



## Full wwPDB EM Validation Report ⓘ

Jan 30, 2025 – 02:28 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 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>.

---

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

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

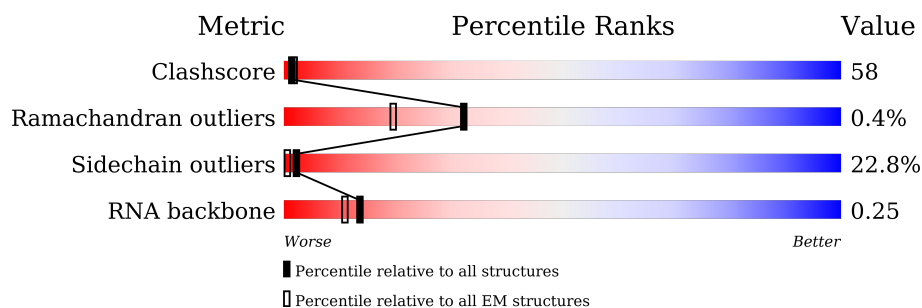
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.62 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.





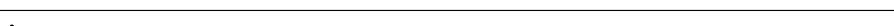


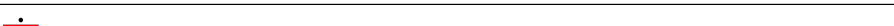






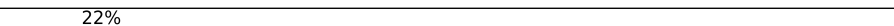



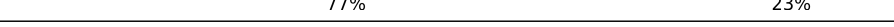




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
2	VTRF	26	
3	AS2P	196	
4	AS4E	240	
5	AS4P	166	
6	AS5P	204	
7	AS6E	105	

Continued on next page...

Continued from previous page...

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called RNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	VTRF	25	Total	C	N	O	P	0	0
			536	238	91	182	25		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 25 is a protein called 30S ribosomal protein S28e.

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

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

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

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

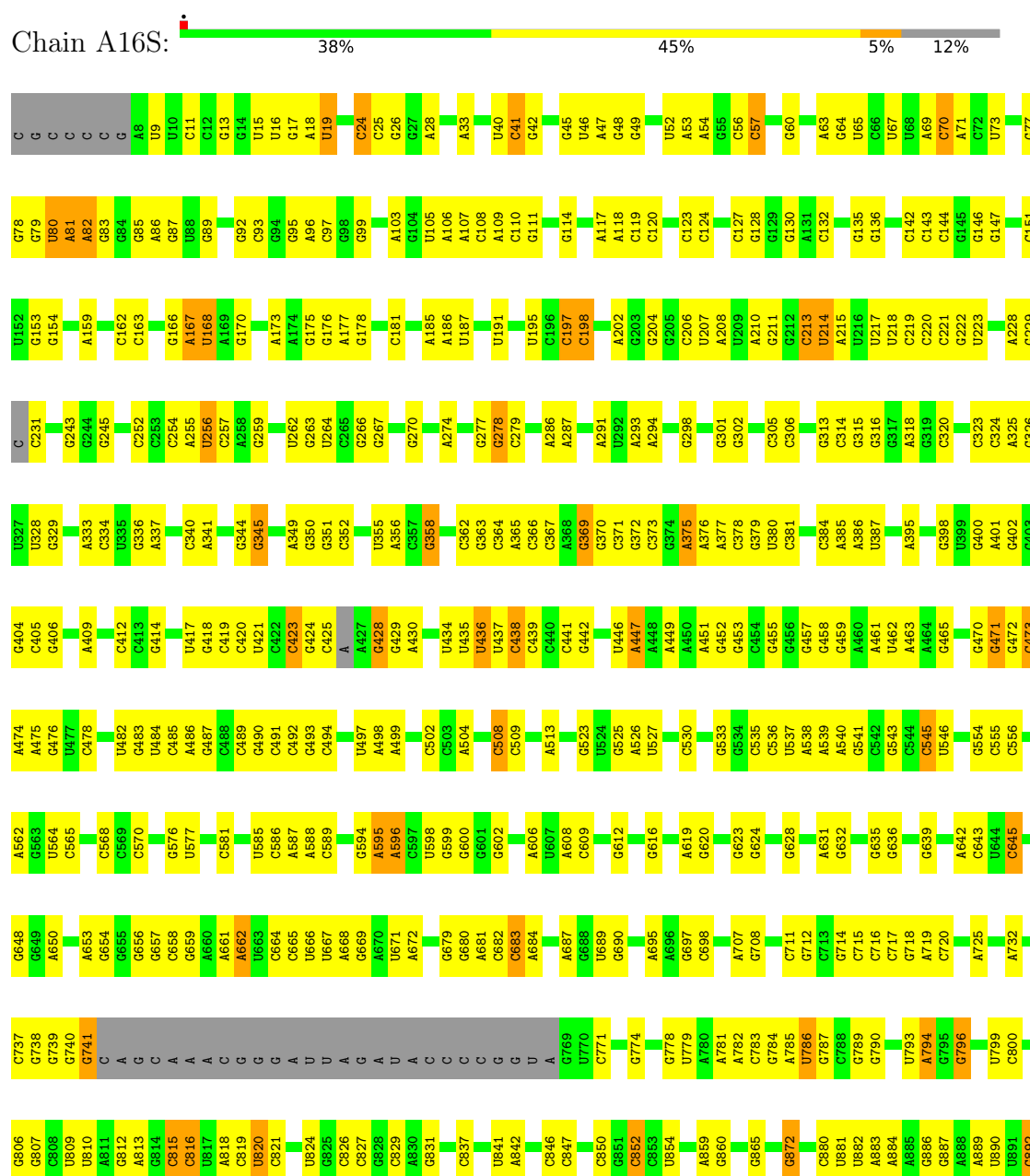
Mol	Chain	Residues	Atoms				AltConf
29	A16S	4	Total	C	N	O	0
			20	12	4	4	
29	AS2P	34	Total	C	N	O	0
			171	102	34	35	
29	AS5P	13	Total	C	N	O	0
			65	39	13	13	
29	AS8P	6	Total	C	N	O	0
			30	18	6	6	



### 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)

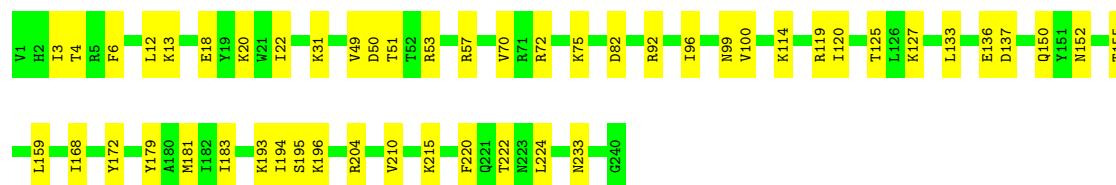






- Molecule 4: 30S ribosomal protein S4e

Chain AS4E:   79% 21%



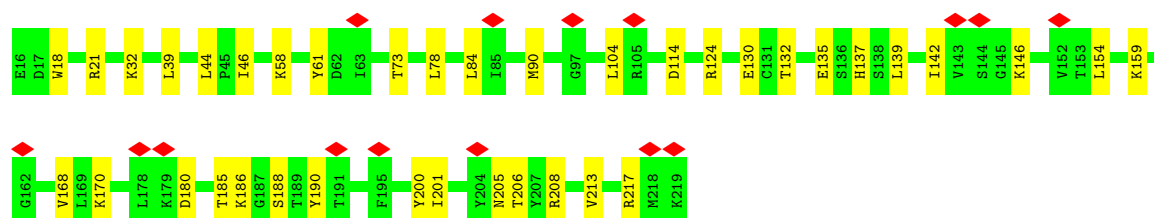
- Molecule 5: 30S ribosomal protein S4

Chain AS4P:   76% 23%



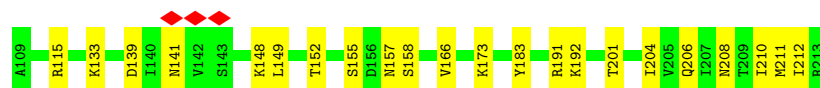
- Molecule 6: 30S ribosomal protein S5

Chain AS5P:    7% 81% 19%



- Molecule 7: 30S ribosomal protein S6e

Chain AS6E:   79% 21%

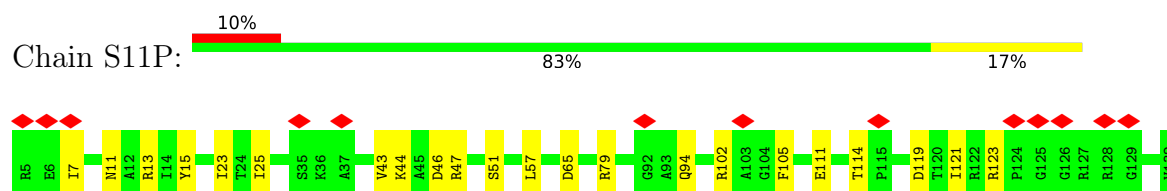


- Molecule 8: 30S ribosomal protein S8e

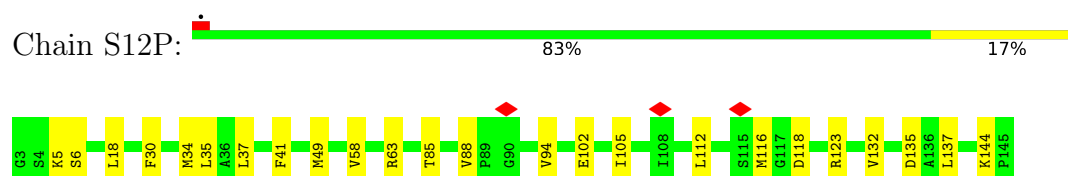
Chain AS8E:   82% 18%



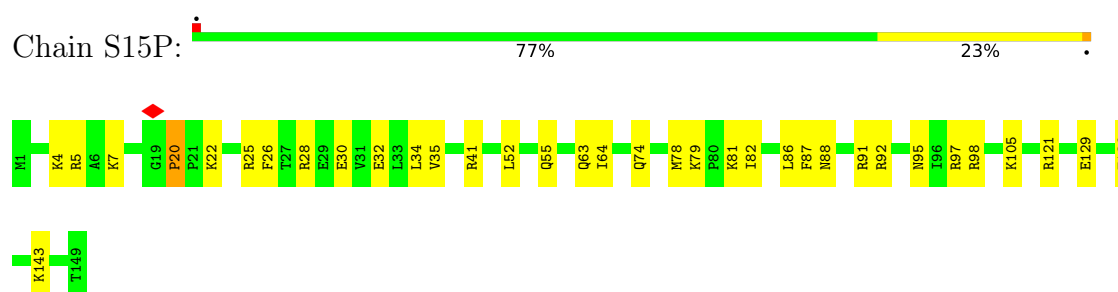
- Molecule 9: 30S ribosomal protein S11



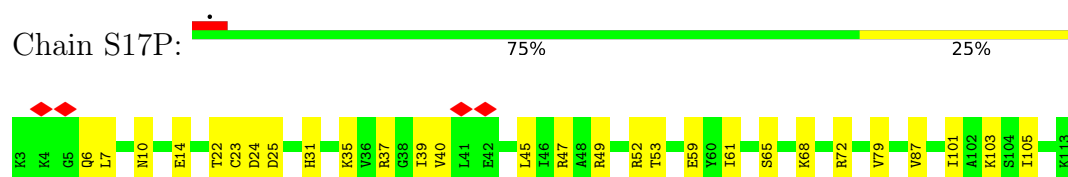
- Molecule 10: 30S ribosomal protein S12



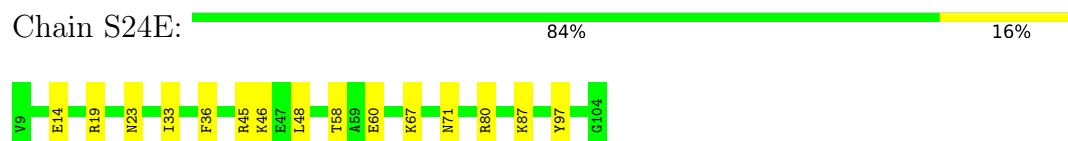
- Molecule 11: 30S ribosomal protein S15



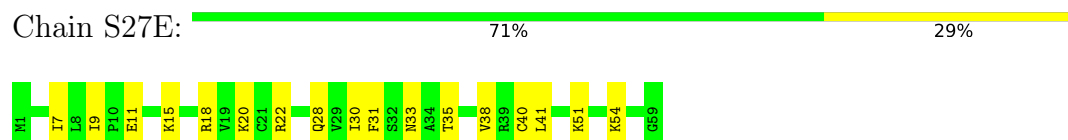
- Molecule 12: 30S ribosomal protein S17




- Molecule 13: 30S ribosomal protein S24e

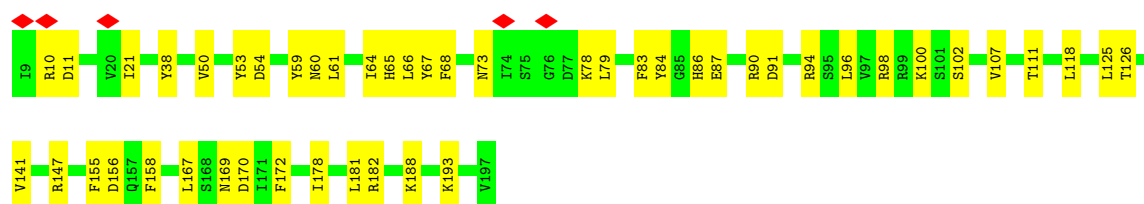


- Molecule 14: 30S ribosomal protein S27e




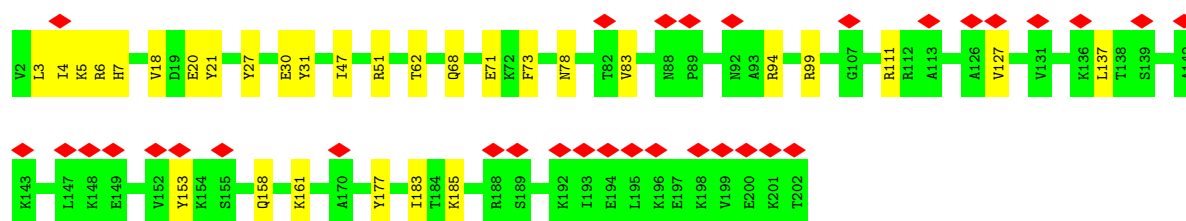
- Molecule 15: 30S ribosomal protein S3Ae

Chain S3AE:  75% 25%




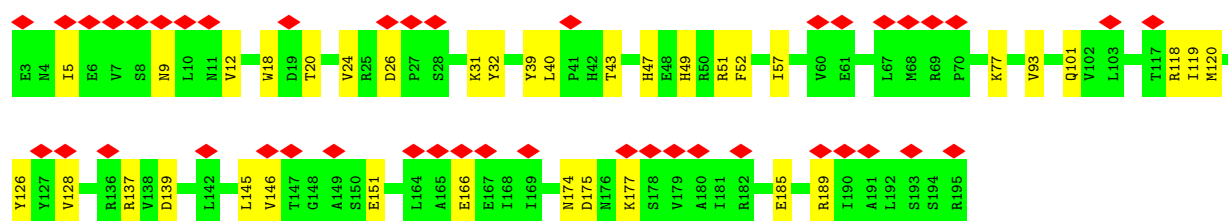
- Molecule 16: 30S ribosomal protein S3

Chain AS3P:  16% 85% 15%




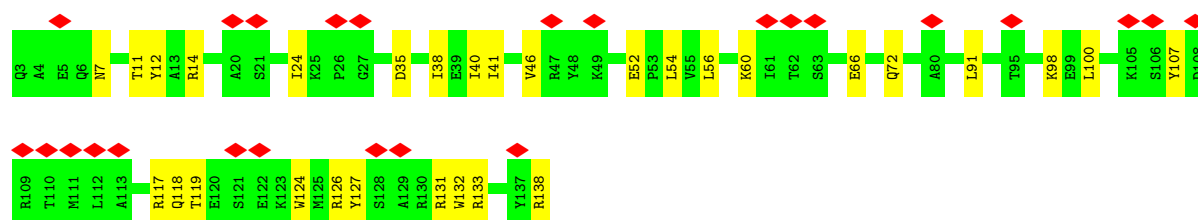
- Molecule 17: 30S ribosomal protein S7

Chain AS7P:  22% 81% 19%




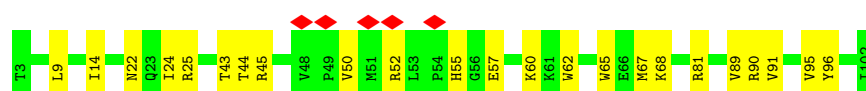
- Molecule 18: 30S ribosomal protein S9

Chain AS9P:  18% 78% 22%

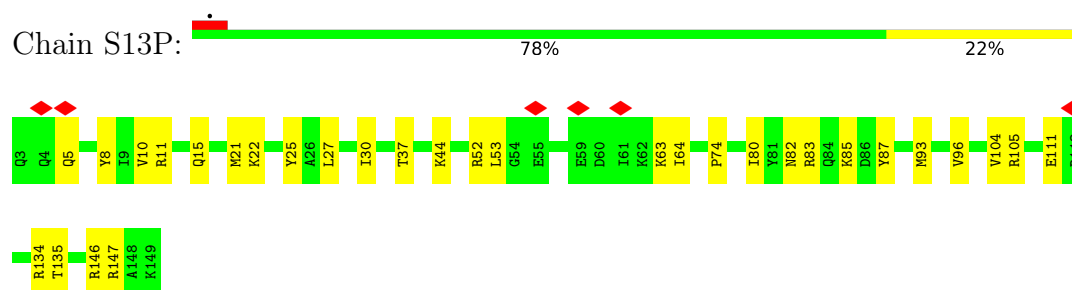


- Molecule 19: 30S ribosomal protein S10

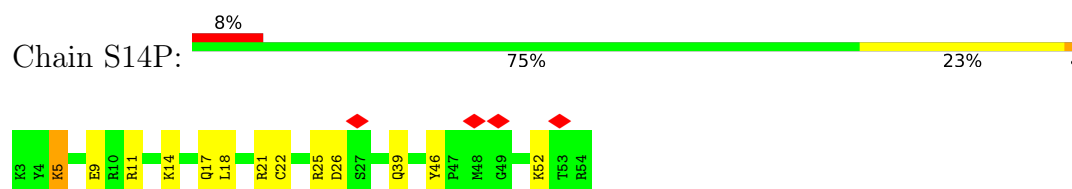
Chain S10P:  5% 77% 23%



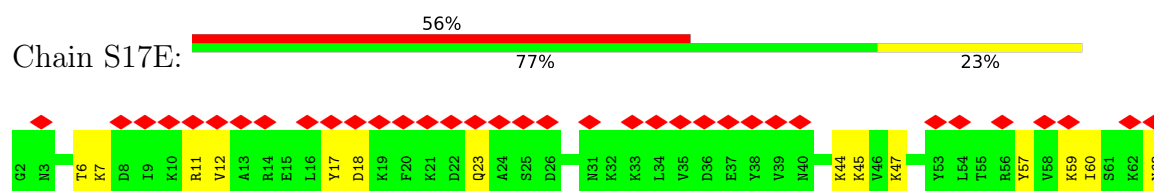
- Molecule 20: 30S ribosomal protein S13



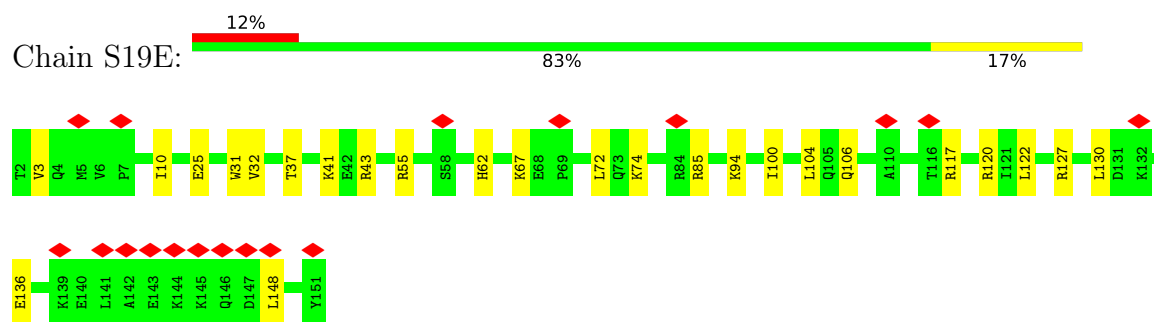
- Molecule 21: 30S ribosomal protein S14 type Z



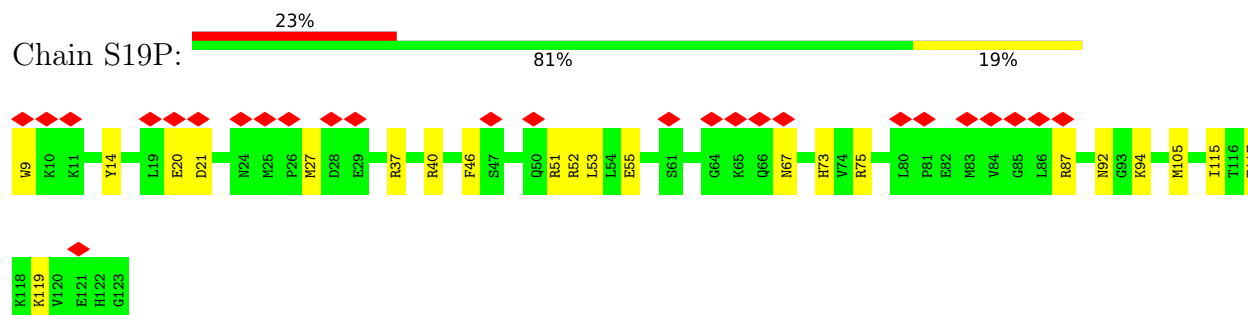
- Molecule 22: 30S ribosomal protein S17e



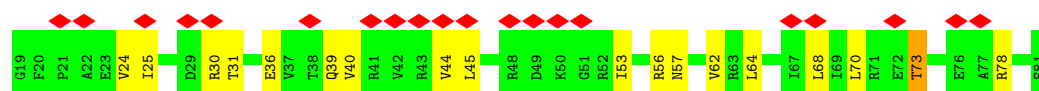
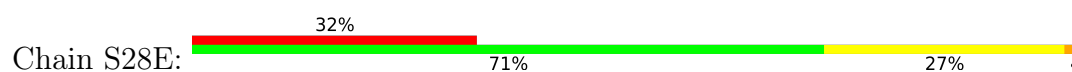
- Molecule 23: 30S ribosomal protein S19e



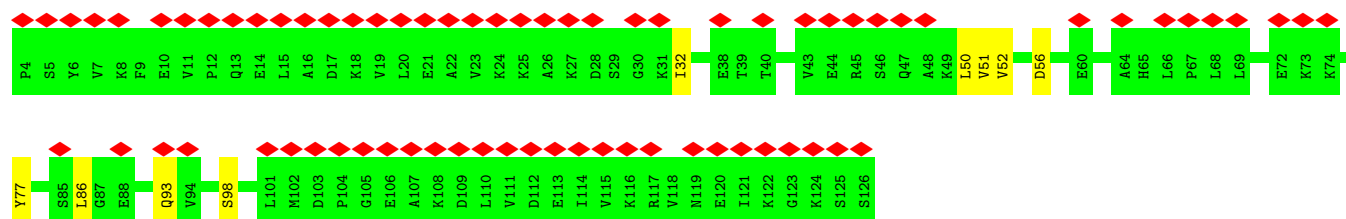
- Molecule 24: 30S ribosomal protein S19



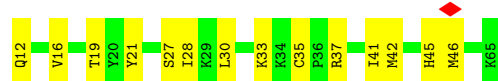
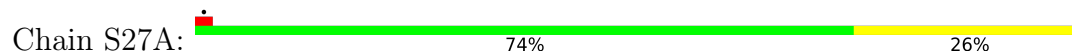
- Molecule 25: 30S ribosomal protein S28e



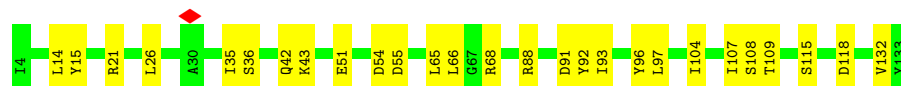
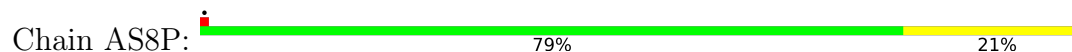
- Molecule 26: 50S ribosomal protein L7Ae



- 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A16S	0.77	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

All (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
1	A16S	375	A	N9-C4	-5.79	1.34	1.37
1	A16S	81	A	O3'-P	5.41	1.67	1.61
2	VTRF	25	G	N9-C4	-5.15	1.33	1.38

All (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
1	A16S	1107	G	O4'-C1'-N9	9.83	116.07	108.20
1	A16S	231	C	O5'-P-OP2	-9.40	97.24	105.70
1	A16S	231	C	C2'-C3'-O3'	9.32	130.00	109.50
1	A16S	1261	C	N3-C2-O2	-8.82	115.72	121.90
1	A16S	369	G	C6-C5-N7	-8.66	125.20	130.40
2	VTRF	25	G	N3-C4-C5	8.64	132.92	128.60
1	A16S	1157	G	N3-C4-N9	-8.61	120.83	126.00
1	A16S	369	G	C4-N9-C1'	8.60	137.68	126.50
1	A16S	168	U	N3-C2-O2	-8.58	116.19	122.20
1	A16S	1261	C	N1-C2-O2	8.57	124.04	118.90
1	A16S	369	G	C8-N9-C1'	-8.53	115.91	127.00
1	A16S	41	C	N1-C2-O2	8.47	123.98	118.90
1	A16S	938	C	C2-N1-C1'	8.25	127.88	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	369	G	N3-C4-N9	8.19	130.92	126.00
2	VTRF	25	G	N3-C4-N9	-8.08	121.15	126.00
1	A16S	997	C	N1-C2-O2	8.06	123.73	118.90
1	A16S	1180	C	C6-N1-C2	-8.02	117.09	120.30
1	A16S	423	C	N3-C2-O2	-7.91	116.37	121.90
1	A16S	1180	C	N3-C2-O2	-7.78	116.45	121.90
1	A16S	1219	C	N1-C2-O2	7.64	123.49	118.90
1	A16S	41	C	C6-N1-C2	-7.62	117.25	120.30
1	A16S	1215	G	C5-C6-O6	7.59	133.15	128.60
1	A16S	1129	C	C2-N1-C1'	7.57	127.13	118.80
1	A16S	938	C	C6-N1-C2	-7.57	117.27	120.30
1	A16S	423	C	C2-N1-C1'	7.54	127.09	118.80
1	A16S	41	C	C2-N1-C1'	7.53	127.08	118.80
1	A16S	1358	C	N1-C2-O2	7.51	123.41	118.90
1	A16S	938	C	N1-C2-O2	7.49	123.39	118.90
1	A16S	57	C	N3-C2-O2	-7.46	116.68	121.90
1	A16S	41	C	N3-C2-O2	-7.41	116.72	121.90
1	A16S	662	A	N1-C6-N6	7.40	123.04	118.60
1	A16S	1006	G	N1-C2-N2	-7.39	109.55	116.20
1	A16S	938	C	N3-C2-O2	-7.37	116.74	121.90
1	A16S	816	C	N3-C2-O2	-7.37	116.74	121.90
1	A16S	168	U	C2-N1-C1'	7.34	126.50	117.70
1	A16S	70	C	C2-N1-C1'	7.33	126.86	118.80
1	A16S	428	G	C5-C6-O6	7.32	132.99	128.60
1	A16S	1215	G	N1-C6-O6	-7.30	115.52	119.90
1	A16S	595	A	C4'-C3'-O3'	7.28	127.56	113.00
1	A16S	997	C	C2-N1-C1'	7.24	126.77	118.80
1	A16S	144	C	N3-C2-O2	-7.12	116.92	121.90
1	A16S	213	C	C2'-C3'-O3'	7.09	125.11	109.50
1	A16S	996	C	C2-N1-C1'	7.09	126.61	118.80
1	A16S	771	C	N1-C2-O2	7.05	123.13	118.90
1	A16S	965	C	C6-N1-C2	-6.99	117.50	120.30
1	A16S	771	C	N3-C2-O2	-6.98	117.01	121.90
1	A16S	1179	C	C2-N1-C1'	6.96	126.46	118.80
1	A16S	999	G	O5'-P-OP1	-6.92	99.48	105.70
1	A16S	214	U	C5'-C4'-O4'	6.90	117.38	109.10
1	A16S	997	C	N3-C2-O2	-6.90	117.07	121.90
1	A16S	1228	G	O4'-C1'-N9	6.88	113.70	108.20
1	A16S	471	G	C6-C5-N7	-6.82	126.31	130.40
1	A16S	369	G	N9-C4-C5	-6.80	102.68	105.40
1	A16S	1358	C	N3-C2-O2	-6.80	117.14	121.90
1	A16S	1348	G	C6-C5-N7	-6.79	126.33	130.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	461	A	N7-C8-N9	6.78	117.19	113.80
1	A16S	909	A	N1-C6-N6	-6.74	114.55	118.60
2	VTRF	8	U	O4'-C1'-N1	6.72	113.58	108.20
1	A16S	471	G	N1-C2-N2	-6.72	110.15	116.20
1	A16S	1157	G	N3-C4-C5	6.67	131.94	128.60
1	A16S	1348	G	C8-N9-C1'	-6.57	118.46	127.00
2	VTRF	25	G	N3-C2-N2	-6.53	115.33	119.90
1	A16S	436	U	N3-C2-O2	-6.47	117.67	122.20
1	A16S	438	C	N1-C2-O2	6.47	122.78	118.90
1	A16S	741	G	N3-C4-C5	6.47	131.84	128.60
1	A16S	70	C	N1-C2-O2	6.46	122.78	118.90
1	A16S	168	U	N1-C2-O2	6.46	127.32	122.80
1	A16S	1207	C	N3-C2-O2	-6.45	117.39	121.90
2	VTRF	11	U	C5-C4-O4	6.44	129.76	125.90
1	A16S	314	C	C2-N1-C1'	6.41	125.85	118.80
1	A16S	658	C	N3-C4-C5	6.40	124.46	121.90
1	A16S	41	C	C5-C6-N1	6.39	124.19	121.00
1	A16S	1157	G	C4-N9-C1'	-6.39	118.20	126.50
1	A16S	1348	G	C4-N9-C1'	6.35	134.76	126.50
2	VTRF	25	G	N1-C2-N2	6.35	121.92	116.20
1	A16S	1006	G	C4-N9-C1'	6.34	134.74	126.50
1	A16S	369	G	C4-C5-N7	6.31	113.32	110.80
1	A16S	213	C	C4'-C3'-O3'	6.29	125.58	113.00
1	A16S	1006	G	N3-C2-N2	6.25	124.28	119.90
1	A16S	1156	G	C5-C6-O6	6.24	132.35	128.60
1	A16S	965	C	C5-C6-N1	6.23	124.11	121.00
1	A16S	1213	C	N1-C2-O2	6.23	122.64	118.90
1	A16S	1076	C	C2-N1-C1'	-6.22	111.95	118.80
1	A16S	56	C	N1-C2-O2	6.22	122.63	118.90
1	A16S	1195	G	N1-C6-O6	-6.21	116.18	119.90
1	A16S	1219	C	C2-N1-C1'	6.19	125.61	118.80
1	A16S	428	G	N3-C4-N9	-6.19	122.29	126.00
1	A16S	892	G	N3-C4-C5	6.18	131.69	128.60
1	A16S	923	C	C2-N1-C1'	6.18	125.59	118.80
1	A16S	852	C	C2-N1-C1'	-6.17	112.02	118.80
1	A16S	1078	C	C5-C4-N4	6.15	124.51	120.20
1	A16S	473	C	N1-C2-O2	6.14	122.59	118.90
1	A16S	1157	G	C5-C6-O6	6.14	132.28	128.60
1	A16S	471	G	N3-C2-N2	6.09	124.17	119.90
1	A16S	1006	G	C6-C5-N7	-6.08	126.75	130.40
1	A16S	214	U	C1'-O4'-C4'	-6.07	105.05	109.90
1	A16S	1157	G	C8-N9-C1'	6.06	134.88	127.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	892	G	N3-C4-N9	-6.05	122.37	126.00
1	A16S	996	C	C6-N1-C2	-6.05	117.88	120.30
1	A16S	70	C	C6-N1-C1'	-6.03	113.57	120.80
1	A16S	198	C	N3-C2-O2	-6.02	117.69	121.90
1	A16S	267	G	N9-C4-C5	-6.01	103.00	105.40
1	A16S	1007	G	C5-C6-O6	5.99	132.20	128.60
1	A16S	77	G	C4'-C3'-O3'	5.98	124.97	113.00
1	A16S	536	C	C2-N1-C1'	5.97	125.37	118.80
1	A16S	953	U	C2-N1-C1'	5.97	124.86	117.70
1	A16S	716	C	C2-N1-C1'	5.95	125.34	118.80
1	A16S	662	A	C8-N9-C4	5.93	108.17	105.80
1	A16S	428	G	N1-C6-O6	-5.93	116.34	119.90
1	A16S	658	C	C6-N1-C2	5.92	122.67	120.30
1	A16S	1090	U	C2-N1-C1'	5.92	124.81	117.70
1	A16S	1195	G	C5-C6-O6	5.92	132.15	128.60
1	A16S	807	G	N7-C8-N9	5.92	116.06	113.10
1	A16S	1157	G	N1-C6-O6	-5.91	116.35	119.90
1	A16S	711	C	N3-C2-O2	-5.91	117.77	121.90
1	A16S	154	G	N1-C2-N2	-5.88	110.91	116.20
1	A16S	680	G	N3-C4-N9	-5.87	122.48	126.00
1	A16S	508	C	C2-N1-C1'	5.87	125.25	118.80
1	A16S	1272	G	C4-N9-C1'	5.85	134.10	126.50
1	A16S	786	U	N3-C4-O4	5.85	123.49	119.40
1	A16S	1272	G	C8-N9-C1'	-5.85	119.40	127.00
1	A16S	314	C	C6-N1-C1'	-5.83	113.81	120.80
1	A16S	1261	C	C5-C4-N4	5.82	124.27	120.20
1	A16S	19	U	O4'-C1'-N1	5.80	112.84	108.20
2	VTRF	19	G	C5-C6-N1	5.78	114.39	111.50
1	A16S	1006	G	N3-C4-N9	5.77	129.46	126.00
1	A16S	1006	G	C8-N9-C1'	-5.76	119.51	127.00
1	A16S	1189	C	C6-N1-C2	-5.76	118.00	120.30
1	A16S	167	A	N1-C6-N6	-5.75	115.15	118.60
1	A16S	807	G	C5-N7-C8	-5.75	101.42	104.30
1	A16S	70	C	C5-C6-N1	5.73	123.86	121.00
1	A16S	794	A	O4'-C1'-N9	5.72	112.78	108.20
1	A16S	1314	U	C2-N3-C4	5.72	130.43	127.00
1	A16S	423	C	C6-N1-C1'	-5.71	113.94	120.80
1	A16S	1351	C	N1-C2-O2	5.71	122.33	118.90
1	A16S	1157	G	C6-C5-N7	5.70	133.82	130.40
1	A16S	1078	C	N3-C4-N4	-5.70	114.01	118.00
1	A16S	816	C	C2-N3-C4	-5.68	117.06	119.90
1	A16S	82	A	C4'-C3'-O3'	5.67	124.33	113.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	997	C	C6-N1-C2	-5.65	118.04	120.30
1	A16S	717	C	N3-C2-O2	-5.65	117.94	121.90
1	A16S	1348	G	N9-C4-C5	-5.65	103.14	105.40
1	A16S	1263	G	N9-C4-C5	-5.65	103.14	105.40
1	A16S	256	U	O4'-C1'-N1	-5.63	103.69	108.20
1	A16S	24	C	N1-C2-O2	5.62	122.27	118.90
1	A16S	508	C	C6-N1-C1'	-5.61	114.06	120.80
1	A16S	168	U	O4'-C1'-N1	5.57	112.66	108.20
1	A16S	1061	C	N1-C2-O2	5.56	122.24	118.90
1	A16S	1272	G	N3-C4-N9	5.55	129.33	126.00
1	A16S	965	C	N1-C2-O2	5.54	122.22	118.90
1	A16S	786	U	C5-C4-O4	-5.53	122.58	125.90
1	A16S	1179	C	C6-N1-C1'	-5.53	114.17	120.80
1	A16S	358	G	N3-C4-N9	5.52	129.31	126.00
1	A16S	438	C	N3-C2-O2	-5.51	118.04	121.90
1	A16S	1207	C	C6-N1-C2	-5.49	118.11	120.30
1	A16S	1129	C	C6-N1-C1'	-5.48	114.22	120.80
1	A16S	1207	C	N1-C2-O2	5.48	122.19	118.90
1	A16S	555	C	N1-C2-O2	5.48	122.19	118.90
1	A16S	816	C	N3-C4-N4	-5.48	114.16	118.00
1	A16S	170	G	N7-C8-N9	5.48	115.84	113.10
1	A16S	536	C	C6-N1-C1'	-5.48	114.23	120.80
1	A16S	1263	G	N3-C4-N9	5.47	129.28	126.00
1	A16S	741	G	C4-N9-C1'	-5.45	119.41	126.50
1	A16S	1129	C	N1-C2-O2	5.44	122.17	118.90
1	A16S	267	G	C8-N9-C4	5.42	108.57	106.40
1	A16S	1179	C	N1-C2-O2	5.41	122.14	118.90
1	A16S	662	A	N9-C4-C5	-5.40	103.64	105.80
1	A16S	1263	G	C8-N9-C1'	-5.38	120.00	127.00
1	A16S	471	G	C4-C5-N7	5.38	112.95	110.80
1	A16S	213	C	O4'-C4'-C3'	-5.35	98.65	104.00
1	A16S	796	G	O4'-C1'-N9	5.35	112.48	108.20
1	A16S	683	C	C2-N1-C1'	5.35	124.68	118.80
1	A16S	926	C	C5-C4-N4	5.34	123.94	120.20
1	A16S	1007	G	N1-C2-N2	-5.32	111.41	116.20
1	A16S	1176	G	C4-N9-C1'	5.32	133.41	126.50
1	A16S	716	C	C6-N1-C1'	-5.31	114.42	120.80
1	A16S	806	G	C8-N9-C4	-5.30	104.28	106.40
1	A16S	1311	C	C2-N1-C1'	5.30	124.63	118.80
1	A16S	815	C	N3-C4-N4	-5.29	114.30	118.00
1	A16S	278	G	N3-C4-C5	5.27	131.23	128.60
1	A16S	872	G	C2-N3-C4	-5.26	109.27	111.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A16S	555	C	N3-C2-O2	-5.25	118.23	121.90
1	A16S	1176	G	C8-N9-C1'	-5.24	120.19	127.00
1	A16S	786	U	C2-N1-C1'	5.23	123.97	117.70
2	VTRF	19	G	O4'-C1'-N9	-5.23	104.02	108.20
2	VTRF	12	C	N3-C2-O2	-5.21	118.25	121.90
2	VTRF	12	C	N3-C4-N4	-5.21	114.36	118.00
1	A16S	645	C	C5-C6-N1	5.21	123.60	121.00
1	A16S	680	G	N9-C4-C5	5.20	107.48	105.40
1	A16S	1219	C	N3-C2-O2	-5.19	118.27	121.90
1	A16S	56	C	N3-C2-O2	-5.19	118.27	121.90
1	A16S	1180	C	N1-C2-N3	5.19	122.83	119.20
1	A16S	1039	U	C2-N1-C1'	5.18	123.91	117.70
1	A16S	852	C	C6-N1-C1'	5.17	127.00	120.80
1	A16S	197	C	N3-C2-O2	-5.16	118.28	121.90
1	A16S	1348	G	N3-C4-N9	5.16	129.10	126.00
1	A16S	1262	U	C2-N1-C1'	5.16	123.89	117.70
1	A16S	447	A	O4'-C1'-N9	5.16	112.33	108.20
1	A16S	565	C	N1-C2-O2	5.16	122.00	118.90
1	A16S	949	A	N9-C4-C5	5.16	107.86	105.80
1	A16S	375	A	C8-N9-C4	5.15	107.86	105.80
1	A16S	471	G	N3-C4-N9	5.15	129.09	126.00
1	A16S	81	A	O5'-P-OP2	-5.14	101.07	105.70
1	A16S	1263	G	C4-N9-C1'	5.13	133.17	126.50
2	VTRF	18	U	OP1-P-O3'	5.13	116.48	105.20
1	A16S	545	C	N1-C2-O2	5.12	121.97	118.90
1	A16S	436	U	N1-C2-O2	5.11	126.38	122.80
2	VTRF	11	U	O4'-C1'-N1	5.11	112.29	108.20
1	A16S	1129	C	N3-C2-O2	-5.10	118.33	121.90
1	A16S	470	G	N9-C4-C5	-5.10	103.36	105.40
1	A16S	1261	C	N3-C4-N4	-5.09	114.44	118.00
1	A16S	852	C	O4'-C1'-N1	5.07	112.26	108.20
1	A16S	1281	G	N3-C4-N9	-5.06	122.96	126.00
1	A16S	345	G	N9-C4-C5	-5.06	103.38	105.40
1	A16S	981	A	C6-N1-C2	-5.04	115.58	118.60
1	A16S	1277	C	N1-C2-O2	5.04	121.92	118.90
1	A16S	1223	G	C4-N9-C1'	5.03	133.04	126.50
1	A16S	965	C	N3-C2-O2	-5.03	118.38	121.90
1	A16S	966	C	N1-C2-O2	5.03	121.92	118.90
1	A16S	1200	C	C6-N1-C2	-5.02	118.29	120.30
1	A16S	820	U	N1-C2-O2	5.02	126.31	122.80
1	A16S	1191	G	N1-C6-O6	-5.02	116.89	119.90
1	A16S	81	A	C4'-C3'-O3'	5.01	123.02	113.00



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

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	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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%)	22	59
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%)	19	56
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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	S3AE	187/189 (99%)	156 (83%)	31 (17%)	0	100	100
16	AS3P	199/201 (99%)	169 (85%)	27 (14%)	3 (2%)	8	39
17	AS7P	191/193 (99%)	157 (82%)	33 (17%)	1 (0%)	25	64
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%)	9	40
21	S14P	50/52 (96%)	33 (66%)	16 (32%)	1 (2%)	6	32
22	S17E	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
23	S19E	148/150 (99%)	128 (86%)	19 (13%)	1 (1%)	19	56
24	S19P	113/115 (98%)	91 (80%)	22 (20%)	0	100	100
25	S28E	61/63 (97%)	41 (67%)	17 (28%)	3 (5%)	2	16
26	SL7A	121/123 (98%)	105 (87%)	15 (12%)	1 (1%)	16	54
27	S27A	52/54 (96%)	37 (71%)	14 (27%)	1 (2%)	6	33
28	AS8P	128/130 (98%)	107 (84%)	21 (16%)	0	100	100
All	All	3386/3438 (98%)	2853 (84%)	518 (15%)	15 (0%)	32	68

All (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
25	S28E	24	VAL
16	AS3P	30	GLU
27	S27A	41	ILE
5	AS4P	166	PRO
25	S28E	73	THR
20	S13P	22	LYS
20	S13P	74	PRO
23	S19E	3	VAL
11	S15P	20	PRO
26	SL7A	52	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AS2P	174/174 (100%)	137 (79%)	37 (21%)	1	5
4	AS4E	210/210 (100%)	160 (76%)	50 (24%)	0	4
5	AS4P	149/149 (100%)	110 (74%)	39 (26%)	0	3
6	AS5P	174/174 (100%)	136 (78%)	38 (22%)	1	5
7	AS6E	88/88 (100%)	66 (75%)	22 (25%)	0	3
8	AS8E	106/106 (100%)	83 (78%)	23 (22%)	1	5
9	S11P	94/94 (100%)	72 (77%)	22 (23%)	0	4
10	S12P	116/116 (100%)	92 (79%)	24 (21%)	1	6
11	S15P	133/133 (100%)	99 (74%)	34 (26%)	0	3
12	S17P	97/97 (100%)	69 (71%)	28 (29%)	0	2
13	S24E	84/84 (100%)	69 (82%)	15 (18%)	1	8
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	11
17	AS7P	166/166 (100%)	131 (79%)	35 (21%)	1	5
18	AS9P	113/113 (100%)	83 (74%)	30 (26%)	0	3
19	S10P	92/92 (100%)	69 (75%)	23 (25%)	0	3
20	S13P	129/129 (100%)	98 (76%)	31 (24%)	0	4
21	S14P	45/45 (100%)	32 (71%)	13 (29%)	0	2
22	S17E	57/57 (100%)	43 (75%)	14 (25%)	0	3
23	S19E	134/134 (100%)	110 (82%)	24 (18%)	1	8
24	S19P	106/106 (100%)	84 (79%)	22 (21%)	1	6
25	S28E	54/54 (100%)	38 (70%)	16 (30%)	0	2
26	SL7A	104/104 (100%)	96 (92%)	8 (8%)	10	30
27	S27A	47/47 (100%)	34 (72%)	13 (28%)	0	3
28	AS8P	111/111 (100%)	84 (76%)	27 (24%)	0	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2969/2969 (100%)	2291 (77%)	678 (23%)	<b>2</b> <b>4</b>

All (678) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AS2P	29	LEU
3	AS2P	46	HIS
3	AS2P	50	ARG
3	AS2P	52	MET
3	AS2P	53	GLU
3	AS2P	73	ASP
3	AS2P	76	LEU
3	AS2P	77	ARG
3	AS2P	85	ARG
3	AS2P	101	PHE
3	AS2P	105	GLN
3	AS2P	106	LYS
3	AS2P	107	PHE
3	AS2P	111	VAL
3	AS2P	112	ARG
3	AS2P	114	LYS
3	AS2P	120	PHE
3	AS2P	124	THR
3	AS2P	125	LEU
3	AS2P	127	ASN
3	AS2P	131	ASP
3	AS2P	145	ARG
3	AS2P	152	LYS
3	AS2P	164	PHE
3	AS2P	165	THR
3	AS2P	173	PHE
3	AS2P	175	ASP
3	AS2P	176	VAL
3	AS2P	186	LYS
3	AS2P	191	LEU
3	AS2P	200	LEU
3	AS2P	202	GLU
3	AS2P	206	ILE
3	AS2P	212	ILE
3	AS2P	214	LEU
3	AS2P	220	GLU
3	AS2P	222	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	AS4E	3	ILE
4	AS4E	4	THR
4	AS4E	6	PHE
4	AS4E	12	LEU
4	AS4E	13	LYS
4	AS4E	18	GLU
4	AS4E	20	LYS
4	AS4E	22	ILE
4	AS4E	31	LYS
4	AS4E	49	VAL
4	AS4E	50	ASP
4	AS4E	51	THR
4	AS4E	53	ARG
4	AS4E	57	ARG
4	AS4E	70	VAL
4	AS4E	72	ARG
4	AS4E	75	LYS
4	AS4E	82	ASP
4	AS4E	92	ARG
4	AS4E	96	ILE
4	AS4E	99	ASN
4	AS4E	100	VAL
4	AS4E	114	LYS
4	AS4E	119	ARG
4	AS4E	120	ILE
4	AS4E	125	THR
4	AS4E	127	LYS
4	AS4E	133	LEU
4	AS4E	136	GLU
4	AS4E	137	ASP
4	AS4E	150	GLN
4	AS4E	152	ASN
4	AS4E	155	THR
4	AS4E	159	LEU
4	AS4E	168	ILE
4	AS4E	172	TYR
4	AS4E	179	TYR
4	AS4E	181	MET
4	AS4E	183	ILE
4	AS4E	193	LYS
4	AS4E	194	ILE
4	AS4E	195	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	AS4E	196	LYS
4	AS4E	204	ARG
4	AS4E	210	VAL
4	AS4E	215	LYS
4	AS4E	220	PHE
4	AS4E	222	THR
4	AS4E	224	LEU
4	AS4E	233	ASN
5	AS4P	5	ARG
5	AS4P	20	LYS
5	AS4P	23	LEU
5	AS4P	29	LEU
5	AS4P	38	LYS
5	AS4P	40	GLU
5	AS4P	42	TRP
5	AS4P	46	THR
5	AS4P	47	MET
5	AS4P	50	ASN
5	AS4P	53	HIS
5	AS4P	56	ARG
5	AS4P	58	LEU
5	AS4P	59	LEU
5	AS4P	69	ARG
5	AS4P	71	LYS
5	AS4P	77	LEU
5	AS4P	78	TYR
5	AS4P	82	ILE
5	AS4P	85	LYS
5	AS4P	94	LEU
5	AS4P	97	THR
5	AS4P	103	GLU
5	AS4P	111	TYR
5	AS4P	115	LEU
5	AS4P	117	ARG
5	AS4P	124	GLN
5	AS4P	125	LEU
5	AS4P	131	ILE
5	AS4P	133	ILE
5	AS4P	136	ARG
5	AS4P	143	TYR
5	AS4P	147	ARG
5	AS4P	149	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AS4P	151	ASP
5	AS4P	153	ILE
5	AS4P	155	TYR
5	AS4P	161	PHE
5	AS4P	162	LYS
6	AS5P	18	TRP
6	AS5P	21	ARG
6	AS5P	32	LYS
6	AS5P	39	LEU
6	AS5P	44	LEU
6	AS5P	46	ILE
6	AS5P	58	LYS
6	AS5P	61	TYR
6	AS5P	73	THR
6	AS5P	78	LEU
6	AS5P	84	LEU
6	AS5P	90	MET
6	AS5P	104	LEU
6	AS5P	114	ASP
6	AS5P	124	ARG
6	AS5P	130	GLU
6	AS5P	132	THR
6	AS5P	135	GLU
6	AS5P	137	HIS
6	AS5P	139	LEU
6	AS5P	142	ILE
6	AS5P	146	LYS
6	AS5P	154	LEU
6	AS5P	159	LYS
6	AS5P	168	VAL
6	AS5P	170	LYS
6	AS5P	180	ASP
6	AS5P	185	THR
6	AS5P	186	LYS
6	AS5P	188	SER
6	AS5P	190	TYR
6	AS5P	200	TYR
6	AS5P	201	ILE
6	AS5P	205	ASN
6	AS5P	206	THR
6	AS5P	208	ARG
6	AS5P	213	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	AS5P	217	ARG
7	AS6E	115	ARG
7	AS6E	133	LYS
7	AS6E	139	ASP
7	AS6E	141	ASN
7	AS6E	148	LYS
7	AS6E	149	LEU
7	AS6E	152	THR
7	AS6E	155	SER
7	AS6E	157	ASN
7	AS6E	158	SER
7	AS6E	166	VAL
7	AS6E	173	LYS
7	AS6E	183	TYR
7	AS6E	191	ARG
7	AS6E	192	LYS
7	AS6E	201	THR
7	AS6E	204	ILE
7	AS6E	206	GLN
7	AS6E	208	ASN
7	AS6E	210	ILE
7	AS6E	211	MET
7	AS6E	212	ILE
8	AS8E	4	TYR
8	AS8E	5	GLN
8	AS8E	7	ASN
8	AS8E	11	LYS
8	AS8E	21	ARG
8	AS8E	22	ASP
8	AS8E	24	ARG
8	AS8E	30	SER
8	AS8E	36	LYS
8	AS8E	44	GLU
8	AS8E	48	VAL
8	AS8E	53	PHE
8	AS8E	67	ASP
8	AS8E	69	GLN
8	AS8E	71	LYS
8	AS8E	82	LEU
8	AS8E	88	ARG
8	AS8E	89	GLU
8	AS8E	96	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
8	AS8E	101	LEU
8	AS8E	102	ILE
8	AS8E	120	ILE
8	AS8E	124	LEU
9	S11P	7	ILE
9	S11P	11	ASN
9	S11P	13	ARG
9	S11P	15	TYR
9	S11P	23	ILE
9	S11P	25	ILE
9	S11P	43	VAL
9	S11P	44	LYS
9	S11P	46	ASP
9	S11P	47	ARG
9	S11P	51	SER
9	S11P	57	LEU
9	S11P	65	ASP
9	S11P	79	ARG
9	S11P	94	GLN
9	S11P	102	ARG
9	S11P	105	PHE
9	S11P	111	GLU
9	S11P	114	THR
9	S11P	119	ASP
9	S11P	121	ILE
9	S11P	123	ARG
10	S12P	5	LYS
10	S12P	6	SER
10	S12P	18	LEU
10	S12P	30	PHE
10	S12P	34	MET
10	S12P	35	LEU
10	S12P	37	LEU
10	S12P	41	PHE
10	S12P	49	MET
10	S12P	58	VAL
10	S12P	63	ARG
10	S12P	85	THR
10	S12P	88	VAL
10	S12P	94	VAL
10	S12P	102	GLU
10	S12P	105	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	S12P	112	LEU
10	S12P	116	MET
10	S12P	118	ASP
10	S12P	123	ARG
10	S12P	132	VAL
10	S12P	135	ASP
10	S12P	137	LEU
10	S12P	144	LYS
11	S15P	4	LYS
11	S15P	5	ARG
11	S15P	7	LYS
11	S15P	22	LYS
11	S15P	25	ARG
11	S15P	26	PHE
11	S15P	28	ARG
11	S15P	30	GLU
11	S15P	32	GLU
11	S15P	34	LEU
11	S15P	35	VAL
11	S15P	41	ARG
11	S15P	52	LEU
11	S15P	55	GLN
11	S15P	63	GLN
11	S15P	64	ILE
11	S15P	74	GLN
11	S15P	78	MET
11	S15P	79	LYS
11	S15P	81	LYS
11	S15P	82	ILE
11	S15P	86	LEU
11	S15P	87	PHE
11	S15P	88	ASN
11	S15P	91	ARG
11	S15P	92	ARG
11	S15P	95	ASN
11	S15P	97	ARG
11	S15P	98	ARG
11	S15P	105	LYS
11	S15P	121	ARG
11	S15P	129	GLU
11	S15P	136	GLU
11	S15P	143	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	S17P	6	GLN
12	S17P	7	LEU
12	S17P	10	ASN
12	S17P	14	GLU
12	S17P	22	THR
12	S17P	23	CYS
12	S17P	24	ASP
12	S17P	25	ASP
12	S17P	31	HIS
12	S17P	35	LYS
12	S17P	37	ARG
12	S17P	39	ILE
12	S17P	40	VAL
12	S17P	45	LEU
12	S17P	47	ARG
12	S17P	49	ARG
12	S17P	52	ARG
12	S17P	53	THR
12	S17P	59	GLU
12	S17P	61	ILE
12	S17P	65	SER
12	S17P	68	LYS
12	S17P	72	ARG
12	S17P	79	VAL
12	S17P	87	VAL
12	S17P	101	ILE
12	S17P	103	LYS
12	S17P	105	ILE
13	S24E	14	GLU
13	S24E	19	ARG
13	S24E	23	ASN
13	S24E	33	ILE
13	S24E	36	PHE
13	S24E	45	ARG
13	S24E	46	LYS
13	S24E	48	LEU
13	S24E	58	THR
13	S24E	60	GLU
13	S24E	67	LYS
13	S24E	71	ASN
13	S24E	80	ARG
13	S24E	87	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	S24E	97	TYR
14	S27E	7	ILE
14	S27E	9	ILE
14	S27E	11	GLU
14	S27E	15	LYS
14	S27E	18	ARG
14	S27E	20	LYS
14	S27E	22	ARG
14	S27E	28	GLN
14	S27E	30	ILE
14	S27E	31	PHE
14	S27E	33	ASN
14	S27E	35	THR
14	S27E	38	VAL
14	S27E	40	CYS
14	S27E	41	LEU
14	S27E	51	LYS
14	S27E	54	LYS
15	S3AE	10	ARG
15	S3AE	11	ASP
15	S3AE	21	ILE
15	S3AE	38	TYR
15	S3AE	50	VAL
15	S3AE	53	TYR
15	S3AE	54	ASP
15	S3AE	59	TYR
15	S3AE	60	ASN
15	S3AE	61	LEU
15	S3AE	64	ILE
15	S3AE	65	HIS
15	S3AE	66	LEU
15	S3AE	67	TYR
15	S3AE	68	PHE
15	S3AE	73	ASN
15	S3AE	78	LYS
15	S3AE	79	LEU
15	S3AE	83	PHE
15	S3AE	84	TYR
15	S3AE	86	HIS
15	S3AE	87	GLU
15	S3AE	90	ARG
15	S3AE	91	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	S3AE	94	ARG
15	S3AE	96	LEU
15	S3AE	98	ARG
15	S3AE	100	LYS
15	S3AE	102	SER
15	S3AE	107	VAL
15	S3AE	111	THR
15	S3AE	118	LEU
15	S3AE	125	LEU
15	S3AE	126	THR
15	S3AE	141	VAL
15	S3AE	147	ARG
15	S3AE	155	PHE
15	S3AE	156	ASP
15	S3AE	158	PHE
15	S3AE	167	LEU
15	S3AE	169	ASN
15	S3AE	170	ASP
15	S3AE	172	PHE
15	S3AE	178	ILE
15	S3AE	182	ARG
15	S3AE	188	LYS
15	S3AE	193	LYS
16	AS3P	3	LEU
16	AS3P	4	ILE
16	AS3P	5	LYS
16	AS3P	6	ARG
16	AS3P	7	HIS
16	AS3P	18	VAL
16	AS3P	20	GLU
16	AS3P	21	TYR
16	AS3P	27	TYR
16	AS3P	31	TYR
16	AS3P	47	ILE
16	AS3P	51	ARG
16	AS3P	62	THR
16	AS3P	68	GLN
16	AS3P	71	GLU
16	AS3P	73	PHE
16	AS3P	94	ARG
16	AS3P	99	ARG
16	AS3P	111	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	AS3P	127	VAL
16	AS3P	137	LEU
16	AS3P	153	TYR
16	AS3P	158	GLN
16	AS3P	161	LYS
16	AS3P	177	TYR
16	AS3P	185	LYS
17	AS7P	5	ILE
17	AS7P	9	ASN
17	AS7P	12	VAL
17	AS7P	18	TRP
17	AS7P	20	THR
17	AS7P	24	VAL
17	AS7P	26	ASP
17	AS7P	31	LYS
17	AS7P	32	TYR
17	AS7P	39	TYR
17	AS7P	40	LEU
17	AS7P	43	THR
17	AS7P	47	HIS
17	AS7P	49	HIS
17	AS7P	51	ARG
17	AS7P	52	PHE
17	AS7P	57	ILE
17	AS7P	77	LYS
17	AS7P	93	VAL
17	AS7P	101	GLN
17	AS7P	118	ARG
17	AS7P	119	ILE
17	AS7P	120	MET
17	AS7P	126	TYR
17	AS7P	137	ARG
17	AS7P	139	ASP
17	AS7P	145	LEU
17	AS7P	146	VAL
17	AS7P	151	GLU
17	AS7P	166	GLU
17	AS7P	174	ASN
17	AS7P	175	ASP
17	AS7P	177	LYS
17	AS7P	185	GLU
17	AS7P	189	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	AS9P	7	ASN
18	AS9P	11	THR
18	AS9P	12	TYR
18	AS9P	14	ARG
18	AS9P	24	ILE
18	AS9P	35	ASP
18	AS9P	38	ILE
18	AS9P	40	ILE
18	AS9P	41	ILE
18	AS9P	46	VAL
18	AS9P	52	GLU
18	AS9P	54	LEU
18	AS9P	56	LEU
18	AS9P	60	LYS
18	AS9P	66	GLU
18	AS9P	72	GLN
18	AS9P	91	LEU
18	AS9P	98	LYS
18	AS9P	100	LEU
18	AS9P	107	TYR
18	AS9P	117	ARG
18	AS9P	118	GLN
18	AS9P	119	THR
18	AS9P	124	TRP
18	AS9P	126	ARG
18	AS9P	127	TYR
18	AS9P	131	ARG
18	AS9P	132	TRP
18	AS9P	133	ARG
18	AS9P	138	ARG
19	S10P	9	LEU
19	S10P	14	ILE
19	S10P	22	ASN
19	S10P	24	ILE
19	S10P	25	ARG
19	S10P	43	THR
19	S10P	44	THR
19	S10P	45	ARG
19	S10P	50	VAL
19	S10P	52	ARG
19	S10P	55	HIS
19	S10P	57	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	S10P	60	LYS
19	S10P	62	TRP
19	S10P	65	TRP
19	S10P	67	MET
19	S10P	68	LYS
19	S10P	81	ARG
19	S10P	89	VAL
19	S10P	90	ARG
19	S10P	91	VAL
19	S10P	95	VAL
19	S10P	96	TYR
20	S13P	5	GLN
20	S13P	8	TYR
20	S13P	10	VAL
20	S13P	11	ARG
20	S13P	15	GLN
20	S13P	21	MET
20	S13P	25	TYR
20	S13P	27	LEU
20	S13P	30	ILE
20	S13P	37	THR
20	S13P	44	LYS
20	S13P	52	ARG
20	S13P	53	LEU
20	S13P	63	LYS
20	S13P	64	ILE
20	S13P	80	ILE
20	S13P	82	ASN
20	S13P	83	ARG
20	S13P	85	LYS
20	S13P	87	TYR
20	S13P	93	MET
20	S13P	96	VAL
20	S13P	104	VAL
20	S13P	105	ARG
20	S13P	111	GLU
20	S13P	115	ARG
20	S13P	117	TRP
20	S13P	134	ARG
20	S13P	135	THR
20	S13P	146	ARG
20	S13P	147	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
21	S14P	5	LYS
21	S14P	9	GLU
21	S14P	11	ARG
21	S14P	14	LYS
21	S14P	17	GLN
21	S14P	18	LEU
21	S14P	21	ARG
21	S14P	22	CYS
21	S14P	25	ARG
21	S14P	26	ASP
21	S14P	39	GLN
21	S14P	46	TYR
21	S14P	52	LYS
22	S17E	6	THR
22	S17E	7	LYS
22	S17E	11	ARG
22	S17E	12	VAL
22	S17E	17	TYR
22	S17E	18	ASP
22	S17E	23	GLN
22	S17E	44	LYS
22	S17E	45	LYS
22	S17E	47	LYS
22	S17E	57	TYR
22	S17E	59	LYS
22	S17E	60	ILE
22	S17E	63	ASN
23	S19E	10	ILE
23	S19E	25	GLU
23	S19E	31	TRP
23	S19E	32	VAL
23	S19E	37	THR
23	S19E	41	LYS
23	S19E	43	ARG
23	S19E	55	ARG
23	S19E	62	HIS
23	S19E	67	LYS
23	S19E	72	LEU
23	S19E	74	LYS
23	S19E	85	ARG
23	S19E	94	LYS
23	S19E	100	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
23	S19E	104	LEU
23	S19E	106	GLN
23	S19E	117	ARG
23	S19E	120	ARG
23	S19E	122	LEU
23	S19E	127	ARG
23	S19E	130	LEU
23	S19E	136	GLU
23	S19E	148	LEU
24	S19P	9	TRP
24	S19P	14	TYR
24	S19P	20	GLU
24	S19P	21	ASP
24	S19P	27	MET
24	S19P	37	ARG
24	S19P	40	ARG
24	S19P	46	PHE
24	S19P	51	ARG
24	S19P	52	ARG
24	S19P	53	LEU
24	S19P	55	GLU
24	S19P	67	ASN
24	S19P	73	HIS
24	S19P	75	ARG
24	S19P	87	ARG
24	S19P	92	ASN
24	S19P	94	LYS
24	S19P	105	MET
24	S19P	115	ILE
24	S19P	117	THR
24	S19P	119	LYS
25	S28E	25	ILE
25	S28E	30	ARG
25	S28E	31	THR
25	S28E	36	GLU
25	S28E	39	GLN
25	S28E	40	VAL
25	S28E	45	LEU
25	S28E	53	ILE
25	S28E	56	ARG
25	S28E	57	ASN
25	S28E	62	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
25	S28E	64	LEU
25	S28E	68	LEU
25	S28E	70	LEU
25	S28E	73	THR
25	S28E	78	ARG
26	SL7A	32	ILE
26	SL7A	50	LEU
26	SL7A	51	VAL
26	SL7A	56	ASP
26	SL7A	77	TYR
26	SL7A	86	LEU
26	SL7A	93	GLN
26	SL7A	98	SER
27	S27A	12	GLN
27	S27A	16	VAL
27	S27A	19	THR
27	S27A	21	TYR
27	S27A	27	SER
27	S27A	28	ILE
27	S27A	30	LEU
27	S27A	33	LYS
27	S27A	35	CYS
27	S27A	37	ARG
27	S27A	42	MET
27	S27A	45	HIS
27	S27A	46	MET
28	AS8P	14	LEU
28	AS8P	15	TYR
28	AS8P	21	ARG
28	AS8P	26	LEU
28	AS8P	35	ILE
28	AS8P	36	SER
28	AS8P	42	GLN
28	AS8P	43	LYS
28	AS8P	51	GLU
28	AS8P	54	ASP
28	AS8P	55	ASP
28	AS8P	65	LEU
28	AS8P	66	LEU
28	AS8P	68	ARG
28	AS8P	88	ARG
28	AS8P	91	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
28	AS8P	92	TYR
28	AS8P	93	ILE
28	AS8P	96	TYR
28	AS8P	97	LEU
28	AS8P	104	ILE
28	AS8P	107	ILE
28	AS8P	108	SER
28	AS8P	109	THR
28	AS8P	115	SER
28	AS8P	118	ASP
28	AS8P	132	VAL

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%)

All (723) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A16S	9	U
1	A16S	11	C
1	A16S	13	G
1	A16S	15	U
1	A16S	16	U
1	A16S	17	G
1	A16S	18	A
1	A16S	19	U
1	A16S	24	C
1	A16S	26	G
1	A16S	28	A
1	A16S	33	A
1	A16S	40	U
1	A16S	41	C
1	A16S	42	G
1	A16S	45	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	47	A
1	A16S	48	G
1	A16S	49	G
1	A16S	52	U
1	A16S	53	A
1	A16S	54	A
1	A16S	57	C
1	A16S	60	G
1	A16S	63	A
1	A16S	64	G
1	A16S	65	U
1	A16S	67	U
1	A16S	69	A
1	A16S	70	C
1	A16S	71	A
1	A16S	73	U
1	A16S	78	G
1	A16S	79	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	87	G
1	A16S	89	G
1	A16S	92	G
1	A16S	93	C
1	A16S	95	G
1	A16S	96	A
1	A16S	97	C
1	A16S	99	G
1	A16S	103	A
1	A16S	105	U
1	A16S	106	A
1	A16S	107	A
1	A16S	108	C
1	A16S	110	C
1	A16S	111	G
1	A16S	114	G
1	A16S	117	A
1	A16S	118	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	119	C
1	A16S	120	C
1	A16S	123	C
1	A16S	124	C
1	A16S	127	C
1	A16S	128	G
1	A16S	130	G
1	A16S	132	C
1	A16S	135	G
1	A16S	136	G
1	A16S	142	C
1	A16S	143	C
1	A16S	146	G
1	A16S	147	G
1	A16S	151	C
1	A16S	153	G
1	A16S	159	A
1	A16S	162	C
1	A16S	163	C
1	A16S	166	G
1	A16S	167	A
1	A16S	168	U
1	A16S	173	A
1	A16S	175	G
1	A16S	176	G
1	A16S	177	A
1	A16S	178	G
1	A16S	181	C
1	A16S	185	A
1	A16S	187	U
1	A16S	191	U
1	A16S	195	U
1	A16S	197	C
1	A16S	198	C
1	A16S	202	A
1	A16S	204	G
1	A16S	206	C
1	A16S	207	U
1	A16S	208	A
1	A16S	210	A
1	A16S	211	G
1	A16S	213	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	214	U
1	A16S	215	A
1	A16S	217	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	228	A
1	A16S	229	G
1	A16S	243	G
1	A16S	245	G
1	A16S	252	C
1	A16S	254	C
1	A16S	255	A
1	A16S	256	U
1	A16S	257	C
1	A16S	259	G
1	A16S	263	G
1	A16S	264	U
1	A16S	266	G
1	A16S	270	G
1	A16S	274	A
1	A16S	277	G
1	A16S	278	G
1	A16S	279	C
1	A16S	287	A
1	A16S	291	A
1	A16S	293	A
1	A16S	294	A
1	A16S	298	G
1	A16S	301	G
1	A16S	302	G
1	A16S	305	C
1	A16S	306	C
1	A16S	313	G
1	A16S	315	G
1	A16S	316	G
1	A16S	318	A
1	A16S	320	C
1	A16S	323	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	324	C
1	A16S	325	A
1	A16S	326	G
1	A16S	328	U
1	A16S	329	G
1	A16S	333	A
1	A16S	334	C
1	A16S	336	G
1	A16S	337	A
1	A16S	340	C
1	A16S	341	A
1	A16S	344	G
1	A16S	345	G
1	A16S	349	A
1	A16S	350	G
1	A16S	351	G
1	A16S	352	C
1	A16S	355	U
1	A16S	356	A
1	A16S	358	G
1	A16S	362	C
1	A16S	363	G
1	A16S	364	C
1	A16S	365	A
1	A16S	366	C
1	A16S	367	C
1	A16S	369	G
1	A16S	370	G
1	A16S	371	C
1	A16S	372	G
1	A16S	373	C
1	A16S	375	A
1	A16S	376	A
1	A16S	377	A
1	A16S	378	C
1	A16S	379	G
1	A16S	380	U
1	A16S	381	C
1	A16S	385	A
1	A16S	386	A
1	A16S	387	U
1	A16S	395	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	398	G
1	A16S	400	G
1	A16S	401	A
1	A16S	402	G
1	A16S	404	G
1	A16S	405	C
1	A16S	406	G
1	A16S	409	A
1	A16S	412	C
1	A16S	414	G
1	A16S	417	U
1	A16S	418	G
1	A16S	419	C
1	A16S	420	C
1	A16S	421	U
1	A16S	423	C
1	A16S	424	G
1	A16S	425	C
1	A16S	428	G
1	A16S	430	A
1	A16S	434	U
1	A16S	435	U
1	A16S	436	U
1	A16S	437	U
1	A16S	438	C
1	A16S	439	C
1	A16S	441	C
1	A16S	442	G
1	A16S	446	U
1	A16S	447	A
1	A16S	449	A
1	A16S	451	A
1	A16S	452	G
1	A16S	453	G
1	A16S	455	G
1	A16S	457	G
1	A16S	458	G
1	A16S	459	G
1	A16S	462	U
1	A16S	463	A
1	A16S	465	G
1	A16S	471	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	482	U
1	A16S	483	G
1	A16S	484	U
1	A16S	485	C
1	A16S	486	A
1	A16S	487	G
1	A16S	489	C
1	A16S	490	G
1	A16S	491	C
1	A16S	492	C
1	A16S	493	G
1	A16S	494	C
1	A16S	497	U
1	A16S	498	A
1	A16S	499	A
1	A16S	502	C
1	A16S	504	A
1	A16S	508	C
1	A16S	509	C
1	A16S	513	A
1	A16S	523	G
1	A16S	525	G
1	A16S	526	A
1	A16S	527	U
1	A16S	530	C
1	A16S	533	G
1	A16S	535	C
1	A16S	537	U
1	A16S	538	A
1	A16S	539	A
1	A16S	540	A
1	A16S	541	G
1	A16S	543	G
1	A16S	545	C
1	A16S	546	U
1	A16S	554	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	556	C
1	A16S	562	A
1	A16S	564	U
1	A16S	568	C
1	A16S	570	C
1	A16S	576	G
1	A16S	577	U
1	A16S	581	C
1	A16S	585	U
1	A16S	586	C
1	A16S	587	A
1	A16S	588	A
1	A16S	589	C
1	A16S	595	A
1	A16S	596	A
1	A16S	598	U
1	A16S	599	G
1	A16S	600	G
1	A16S	602	G
1	A16S	606	A
1	A16S	608	A
1	A16S	609	C
1	A16S	612	G
1	A16S	616	G
1	A16S	619	A
1	A16S	620	G
1	A16S	623	G
1	A16S	624	G
1	A16S	628	G
1	A16S	631	A
1	A16S	632	G
1	A16S	635	G
1	A16S	636	G
1	A16S	639	G
1	A16S	642	A
1	A16S	643	C
1	A16S	645	C
1	A16S	648	G
1	A16S	650	A
1	A16S	653	A
1	A16S	654	G
1	A16S	656	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	657	G
1	A16S	659	G
1	A16S	661	A
1	A16S	662	A
1	A16S	664	C
1	A16S	665	C
1	A16S	666	U
1	A16S	667	U
1	A16S	668	A
1	A16S	669	G
1	A16S	671	U
1	A16S	672	A
1	A16S	679	G
1	A16S	681	A
1	A16S	682	C
1	A16S	683	C
1	A16S	684	A
1	A16S	687	A
1	A16S	689	U
1	A16S	690	G
1	A16S	695	A
1	A16S	697	G
1	A16S	698	C
1	A16S	707	A
1	A16S	708	G
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	725	A
1	A16S	732	A
1	A16S	737	C
1	A16S	738	G
1	A16S	739	G
1	A16S	740	G
1	A16S	741	G
1	A16S	774	G
1	A16S	778	G
1	A16S	779	U
1	A16S	781	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	789	G
1	A16S	790	G
1	A16S	793	U
1	A16S	794	A
1	A16S	796	G
1	A16S	799	U
1	A16S	800	C
1	A16S	809	U
1	A16S	810	U
1	A16S	812	G
1	A16S	813	A
1	A16S	815	C
1	A16S	816	C
1	A16S	818	A
1	A16S	819	C
1	A16S	820	U
1	A16S	821	C
1	A16S	824	U
1	A16S	826	C
1	A16S	827	C
1	A16S	829	C
1	A16S	831	G
1	A16S	837	C
1	A16S	841	U
1	A16S	842	A
1	A16S	846	C
1	A16S	847	C
1	A16S	850	C
1	A16S	852	C
1	A16S	854	U
1	A16S	860	G
1	A16S	865	G
1	A16S	872	G
1	A16S	880	C
1	A16S	881	U
1	A16S	882	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	883	A
1	A16S	884	A
1	A16S	886	G
1	A16S	887	G
1	A16S	889	A
1	A16S	890	U
1	A16S	892	G
1	A16S	893	G
1	A16S	894	C
1	A16S	895	G
1	A16S	896	G
1	A16S	898	G
1	A16S	899	G
1	A16S	900	A
1	A16S	901	G
1	A16S	903	A
1	A16S	904	C
1	A16S	905	C
1	A16S	906	A
1	A16S	909	A
1	A16S	910	G
1	A16S	911	G
1	A16S	912	G
1	A16S	915	G
1	A16S	916	G
1	A16S	917	A
1	A16S	918	A
1	A16S	919	C
1	A16S	922	G
1	A16S	924	G
1	A16S	926	C
1	A16S	928	C
1	A16S	929	A
1	A16S	930	A
1	A16S	931	U
1	A16S	932	U
1	A16S	936	G
1	A16S	937	U
1	A16S	938	C
1	A16S	939	A
1	A16S	940	A
1	A16S	942	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	943	C
1	A16S	945	U
1	A16S	946	G
1	A16S	947	G
1	A16S	948	A
1	A16S	950	U
1	A16S	951	C
1	A16S	952	U
1	A16S	953	U
1	A16S	955	C
1	A16S	957	G
1	A16S	961	G
1	A16S	962	A
1	A16S	963	G
1	A16S	964	A
1	A16S	966	C
1	A16S	967	G
1	A16S	968	C
1	A16S	971	U
1	A16S	972	A
1	A16S	973	U
1	A16S	974	G
1	A16S	975	A
1	A16S	976	C
1	A16S	978	G
1	A16S	981	A
1	A16S	982	G
1	A16S	983	G
1	A16S	986	A
1	A16S	987	A
1	A16S	988	C
1	A16S	989	G
1	A16S	990	A
1	A16S	992	C
1	A16S	993	U
1	A16S	994	U
1	A16S	996	C
1	A16S	997	C
1	A16S	998	U
1	A16S	999	G
1	A16S	1000	A
1	A16S	1001	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	1002	U
1	A16S	1003	C
1	A16S	1005	C
1	A16S	1006	G
1	A16S	1007	G
1	A16S	1009	G
1	A16S	1010	A
1	A16S	1014	G
1	A16S	1017	G
1	A16S	1018	C
1	A16S	1019	A
1	A16S	1020	U
1	A16S	1022	G
1	A16S	1027	C
1	A16S	1028	G
1	A16S	1029	C
1	A16S	1030	C
1	A16S	1031	A
1	A16S	1032	G
1	A16S	1034	U
1	A16S	1035	C
1	A16S	1036	G
1	A16S	1037	U
1	A16S	1039	U
1	A16S	1040	U
1	A16S	1041	G
1	A16S	1044	A
1	A16S	1045	A
1	A16S	1046	A
1	A16S	1047	U
1	A16S	1048	G
1	A16S	1050	C
1	A16S	1052	G
1	A16S	1056	A
1	A16S	1058	G
1	A16S	1059	U
1	A16S	1060	C
1	A16S	1063	G
1	A16S	1065	A
1	A16S	1066	A
1	A16S	1068	G
1	A16S	1071	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	1073	A
1	A16S	1074	G
1	A16S	1075	A
1	A16S	1076	C
1	A16S	1077	C
1	A16S	1078	C
1	A16S	1080	C
1	A16S	1082	C
1	A16S	1086	U
1	A16S	1088	G
1	A16S	1089	U
1	A16S	1090	U
1	A16S	1091	G
1	A16S	1092	G
1	A16S	1093	U
1	A16S	1094	A
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	1106	G
1	A16S	1107	G
1	A16S	1108	U
1	A16S	1109	C
1	A16S	1113	A
1	A16S	1114	A
1	A16S	1115	C
1	A16S	1116	C
1	A16S	1117	A
1	A16S	1118	C
1	A16S	1120	C
1	A16S	1121	U
1	A16S	1122	A
1	A16S	1123	G
1	A16S	1124	G
1	A16S	1128	A
1	A16S	1130	U
1	A16S	1131	G
1	A16S	1132	C
1	A16S	1136	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	1137	G
1	A16S	1138	U
1	A16S	1139	A
1	A16S	1140	A
1	A16S	1141	G
1	A16S	1142	C
1	A16S	1143	C
1	A16S	1148	G
1	A16S	1149	A
1	A16S	1150	A
1	A16S	1152	G
1	A16S	1153	A
1	A16S	1154	G
1	A16S	1157	G
1	A16S	1158	G
1	A16S	1159	C
1	A16S	1160	C
1	A16S	1163	G
1	A16S	1164	G
1	A16S	1165	C
1	A16S	1166	A
1	A16S	1167	G
1	A16S	1168	G
1	A16S	1169	U
1	A16S	1177	C
1	A16S	1179	C
1	A16S	1180	C
1	A16S	1182	A
1	A16S	1183	A
1	A16S	1184	A
1	A16S	1190	G
1	A16S	1191	G
1	A16S	1192	G
1	A16S	1193	C
1	A16S	1194	C
1	A16S	1195	G
1	A16S	1196	C
1	A16S	1201	G
1	A16S	1204	U
1	A16S	1205	U
1	A16S	1207	C
1	A16S	1208	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	1210	U
1	A16S	1211	G
1	A16S	1214	A
1	A16S	1216	G
1	A16S	1217	G
1	A16S	1218	A
1	A16S	1219	C
1	A16S	1220	A
1	A16S	1221	A
1	A16S	1223	G
1	A16S	1224	G
1	A16S	1226	A
1	A16S	1227	U
1	A16S	1228	G
1	A16S	1229	C
1	A16S	1230	U
1	A16S	1231	A
1	A16S	1232	C
1	A16S	1233	C
1	A16S	1236	G
1	A16S	1237	A
1	A16S	1238	A
1	A16S	1242	G
1	A16S	1244	G
1	A16S	1245	A
1	A16S	1246	G
1	A16S	1249	A
1	A16S	1250	A
1	A16S	1251	U
1	A16S	1252	C
1	A16S	1254	U
1	A16S	1255	U
1	A16S	1256	A
1	A16S	1259	C
1	A16S	1261	C
1	A16S	1262	U
1	A16S	1264	C
1	A16S	1265	C
1	A16S	1266	G
1	A16S	1267	C
1	A16S	1269	G
1	A16S	1272	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	1273	G
1	A16S	1274	G
1	A16S	1275	A
1	A16S	1276	U
1	A16S	1278	G
1	A16S	1280	G
1	A16S	1283	C
1	A16S	1284	U
1	A16S	1286	A
1	A16S	1287	A
1	A16S	1288	A
1	A16S	1289	C
1	A16S	1290	C
1	A16S	1293	C
1	A16S	1294	C
1	A16S	1296	U
1	A16S	1298	G
1	A16S	1300	G
1	A16S	1301	A
1	A16S	1302	A
1	A16S	1304	G
1	A16S	1305	A
1	A16S	1306	G
1	A16S	1307	G
1	A16S	1309	A
1	A16S	1310	U
1	A16S	1311	C
1	A16S	1314	U
1	A16S	1315	A
1	A16S	1316	G
1	A16S	1317	U
1	A16S	1320	C
1	A16S	1323	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	1337	G
1	A16S	1339	G
1	A16S	1343	A
1	A16S	1344	A
1	A16S	1345	U
1	A16S	1347	C
1	A16S	1350	C
1	A16S	1351	C
1	A16S	1354	G
1	A16S	1356	U
1	A16S	1357	C
1	A16S	1361	G
1	A16S	1363	A
1	A16S	1364	C
1	A16S	1365	A
2	VTRF	3	G
2	VTRF	4	U
2	VTRF	5	U
2	VTRF	6	G
2	VTRF	7	G
2	VTRF	8	U
2	VTRF	9	G
2	VTRF	10	G
2	VTRF	11	U
2	VTRF	15	G
2	VTRF	17	C
2	VTRF	18	U
2	VTRF	19	G
2	VTRF	20	G
2	VTRF	21	U
2	VTRF	22	U
2	VTRF	23	A
2	VTRF	24	U
2	VTRF	25	G
2	VTRF	26	A

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A16S	25	C
1	A16S	46	U
1	A16S	47	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	63	A
1	A16S	78	G
1	A16S	92	G
1	A16S	167	A
1	A16S	186	A
1	A16S	213	C
1	A16S	214	U
1	A16S	220	C
1	A16S	221	C
1	A16S	222	G
1	A16S	255	A
1	A16S	262	U
1	A16S	286	A
1	A16S	324	C
1	A16S	340	C
1	A16S	384	C
1	A16S	400	G
1	A16S	401	A
1	A16S	429	G
1	A16S	462	U
1	A16S	471	G
1	A16S	474	A
1	A16S	475	A
1	A16S	484	U
1	A16S	526	A
1	A16S	587	A
1	A16S	664	C
1	A16S	697	G
1	A16S	719	A
1	A16S	781	A
1	A16S	785	A
1	A16S	859	A
1	A16S	883	A
1	A16S	889	A
1	A16S	892	G
1	A16S	903	A
1	A16S	947	G
1	A16S	960	G
1	A16S	973	U
1	A16S	998	U
1	A16S	999	G
1	A16S	1009	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A16S	1013	A
1	A16S	1017	G
1	A16S	1029	C
1	A16S	1065	A
1	A16S	1088	G
1	A16S	1091	G
1	A16S	1093	U
1	A16S	1107	G
1	A16S	1127	G
1	A16S	1149	A
1	A16S	1158	G
1	A16S	1203	G
1	A16S	1204	U
1	A16S	1207	C
1	A16S	1228	G
1	A16S	1237	A
1	A16S	1254	U
1	A16S	1265	C
1	A16S	1271	U
1	A16S	1274	G
1	A16S	1286	A
1	A16S	1287	A
1	A16S	1288	A
1	A16S	1329	A
1	A16S	1360	U
1	A16S	1363	A
1	A16S	1364	C
2	VTRF	18	U
2	VTRF	20	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 57 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



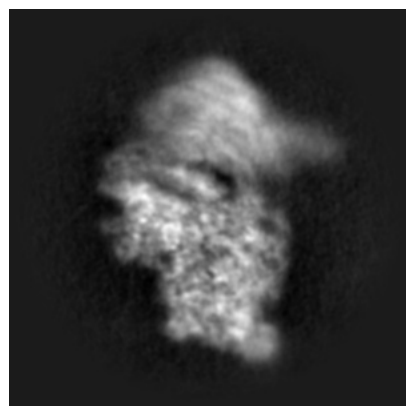
## 6 Map visualisation [i](#)

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

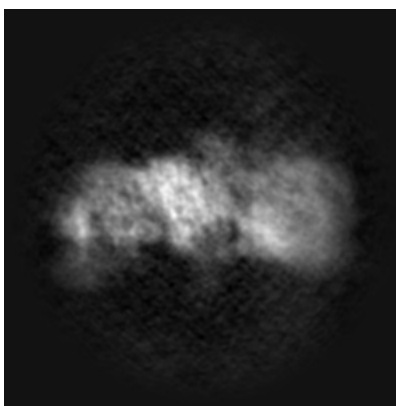
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

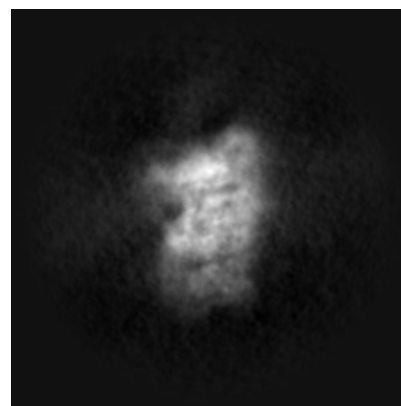
#### 6.1.1 Primary map



X

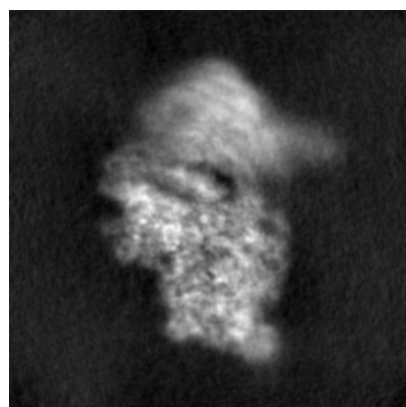


Y

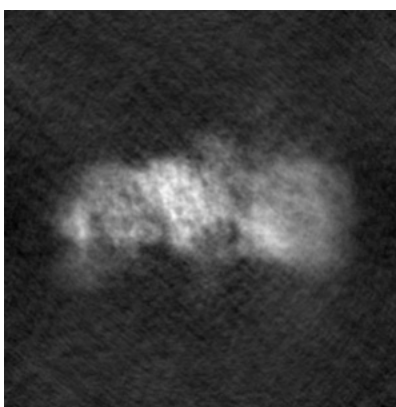


Z

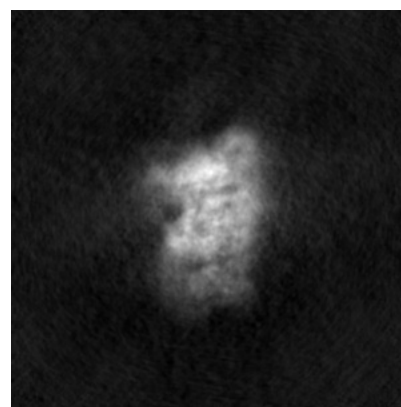
#### 6.1.2 Raw map



X



Y

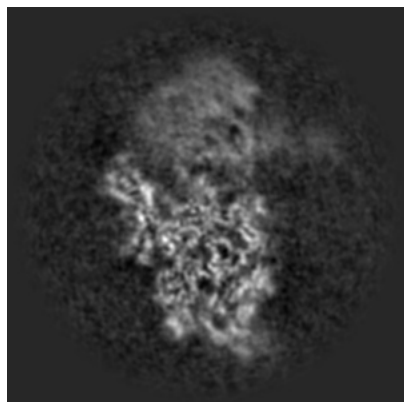


Z

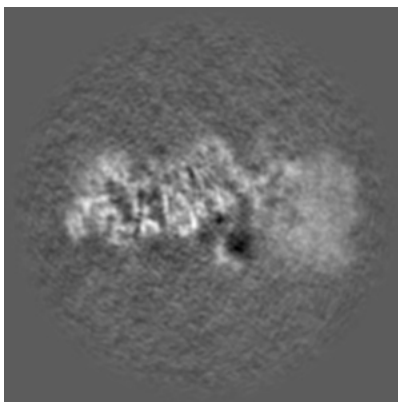
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

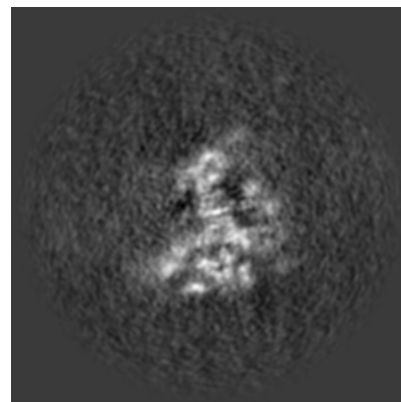
### 6.2.1 Primary map



X Index: 150

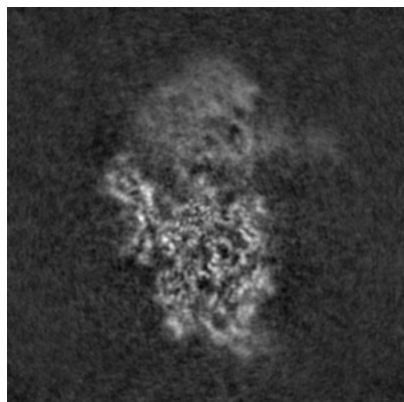


Y Index: 150

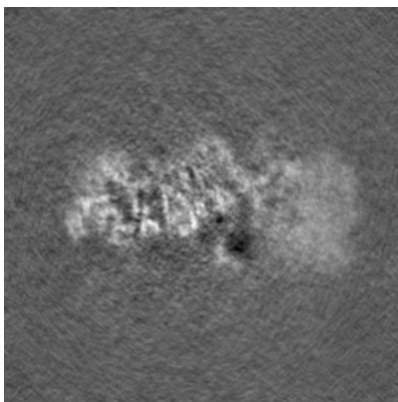


Z Index: 150

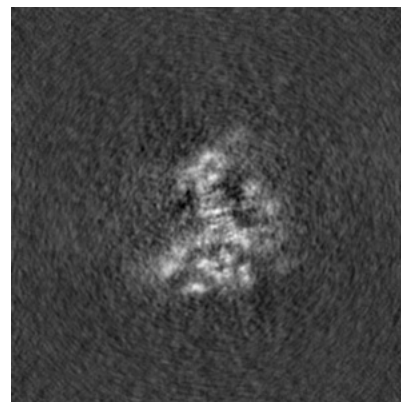
### 6.2.2 Raw map



X Index: 150



Y Index: 150

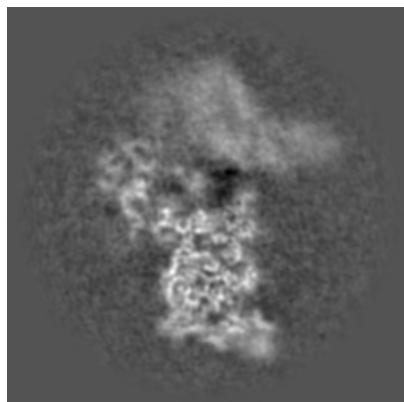


Z Index: 150

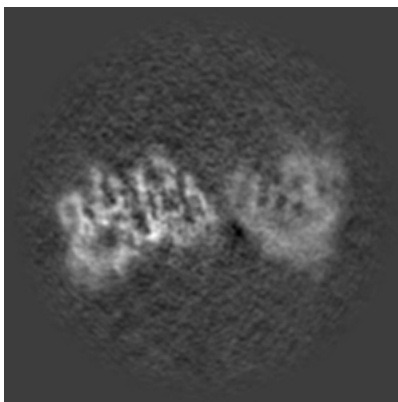
The images above show central slices of the map in three orthogonal directions.

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

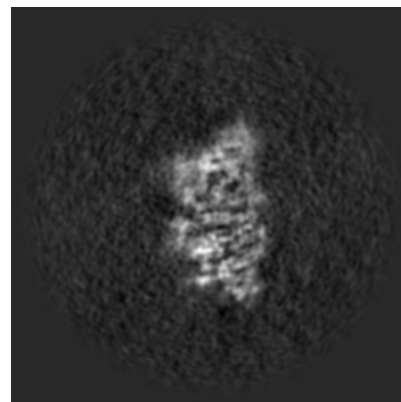
### 6.3.1 Primary map



X Index: 133

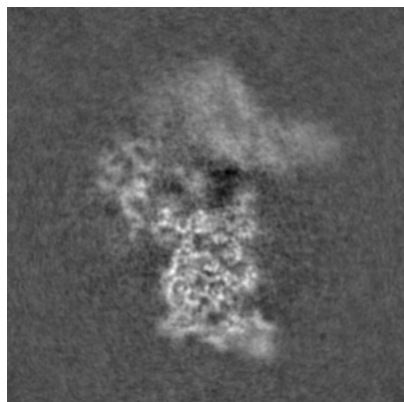


Y Index: 173

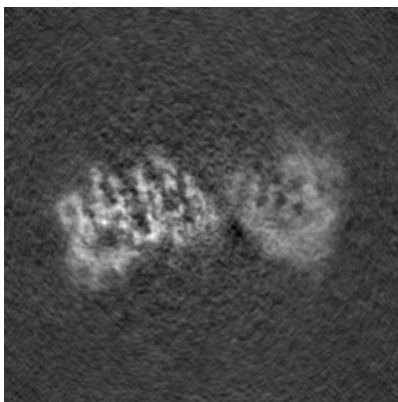


Z Index: 127

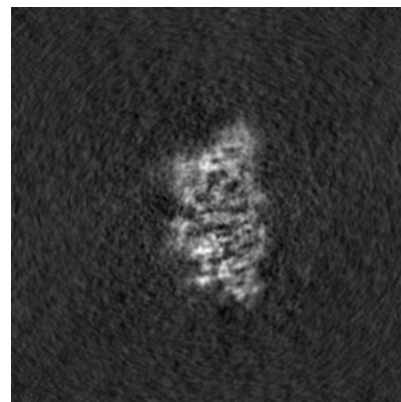
### 6.3.2 Raw map



X Index: 133



Y Index: 174

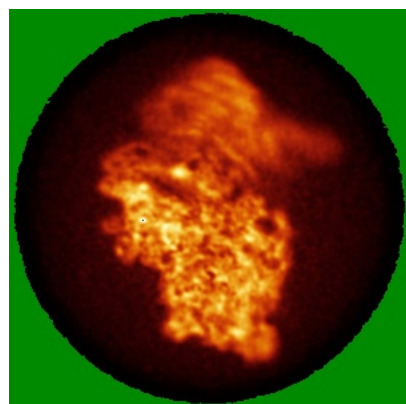


Z Index: 127

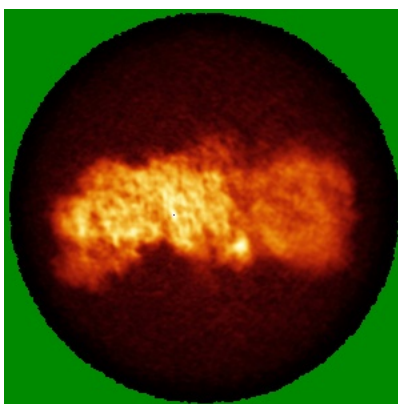
The images above show the largest variance slices of the map in three orthogonal directions.

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

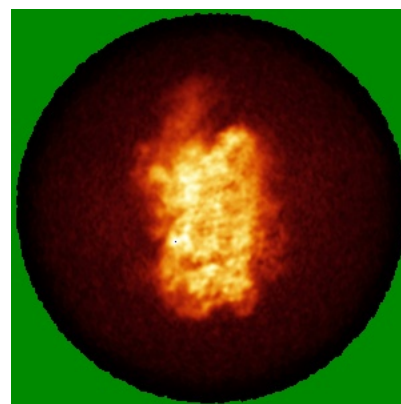
### 6.4.1 Primary map



X

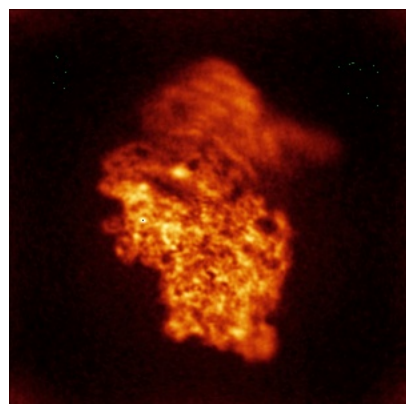


Y

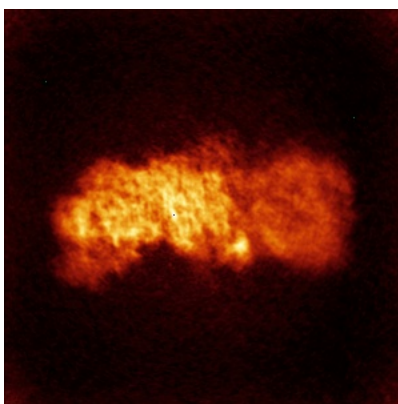


Z

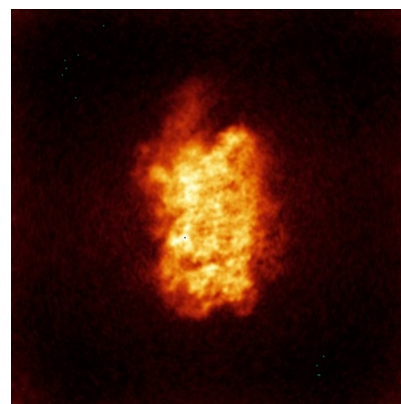
### 6.4.2 Raw map



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.

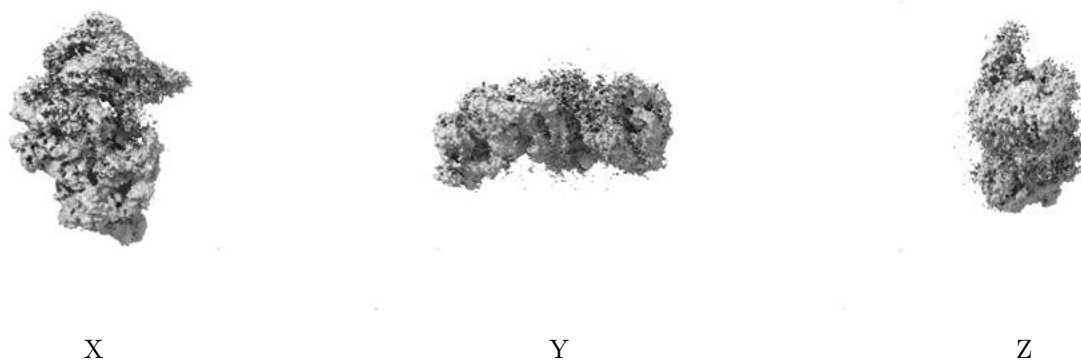
## 6.5 Orthogonal surface views [i](#)

### 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.

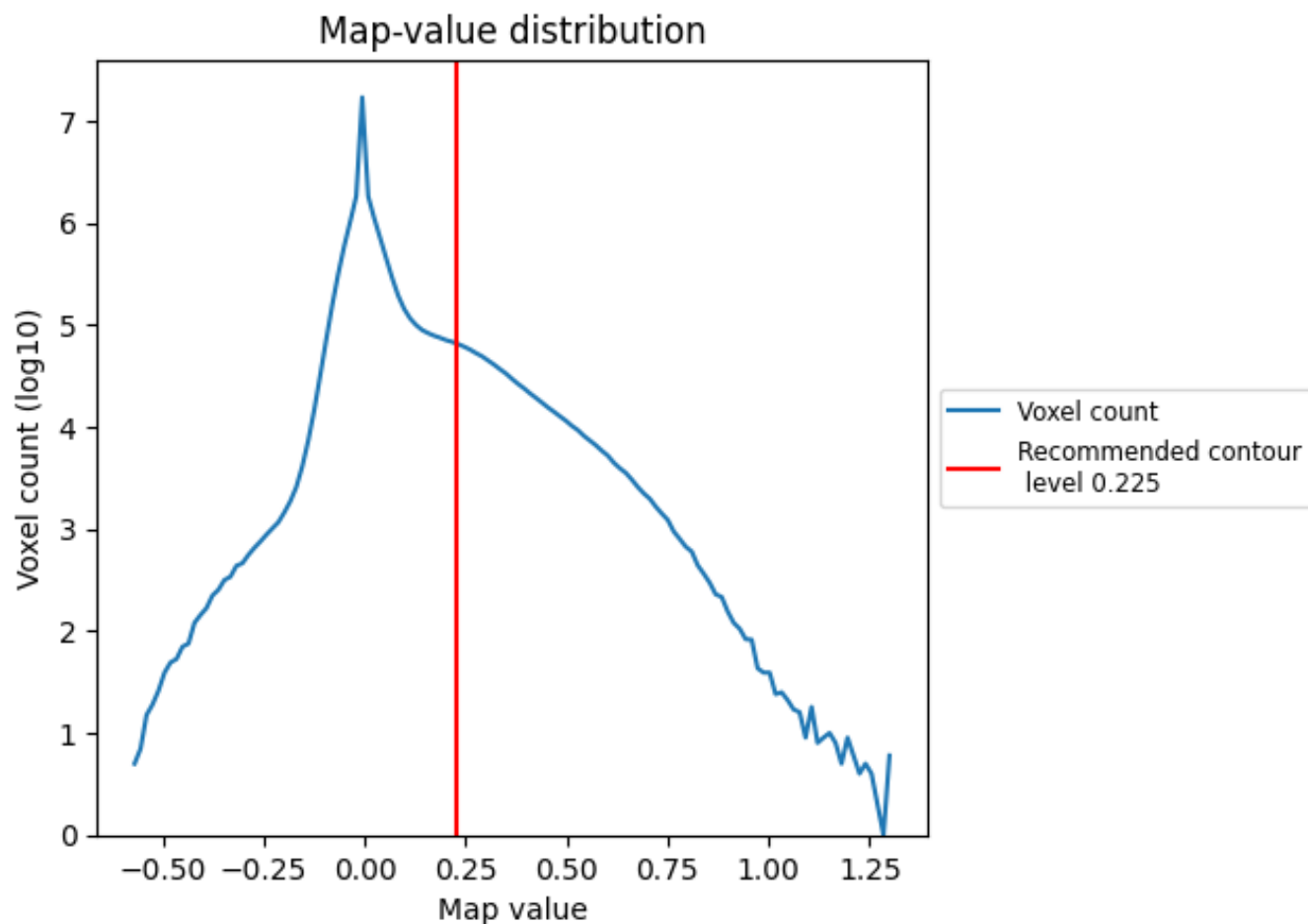
## 6.6 Mask visualisation [i](#)

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.

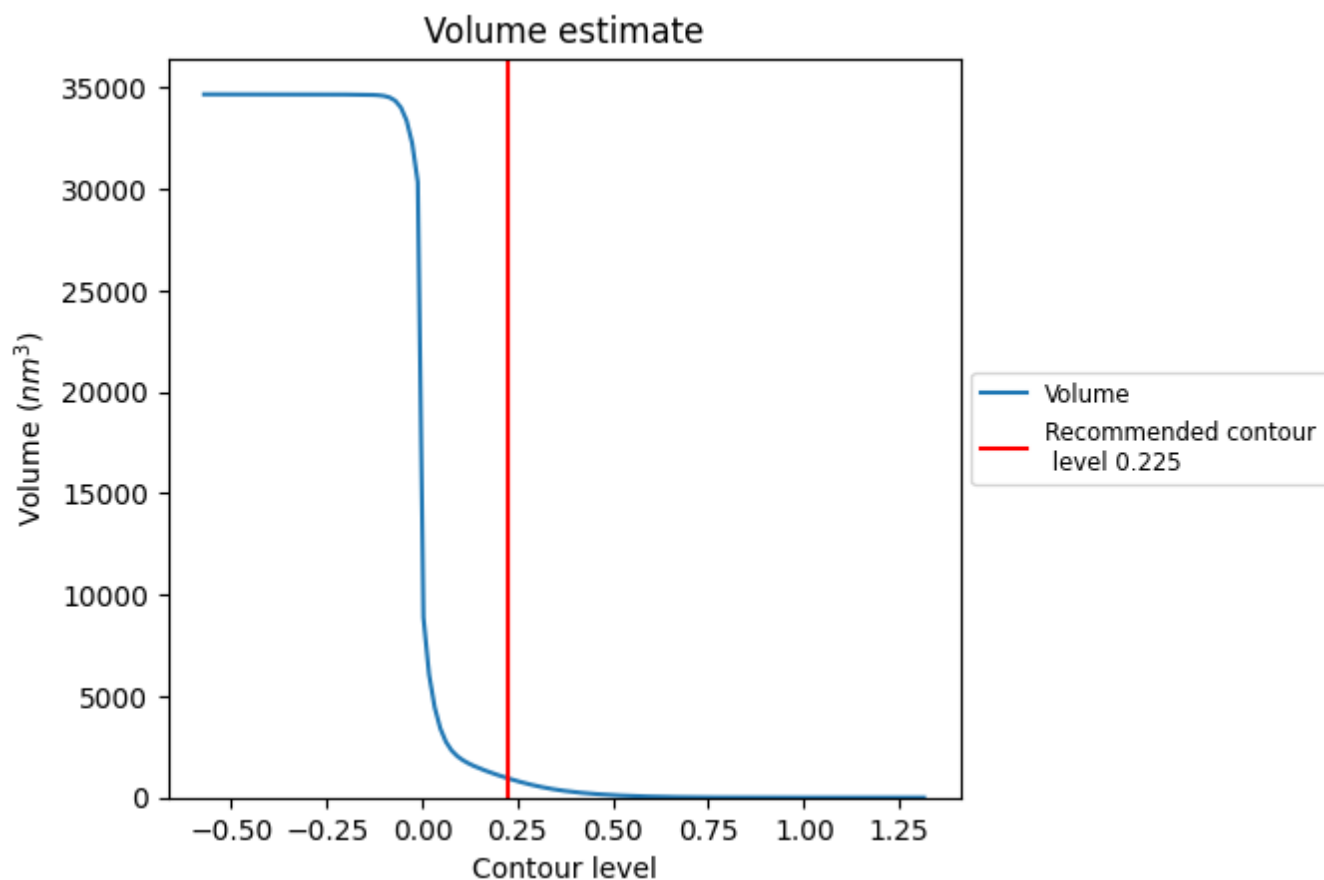
### 7.1 Map-value distribution [i](#)



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.



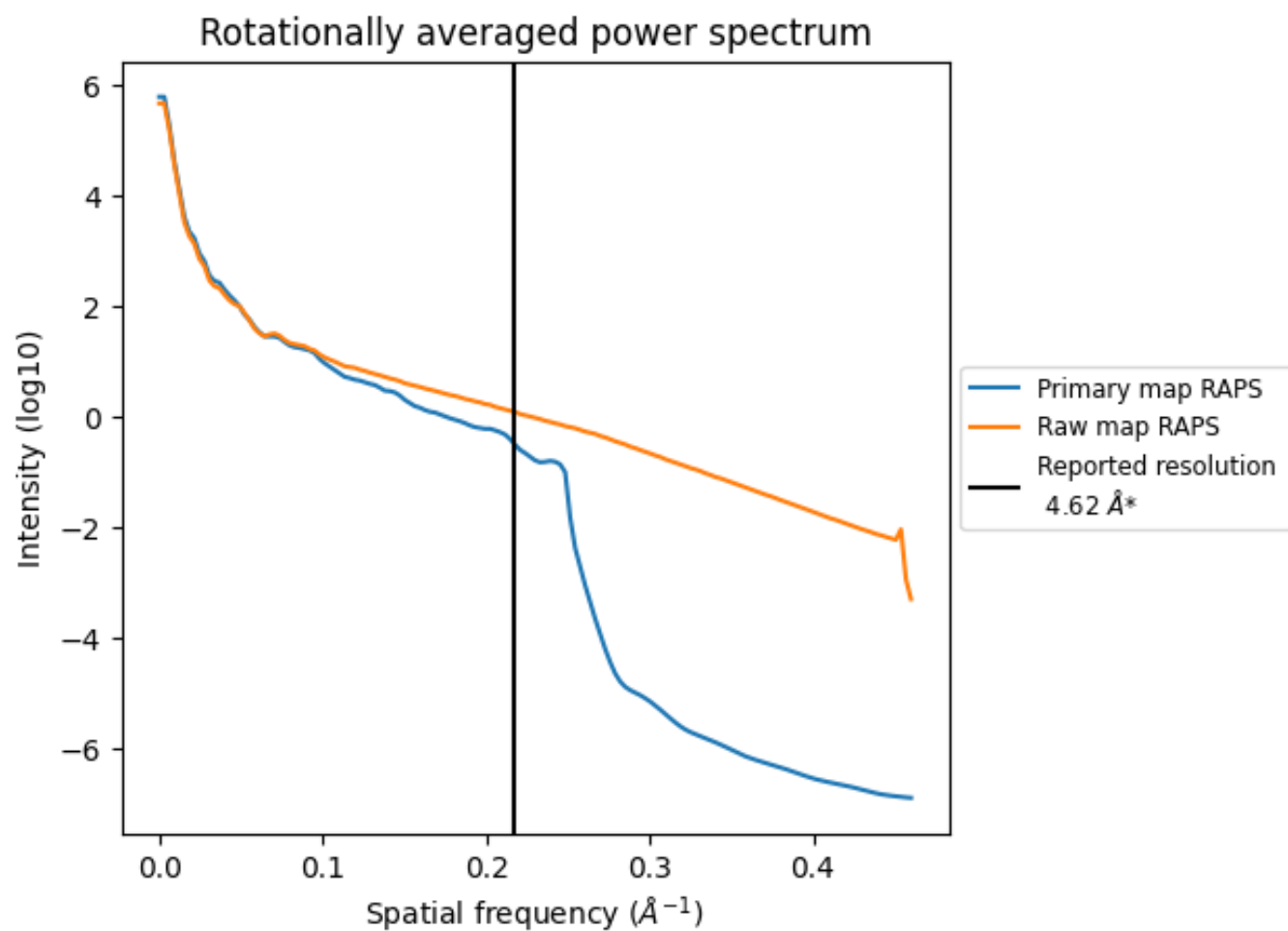
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 951 nm<sup>3</sup>; 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 ⓘ



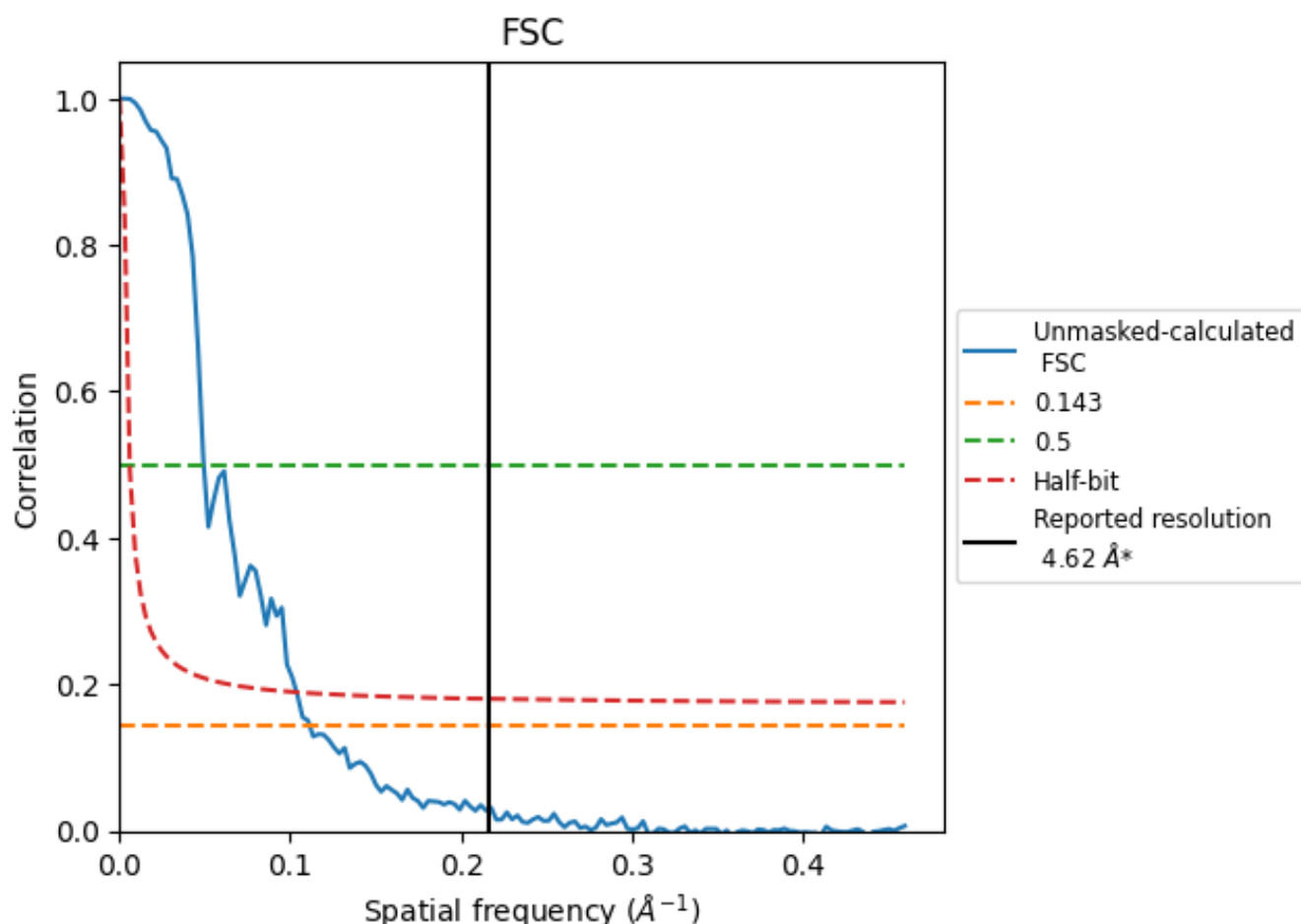
\*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹



## 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  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

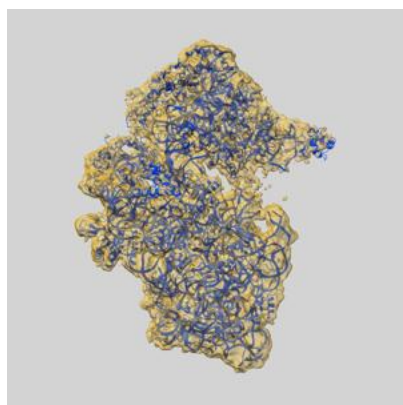
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.97	20.28	9.64

\*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 %

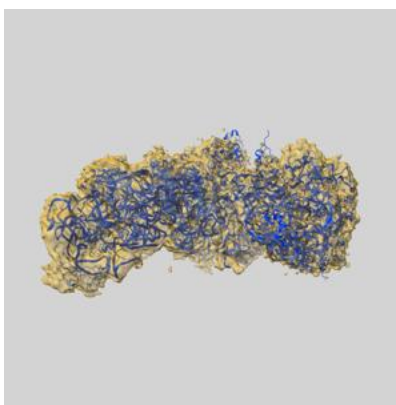
## 9 Map-model fit [i](#)

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](#).

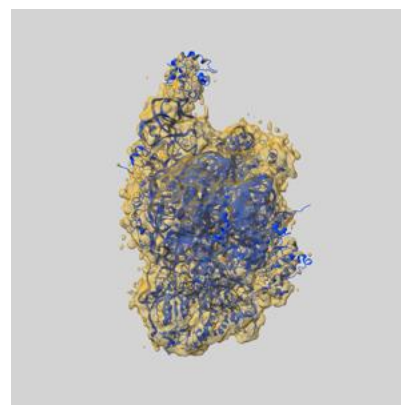
### 9.1 Map-model overlay [i](#)



X



Y



Z

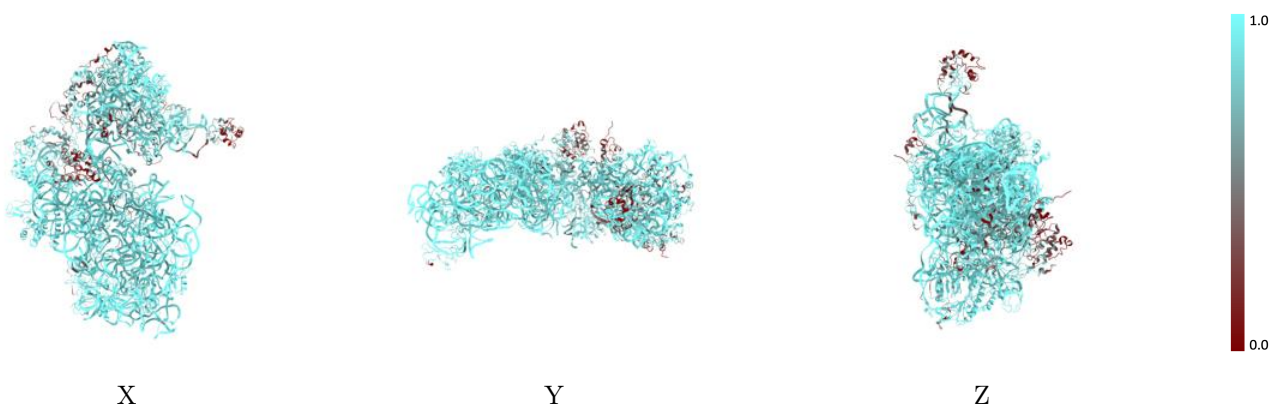
The images above show the 3D surface view of the map at the recommended contour level 0.225 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



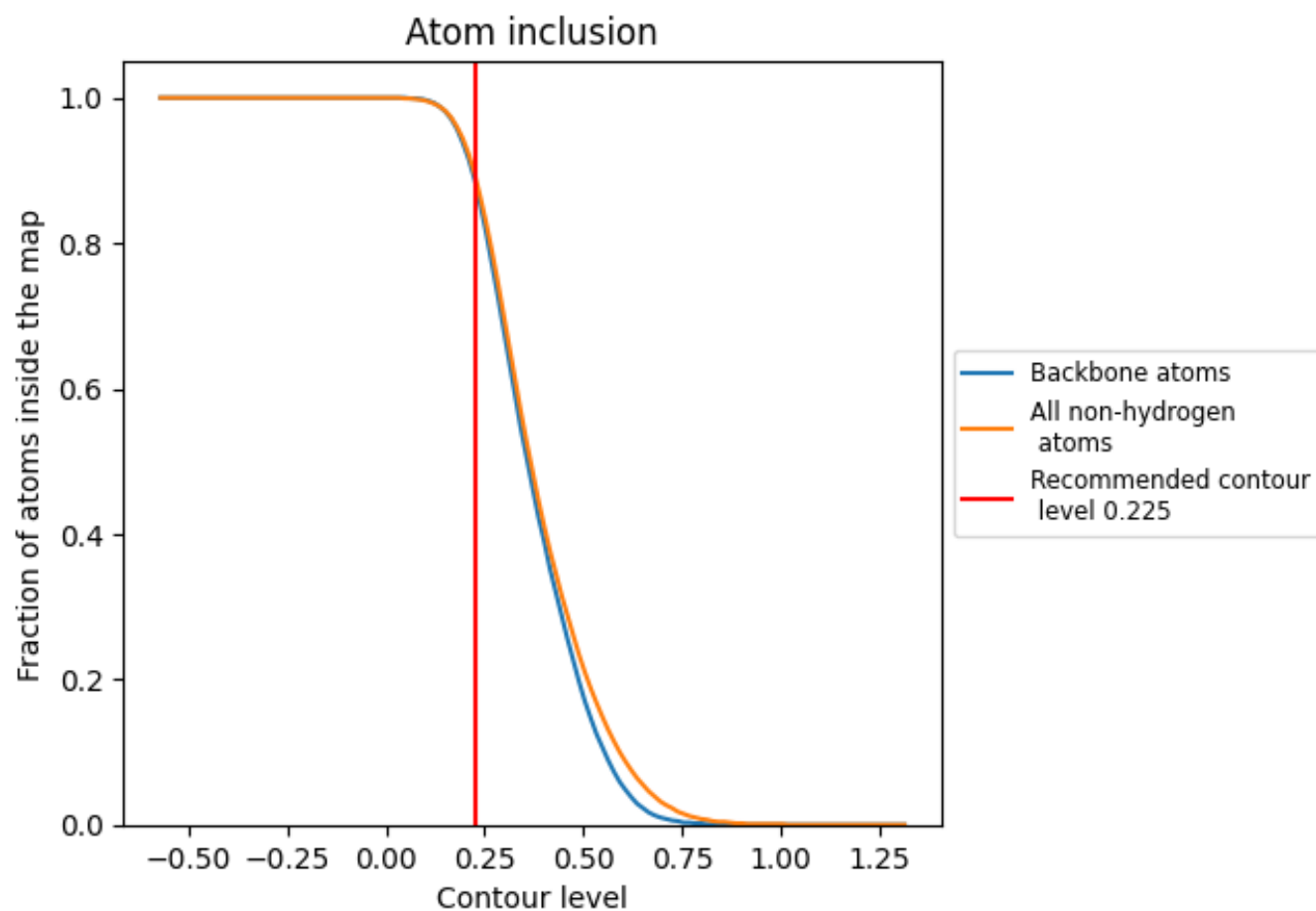
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

