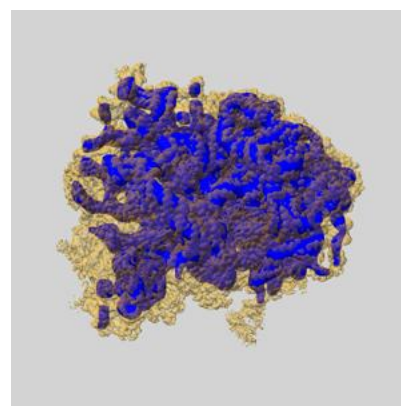
### 6.6.1 emd\_52418\_msk\_1.map [i](#)



X



Y

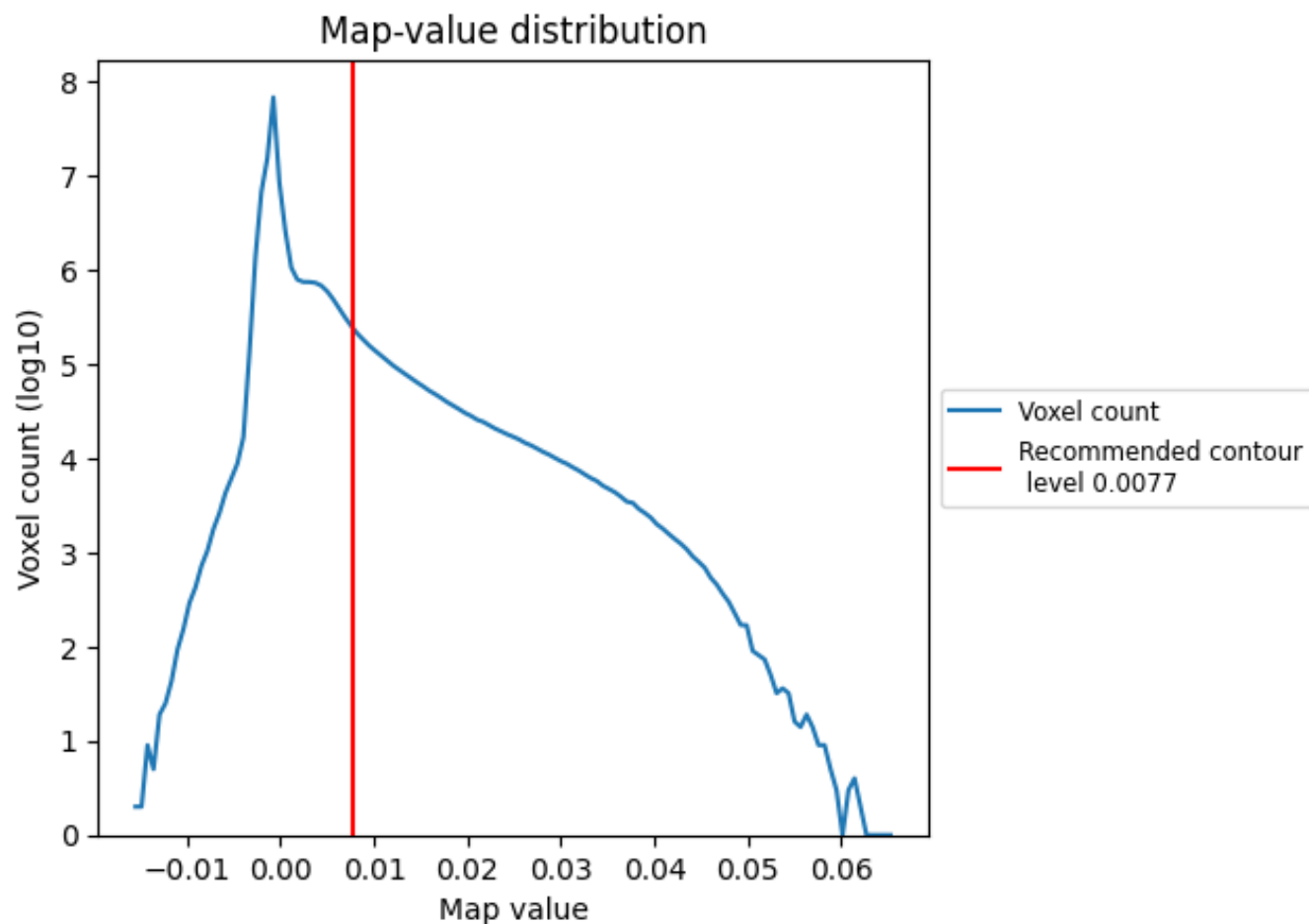


Z

## 7 Map analysis [i](#)

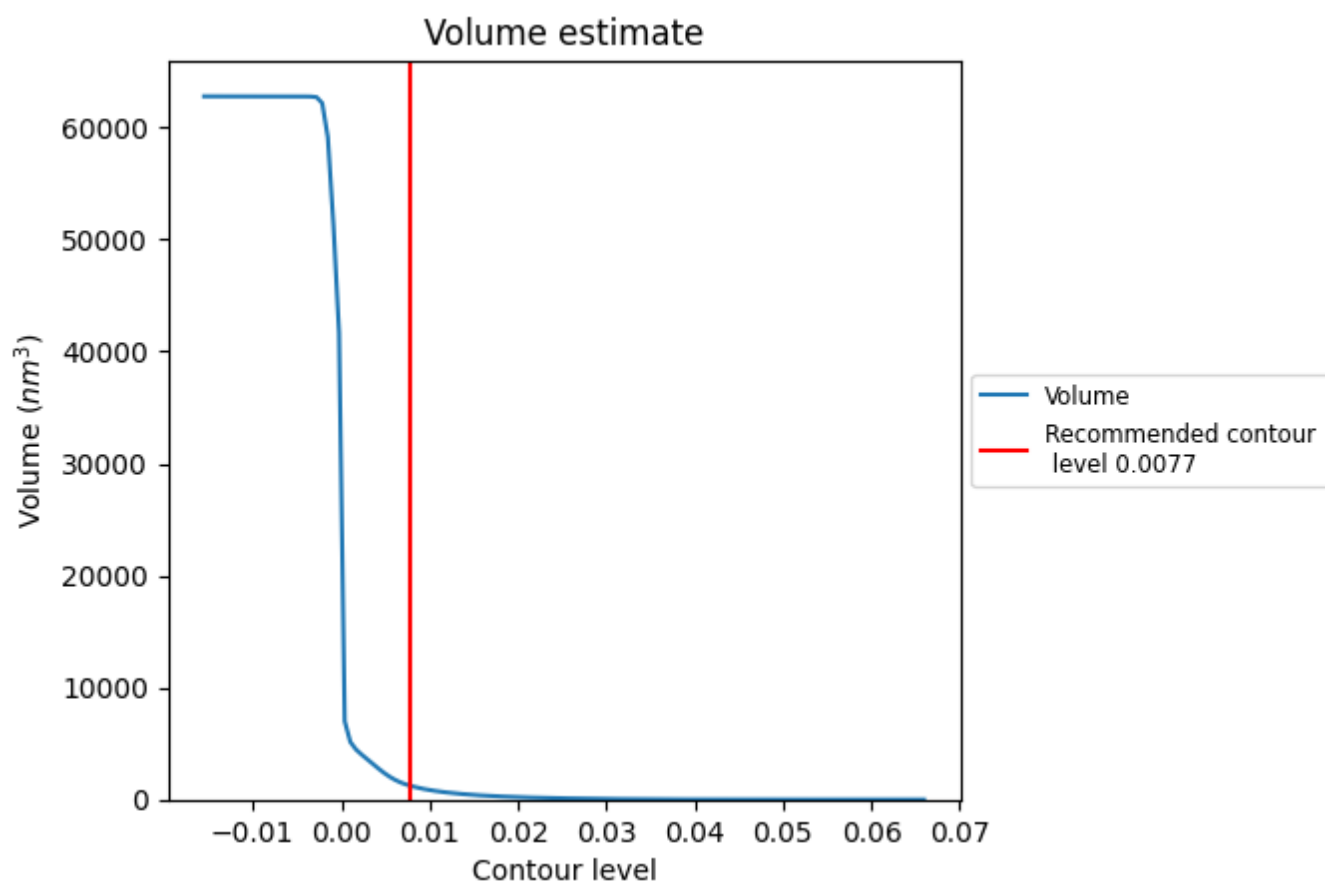
This section contains the results of statistical analysis of the map.

### 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.

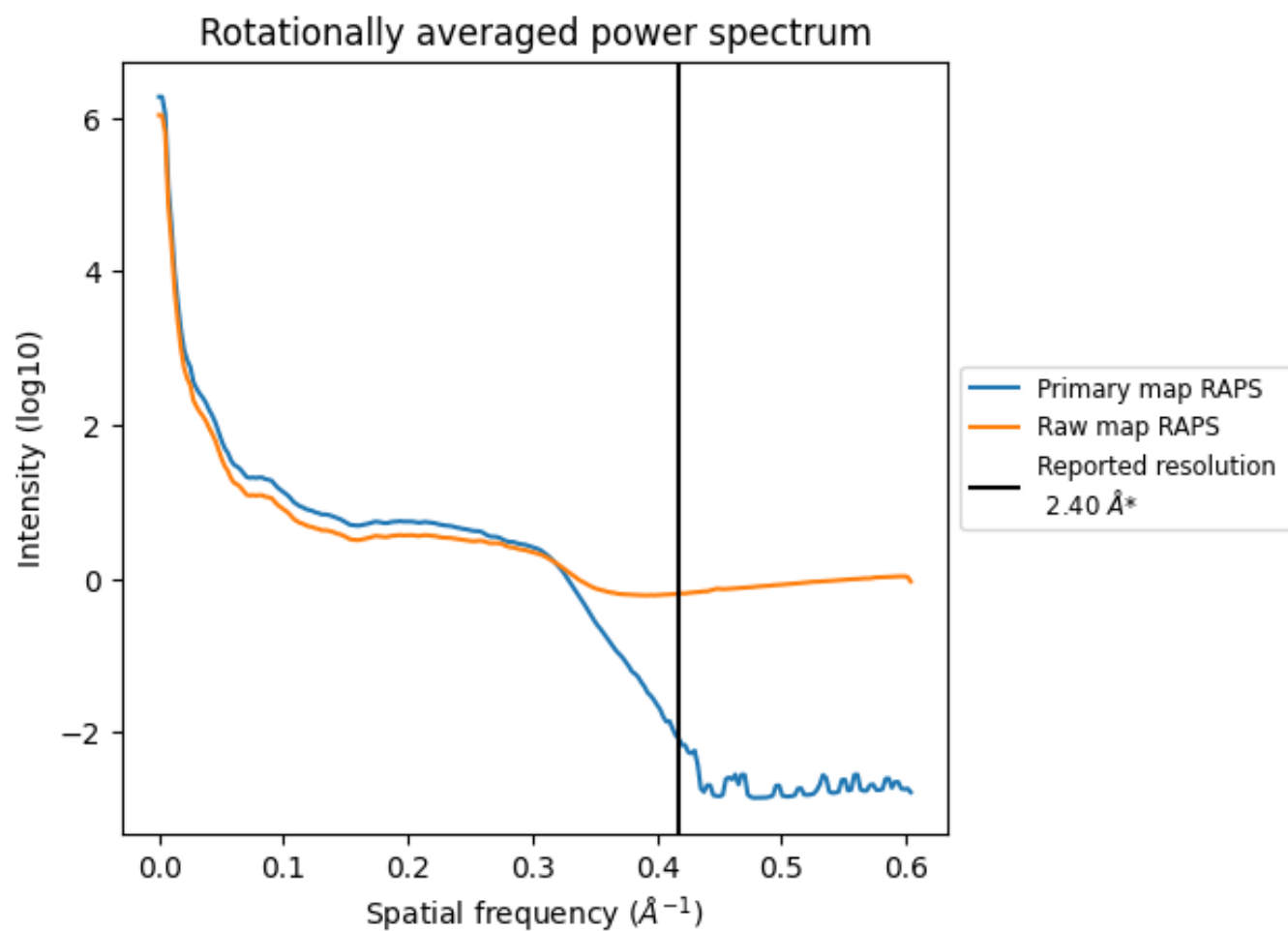
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1259 nm<sup>3</sup>; this corresponds to an approximate mass of 1137 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 ⓘ

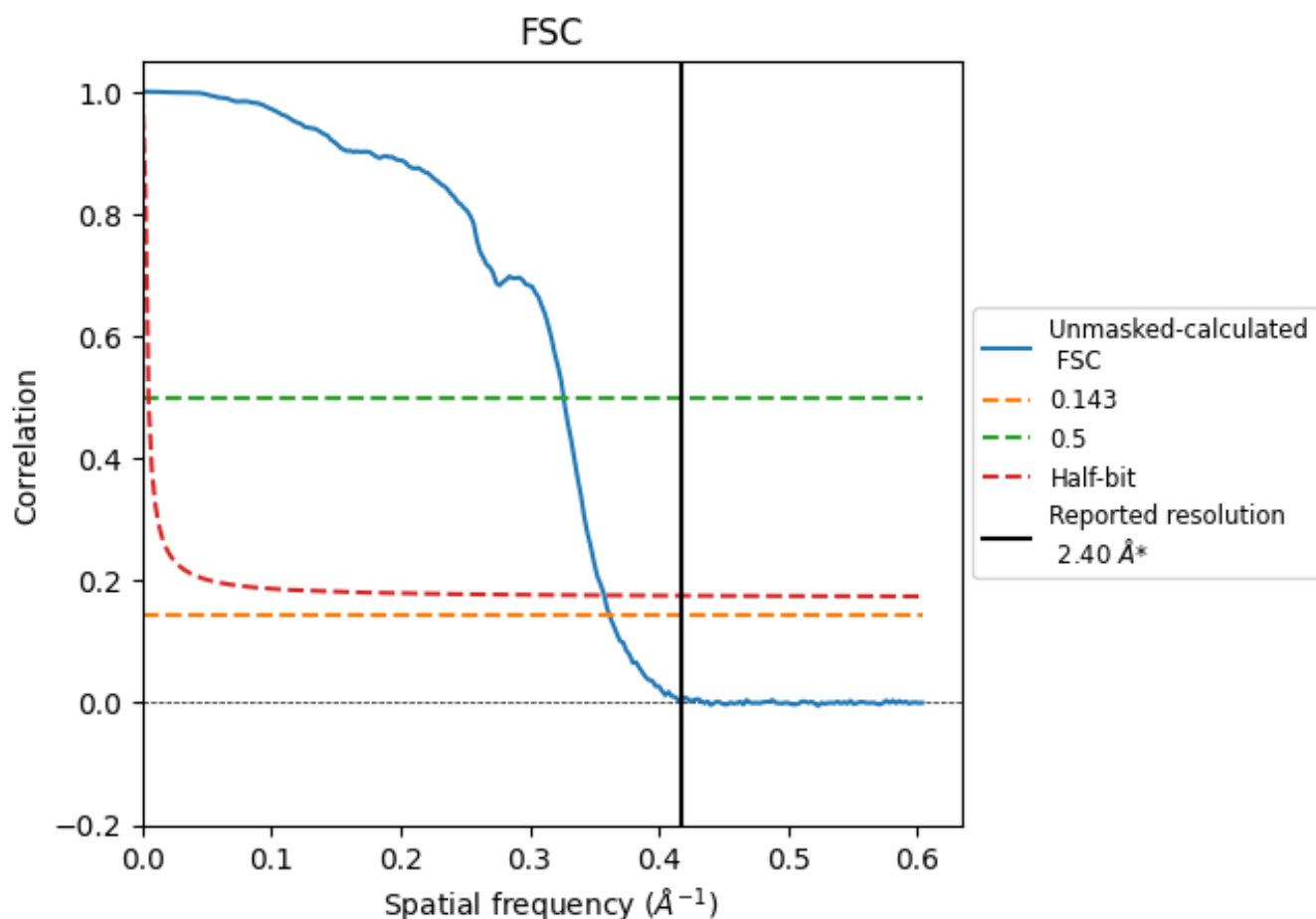


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 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 0.417 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

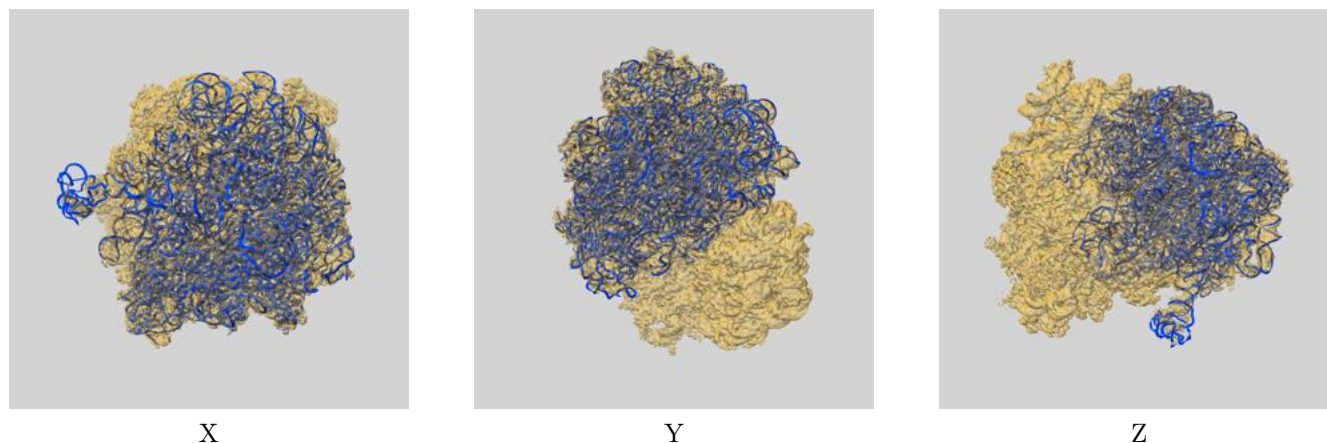
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.76	3.06	2.80

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.76 differs from the reported value 2.4 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-52418 and PDB model 9HUS. Per-residue inclusion information can be found in section 3 on page 11.

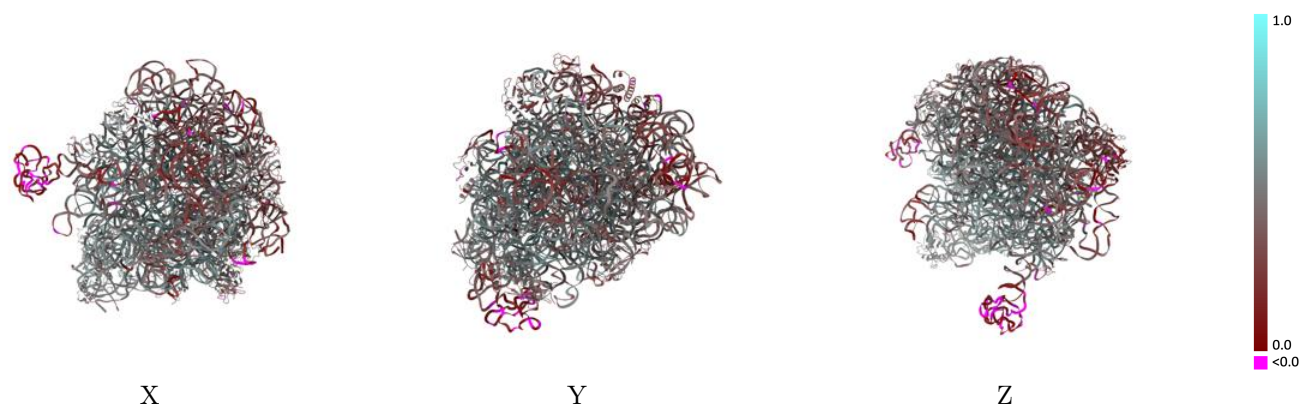
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0077 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.

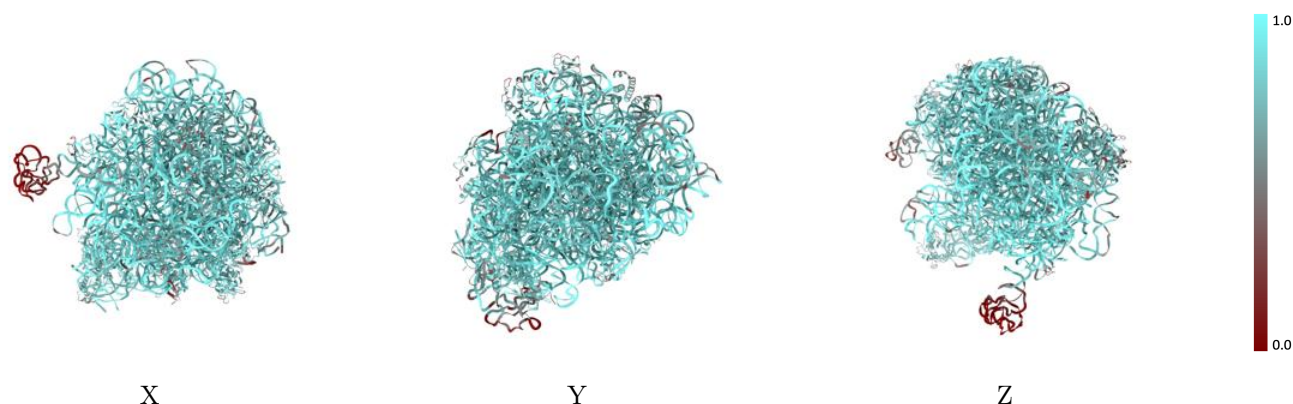


## 9.2 Q-score mapped to coordinate model [i](#)



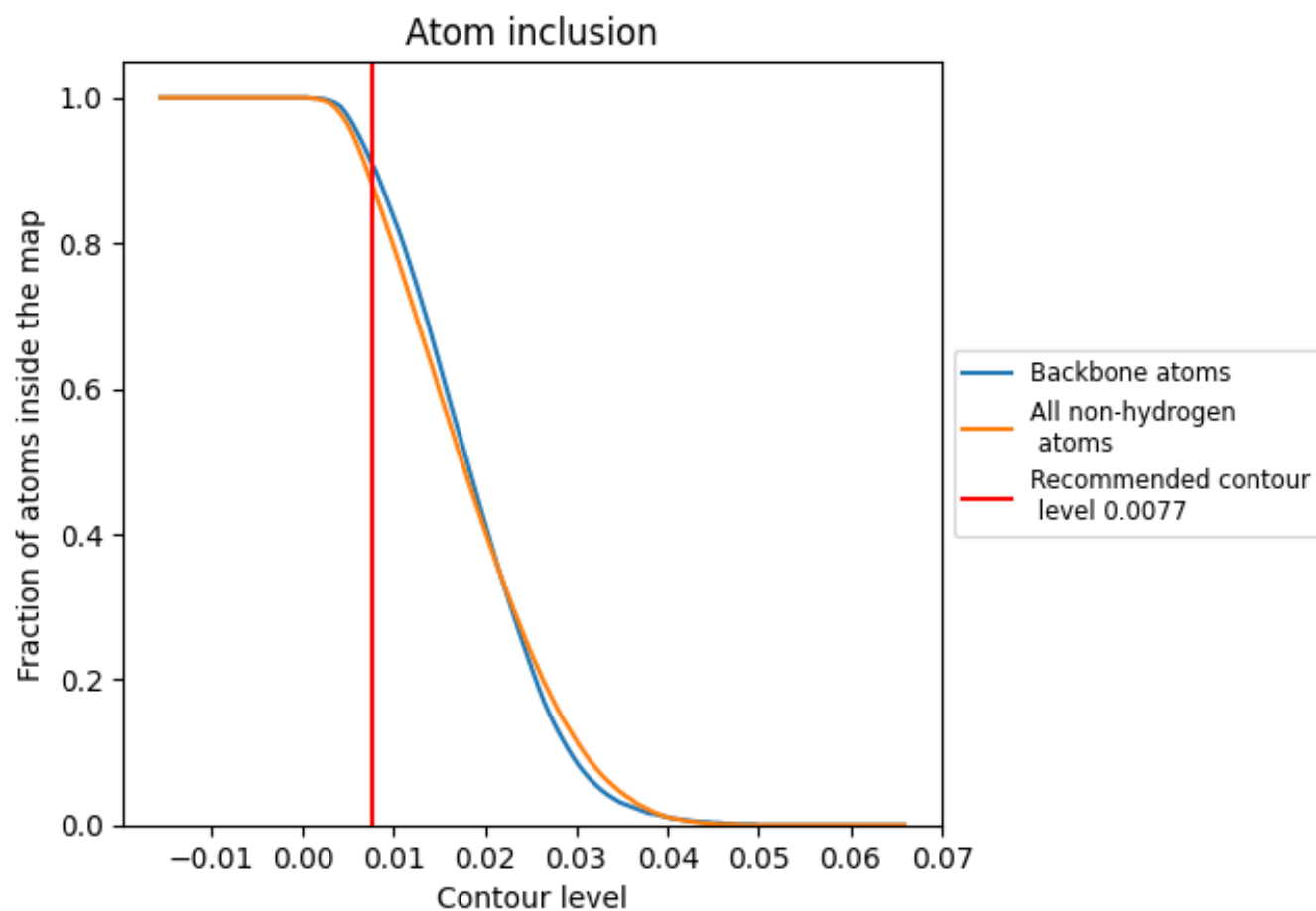
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0077).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (0.0077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8800	 0.4380
0	 0.9180	 0.5320
1	 0.6710	 0.2780
2	 0.8880	 0.5060
3	 0.8180	 0.4010
4	 0.8730	 0.5370
6	 0.9690	 0.5090
7	 0.9820	 0.5870
8	 0.9280	 0.5030
a	 0.9350	 0.4780
b	 0.8940	 0.4330
c	 0.9310	 0.4910
d	 0.8360	 0.4340
e	 0.7790	 0.4220
f	 0.7610	 0.4550
g	 0.6990	 0.3640
h	 0.6370	 0.4060
j	 0.8610	 0.4570
k	 0.8690	 0.4670
l	 0.8760	 0.5150
m	 0.9360	 0.5650
n	 0.8130	 0.3740
o	 0.8110	 0.4630
p	 0.8100	 0.3840
q	 0.8930	 0.4880
r	 0.7790	 0.4280
s	 0.8460	 0.4530
t	 0.7240	 0.3130
u	 0.6710	 0.3110
v	 0.9440	 0.4390
w	 0.8140	 0.4850
y	 0.9140	 0.5410
z	 0.7860	 0.2760

