



wwPDB EM Validation Summary Report ⓘ

May 14, 2024 – 12:40 PM JST

PDB ID : 8WKP
EMDB ID : EMD-37604
Title : Structural basis of translation inhibition by a valine tRNA-derived fragment
Authors : Wang, Y.H.; Zhou, J.
Deposited on : 2023-09-28
Resolution : 4.62 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:

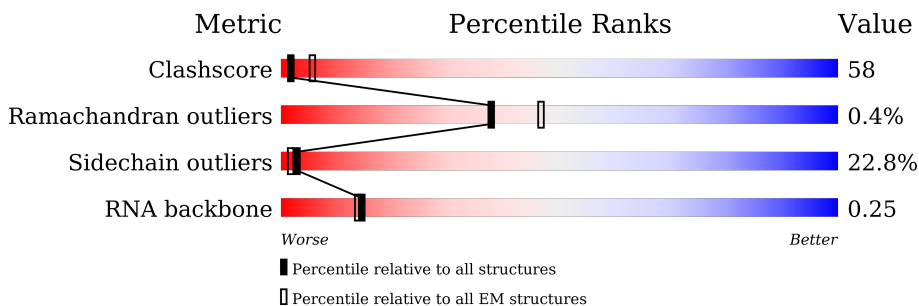
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 4.62 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.









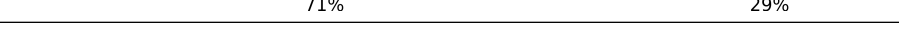
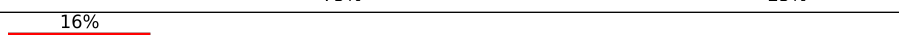
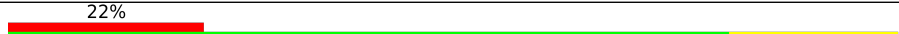












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 ≥ 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	
2	VTRF	26	
3	AS2P	196	
4	AS4E	240	
5	AS4P	166	
6	AS5P	204	
7	AS6E	105	

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Mol	Chain	Length	Quality of chain
8	AS8E	126	 82% 18%
9	S11P	128	 10% 83% 17%
10	S12P	143	 83% 17%
11	S15P	149	 77% 23%
12	S17P	111	 75% 25%
13	S24E	96	 84% 16%
14	S27E	59	 71% 29%
15	S3AE	189	 75% 25%
16	AS3P	201	 16% 85% 15%
17	AS7P	193	 22% 81% 19%
18	AS9P	136	 18% 78% 22%
19	S10P	100	 5% 77% 23%
20	S13P	147	 78% 22%
21	S14P	52	 8% 75% 23%
22	S17E	62	 56% 77% 23%
23	S19E	150	 12% 83% 17%
24	S19P	115	 23% 81% 19%
25	S28E	63	 32% 71% 27%
26	SL7A	123	 59% 93% 7%
27	S27A	54	 74% 26%
28	AS8P	130	 79% 21%

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 56789 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 (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	VTRF	25	536	238	91	182	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 S28e.

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

- Molecule 26 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 27 is a protein called 30S ribosomal protein S27ae.

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

- 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		

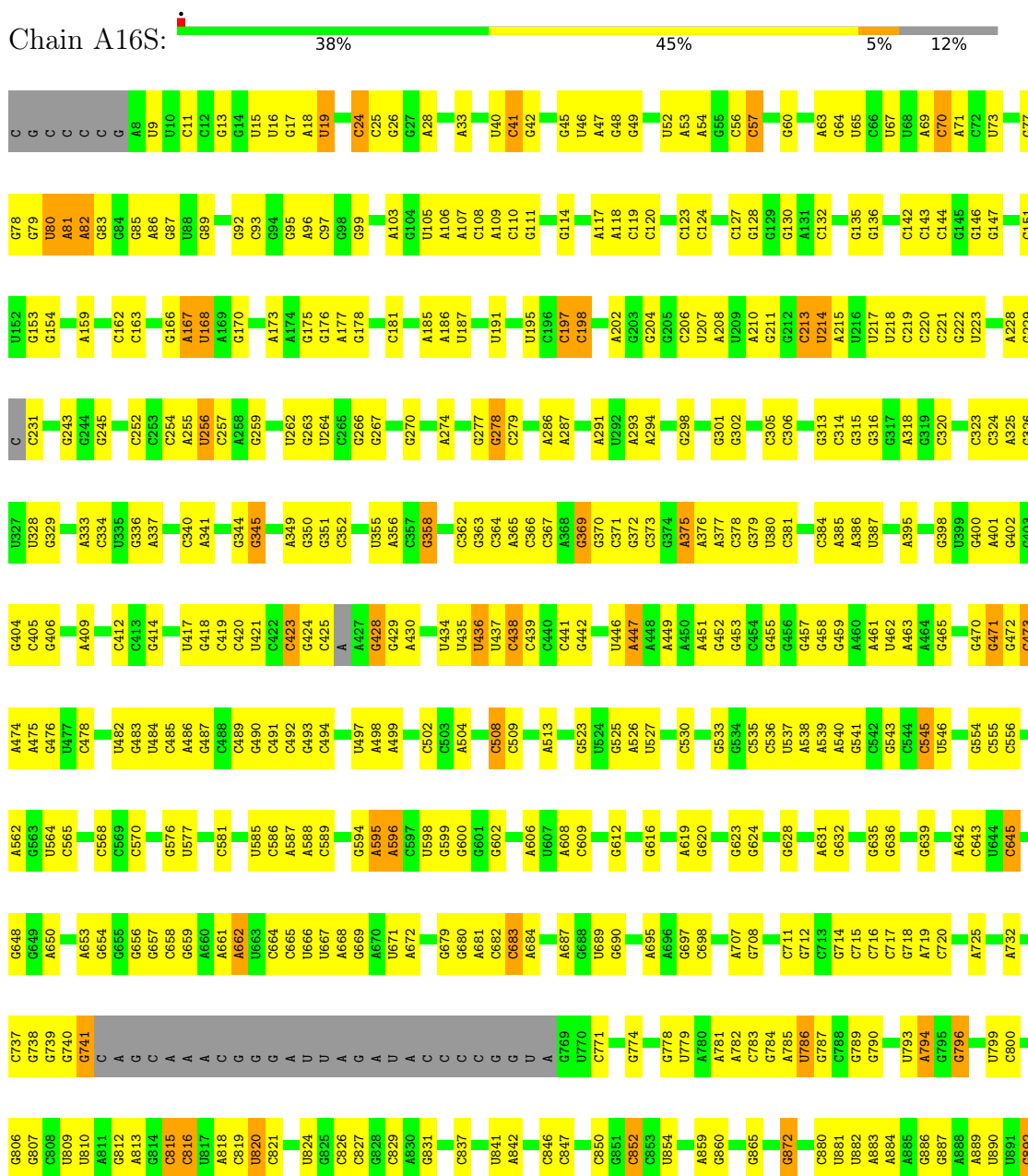
- Molecule 29 is UNKNOWN (three-letter code: UNK) (formula: C₄H₉NO₂) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
29	A16S	4	Total	C	N	O	0
			20	12	4	4	
29	AS2P	34	Total	C	N	O	0
			171	102	34	35	
29	AS5P	13	Total	C	N	O	0
			65	39	13	13	
29	AS8P	6	Total	C	N	O	0
			30	18	6	6	

3 Residue-property plots

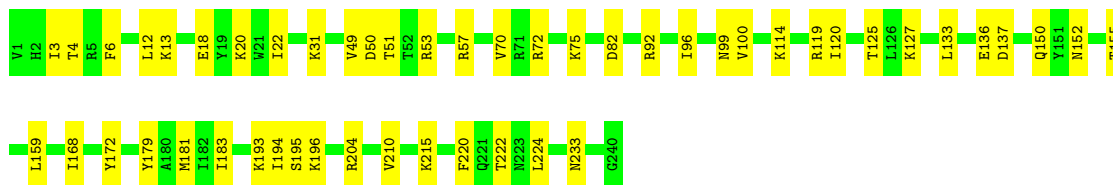
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: RNA (1328-MER)

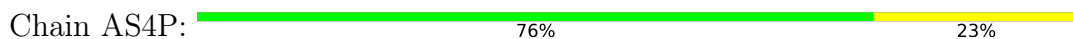




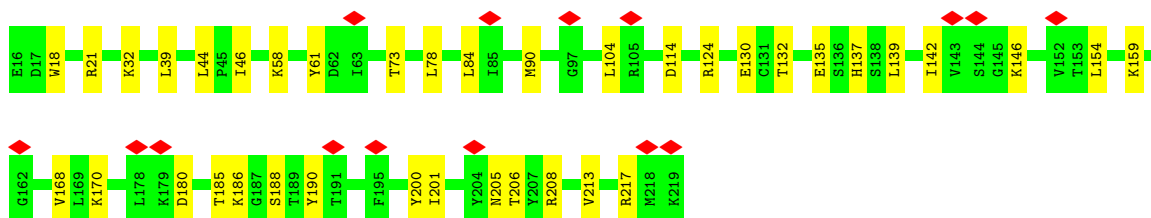
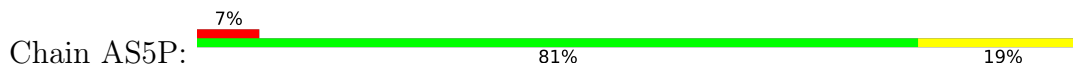
- Molecule 4: 30S ribosomal protein S4e



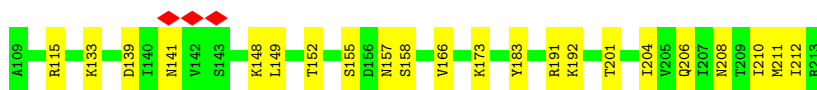
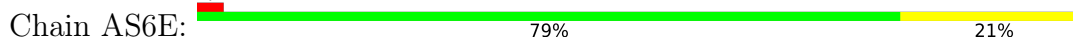
- Molecule 5: 30S ribosomal protein S4



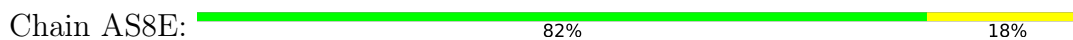
- Molecule 6: 30S ribosomal protein S5



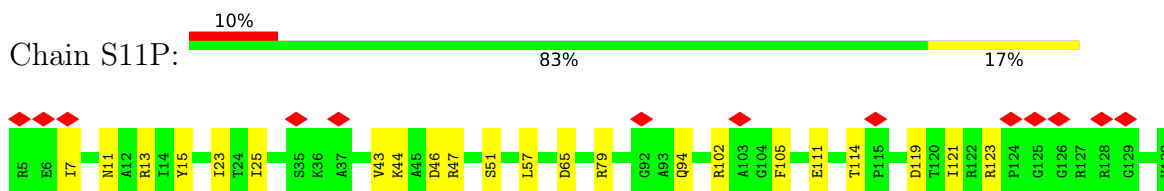
- Molecule 7: 30S ribosomal protein S6e



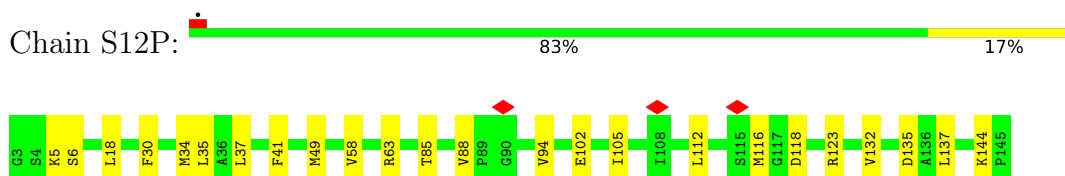
- Molecule 8: 30S ribosomal protein S8e



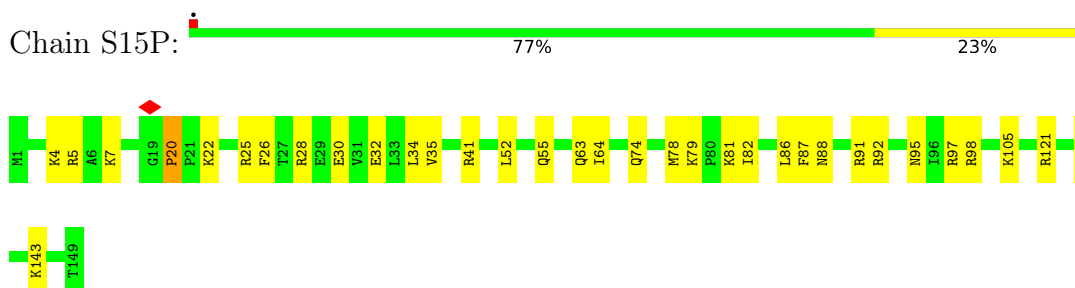
- Molecule 9: 30S ribosomal protein S11



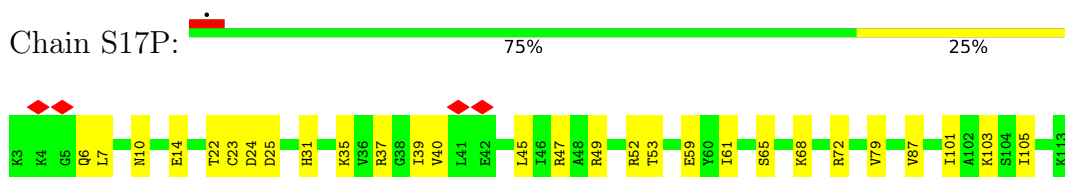
- Molecule 10: 30S ribosomal protein S12



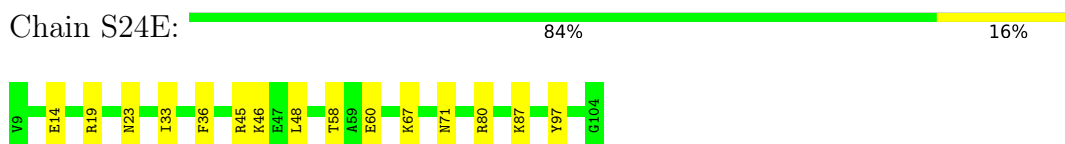
- Molecule 11: 30S ribosomal protein S15



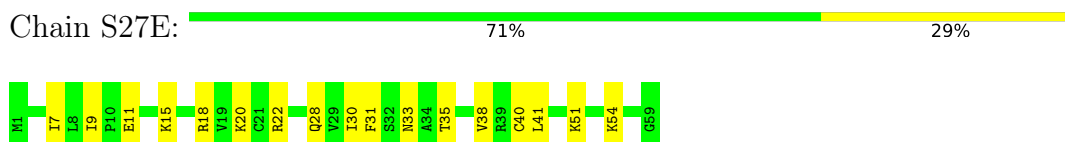
- Molecule 12: 30S ribosomal protein S17




- Molecule 13: 30S ribosomal protein S24e

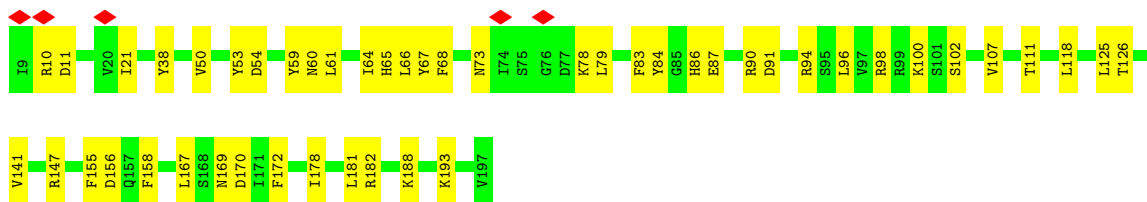


- Molecule 14: 30S ribosomal protein S27e




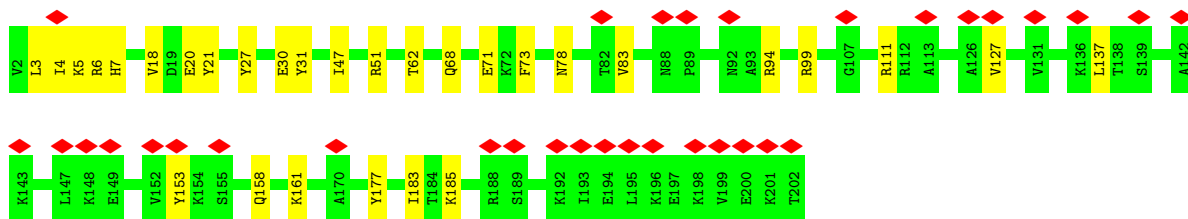
- Molecule 15: 30S ribosomal protein S3Ae

Chain S3AE:  75% 25%




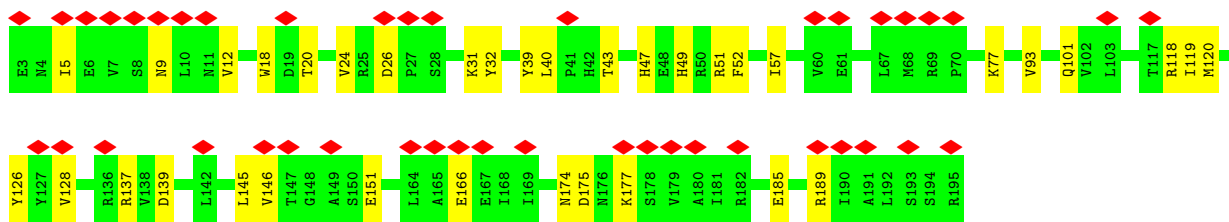
- Molecule 16: 30S ribosomal protein S3

Chain AS3P:  16% 85% 15%




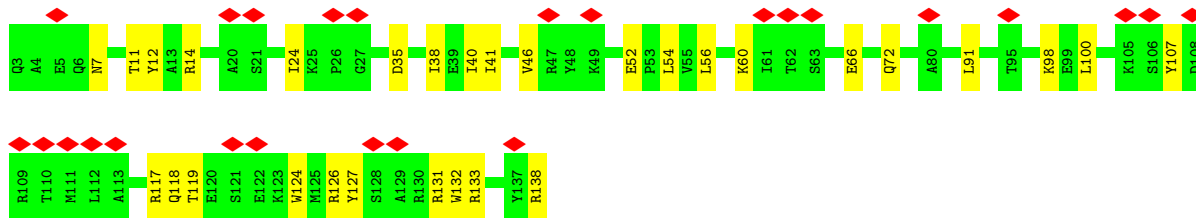
- Molecule 17: 30S ribosomal protein S7

Chain AS7P:  22% 81% 19%




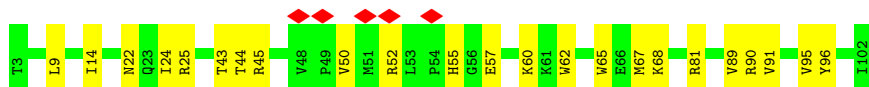
- Molecule 18: 30S ribosomal protein S9

Chain AS9P:  18% 78% 22%

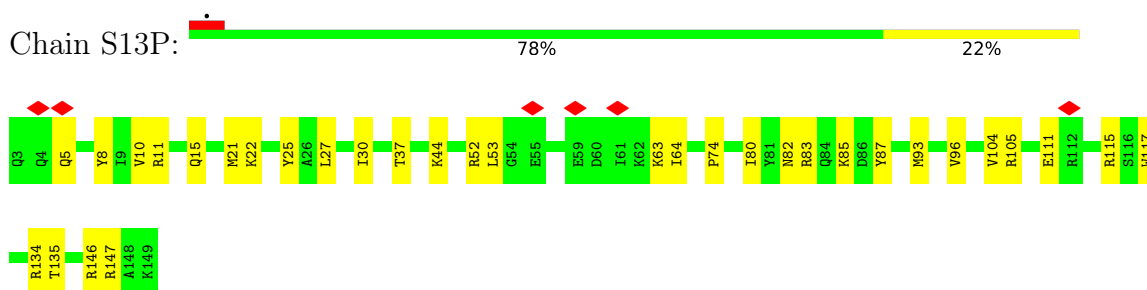


- Molecule 19: 30S ribosomal protein S10

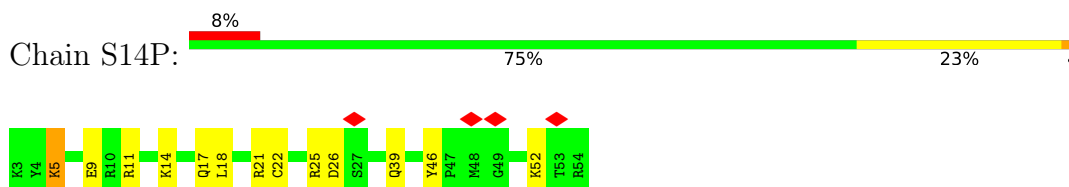
Chain S10P:  5% 77% 23%



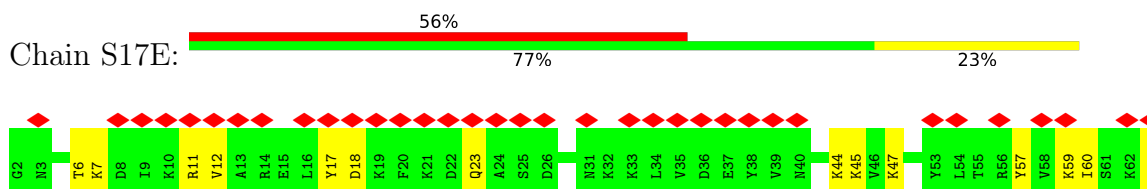
- Molecule 20: 30S ribosomal protein S13



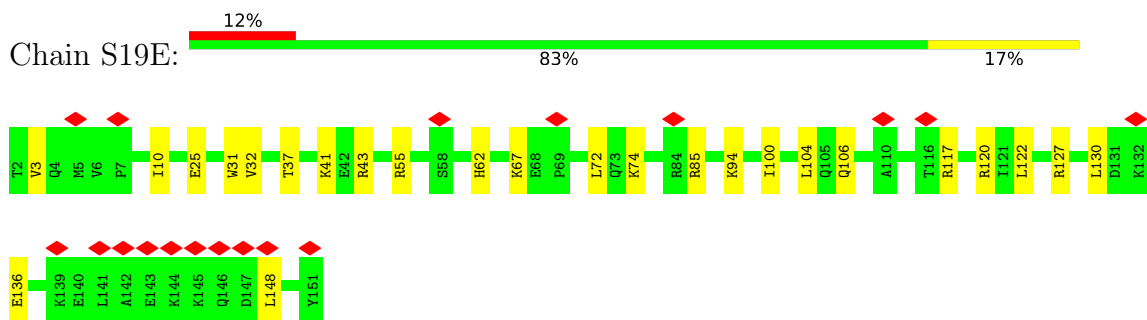
- Molecule 21: 30S ribosomal protein S14 type Z



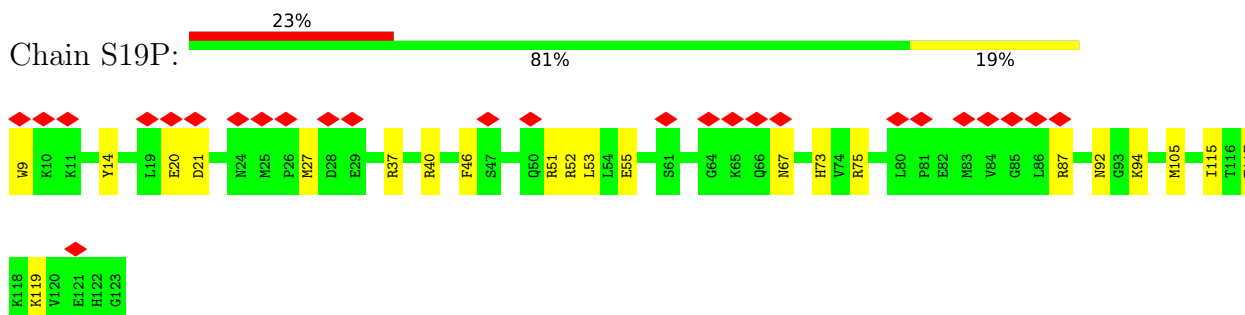
- Molecule 22: 30S ribosomal protein S17e



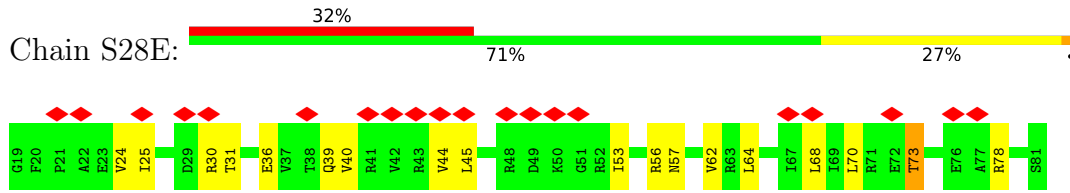
- Molecule 23: 30S ribosomal protein S19e



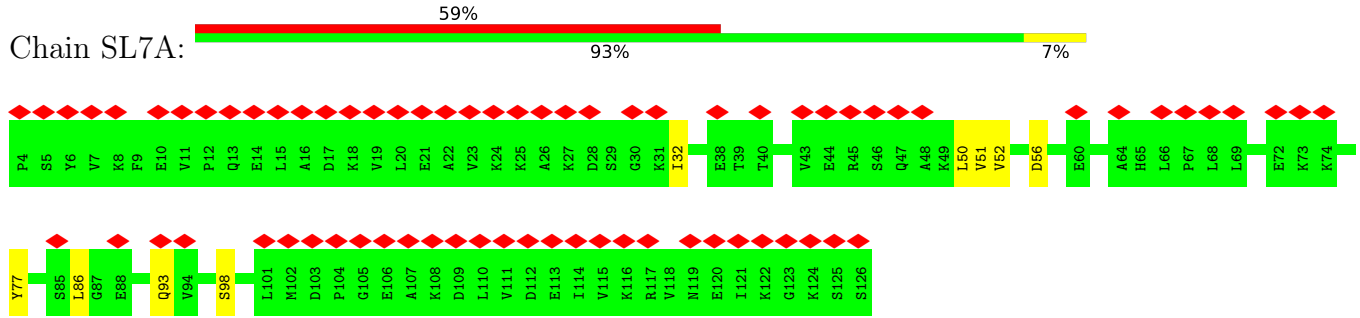
- Molecule 24: 30S ribosomal protein S19



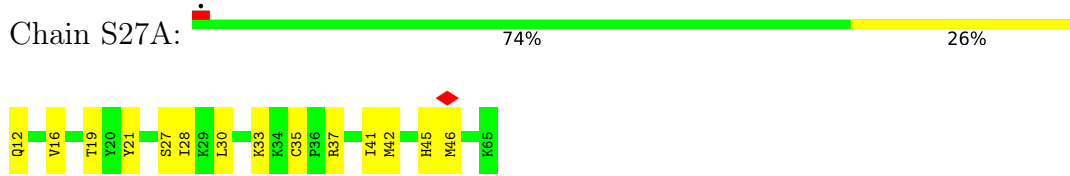
- Molecule 25: 30S ribosomal protein S28e



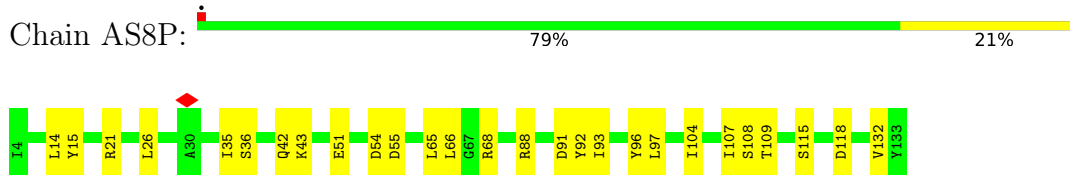
• Molecule 26: 50S ribosomal protein L7Ae



• Molecule 27: 30S ribosomal protein S27ae



• 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	5357	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	1.315	Depositor
Minimum map value	-0.571	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.225	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	0.77	7/31855 (0.0%)	1.23	216/49699 (0.4%)
2	VTRF	0.74	1/598 (0.2%)	1.40	12/931 (1.3%)
3	AS2P	0.30	0/1621	0.56	0/2202
4	AS4E	0.35	0/1956	0.59	0/2635
5	AS4P	0.35	0/1399	0.58	0/1883
6	AS5P	0.34	0/1631	0.58	0/2200
7	AS6E	0.31	0/815	0.61	0/1093
8	AS8E	0.37	0/1005	0.59	0/1342
9	S11P	0.32	0/976	0.61	0/1315
10	S12P	0.35	0/1120	0.60	0/1495
11	S15P	0.36	0/1250	0.60	0/1677
12	S17P	0.38	0/899	0.60	0/1203
13	S24E	0.33	0/769	0.52	0/1034
14	S27E	0.33	0/465	0.57	0/618
15	S3AE	0.34	0/1573	0.58	0/2115
16	AS3P	0.29	0/1599	0.55	0/2147
17	AS7P	0.26	0/1561	0.55	0/2105
18	AS9P	0.27	0/1115	0.59	0/1496
19	S10P	0.26	0/840	0.56	0/1132
20	S13P	0.26	0/1221	0.59	0/1634
21	S14P	0.32	0/441	0.61	0/583
22	S17E	0.28	0/523	0.50	0/696
23	S19E	0.28	0/1267	0.53	0/1705
24	S19P	0.28	0/986	0.60	0/1310
25	S28E	0.26	0/500	0.63	0/669
26	SL7A	0.26	0/946	0.51	0/1272
27	S27A	0.34	0/444	0.61	0/590
28	AS8P	0.38	0/1046	0.58	0/1410
All	All	0.60	8/60421 (0.0%)	1.01	228/88191 (0.3%)

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
5	AS4P	0	1
11	S15P	0	1
15	S3AE	0	1
16	AS3P	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A16S	594	G	O3'-P	7.35	1.70	1.61
1	A16S	80	U	O3'-P	7.32	1.70	1.61
1	A16S	231	C	O3'-P	7.31	1.70	1.61
1	A16S	596	A	O3'-P	6.58	1.69	1.61
1	A16S	109	A	N9-C4	-6.48	1.33	1.37

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	1314	U	C5-C4-O4	12.99	133.69	125.90
1	A16S	996	C	N1-C2-O2	11.65	125.89	118.90
1	A16S	996	C	N3-C2-O2	-11.64	113.75	121.90
1	A16S	423	C	N1-C2-O2	10.09	124.96	118.90
1	A16S	1314	U	N3-C4-O4	-10.01	112.39	119.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	AS3P	78	ASN	Peptide
5	AS4P	162	LYS	Peptide
11	S15P	20	PRO	Peptide
15	S3AE	181	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A16S	28462	0	0	0	0
2	VTRF	536	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	S28E	498	0	0	0	0
26	SL7A	935	0	0	0	0
27	S27A	435	0	0	0	0
28	AS8P	1028	0	0	0	0
29	A16S	20	0	0	0	0
29	AS2P	171	0	0	0	0
29	AS5P	65	0	0	0	0
29	AS8P	30	0	0	0	0
All	All	56789	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 58.

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%)	177 (91%)	17 (9%)	0	100	100
4	AS4E	238/240 (99%)	201 (84%)	37 (16%)	0	100	100
5	AS4P	164/166 (99%)	137 (84%)	26 (16%)	1 (1%)	25	65
6	AS5P	202/204 (99%)	174 (86%)	28 (14%)	0	100	100
7	AS6E	103/105 (98%)	87 (84%)	16 (16%)	0	100	100
8	AS8E	124/126 (98%)	112 (90%)	12 (10%)	0	100	100
9	S11P	126/128 (98%)	98 (78%)	28 (22%)	0	100	100
10	S12P	141/143 (99%)	117 (83%)	24 (17%)	0	100	100
11	S15P	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22	62
12	S17P	109/111 (98%)	94 (86%)	15 (14%)	0	100	100
13	S24E	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
14	S27E	57/59 (97%)	46 (81%)	11 (19%)	0	100	100
15	S3AE	187/189 (99%)	156 (83%)	31 (17%)	0	100	100
16	AS3P	199/201 (99%)	169 (85%)	27 (14%)	3 (2%)	10	46
17	AS7P	191/193 (99%)	157 (82%)	33 (17%)	1 (0%)	29	68
18	AS9P	134/136 (98%)	110 (82%)	24 (18%)	0	100	100
19	S10P	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
20	S13P	145/147 (99%)	124 (86%)	19 (13%)	2 (1%)	11	47
21	S14P	50/52 (96%)	33 (66%)	16 (32%)	1 (2%)	7	40
22	S17E	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
23	S19E	148/150 (99%)	128 (86%)	19 (13%)	1 (1%)	22	62
24	S19P	113/115 (98%)	91 (80%)	22 (20%)	0	100	100
25	S28E	61/63 (97%)	41 (67%)	17 (28%)	3 (5%)	2	23
26	SL7A	121/123 (98%)	105 (87%)	15 (12%)	1 (1%)	19	60
27	S27A	52/54 (96%)	37 (71%)	14 (27%)	1 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	AS8P	128/130 (98%)	107 (84%)	21 (16%)	0	100	100
All	All	3386/3438 (98%)	2853 (84%)	518 (15%)	15 (0%)	38	72

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	AS3P	83	VAL
21	S14P	5	LYS
16	AS3P	183	ILE
17	AS7P	128	VAL
25	S28E	44	VAL

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%)	137 (79%)	37 (21%)	1	6
4	AS4E	210/210 (100%)	160 (76%)	50 (24%)	0	5
5	AS4P	149/149 (100%)	110 (74%)	39 (26%)	0	4
6	AS5P	174/174 (100%)	136 (78%)	38 (22%)	1	6
7	AS6E	88/88 (100%)	66 (75%)	22 (25%)	0	4
8	AS8E	106/106 (100%)	83 (78%)	23 (22%)	1	6
9	S11P	94/94 (100%)	72 (77%)	22 (23%)	1	5
10	S12P	116/116 (100%)	92 (79%)	24 (21%)	1	7
11	S15P	133/133 (100%)	99 (74%)	34 (26%)	0	4
12	S17P	97/97 (100%)	69 (71%)	28 (29%)	0	3
13	S24E	84/84 (100%)	69 (82%)	15 (18%)	2	11
14	S27E	51/51 (100%)	34 (67%)	17 (33%)	0	2
15	S3AE	170/170 (100%)	123 (72%)	47 (28%)	0	3
16	AS3P	165/165 (100%)	139 (84%)	26 (16%)	2	15
17	AS7P	166/166 (100%)	131 (79%)	35 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AS9P	113/113 (100%)	83 (74%)	30 (26%)	0	4
19	S10P	92/92 (100%)	69 (75%)	23 (25%)	0	4
20	S13P	129/129 (100%)	98 (76%)	31 (24%)	0	5
21	S14P	45/45 (100%)	32 (71%)	13 (29%)	0	3
22	S17E	57/57 (100%)	43 (75%)	14 (25%)	0	4
23	S19E	134/134 (100%)	110 (82%)	24 (18%)	2	11
24	S19P	106/106 (100%)	84 (79%)	22 (21%)	1	7
25	S28E	54/54 (100%)	38 (70%)	16 (30%)	0	2
26	SL7A	104/104 (100%)	96 (92%)	8 (8%)	13	39
27	S27A	47/47 (100%)	34 (72%)	13 (28%)	0	3
28	AS8P	111/111 (100%)	84 (76%)	27 (24%)	0	4
All	All	2969/2969 (100%)	2291 (77%)	678 (23%)	3	6

5 of 678 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	AS9P	38	ILE
23	S19E	41	LYS
18	AS9P	107	TYR
18	AS9P	35	ASP
20	S13P	44	LYS

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A16S	1319/1501 (87%)	703 (53%)	72 (5%)
2	VTRF	24/26 (92%)	20 (83%)	2 (8%)
All	All	1343/1527 (87%)	723 (53%)	74 (5%)

5 of 723 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A16S	9	U
1	A16S	11	C

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Mol	Chain	Res	Type
1	A16S	13	G
1	A16S	15	U
1	A16S	16	U

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A16S	1204	U
1	A16S	1364	C
1	A16S	1228	G
1	A16S	1286	A
1	A16S	474	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

There are no chain breaks in this entry.

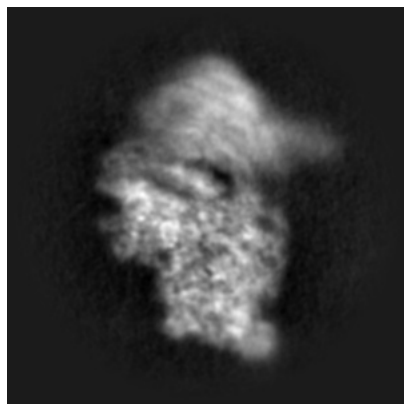
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37604. These allow visual inspection of the internal detail of the map and identification of artifacts.

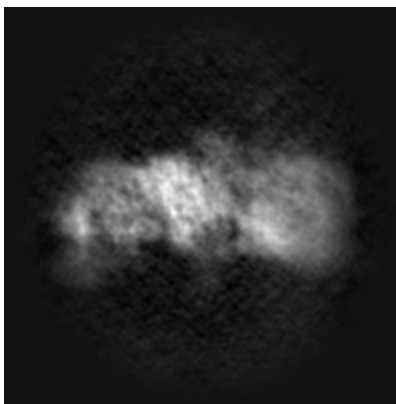
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

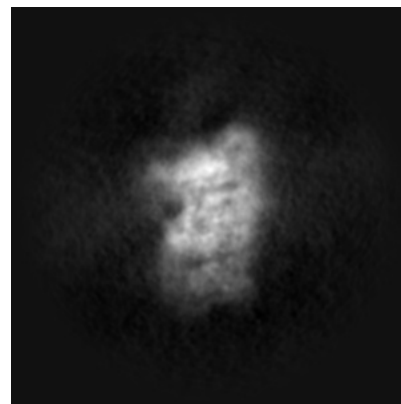
6.1.1 Primary map



X

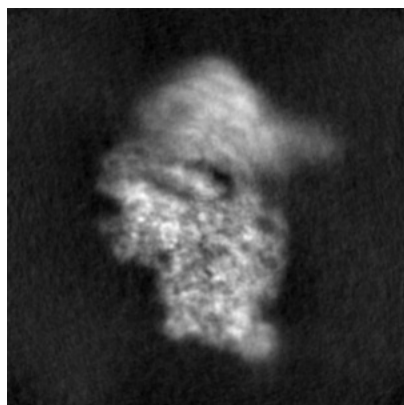


Y

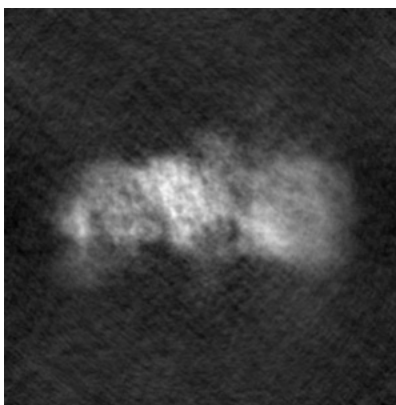


Z

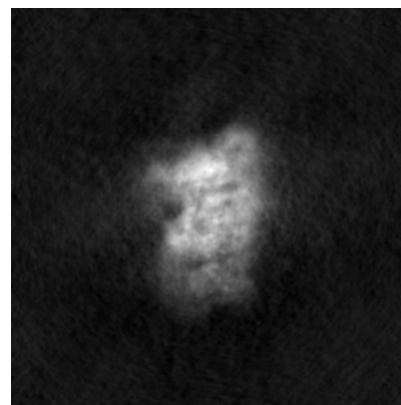
6.1.2 Raw map



X



Y

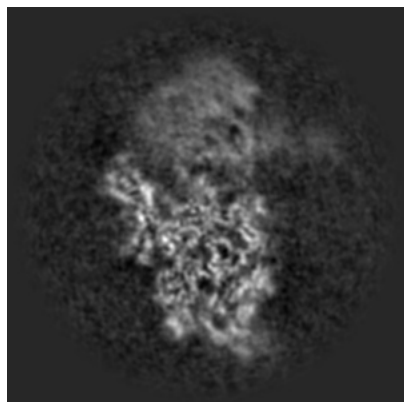


Z

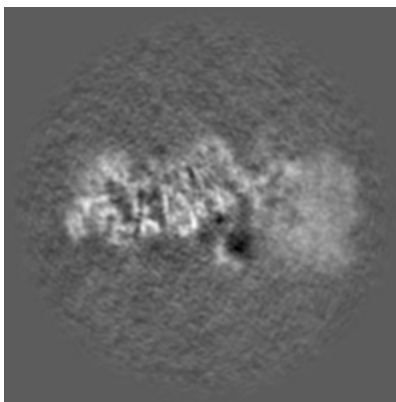
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

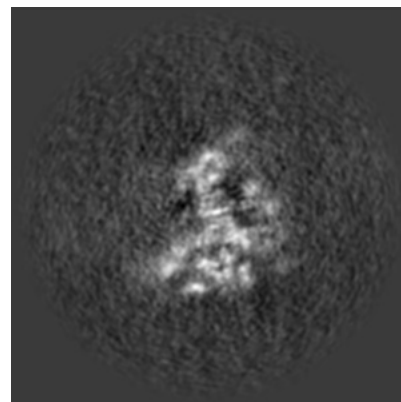
6.2.1 Primary map



X Index: 150

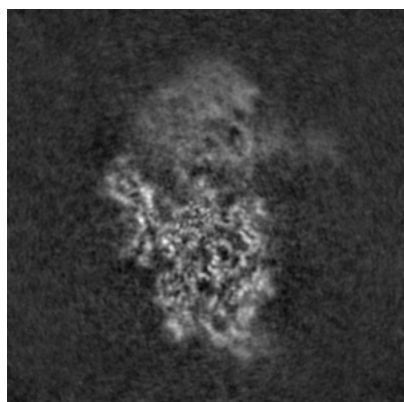


Y Index: 150

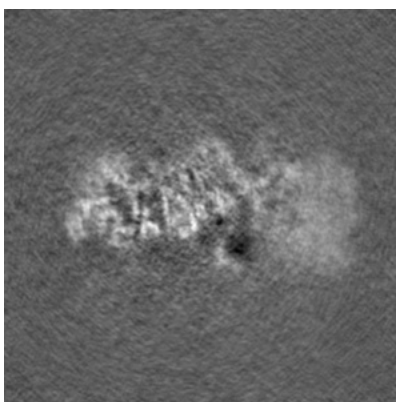


Z Index: 150

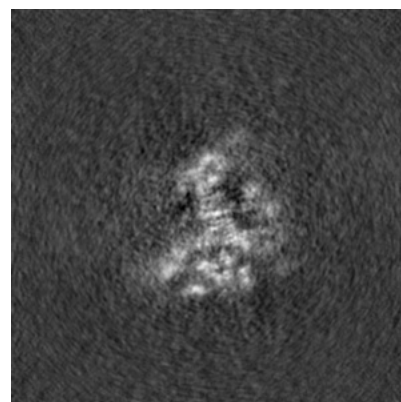
6.2.2 Raw map



X Index: 150



Y Index: 150

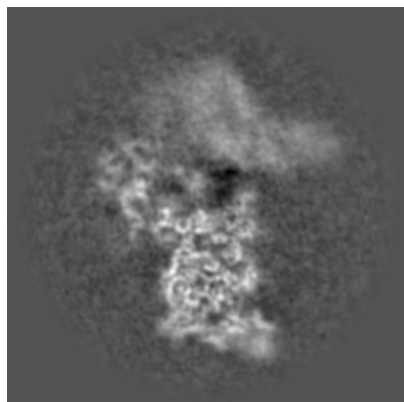


Z Index: 150

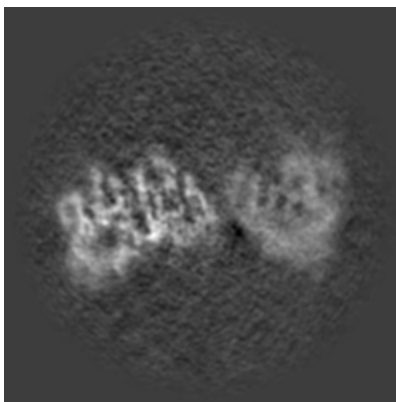
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

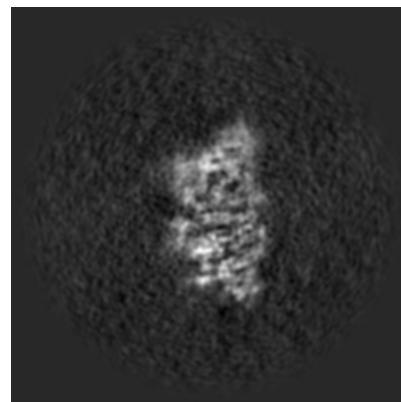
6.3.1 Primary map



X Index: 133

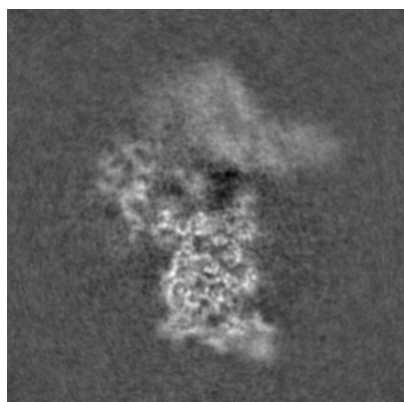


Y Index: 173

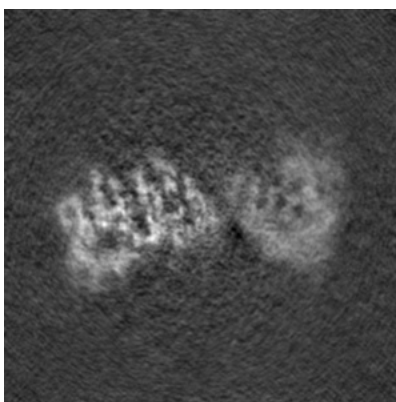


Z Index: 127

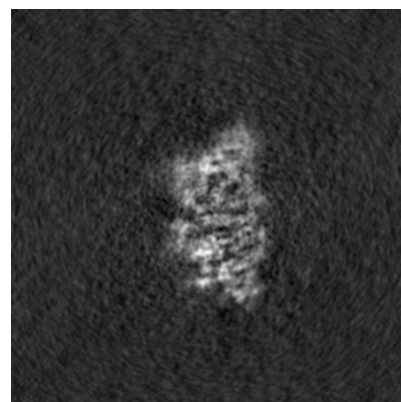
6.3.2 Raw map



X Index: 133



Y Index: 174

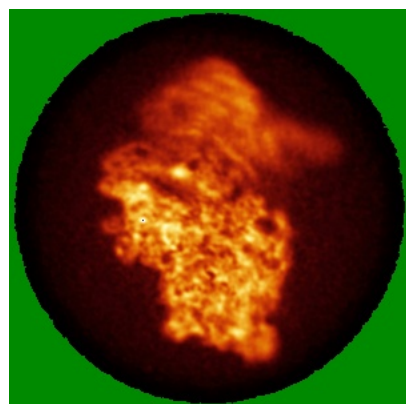


Z Index: 127

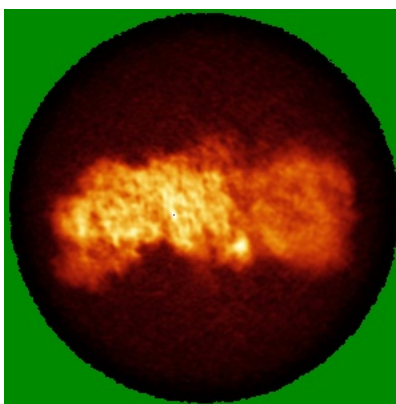
The images above show the largest variance slices of the map in three orthogonal directions.

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

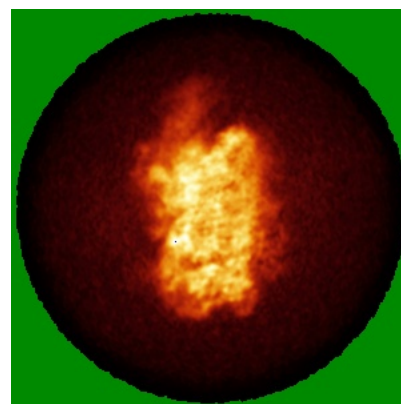
6.4.1 Primary map



X

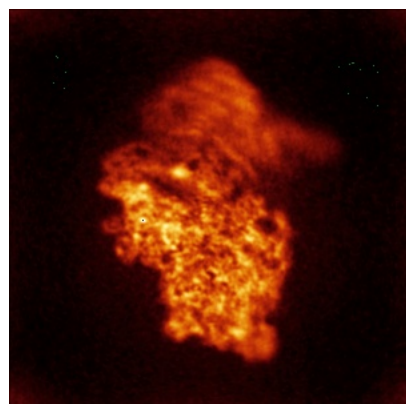


Y

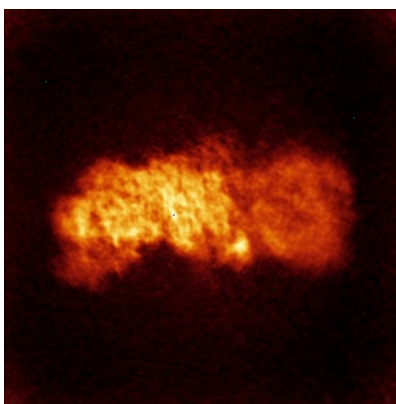


Z

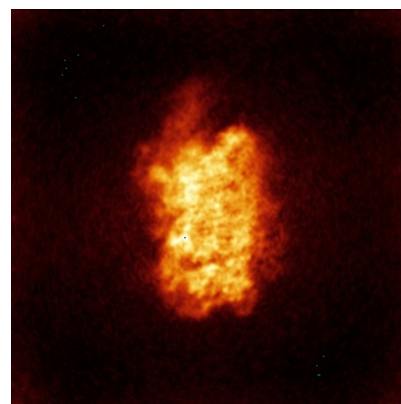
6.4.2 Raw map



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.

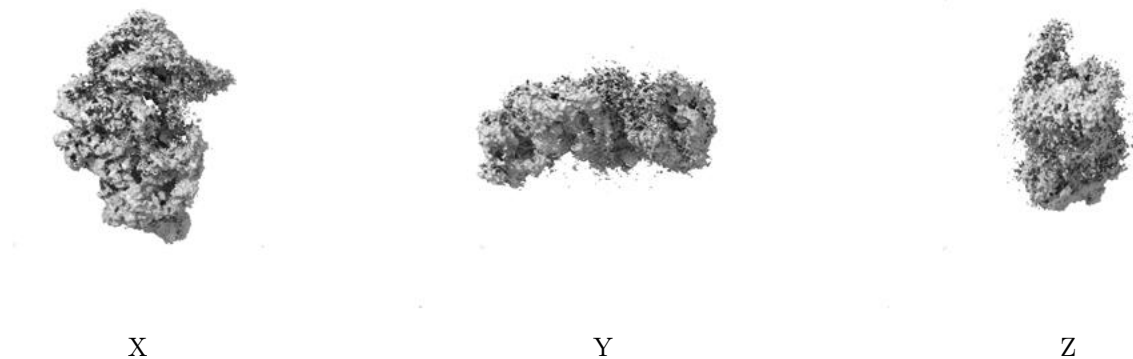
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.225. 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.

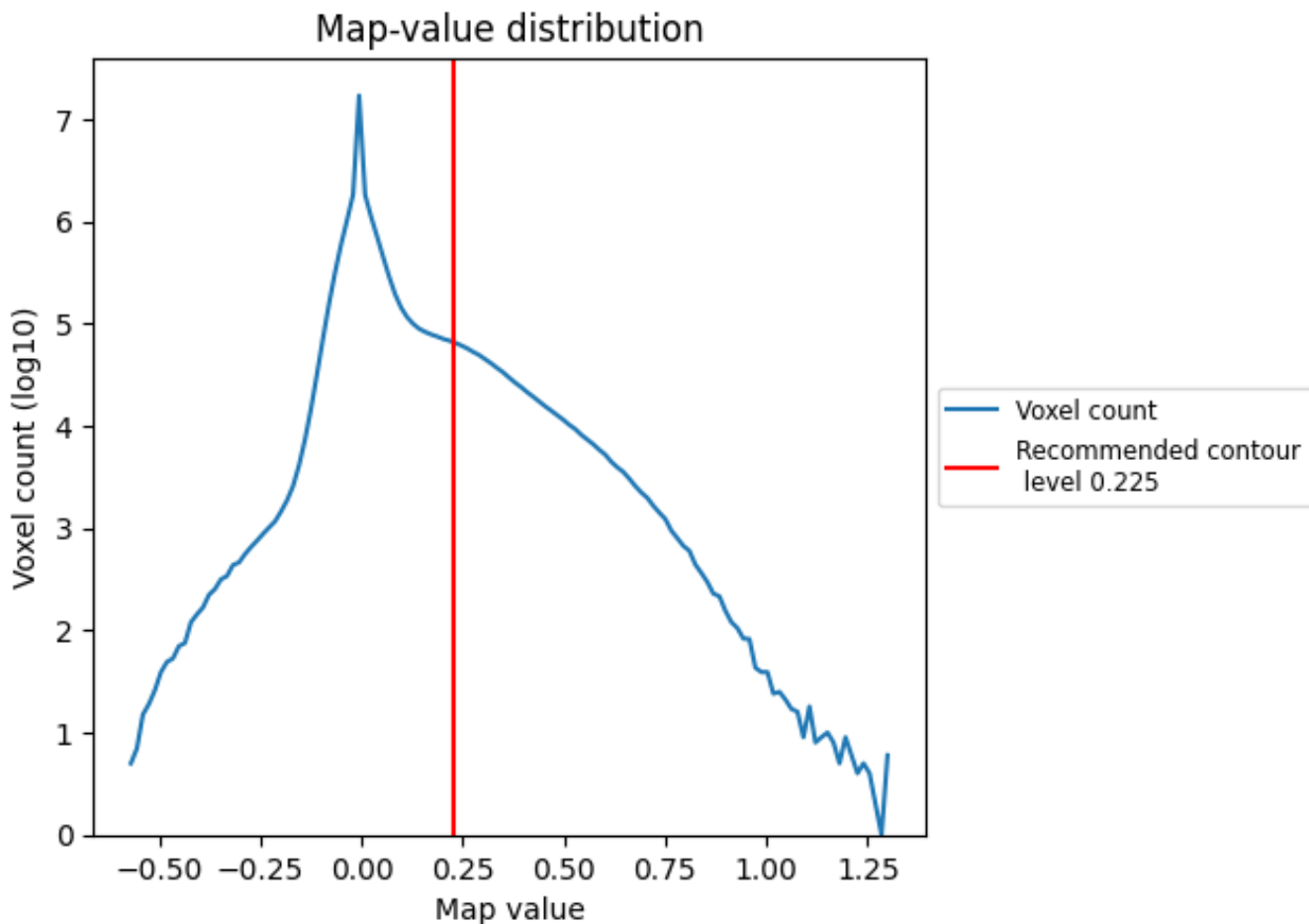
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

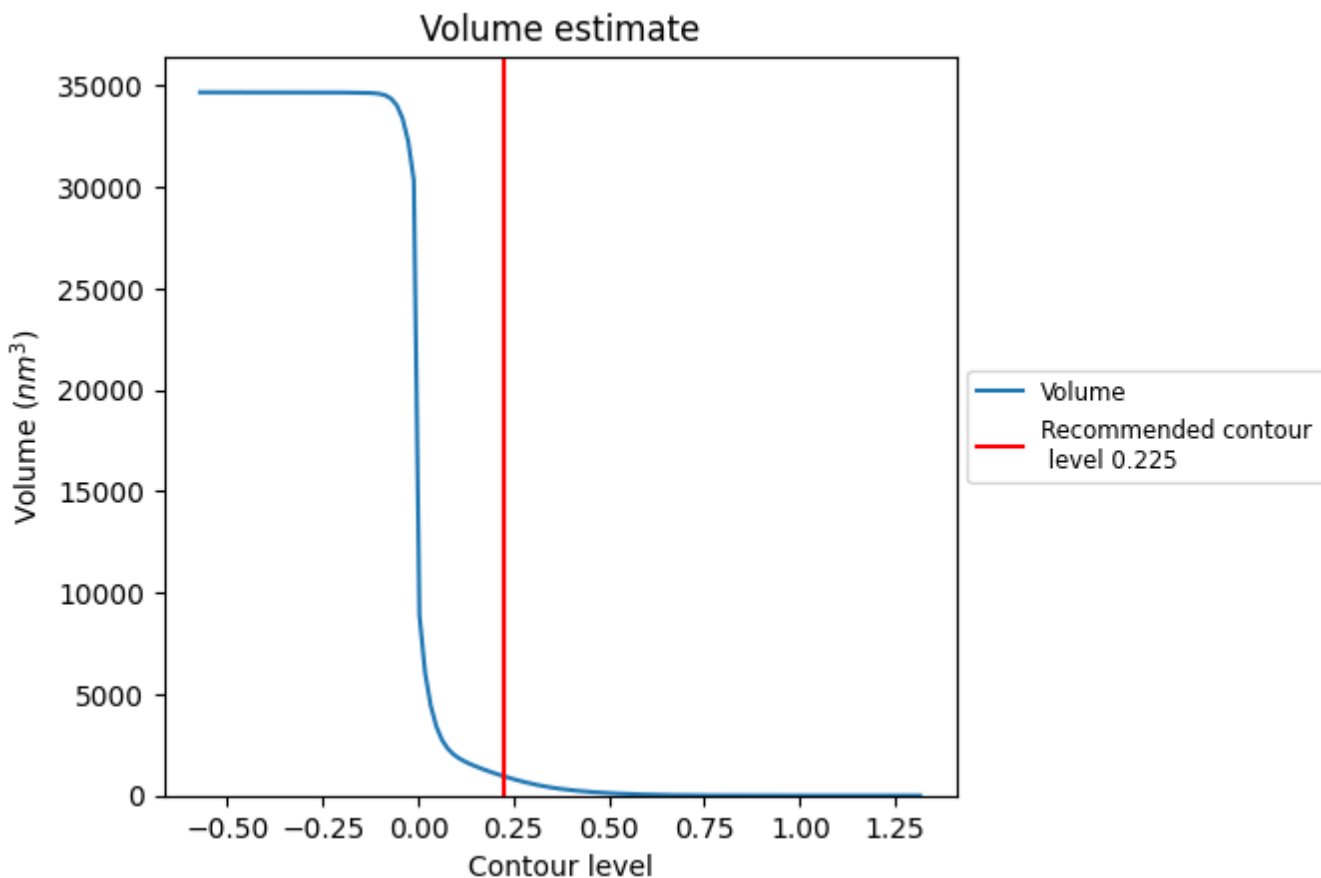
This section contains the results of statistical analysis of the map.

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.

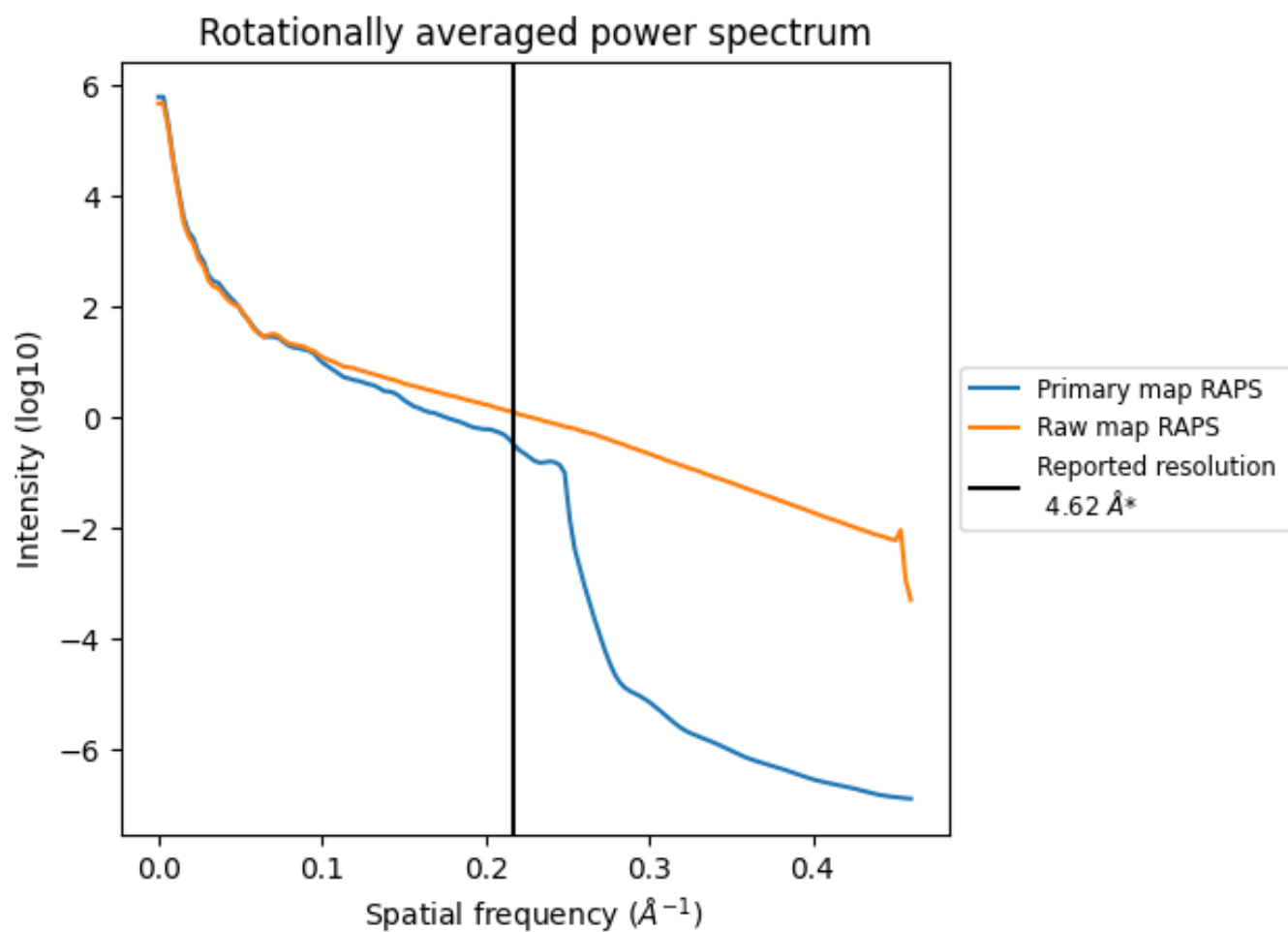
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 951 nm³; this corresponds to an approximate mass of 859 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

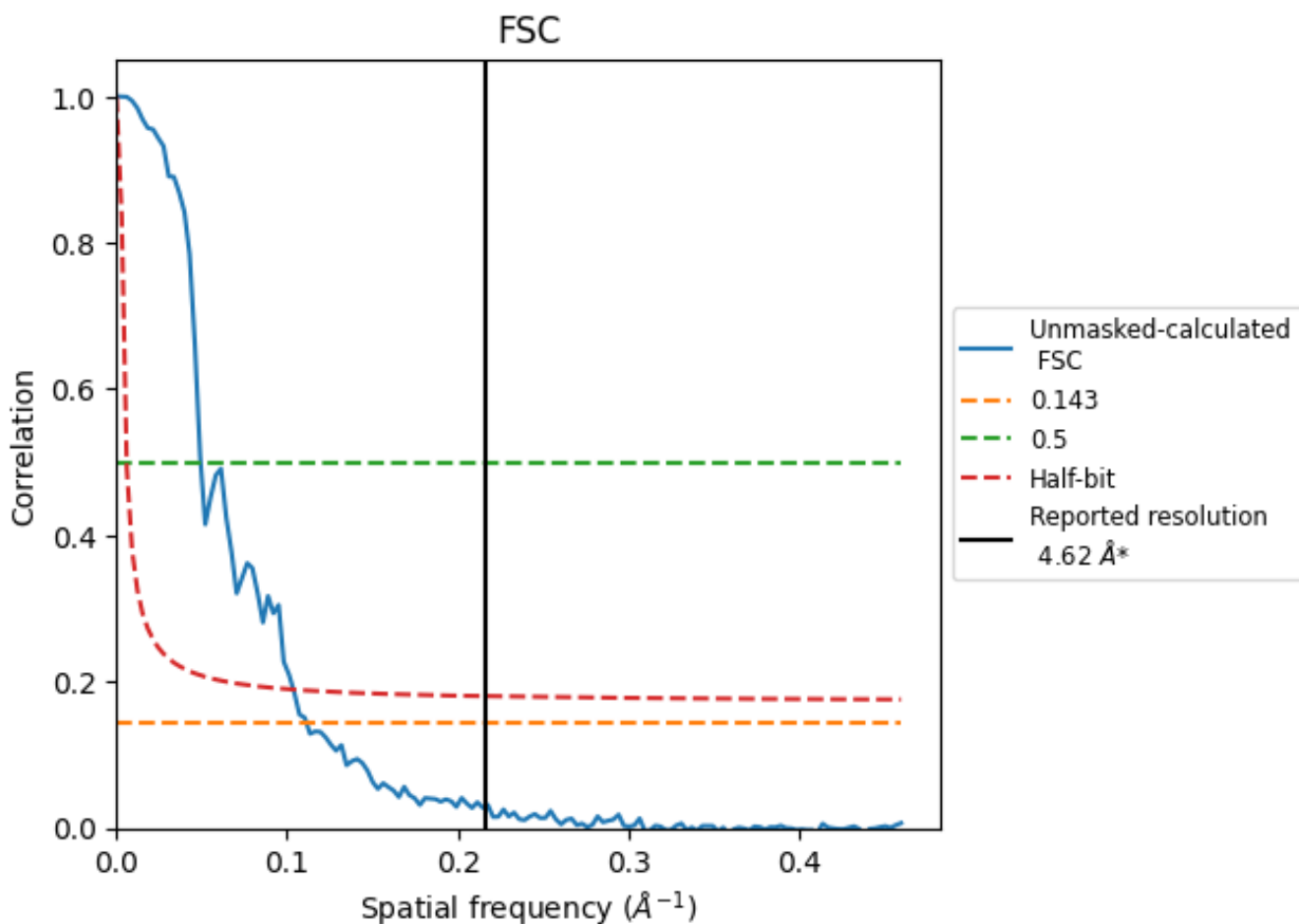


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

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 0.216 Å⁻¹

8.2 Resolution estimates [i](#)

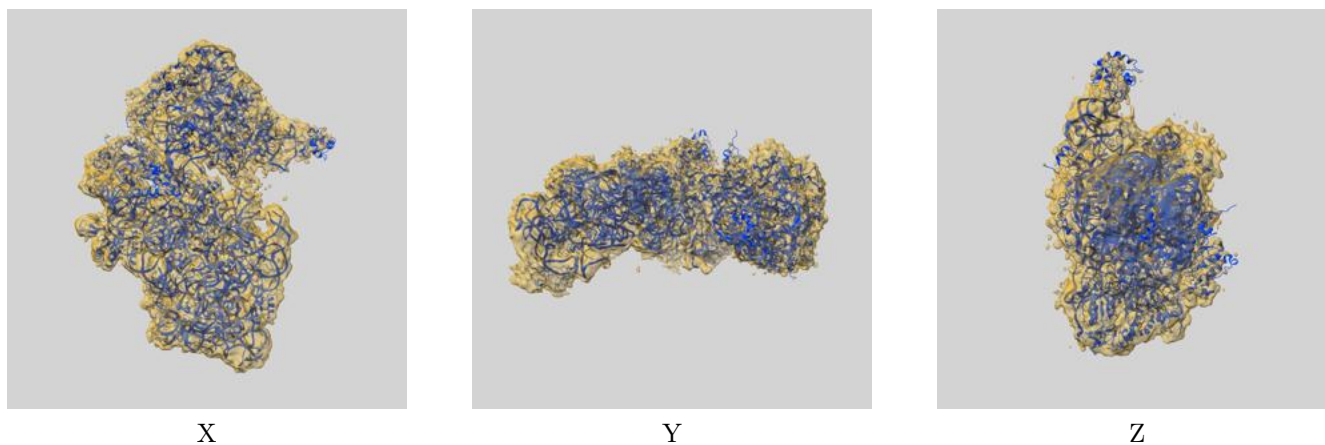
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.97	20.28	9.64

*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 8.97 differs from the reported value 4.62 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37604 and PDB model 8WKP. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



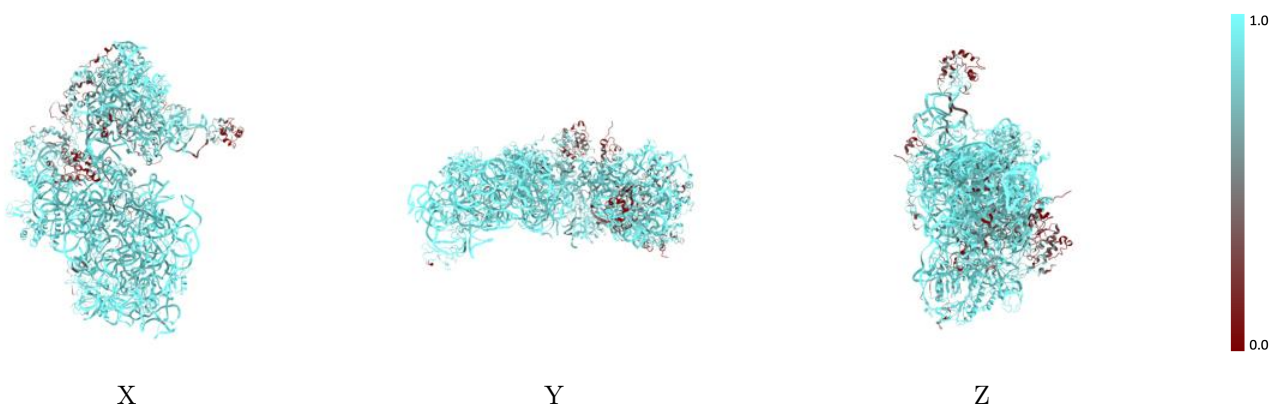
The images above show the 3D surface view of the map at the recommended contour level 0.225 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



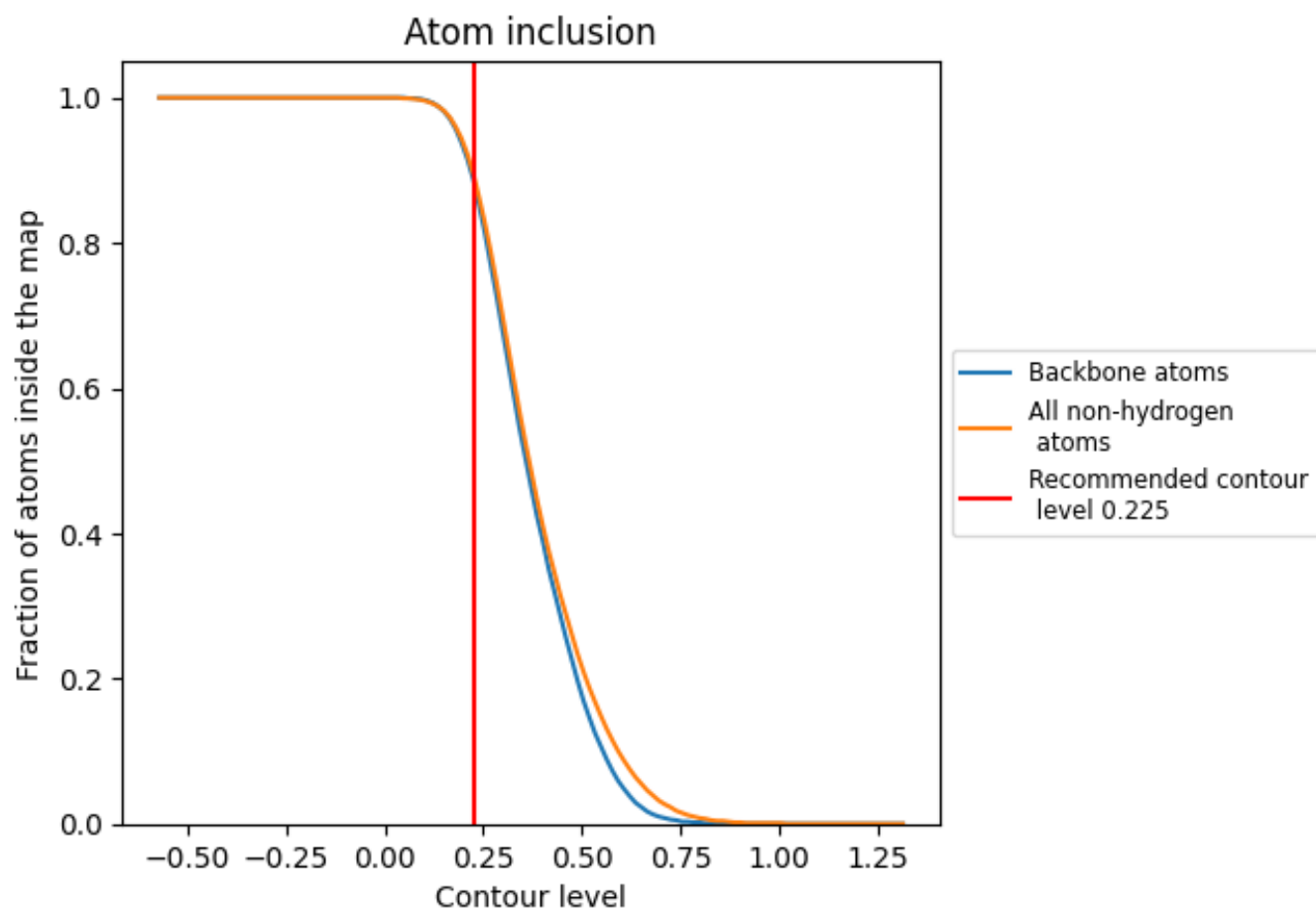
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.225).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.225) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.2420
A16S	 0.9710	 0.2470
AS2P	 0.4030	 0.2570
AS3P	 0.7430	 0.2330
AS4E	 0.9890	 0.2860
AS4P	 0.9500	 0.2820
AS5P	 0.8210	 0.2850
AS6E	 0.9080	 0.2080
AS7P	 0.7020	 0.2030
AS8E	 0.9940	 0.2820
AS8P	 0.9530	 0.3180
AS9P	 0.7410	 0.1870
S10P	 0.9140	 0.1840
S11P	 0.7930	 0.2040
S12P	 0.9560	 0.3110
S13P	 0.9210	 0.1420
S14P	 0.8540	 0.2150
S15P	 0.9680	 0.2820
S17E	 0.4040	 0.2030
S17P	 0.9250	 0.3170
S19E	 0.8200	 0.1490
S19P	 0.6810	 0.1440
S24E	 0.9990	 0.2600
S27A	 0.9360	 0.1720
S27E	 0.9600	 0.2910
S28E	 0.5710	 0.2020
S3AE	 0.9420	 0.2480
SL7A	 0.3840	 0.1620
VTRF	 0.9200	 0.2270

