



## wwPDB EM Validation Summary Report ⓘ

Nov 17, 2025 – 07:02 PM JST

PDB ID : 9KMY / pdb\_00009kmy  
EMDB ID : EMD-62449  
Title : Bat MERsSr-CoV NeoCoV Nsp1 bound to the Human 40S Ribosomal subunit-State2  
Authors : Yuan, S.; Yan, R.; Wu, M.  
Deposited on : 2024-11-18  
Resolution : 2.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

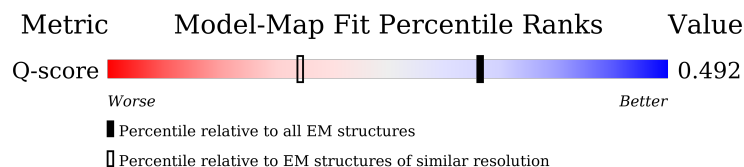
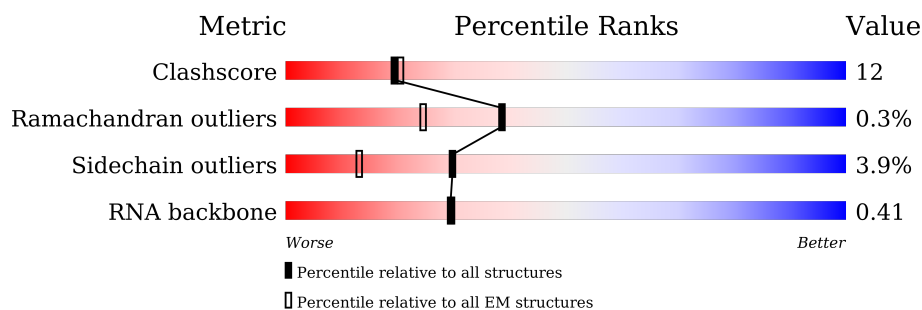
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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.






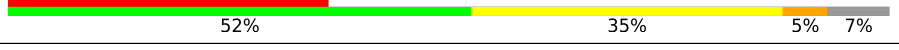


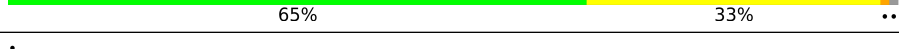
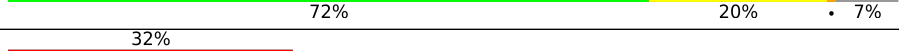
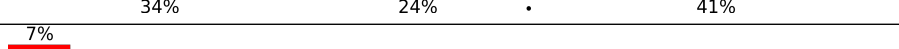

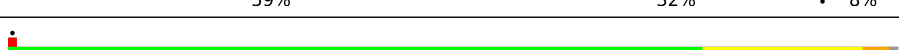



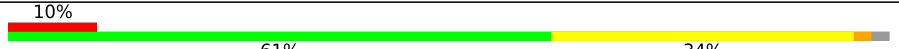





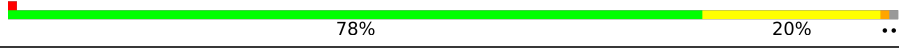
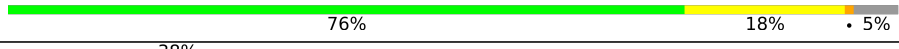
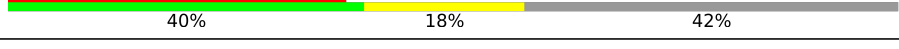


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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	2	1869	<div> <div>6%</div> <div>35%</div> <div>40%</div> <div>13%</div> <div>11%</div> </div>
2	A	295	<div> <div>54%</div> <div>18%</div> <div>28%</div> </div>
3	B	264	<div> <div>61%</div> <div>18%</div> <div>19%</div> </div>



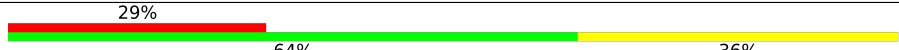
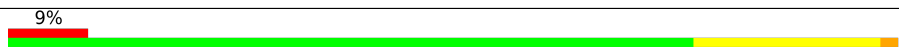
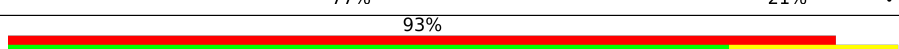
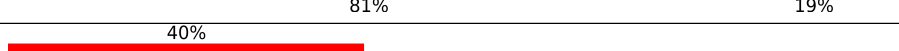
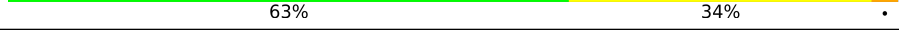

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Mol	Chain	Length	Quality of chain
4	C	293	
5	D	243	
6	E	263	
7	F	204	
8	G	249	
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	130	
27	Z	125	
28	a	100	

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Mol	Chain	Length	Quality of chain
29	b	82	
30	c	62	
31	d	55	
32	e	56	
33	f	74	
34	g	315	
35	h	25	
36	n	193	

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 74514 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1659	Total	C	N	O	P	0	0
			35392	15811	6360	11571	1650		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	213	Total	C	N	O	S	0	0
			1686	1072	295	311	8		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	230	Total	C	N	O	S	0	0
			1864	1164	373	320	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	221	ARG	LYS	variant	UNP P62753

- Molecule 9 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 10 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 11 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 12 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 13 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	121	Total	C	N	O	S	0	0
			935	586	165	175	9		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 17 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	126	Total	C	N	O	S	0	0
			1037	659	196	175	7		

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	138	Total	C	N	O	S	0	0
			1097	698	206	190	3		

- Molecule 19 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 21 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	144	Total	C	N	O	S	0	0
			1123	703	217	200	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 23 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 27 is a protein called Small ribosomal subunit protein eS25.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 28 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	99	Total	C	N	O	S	0	0
			794	494	165	130	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	78	VAL	ALA	conflict	UNP P62854

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	82	Total	C	N	O	S	0	0
			641	402	118	114	7		

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			489	297	97	93	2		

- Molecule 31 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 33 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	74	Total	C	N	O	S	0	0
			611	385	117	102	7		

- Molecule 34 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2441	1537	425	467	12		

- Molecule 35 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	22	Total	C	N	O	S	0	0
			213	130	57	23	3		

- Molecule 36 is a protein called ORF1ab polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	26	Total	C	N	O		0	0
			209	136	33	40			

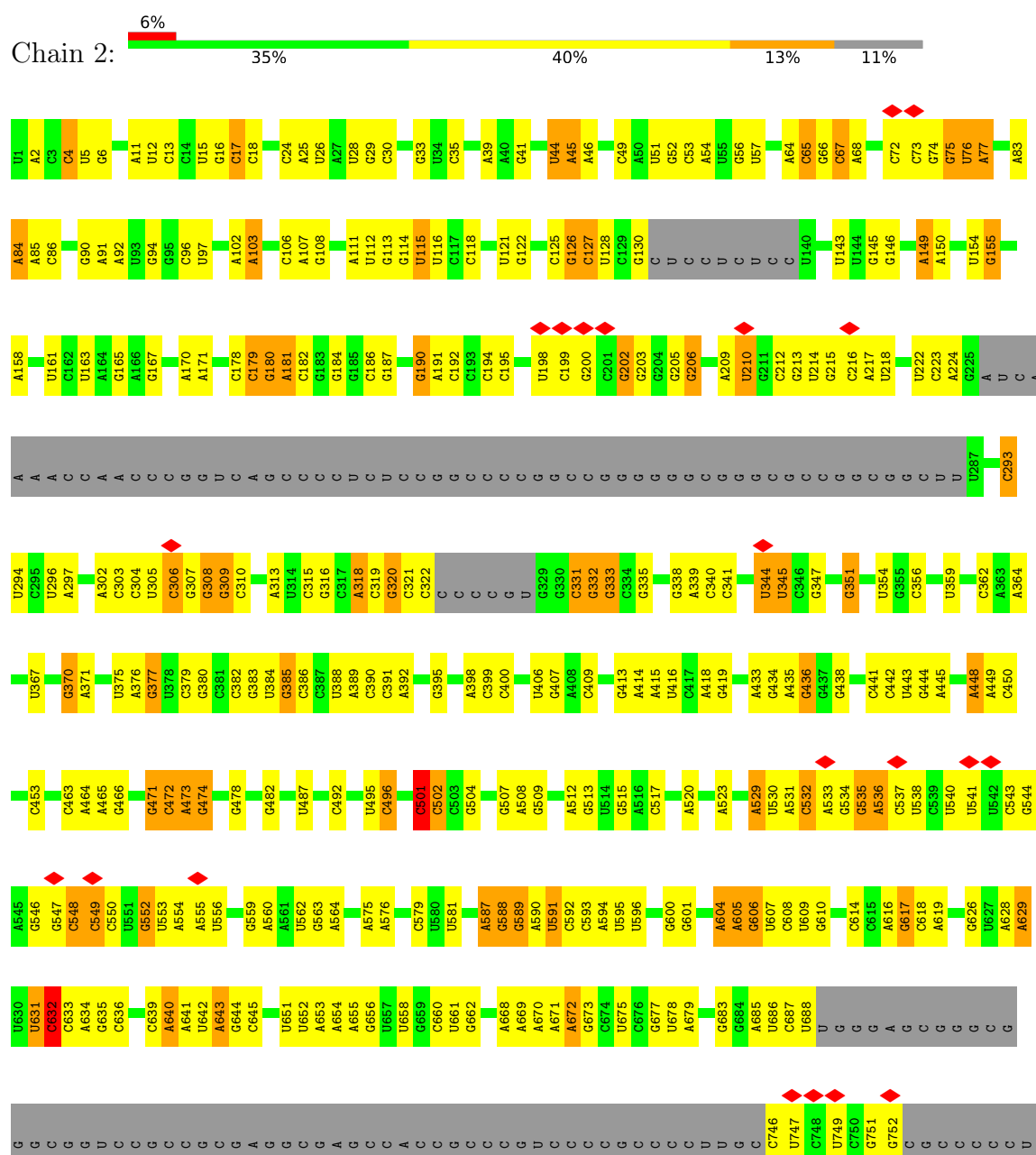
There are 3 discrepancies between the modelled and reference sequences:

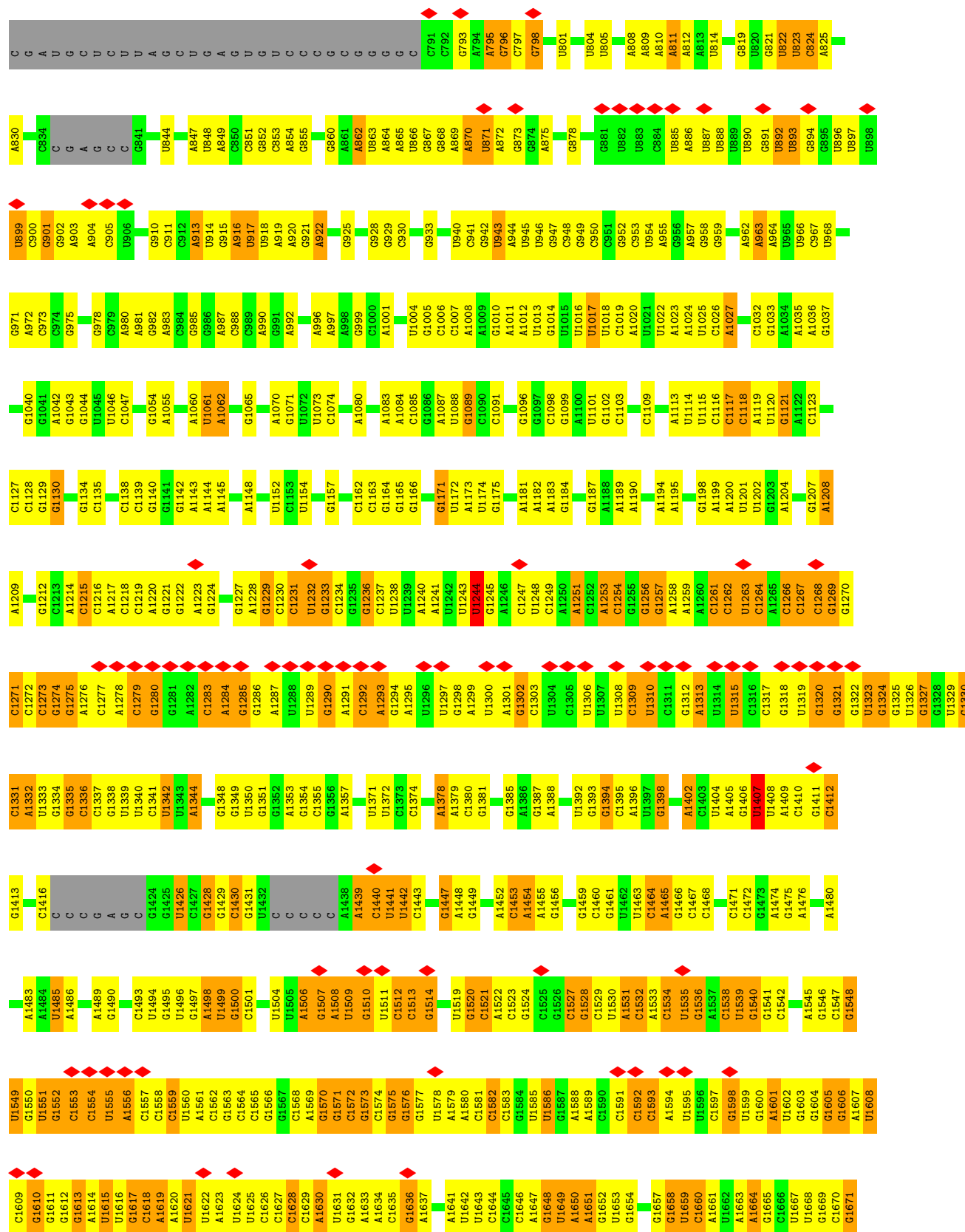
Chain	Residue	Modelled	Actual	Comment	Reference
n	77	VAL	ALA	conflict	UNP A0A2R2YRH0
n	168	SER	PRO	conflict	UNP A0A2R2YRH0
n	182	PHE	TYR	conflict	UNP A0A2R2YRH0

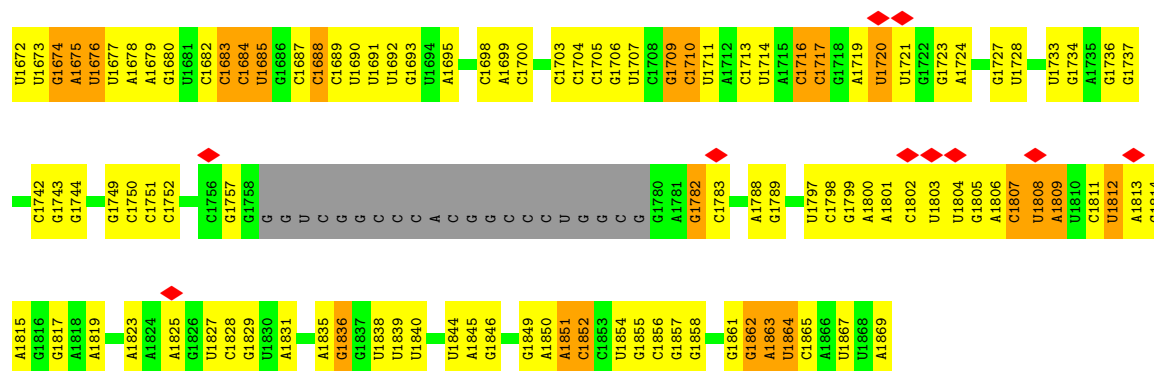
### 3 Residue-property plots

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.

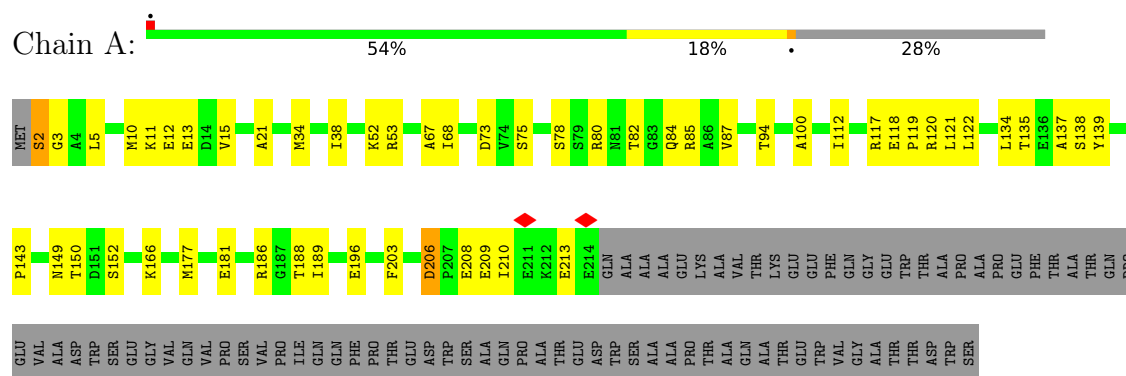
#### • Molecule 1: 18S ribosomal RNA



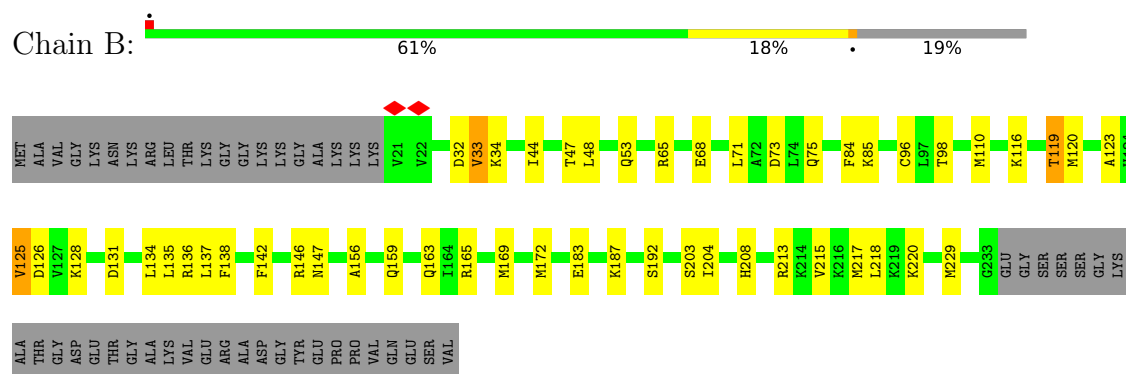




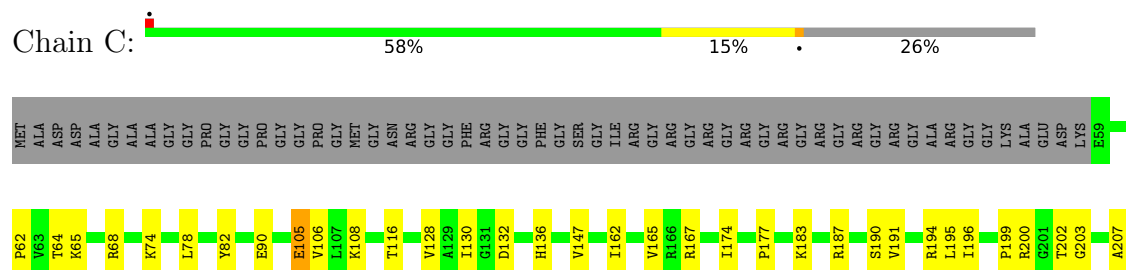
• Molecule 2: Small ribosomal subunit protein uS2

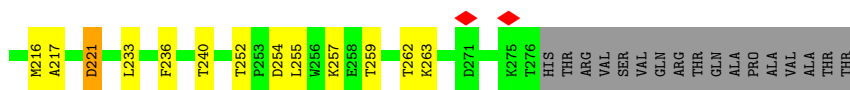


• Molecule 3: Small ribosomal subunit protein eS1

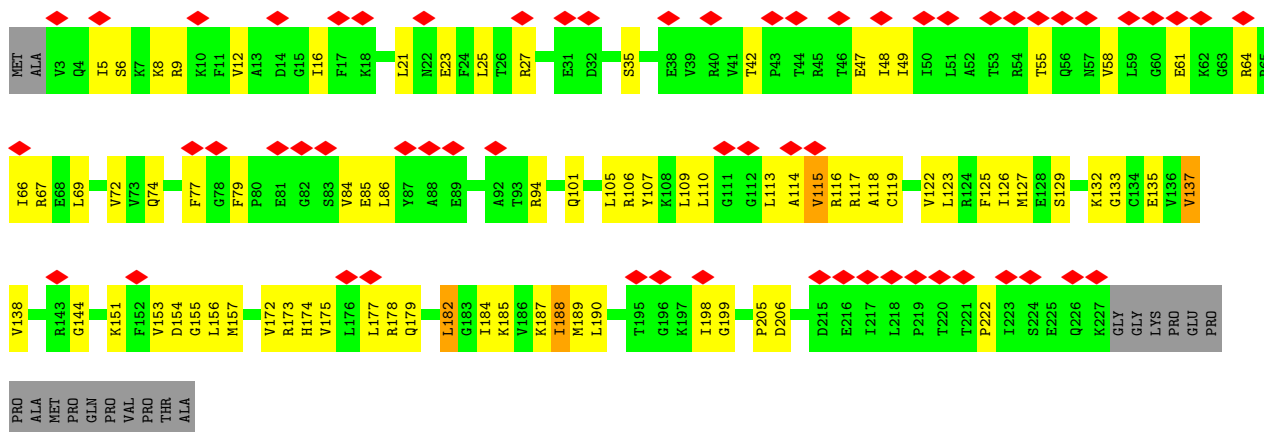


• Molecule 4: Small ribosomal subunit protein uS5

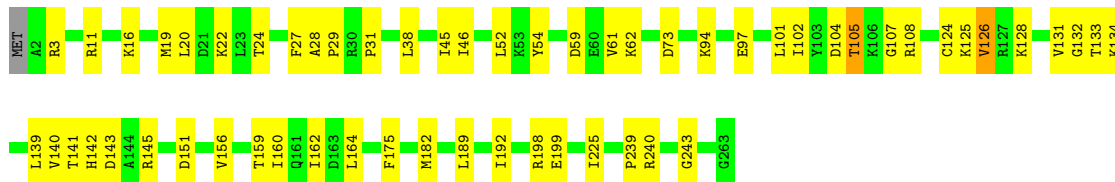
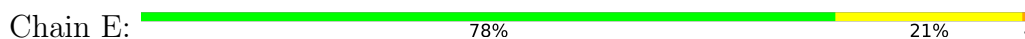




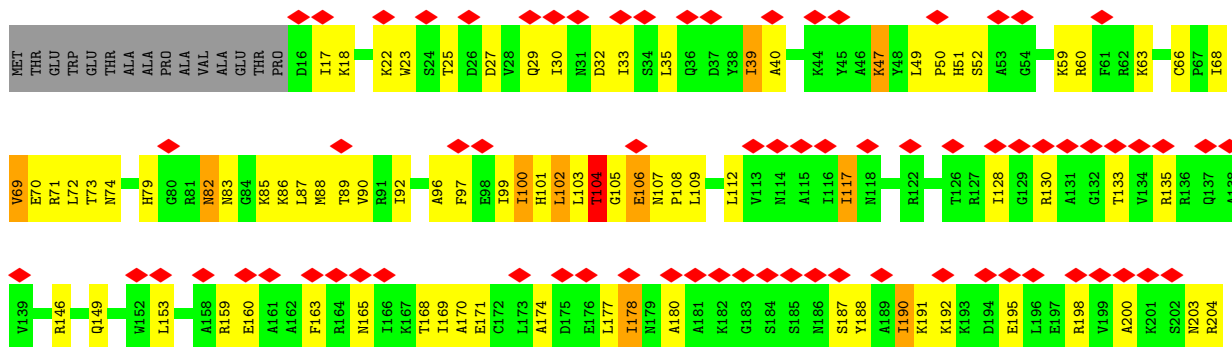
• Molecule 5: Small ribosomal subunit protein uS3



• Molecule 6: Small ribosomal subunit protein eS4, X isoform

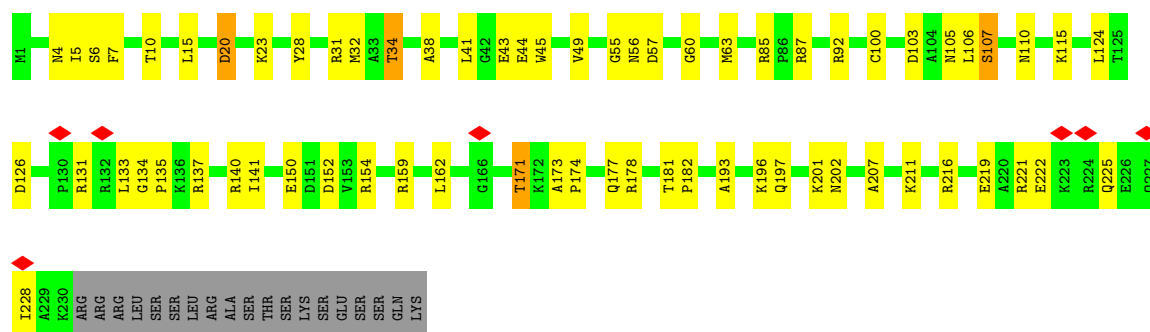


• Molecule 7: Small ribosomal subunit protein uS7

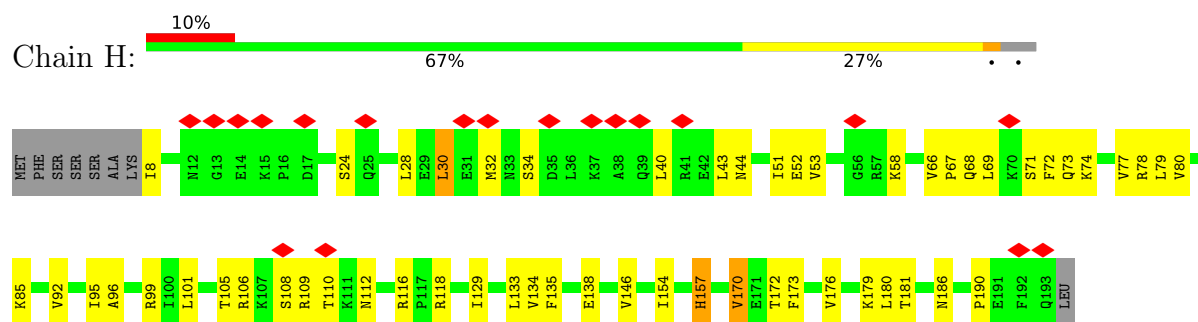


• Molecule 8: Small ribosomal subunit protein eS6

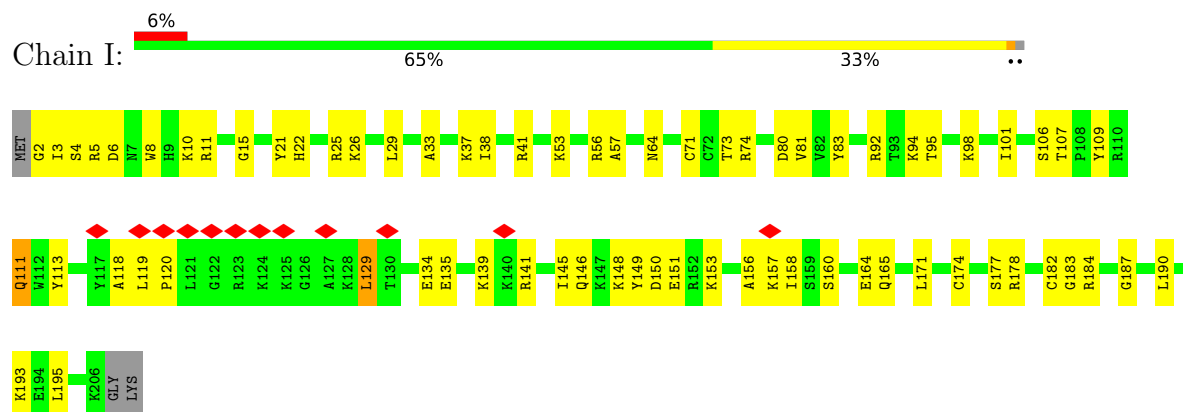




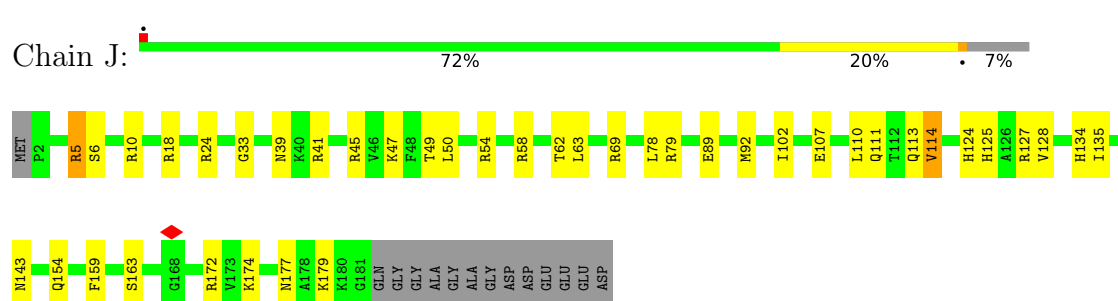
- Molecule 9: Small ribosomal subunit protein eS7



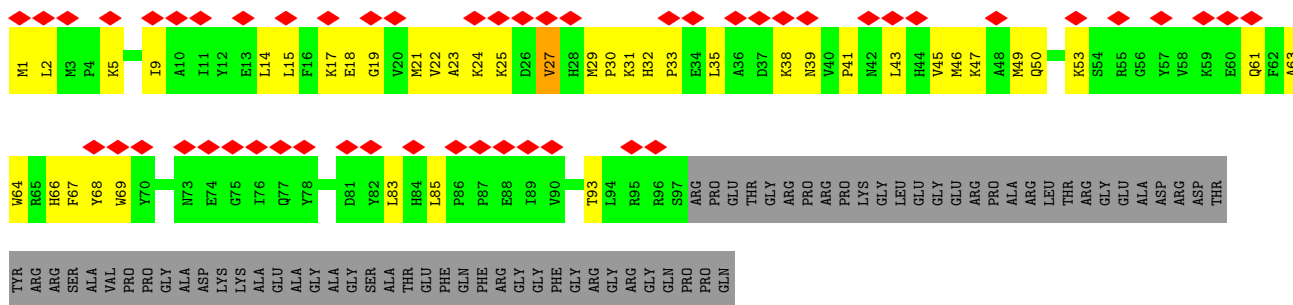
- Molecule 10: Small ribosomal subunit protein eS8



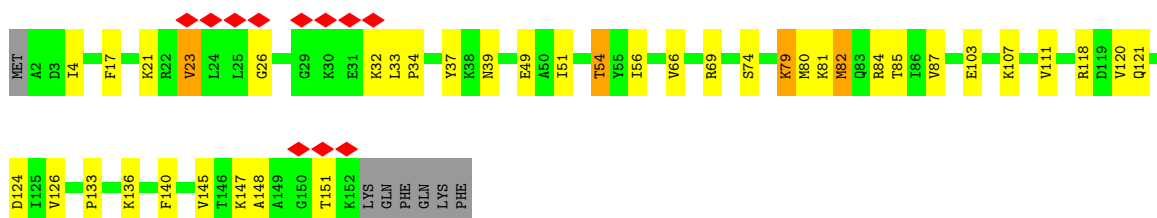
- Molecule 11: Small ribosomal subunit protein uS4



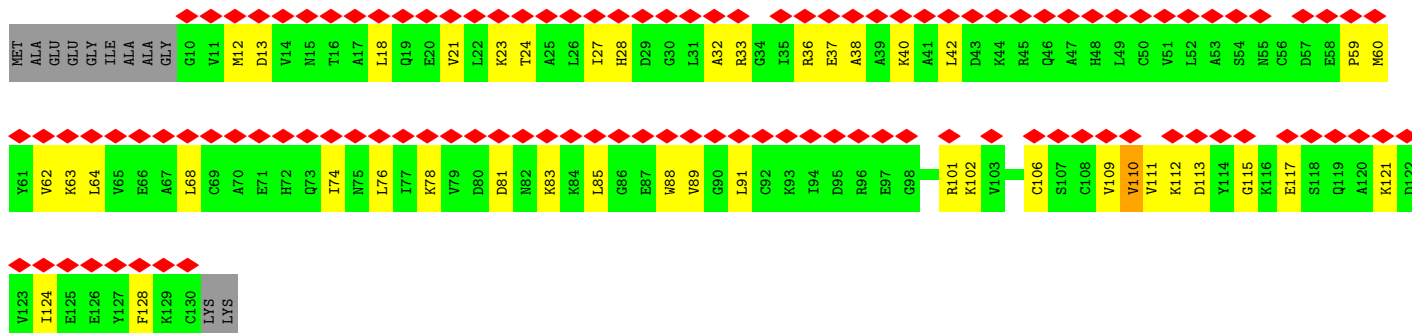
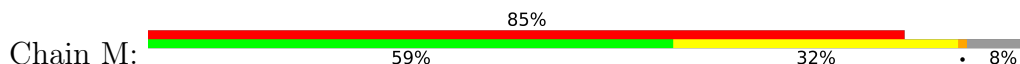
- Molecule 12: Small ribosomal subunit protein eS10



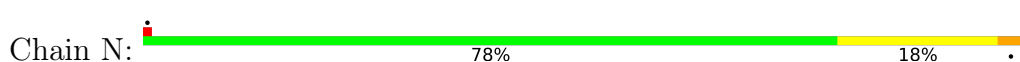
- Molecule 13: Small ribosomal subunit protein uS17



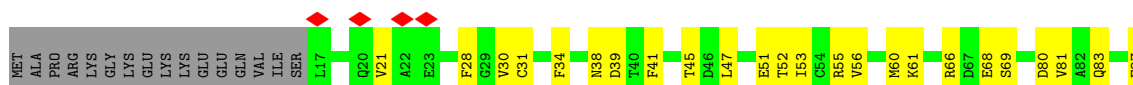
- Molecule 14: Small ribosomal subunit protein eS12



- Molecule 15: Small ribosomal subunit protein uS15



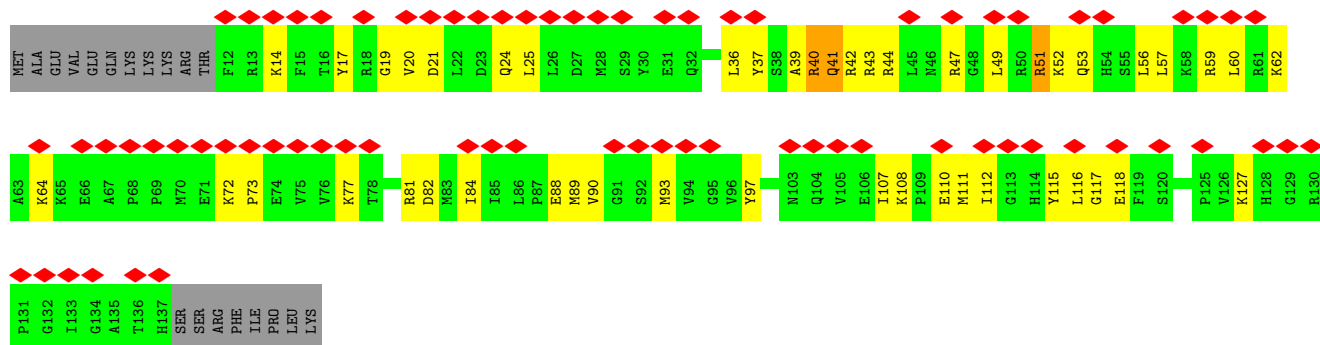
- Molecule 16: Small ribosomal subunit protein uS11



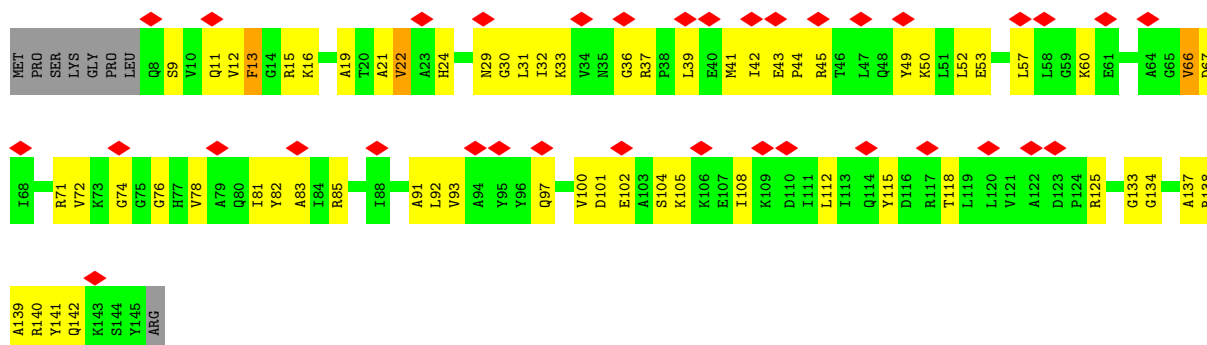




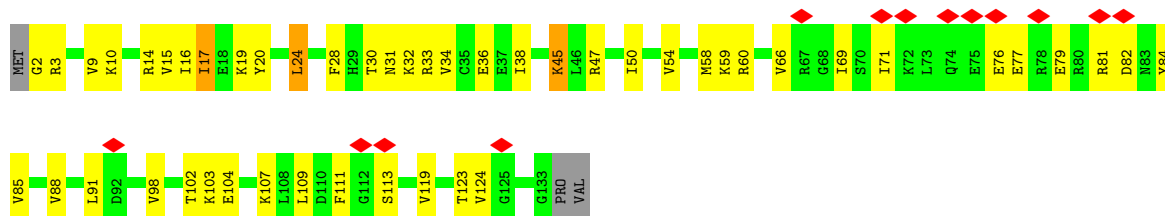
• Molecule 17: Small ribosomal subunit protein uS19



• Molecule 18: Small ribosomal subunit protein uS9

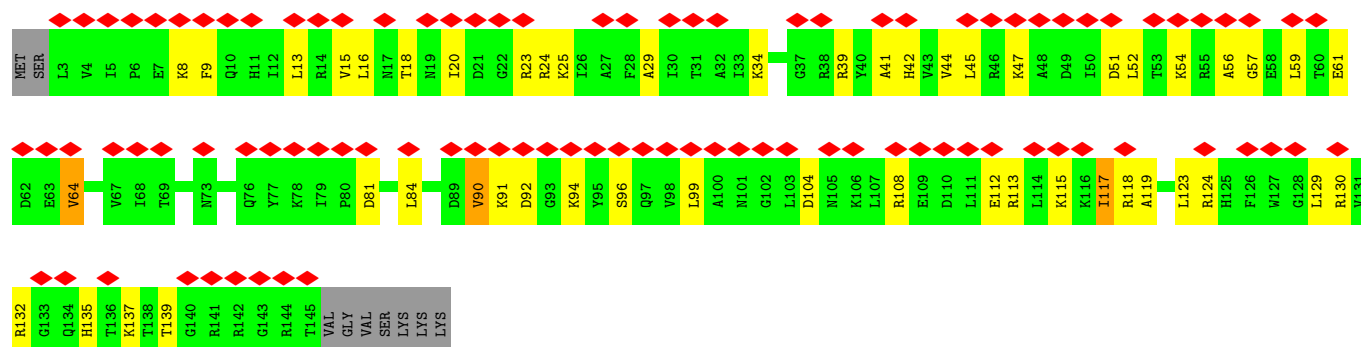


• Molecule 19: Small ribosomal subunit protein eS17

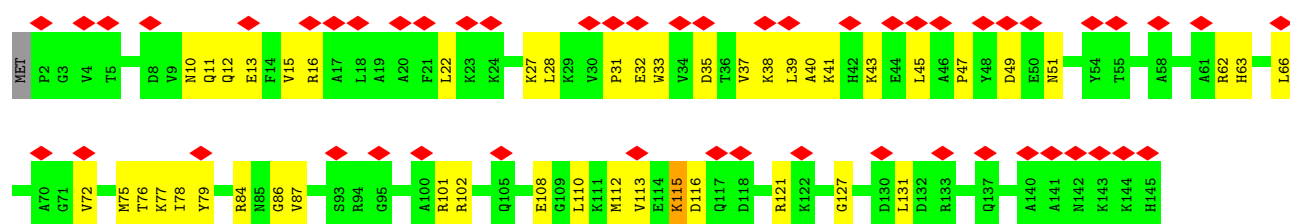


• Molecule 20: Small ribosomal subunit protein uS13

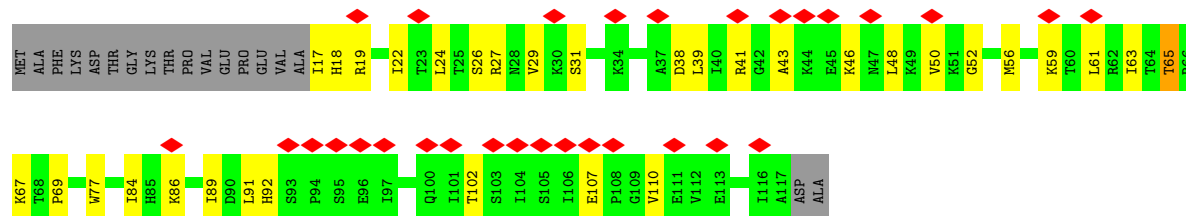




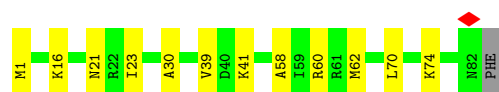
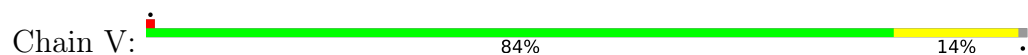
- Molecule 21: Small ribosomal subunit protein eS19



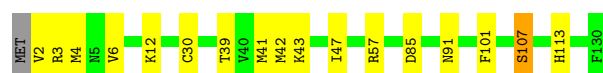
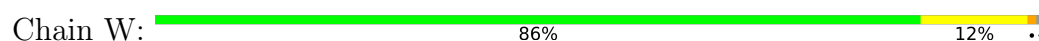
- Molecule 22: Small ribosomal subunit protein uS10



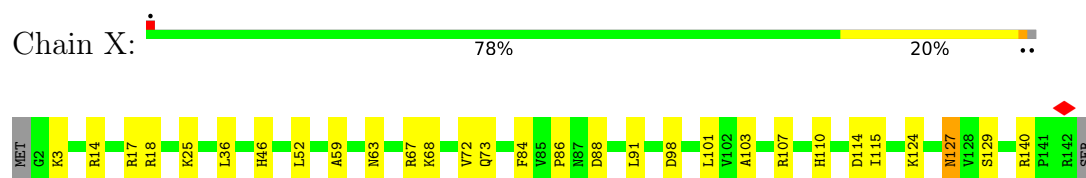
- Molecule 23: Small ribosomal subunit protein eS21



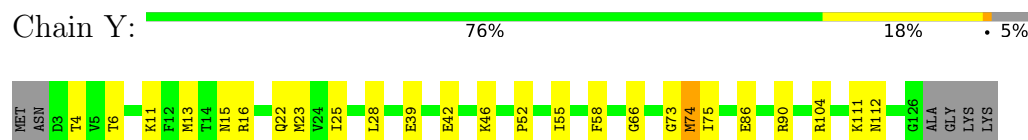
- Molecule 24: Small ribosomal subunit protein uS8



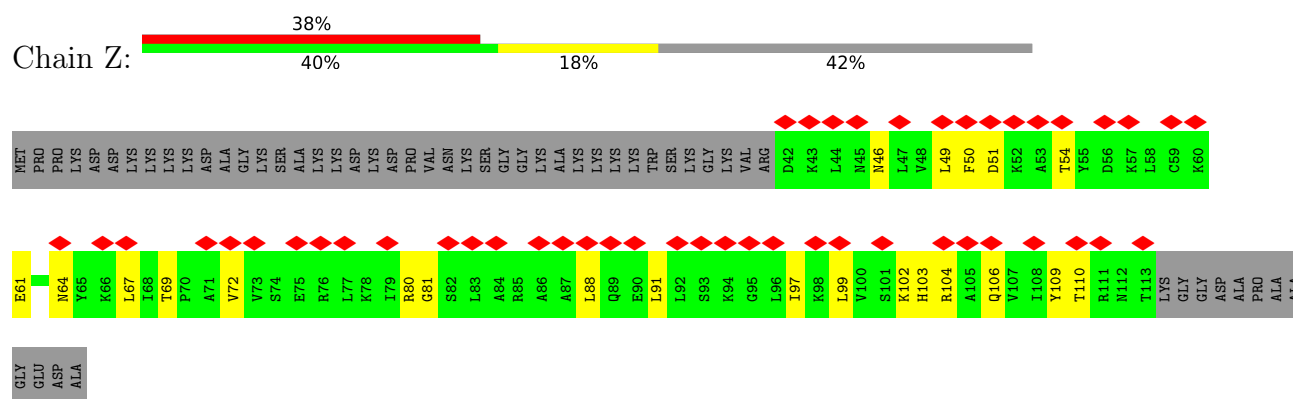
- Molecule 25: Small ribosomal subunit protein uS12



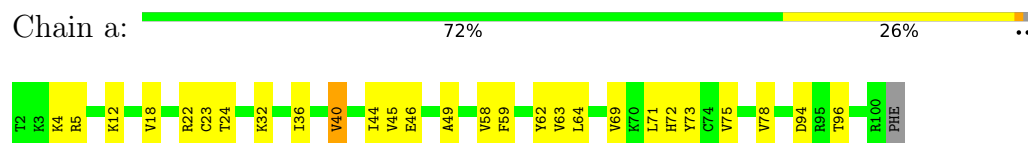
- Molecule 26: Small ribosomal subunit protein eS24



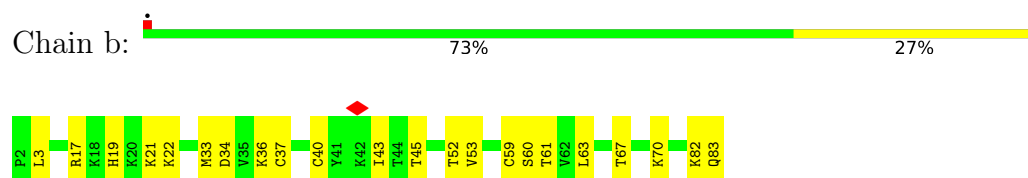
- Molecule 27: Small ribosomal subunit protein eS25



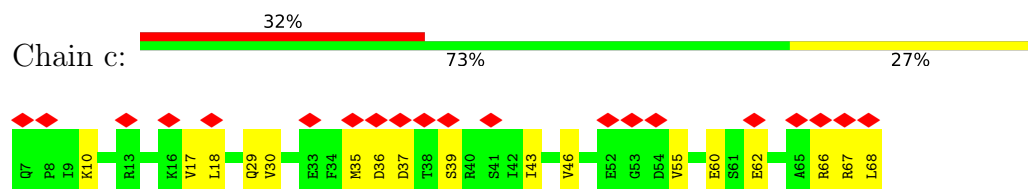
- Molecule 28: Small ribosomal subunit protein eS26



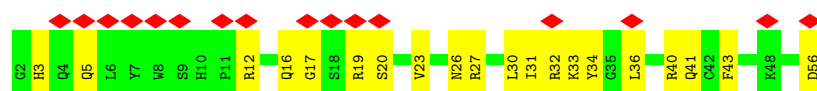
- Molecule 29: Small ribosomal subunit protein eS27



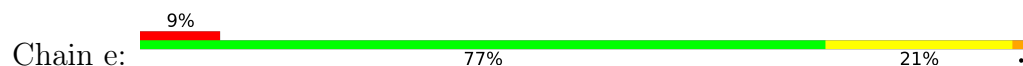
- Molecule 30: Small ribosomal subunit protein eS28



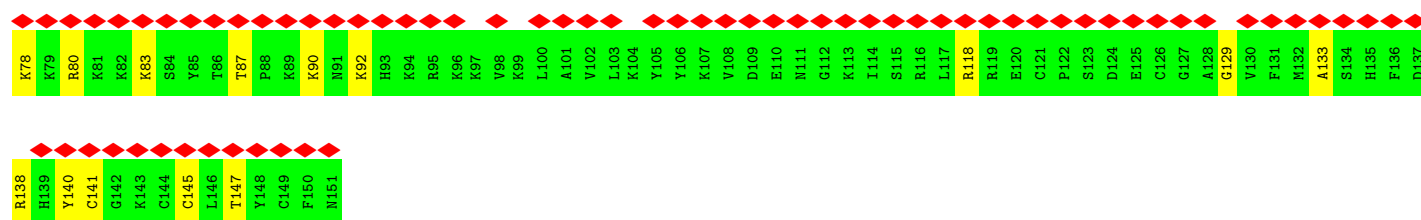
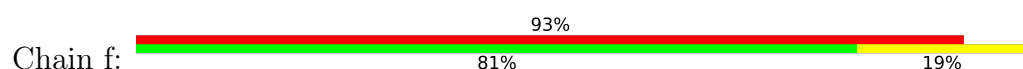
- Molecule 31: Small ribosomal subunit protein uS14



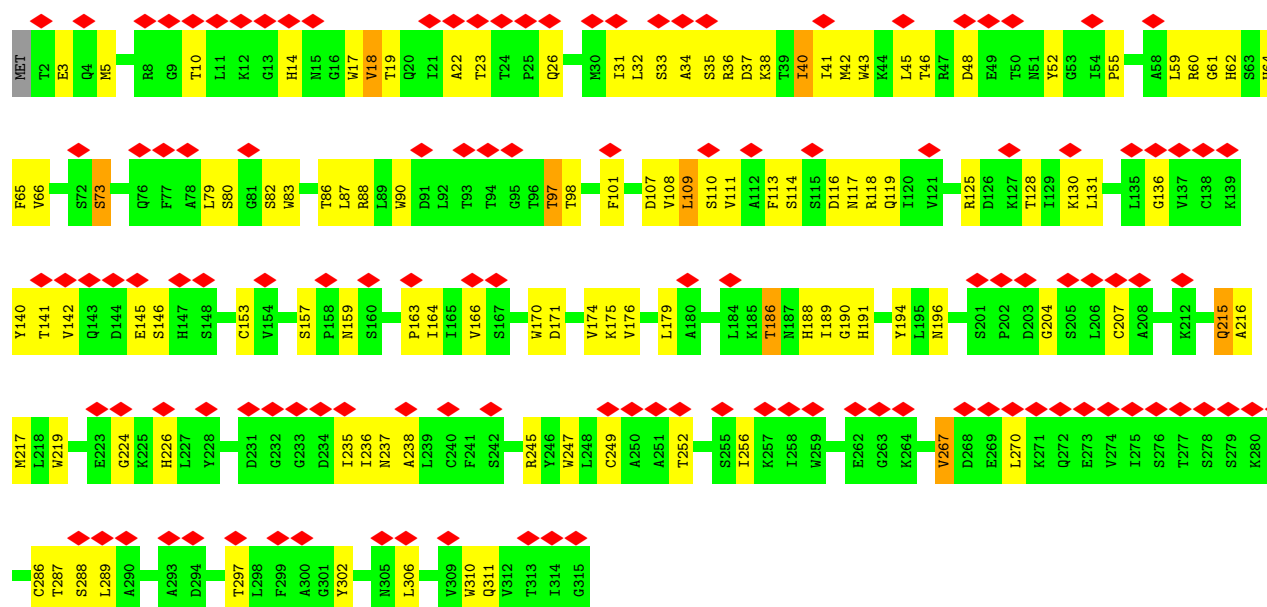
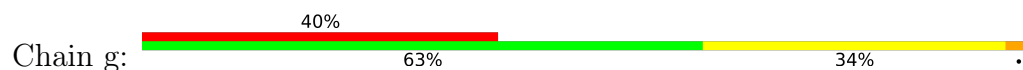
- Molecule 32: Small ribosomal subunit protein eS30



- Molecule 33: Small ribosomal subunit protein eS31



- Molecule 34: Small ribosomal subunit protein RACK1

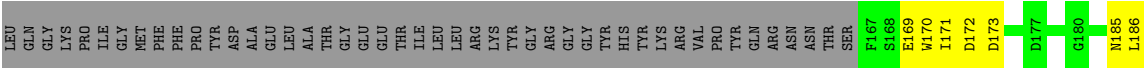
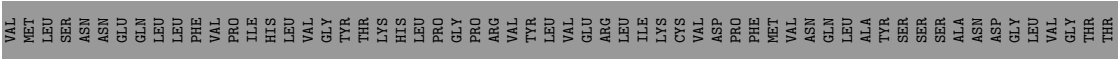
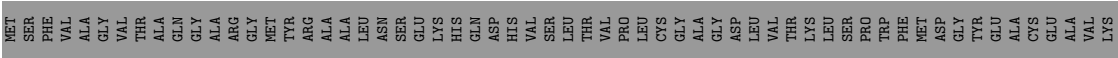


- Molecule 35: Small ribosomal subunit protein eS32





● Molecule 36: ORF1ab polypeptide



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104004	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.834	Depositor
Minimum map value	-1.311	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.181	Depositor
Map size ( $\text{\AA}$ )	486.4, 486.4, 486.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.95, 0.95, 0.95	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	2	0.26	0/39580	0.31	7/61688 (0.0%)
2	A	0.21	0/1723	0.31	0/2341
3	B	0.21	0/1756	0.31	0/2350
4	C	0.23	0/1726	0.34	0/2332
5	D	0.25	0/1780	0.43	0/2397
6	E	0.29	0/2118	0.39	0/2849
7	F	0.30	0/1516	0.54	0/2037
8	G	0.17	0/1887	0.29	0/2513
9	H	0.16	0/1524	0.35	0/2042
10	I	0.22	0/1711	0.36	0/2282
11	J	0.25	0/1524	0.35	0/2035
12	K	0.51	0/840	0.67	1/1133 (0.1%)
13	L	0.29	0/1250	0.35	0/1673
14	M	0.14	0/945	0.35	0/1269
15	N	0.20	0/1226	0.27	0/1649
16	O	0.22	0/1023	0.36	0/1372
17	P	0.15	0/1058	0.43	0/1414
18	Q	0.19	0/1114	0.40	0/1492
19	R	0.18	0/1082	0.31	0/1452
20	S	0.14	0/1202	0.37	0/1610
21	T	0.17	0/1143	0.35	0/1530
22	U	0.30	0/813	0.54	0/1092
23	V	0.20	0/631	0.29	0/844
24	W	0.26	0/1051	0.34	0/1406
25	X	0.23	0/1116	0.29	0/1490
26	Y	0.22	0/1031	0.30	0/1370
27	Z	0.10	0/580	0.30	0/780
28	a	0.25	0/807	0.34	0/1082
29	b	0.22	0/654	0.34	0/876
30	c	0.13	0/491	0.35	0/656
31	d	0.11	0/470	0.33	0/623
32	e	0.19	0/447	0.32	0/587
33	f	0.11	0/623	0.37	0/822
34	g	0.13	0/2498	0.36	0/3399

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	h	0.27	0/214	0.31	0/272
36	n	0.12	0/213	0.23	0/285
All	All	0.24	0/79367	0.34	8/115044 (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
11	J	0	1
17	P	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	O3'-P-O5'	-8.10	91.85	104.00
1	2	1684	C	O3'-P-O5'	5.73	112.59	104.00
1	2	1244	U	O3'-P-O5'	5.67	112.50	104.00
1	2	632	C	O3'-P-O5'	-5.60	95.60	104.00
12	K	27	VAL	N-CA-C	-5.51	108.12	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	5	ARG	Sidechain
17	P	40	ARG	Peptide

## 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	2	35392	0	17891	716	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1686	0	1688	36	0
3	B	1729	0	1803	35	0
4	C	1690	0	1777	35	0
5	D	1752	0	1848	74	0
6	E	2076	0	2177	44	0
7	F	1495	0	1549	83	0
8	G	1864	0	2018	51	0
9	H	1501	0	1593	43	0
10	I	1682	0	1769	57	0
11	J	1499	0	1618	33	0
12	K	816	0	841	42	0
13	L	1229	0	1302	34	0
14	M	935	0	964	30	0
15	N	1202	0	1289	24	0
16	O	1010	0	1034	39	0
17	P	1037	0	1082	43	0
18	Q	1097	0	1161	59	0
19	R	1068	0	1121	43	0
20	S	1184	0	1244	45	0
21	T	1123	0	1153	46	0
22	U	803	0	873	23	0
23	V	625	0	628	9	0
24	W	1034	0	1080	12	0
25	X	1098	0	1167	21	0
26	Y	1014	0	1082	17	0
27	Z	574	0	627	20	0
28	a	794	0	849	23	0
29	b	641	0	665	16	0
30	c	489	0	514	12	0
31	d	459	0	452	20	0
32	e	442	0	487	9	0
33	f	611	0	638	12	0
34	g	2441	0	2396	73	0
35	h	213	0	258	11	0
36	n	209	0	207	8	0
All	All	74514	0	58845	1606	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 1606 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)
12:K:31:LYS:HA	12:K:41:PRO:HA	1.15	1.07
2:A:10:MET:HE2	2:A:15:VAL:HG22	1.36	1.05
1:2:1513:C:O2	1:2:1513:C:OP1	1.75	1.04
12:K:43:LEU:HA	12:K:46:MET:HE3	1.41	1.03
12:K:32:HIS:HB3	12:K:35:LEU:HB2	1.45	0.97

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	A	211/295 (72%)	205 (97%)	5 (2%)	1 (0%)	25	49
3	B	211/264 (80%)	209 (99%)	2 (1%)	0	100	100
4	C	216/293 (74%)	210 (97%)	6 (3%)	0	100	100
5	D	223/243 (92%)	215 (96%)	8 (4%)	0	100	100
6	E	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
7	F	187/204 (92%)	161 (86%)	23 (12%)	3 (2%)	8	21
8	G	228/249 (92%)	224 (98%)	4 (2%)	0	100	100
9	H	184/194 (95%)	178 (97%)	6 (3%)	0	100	100
10	I	203/208 (98%)	194 (96%)	8 (4%)	1 (0%)	25	49
11	J	178/194 (92%)	174 (98%)	4 (2%)	0	100	100
12	K	95/165 (58%)	88 (93%)	6 (6%)	1 (1%)	12	30
13	L	149/158 (94%)	146 (98%)	2 (1%)	1 (1%)	19	42
14	M	119/132 (90%)	107 (90%)	10 (8%)	2 (2%)	7	20
15	N	147/151 (97%)	147 (100%)	0	0	100	100
16	O	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
17	P	124/145 (86%)	111 (90%)	12 (10%)	1 (1%)	16	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Q	136/146 (93%)	123 (90%)	12 (9%)	1 (1%)	19	42
19	R	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
20	S	141/152 (93%)	129 (92%)	12 (8%)	0	100	100
21	T	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
22	U	99/119 (83%)	93 (94%)	6 (6%)	0	100	100
23	V	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
24	W	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
25	X	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
26	Y	122/130 (94%)	121 (99%)	1 (1%)	0	100	100
27	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
28	a	97/100 (97%)	96 (99%)	0	1 (1%)	13	33
29	b	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
30	c	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
31	d	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
32	e	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
33	f	72/74 (97%)	60 (83%)	12 (17%)	0	100	100
34	g	312/315 (99%)	289 (93%)	22 (7%)	1 (0%)	37	61
35	h	20/25 (80%)	20 (100%)	0	0	100	100
36	n	24/193 (12%)	22 (92%)	2 (8%)	0	100	100
All	All	4826/5579 (86%)	4603 (95%)	210 (4%)	13 (0%)	38	61

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	189	ILE
7	F	100	ILE
10	I	129	LEU
14	M	109	VAL
14	M	110	VAL

### 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	
2	A	179/243 (74%)	172 (96%)	7 (4%)	27	56
3	B	194/231 (84%)	184 (95%)	10 (5%)	19	44
4	C	184/225 (82%)	179 (97%)	5 (3%)	40	69
5	D	189/202 (94%)	180 (95%)	9 (5%)	21	48
6	E	224/225 (100%)	219 (98%)	5 (2%)	47	76
7	F	159/170 (94%)	147 (92%)	12 (8%)	11	28
8	G	200/218 (92%)	192 (96%)	8 (4%)	27	55
9	H	167/174 (96%)	159 (95%)	8 (5%)	21	48
10	I	178/180 (99%)	173 (97%)	5 (3%)	38	68
11	J	160/168 (95%)	155 (97%)	5 (3%)	35	64
12	K	88/136 (65%)	88 (100%)	0	100	100
13	L	135/142 (95%)	127 (94%)	8 (6%)	16	38
14	M	102/108 (94%)	100 (98%)	2 (2%)	50	78
15	N	130/131 (99%)	124 (95%)	6 (5%)	23	49
16	O	105/119 (88%)	102 (97%)	3 (3%)	37	67
17	P	112/130 (86%)	110 (98%)	2 (2%)	54	80
18	Q	114/121 (94%)	111 (97%)	3 (3%)	41	70
19	R	119/122 (98%)	107 (90%)	12 (10%)	6	15
20	S	124/132 (94%)	121 (98%)	3 (2%)	44	73
21	T	114/115 (99%)	112 (98%)	2 (2%)	54	80
22	U	93/107 (87%)	89 (96%)	4 (4%)	25	52
23	V	66/67 (98%)	64 (97%)	2 (3%)	36	65
24	W	112/113 (99%)	108 (96%)	4 (4%)	30	59
25	X	113/115 (98%)	109 (96%)	4 (4%)	31	60
26	Y	108/112 (96%)	104 (96%)	4 (4%)	29	58
27	Z	64/103 (62%)	64 (100%)	0	100	100
28	a	87/88 (99%)	85 (98%)	2 (2%)	45	74
29	b	74/74 (100%)	71 (96%)	3 (4%)	26	54
30	c	55/55 (100%)	53 (96%)	2 (4%)	30	59
31	d	48/48 (100%)	46 (96%)	2 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	e	45/45 (100%)	41 (91%)	4 (9%)	8	20
33	f	67/67 (100%)	66 (98%)	1 (2%)	60	83
34	g	272/273 (100%)	255 (94%)	17 (6%)	15	35
35	h	21/24 (88%)	21 (100%)	0	100	100
36	n	22/160 (14%)	21 (96%)	1 (4%)	23	50
All	All	4224/4743 (89%)	4059 (96%)	165 (4%)	30	56

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	U	24	LEU
32	e	8	ARG
23	V	1	MET
26	Y	46	LYS
34	g	73	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
26	Y	85	ASN
34	g	215	GLN
27	Z	103	HIS
30	c	29	GLN
8	G	163	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1649/1869 (88%)	492 (29%)	30 (1%)

5 of 492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	11	A
1	2	17	C
1	2	33	G

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1244	U
1	2	1610	G
1	2	1271	C
1	2	1801	A
1	2	1464	C

## 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 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](#)

There are no chain breaks in this entry.

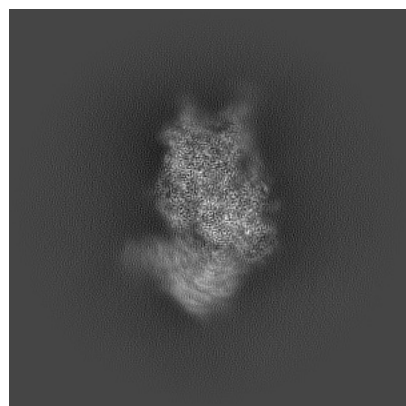
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62449. These allow visual inspection of the internal detail of the map and identification of artifacts.

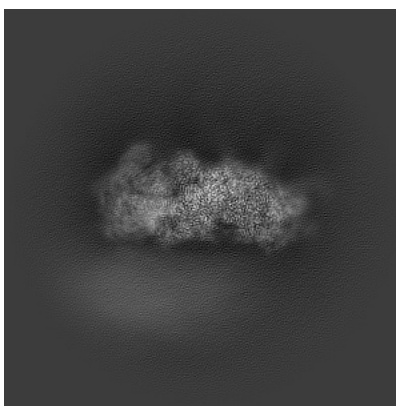
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

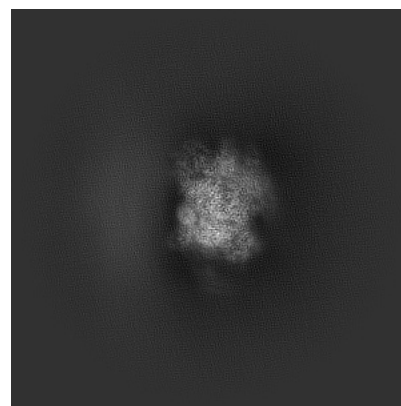
#### 6.1.1 Primary map



X

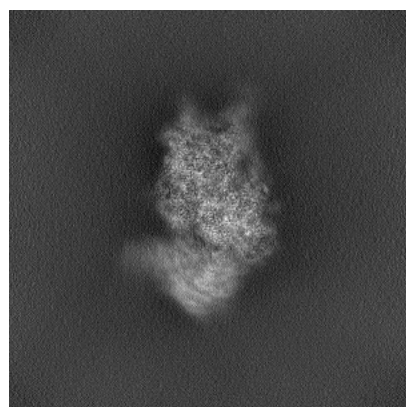


Y

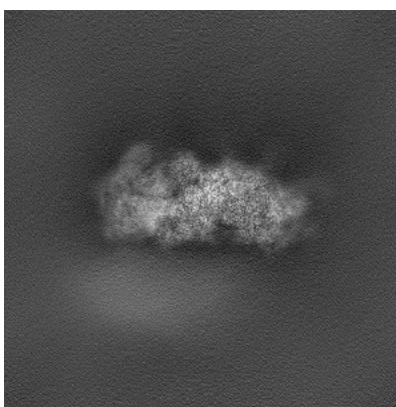


Z

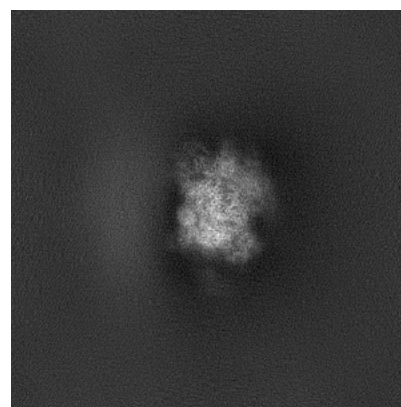
#### 6.1.2 Raw map



X



Y



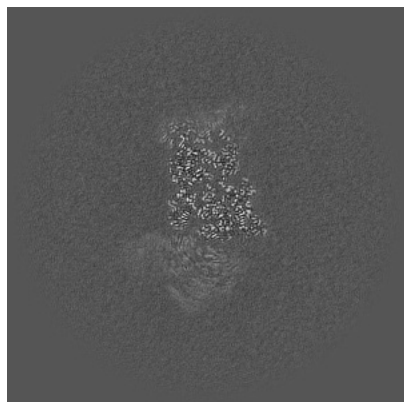
Z

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

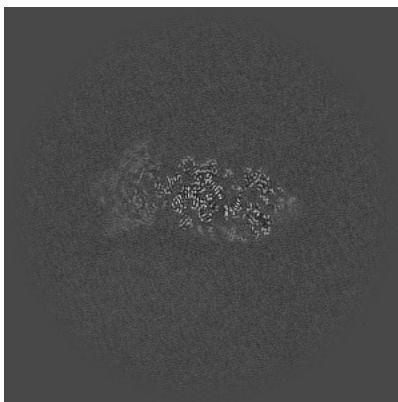


## 6.2 Central slices [i](#)

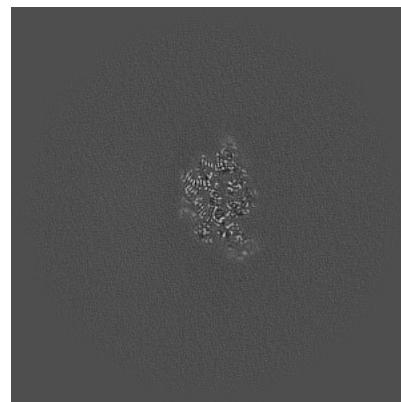
### 6.2.1 Primary map



X Index: 256

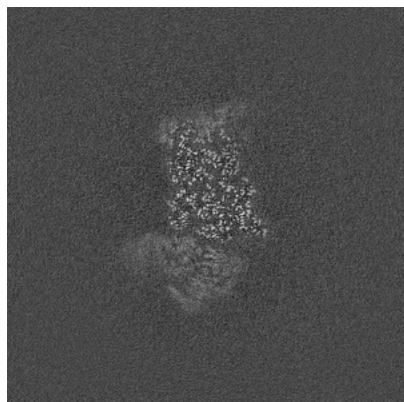


Y Index: 256

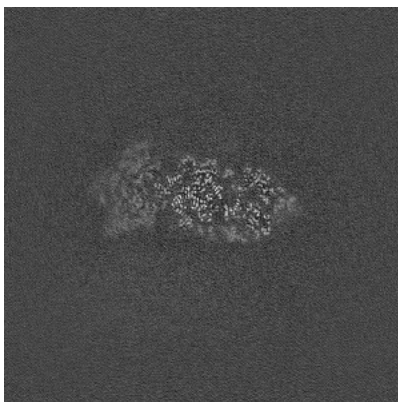


Z Index: 256

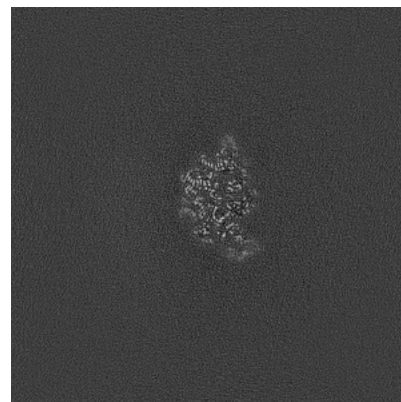
### 6.2.2 Raw map



X Index: 256



Y Index: 256



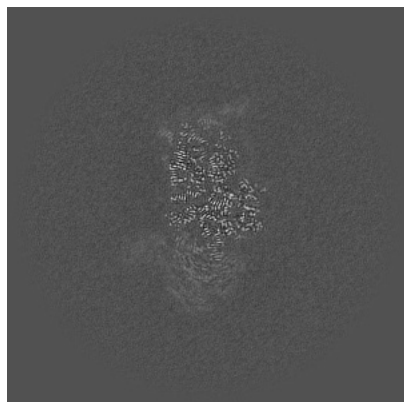
Z Index: 256

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

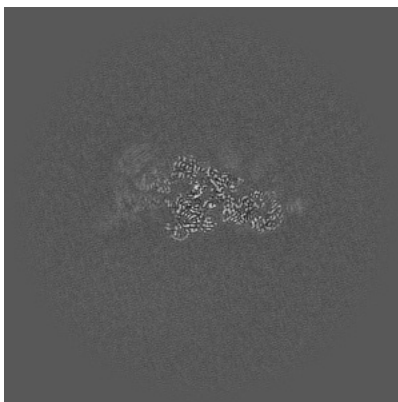


## 6.3 Largest variance slices [i](#)

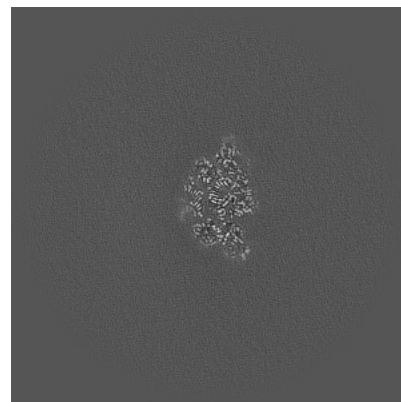
### 6.3.1 Primary map



X Index: 262

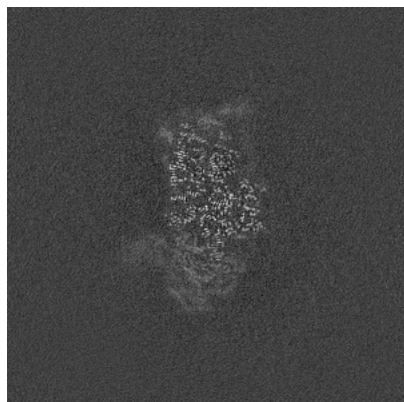


Y Index: 276

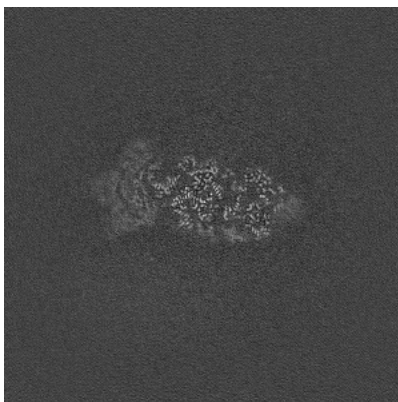


Z Index: 262

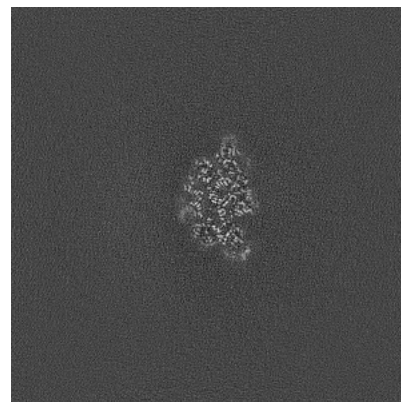
### 6.3.2 Raw map



X Index: 262



Y Index: 255

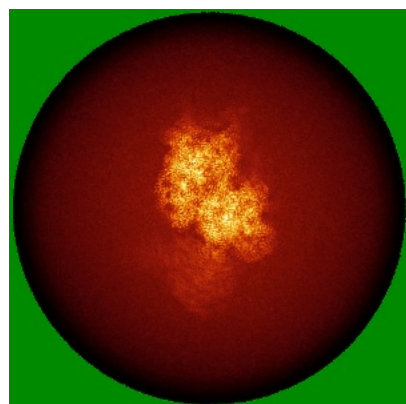


Z Index: 262

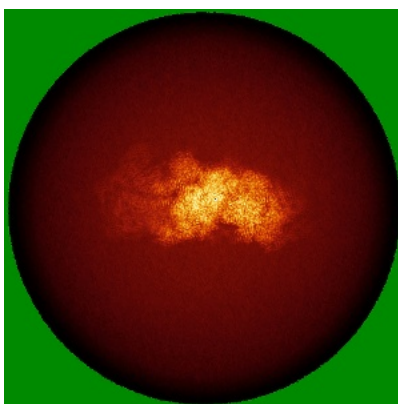
The images above show the largest variance slices of the map in three orthogonal directions.

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

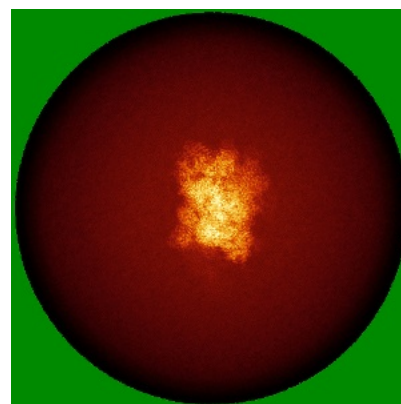
### 6.4.1 Primary map



X

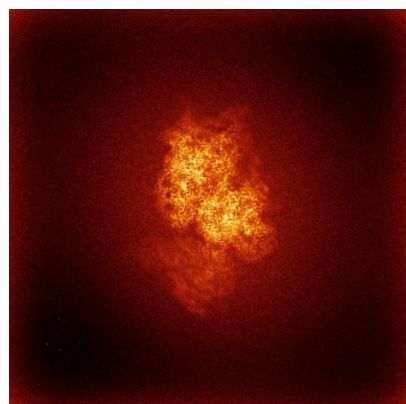


Y

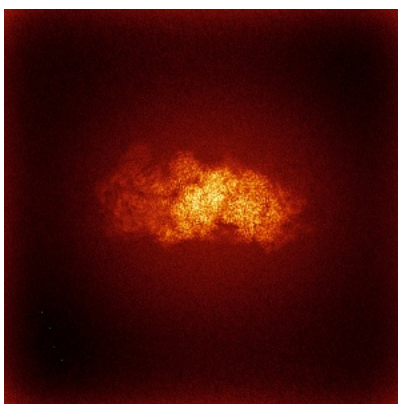


Z

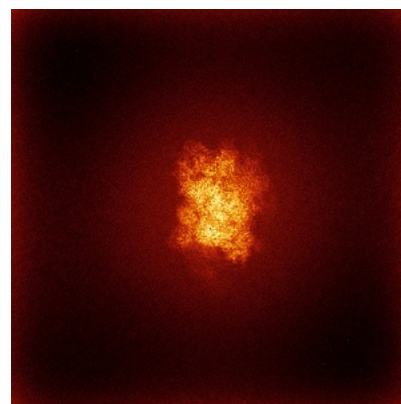
### 6.4.2 Raw map



X



Y

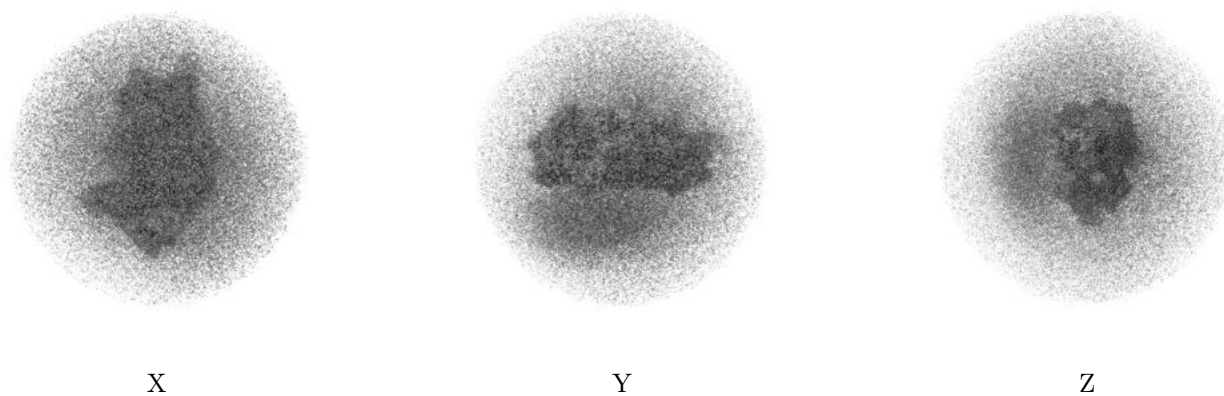


Z

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.

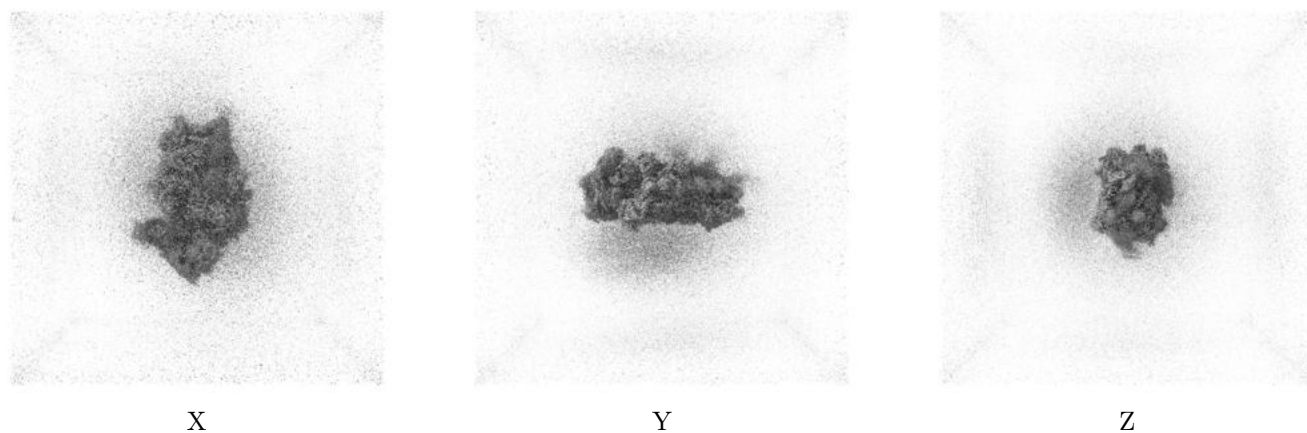
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.181. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

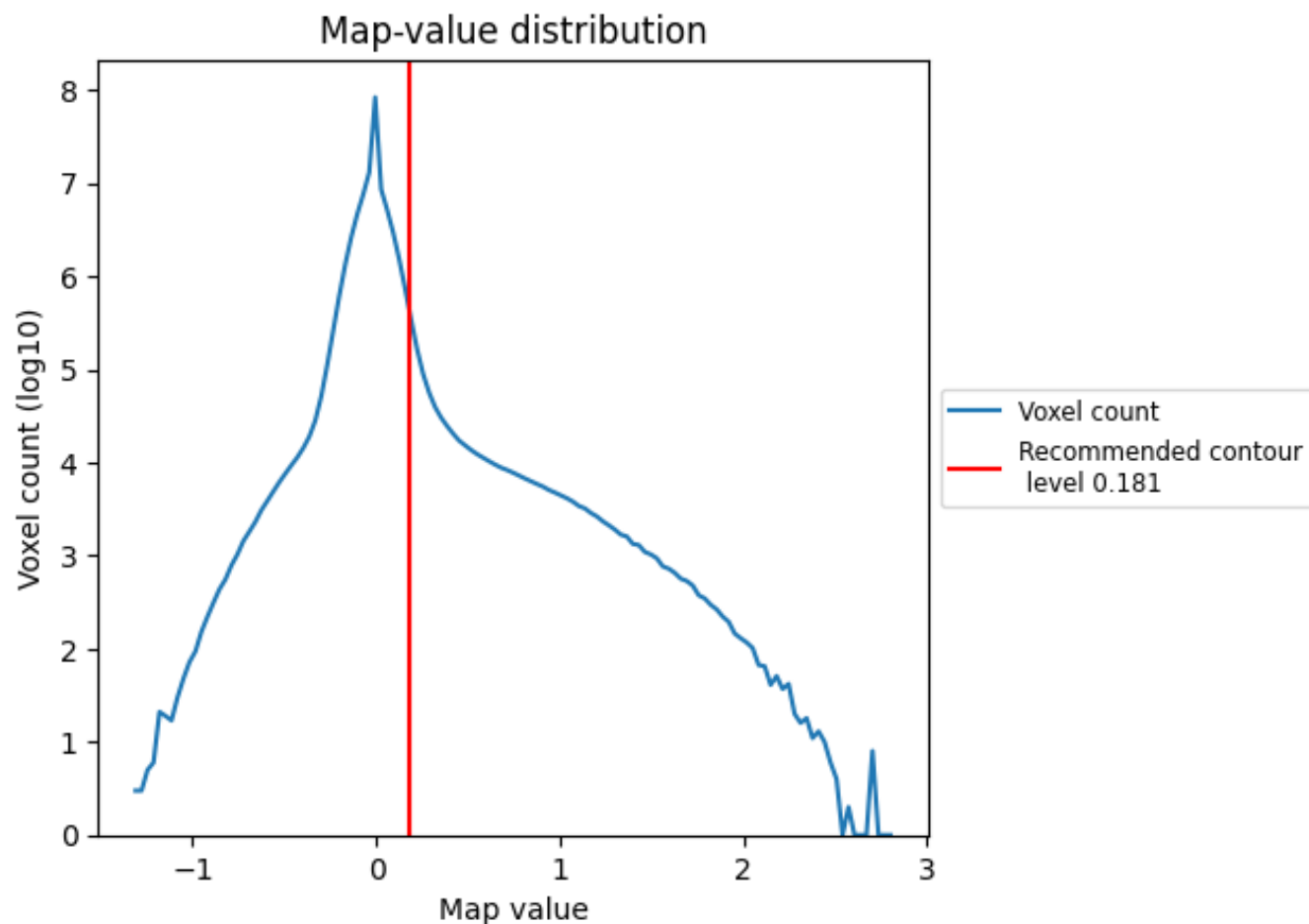
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

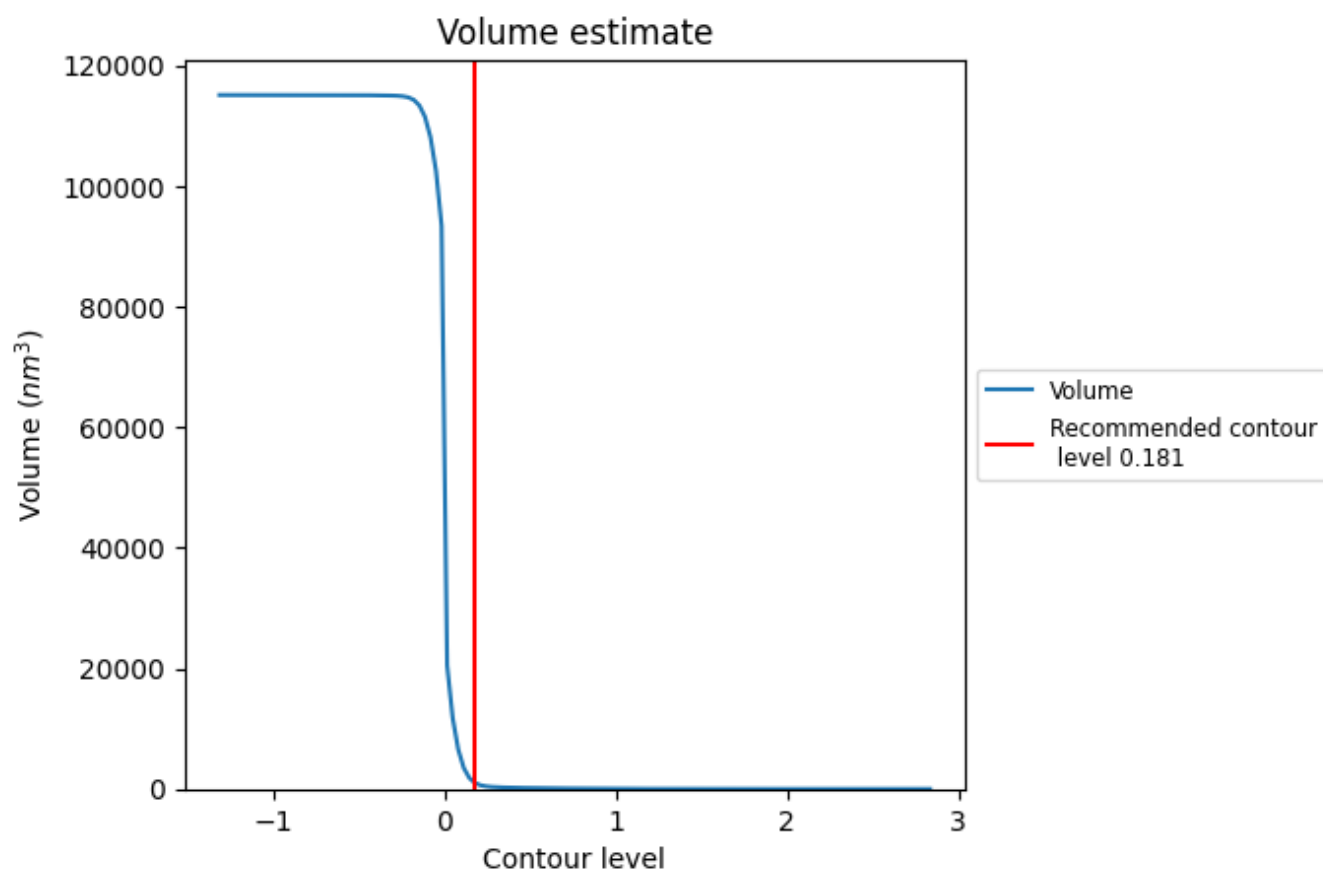
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

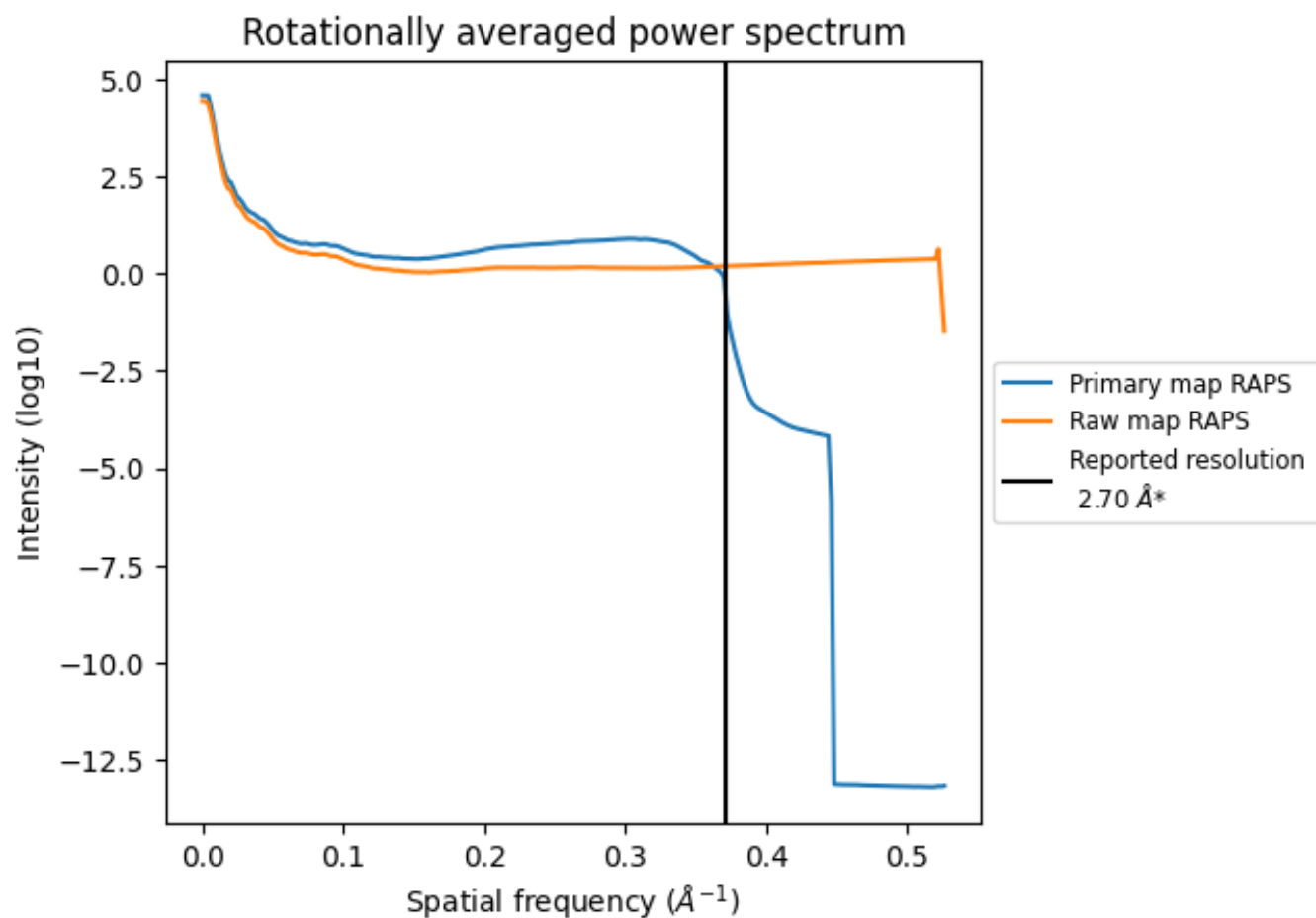
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 976 nm<sup>3</sup>; this corresponds to an approximate mass of 881 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 ⓘ

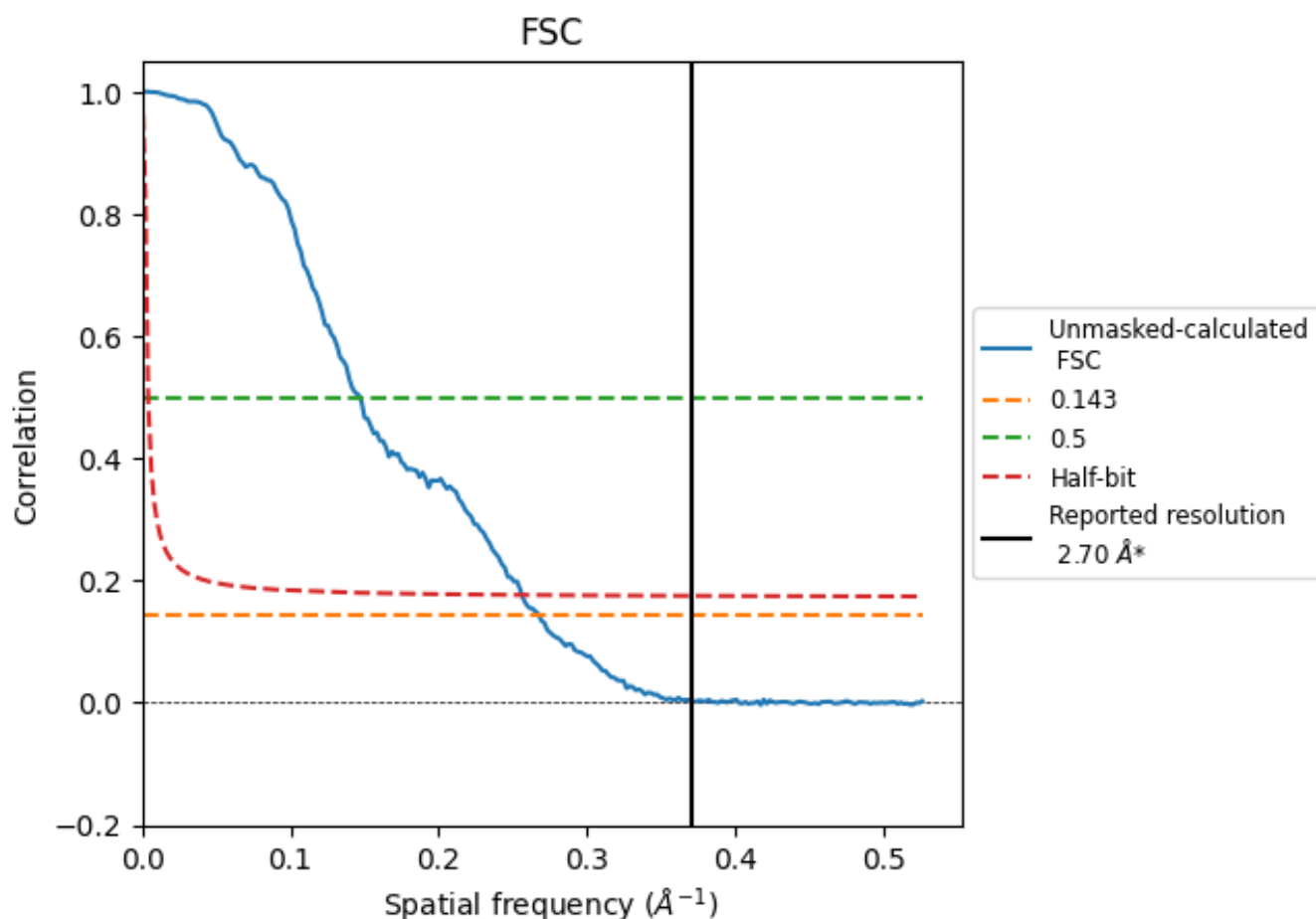


\*Reported resolution corresponds to spatial frequency of 0.370  $\text{\AA}^{-1}$

## 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 0.370 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	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	6.82	3.90

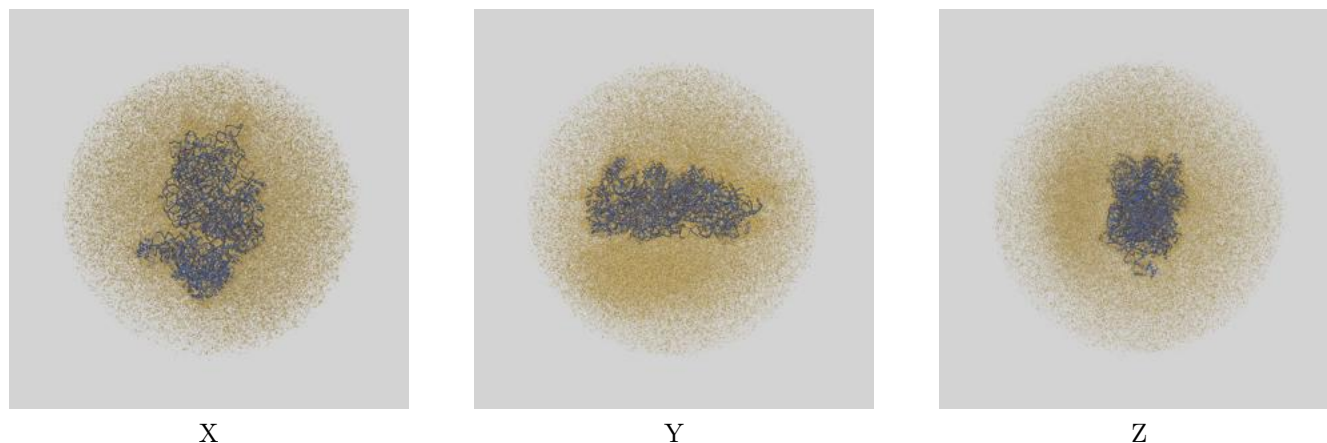
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.7 by more than 10 %



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

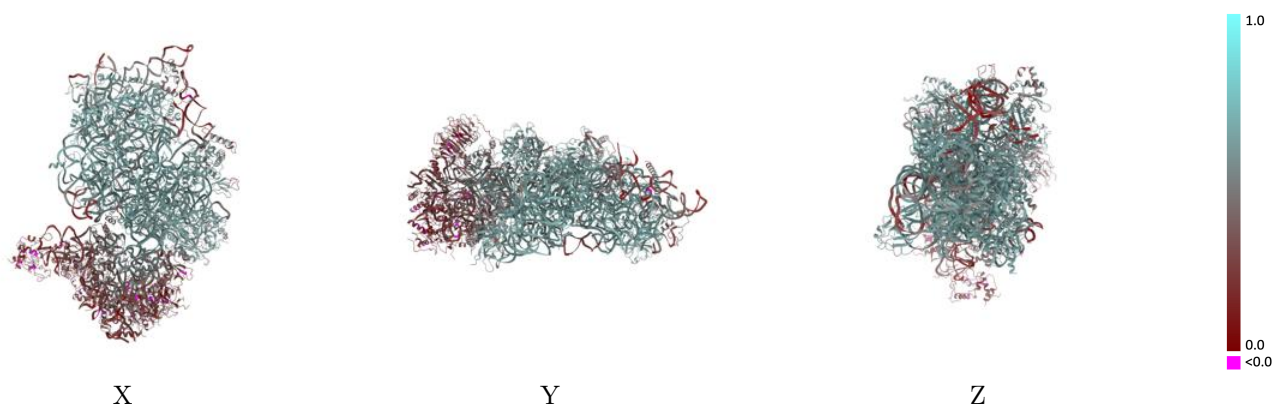
This section contains information regarding the fit between EMDB map EMD-62449 and PDB model 9KMY. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



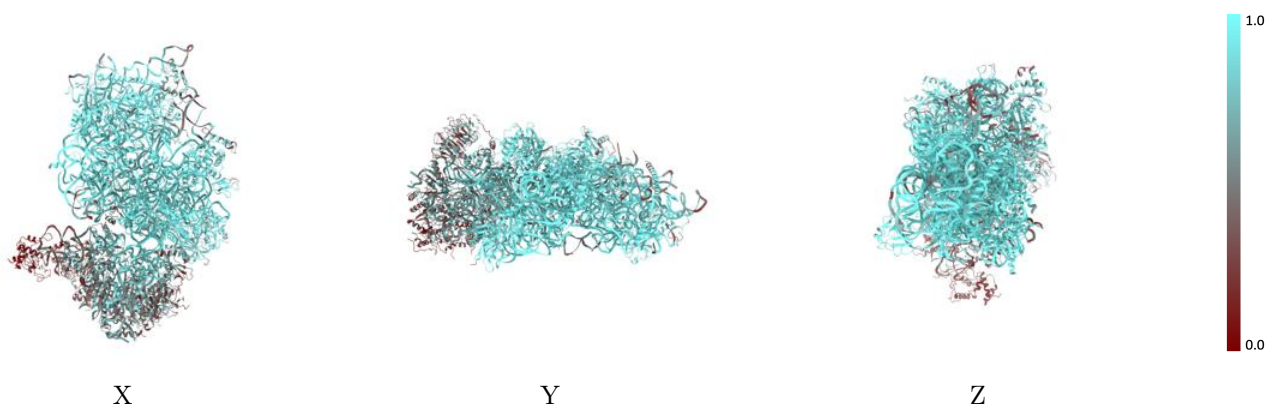
The images above show the 3D surface view of the map at the recommended contour level 0.181 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



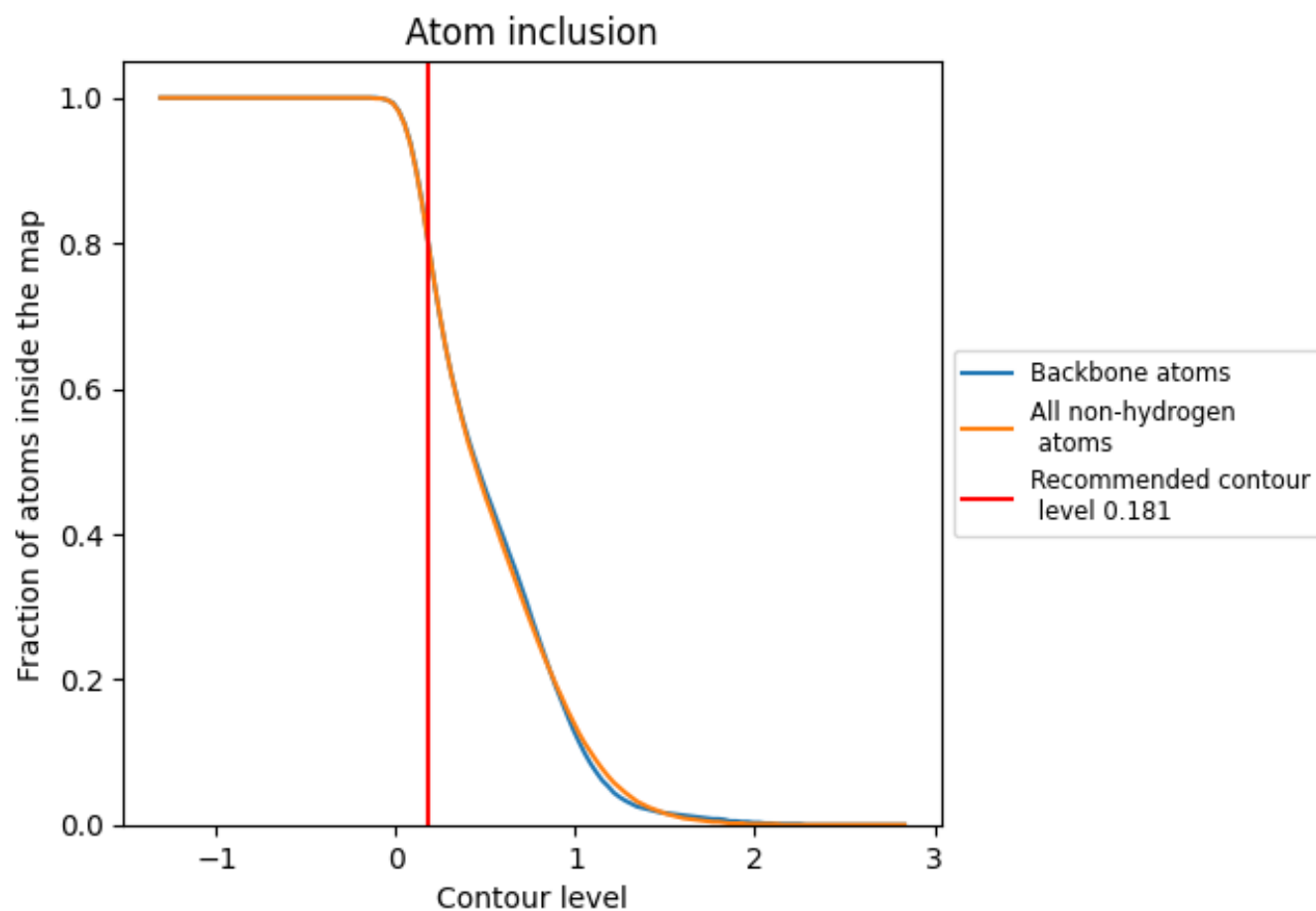
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.181).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.181) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.4920
2	 0.8620	 0.5040
A	 0.9430	 0.6010
B	 0.9280	 0.5980
C	 0.9580	 0.6280
D	 0.5960	 0.3890
E	 0.9680	 0.6310
F	 0.5060	 0.3130
G	 0.9080	 0.5700
H	 0.7910	 0.5100
I	 0.8950	 0.5740
J	 0.9670	 0.6300
K	 0.3950	 0.2540
L	 0.9180	 0.6120
M	 0.1450	 0.2240
N	 0.9540	 0.6080
O	 0.9070	 0.5890
P	 0.3460	 0.2520
Q	 0.5850	 0.3390
R	 0.7530	 0.4910
S	 0.3180	 0.2470
T	 0.4780	 0.2840
U	 0.5470	 0.3440
V	 0.9570	 0.6170
W	 0.9820	 0.6400
X	 0.9690	 0.6310
Y	 0.9670	 0.6220
Z	 0.3280	 0.2230
a	 0.9480	 0.6100
b	 0.9060	 0.5610
c	 0.5410	 0.3320
d	 0.5580	 0.3540
e	 0.8430	 0.5730
f	 0.1280	 0.2040
g	 0.4850	 0.2980



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Chain	Atom inclusion	Q-score
h	 0.8870	 0.5900
n	 0.5670	 0.4730