



## wwPDB EM Validation Summary Report ⓘ

Feb 10, 2025 – 01:38 PM EST

PDB ID : 9C8K  
EMDB ID : EMD-45307  
Title : Rabbit Hemorrhagic Disease Virus reinitiation stimulating TURBS RNA bound to rabbit ribosome  
Authors : Sherlock, M.E.; Kieft, J.S.  
Deposited on : 2024-06-12  
Resolution : 3.10 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:

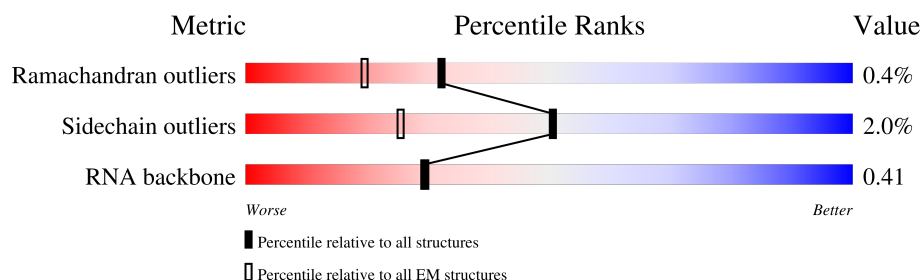
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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.



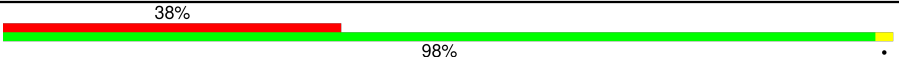


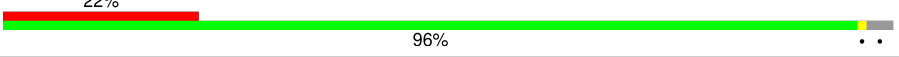

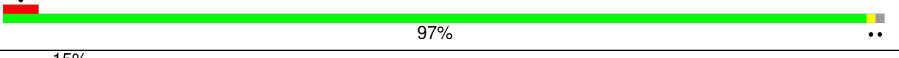
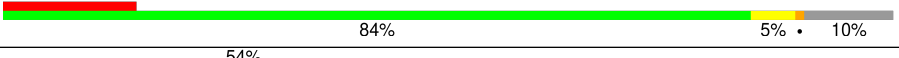

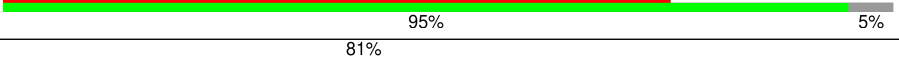


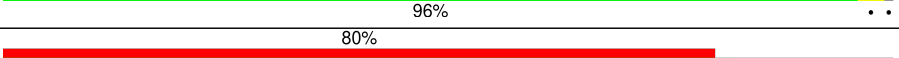
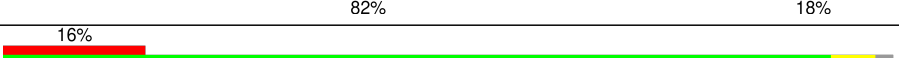
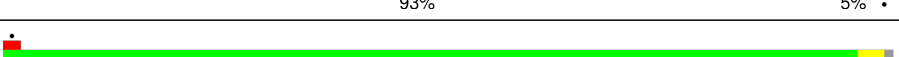
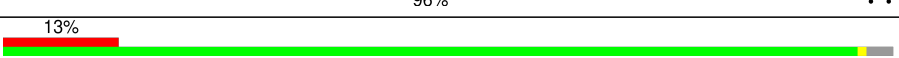
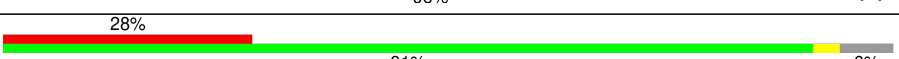
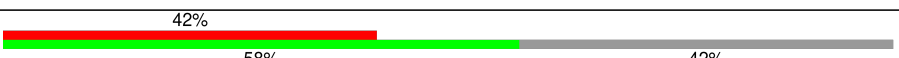
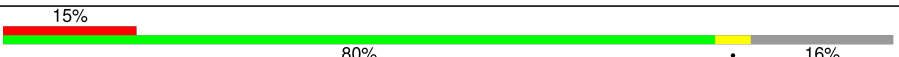
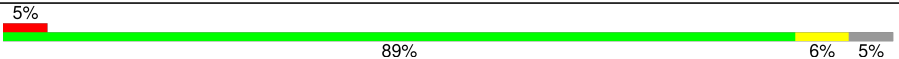


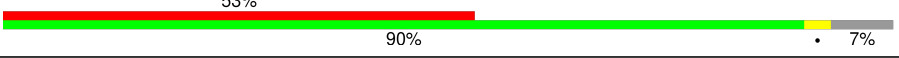

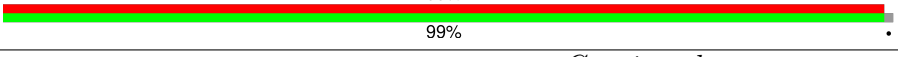

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	
2	B	264	
3	C	293	
4	D	243	
5	E	263	
6	F	204	
7	G	249	
8	H	194	

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Mol	Chain	Length	Quality of chain
9	I	208	
10	J	194	
11	K	165	
12	L	158	
13	M	132	
14	N	151	
15	O	151	
16	P	145	
17	Q	146	
18	R	135	
19	S	152	
20	T	145	
21	U	119	
22	V	83	
23	W	130	
24	X	143	
25	Y	133	
26	Z	125	
27	a	115	
28	b	84	
29	c	69	
30	d	56	
31	e	59	
32	f	156	
33	g	317	

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Mol	Chain	Length	Quality of chain
34	1	1869	<div><div></div><div>25%</div><div></div><div>70%</div><div></div><div>22%</div><div></div><div>9%</div></div>
35	2	91	<div><div></div><div>5%</div><div></div><div>26%</div><div></div><div>70%</div></div>

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 134479 atoms, of which 58947 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 Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	215	Total	C	H	N	O	S	0	0
			3409	1083	1705	298	315	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	THR	conflict	UNP G1TLT8
A	293	ASP	GLU	conflict	UNP G1TLT8

- Molecule 2 is a protein called eS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	212	Total	C	H	N	O	S	0	0
			3517	1093	1795	308	307	14		

- Molecule 3 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	222	Total	C	H	N	O	S	0	0
			3533	1114	1809	296	304	10		

- Molecule 4 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	220	Total	C	H	N	O	S	0	0
			3513	1090	1804	308	304	7		

- Molecule 5 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	257	Total	C	H	N	O	S	0	0
			4170	1298	2139	381	344	8		

- Molecule 6 is a protein called uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	190	Total	C	H	N	O	S	0	0
			3060	939	1558	285	271	7		

- Molecule 7 is a protein called eS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	232	Total	C	H	N	O	S	0	0
			3929	1176	2045	379	322	7		

- Molecule 8 is a protein called eS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	183	Total	C	H	N	O	S	0	0
			3045	941	1566	272	265	1		

- Molecule 9 is a protein called eS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	207	Total	C	H	N	O	S	0	0
			3482	1064	1786	334	293	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 10 is a protein called uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	179	Total	C	H	N	O	S	0	0
			3110	953	1615	299	241	2		

- Molecule 11 is a protein called S10\_pectin domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	98	Total	C	H	N	O	S	0	0
			1681	539	854	148	134	6		

- Molecule 12 is a protein called uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	153	Total	C	H	N	O	S	0	0
			2593	804	1335	235	213	6		

- Molecule 13 is a protein called eS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	120	Total	C	H	N	O	S	0	0
			1893	584	962	164	174	9		

- Molecule 14 is a protein called uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	149	Total	C	H	N	O	S	0	0
			2492	770	1290	228	203	1		

- Molecule 15 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	136	Total	C	H	N	O	S	0	0
			2056	621	1040	199	190	6		

- Molecule 16 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	120	Total	C	H	N	O	S	0	0
			2046	636	1047	188	168	7		

- Molecule 17 is a protein called uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	139	Total	C	H	N	O	S	0	0
			2284	704	1175	210	192	3		

- Molecule 18 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	121	Total	C	H	N	O	S	0	0
			2021	618	1036	183	181	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	134	PRO	ALA	conflict	UNP G1TU13

- Molecule 19 is a protein called uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	139	Total	C	H	N	O	S	0	0
			2365	725	1211	233	195	1		

- Molecule 20 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	143	Total	C	H	N	O	S	0	0
			2258	697	1146	214	198	3		

- Molecule 21 is a protein called uS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	97	Total	C	H	N	O	S	0	0
			1607	483	838	144	138	4		

- Molecule 22 is a protein called eS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	81	Total	C	H	N	O	S	0	0
			1239	380	622	114	118	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	3	ASN	SER	conflict	UNP G1TM82
V	4	ASP	ASN	conflict	UNP G1TM82
V	33	GLN	PRO	conflict	UNP G1TM82
V	50	PHE	SER	conflict	UNP G1TM82
V	75	ALA	SER	conflict	UNP G1TM82
V	76	ASP	HIS	conflict	UNP G1TM82
V	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 23 is a protein called uS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	129	Total	C	H	N	O	S	0	0
			2115	659	1081	193	176	6		



- Molecule 24 is a protein called uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	139	Total	C	H	N	O	S	0	0
			2228	682	1148	214	181	3		

- Molecule 25 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	125	Total	C	H	N	O	S	0	0
			2102	642	1087	199	169	5		

- Molecule 26 is a protein called eS25.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	73	Total	C	H	N	O	S	0	0
			1226	374	641	108	102	1		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	97	Total	C	H	N	O	S	0	0
			1598	481	824	160	128	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	28	ARG	CYS	conflict	UNP G1TFE8
a	56	ALA	VAL	conflict	UNP G1TFE8
a	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 28 is a protein called eS27.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	80	Total	C	H	N	O	S	0	0
			1272	391	647	116	111	7		

- Molecule 29 is a protein called eS28.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	61	Total	C	H	N	O	S	0	0
			984	291	504	96	91	2		

- Molecule 30 is a protein called uS14.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	51	Total	C	H	N	O	S	0	0
			858	269	431	87	66	5		

- Molecule 31 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	e	55	Total	C	H	N	O	S	0	0
			921	272	484	96	68	1		

- Molecule 32 is a protein called eS31.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	f	73	Total	C	H	N	O	S	0	0
			1224	379	623	115	100	7		

- Molecule 33 is a protein called Receptor for Activated C Kinase 1 (RACK1).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	g	314	Total	C	H	N	O	S	0	0
			4839	1537	2399	425	466	12		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	1	1708	Total	C	H	N	O	P	0	0
			54862	16274	18406	6546	11928	1708		

- Molecule 35 is a RNA chain called RHDV Reinitiation stimulating element RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	2	27	Total	C	H	N	O	P	0	0
			871	258	294	108	186	25		

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	Q	2	Total	Mg	0
			2	2	
36	X	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
36	1	71	Total	Mg	0
			71	71	

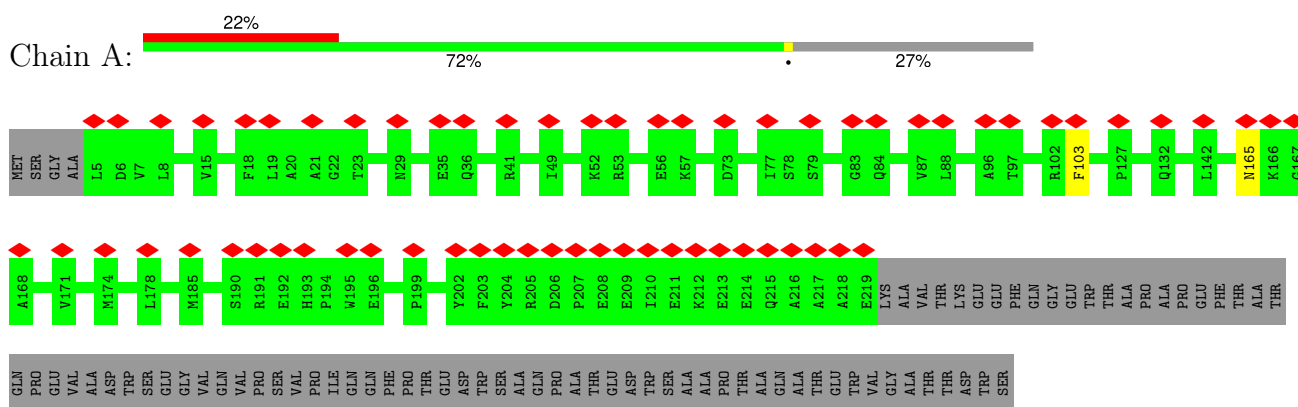
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	a	1	Total	Zn	0
			1	1	
37	d	1	Total	Zn	0
			1	1	

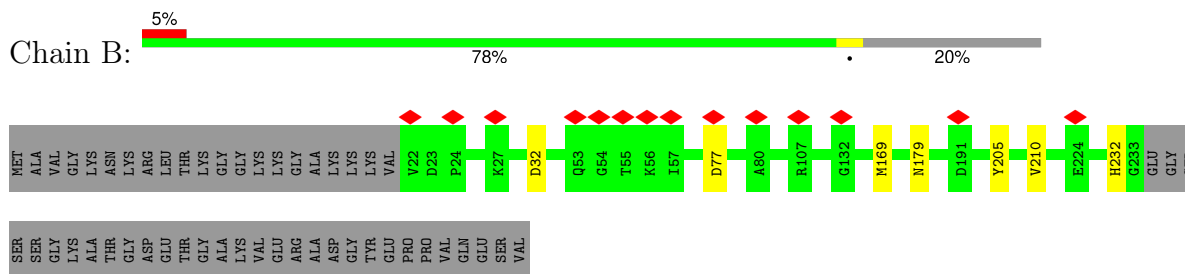
### 3 Residue-property plots

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.

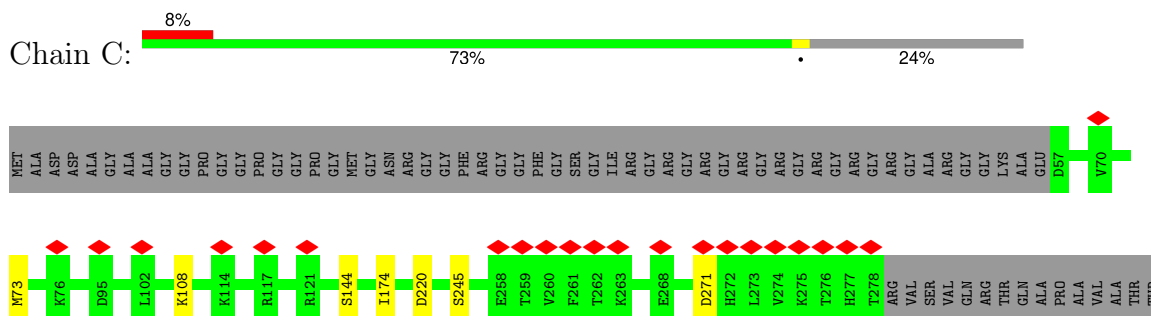
- Molecule 1: Small ribosomal subunit protein uS2




- Molecule 2: eS1

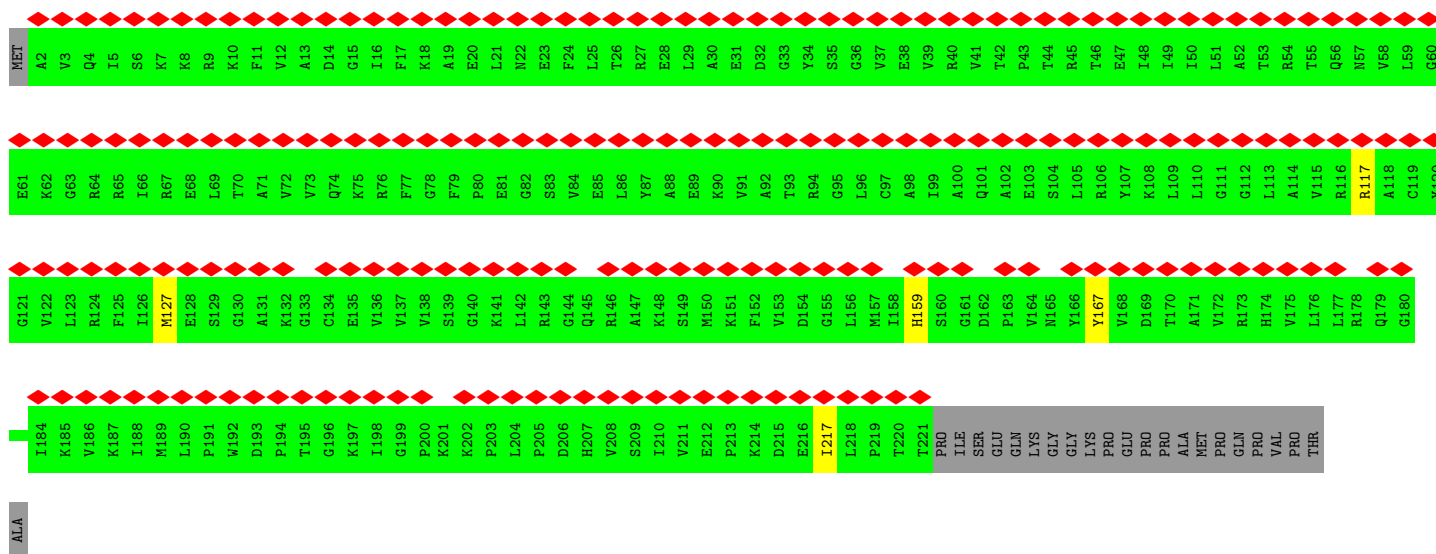


- Molecule 3: 40S ribosomal protein uS5



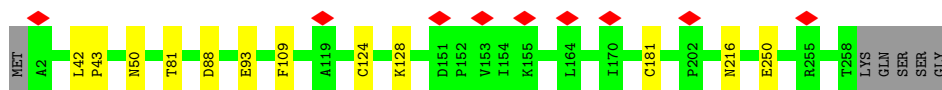
- Molecule 4: 40S ribosomal protein uS3

Chain D: 

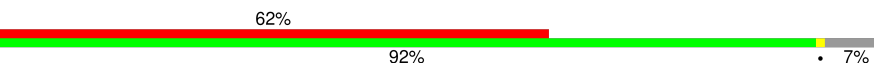


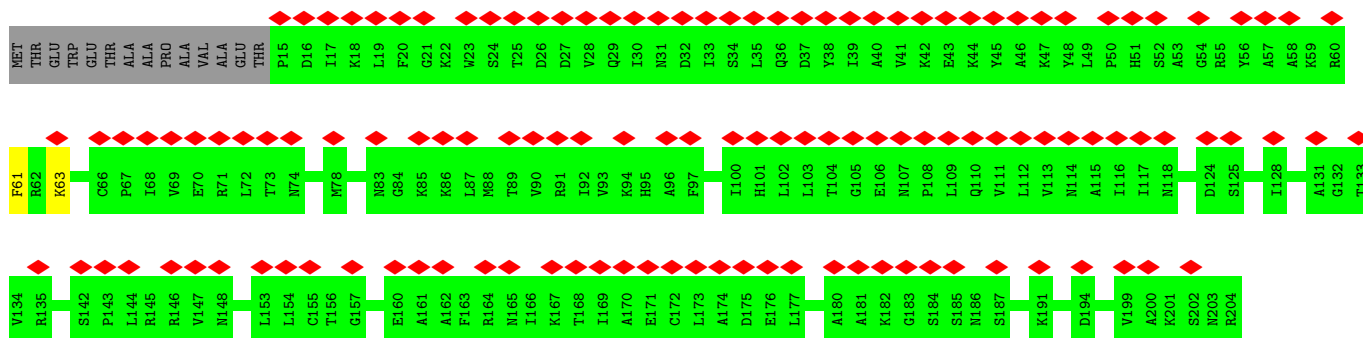
- Molecule 5: 40S ribosomal protein eS4

Chain E: 



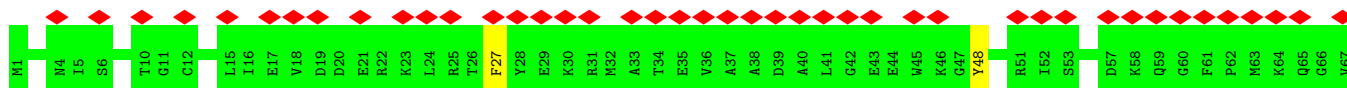
- Molecule 6: uS7

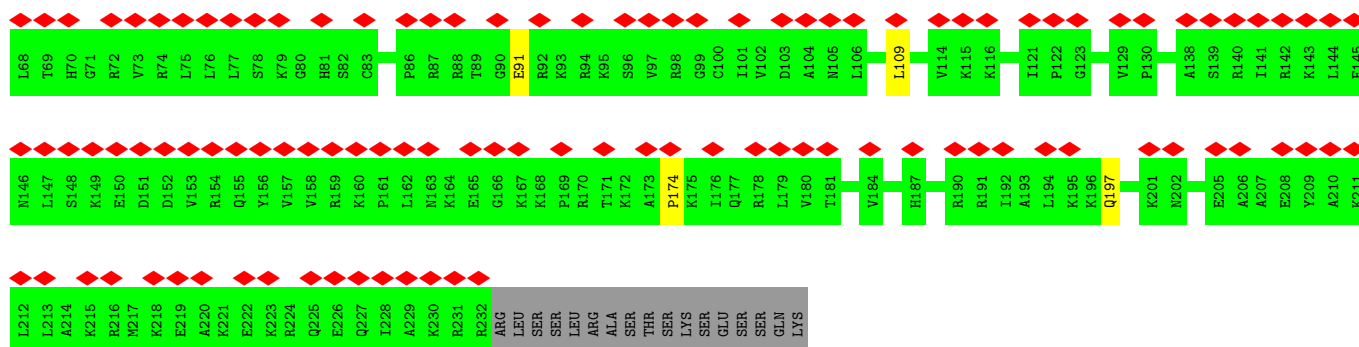
Chain F: 



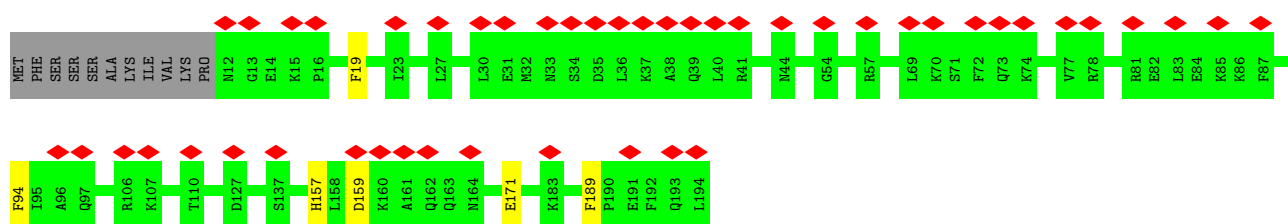
- Molecule 7: eS6

Chain G: 





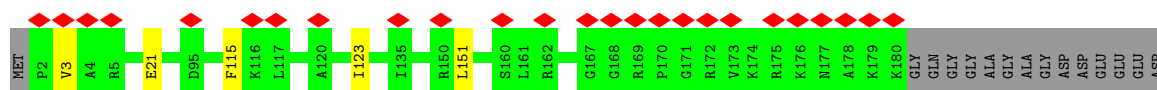
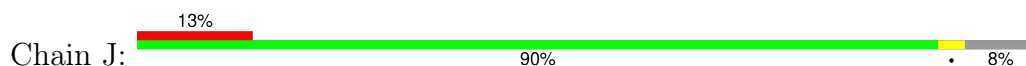
- Molecule 8: eS7



- Molecule 9: eS8

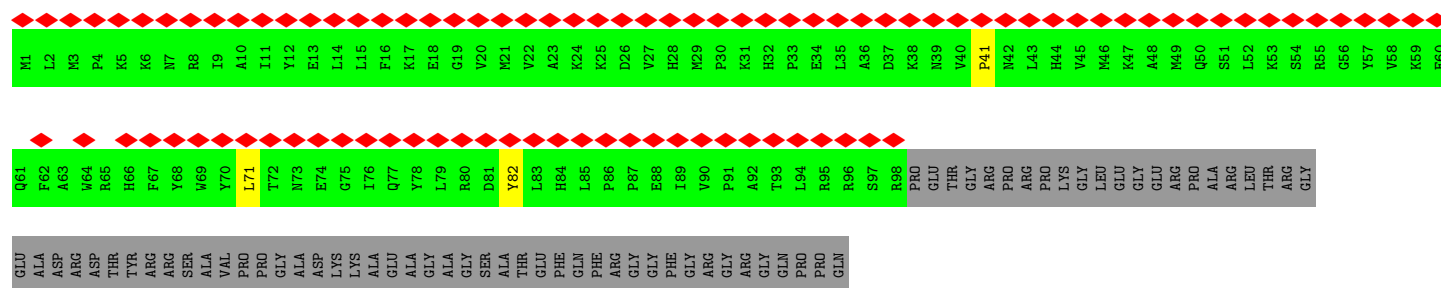


- Molecule 10: uS4

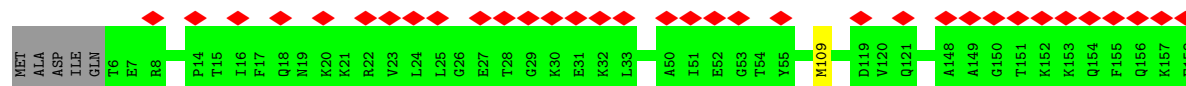


- Molecule 11: S10\_pectin domain-containing protein

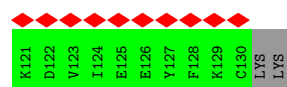
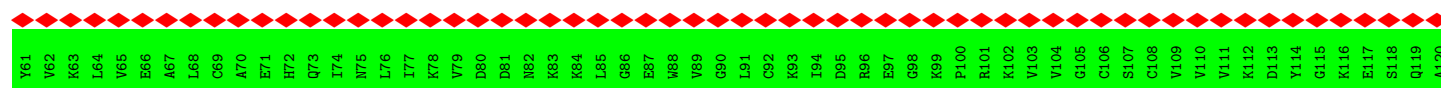
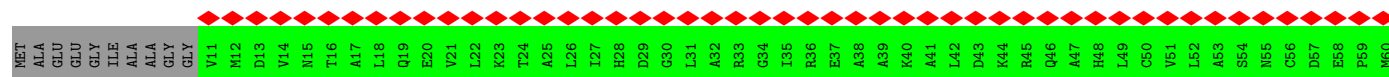




- Molecule 12: uS17



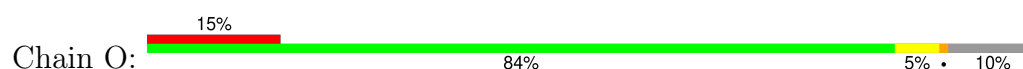
- Molecule 13: eS12



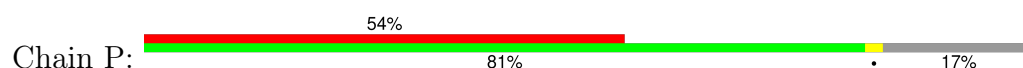
- Molecule 14: uS15

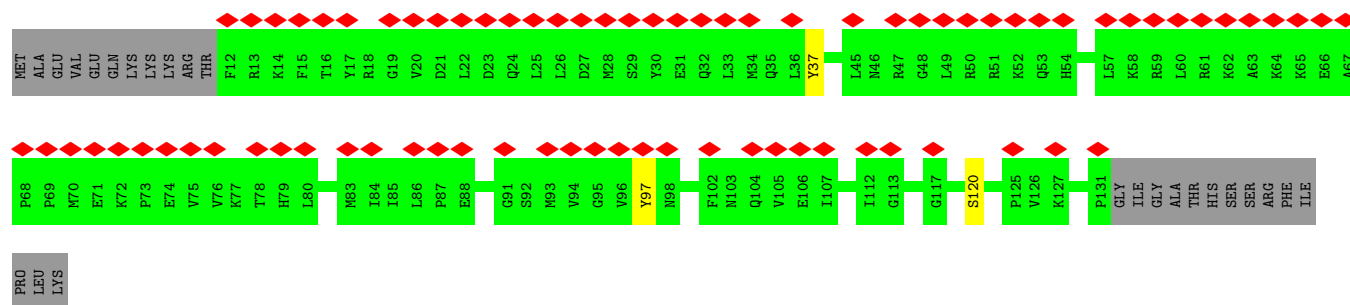


- Molecule 15: Small ribosomal subunit protein uS11

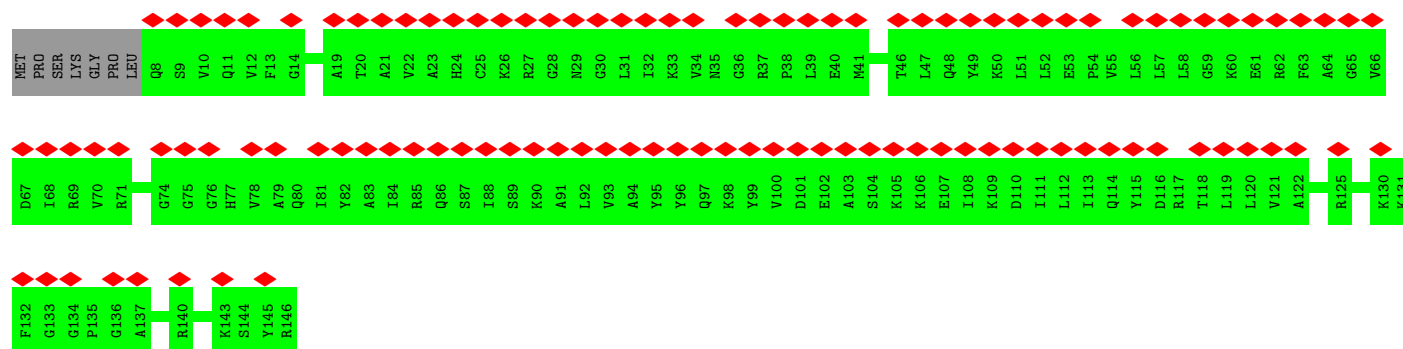
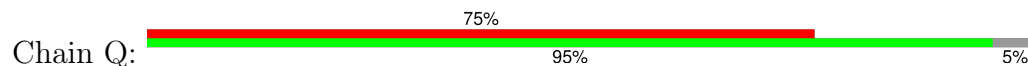


- Molecule 16: 40S ribosomal protein uS19

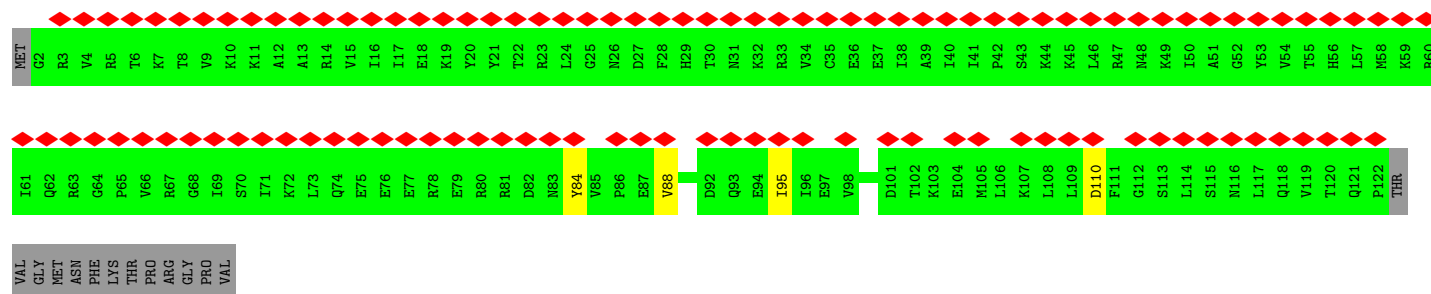
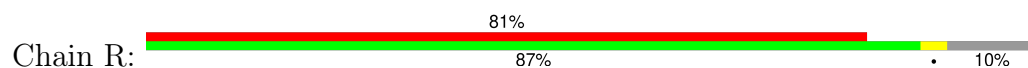




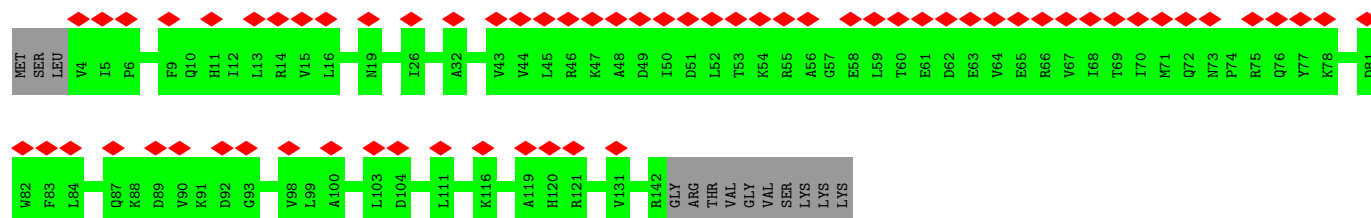
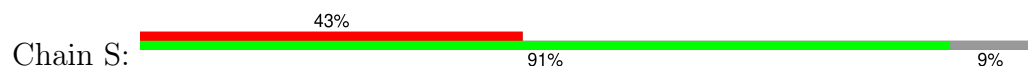
• Molecule 17: uS9



• Molecule 18: Small ribosomal subunit protein eS17

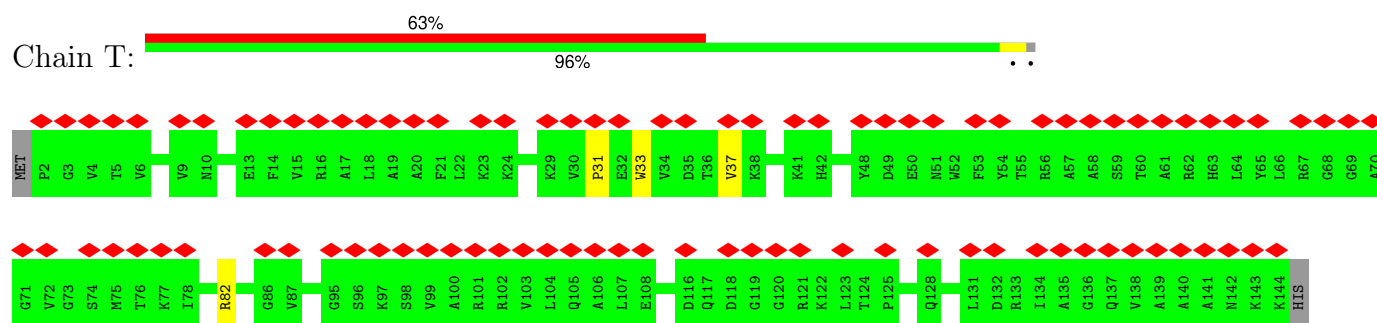


• Molecule 19: uS13

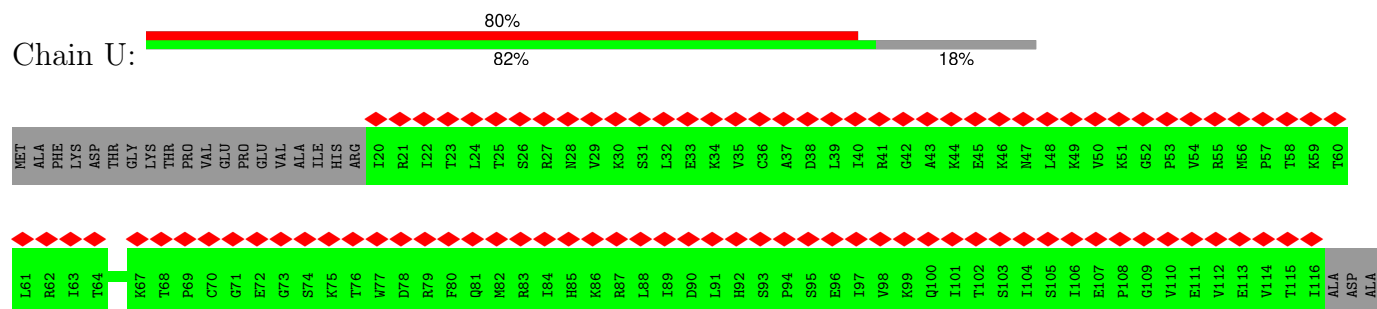


• Molecule 20: 40S ribosomal protein eS19

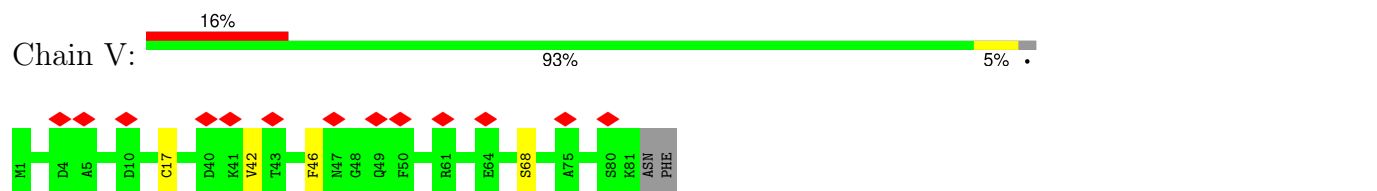




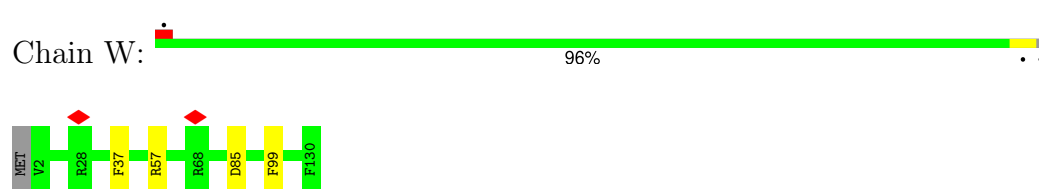
- Molecule 21: uS10



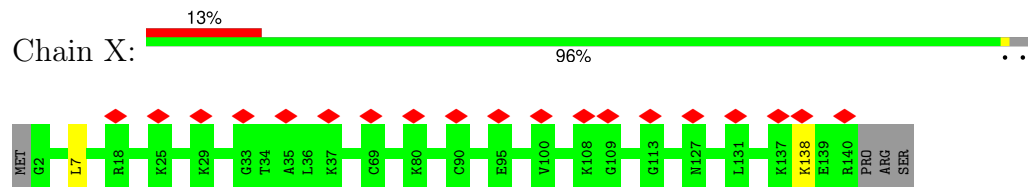
- Molecule 22: eS21



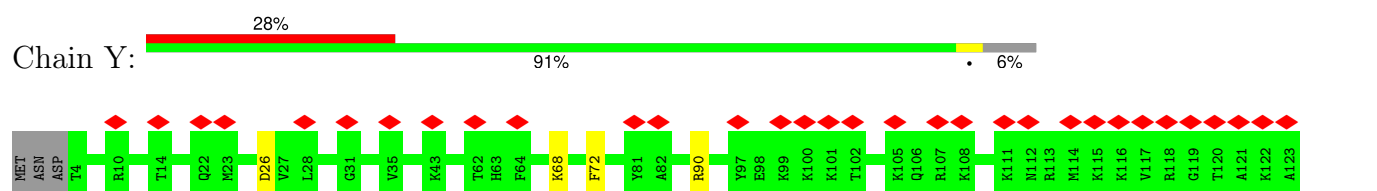
- Molecule 23: uS8

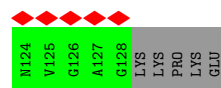


- Molecule 24: uS12

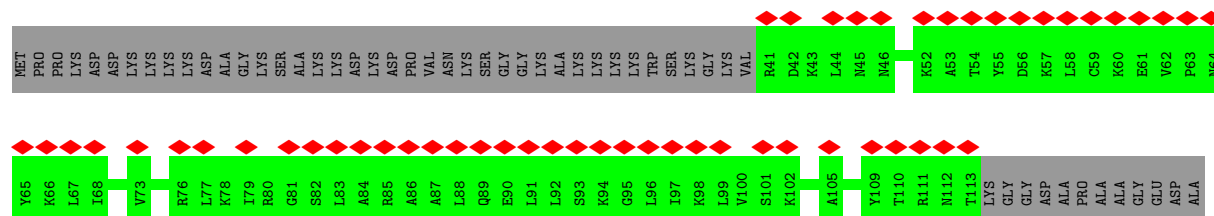


- Molecule 25: Small ribosomal subunit protein eS24

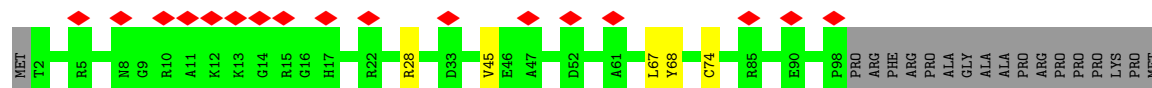




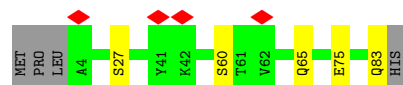
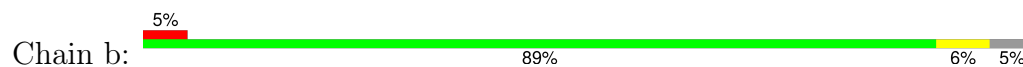
• Molecule 26: eS25



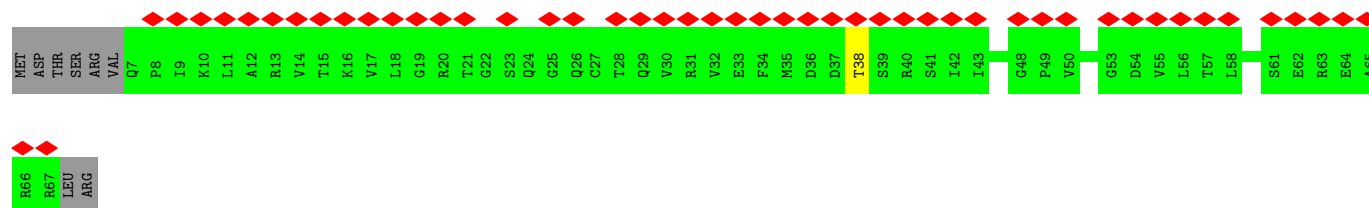
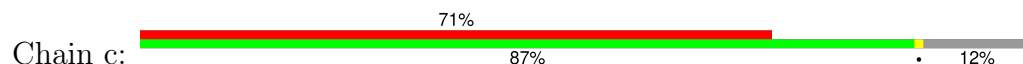
• Molecule 27: 40S ribosomal protein S26



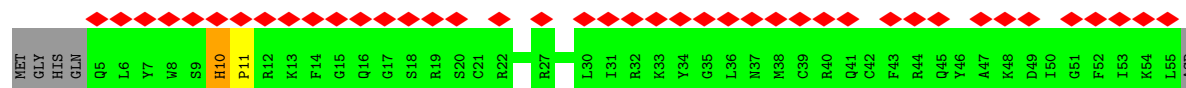
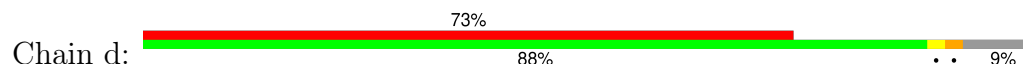
• Molecule 28: eS27



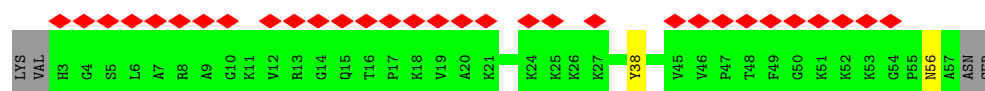
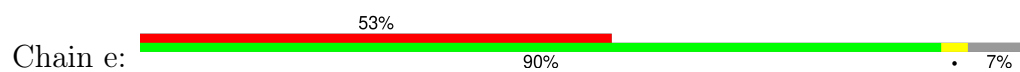
• Molecule 29: eS28



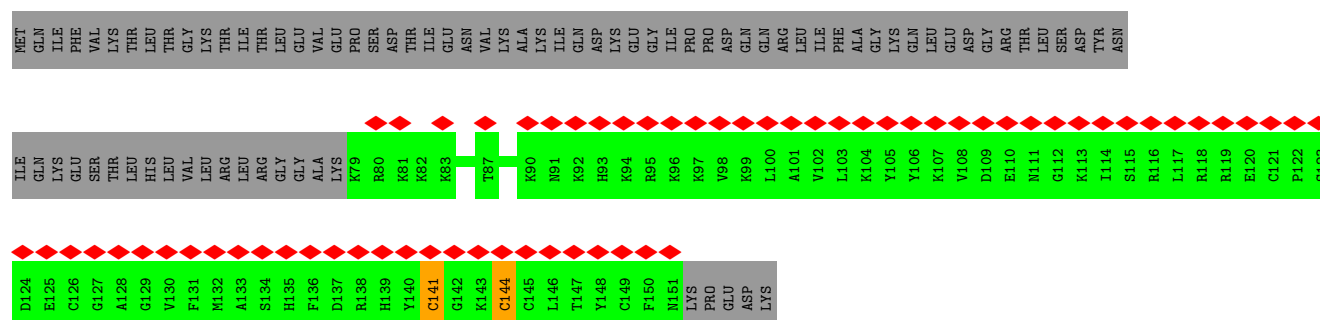
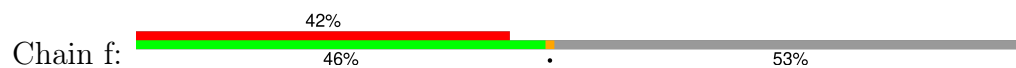
• Molecule 30: uS14



• Molecule 31: 40S ribosomal protein eS30



• Molecule 32: eS31



• Molecule 33: Receptor for Activated C Kinase 1 (RACK1)



• Molecule 34: 18S ribosomal RNA







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61643	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.94	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.029	Depositor
Minimum map value	-1.682	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	388.0, 388.0, 388.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.29	0/1741	0.60	0/2366
2	B	0.27	0/1749	0.60	0/2340
3	C	0.26	0/1761	0.54	0/2379
4	D	0.25	0/1736	0.53	0/2338
5	E	0.64	3/2072 (0.1%)	0.79	4/2793 (0.1%)
6	F	0.24	0/1524	0.54	0/2048
7	G	0.73	3/1907 (0.2%)	0.92	5/2538 (0.2%)
8	H	0.26	0/1501	0.59	0/2009
9	I	0.77	2/1725 (0.1%)	0.93	5/2298 (0.2%)
10	J	0.28	0/1520	0.64	0/2030
11	K	0.26	0/851	0.51	0/1147
12	L	0.27	0/1281	0.60	0/1710
13	M	0.23	0/941	0.45	0/1264
14	N	0.27	0/1226	0.58	0/1649
15	O	1.00	4/1029 (0.4%)	1.04	6/1380 (0.4%)
16	P	0.27	0/1019	0.59	0/1361
17	Q	0.25	0/1126	0.55	0/1506
18	R	0.25	0/997	0.54	0/1338
19	S	0.24	0/1172	0.57	0/1570
20	T	0.25	0/1131	0.52	0/1515
21	U	0.23	0/778	0.53	0/1045
22	V	0.27	0/623	0.54	0/833
23	W	0.27	0/1051	0.63	1/1406 (0.1%)
24	X	0.25	0/1097	0.55	0/1464
25	Y	0.29	0/1032	0.59	0/1371
26	Z	0.24	0/591	0.54	0/794
27	a	0.26	0/786	0.62	0/1053
28	b	0.28	0/637	0.62	0/854
29	c	0.24	0/482	0.63	0/645
30	d	0.94	3/437 (0.7%)	1.50	4/580 (0.7%)
31	e	0.25	0/443	0.57	0/583
32	f	0.41	1/613 (0.2%)	0.73	2/811 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g	0.23	0/2497	0.49	0/3399
34	1	0.21	1/40767 (0.0%)	0.77	5/63536 (0.0%)
35	2	0.19	0/644	0.80	0/1003
All	All	0.32	17/80487 (0.0%)	0.72	32/116956 (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
15	O	0	2
28	b	0	1
30	d	0	1
32	f	0	1
All	All	0	5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	71	PRO	CB-CG	22.51	2.62	1.50
9	I	179	PRO	CB-CG	22.29	2.61	1.50
5	E	43	PRO	CG-CD	-22.27	0.77	1.50
7	G	174	PRO	CB-CG	21.98	2.59	1.50
15	O	71	PRO	CG-CD	-18.77	0.88	1.50

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	179	PRO	CB-CG-CD	-25.48	7.13	106.50
7	G	174	PRO	CB-CG-CD	-24.17	12.24	106.50
5	E	43	PRO	N-CD-CG	-22.69	69.16	103.20
15	O	71	PRO	CB-CG-CD	-20.28	27.42	106.50
30	d	11	PRO	N-CD-CG	-18.81	74.98	103.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	O	141	ARG	Peptide
15	O	142	ARG	Peptide

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Mol	Chain	Res	Type	Group
28	b	65	GLN	Peptide
30	d	10	HIS	Peptide
32	f	141	CYS	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	A	213/295 (72%)	188 (88%)	25 (12%)	0	100	100
2	B	210/264 (80%)	160 (76%)	47 (22%)	3 (1%)	9	34
3	C	220/293 (75%)	196 (89%)	23 (10%)	1 (0%)	25	58
4	D	218/243 (90%)	204 (94%)	13 (6%)	1 (0%)	25	58
5	E	255/263 (97%)	217 (85%)	37 (14%)	1 (0%)	30	63
6	F	188/204 (92%)	162 (86%)	25 (13%)	1 (0%)	25	58
7	G	230/249 (92%)	202 (88%)	28 (12%)	0	100	100
8	H	181/194 (93%)	162 (90%)	19 (10%)	0	100	100
9	I	205/208 (99%)	167 (82%)	38 (18%)	0	100	100
10	J	177/194 (91%)	156 (88%)	19 (11%)	2 (1%)	12	39
11	K	96/165 (58%)	85 (88%)	10 (10%)	1 (1%)	13	42
12	L	151/158 (96%)	133 (88%)	18 (12%)	0	100	100
13	M	118/132 (89%)	112 (95%)	6 (5%)	0	100	100
14	N	147/151 (97%)	126 (86%)	20 (14%)	1 (1%)	19	51
15	O	134/151 (89%)	111 (83%)	21 (16%)	2 (2%)	8	33
16	P	118/145 (81%)	98 (83%)	20 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	137/146 (94%)	126 (92%)	11 (8%)	0	100	100
18	R	119/135 (88%)	111 (93%)	6 (5%)	2 (2%)	7	30
19	S	137/152 (90%)	125 (91%)	12 (9%)	0	100	100
20	T	141/145 (97%)	133 (94%)	6 (4%)	2 (1%)	9	34
21	U	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
22	V	79/83 (95%)	76 (96%)	2 (2%)	1 (1%)	10	36
23	W	127/130 (98%)	112 (88%)	15 (12%)	0	100	100
24	X	137/143 (96%)	123 (90%)	14 (10%)	0	100	100
25	Y	123/133 (92%)	115 (94%)	8 (6%)	0	100	100
26	Z	71/125 (57%)	68 (96%)	3 (4%)	0	100	100
27	a	95/115 (83%)	80 (84%)	14 (15%)	1 (1%)	12	39
28	b	78/84 (93%)	56 (72%)	21 (27%)	1 (1%)	10	36
29	c	59/69 (86%)	52 (88%)	6 (10%)	1 (2%)	7	30
30	d	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
31	e	53/59 (90%)	47 (89%)	6 (11%)	0	100	100
32	f	71/156 (46%)	66 (93%)	5 (7%)	0	100	100
33	g	312/317 (98%)	292 (94%)	20 (6%)	0	100	100
All	All	4744/5476 (87%)	4200 (88%)	523 (11%)	21 (0%)	32	63

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	93	GLU
6	F	63	LYS
10	J	3	VAL
22	V	42	VAL
3	C	174	ILE

### 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	A	180/243 (74%)	178 (99%)	2 (1%)	70	84
2	B	193/231 (84%)	189 (98%)	4 (2%)	48	72
3	C	188/225 (84%)	182 (97%)	6 (3%)	34	63
4	D	183/202 (91%)	179 (98%)	4 (2%)	47	71
5	E	220/225 (98%)	211 (96%)	9 (4%)	26	57
6	F	160/170 (94%)	159 (99%)	1 (1%)	84	91
7	G	202/218 (93%)	197 (98%)	5 (2%)	42	69
8	H	164/174 (94%)	158 (96%)	6 (4%)	29	59
9	I	179/180 (99%)	176 (98%)	3 (2%)	56	78
10	J	160/168 (95%)	157 (98%)	3 (2%)	52	75
11	K	89/136 (65%)	87 (98%)	2 (2%)	47	71
12	L	138/142 (97%)	137 (99%)	1 (1%)	81	90
13	M	102/108 (94%)	102 (100%)	0	100	100
14	N	130/131 (99%)	129 (99%)	1 (1%)	79	89
15	O	106/119 (89%)	101 (95%)	5 (5%)	22	52
16	P	109/130 (84%)	106 (97%)	3 (3%)	38	66
17	Q	115/121 (95%)	115 (100%)	0	100	100
18	R	110/122 (90%)	108 (98%)	2 (2%)	54	76
19	S	121/132 (92%)	121 (100%)	0	100	100
20	T	113/115 (98%)	111 (98%)	2 (2%)	54	76
21	U	90/107 (84%)	90 (100%)	0	100	100
22	V	65/67 (97%)	62 (95%)	3 (5%)	23	52
23	W	112/113 (99%)	109 (97%)	3 (3%)	40	67
24	X	111/115 (96%)	109 (98%)	2 (2%)	54	76
25	Y	107/115 (93%)	103 (96%)	4 (4%)	29	59
26	Z	65/103 (63%)	65 (100%)	0	100	100
27	a	84/98 (86%)	80 (95%)	4 (5%)	21	51
28	b	72/76 (95%)	69 (96%)	3 (4%)	25	56
29	c	54/62 (87%)	54 (100%)	0	100	100
30	d	45/49 (92%)	45 (100%)	0	100	100
31	e	44/48 (92%)	42 (96%)	2 (4%)	23	53
32	f	66/140 (47%)	65 (98%)	1 (2%)	60	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	g	272/275 (99%)	271 (100%)	1 (0%)	89	94
All	All	4149/4660 (89%)	4067 (98%)	82 (2%)	50	74

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	33	TRP
27	a	28	ARG
22	V	17	CYS
24	X	7	LEU
28	b	27	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
28	b	26	GLN
19	S	42	HIS
9	I	22	HIS
7	G	187	HIS
15	O	43	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	1	1701/1869 (91%)	393 (23%)	16 (0%)
35	2	25/91 (27%)	3 (12%)	1 (4%)
All	All	1726/1960 (88%)	396 (22%)	17 (0%)

5 of 396 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	1	4	C
34	1	9	U
34	1	11	A
34	1	13	C
34	1	17	C

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	1	1554	C
35	2	5	U
34	1	561	A
34	1	797	C
34	1	822	U

## 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](#)

Of 76 ligands modelled in this entry, 76 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
30	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	10:HIS	C	11:PRO	N	1.10

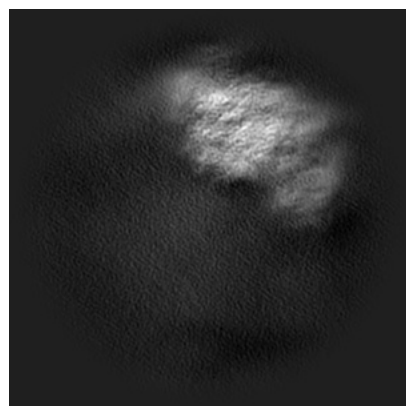
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45307. These allow visual inspection of the internal detail of the map and identification of artifacts.

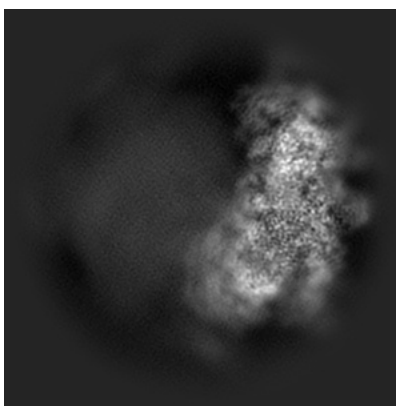
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

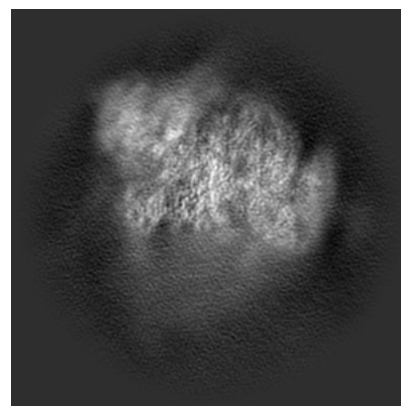
#### 6.1.1 Primary map



X

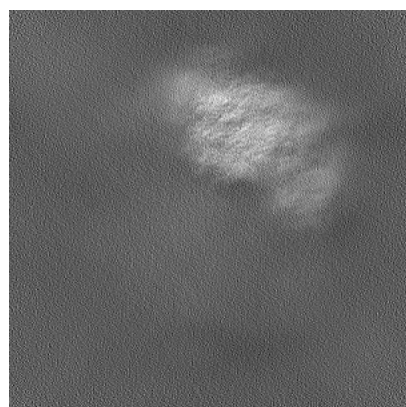


Y

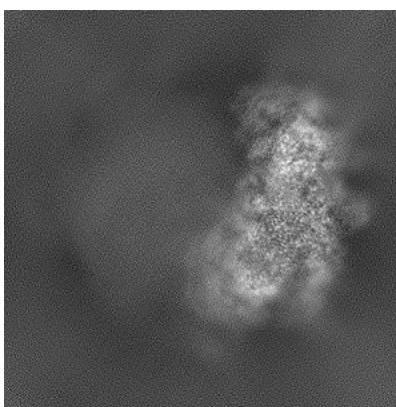


Z

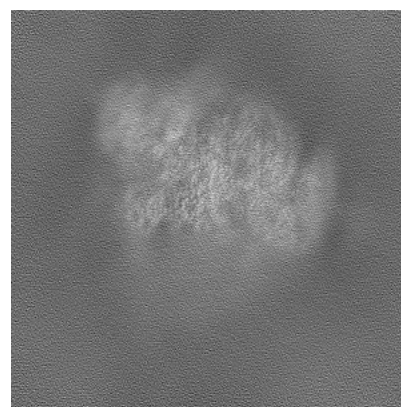
#### 6.1.2 Raw map



X



Y



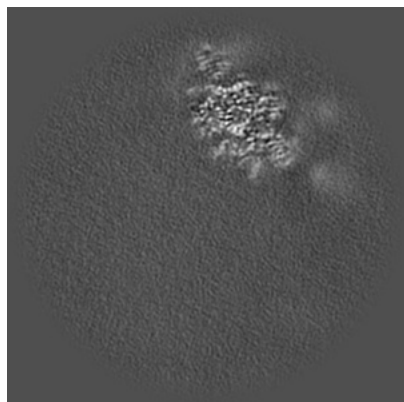
Z

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

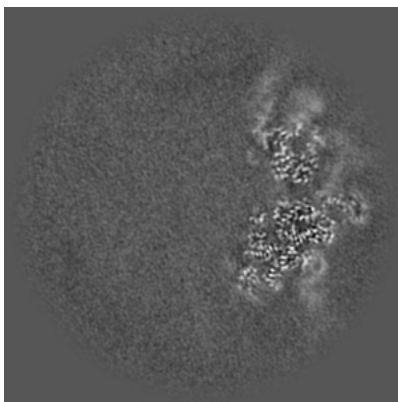


## 6.2 Central slices [i](#)

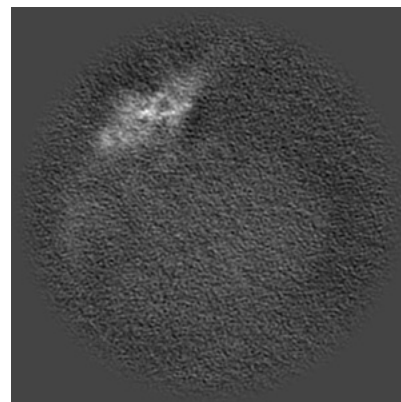
### 6.2.1 Primary map



X Index: 200

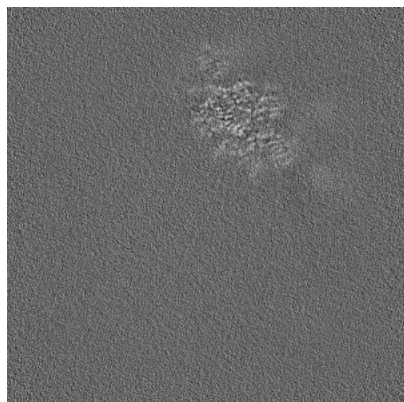


Y Index: 200

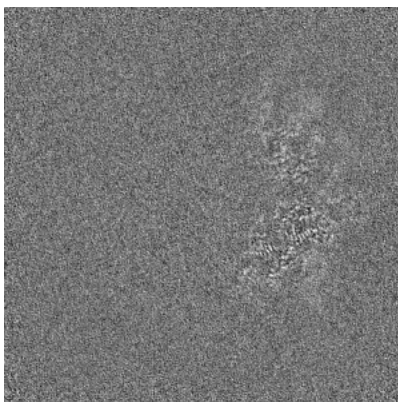


Z Index: 200

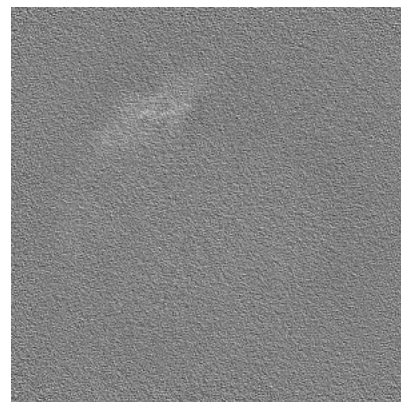
### 6.2.2 Raw map



X Index: 200



Y Index: 200



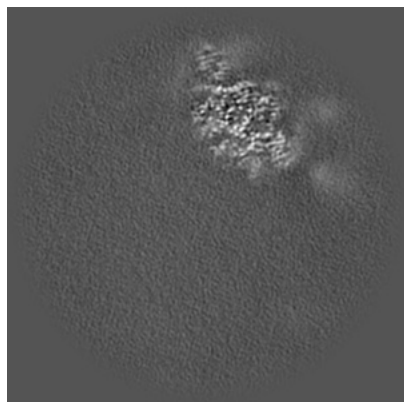
Z Index: 200

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

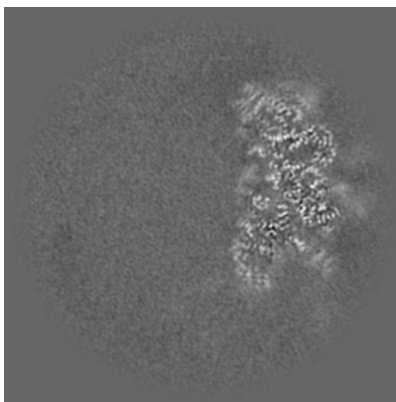


## 6.3 Largest variance slices [i](#)

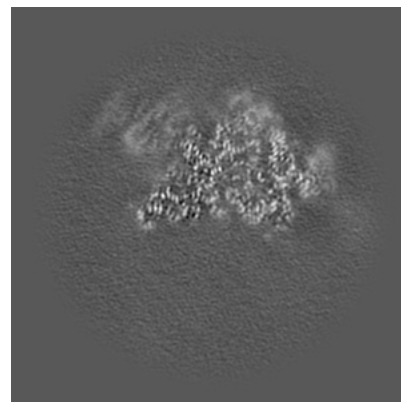
### 6.3.1 Primary map



X Index: 201

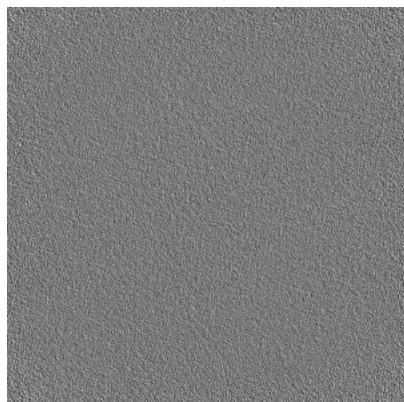


Y Index: 226

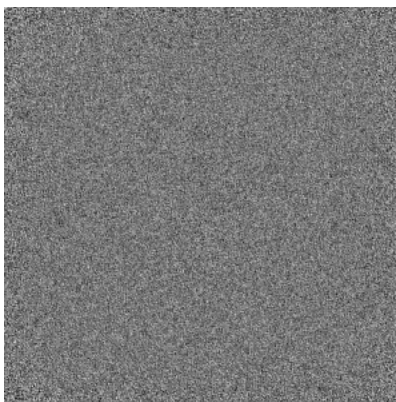


Z Index: 277

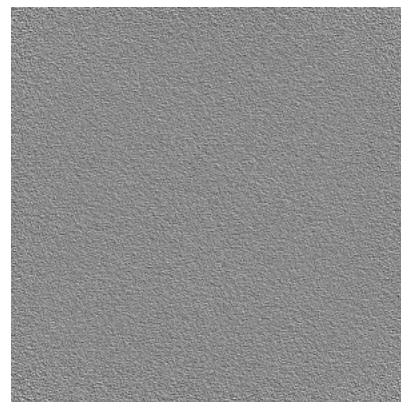
### 6.3.2 Raw map



X Index: 0



Y Index: 0

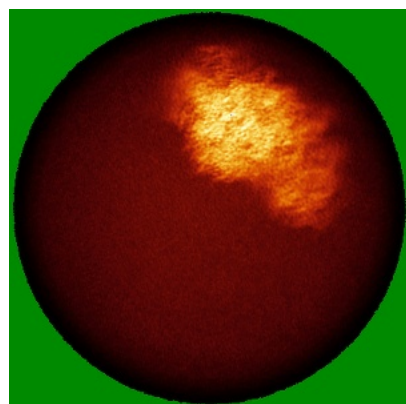


Z Index: 0

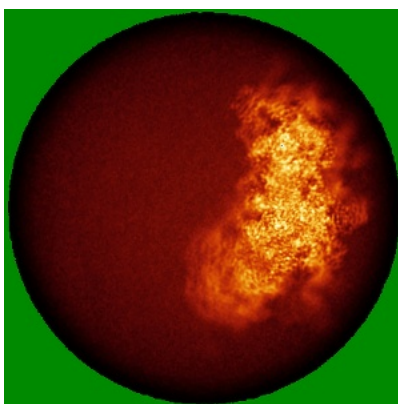
The images above show the largest variance slices of the map in three orthogonal directions.

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

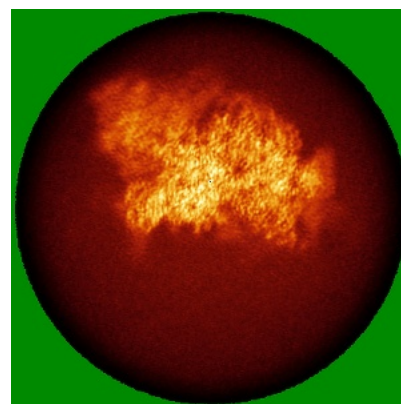
### 6.4.1 Primary map



X

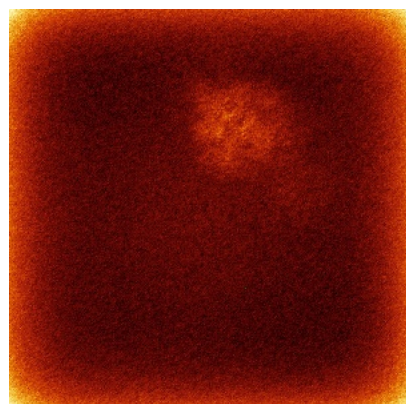


Y

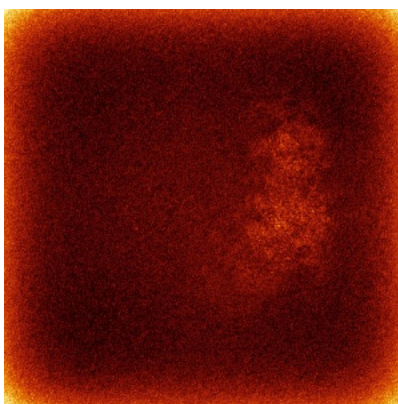


Z

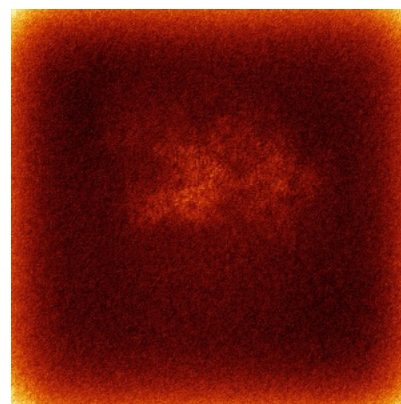
### 6.4.2 Raw map



X



Y

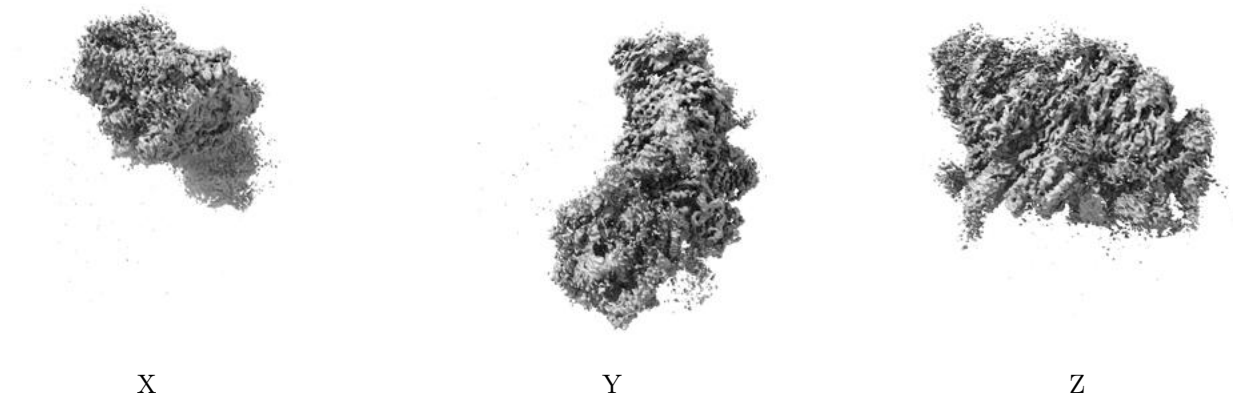


Z

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.

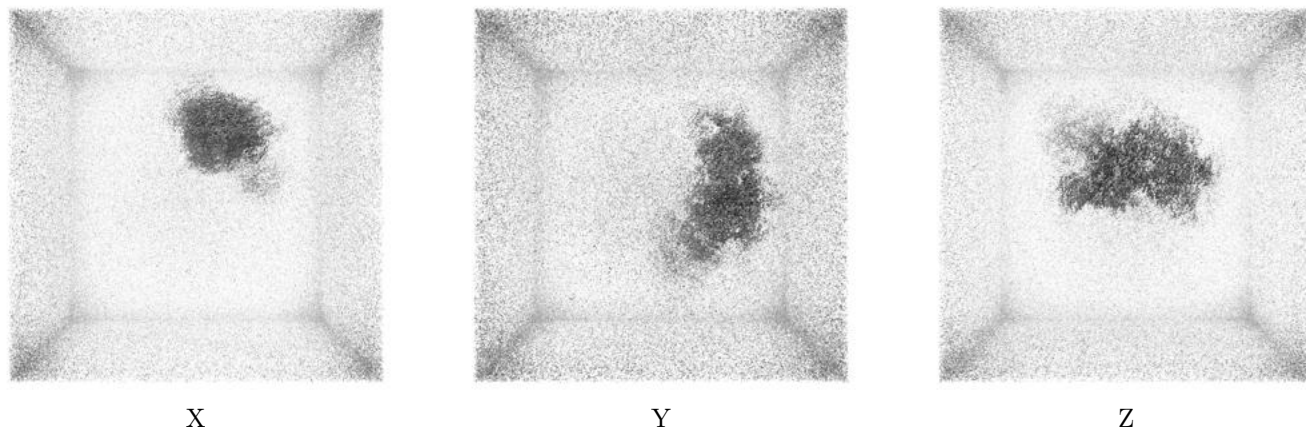
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.43. 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.

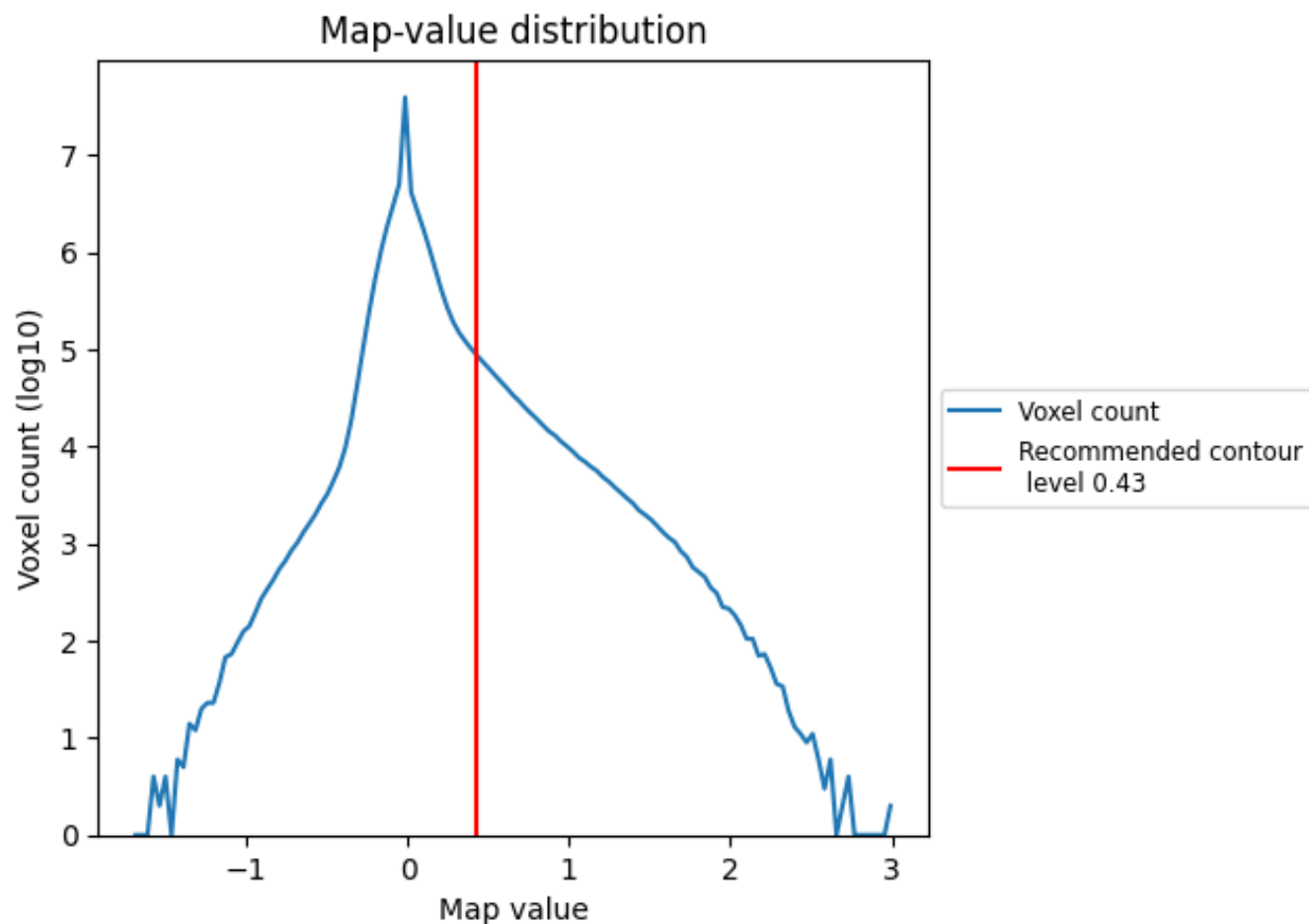
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

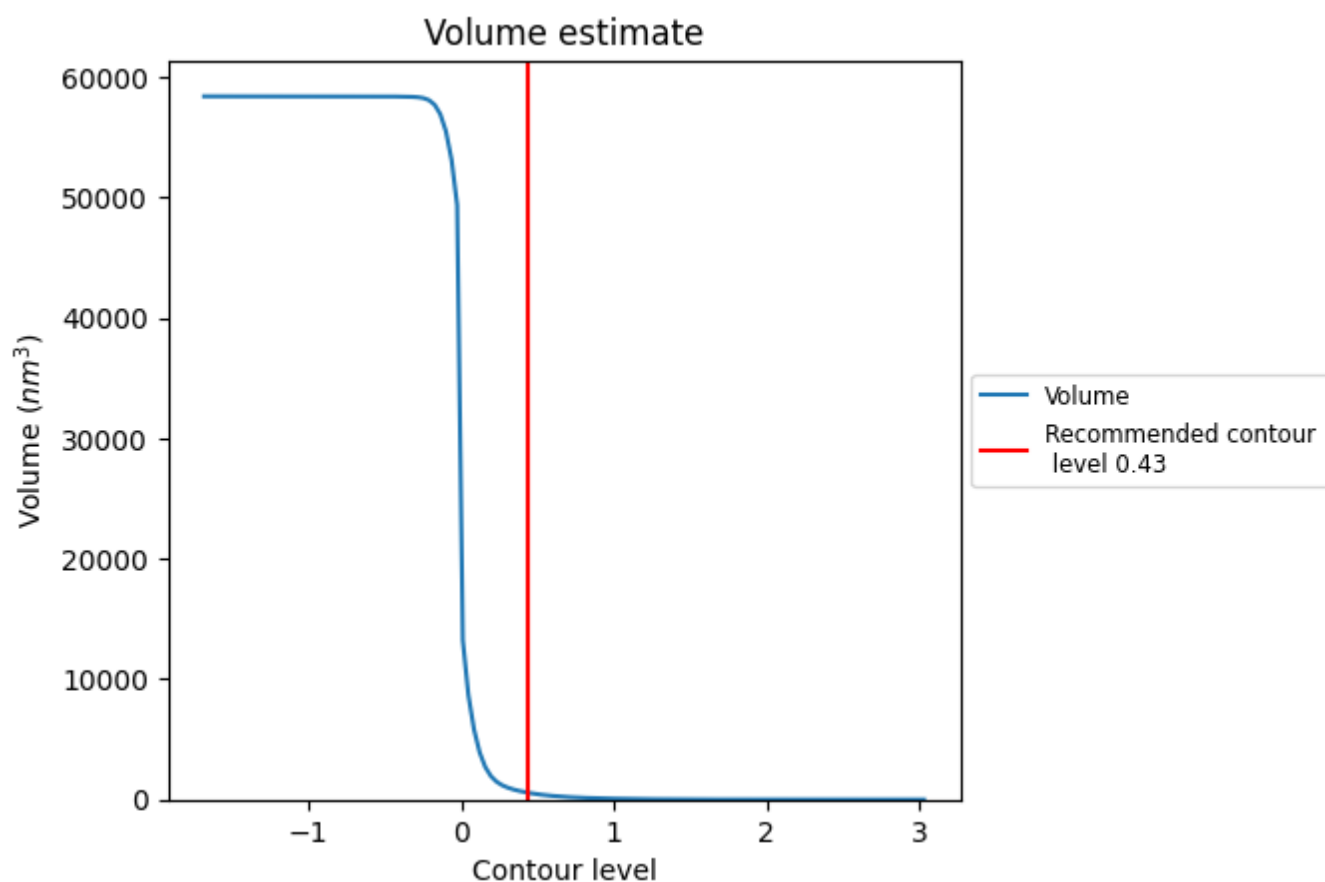
This section contains the results of statistical analysis of the map.

### 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](#)

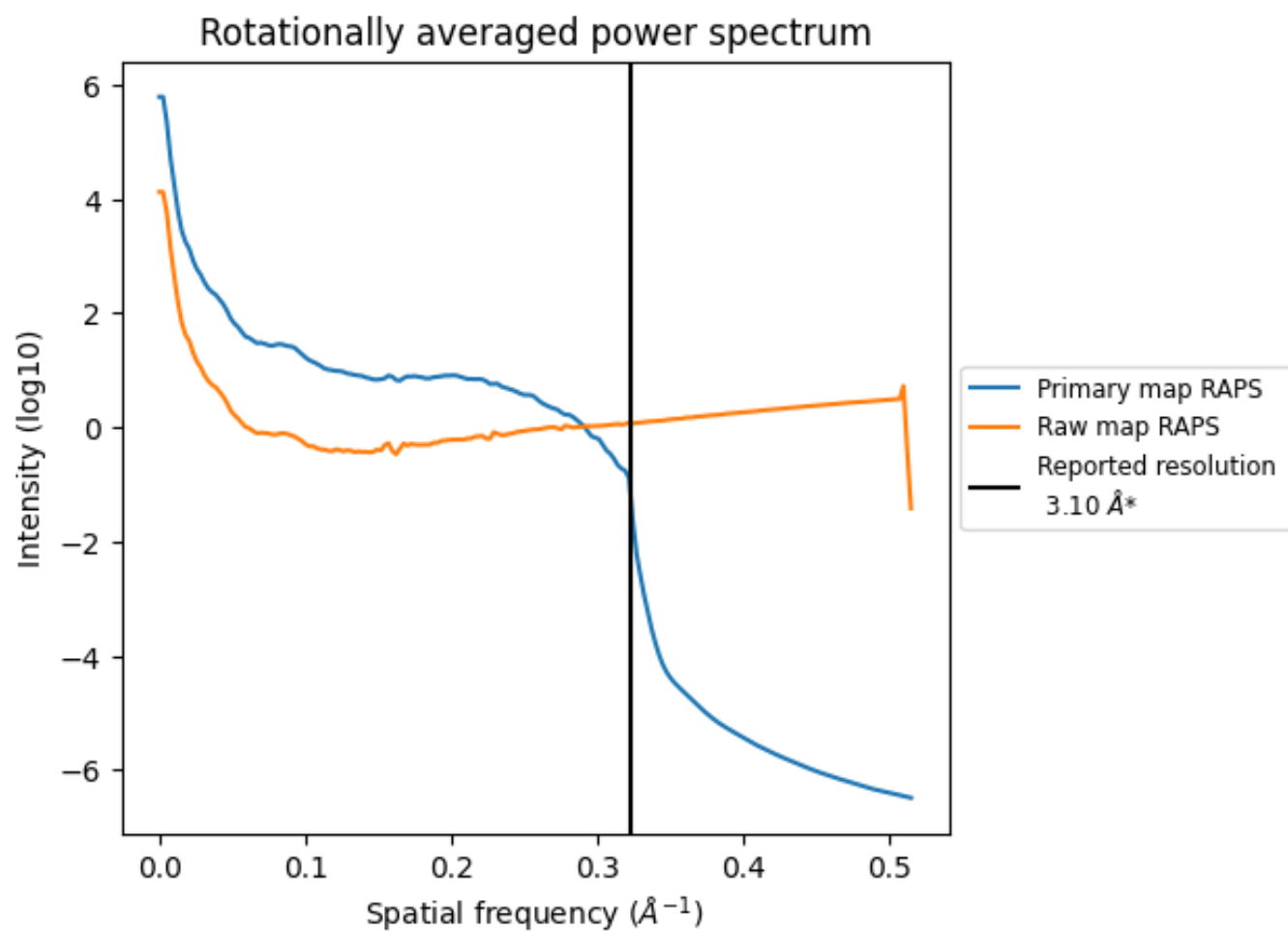


The volume at the recommended contour level is 586 nm<sup>3</sup>; this corresponds to an approximate mass of 529 kDa.

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 ⓘ

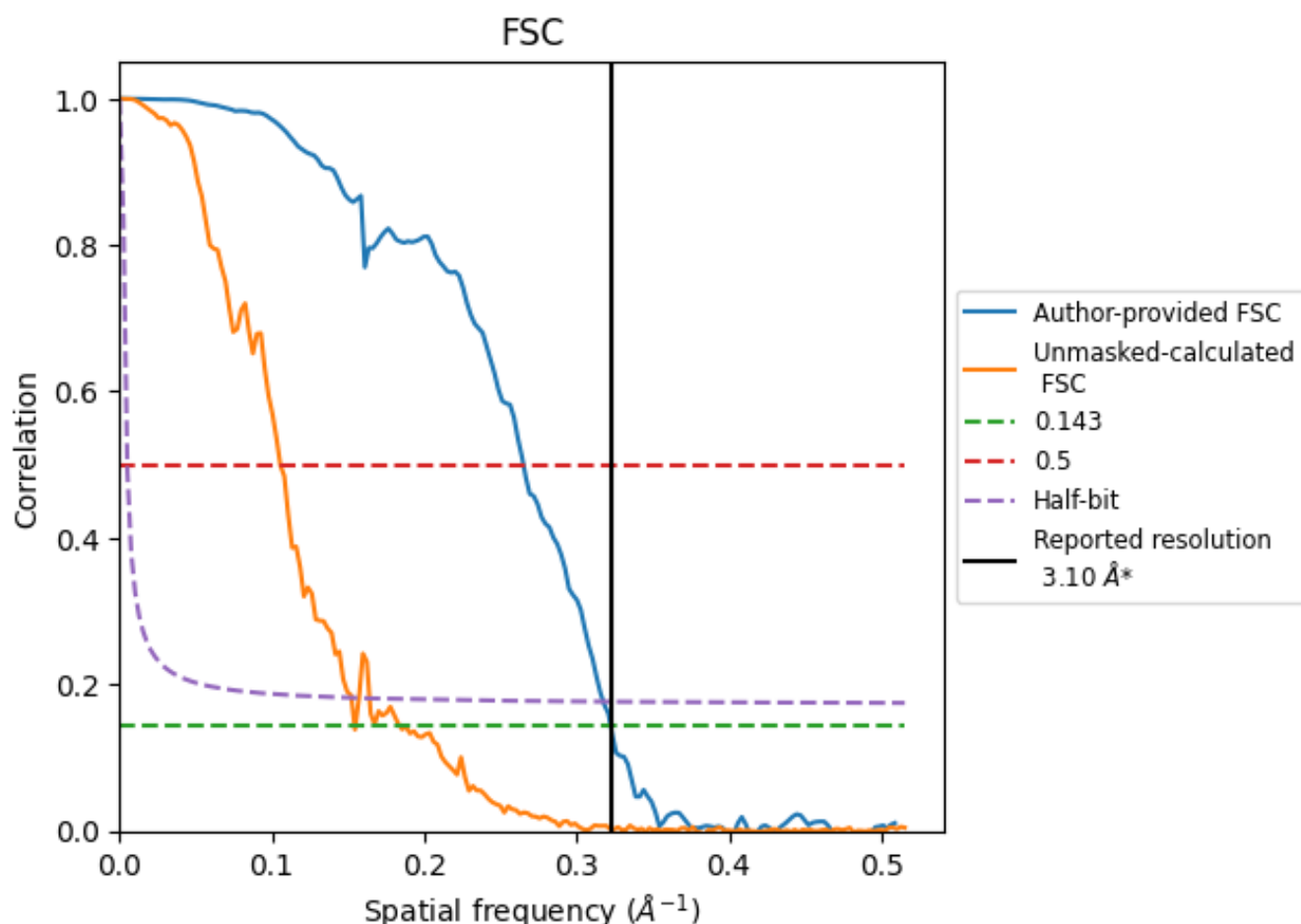


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.77	3.15
Unmasked-calculated*	6.48	9.47	6.57

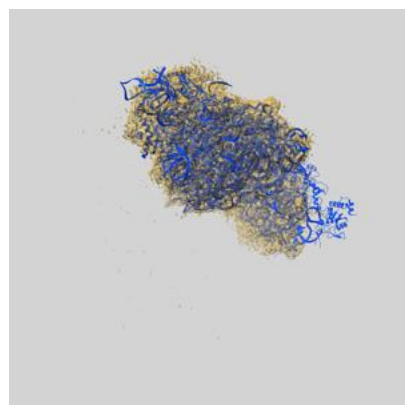
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.48 differs from the reported value 3.1 by more than 10 %



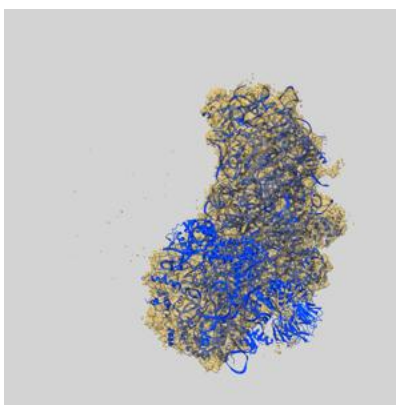
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45307 and PDB model 9C8K. Per-residue inclusion information can be found in section [3](#) on page [12](#).

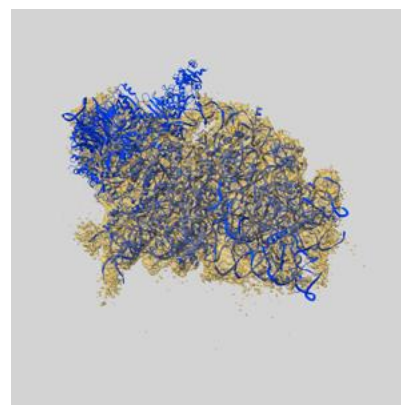
### 9.1 Map-model overlay [i](#)



X



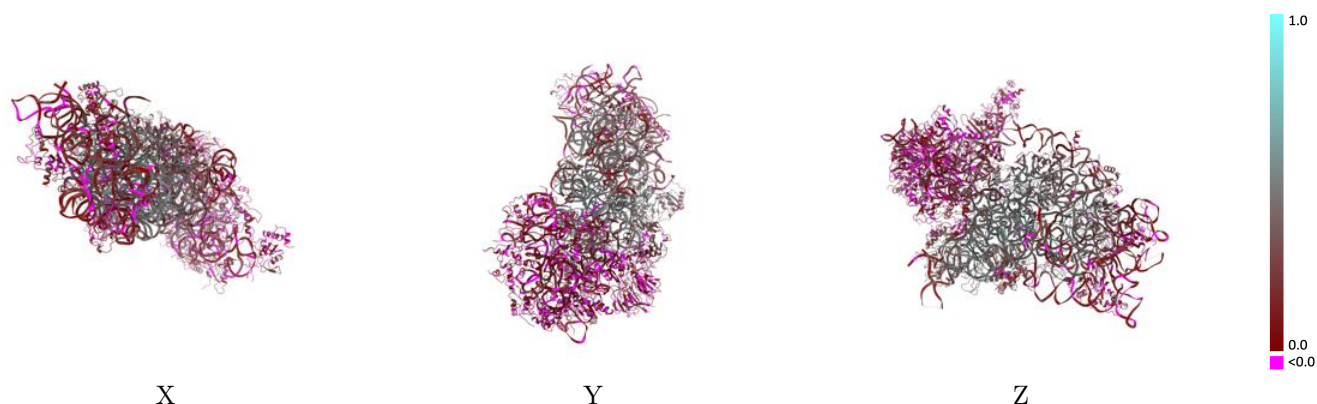
Y



Z

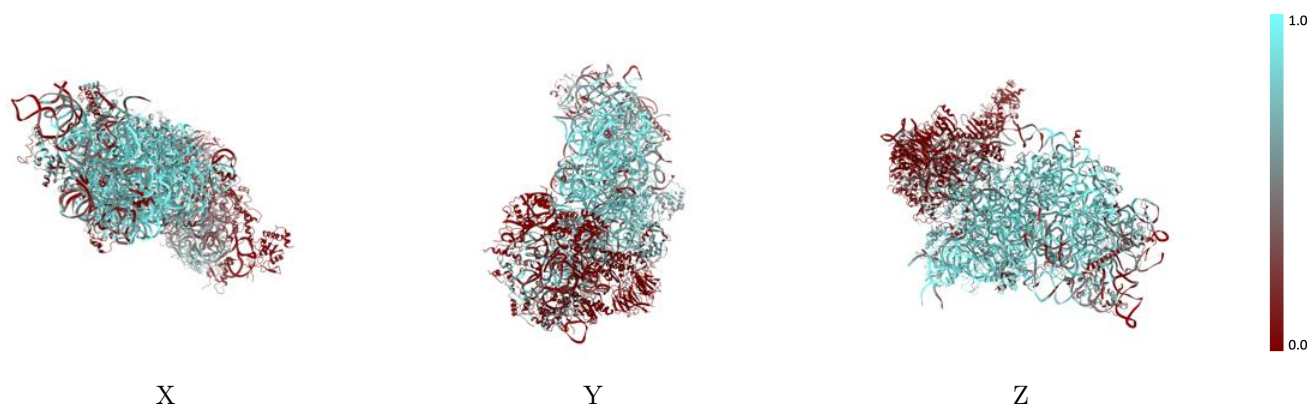
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



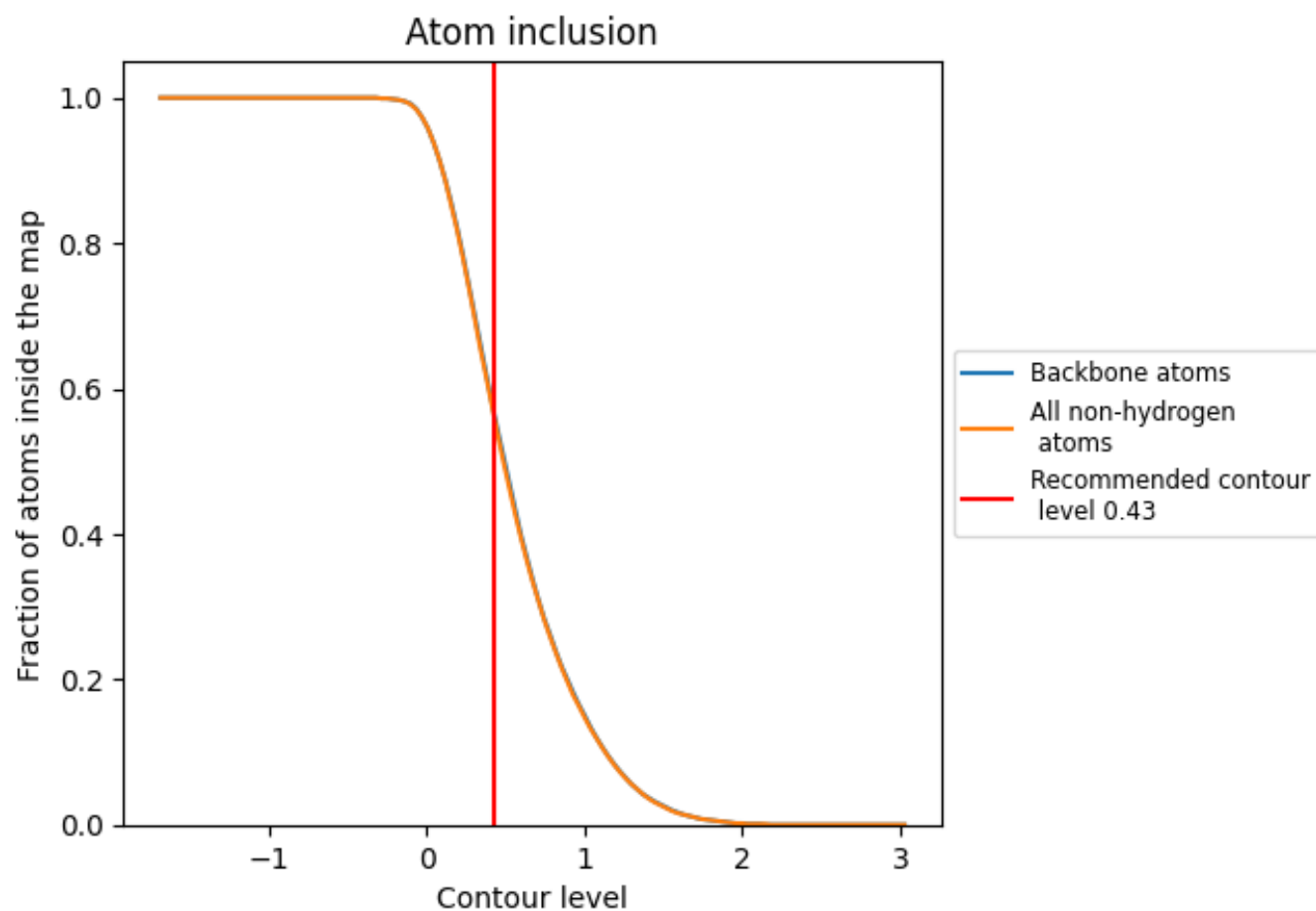
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.43).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5610	 0.2560
1	 0.6570	 0.2800
2	 0.7180	 0.1940
A	 0.5930	 0.2380
B	 0.8190	 0.4000
C	 0.7400	 0.4020
D	 0.0700	 0.1280
E	 0.8180	 0.4050
F	 0.3000	 0.0800
G	 0.3060	 0.0770
H	 0.5820	 0.2850
I	 0.5310	 0.1780
J	 0.7140	 0.3400
K	 0.0370	 0.0900
L	 0.6560	 0.3760
M	 0.0000	 0.0720
N	 0.8100	 0.4510
O	 0.7160	 0.3500
P	 0.3050	 0.1080
Q	 0.1900	 0.1120
R	 0.1010	 0.0830
S	 0.4720	 0.1330
T	 0.3280	 0.0930
U	 0.0320	 0.0800
V	 0.6830	 0.3720
W	 0.8470	 0.4820
X	 0.6800	 0.4350
Y	 0.5520	 0.2210
Z	 0.2630	 0.1080
a	 0.6630	 0.3930
b	 0.8010	 0.4010
c	 0.1910	 0.0890
d	 0.2020	 0.0940
e	 0.4290	 0.2600
f	 0.0920	 0.0660
g	 0.0080	 0.0990

