



wwPDB EM Validation Summary Report ⓘ

Jan 30, 2025 – 02:27 PM JST

PDB ID : 8WQ4
EMDB ID : EMD-37734
Title : Structural basis of translation inhibition by a valine tRNA-derived fragment
Authors : Wang, Y.H.; Zhou, J.
Deposited on : 2023-10-11
Resolution : 4.53 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

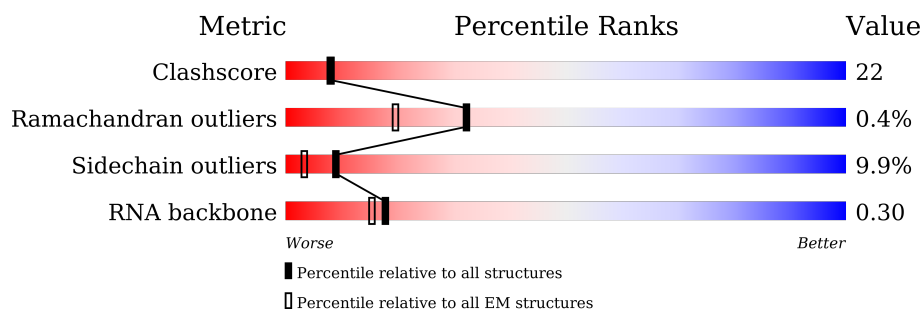
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.53 Å.

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




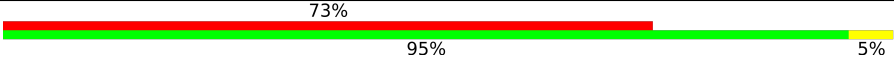
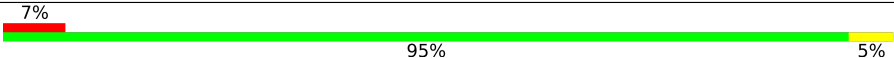
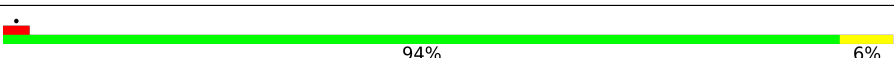
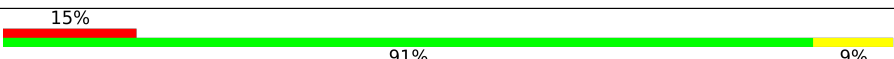
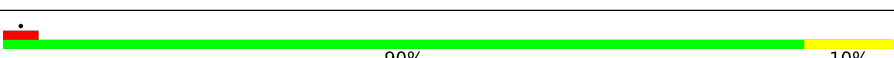
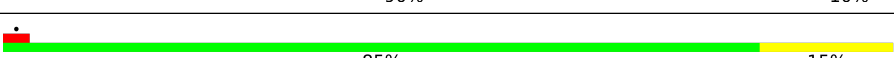
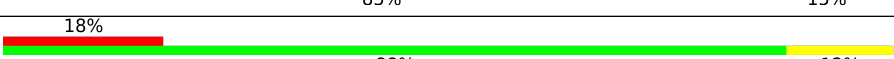

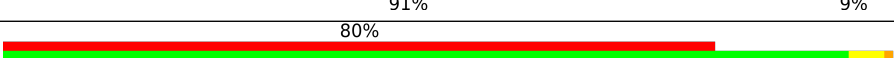


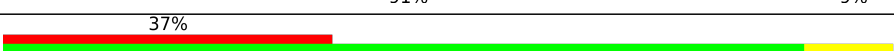
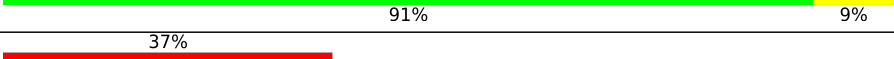
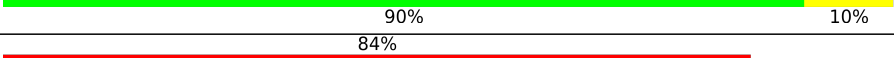

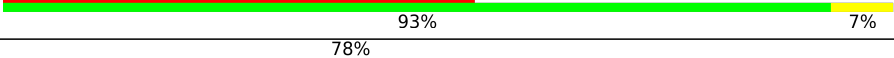
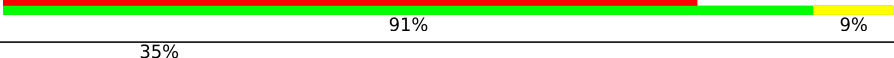
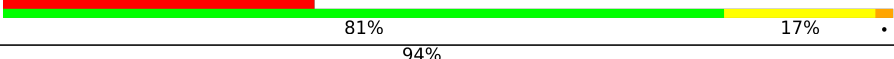
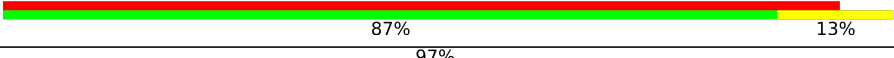
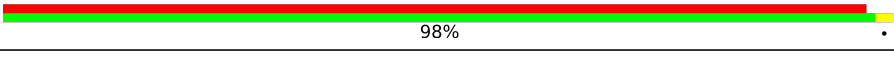
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 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	A16S	1501	<div> <div>5%</div> <div>45%</div> <div>41%</div> <div>12%</div> </div>
2	VTRF	26	<div> <div>23%</div> <div>73%</div> <div>.</div> </div>
3	AS2P	196	<div> <div>90%</div> <div>90%</div> <div>10%</div> </div>
4	AS4E	240	<div> <div>88%</div> <div>12%</div> </div>
5	AS4P	166	<div> <div>8%</div> <div>87%</div> <div>13%</div> </div>
6	AS5P	204	<div> <div>36%</div> <div>94%</div> <div>6%</div> </div>
7	AS6E	105	<div> <div>30%</div> <div>90%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
8	AS8E	126	
9	S11P	128	
10	S12P	143	
11	S15P	149	
12	S17P	111	
13	S24E	96	
14	S27E	59	
15	S3AE	189	
16	AS3P	201	
17	AS7P	193	
18	AS9P	136	
19	S10P	100	
20	S13P	147	
21	S14P	52	
22	S17E	62	
23	S19E	150	
24	S19P	115	
25	S27A	54	
26	S28E	63	
27	SL7A	123	
28	AS8P	130	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 56809 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA (1328-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A16S	1325	Total	C	N	O	P	0	0
			28462	12674	5267	9196	1325		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A16S	?	-	U	deletion	GB 2440479486
A16S	?	-	C	deletion	GB 2440479486
A16S	1450	G	-	insertion	GB 2440479486

- Molecule 2 is a RNA chain called RNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	VTRF	26	Total	C	N	O	P	0	0
			556	248	96	187	25		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AS2P	196	Total	C	N	O	S	0	0
			1587	1022	277	286	2		

- Molecule 4 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AS4E	240	Total	C	N	O	S	0	0
			1925	1238	335	348	4		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AS4P	166	Total	C	N	O	S	0	0
			1370	874	252	241	3		

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AS5P	204	Total	C	N	O	S	0	0
			1600	1028	277	287	8		

- Molecule 7 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AS6E	105	Total	C	N	O	S	0	0
			805	506	149	147	3		

- Molecule 8 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AS8E	126	Total	C	N	O	S	0	0
			993	619	187	187			

- Molecule 9 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S11P	128	Total	C	N	O	S	0	0
			960	595	190	173	2		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S12P	143	Total	C	N	O	S	0	0
			1103	701	209	189	4		

- Molecule 11 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S15P	149	Total	C	N	O	S	0	0
			1225	778	228	214	5		

- Molecule 12 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S17P	111	Total	C	N	O	S	0	0
			885	557	165	160	3		

- Molecule 13 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	S24E	96	Total	C	N	O		
			759	479	133	147	0	0

- Molecule 14 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S27E	59	Total	C	N	O	S		
			458	294	83	76	5	0	0

- Molecule 15 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S3AE	189	Total	C	N	O	S		
			1545	1004	264	276	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AS3P	201	Total	C	N	O	S		
			1576	1020	274	278	4	0	0

- Molecule 17 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AS7P	193	Total	C	N	O	S		
			1537	969	285	279	4	0	0

- Molecule 18 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS9P	136	Total	C	N	O	S		
			1096	692	200	197	7	0	0

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S10P	100	Total	C	N	O	S		
			824	522	154	142	6	0	0

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S13P	147	Total	C	N	O	S	0	0
			1204	753	230	217	4		

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S14P	52	Total	C	N	O	S	0	0
			432	273	85	69	5		

- Molecule 22 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S17E	62	Total	C	N	O		0	0
			517	326	92	99			

- Molecule 23 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S19E	150	Total	C	N	O	S	0	0
			1239	801	223	213	2		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S19P	115	Total	C	N	O	S	0	0
			969	620	181	163	5		

- Molecule 25 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S27A	54	Total	C	N	O	S	0	0
			435	274	79	76	6		

- Molecule 26 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S28E	63	Total	C	N	O		0	0
			498	308	99	91			

- Molecule 27 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SL7A	123	Total	C	N	O	S	0	0
			935	593	155	184	3		

- Molecule 28 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AS8P	130	Total	C	N	O	S	0	0
			1028	661	181	182	4		

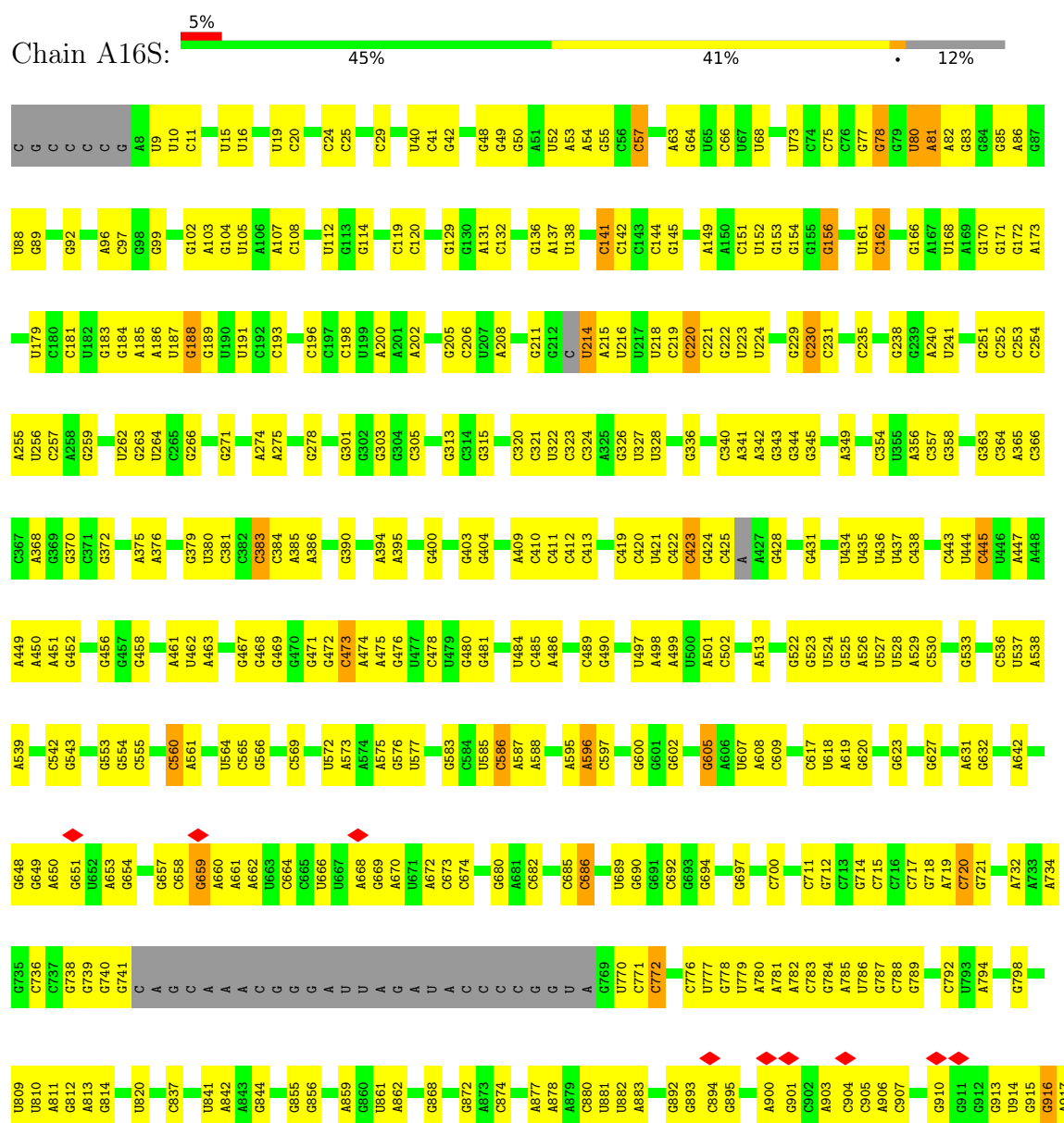
- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

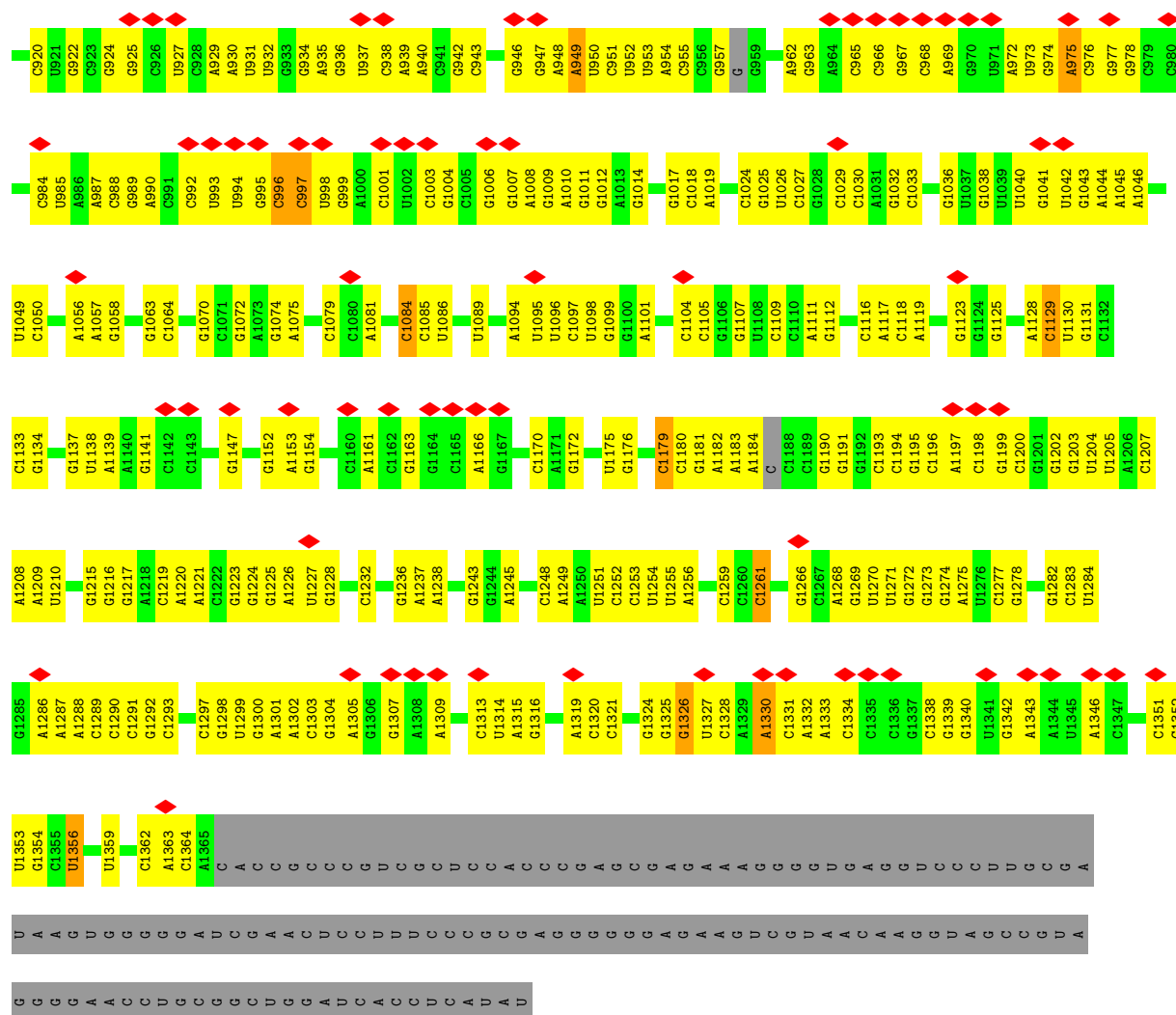
Mol	Chain	Residues	Atoms				AltConf
29	A16S	3	Total	C	N	O	0
			15	9	3	3	
29	AS2P	28	Total	C	N	O	0
			141	84	28	29	
29	AS5P	21	Total	C	N	O	0
			105	63	21	21	
29	AS8P	5	Total	C	N	O	0
			25	15	5	5	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA (1328-MER)





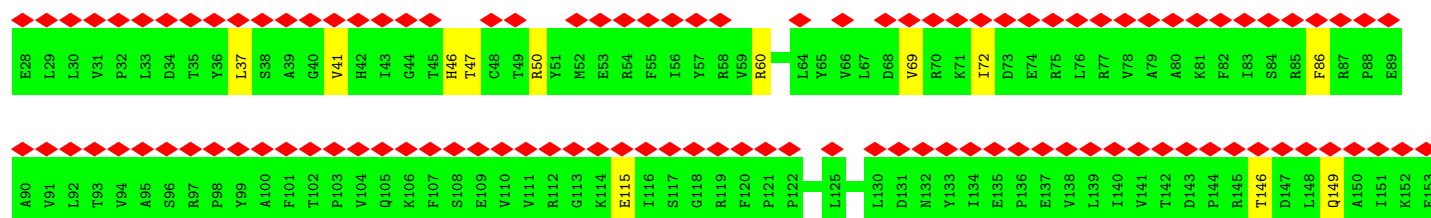
• Molecule 2: RNA (26-MER)

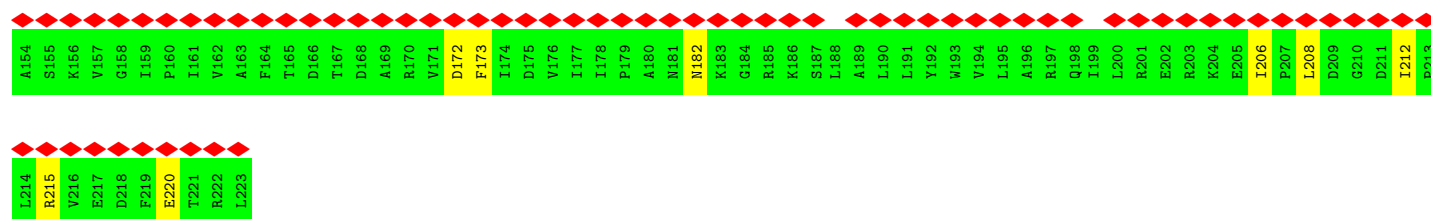
Chain VTRF: 23% 73%



• Molecule 3: 30S ribosomal protein S2

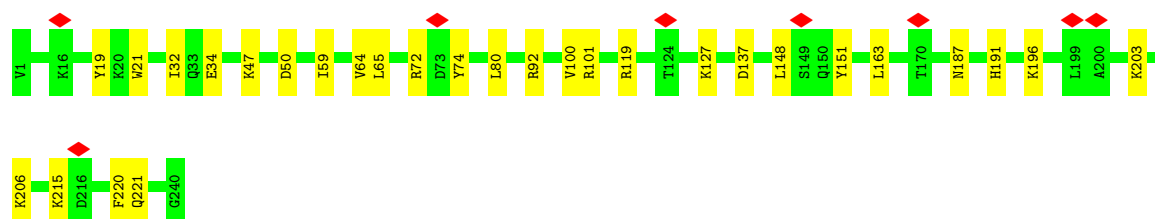
Chain AS2P: 90% 90% 10%





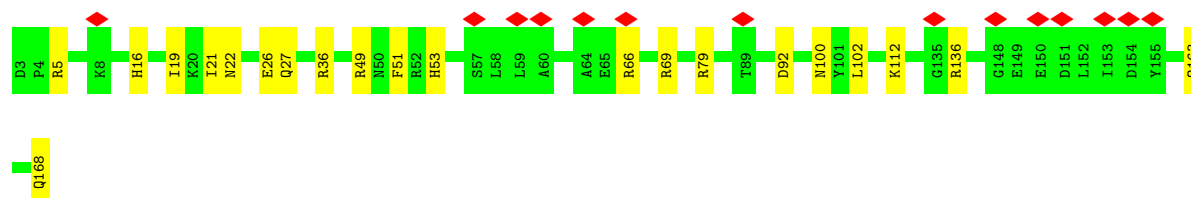
• Molecule 4: 30S ribosomal protein S4e

Chain AS4E: 88% 12%



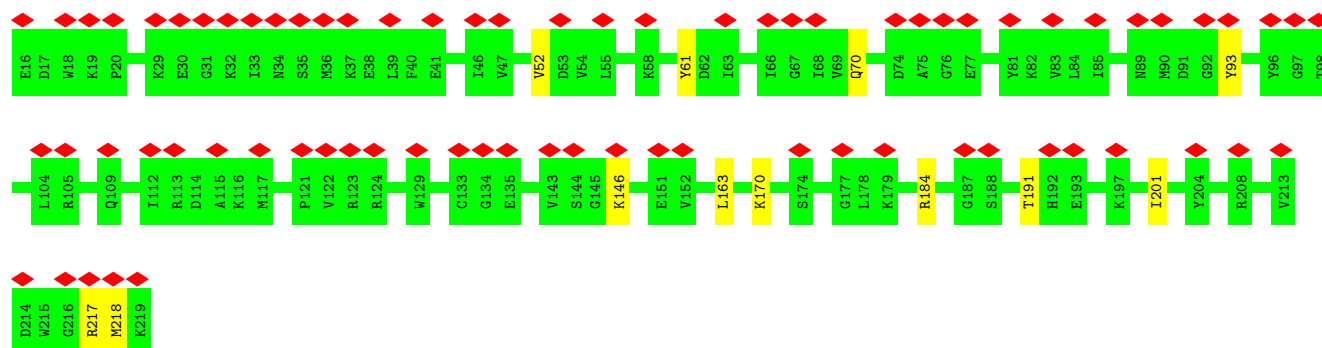
• Molecule 5: 30S ribosomal protein S4

Chain AS4P: 8% 87% 13%



• Molecule 6: 30S ribosomal protein S5

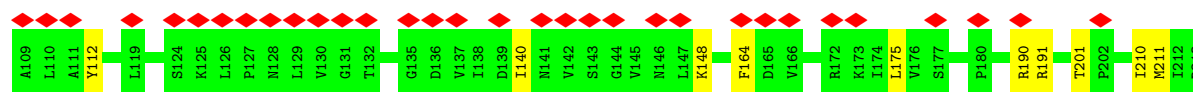
Chain AS5P: 36% 94% 6%



• Molecule 7: 30S ribosomal protein S6e

Chain AS6E: 30% 90% 10%

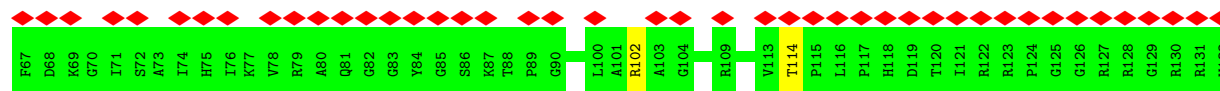
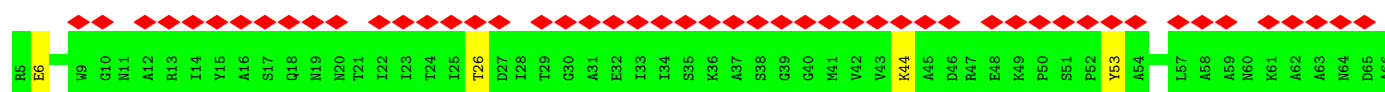
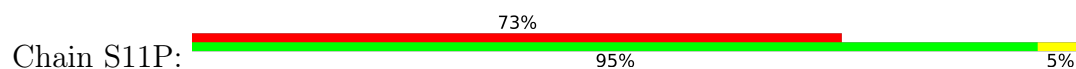




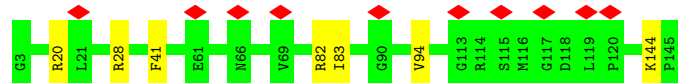
- Molecule 8: 30S ribosomal protein S8e



- Molecule 9: 30S ribosomal protein S11



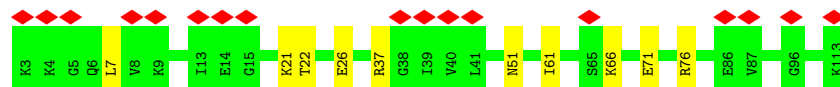
- Molecule 10: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S15

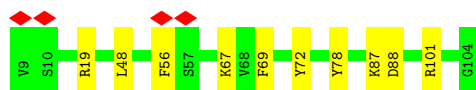


- Molecule 12: 30S ribosomal protein S17

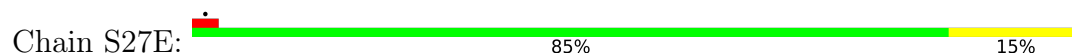


- Molecule 13: 30S ribosomal protein S24e

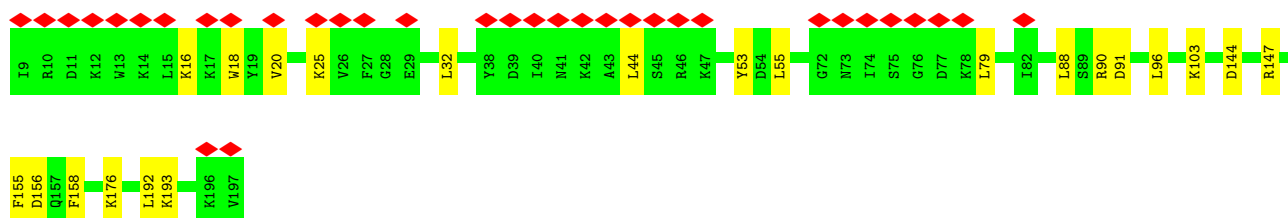




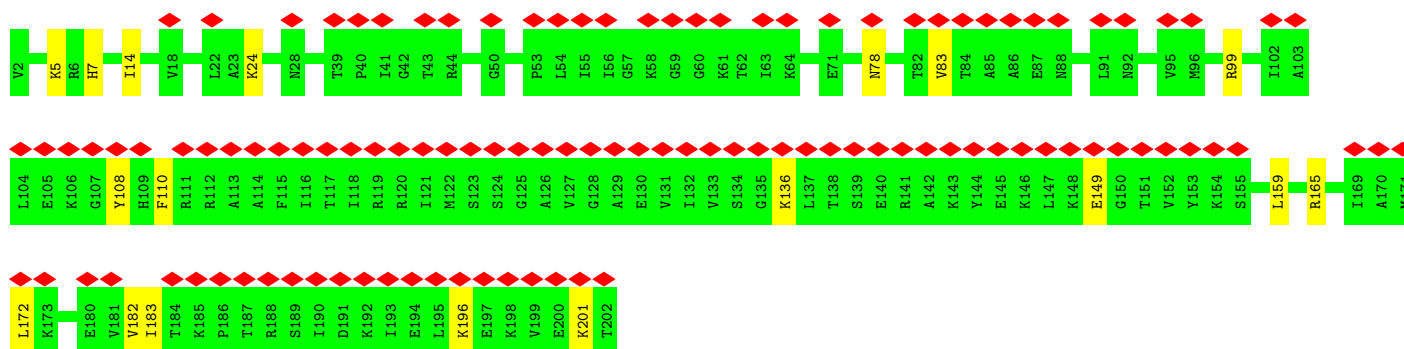
- Molecule 14: 30S ribosomal protein S27e



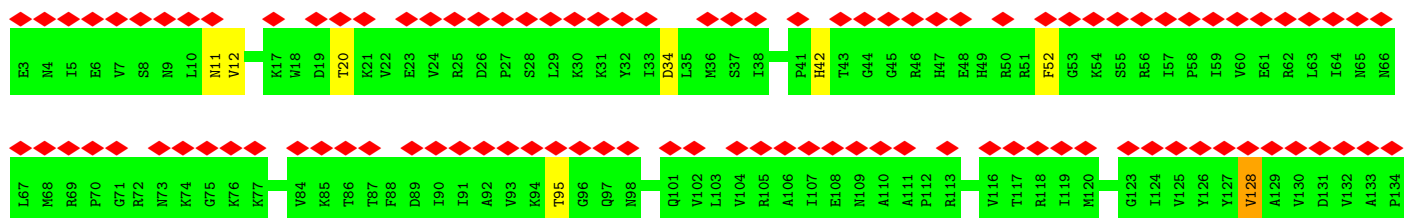
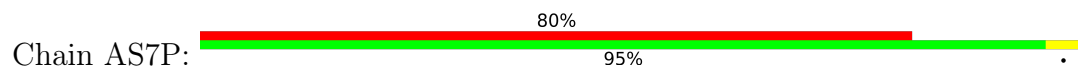
- Molecule 15: 30S ribosomal protein S3Ae

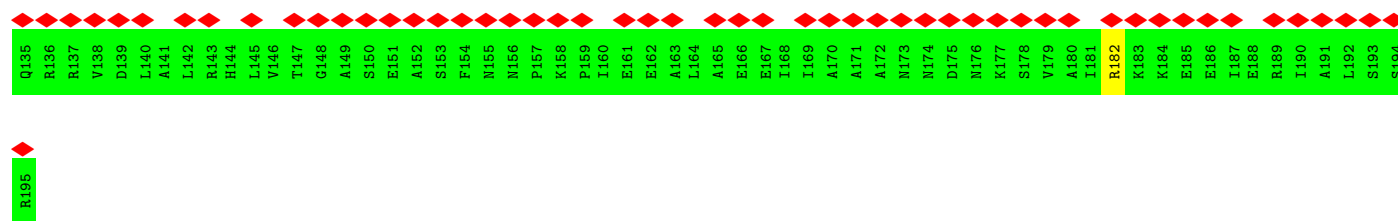


- Molecule 16: 30S ribosomal protein S3



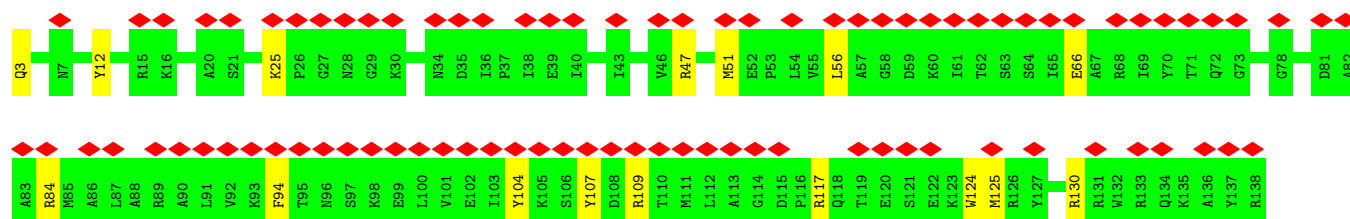
- Molecule 17: 30S ribosomal protein S7





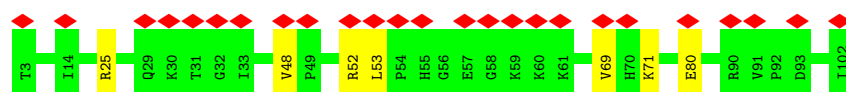
- Molecule 18: 30S ribosomal protein S9

Chain AS9P: 




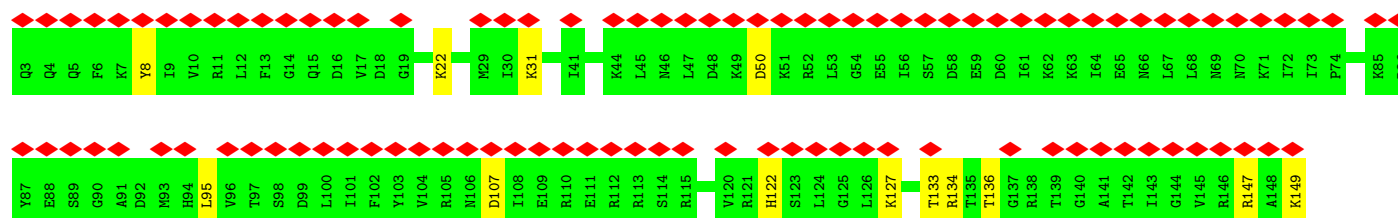
- Molecule 19: 30S ribosomal protein S10

Chain S10P: 

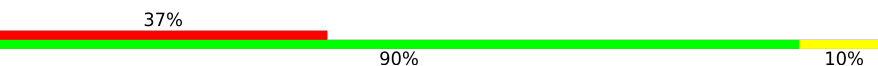


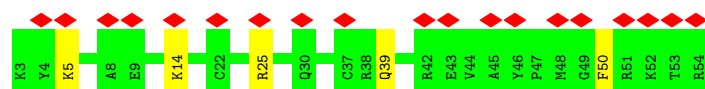
- Molecule 20: 30S ribosomal protein S13

Chain S13P: 




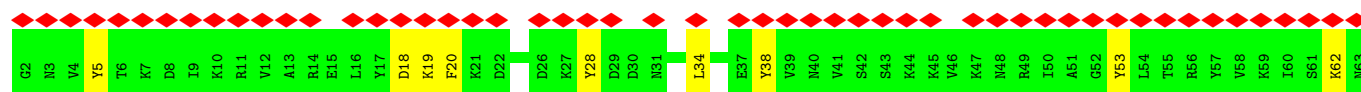
- Molecule 21: 30S ribosomal protein S14 type Z

Chain S14P: 

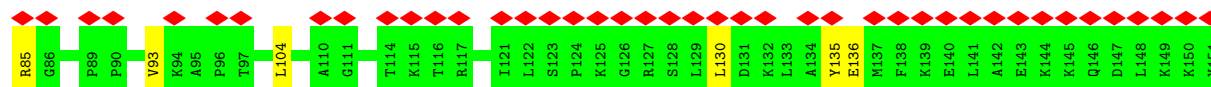
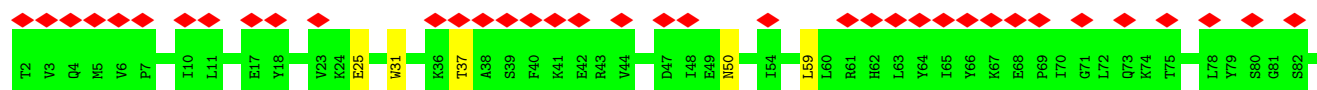


- Molecule 22: 30S ribosomal protein S17e

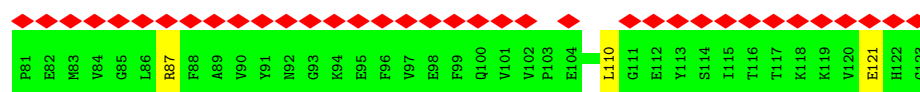
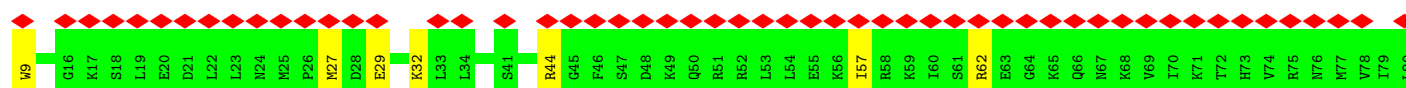
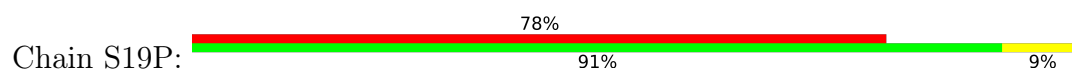
Chain S17E: 



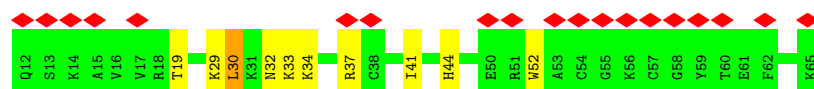
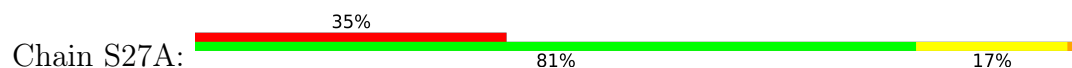
- Molecule 23: 30S ribosomal protein S19e



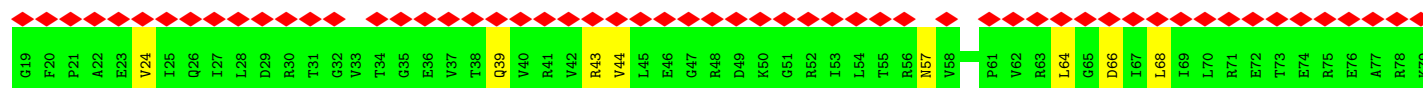
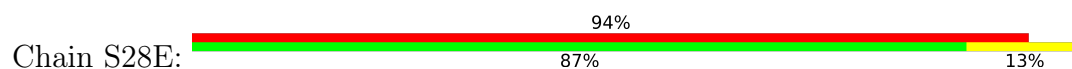
- Molecule 24: 30S ribosomal protein S19



- Molecule 25: 30S ribosomal protein S27ae

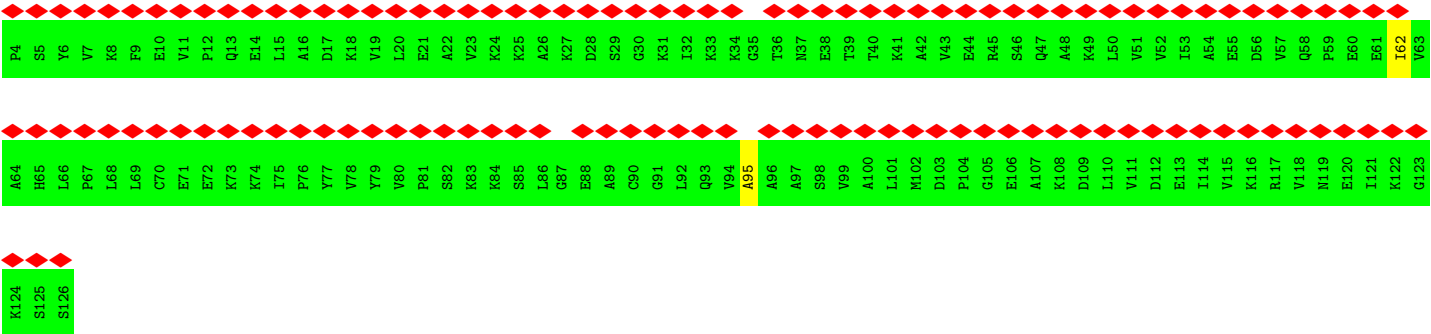


- Molecule 26: 30S ribosomal protein S28e

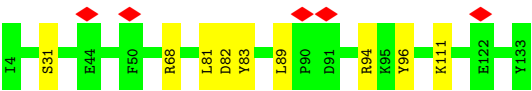


- Molecule 27: 50S ribosomal protein L7Ae





● Molecule 28: Small ribosomal subunit protein uS8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5281	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 ($e^-/\text{\AA}^2$)	26.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.079	Depositor
Minimum map value	-0.592	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.267	Depositor
Map size (\AA)	326.1, 326.1, 326.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	A16S	0.34	3/31855 (0.0%)	0.98	112/49699 (0.2%)
2	VTRF	0.47	0/621	1.03	2/968 (0.2%)
3	AS2P	0.26	0/1621	0.52	0/2202
4	AS4E	0.26	0/1956	0.52	0/2635
5	AS4P	0.25	0/1399	0.51	0/1883
6	AS5P	0.26	0/1631	0.50	0/2200
7	AS6E	0.26	0/815	0.53	0/1093
8	AS8E	0.26	0/1005	0.53	0/1342
9	S11P	0.25	0/976	0.56	0/1315
10	S12P	0.26	0/1120	0.52	0/1495
11	S15P	0.26	0/1250	0.52	0/1677
12	S17P	0.28	0/899	0.55	0/1203
13	S24E	0.26	0/769	0.49	0/1034
14	S27E	0.26	0/465	0.48	0/618
15	S3AE	0.26	0/1573	0.50	0/2115
16	AS3P	0.25	0/1599	0.50	0/2147
17	AS7P	0.24	0/1561	0.52	0/2105
18	AS9P	0.25	0/1115	0.56	0/1496
19	S10P	0.24	0/840	0.52	0/1132
20	S13P	0.24	0/1221	0.54	0/1634
21	S14P	0.25	0/441	0.57	0/583
22	S17E	0.24	0/523	0.46	0/696
23	S19E	0.25	0/1267	0.49	0/1705
24	S19P	0.25	0/986	0.53	0/1310
25	S27A	0.29	0/444	0.60	1/590 (0.2%)
26	S28E	0.24	0/500	0.62	0/669
27	SL7A	0.24	0/946	0.46	0/1272
28	AS8P	0.27	0/1046	0.51	0/1410
All	All	0.31	3/60444 (0.0%)	0.82	115/88228 (0.1%)

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
4	AS4E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A16S	80	U	O3'-P	6.24	1.68	1.61
1	A16S	78	G	O3'-P	5.62	1.67	1.61
1	A16S	596	A	O3'-P	5.20	1.67	1.61

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	81	A	C4'-C3'-O3'	12.78	138.55	113.00
1	A16S	1261	C	N1-C2-O2	12.23	126.24	118.90
1	A16S	80	U	C4'-C3'-O3'	11.97	136.95	113.00
1	A16S	29	C	N3-C2-O2	-11.09	114.14	121.90
1	A16S	29	C	N1-C2-O2	10.70	125.32	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AS4E	163	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A16S	28462	0	0	0	0
2	VTRF	556	0	0	0	0
3	AS2P	1587	0	0	0	0
4	AS4E	1925	0	0	0	0
5	AS4P	1370	0	0	0	0
6	AS5P	1600	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AS6E	805	0	0	0	0
8	AS8E	993	0	0	0	0
9	S11P	960	0	0	0	0
10	S12P	1103	0	0	0	0
11	S15P	1225	0	0	0	0
12	S17P	885	0	0	0	0
13	S24E	759	0	0	0	0
14	S27E	458	0	0	0	0
15	S3AE	1545	0	0	0	0
16	AS3P	1576	0	0	0	0
17	AS7P	1537	0	0	0	0
18	AS9P	1096	0	0	0	0
19	S10P	824	0	0	0	0
20	S13P	1204	0	0	0	0
21	S14P	432	0	0	0	0
22	S17E	517	0	0	0	0
23	S19E	1239	0	0	0	0
24	S19P	969	0	0	0	0
25	S27A	435	0	0	0	0
26	S28E	498	0	0	0	0
27	SL7A	935	0	0	0	0
28	AS8P	1028	0	0	0	0
29	A16S	15	0	0	0	0
29	AS2P	141	0	0	0	0
29	AS5P	105	0	0	0	0
29	AS8P	25	0	0	0	0
All	All	56809	0	0	0	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 22.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
3	AS2P	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
4	AS4E	238/240 (99%)	222 (93%)	16 (7%)	0	100	100
5	AS4P	164/166 (99%)	147 (90%)	17 (10%)	0	100	100
6	AS5P	202/204 (99%)	189 (94%)	13 (6%)	0	100	100
7	AS6E	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
8	AS8E	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
9	S11P	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
10	S12P	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
11	S15P	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
12	S17P	109/111 (98%)	107 (98%)	2 (2%)	0	100	100
13	S24E	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
14	S27E	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
15	S3AE	187/189 (99%)	168 (90%)	19 (10%)	0	100	100
16	AS3P	199/201 (99%)	180 (90%)	17 (8%)	2 (1%)	13	48
17	AS7P	191/193 (99%)	162 (85%)	28 (15%)	1 (0%)	25	64
18	AS9P	134/136 (98%)	115 (86%)	19 (14%)	0	100	100
19	S10P	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
20	S13P	145/147 (99%)	134 (92%)	10 (7%)	1 (1%)	19	56
21	S14P	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	6	32
22	S17E	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
23	S19E	148/150 (99%)	134 (90%)	14 (10%)	0	100	100
24	S19P	113/115 (98%)	105 (93%)	7 (6%)	1 (1%)	14	51
25	S27A	52/54 (96%)	42 (81%)	7 (14%)	3 (6%)	1	14
26	S28E	61/63 (97%)	51 (84%)	8 (13%)	2 (3%)	3	21
27	SL7A	121/123 (98%)	111 (92%)	9 (7%)	1 (1%)	16	54
28	AS8P	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
All	All	3386/3438 (98%)	3081 (91%)	293 (9%)	12 (0%)	32	68

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	AS3P	83	VAL
17	AS7P	128	VAL
21	S14P	5	LYS
16	AS3P	183	ILE
26	S28E	44	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	
3	AS2P	174/174 (100%)	154 (88%)	20 (12%)	4	17
4	AS4E	210/210 (100%)	182 (87%)	28 (13%)	3	15
5	AS4P	149/149 (100%)	128 (86%)	21 (14%)	3	14
6	AS5P	174/174 (100%)	162 (93%)	12 (7%)	13	33
7	AS6E	88/88 (100%)	78 (89%)	10 (11%)	4	17
8	AS8E	106/106 (100%)	92 (87%)	14 (13%)	3	15
9	S11P	94/94 (100%)	88 (94%)	6 (6%)	14	36
10	S12P	116/116 (100%)	109 (94%)	7 (6%)	16	38
11	S15P	133/133 (100%)	124 (93%)	9 (7%)	13	34
12	S17P	97/97 (100%)	87 (90%)	10 (10%)	6	20
13	S24E	84/84 (100%)	74 (88%)	10 (12%)	4	17
14	S27E	51/51 (100%)	42 (82%)	9 (18%)	1	9
15	S3AE	170/170 (100%)	148 (87%)	22 (13%)	3	15
16	AS3P	165/165 (100%)	149 (90%)	16 (10%)	6	22
17	AS7P	166/166 (100%)	157 (95%)	9 (5%)	18	40
18	AS9P	113/113 (100%)	97 (86%)	16 (14%)	2	14
19	S10P	92/92 (100%)	85 (92%)	7 (8%)	11	30
20	S13P	129/129 (100%)	117 (91%)	12 (9%)	7	23
21	S14P	45/45 (100%)	41 (91%)	4 (9%)	8	25
22	S17E	57/57 (100%)	48 (84%)	9 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	S19E	134/134 (100%)	123 (92%)	11 (8%)	9	28
24	S19P	106/106 (100%)	97 (92%)	9 (8%)	8	27
25	S27A	47/47 (100%)	40 (85%)	7 (15%)	2	12
26	S28E	54/54 (100%)	48 (89%)	6 (11%)	5	18
27	SL7A	104/104 (100%)	103 (99%)	1 (1%)	73	81
28	AS8P	111/111 (100%)	102 (92%)	9 (8%)	9	29
All	All	2969/2969 (100%)	2675 (90%)	294 (10%)	9	21

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	S13P	122	HIS
28	AS8P	68	ARG
21	S14P	14	LYS
23	S19E	135	TYR
8	AS8E	69	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A16S	1320/1501 (87%)	611 (46%)	51 (3%)
2	VTRF	25/26 (96%)	20 (80%)	2 (8%)
All	All	1345/1527 (88%)	631 (46%)	53 (3%)

5 of 631 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A16S	9	U
1	A16S	10	U
1	A16S	11	C
1	A16S	15	U
1	A16S	16	U

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A16S	595	A
1	A16S	965	C
1	A16S	1272	G
1	A16S	650	A
1	A16S	880	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](#)

Of 57 ligands modelled in this entry, 57 are unknown - 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](#)

There are no chain breaks in this entry.

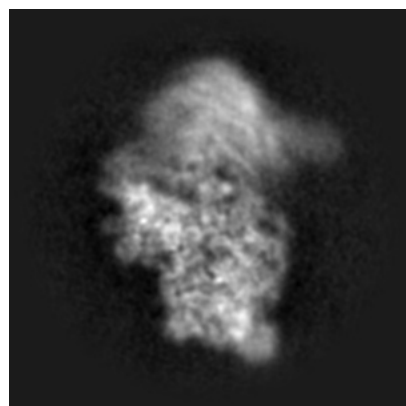
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37734. These allow visual inspection of the internal detail of the map and identification of artifacts.

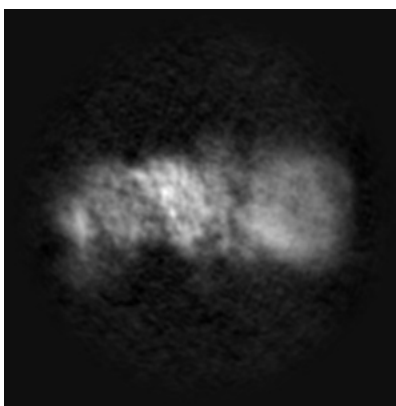
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

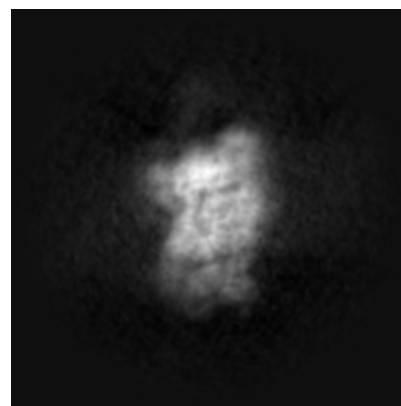
6.1.1 Primary map



X

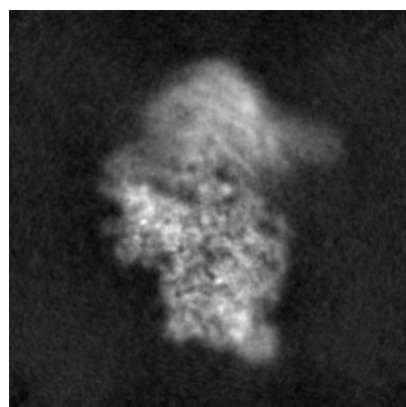


Y

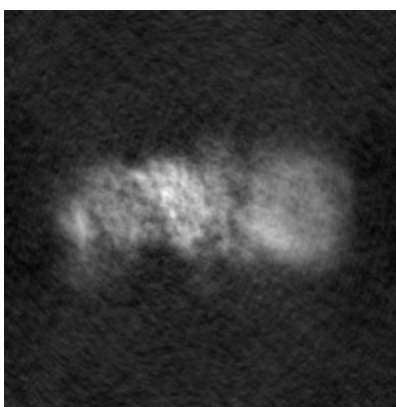


Z

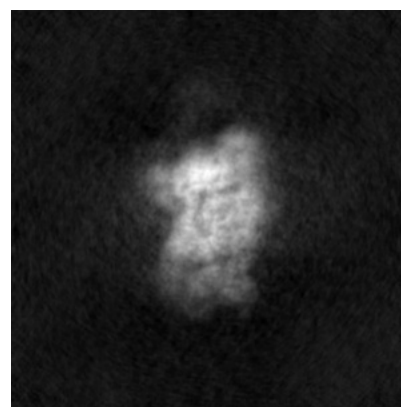
6.1.2 Raw map



X



Y

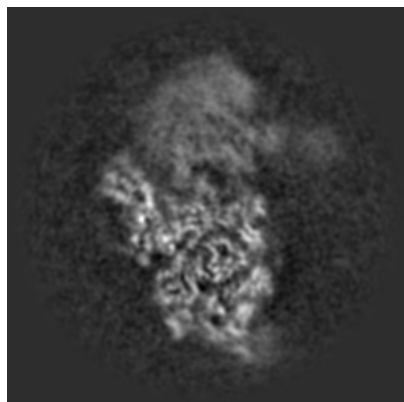


Z

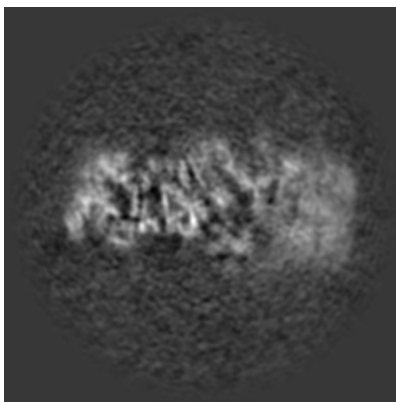
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

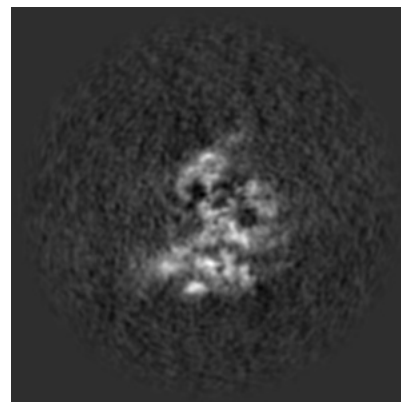
6.2.1 Primary map



X Index: 150

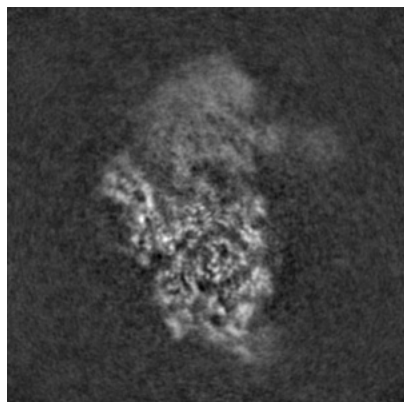


Y Index: 150

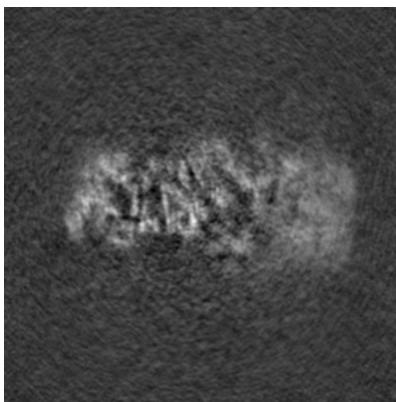


Z Index: 150

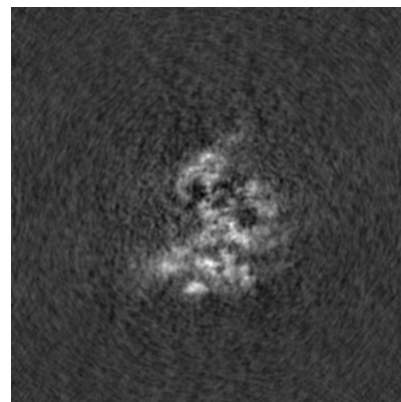
6.2.2 Raw map



X Index: 150



Y Index: 150

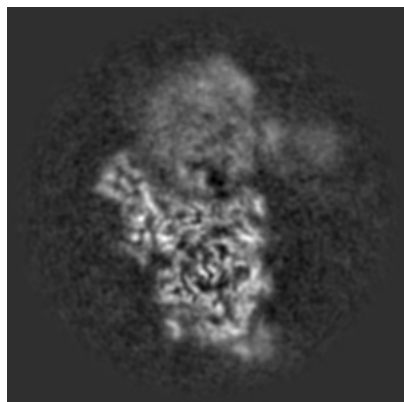


Z Index: 150

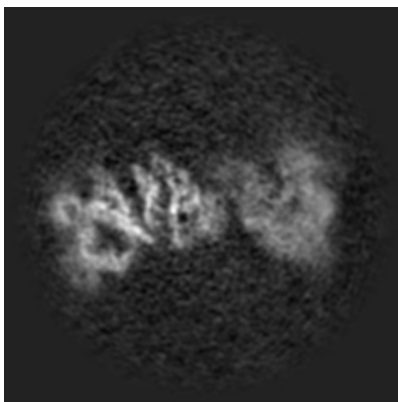
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

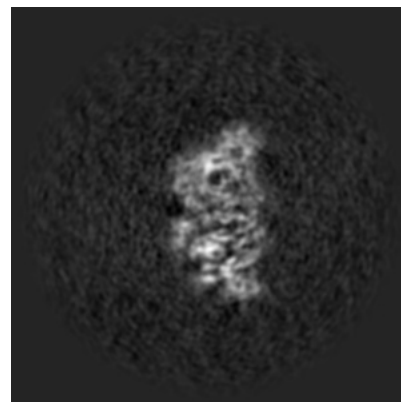
6.3.1 Primary map



X Index: 147

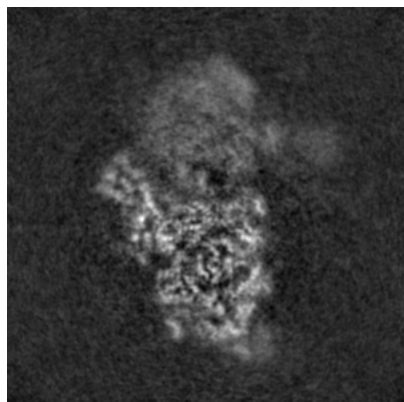


Y Index: 178

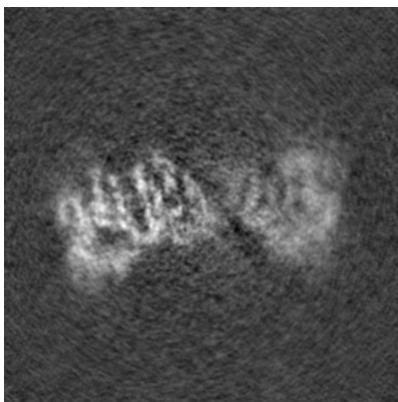


Z Index: 126

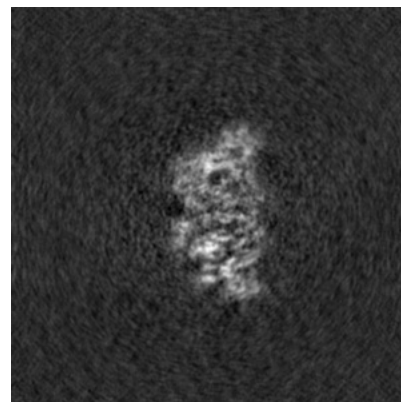
6.3.2 Raw map



X Index: 148



Y Index: 174

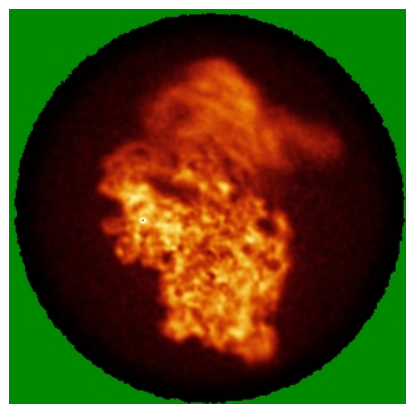


Z Index: 126

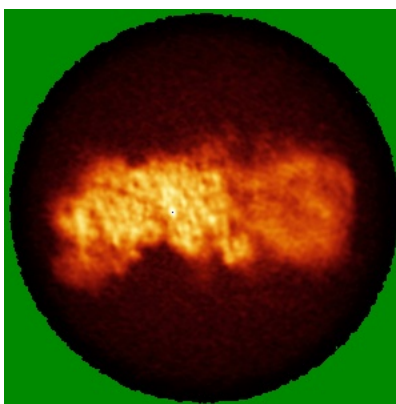
The images above show the largest variance slices of the map in three orthogonal directions.

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

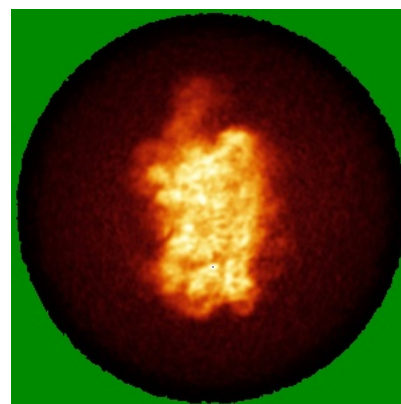
6.4.1 Primary map



X

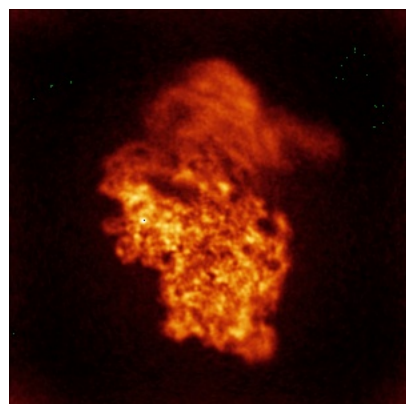


Y

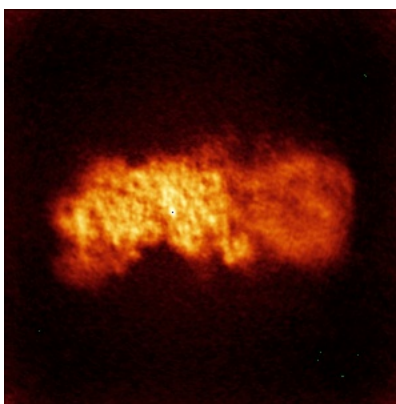


Z

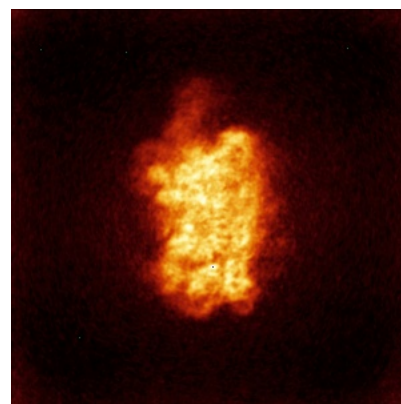
6.4.2 Raw map



X



Y

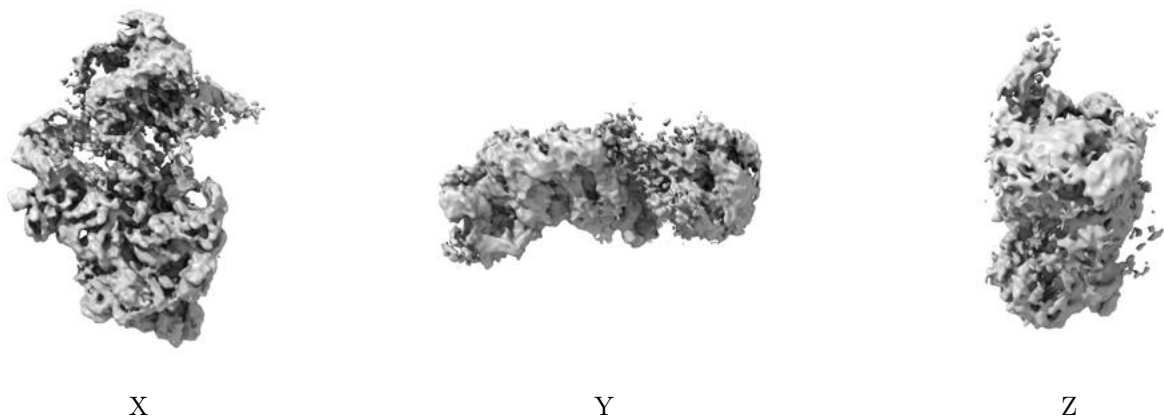


Z

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.

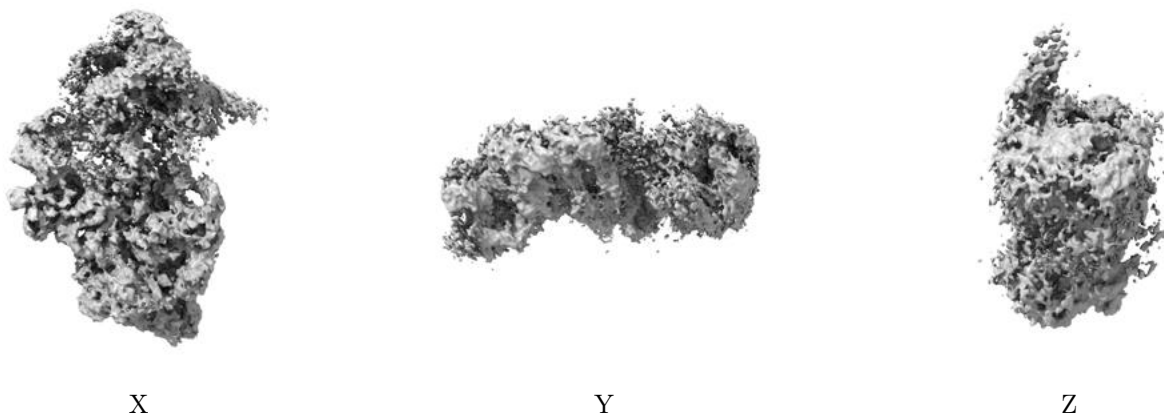
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.267. 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.

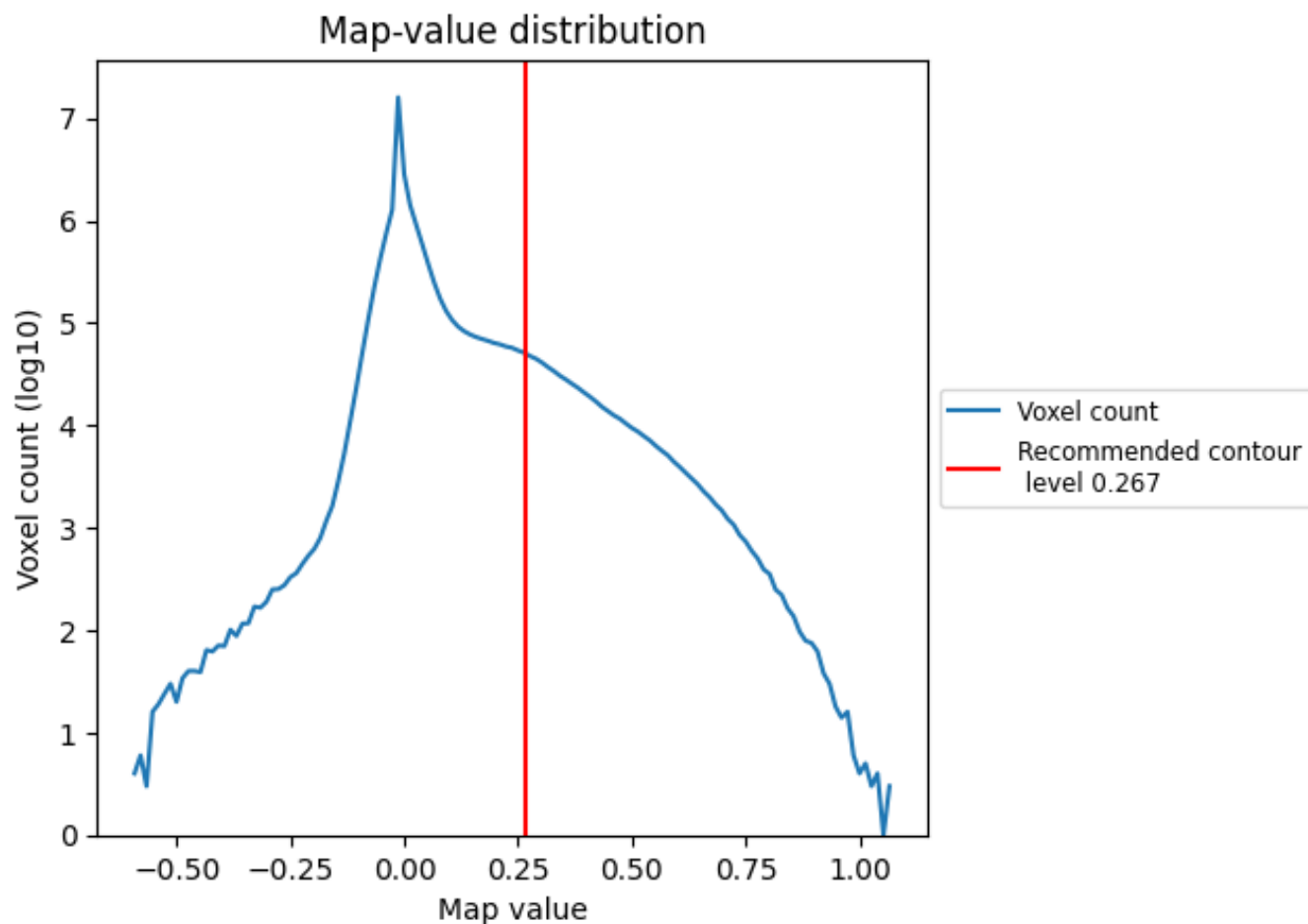
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

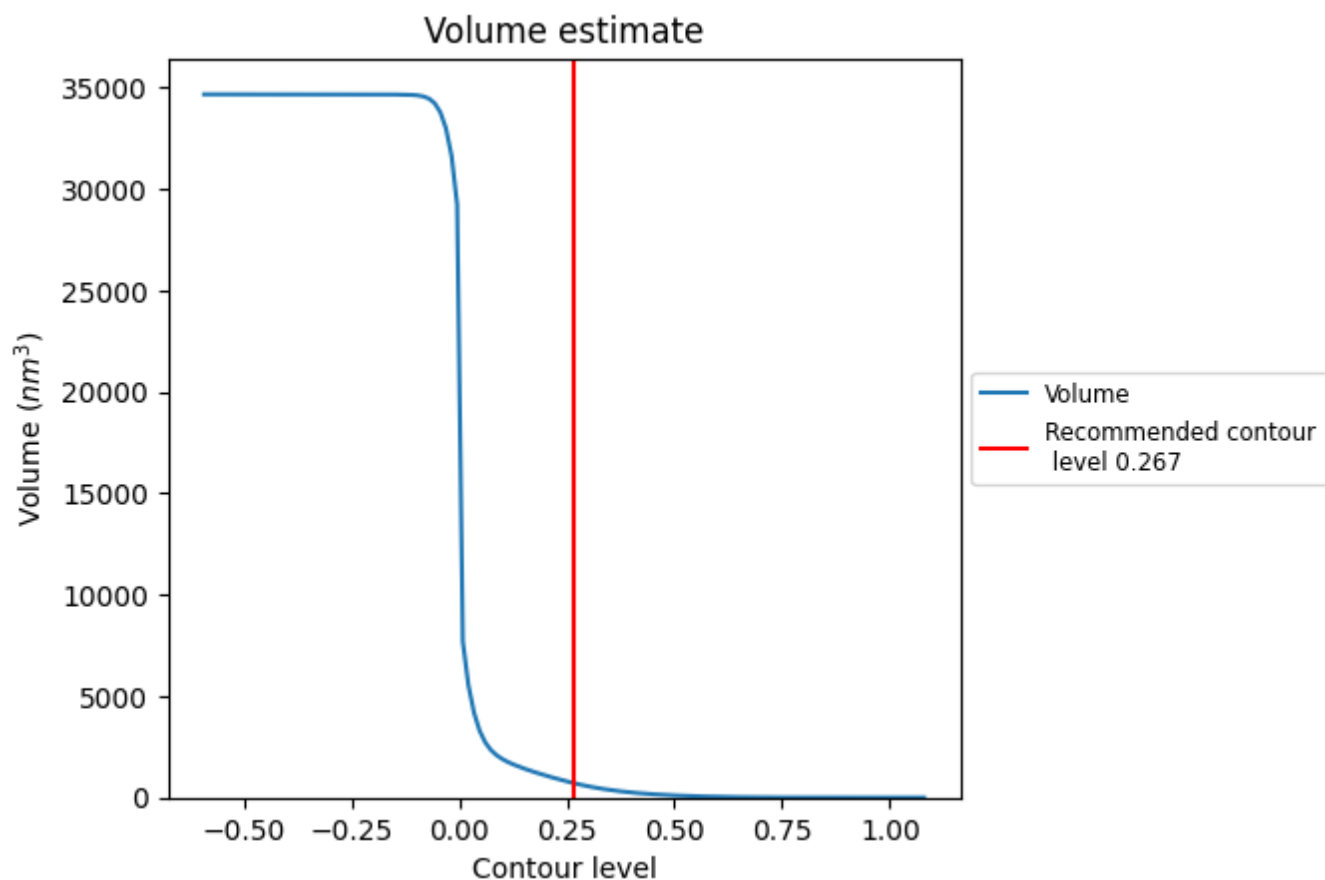
This section contains the results of statistical analysis of the map.

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.

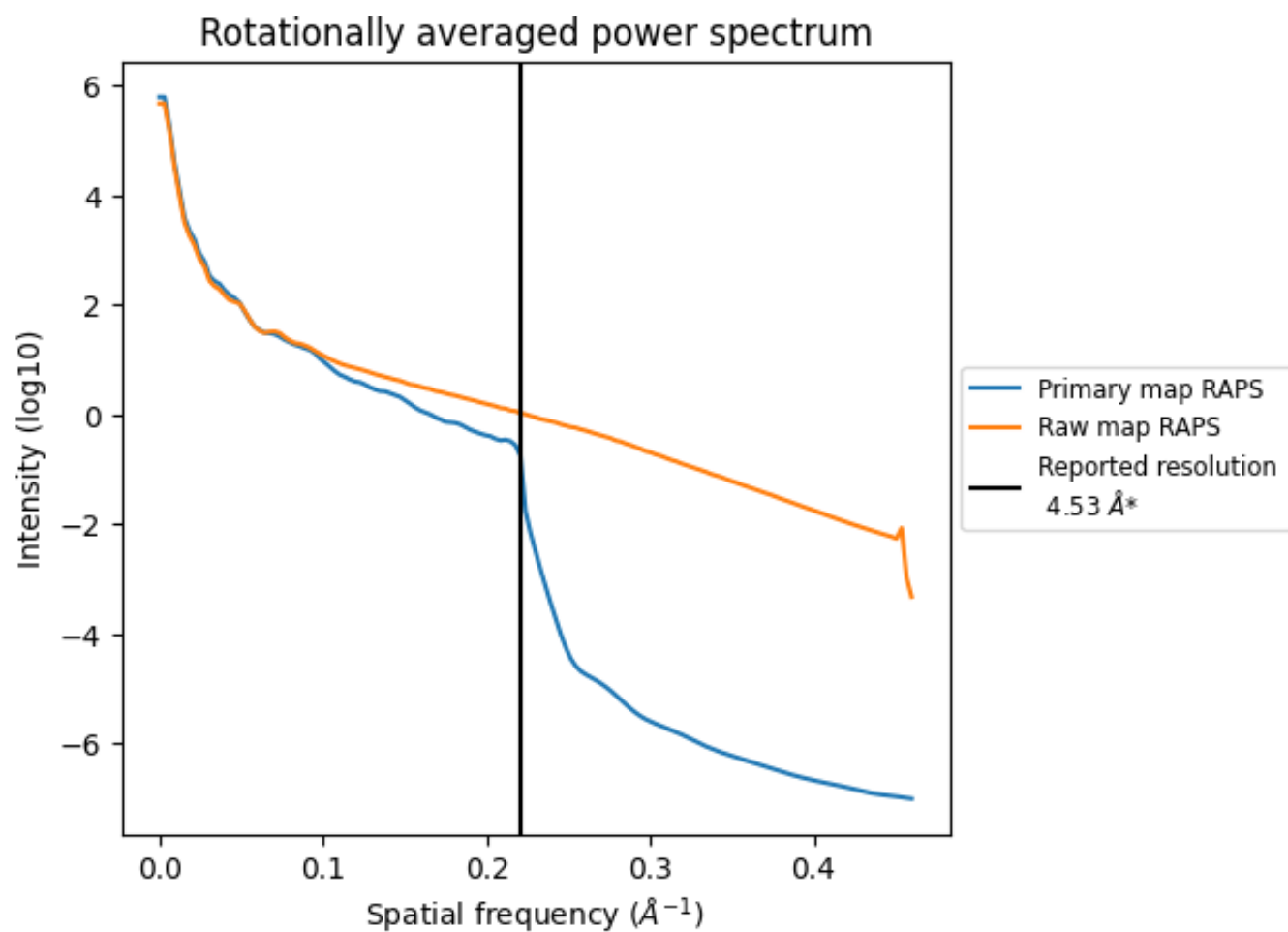
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 708 nm³; this corresponds to an approximate mass of 640 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 ⓘ

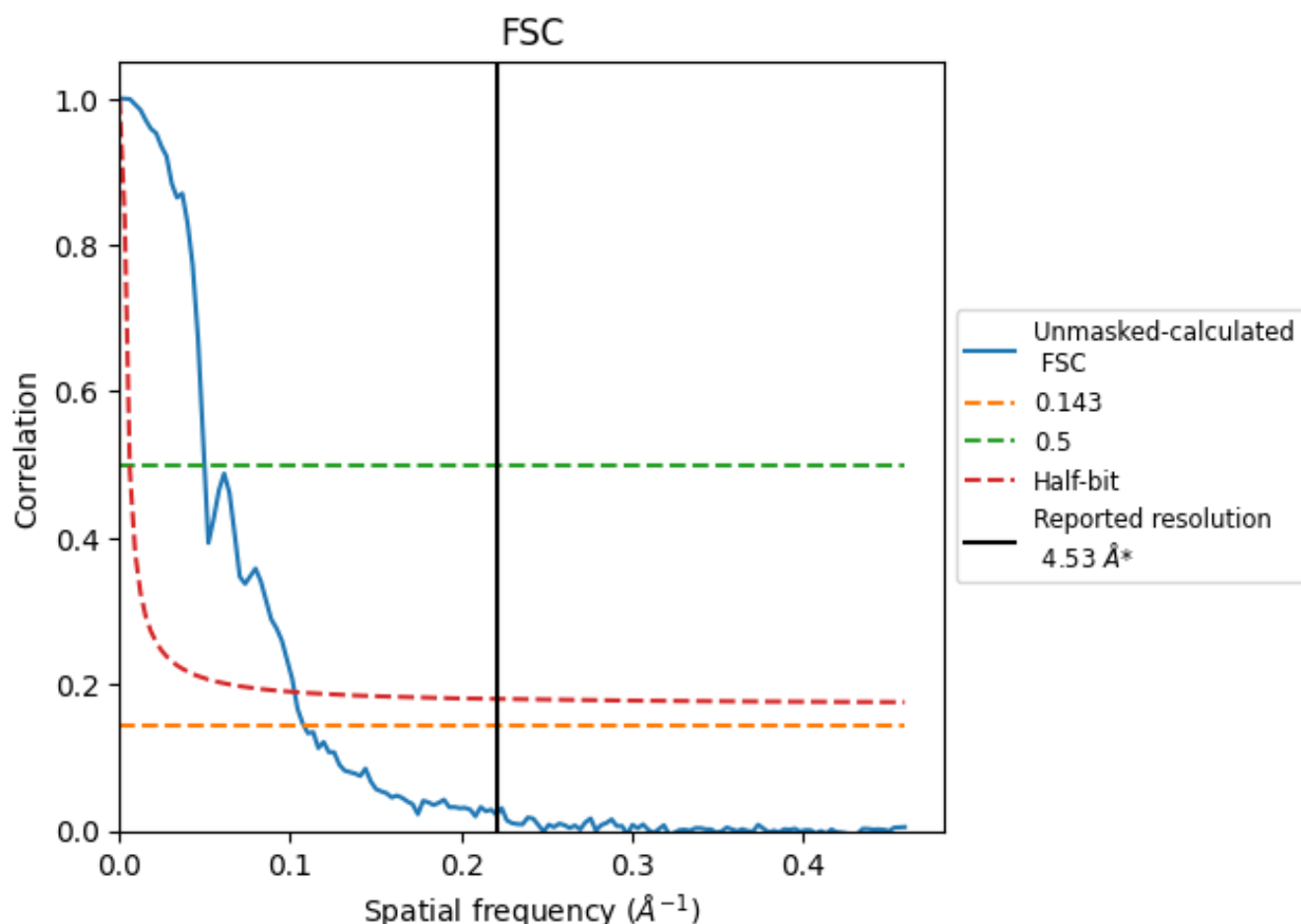


*Reported resolution corresponds to spatial frequency of 0.221 \AA^{-1}

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 0.221 Å⁻¹

8.2 Resolution estimates [i](#)

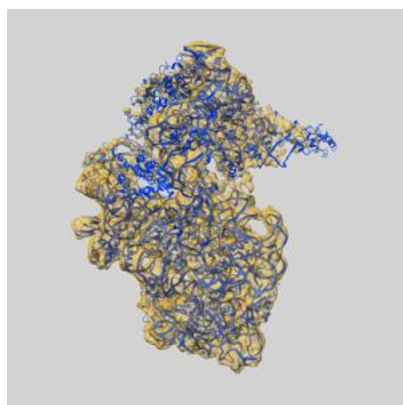
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.25	20.12	9.75

*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 9.25 differs from the reported value 4.53 by more than 10 %

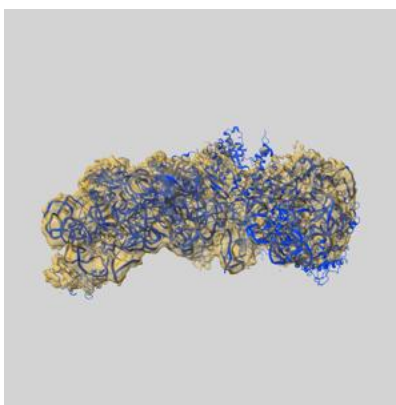
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37734 and PDB model 8WQ4. Per-residue inclusion information can be found in section [3](#) on page [9](#).

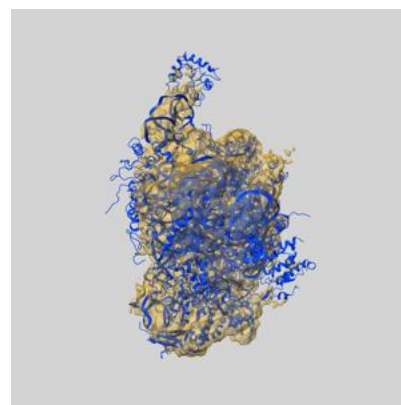
9.1 Map-model overlay [i](#)



X



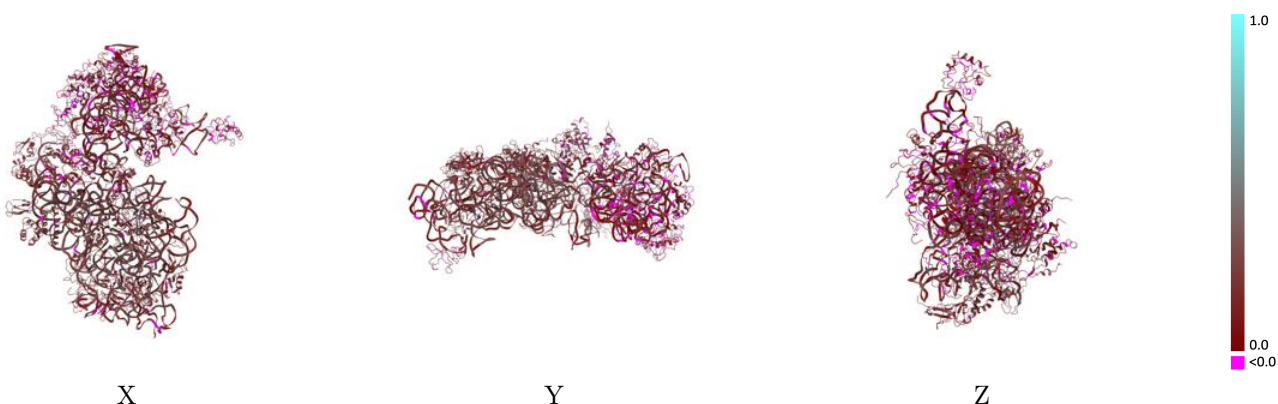
Y



Z

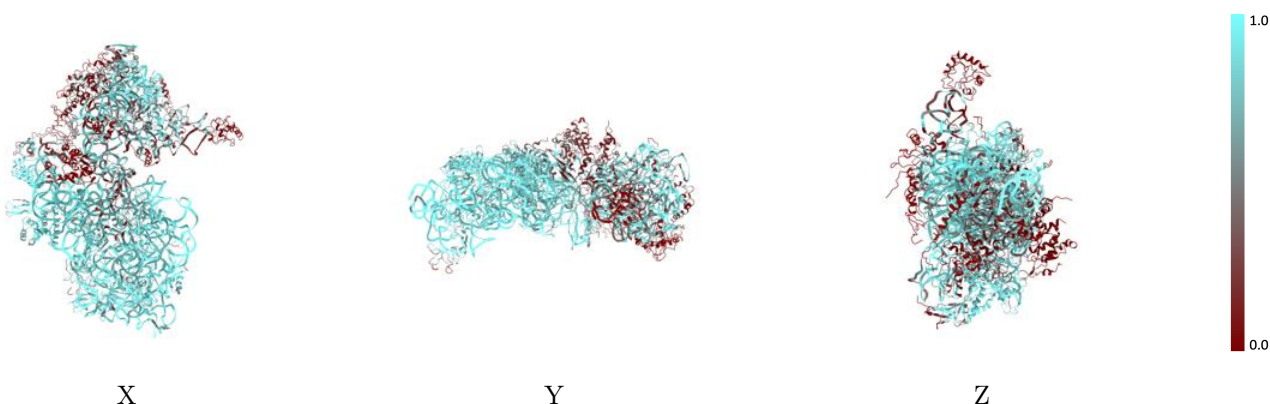
The images above show the 3D surface view of the map at the recommended contour level 0.267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



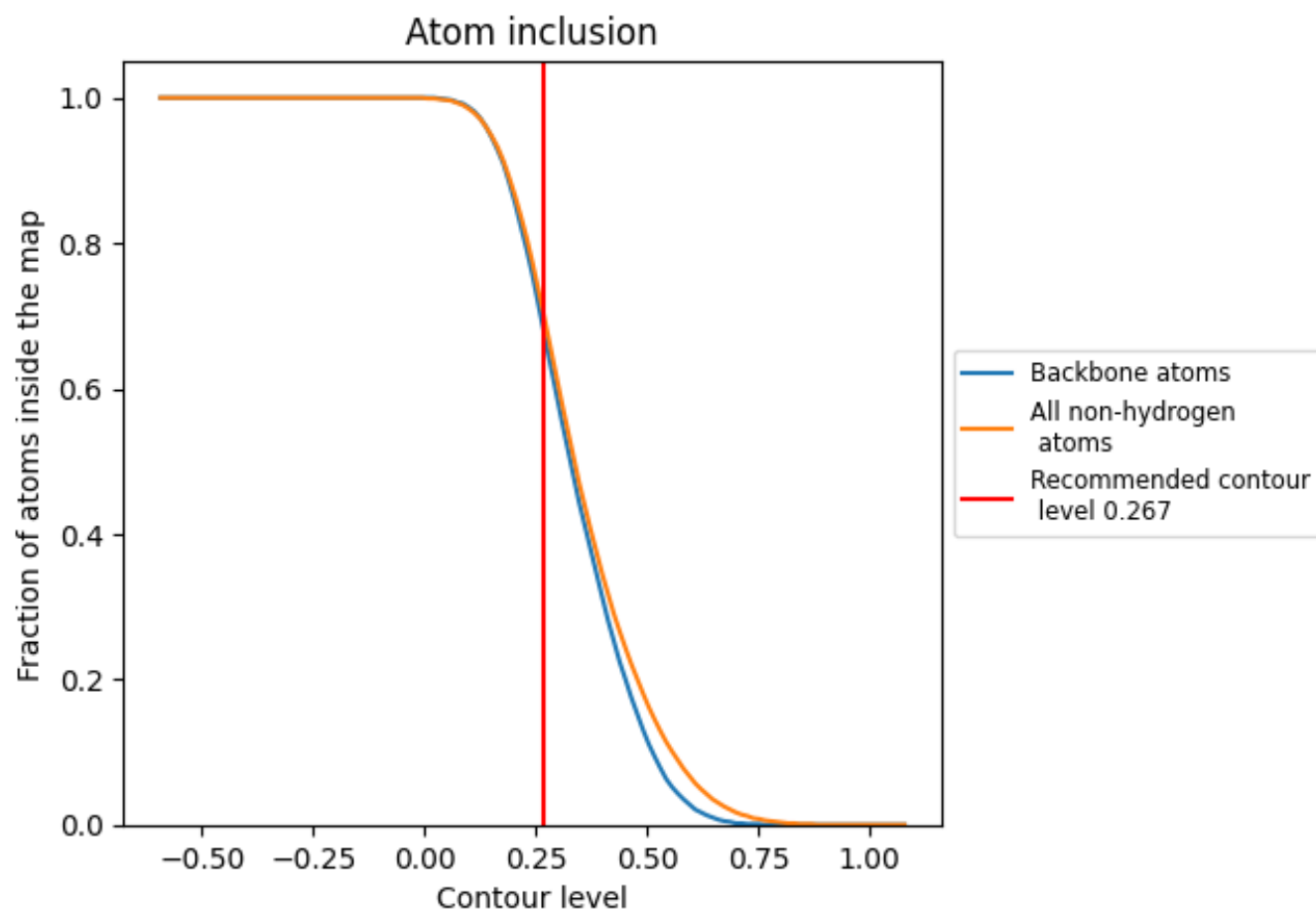
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.267).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 71% 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 (0.267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.1890
A16S	 0.8710	 0.2040
AS2P	 0.1140	 0.1730
AS3P	 0.4100	 0.1540
AS4E	 0.8720	 0.2120
AS4P	 0.7880	 0.2380
AS5P	 0.5120	 0.2050
AS6E	 0.5870	 0.1440
AS7P	 0.2090	 0.1080
AS8E	 0.9030	 0.2310
AS8P	 0.8090	 0.2510
AS9P	 0.3310	 0.1400
S10P	 0.6760	 0.1400
S11P	 0.2680	 0.1590
S12P	 0.8000	 0.2260
S13P	 0.3200	 0.1010
S14P	 0.5660	 0.1800
S15P	 0.8470	 0.2310
S17E	 0.1750	 0.1080
S17P	 0.7620	 0.2490
S19E	 0.4180	 0.0750
S19P	 0.2040	 0.1080
S24E	 0.8810	 0.2010
S27A	 0.5690	 0.1230
S27E	 0.8340	 0.2480
S28E	 0.0670	 0.1310
S3AE	 0.7170	 0.1990
SL7A	 0.0540	 0.1020
VTRF	 0.8990	 0.1890

