



## Full wwPDB EM Validation Report ⓘ

Apr 2, 2024 – 04:30 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 Full wwPDB EM Validation 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:

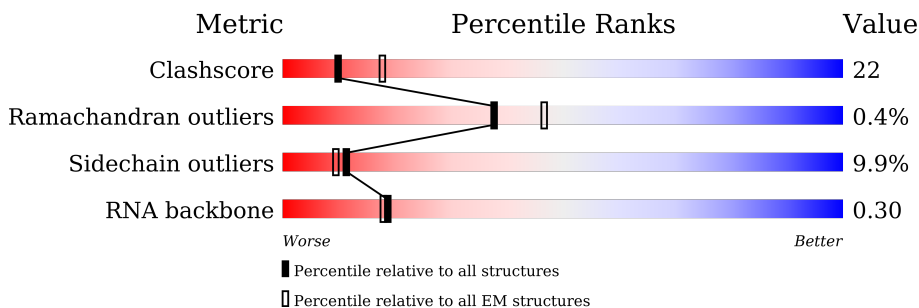
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A16S	1501	5% (red), 45% (green), 41% (yellow), 12% (grey)
2	VTRF	26	23% (green), 73% (yellow), 4% (orange)
3	AS2P	196	90% (red), 90% (green), 10% (yellow)
4	AS4E	240	88% (green), 12% (yellow)
5	AS4P	166	8% (red), 87% (green), 13% (yellow)
6	AS5P	204	36% (red), 94% (green), 6% (yellow)
7	AS6E	105	30% (red), 90% (green), 10% (yellow)

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Mol	Chain	Length	Quality of chain
8	AS8E	126	89% 11%
9	S11P	128	73% 95% 5%
10	S12P	143	7% 95% 5%
11	S15P	149	94% 6%
12	S17P	111	15% 91% 9%
13	S24E	96	90% 10%
14	S27E	59	85% 15%
15	S3AE	189	18% 88% 12%
16	AS3P	201	55% 91% 9%
17	AS7P	193	80% 95% 5%
18	AS9P	136	63% 88% 12%
19	S10P	100	25% 93% 7%
20	S13P	147	68% 91% 9%
21	S14P	52	37% 90% 10%
22	S17E	62	84% 85% 15%
23	S19E	150	53% 93% 7%
24	S19P	115	78% 91% 9%
25	S27A	54	35% 81% 17%
26	S28E	63	94% 87% 13%
27	SL7A	123	97% 98%
28	AS8P	130	93% 7%

## 2 Entry composition i

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
			Total	C	N	O	P		
1	A16S	1325	28462	12674	5267	9196	1325	0	0

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
			Total	C	N	O	P		
2	VTRF	26	556	248	96	187	25	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 29 is UNKNOWN (three-letter code: UNK) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

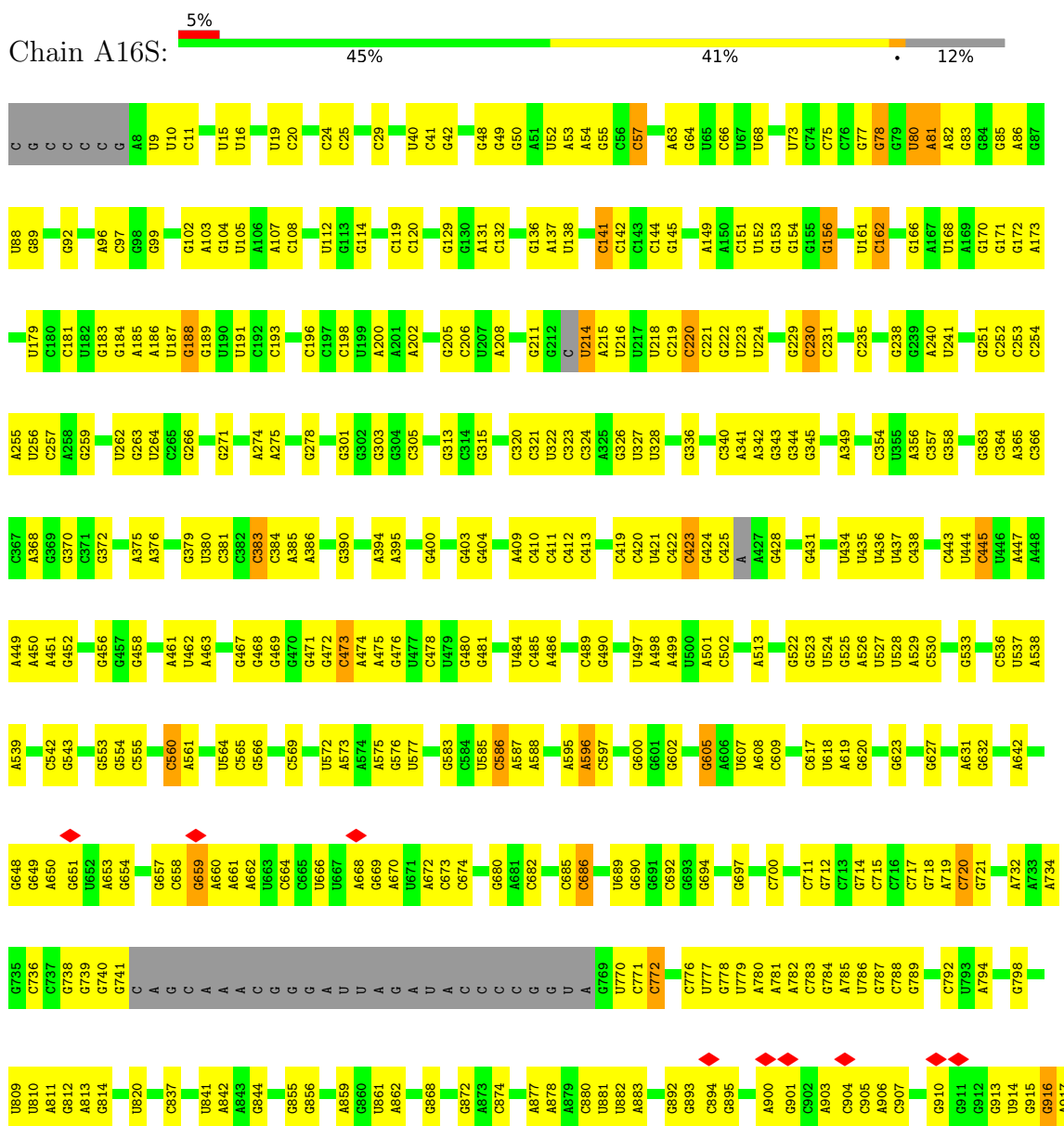
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	A16S	3	15	9	3	3	0
29	AS2P	28	141	84	28	29	0
29	AS5P	21	105	63	21	21	0
29	AS8P	5	25	15	5	5	0

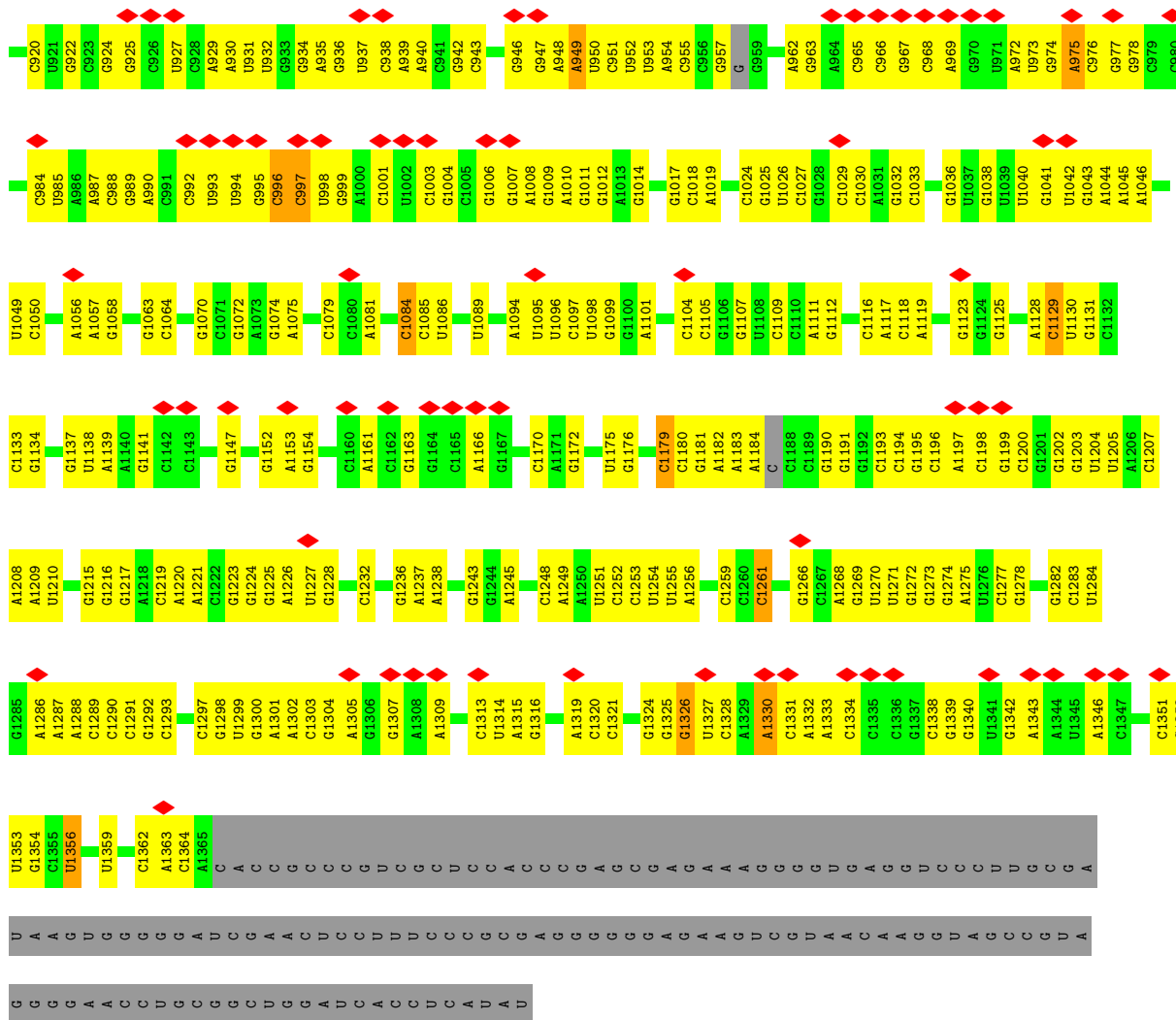


### 3 Residue-property plots i

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)

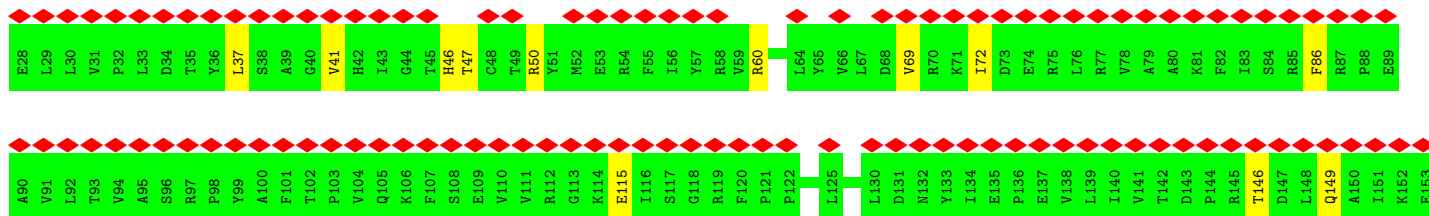


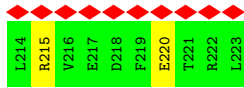
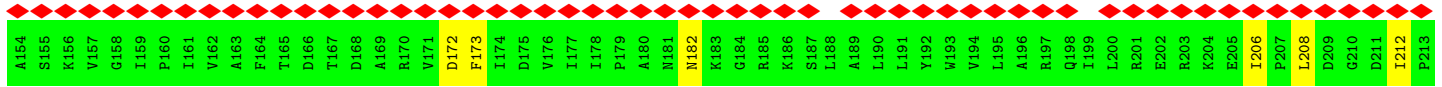


• Molecule 2: RNA (26-MER)



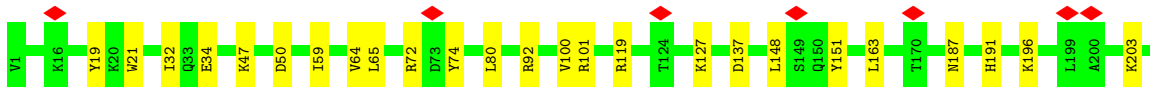
• Molecule 3: 30S ribosomal protein S2





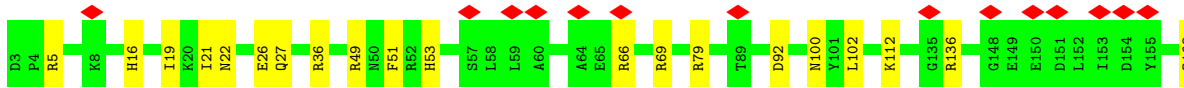
- Molecule 4: 30S ribosomal protein S4e

Chain AS4E: 88% 12%



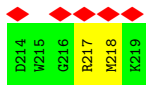
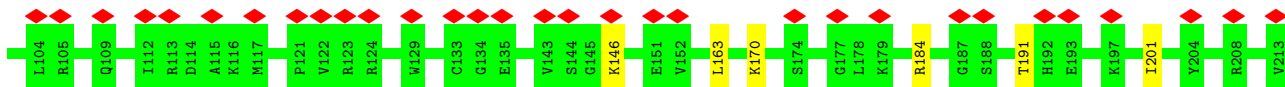
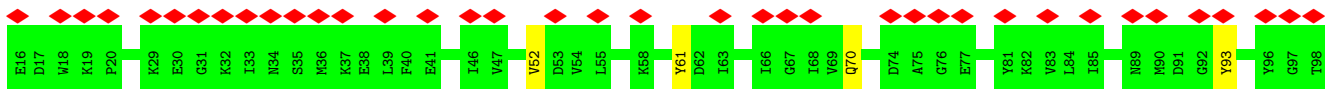
- Molecule 5: 30S ribosomal protein S4

Chain AS4P: 8% 87% 13%



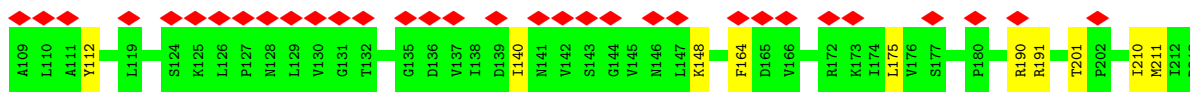
- Molecule 6: 30S ribosomal protein S5

Chain AS5P: 36% 94% 6%



- Molecule 7: 30S ribosomal protein S6e

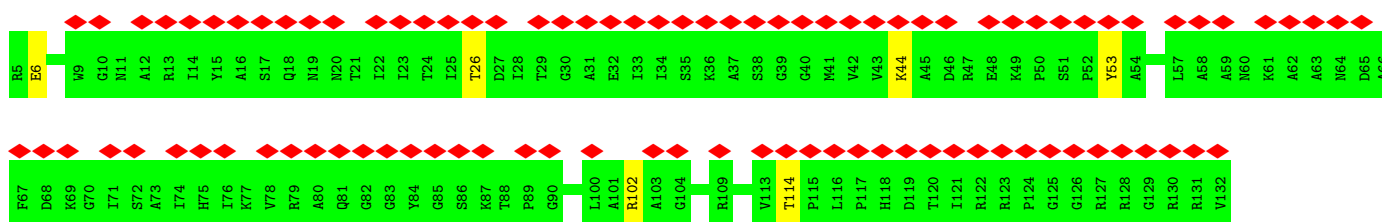
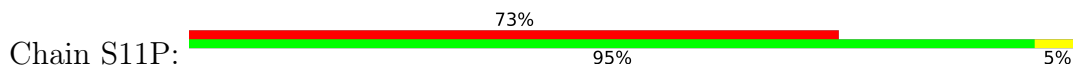
Chain AS6E: 30% 90% 10%



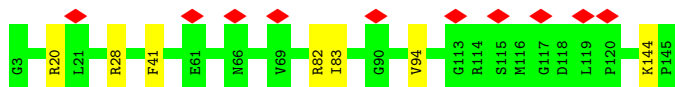
- Molecule 8: 30S ribosomal protein S8e



- Molecule 9: 30S ribosomal protein S11



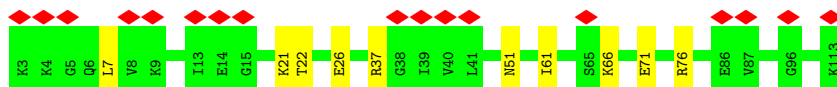
- Molecule 10: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S15

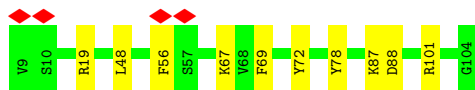


- Molecule 12: 30S ribosomal protein S17

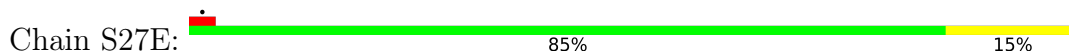


- Molecule 13: 30S ribosomal protein S24e

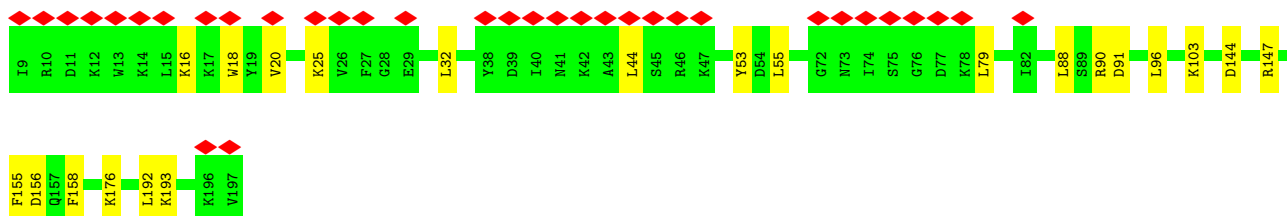




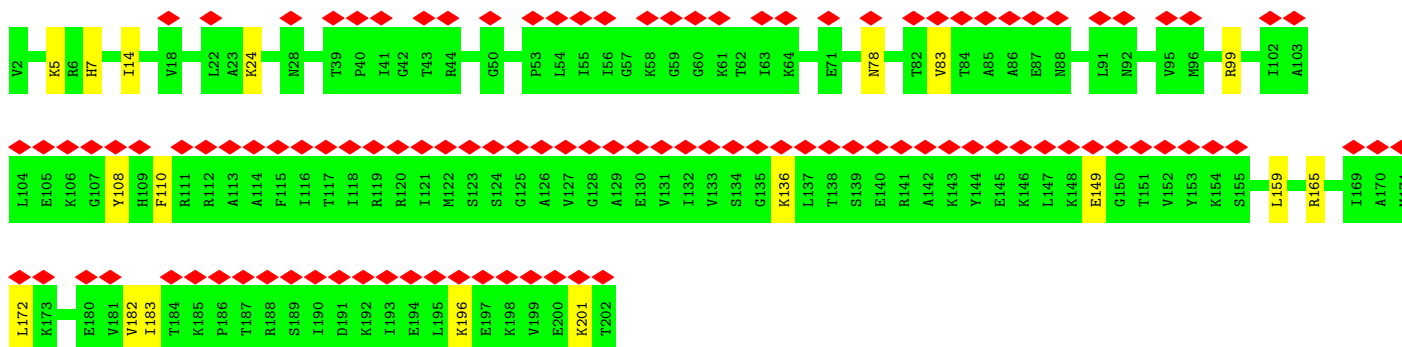
- Molecule 14: 30S ribosomal protein S27e



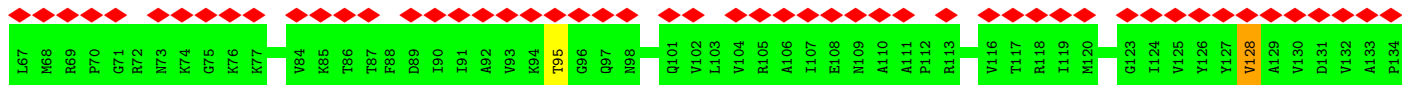
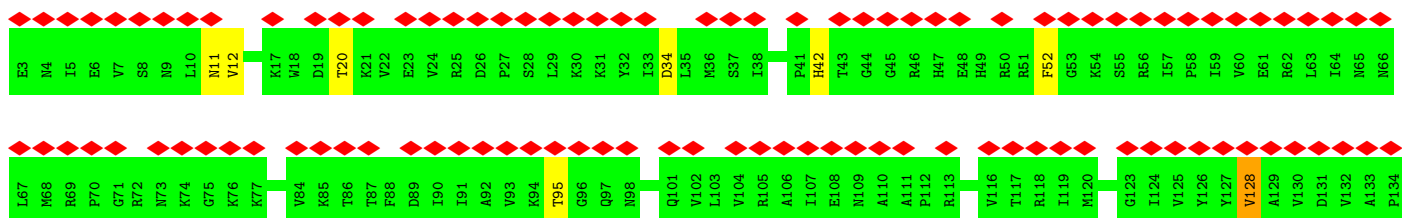
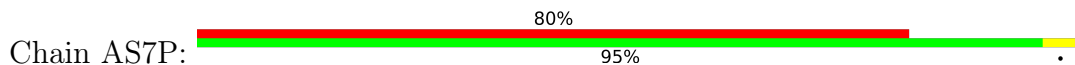
- Molecule 15: 30S ribosomal protein S3Ae

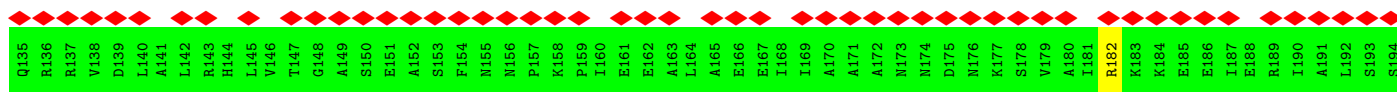


- Molecule 16: 30S ribosomal protein S3

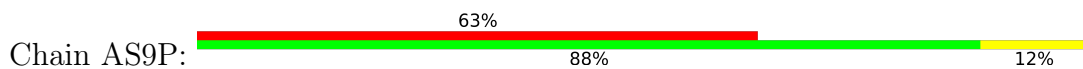


- Molecule 17: 30S ribosomal protein S7

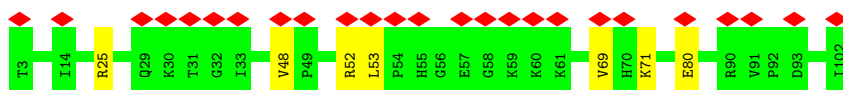




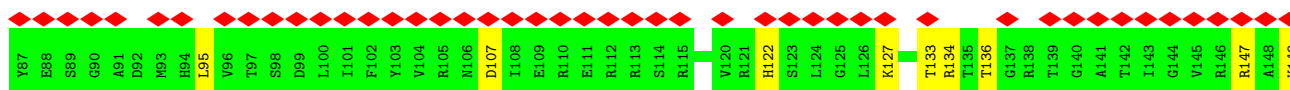
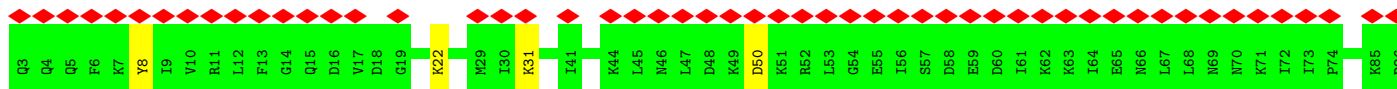
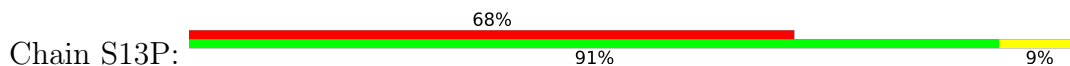
• Molecule 18: 30S ribosomal protein S9



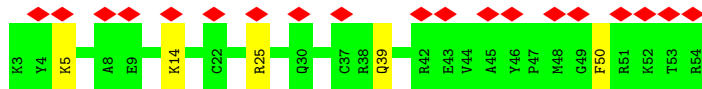
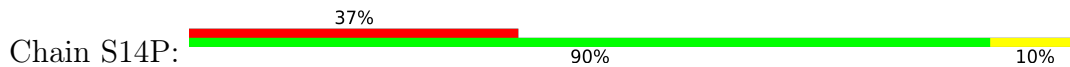
• Molecule 19: 30S ribosomal protein S10



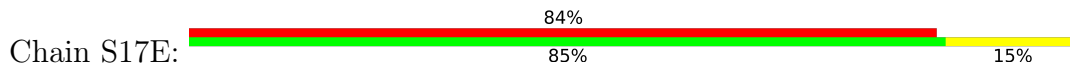
• Molecule 20: 30S ribosomal protein S13



• Molecule 21: 30S ribosomal protein S14 type Z

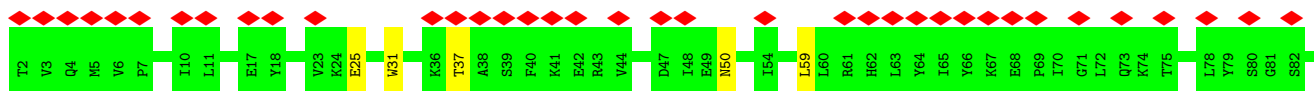


• Molecule 22: 30S ribosomal protein S17e

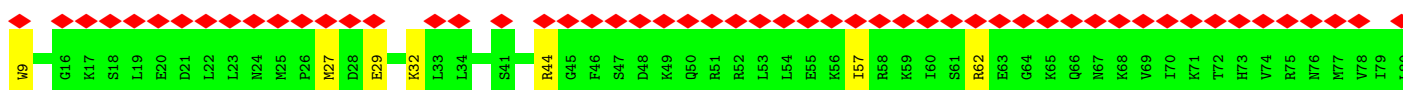
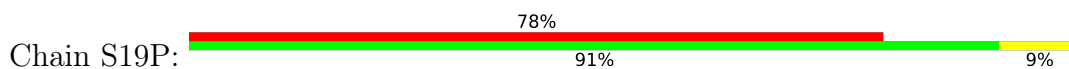




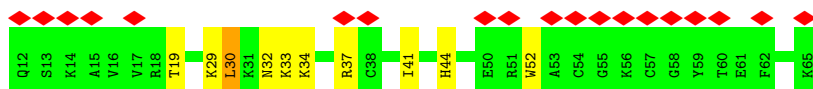
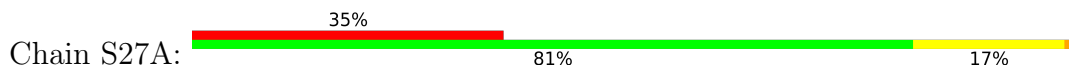
- Molecule 23: 30S ribosomal protein S19e



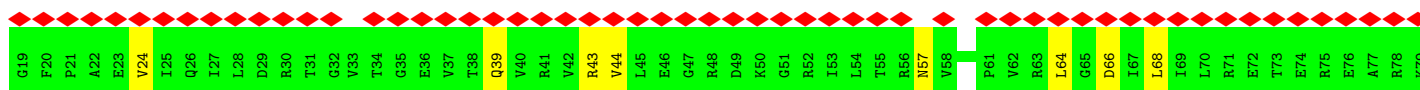
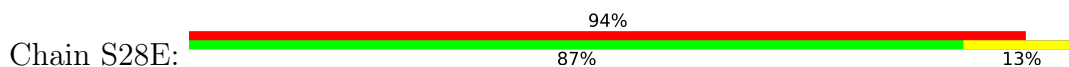
- Molecule 24: 30S ribosomal protein S19



- Molecule 25: 30S ribosomal protein S27ae

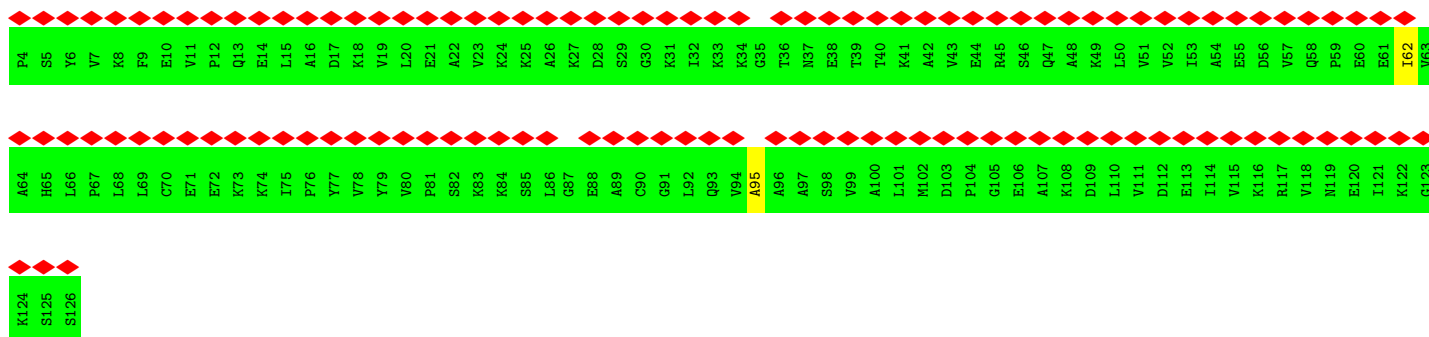


- Molecule 26: 30S ribosomal protein S28e



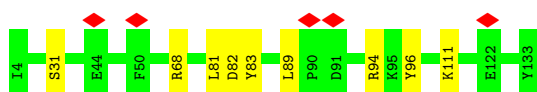
- Molecule 27: 50S ribosomal protein L7Ae





● Molecule 28: Small ribosomal subunit protein uS8

Chain AS8P: 93% 7%





## 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 (Å)	326.1, 326.1, 326.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

All (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
1	A16S	772	C	N1-C2-O2	9.99	124.89	118.90
1	A16S	560	C	N1-C2-O2	9.91	124.85	118.90
1	A16S	156	G	C5-C6-O6	9.81	134.49	128.60
1	A16S	141	C	N3-C2-O2	-9.56	115.21	121.90
1	A16S	156	G	N1-C6-O6	-9.04	114.48	119.90
1	A16S	141	C	N1-C2-O2	8.94	124.26	118.90
1	A16S	1334	C	N1-C2-O2	8.91	124.24	118.90
1	A16S	1261	C	N3-C2-O2	-8.60	115.88	121.90
1	A16S	772	C	N3-C2-O2	-8.59	115.88	121.90
1	A16S	1180	C	N3-C2-O2	-8.55	115.91	121.90
1	A16S	321	C	N3-C2-O2	-8.33	116.07	121.90
1	A16S	321	C	N1-C2-O2	8.32	123.89	118.90
1	A16S	673	C	N1-C2-O2	8.10	123.76	118.90
1	A16S	29	C	C5-C4-N4	7.96	125.77	120.20
1	A16S	81	A	O4'-C4'-C3'	-7.93	96.07	104.00
1	A16S	673	C	N3-C2-O2	-7.87	116.39	121.90
1	A16S	423	C	N1-C2-O2	7.86	123.61	118.90
1	A16S	29	C	N3-C4-N4	-7.79	112.55	118.00
1	A16S	522	G	C5-C6-O6	7.75	133.25	128.60
1	A16S	141	C	C5-C4-N4	7.71	125.60	120.20
1	A16S	739	G	C5-C6-O6	7.61	133.16	128.60
1	A16S	1334	C	N3-C2-O2	-7.57	116.60	121.90
1	A16S	560	C	N3-C2-O2	-7.45	116.69	121.90
1	A16S	1326	G	C5-C6-O6	7.44	133.06	128.60
1	A16S	772	C	N3-C4-N4	-7.42	112.81	118.00
1	A16S	586	C	C2-N1-C1'	7.28	126.80	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	214	U	N1-C1'-C2'	7.27	123.45	114.00
1	A16S	772	C	C5-C4-N4	7.27	125.29	120.20
1	A16S	214	U	C4'-C3'-O3'	7.26	127.52	113.00
1	A16S	1084	C	C2-N1-C1'	7.24	126.77	118.80
1	A16S	711	C	N3-C2-O2	-7.19	116.86	121.90
1	A16S	522	G	N1-C2-N2	-7.16	109.75	116.20
1	A16S	717	C	N3-C2-O2	-7.15	116.90	121.90
1	A16S	57	C	N3-C2-O2	-7.07	116.95	121.90
1	A16S	586	C	N1-C2-O2	7.05	123.13	118.90
1	A16S	739	G	N1-C6-O6	-7.00	115.70	119.90
1	A16S	522	G	N3-C2-N2	6.98	124.79	119.90
1	A16S	144	C	N3-C2-O2	-6.83	117.12	121.90
1	A16S	949	A	N1-C6-N6	-6.80	114.52	118.60
1	A16S	206	C	C2-N1-C1'	6.74	126.21	118.80
1	A16S	1326	G	N1-C6-O6	-6.62	115.92	119.90
1	A16S	1334	C	C5-C4-N4	6.60	124.82	120.20
1	A16S	141	C	N3-C4-N4	-6.59	113.39	118.00
1	A16S	25	C	N3-C2-O2	-6.52	117.34	121.90
1	A16S	771	C	N3-C2-O2	-6.48	117.36	121.90
1	A16S	1334	C	N3-C4-N4	-6.42	113.51	118.00
1	A16S	1356	U	C5-C4-O4	6.40	129.74	125.90
1	A16S	739	G	N3-C2-N2	6.31	124.31	119.90
1	A16S	984	C	N1-C2-O2	6.29	122.67	118.90
1	A16S	214	U	C5'-C4'-C3'	6.26	126.02	116.00
25	S27A	30	LEU	CA-CB-CG	6.26	129.70	115.30
1	A16S	198	C	N3-C2-O2	-6.25	117.53	121.90
1	A16S	383	C	N1-C2-O2	6.14	122.59	118.90
1	A16S	214	U	C2'-C3'-O3'	-6.10	96.08	109.50
1	A16S	522	G	N1-C6-O6	-6.02	116.29	119.90
1	A16S	771	C	N1-C2-O2	5.78	122.37	118.90
1	A16S	776	C	N3-C2-O2	-5.77	117.86	121.90
1	A16S	586	C	C6-N1-C1'	-5.74	113.91	120.80
1	A16S	984	C	C2-N1-C1'	5.73	125.11	118.80
2	VTRF	25	G	C4-N9-C1'	5.72	133.94	126.50
1	A16S	473	C	N1-C2-O2	5.69	122.31	118.90
1	A16S	1330	A	N9-C1'-C2'	-5.65	105.78	112.00
2	VTRF	25	G	N3-C4-N9	5.62	129.37	126.00
1	A16S	711	C	N1-C2-O2	5.60	122.26	118.90
1	A16S	997	C	N1-C2-O2	5.55	122.23	118.90
1	A16S	220	C	C3'-C2'-C1'	-5.55	97.06	101.50
1	A16S	1338	C	N3-C2-O2	-5.55	118.02	121.90
1	A16S	900	A	C6-N1-C2	-5.54	115.28	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	900	A	N1-C2-N3	5.54	132.07	129.30
1	A16S	605	G	C5-C6-O6	5.54	131.92	128.60
1	A16S	154	G	N1-C2-N2	-5.53	111.22	116.20
1	A16S	720	C	C2-N1-C1'	5.52	124.87	118.80
1	A16S	1215	G	C5-C6-O6	5.51	131.91	128.60
1	A16S	1326	G	N3-C2-N2	5.51	123.75	119.90
1	A16S	605	G	N3-C4-N9	-5.47	122.72	126.00
1	A16S	1180	C	N1-C2-O2	5.47	122.18	118.90
1	A16S	1129	C	C2-N1-C1'	5.45	124.79	118.80
1	A16S	1338	C	N1-C2-O2	5.39	122.14	118.90
1	A16S	975	A	O4'-C1'-N9	-5.38	103.90	108.20
1	A16S	649	G	C5-C6-O6	5.35	131.81	128.60
1	A16S	659	G	C6-N1-C2	5.34	128.30	125.10
1	A16S	1200	C	N1-C2-O2	5.34	122.10	118.90
1	A16S	996	C	N3-C2-O2	-5.31	118.18	121.90
1	A16S	214	U	O5'-P-OP2	5.29	117.05	110.70
1	A16S	586	C	N3-C2-O2	-5.27	118.21	121.90
1	A16S	154	G	N3-C2-N2	5.27	123.59	119.90
1	A16S	445	C	N1-C2-O2	5.27	122.06	118.90
1	A16S	230	C	C2'-C3'-O3'	5.27	122.13	113.70
1	A16S	1084	C	C6-N1-C1'	-5.26	114.48	120.80
1	A16S	370	G	C5-C6-O6	5.26	131.76	128.60
1	A16S	686	C	C6-N1-C2	-5.26	118.20	120.30
1	A16S	1215	G	N3-C2-N2	5.26	123.58	119.90
1	A16S	214	U	P-O3'-C3'	5.25	126.00	119.70
1	A16S	605	G	N1-C6-O6	-5.25	116.75	119.90
1	A16S	423	C	N3-C2-O2	-5.23	118.24	121.90
1	A16S	1012	G	N1-C2-N2	-5.23	111.49	116.20
1	A16S	187	U	C2-N1-C1'	5.17	123.91	117.70
1	A16S	80	U	C4'-C3'-C2'	-5.17	97.43	102.60
1	A16S	214	U	C1'-O4'-C4'	-5.15	105.78	109.90
1	A16S	162	C	N1-C2-O2	5.14	121.99	118.90
1	A16S	370	G	N1-C6-O6	-5.14	116.82	119.90
1	A16S	536	C	C2-N1-C1'	5.12	124.43	118.80
1	A16S	162	C	N3-C2-O2	-5.10	118.33	121.90
1	A16S	1179	C	N1-C2-O2	5.10	121.96	118.90
1	A16S	997	C	C2-N1-C1'	5.08	124.38	118.80
1	A16S	916	G	C4-N9-C1'	5.06	133.07	126.50
1	A16S	80	U	O4'-C4'-C3'	-5.05	98.95	104.00
1	A16S	188	G	C5-C6-O6	5.04	131.62	128.60
1	A16S	188	G	N1-C6-O6	-5.01	116.89	119.90
1	A16S	920	C	N3-C2-O2	-5.01	118.39	121.90

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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 [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	
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%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AS7P	191/193 (99%)	162 (85%)	28 (15%)	1 (0%)	29	68
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%)	22	62
21	S14P	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	7	40
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%)	17	56
25	S27A	52/54 (96%)	42 (81%)	7 (14%)	3 (6%)	1	20
26	S28E	61/63 (97%)	51 (84%)	8 (13%)	2 (3%)	4	30
27	SL7A	121/123 (98%)	111 (92%)	9 (7%)	1 (1%)	19	60
28	AS8P	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
All	All	3386/3438 (98%)	3081 (91%)	293 (9%)	12 (0%)	38	72

All (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
26	S28E	24	VAL
25	S27A	30	LEU
25	S27A	33	LYS
25	S27A	41	ILE
27	SL7A	95	ALA
20	S13P	22	LYS
24	S19P	121	GLU

### 5.3.2 Protein sidechains [i](#)

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%)	5	23
4	AS4E	210/210 (100%)	182 (87%)	28 (13%)	4	20
5	AS4P	149/149 (100%)	128 (86%)	21 (14%)	3	18
6	AS5P	174/174 (100%)	162 (93%)	12 (7%)	15	42
7	AS6E	88/88 (100%)	78 (89%)	10 (11%)	5	24
8	AS8E	106/106 (100%)	92 (87%)	14 (13%)	4	20
9	S11P	94/94 (100%)	88 (94%)	6 (6%)	17	44
10	S12P	116/116 (100%)	109 (94%)	7 (6%)	19	46
11	S15P	133/133 (100%)	124 (93%)	9 (7%)	16	42
12	S17P	97/97 (100%)	87 (90%)	10 (10%)	7	27
13	S24E	84/84 (100%)	74 (88%)	10 (12%)	5	23
14	S27E	51/51 (100%)	42 (82%)	9 (18%)	2	12
15	S3AE	170/170 (100%)	148 (87%)	22 (13%)	4	20
16	AS3P	165/165 (100%)	149 (90%)	16 (10%)	8	29
17	AS7P	166/166 (100%)	157 (95%)	9 (5%)	22	49
18	AS9P	113/113 (100%)	97 (86%)	16 (14%)	3	18
19	S10P	92/92 (100%)	85 (92%)	7 (8%)	13	39
20	S13P	129/129 (100%)	117 (91%)	12 (9%)	9	30
21	S14P	45/45 (100%)	41 (91%)	4 (9%)	9	33
22	S17E	57/57 (100%)	48 (84%)	9 (16%)	2	15
23	S19E	134/134 (100%)	123 (92%)	11 (8%)	11	37
24	S19P	106/106 (100%)	97 (92%)	9 (8%)	10	36
25	S27A	47/47 (100%)	40 (85%)	7 (15%)	3	17
26	S28E	54/54 (100%)	48 (89%)	6 (11%)	6	25
27	SL7A	104/104 (100%)	103 (99%)	1 (1%)	76	86
28	AS8P	111/111 (100%)	102 (92%)	9 (8%)	11	37
All	All	2969/2969 (100%)	2675 (90%)	294 (10%)	11	28

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AS2P	37	LEU
3	AS2P	41	VAL
3	AS2P	46	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	AS2P	47	THR
3	AS2P	50	ARG
3	AS2P	60	ARG
3	AS2P	69	VAL
3	AS2P	72	ILE
3	AS2P	86	PHE
3	AS2P	115	GLU
3	AS2P	146	THR
3	AS2P	149	GLN
3	AS2P	172	ASP
3	AS2P	173	PHE
3	AS2P	182	ASN
3	AS2P	206	ILE
3	AS2P	208	LEU
3	AS2P	212	ILE
3	AS2P	215	ARG
3	AS2P	220	GLU
4	AS4E	19	TYR
4	AS4E	21	TRP
4	AS4E	32	ILE
4	AS4E	34	GLU
4	AS4E	47	LYS
4	AS4E	50	ASP
4	AS4E	59	ILE
4	AS4E	64	VAL
4	AS4E	65	LEU
4	AS4E	72	ARG
4	AS4E	74	TYR
4	AS4E	80	LEU
4	AS4E	92	ARG
4	AS4E	100	VAL
4	AS4E	101	ARG
4	AS4E	119	ARG
4	AS4E	127	LYS
4	AS4E	137	ASP
4	AS4E	148	LEU
4	AS4E	151	TYR
4	AS4E	187	ASN
4	AS4E	191	HIS
4	AS4E	196	LYS
4	AS4E	203	LYS
4	AS4E	206	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	AS4E	215	LYS
4	AS4E	220	PHE
4	AS4E	221	GLN
5	AS4P	5	ARG
5	AS4P	16	HIS
5	AS4P	19	ILE
5	AS4P	21	ILE
5	AS4P	22	ASN
5	AS4P	26	GLU
5	AS4P	27	GLN
5	AS4P	36	ARG
5	AS4P	49	ARG
5	AS4P	51	PHE
5	AS4P	53	HIS
5	AS4P	66	ARG
5	AS4P	69	ARG
5	AS4P	79	ARG
5	AS4P	92	ASP
5	AS4P	100	ASN
5	AS4P	102	LEU
5	AS4P	112	LYS
5	AS4P	136	ARG
5	AS4P	163	GLN
5	AS4P	168	GLN
6	AS5P	52	VAL
6	AS5P	61	TYR
6	AS5P	70	GLN
6	AS5P	93	TYR
6	AS5P	146	LYS
6	AS5P	163	LEU
6	AS5P	170	LYS
6	AS5P	184	ARG
6	AS5P	191	THR
6	AS5P	201	ILE
6	AS5P	217	ARG
6	AS5P	218	MET
7	AS6E	112	TYR
7	AS6E	140	ILE
7	AS6E	148	LYS
7	AS6E	164	PHE
7	AS6E	175	LEU
7	AS6E	190	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	AS6E	191	ARG
7	AS6E	201	THR
7	AS6E	210	ILE
7	AS6E	211	MET
8	AS8E	17	LYS
8	AS8E	43	LYS
8	AS8E	45	LYS
8	AS8E	47	ARG
8	AS8E	54	LYS
8	AS8E	62	TYR
8	AS8E	69	GLN
8	AS8E	74	LYS
8	AS8E	81	VAL
8	AS8E	88	ARG
8	AS8E	92	ARG
8	AS8E	110	LYS
8	AS8E	118	ASP
8	AS8E	127	ARG
9	S11P	6	GLU
9	S11P	26	THR
9	S11P	44	LYS
9	S11P	53	TYR
9	S11P	102	ARG
9	S11P	114	THR
10	S12P	20	ARG
10	S12P	28	ARG
10	S12P	41	PHE
10	S12P	82	ARG
10	S12P	83	ILE
10	S12P	94	VAL
10	S12P	144	LYS
11	S15P	22	LYS
11	S15P	23	TRP
11	S15P	28	ARG
11	S15P	30	GLU
11	S15P	81	LYS
11	S15P	82	ILE
11	S15P	87	PHE
11	S15P	91	ARG
11	S15P	121	ARG
12	S17P	7	LEU
12	S17P	21	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	S17P	22	THR
12	S17P	26	GLU
12	S17P	37	ARG
12	S17P	51	ASN
12	S17P	61	ILE
12	S17P	66	LYS
12	S17P	71	GLU
12	S17P	76	ARG
13	S24E	19	ARG
13	S24E	48	LEU
13	S24E	56	PHE
13	S24E	67	LYS
13	S24E	69	PHE
13	S24E	72	TYR
13	S24E	78	TYR
13	S24E	87	LYS
13	S24E	88	ASP
13	S24E	101	ARG
14	S27E	4	LYS
14	S27E	8	LEU
14	S27E	18	ARG
14	S27E	19	VAL
14	S27E	22	ARG
14	S27E	23	GLN
14	S27E	25	ASN
14	S27E	31	PHE
14	S27E	48	VAL
15	S3AE	16	LYS
15	S3AE	18	TRP
15	S3AE	20	VAL
15	S3AE	25	LYS
15	S3AE	32	LEU
15	S3AE	44	LEU
15	S3AE	53	TYR
15	S3AE	55	LEU
15	S3AE	79	LEU
15	S3AE	88	LEU
15	S3AE	90	ARG
15	S3AE	91	ASP
15	S3AE	96	LEU
15	S3AE	103	LYS
15	S3AE	144	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	S3AE	147	ARG
15	S3AE	155	PHE
15	S3AE	156	ASP
15	S3AE	158	PHE
15	S3AE	176	LYS
15	S3AE	192	LEU
15	S3AE	193	LYS
16	AS3P	5	LYS
16	AS3P	7	HIS
16	AS3P	14	ILE
16	AS3P	24	LYS
16	AS3P	78	ASN
16	AS3P	99	ARG
16	AS3P	108	TYR
16	AS3P	110	PHE
16	AS3P	136	LYS
16	AS3P	149	GLU
16	AS3P	159	LEU
16	AS3P	165	ARG
16	AS3P	172	LEU
16	AS3P	182	VAL
16	AS3P	196	LYS
16	AS3P	201	LYS
17	AS7P	11	ASN
17	AS7P	12	VAL
17	AS7P	20	THR
17	AS7P	34	ASP
17	AS7P	42	HIS
17	AS7P	52	PHE
17	AS7P	95	THR
17	AS7P	128	VAL
17	AS7P	182	ARG
18	AS9P	3	GLN
18	AS9P	12	TYR
18	AS9P	25	LYS
18	AS9P	47	ARG
18	AS9P	51	MET
18	AS9P	56	LEU
18	AS9P	66	GLU
18	AS9P	84	ARG
18	AS9P	94	PHE
18	AS9P	104	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	AS9P	107	TYR
18	AS9P	109	ARG
18	AS9P	117	ARG
18	AS9P	124	TRP
18	AS9P	125	MET
18	AS9P	130	ARG
19	S10P	25	ARG
19	S10P	48	VAL
19	S10P	52	ARG
19	S10P	53	LEU
19	S10P	69	VAL
19	S10P	71	LYS
19	S10P	80	GLU
20	S13P	8	TYR
20	S13P	31	LYS
20	S13P	50	ASP
20	S13P	95	LEU
20	S13P	107	ASP
20	S13P	122	HIS
20	S13P	127	LYS
20	S13P	133	THR
20	S13P	134	ARG
20	S13P	136	THR
20	S13P	147	ARG
20	S13P	149	LYS
21	S14P	14	LYS
21	S14P	25	ARG
21	S14P	39	GLN
21	S14P	50	PHE
22	S17E	5	TYR
22	S17E	18	ASP
22	S17E	19	LYS
22	S17E	20	PHE
22	S17E	28	TYR
22	S17E	34	LEU
22	S17E	38	TYR
22	S17E	53	TYR
22	S17E	62	LYS
23	S19E	25	GLU
23	S19E	31	TRP
23	S19E	37	THR
23	S19E	50	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	S19E	59	LEU
23	S19E	85	ARG
23	S19E	93	VAL
23	S19E	104	LEU
23	S19E	130	LEU
23	S19E	135	TYR
23	S19E	136	GLU
24	S19P	9	TRP
24	S19P	27	MET
24	S19P	29	GLU
24	S19P	32	LYS
24	S19P	44	ARG
24	S19P	57	ILE
24	S19P	62	ARG
24	S19P	87	ARG
24	S19P	110	LEU
25	S27A	19	THR
25	S27A	29	LYS
25	S27A	32	ASN
25	S27A	34	LYS
25	S27A	37	ARG
25	S27A	44	HIS
25	S27A	52	TRP
26	S28E	39	GLN
26	S28E	43	ARG
26	S28E	57	ASN
26	S28E	64	LEU
26	S28E	66	ASP
26	S28E	68	LEU
27	SL7A	62	ILE
28	AS8P	31	SER
28	AS8P	68	ARG
28	AS8P	81	LEU
28	AS8P	82	ASP
28	AS8P	83	TYR
28	AS8P	89	LEU
28	AS8P	94	ARG
28	AS8P	96	TYR
28	AS8P	111	LYS

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%)

All (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
1	A16S	19	U
1	A16S	20	C
1	A16S	24	C
1	A16S	40	U
1	A16S	41	C
1	A16S	42	G
1	A16S	48	G
1	A16S	49	G
1	A16S	50	G
1	A16S	52	U
1	A16S	53	A
1	A16S	54	A
1	A16S	55	G
1	A16S	57	C
1	A16S	63	A
1	A16S	64	G
1	A16S	66	C
1	A16S	68	U
1	A16S	75	C
1	A16S	77	G
1	A16S	78	G
1	A16S	80	U
1	A16S	81	A
1	A16S	82	A
1	A16S	83	G
1	A16S	85	G
1	A16S	86	A
1	A16S	88	U
1	A16S	89	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	92	G
1	A16S	96	A
1	A16S	97	C
1	A16S	99	G
1	A16S	102	G
1	A16S	103	A
1	A16S	104	G
1	A16S	105	U
1	A16S	107	A
1	A16S	108	C
1	A16S	112	U
1	A16S	114	G
1	A16S	119	C
1	A16S	120	C
1	A16S	129	G
1	A16S	131	A
1	A16S	132	C
1	A16S	136	G
1	A16S	137	A
1	A16S	138	U
1	A16S	141	C
1	A16S	142	C
1	A16S	145	G
1	A16S	149	A
1	A16S	151	C
1	A16S	152	U
1	A16S	153	G
1	A16S	156	G
1	A16S	161	U
1	A16S	162	C
1	A16S	166	G
1	A16S	168	U
1	A16S	170	G
1	A16S	171	G
1	A16S	172	G
1	A16S	173	A
1	A16S	179	U
1	A16S	181	C
1	A16S	183	G
1	A16S	184	G
1	A16S	185	A
1	A16S	186	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	188	G
1	A16S	189	G
1	A16S	191	U
1	A16S	193	C
1	A16S	196	C
1	A16S	200	A
1	A16S	202	A
1	A16S	205	G
1	A16S	208	A
1	A16S	211	G
1	A16S	215	A
1	A16S	216	U
1	A16S	218	U
1	A16S	219	C
1	A16S	220	C
1	A16S	221	C
1	A16S	222	G
1	A16S	223	U
1	A16S	224	U
1	A16S	229	G
1	A16S	230	C
1	A16S	231	C
1	A16S	235	C
1	A16S	238	G
1	A16S	240	A
1	A16S	241	U
1	A16S	251	G
1	A16S	252	C
1	A16S	253	C
1	A16S	254	C
1	A16S	256	U
1	A16S	257	C
1	A16S	259	G
1	A16S	262	U
1	A16S	263	G
1	A16S	264	U
1	A16S	266	G
1	A16S	271	G
1	A16S	274	A
1	A16S	275	A
1	A16S	278	G
1	A16S	301	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	303	G
1	A16S	305	C
1	A16S	313	G
1	A16S	315	G
1	A16S	320	C
1	A16S	323	C
1	A16S	324	C
1	A16S	326	G
1	A16S	327	U
1	A16S	328	U
1	A16S	336	G
1	A16S	340	C
1	A16S	341	A
1	A16S	342	A
1	A16S	343	G
1	A16S	344	G
1	A16S	345	G
1	A16S	349	A
1	A16S	354	C
1	A16S	356	A
1	A16S	357	C
1	A16S	358	G
1	A16S	363	G
1	A16S	364	C
1	A16S	365	A
1	A16S	366	C
1	A16S	368	A
1	A16S	372	G
1	A16S	375	A
1	A16S	376	A
1	A16S	379	G
1	A16S	380	U
1	A16S	381	C
1	A16S	383	C
1	A16S	384	C
1	A16S	385	A
1	A16S	386	A
1	A16S	390	G
1	A16S	394	A
1	A16S	395	A
1	A16S	400	G
1	A16S	403	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	404	G
1	A16S	409	A
1	A16S	410	C
1	A16S	411	C
1	A16S	412	C
1	A16S	413	C
1	A16S	419	C
1	A16S	420	C
1	A16S	421	U
1	A16S	422	C
1	A16S	423	C
1	A16S	424	G
1	A16S	425	C
1	A16S	428	G
1	A16S	431	G
1	A16S	434	U
1	A16S	435	U
1	A16S	436	U
1	A16S	437	U
1	A16S	438	C
1	A16S	443	C
1	A16S	445	C
1	A16S	447	A
1	A16S	449	A
1	A16S	450	A
1	A16S	451	A
1	A16S	452	G
1	A16S	456	G
1	A16S	458	G
1	A16S	461	A
1	A16S	462	U
1	A16S	463	A
1	A16S	467	G
1	A16S	468	G
1	A16S	469	G
1	A16S	472	G
1	A16S	473	C
1	A16S	474	A
1	A16S	475	A
1	A16S	476	G
1	A16S	478	C
1	A16S	480	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	481	G
1	A16S	484	U
1	A16S	485	C
1	A16S	486	A
1	A16S	489	C
1	A16S	490	G
1	A16S	497	U
1	A16S	498	A
1	A16S	499	A
1	A16S	501	A
1	A16S	502	C
1	A16S	513	A
1	A16S	523	G
1	A16S	524	U
1	A16S	525	G
1	A16S	526	A
1	A16S	527	U
1	A16S	528	U
1	A16S	529	A
1	A16S	530	C
1	A16S	533	G
1	A16S	537	U
1	A16S	538	A
1	A16S	539	A
1	A16S	542	C
1	A16S	543	G
1	A16S	553	G
1	A16S	554	G
1	A16S	555	C
1	A16S	560	C
1	A16S	561	A
1	A16S	564	U
1	A16S	565	C
1	A16S	566	G
1	A16S	569	C
1	A16S	572	U
1	A16S	573	A
1	A16S	575	A
1	A16S	576	G
1	A16S	577	U
1	A16S	583	G
1	A16S	585	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	586	C
1	A16S	587	A
1	A16S	588	A
1	A16S	595	A
1	A16S	596	A
1	A16S	597	C
1	A16S	600	G
1	A16S	602	G
1	A16S	605	G
1	A16S	607	U
1	A16S	608	A
1	A16S	609	C
1	A16S	617	C
1	A16S	618	U
1	A16S	619	A
1	A16S	620	G
1	A16S	623	G
1	A16S	627	G
1	A16S	631	A
1	A16S	632	G
1	A16S	642	A
1	A16S	648	G
1	A16S	651	G
1	A16S	653	A
1	A16S	654	G
1	A16S	657	G
1	A16S	658	C
1	A16S	659	G
1	A16S	660	A
1	A16S	661	A
1	A16S	662	A
1	A16S	664	C
1	A16S	666	U
1	A16S	668	A
1	A16S	669	G
1	A16S	670	A
1	A16S	672	A
1	A16S	674	C
1	A16S	680	G
1	A16S	682	C
1	A16S	685	C
1	A16S	686	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	689	U
1	A16S	690	G
1	A16S	692	C
1	A16S	694	G
1	A16S	697	G
1	A16S	700	C
1	A16S	712	G
1	A16S	714	G
1	A16S	715	C
1	A16S	718	G
1	A16S	719	A
1	A16S	720	C
1	A16S	721	G
1	A16S	732	A
1	A16S	734	A
1	A16S	736	C
1	A16S	738	G
1	A16S	740	G
1	A16S	741	G
1	A16S	770	U
1	A16S	772	C
1	A16S	777	U
1	A16S	778	G
1	A16S	779	U
1	A16S	780	A
1	A16S	781	A
1	A16S	782	A
1	A16S	783	C
1	A16S	784	G
1	A16S	785	A
1	A16S	786	U
1	A16S	787	G
1	A16S	788	C
1	A16S	789	G
1	A16S	792	C
1	A16S	794	A
1	A16S	798	G
1	A16S	809	U
1	A16S	810	U
1	A16S	811	A
1	A16S	812	G
1	A16S	813	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	814	G
1	A16S	820	U
1	A16S	837	C
1	A16S	841	U
1	A16S	842	A
1	A16S	844	G
1	A16S	855	G
1	A16S	856	G
1	A16S	859	A
1	A16S	861	U
1	A16S	862	A
1	A16S	868	G
1	A16S	872	G
1	A16S	874	C
1	A16S	877	A
1	A16S	878	A
1	A16S	880	C
1	A16S	881	U
1	A16S	882	U
1	A16S	883	A
1	A16S	892	G
1	A16S	893	G
1	A16S	894	C
1	A16S	895	G
1	A16S	901	G
1	A16S	903	A
1	A16S	904	C
1	A16S	905	C
1	A16S	906	A
1	A16S	907	C
1	A16S	910	G
1	A16S	913	G
1	A16S	914	U
1	A16S	915	G
1	A16S	916	G
1	A16S	917	A
1	A16S	922	G
1	A16S	924	G
1	A16S	925	G
1	A16S	927	U
1	A16S	929	A
1	A16S	930	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	931	U
1	A16S	932	U
1	A16S	934	G
1	A16S	935	A
1	A16S	936	G
1	A16S	937	U
1	A16S	938	C
1	A16S	939	A
1	A16S	940	A
1	A16S	942	G
1	A16S	943	C
1	A16S	946	G
1	A16S	947	G
1	A16S	948	A
1	A16S	949	A
1	A16S	950	U
1	A16S	951	C
1	A16S	952	U
1	A16S	953	U
1	A16S	954	A
1	A16S	955	C
1	A16S	957	G
1	A16S	962	A
1	A16S	963	G
1	A16S	966	C
1	A16S	967	G
1	A16S	968	C
1	A16S	969	A
1	A16S	972	A
1	A16S	973	U
1	A16S	974	G
1	A16S	975	A
1	A16S	976	C
1	A16S	977	G
1	A16S	978	G
1	A16S	985	U
1	A16S	987	A
1	A16S	988	C
1	A16S	989	G
1	A16S	990	A
1	A16S	992	C
1	A16S	993	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	994	U
1	A16S	995	G
1	A16S	996	C
1	A16S	997	C
1	A16S	998	U
1	A16S	999	G
1	A16S	1001	C
1	A16S	1003	C
1	A16S	1004	G
1	A16S	1006	G
1	A16S	1007	G
1	A16S	1008	A
1	A16S	1009	G
1	A16S	1010	A
1	A16S	1011	G
1	A16S	1014	G
1	A16S	1017	G
1	A16S	1018	C
1	A16S	1019	A
1	A16S	1024	C
1	A16S	1025	G
1	A16S	1027	C
1	A16S	1029	C
1	A16S	1030	C
1	A16S	1032	G
1	A16S	1033	C
1	A16S	1036	G
1	A16S	1038	G
1	A16S	1040	U
1	A16S	1041	G
1	A16S	1042	U
1	A16S	1043	G
1	A16S	1044	A
1	A16S	1045	A
1	A16S	1046	A
1	A16S	1049	U
1	A16S	1050	C
1	A16S	1056	A
1	A16S	1057	A
1	A16S	1058	G
1	A16S	1063	G
1	A16S	1064	C

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	1070	G
1	A16S	1072	G
1	A16S	1074	G
1	A16S	1075	A
1	A16S	1079	C
1	A16S	1081	A
1	A16S	1084	C
1	A16S	1085	C
1	A16S	1086	U
1	A16S	1089	U
1	A16S	1094	A
1	A16S	1095	U
1	A16S	1096	U
1	A16S	1097	C
1	A16S	1098	U
1	A16S	1099	G
1	A16S	1101	A
1	A16S	1104	C
1	A16S	1105	C
1	A16S	1107	G
1	A16S	1109	C
1	A16S	1112	G
1	A16S	1116	C
1	A16S	1117	A
1	A16S	1118	C
1	A16S	1119	A
1	A16S	1123	G
1	A16S	1125	G
1	A16S	1128	A
1	A16S	1129	C
1	A16S	1130	U
1	A16S	1131	G
1	A16S	1133	C
1	A16S	1134	G
1	A16S	1137	G
1	A16S	1138	U
1	A16S	1139	A
1	A16S	1141	G
1	A16S	1147	G
1	A16S	1152	G
1	A16S	1153	A
1	A16S	1154	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	1161	A
1	A16S	1163	G
1	A16S	1166	A
1	A16S	1170	C
1	A16S	1172	G
1	A16S	1175	U
1	A16S	1176	G
1	A16S	1179	C
1	A16S	1181	G
1	A16S	1182	A
1	A16S	1183	A
1	A16S	1184	A
1	A16S	1190	G
1	A16S	1191	G
1	A16S	1193	C
1	A16S	1194	C
1	A16S	1195	G
1	A16S	1196	C
1	A16S	1197	A
1	A16S	1198	C
1	A16S	1199	G
1	A16S	1202	G
1	A16S	1203	G
1	A16S	1205	U
1	A16S	1207	C
1	A16S	1209	A
1	A16S	1210	U
1	A16S	1216	G
1	A16S	1217	G
1	A16S	1219	C
1	A16S	1220	A
1	A16S	1221	A
1	A16S	1223	G
1	A16S	1224	G
1	A16S	1225	G
1	A16S	1226	A
1	A16S	1227	U
1	A16S	1228	G
1	A16S	1232	C
1	A16S	1236	G
1	A16S	1237	A
1	A16S	1238	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	1243	G
1	A16S	1245	A
1	A16S	1248	C
1	A16S	1249	A
1	A16S	1251	U
1	A16S	1252	C
1	A16S	1253	C
1	A16S	1254	U
1	A16S	1255	U
1	A16S	1256	A
1	A16S	1259	C
1	A16S	1261	C
1	A16S	1266	G
1	A16S	1268	A
1	A16S	1269	G
1	A16S	1270	U
1	A16S	1271	U
1	A16S	1273	G
1	A16S	1274	G
1	A16S	1275	A
1	A16S	1277	C
1	A16S	1278	G
1	A16S	1282	G
1	A16S	1283	C
1	A16S	1284	U
1	A16S	1287	A
1	A16S	1288	A
1	A16S	1289	C
1	A16S	1290	C
1	A16S	1291	C
1	A16S	1292	G
1	A16S	1293	C
1	A16S	1297	C
1	A16S	1298	G
1	A16S	1299	U
1	A16S	1300	G
1	A16S	1301	A
1	A16S	1302	A
1	A16S	1303	C
1	A16S	1304	G
1	A16S	1305	A
1	A16S	1307	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	1309	A
1	A16S	1313	C
1	A16S	1314	U
1	A16S	1315	A
1	A16S	1316	G
1	A16S	1319	A
1	A16S	1320	C
1	A16S	1321	C
1	A16S	1324	G
1	A16S	1325	G
1	A16S	1326	G
1	A16S	1327	U
1	A16S	1328	C
1	A16S	1330	A
1	A16S	1331	C
1	A16S	1332	A
1	A16S	1333	A
1	A16S	1339	G
1	A16S	1340	G
1	A16S	1342	G
1	A16S	1343	A
1	A16S	1346	A
1	A16S	1351	C
1	A16S	1352	C
1	A16S	1353	U
1	A16S	1354	G
1	A16S	1356	U
1	A16S	1359	U
1	A16S	1362	C
1	A16S	1363	A
1	A16S	1364	C
2	VTRF	2	G
2	VTRF	4	U
2	VTRF	5	U
2	VTRF	6	G
2	VTRF	8	U
2	VTRF	9	G
2	VTRF	10	G
2	VTRF	12	C
2	VTRF	13	U
2	VTRF	14	A
2	VTRF	15	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	VTRF	16	U
2	VTRF	17	C
2	VTRF	18	U
2	VTRF	19	G
2	VTRF	20	G
2	VTRF	23	A
2	VTRF	24	U
2	VTRF	25	G
2	VTRF	26	A

All (53) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A16S	54	A
1	A16S	63	A
1	A16S	73	U
1	A16S	77	G
1	A16S	80	U
1	A16S	81	A
1	A16S	82	A
1	A16S	85	G
1	A16S	137	A
1	A16S	214	U
1	A16S	220	C
1	A16S	221	C
1	A16S	230	C
1	A16S	231	C
1	A16S	255	A
1	A16S	322	U
1	A16S	340	C
1	A16S	380	U
1	A16S	384	C
1	A16S	423	C
1	A16S	444	U
1	A16S	449	A
1	A16S	471	G
1	A16S	475	A
1	A16S	484	U
1	A16S	527	U
1	A16S	564	U
1	A16S	587	A
1	A16S	595	A

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Mol	Chain	Res	Type
1	A16S	650	A
1	A16S	777	U
1	A16S	778	G
1	A16S	880	C
1	A16S	914	U
1	A16S	938	C
1	A16S	965	C
1	A16S	973	U
1	A16S	996	C
1	A16S	1006	G
1	A16S	1026	U
1	A16S	1043	G
1	A16S	1098	U
1	A16S	1111	A
1	A16S	1138	U
1	A16S	1196	C
1	A16S	1204	U
1	A16S	1208	A
1	A16S	1236	G
1	A16S	1254	U
1	A16S	1272	G
1	A16S	1286	A
2	VTRF	8	U
2	VTRF	23	A

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

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.

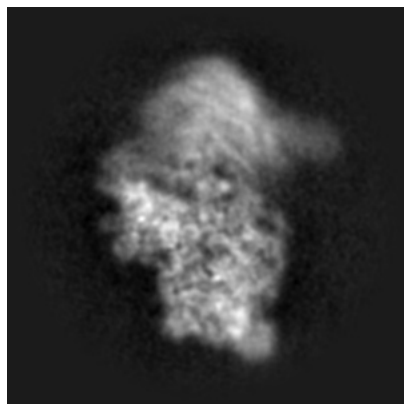
## 6 Map visualisation [i](#)

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.

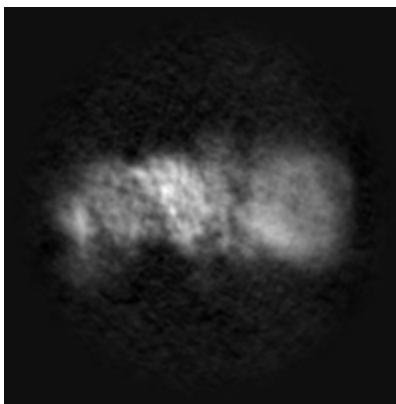
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

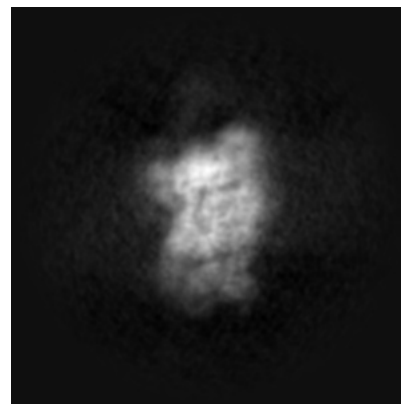
#### 6.1.1 Primary map



X

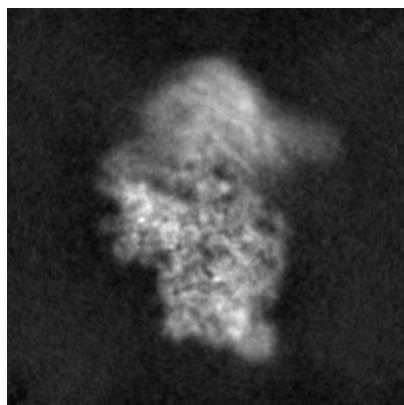


Y

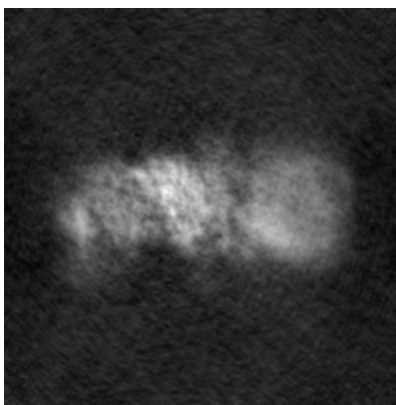


Z

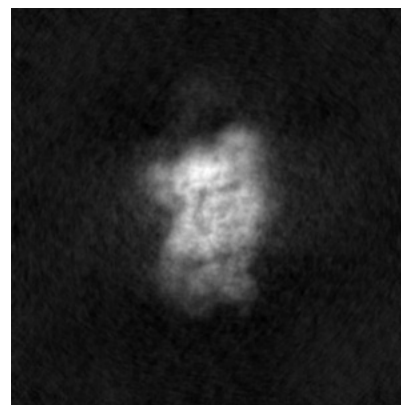
#### 6.1.2 Raw map



X



Y

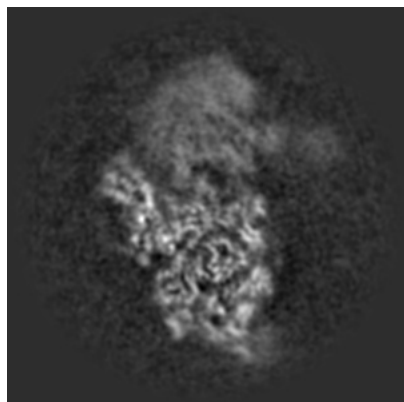


Z

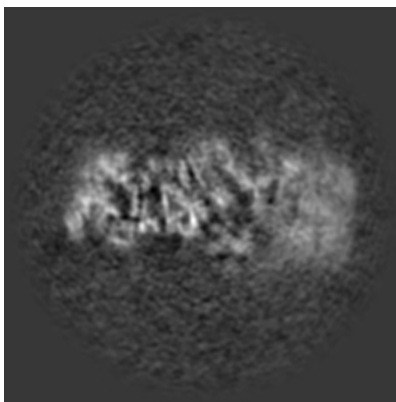
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

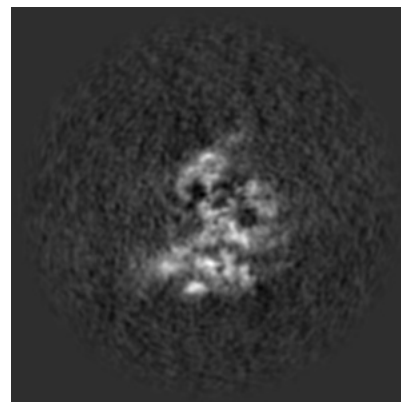
### 6.2.1 Primary map



X Index: 150

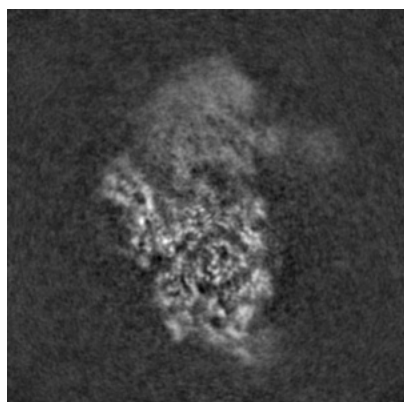


Y Index: 150

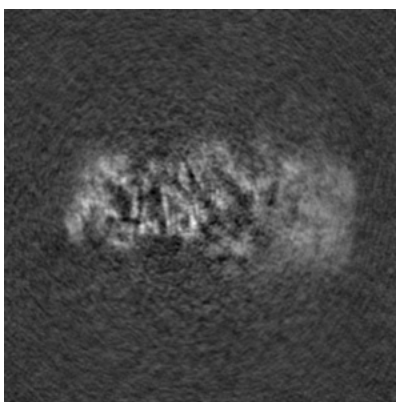


Z Index: 150

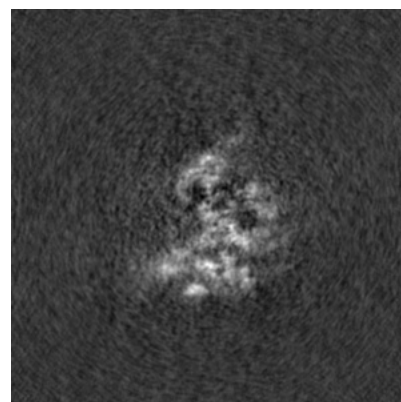
### 6.2.2 Raw map



X Index: 150



Y Index: 150

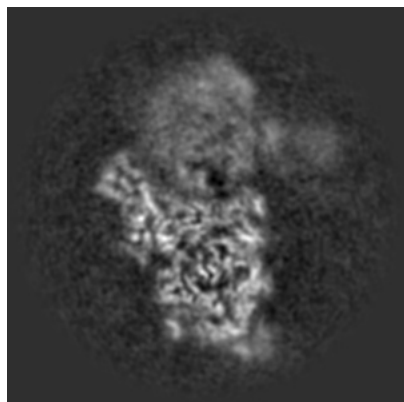


Z Index: 150

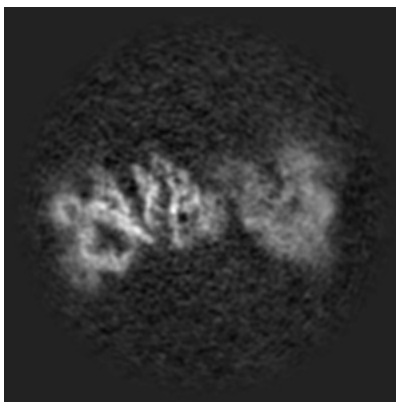
The images above show central slices of the map in three orthogonal directions.

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

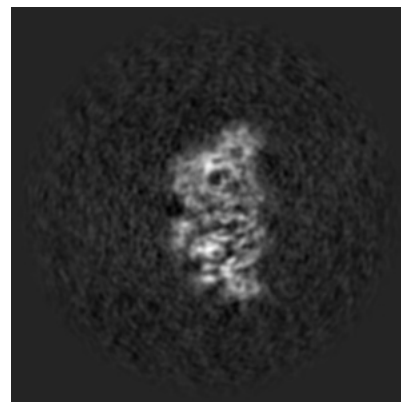
### 6.3.1 Primary map



X Index: 147

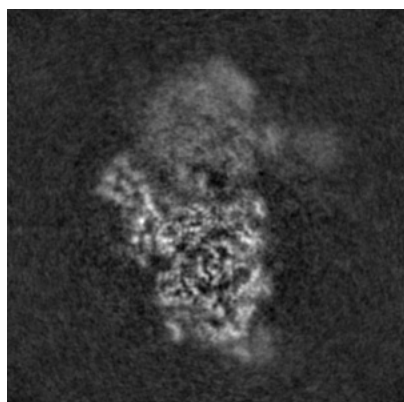


Y Index: 178

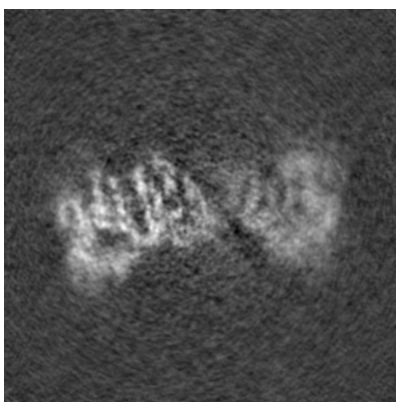


Z Index: 126

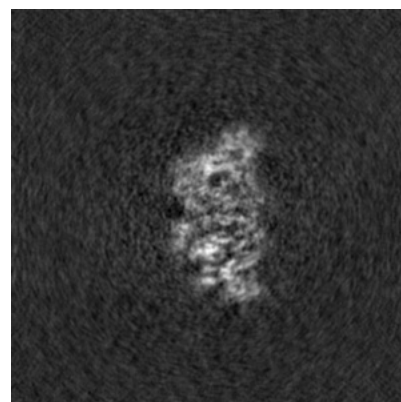
### 6.3.2 Raw map



X Index: 148



Y Index: 174

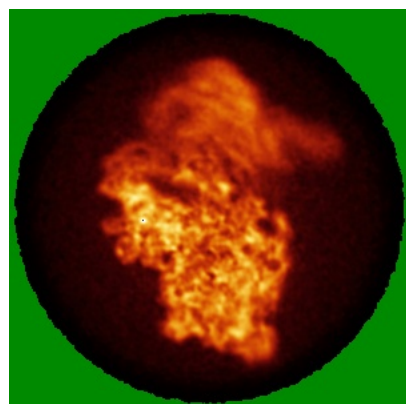


Z Index: 126

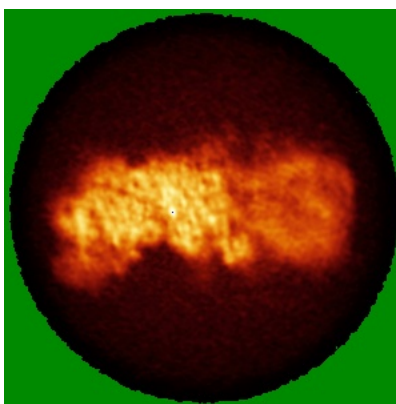
The images above show the largest variance slices of the map in three orthogonal directions.

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

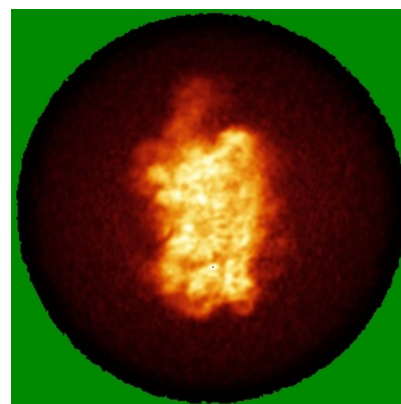
### 6.4.1 Primary map



X



Y

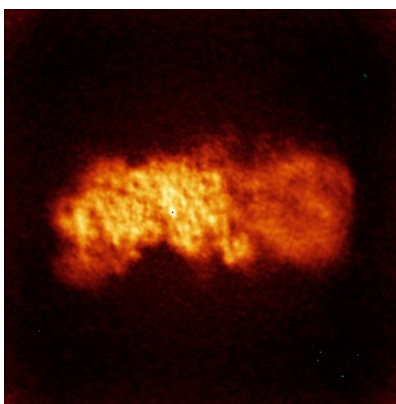


Z

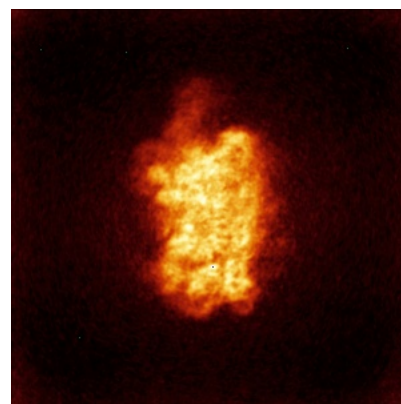
### 6.4.2 Raw map



X



Y



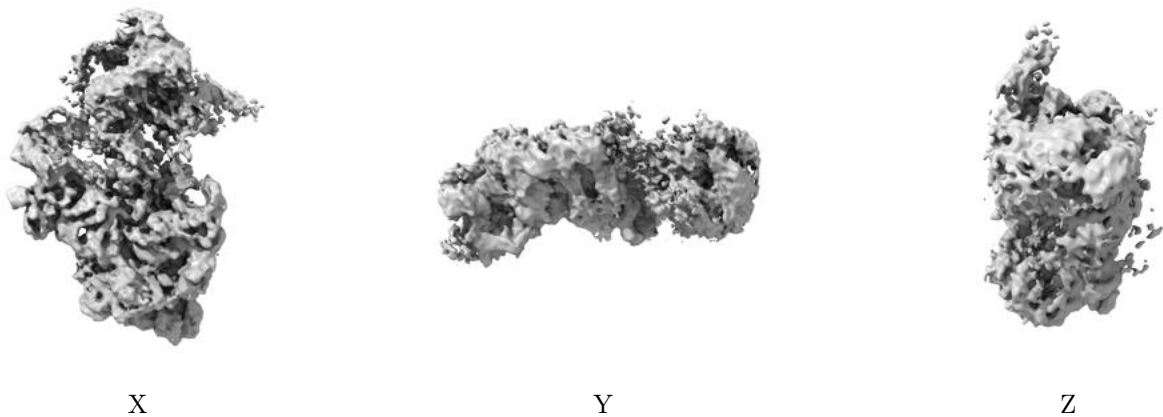
Z

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.



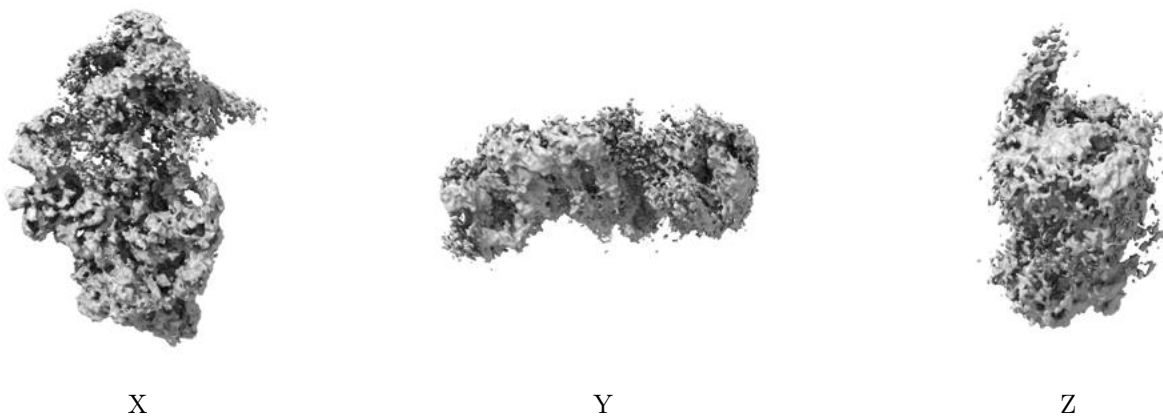
## 6.5 Orthogonal surface views [i](#)

### 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.

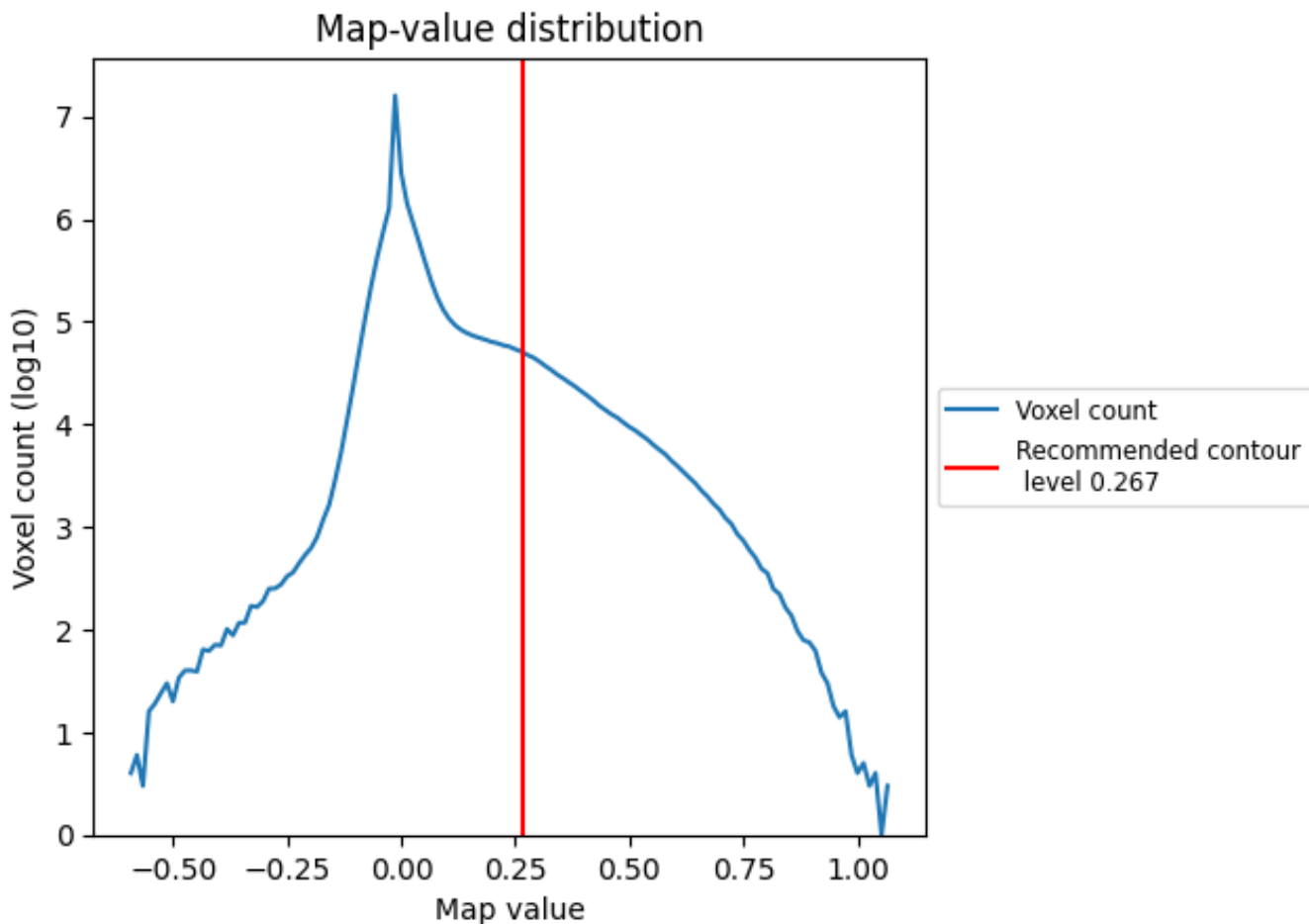
## 6.6 Mask visualisation [i](#)

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.

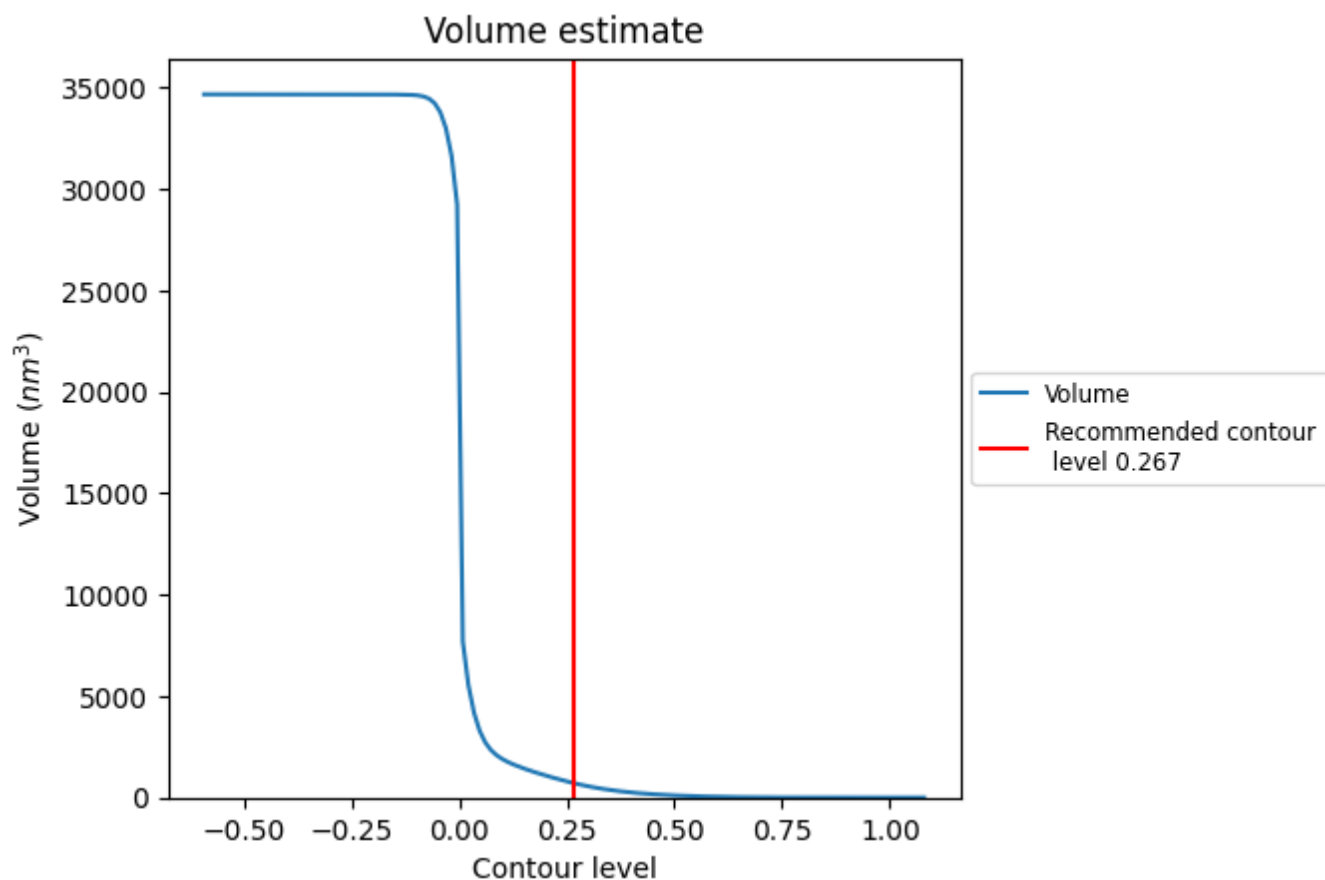
### 7.1 Map-value distribution [i](#)



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.



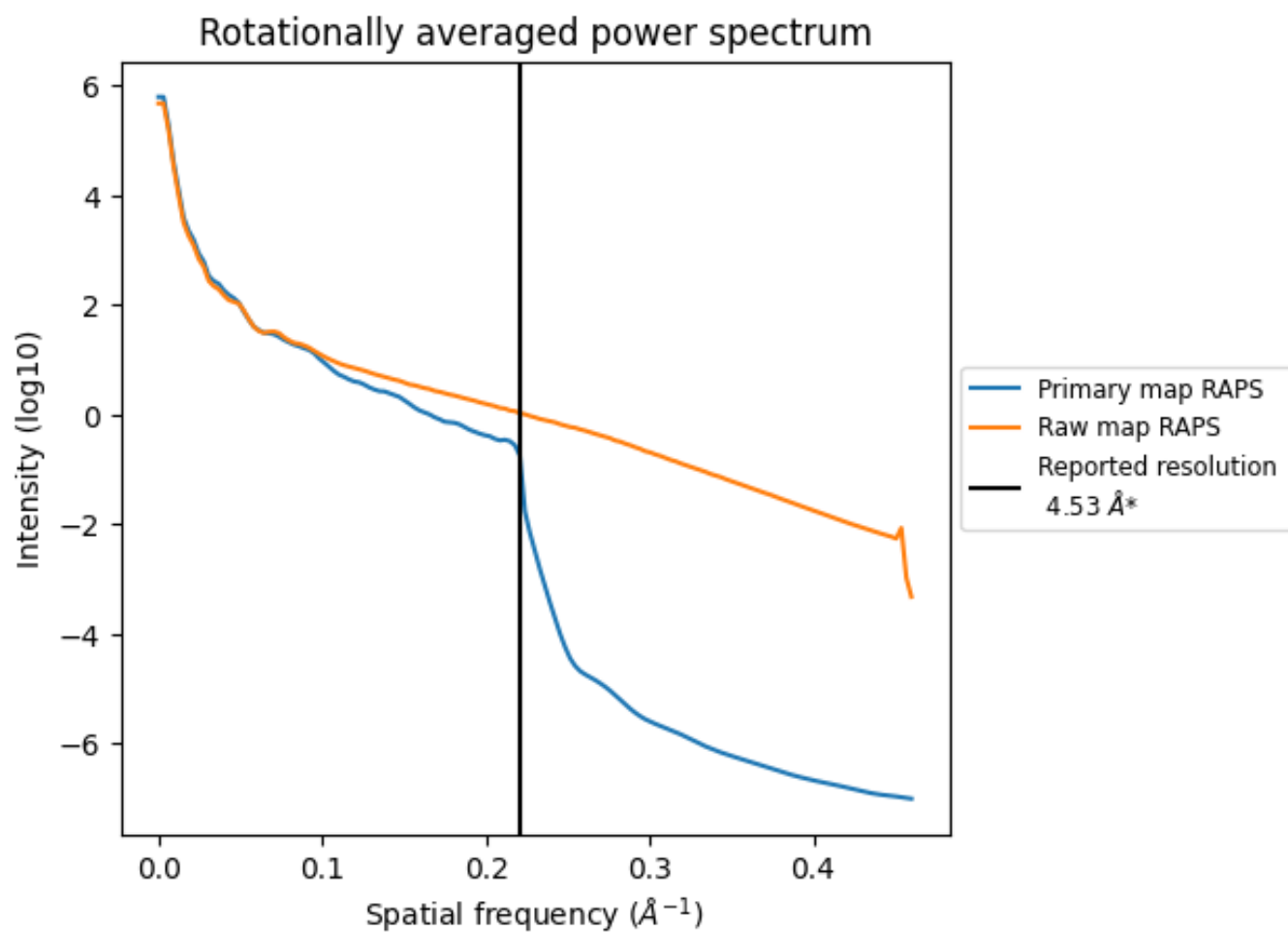
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 708  $\text{nm}^3$ ; 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 i

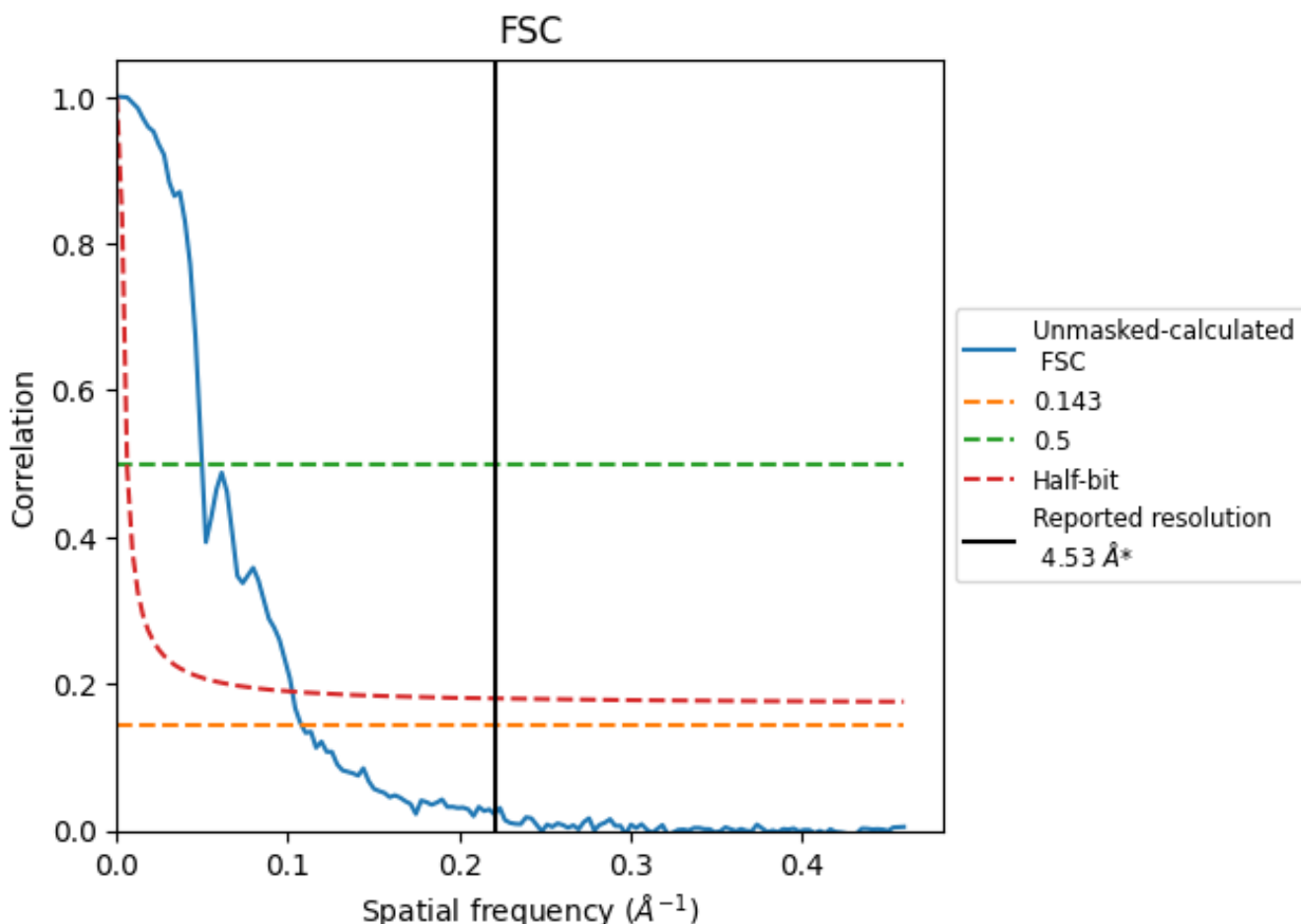


\*Reported resolution corresponds to spatial frequency of 0.221 Å<sup>-1</sup>

## 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 0.221 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

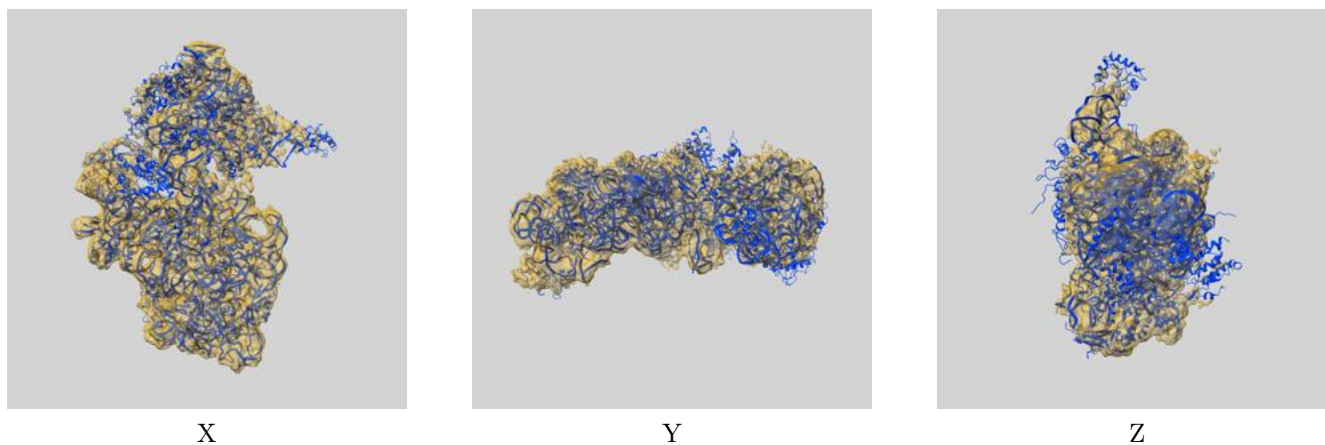
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.25	20.12	9.75

\*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](#)

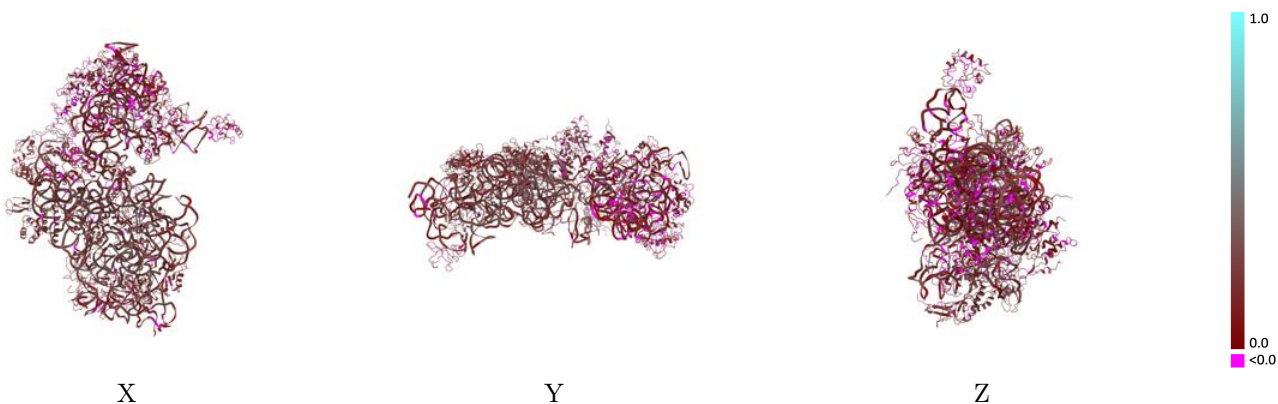
This section contains information regarding the fit between EMDB map EMD-37734 and PDB model 8WQ4. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



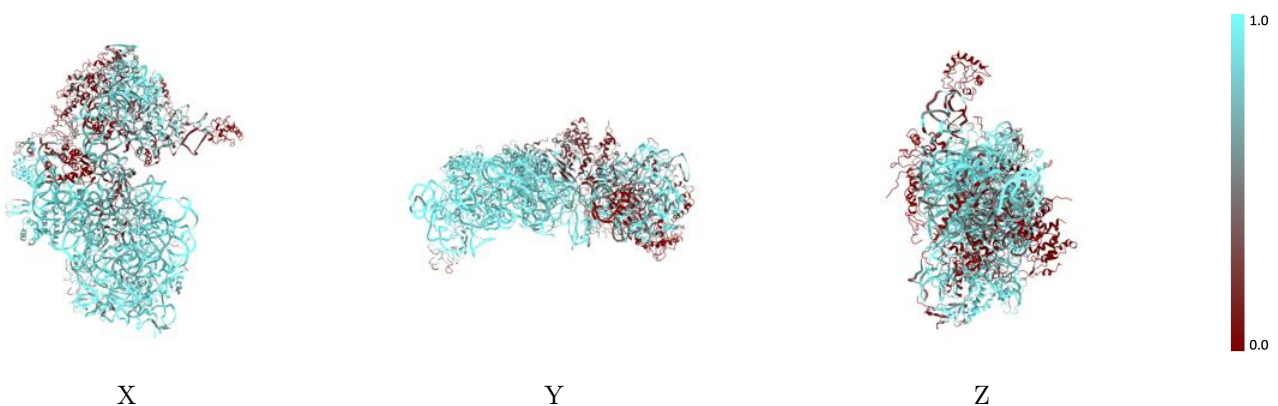
The images above show the 3D surface view of the map at the recommended contour level 0.267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



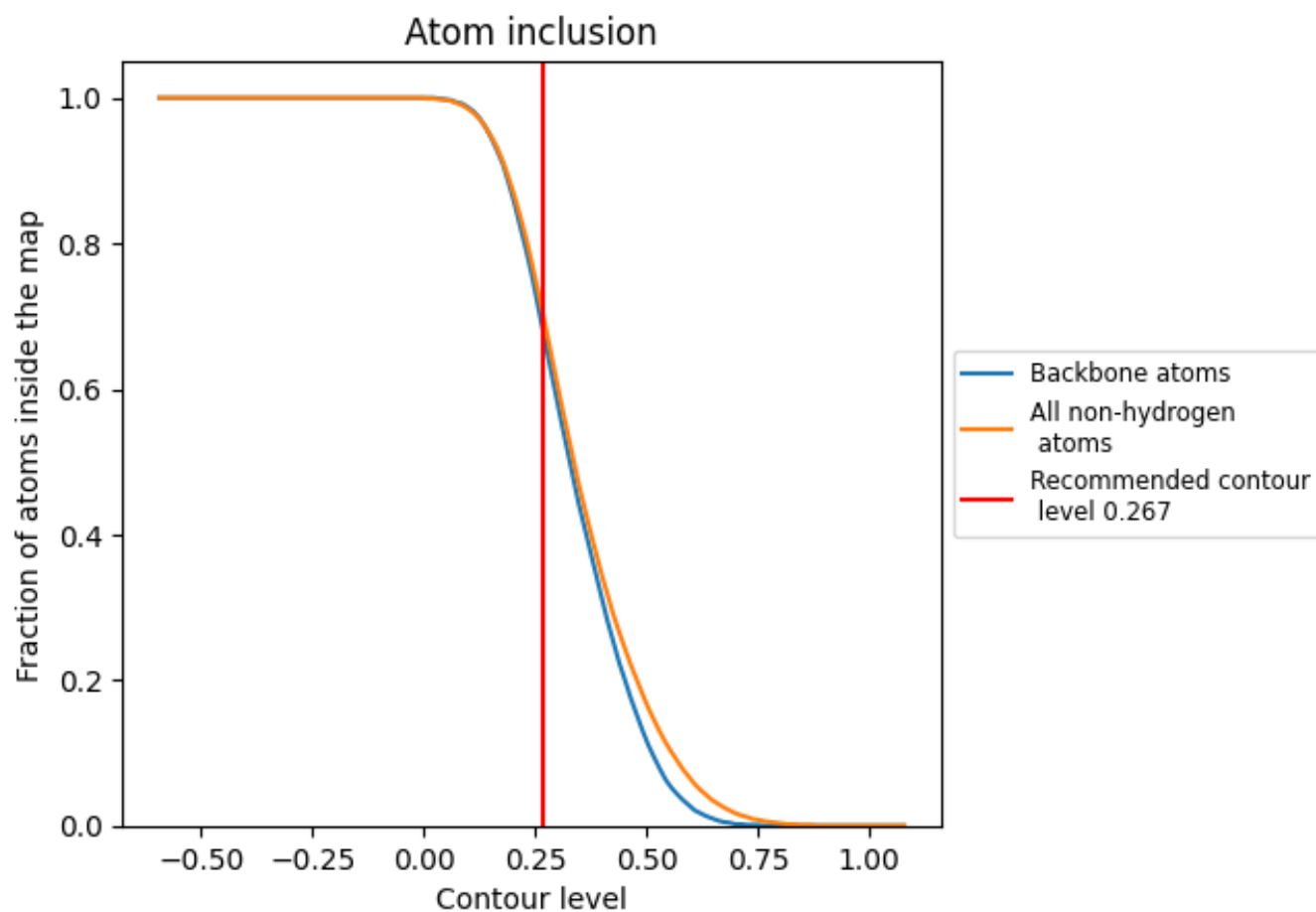
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

