



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:56 AM JST

PDB ID : 7WTT  
EMDB ID : EMD-32800  
Title : Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-A1 (with CK1)  
Authors : Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.  
Deposited on : 2022-02-05  
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

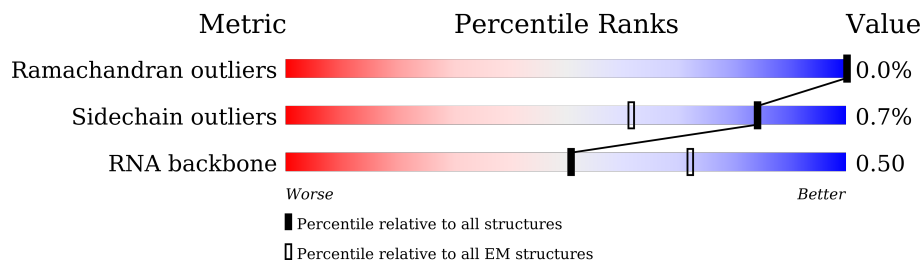
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.10 Å.

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



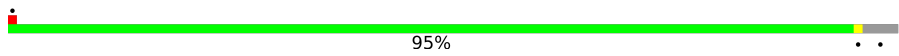
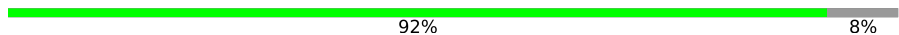
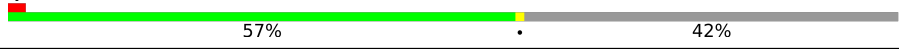
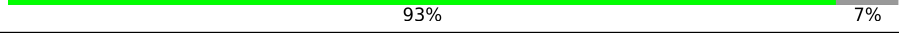

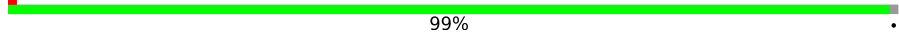

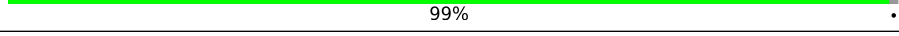

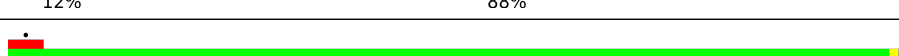



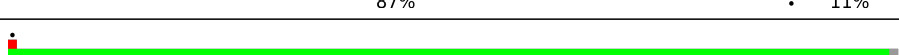
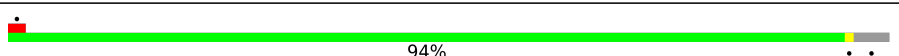
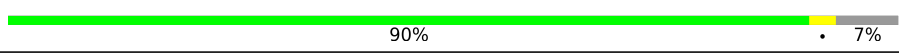
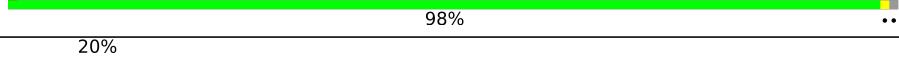
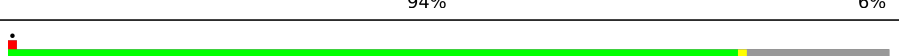
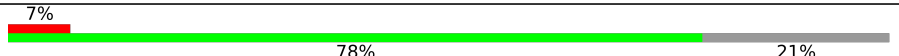


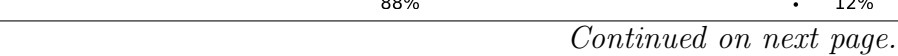



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	2	1873	
2	R	135	
3	b	84	
4	B	264	
5	c	69	
6	E	263	
7	e	59	
8	F	204	


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Mol	Chain	Length	Quality of chain
9	H	194	 95%
10	G	249	 92% 8%
11	Z	125	 57% 42%
12	Y	133	 93% 7%
13	x	252	 69% 31%
14	X	143	 99%
15	w	437	 75% 24%
16	W	130	 99%
17	u	804	 78% 20%
18	t	475	 12% 88%
19	T	145	 99%
20	S	152	 84% 16%
21	Q	146	 85% 14%
22	P	145	 83% 17%
23	O	151	 87% 11%
24	N	151	 99%
25	L	158	 94%
26	J	194	 90% 7%
27	I	208	 98%
28	r	125	 20% 94% 6%
29	q	281	 82% 16%
30	K	1297	 7% 78% 21%
31	M	132	 8% 82% 18%
32	f	156	 37% 63%
33	a	337	 27% 88% 12%

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Mol	Chain	Length	Quality of chain
34	z	230	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '7%', a larger green segment in the middle labeled '36%', and a large grey segment on the right labeled '64%'. The segments are stacked horizontally to represent 100% of the chain's quality.</p>

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 83677 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1575	33634	15011	6036	11012	1575	0	0

- Molecule 2 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	81	673	420	137	114	2	0	0

- Molecule 3 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	b	82	640	402	118	113	7	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	213	1729	1098	309	308	14	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	61	471	288	95	86	2	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	262	2076	1324	386	358	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	e	20	179	110	43	25	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	189	1494	934	284	269	7	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	186	1501	957	276	267	1	0	0

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	230	1862	1164	371	320	7	0	0

- Molecule 11 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Z	72	574	368	104	101	1	0	0

- Molecule 12 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Y	124	1014	641	198	170	5	0	0

- Molecule 13 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	x	175	1372	881	249	238	4	0	0

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	X	141	1098	693	219	183	3	0	0

- Molecule 15 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	w	331	2610	1671	477	453	9	0	0

- Molecule 16 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	W	129	1033	659	193	175	6	0	0

- Molecule 17 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	u	642	5168	3315	928	901	24	0	0

- Molecule 18 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	t	59	520	328	88	101	3	0	0

- Molecule 19 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	144	1122	703	217	199	3	0	0

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	127	1054	669	205	179	1	0	0

- Molecule 21 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	125	Total	C	N	O	S	0	0
			998	637	185	173	3		

- Molecule 22 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	121	Total	C	N	O	S	0	0
			1006	643	186	170	7		

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 28 is a protein called Multifunctional methyltransferase subunit TRM112-like protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	r	118	940	601	166	166	7	0	0

- Molecule 29 is a protein called Probable 18S rRNA (guanine-N(7))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	q	235	1869	1182	333	343	11	0	0

- Molecule 30 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	K	1022	7949	5087	1383	1434	45	0	0

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	M	108	837	530	147	153	7	0	0

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	57	465	295	89	74	7	0	0

- Molecule 33 is a protein called Casein kinase I isoform alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	a	297	2462	1581	432	434	15	1	0

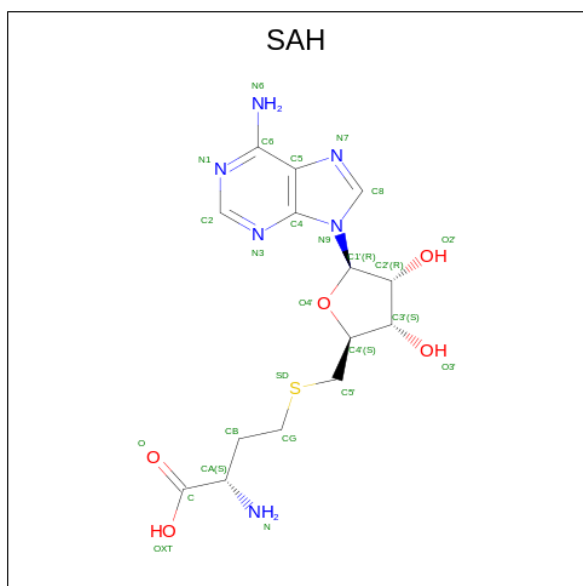
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	20	GLY	VAL	conflict	UNP P48729
a	35	THR	ILE	conflict	UNP P48729
a	58	HIS	LEU	conflict	UNP P48729

- Molecule 34 is a protein called Ribosome biogenesis protein SLX9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	z	82	679	424	132	120	3	0	0

- Molecule 35 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
35	q	1	26	14	6	5	1	0

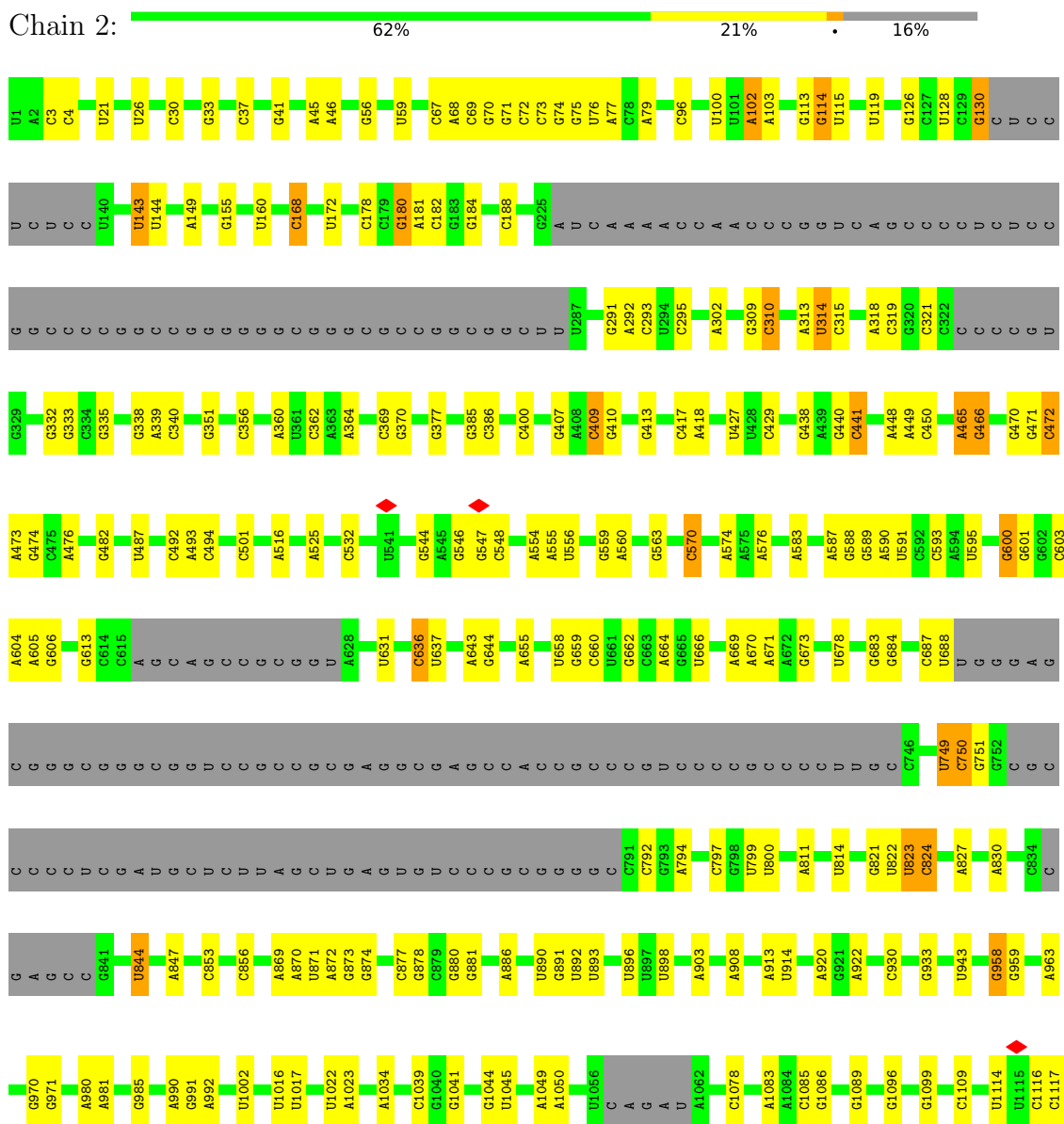
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

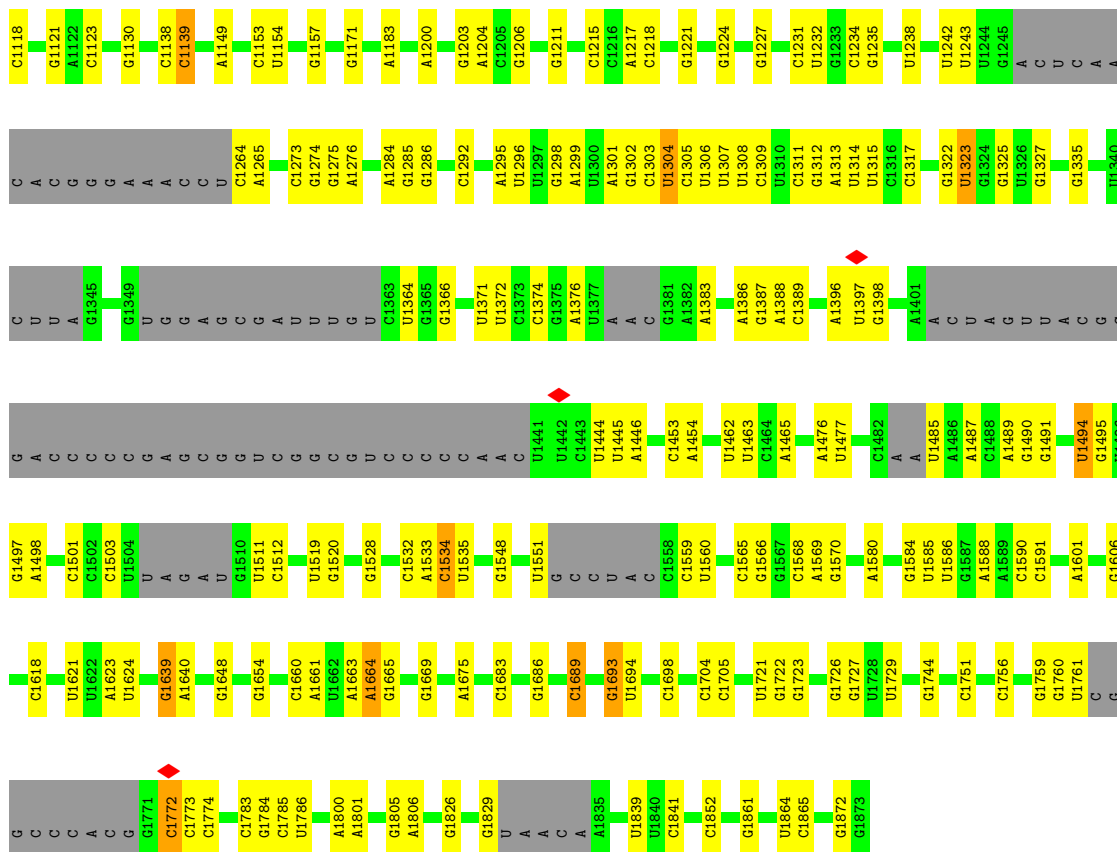
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
36	f	1	1	1	0

### 3 Residue-property plots [i](#)

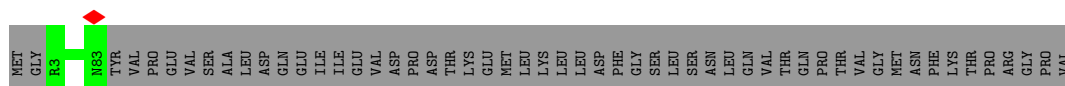
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA

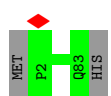




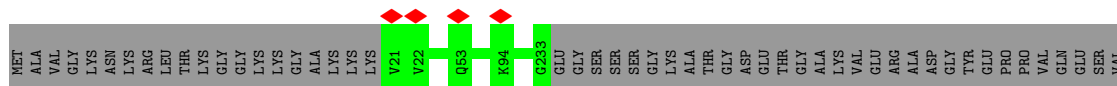
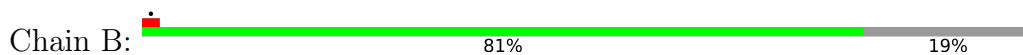
• Molecule 2: 40S ribosomal protein S17



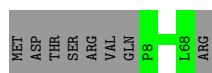
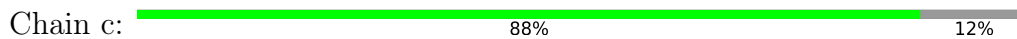
• Molecule 3: 40S ribosomal protein S27



• Molecule 4: 40S ribosomal protein S3a



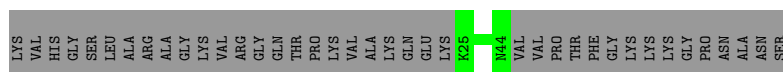
• Molecule 5: 40S ribosomal protein S28



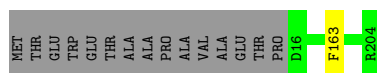
- Molecule 6: 40S ribosomal protein S4, X isoform



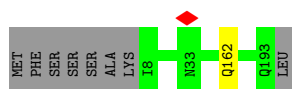
- Molecule 7: 40S ribosomal protein S30



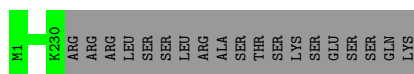
- Molecule 8: 40S ribosomal protein S5



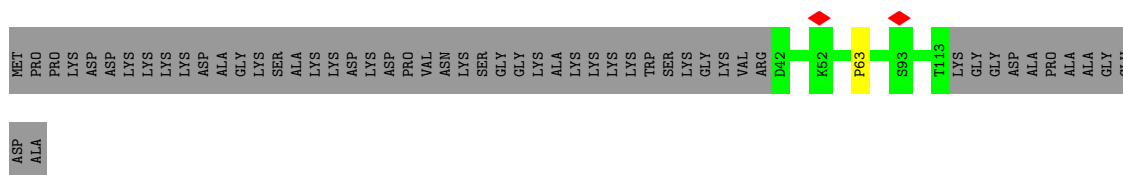
- Molecule 9: 40S ribosomal protein S7



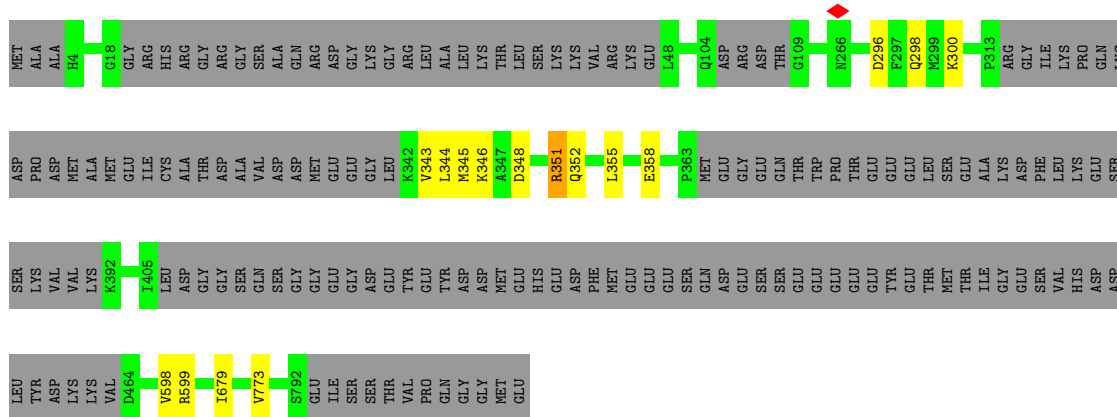
- Molecule 10: 40S ribosomal protein S6



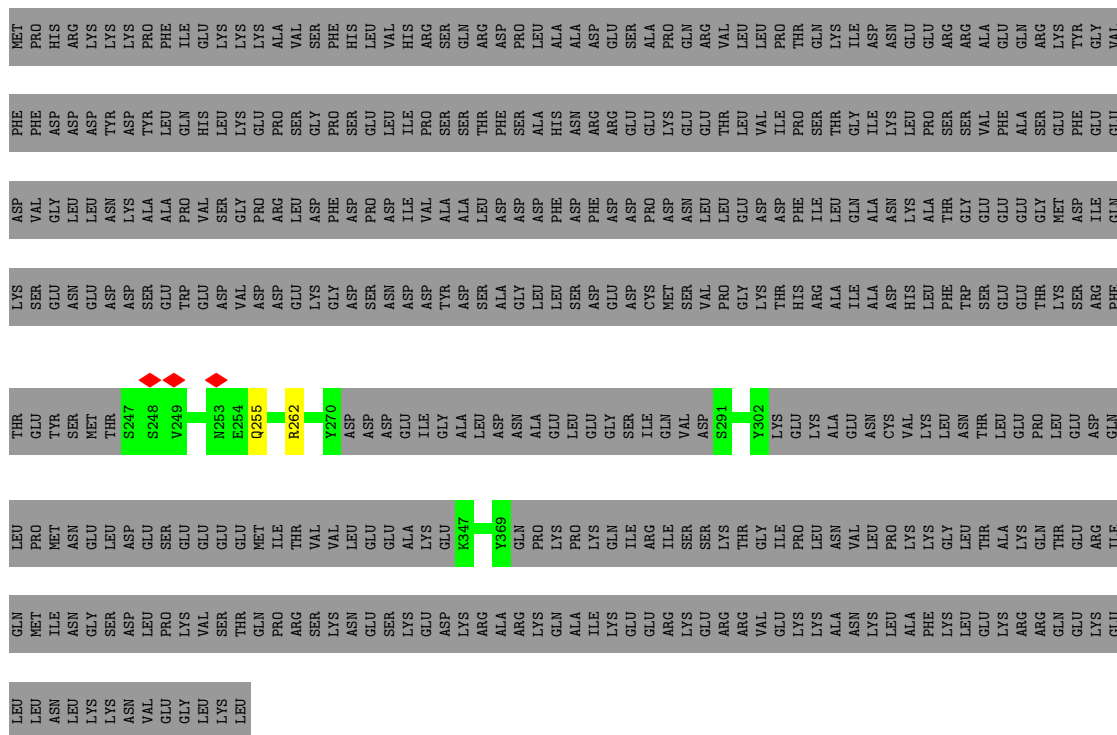
- Molecule 11: 40S ribosomal protein S25



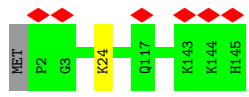




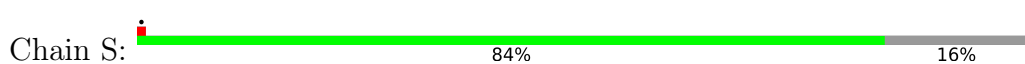
• Molecule 18: Protein LTV1 homolog

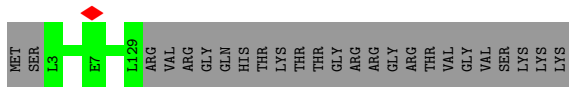


• Molecule 19: 40S ribosomal protein S19

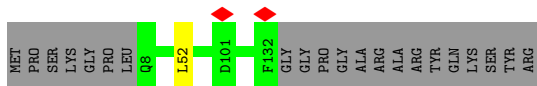
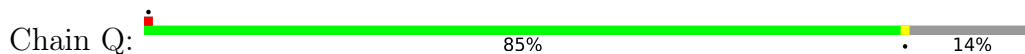


• Molecule 20: 40S ribosomal protein S18

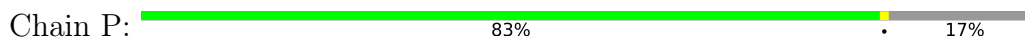




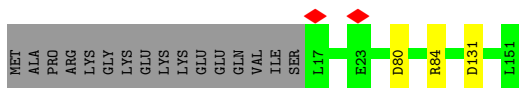
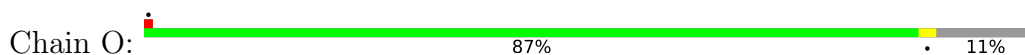
- Molecule 21: 40S ribosomal protein S16



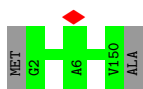
- Molecule 22: 40S ribosomal protein S15



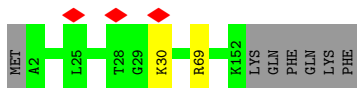
- Molecule 23: 40S ribosomal protein S14



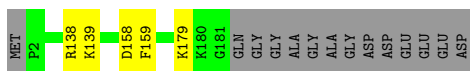
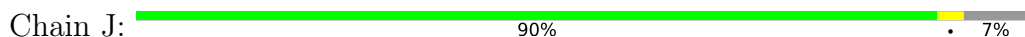
- Molecule 24: 40S ribosomal protein S13



- Molecule 25: 40S ribosomal protein S11



- Molecule 26: 40S ribosomal protein S9

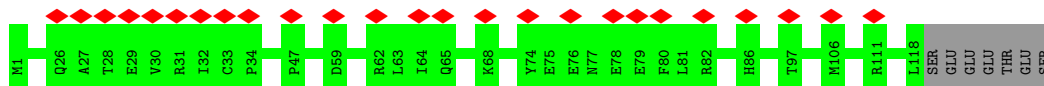
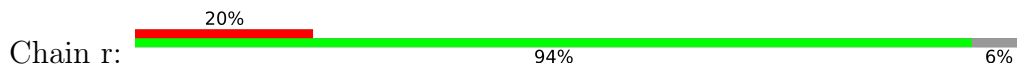


- Molecule 27: 40S ribosomal protein S8

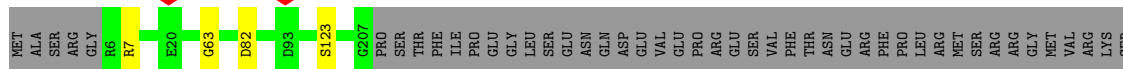
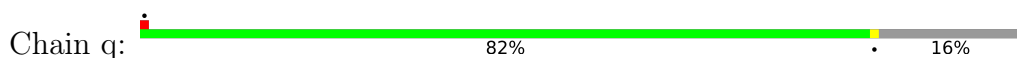




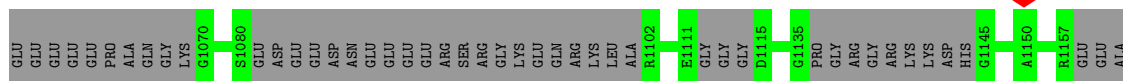
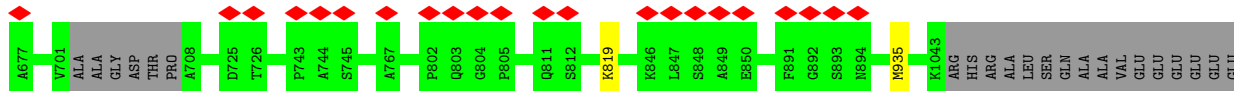
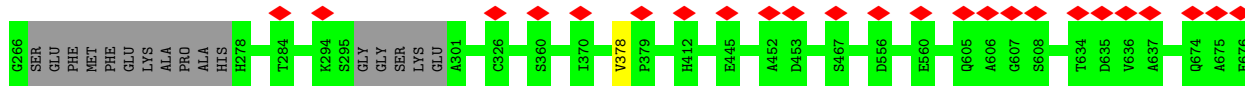
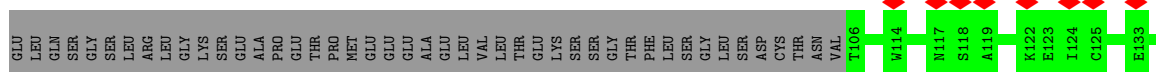
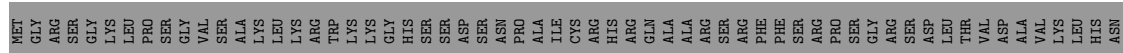
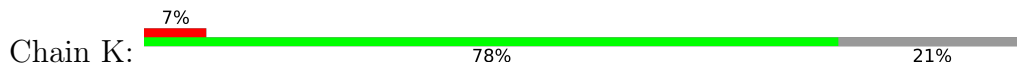
- Molecule 28: Multifunctional methyltransferase subunit TRM112-like protein



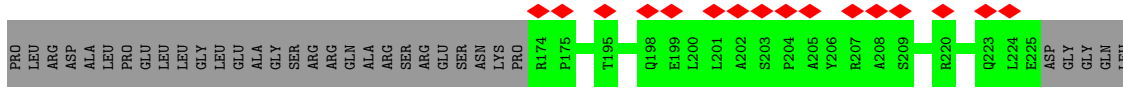
- Molecule 29: Probable 18S rRNA (guanine-N(7))-methyltransferase



- Molecule 30: RRP12-like protein







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103616	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.613	Depositor
Minimum map value	-0.355	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.059, 1.059, 1.059	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, SAH, ZN

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	2	0.65	0/37573	1.07	186/58534 (0.3%)
2	R	0.26	0/680	0.68	0/905
3	b	0.34	0/653	0.56	0/876
4	B	0.31	0/1756	0.61	0/2350
5	c	0.31	0/473	0.72	0/633
6	E	0.42	0/2118	0.66	0/2849
7	e	0.35	0/180	0.67	0/232
8	F	0.30	0/1515	0.60	0/2037
9	H	0.29	0/1524	0.63	1/2042 (0.0%)
10	G	0.34	0/1885	0.65	0/2510
11	Z	0.34	0/580	0.70	2/780 (0.3%)
12	Y	0.42	0/1031	0.64	0/1370
13	x	0.33	0/1394	0.64	1/1880 (0.1%)
14	X	0.39	0/1116	0.63	0/1490
15	w	0.29	0/2656	0.61	1/3586 (0.0%)
16	W	0.36	0/1050	0.62	0/1406
17	u	0.37	0/5296	0.60	1/7154 (0.0%)
18	t	0.29	0/531	0.66	0/713
19	T	0.30	0/1142	0.60	0/1530
20	S	0.30	0/1071	0.63	0/1437
21	Q	0.31	0/1012	0.66	1/1356 (0.1%)
22	P	0.33	0/1025	0.67	1/1369 (0.1%)
23	O	0.32	0/1022	0.74	2/1372 (0.1%)
24	N	0.33	0/1226	0.60	0/1649
25	L	0.42	0/1250	0.65	0/1673
26	J	0.43	0/1524	0.65	0/2035
27	I	0.41	0/1711	0.67	0/2282
28	r	0.27	0/961	0.62	0/1301
29	q	0.36	0/1910	0.61	0/2572
30	K	0.27	0/8097	0.55	0/10950
31	M	0.24	0/845	0.53	0/1134
32	f	0.29	0/474	0.65	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	a	0.28	0/2520	0.63	0/3385
34	z	0.25	0/686	0.57	0/914
All	All	0.49	0/88487	0.85	196/126932 (0.2%)

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
18	t	0	1
30	K	0	1
All	All	0	2

There are no bond length outliers.

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1323	U	N3-C2-O2	-14.51	112.04	122.20
1	2	501	C	N1-C2-O2	13.27	126.86	118.90
1	2	293	C	N1-C2-O2	13.02	126.72	118.90
1	2	501	C	C2-N1-C1'	12.63	132.69	118.80
1	2	356	C	N1-C2-O2	12.14	126.18	118.90
1	2	1773	C	N3-C2-O2	-11.87	113.59	121.90
1	2	356	C	C2-N1-C1'	11.39	131.33	118.80
1	2	501	C	N3-C2-O2	-10.92	114.26	121.90
1	2	356	C	N3-C2-O2	-10.32	114.67	121.90
1	2	1016	U	N3-C2-O2	-10.20	115.06	122.20
1	2	1774	C	N3-C2-O2	-10.07	114.85	121.90
1	2	1016	U	N1-C2-O2	9.87	129.71	122.80
1	2	427	U	N3-C2-O2	-9.70	115.41	122.20
1	2	293	C	C2-N1-C1'	9.25	128.97	118.80
1	2	1773	C	N1-C2-O2	9.23	124.44	118.90
1	2	1865	C	N1-C2-O2	9.23	124.44	118.90
1	2	501	C	C6-N1-C1'	-9.22	109.73	120.80
1	2	1016	U	C2-N1-C1'	9.11	128.63	117.70
1	2	293	C	N3-C2-O2	-9.03	115.58	121.90
1	2	1323	U	N1-C2-O2	8.98	129.09	122.80
1	2	1374	C	N3-C2-O2	-8.97	115.62	121.90
1	2	853	C	C2-N1-C1'	8.83	128.51	118.80
1	2	1453	C	N1-C2-O2	8.74	124.14	118.90
1	2	1453	C	C2-N1-C1'	8.51	128.16	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	356	C	C6-N1-C1'	-8.31	110.83	120.80
1	2	1865	C	N3-C2-O2	-8.23	116.14	121.90
1	2	1306	U	C2-N1-C1'	8.07	127.38	117.70
1	2	1276	A	N1-C6-N6	-8.06	113.77	118.60
1	2	472	C	C6-N1-C2	-8.02	117.09	120.30
1	2	1865	C	C2-N1-C1'	7.97	127.56	118.80
1	2	823	U	N3-C2-O2	-7.83	116.72	122.20
1	2	427	U	C2-N1-C1'	7.80	127.06	117.70
1	2	427	U	N1-C2-O2	7.70	128.19	122.80
23	O	80	ASP	CB-CG-OD1	7.58	125.13	118.30
1	2	1494	U	P-O3'-C3'	7.55	128.76	119.70
1	2	853	C	N1-C2-O2	7.40	123.34	118.90
1	2	1772	C	N1-C2-O2	7.34	123.30	118.90
1	2	1624	U	C2-N1-C1'	7.32	126.48	117.70
1	2	1520	G	C4-N9-C1'	7.18	135.84	126.50
1	2	4	C	C2-N1-C1'	7.09	126.59	118.80
1	2	1022	U	C2-N1-C1'	7.08	126.19	117.70
1	2	1774	C	N1-C2-O2	7.05	123.13	118.90
1	2	1590	C	N1-C2-O2	7.04	123.13	118.90
1	2	293	C	C6-N1-C1'	-6.92	112.49	120.80
1	2	1453	C	N3-C2-O2	-6.90	117.07	121.90
1	2	501	C	C6-N1-C2	-6.87	117.55	120.30
1	2	853	C	N3-C2-O2	-6.84	117.11	121.90
1	2	178	C	N1-C2-O2	6.81	122.98	118.90
1	2	1624	U	N3-C2-O2	-6.76	117.47	122.20
1	2	1624	U	N1-C2-O2	6.70	127.49	122.80
13	x	230	LEU	CA-CB-CG	6.64	130.58	115.30
1	2	856	C	C6-N1-C2	-6.63	117.65	120.30
1	2	1759	G	N1-C2-N2	-6.62	110.25	116.20
1	2	1123	C	N1-C2-O2	6.60	122.86	118.90
1	2	1323	U	N1-C2-N3	6.59	118.86	114.90
1	2	1139	C	C6-N1-C2	-6.55	117.68	120.30
1	2	750	C	C5-C6-N1	6.50	124.25	121.00
1	2	1532	C	N3-C2-O2	-6.48	117.37	121.90
1	2	1532	C	N1-C2-O2	6.40	122.74	118.90
1	2	1292	C	C6-N1-C2	-6.39	117.74	120.30
1	2	356	C	C6-N1-C2	-6.37	117.75	120.30
1	2	1698	C	N1-C2-O2	6.35	122.71	118.90
1	2	1759	G	N1-C6-O6	-6.28	116.13	119.90
1	2	1276	A	C5-C6-N6	6.27	128.71	123.70
1	2	1078	C	N3-C2-O2	-6.26	117.52	121.90
1	2	114	G	P-O3'-C3'	6.24	127.19	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	823	U	N1-C2-O2	6.24	127.17	122.80
1	2	1760	G	N1-C2-N2	-6.22	110.60	116.20
1	2	1590	C	C6-N1-C2	-6.21	117.82	120.30
1	2	659	G	C4-N9-C1'	6.20	134.56	126.50
1	2	1520	G	C8-N9-C1'	-6.14	119.01	127.00
1	2	853	C	C6-N1-C1'	-6.14	113.43	120.80
1	2	102	A	P-O3'-C3'	6.13	127.06	119.70
1	2	119	U	N3-C2-O2	-6.12	117.92	122.20
1	2	314	U	N3-C2-O2	-6.12	117.92	122.20
1	2	824	C	N1-C2-O2	6.06	122.54	118.90
1	2	1123	C	N3-C2-O2	-6.06	117.66	121.90
1	2	4	C	C6-N1-C2	-6.05	117.88	120.30
9	H	162	GLN	CA-CB-CG	6.05	126.70	113.40
1	2	494	C	N1-C2-O2	6.04	122.53	118.90
1	2	877	C	C2-N1-C1'	6.03	125.43	118.80
1	2	1520	G	N3-C4-N9	6.02	129.61	126.00
1	2	1109	C	N1-C2-O2	6.01	122.50	118.90
1	2	1760	G	N3-C2-N2	6.00	124.10	119.90
1	2	1374	C	C6-N1-C2	-6.00	117.90	120.30
1	2	1590	C	N3-C2-O2	-5.99	117.71	121.90
1	2	1139	C	C2-N1-C1'	5.92	125.32	118.80
1	2	1139	C	N3-C2-O2	-5.92	117.75	121.90
1	2	593	C	C2-N1-C1'	5.88	125.27	118.80
1	2	1453	C	C6-N1-C1'	-5.88	113.74	120.80
1	2	1751	C	N1-C2-O2	5.88	122.43	118.90
11	Z	63	PRO	CA-N-CD	-5.88	103.27	111.50
1	2	814	U	N3-C2-O2	-5.86	118.10	122.20
1	2	409	C	C5-C6-N1	5.86	123.93	121.00
1	2	1759	G	N3-C2-N2	5.85	123.99	119.90
1	2	466	G	N3-C4-N9	5.83	129.50	126.00
1	2	143	U	P-O3'-C3'	5.81	126.68	119.70
1	2	21	U	N3-C2-O2	-5.79	118.15	122.20
1	2	30	C	C6-N1-C2	-5.78	117.99	120.30
1	2	1751	C	N3-C2-O2	-5.76	117.87	121.90
21	Q	52	LEU	CA-CB-CG	5.75	128.54	115.30
11	Z	63	PRO	N-CD-CG	-5.75	94.57	103.20
1	2	1016	U	C6-N1-C1'	-5.74	113.16	121.20
1	2	823	U	C2-N1-C1'	5.72	124.56	117.70
1	2	1520	G	N3-C4-C5	-5.72	125.74	128.60
1	2	1485	U	N1-C2-O2	5.71	126.80	122.80
1	2	1591	C	N1-C2-O2	5.71	122.32	118.90
1	2	465	A	P-O3'-C3'	5.68	126.52	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	844	U	N3-C2-O2	-5.68	118.23	122.20
1	2	1852	C	C5-C6-N1	5.64	123.82	121.00
1	2	1311	C	C2-N1-C1'	5.64	125.00	118.80
1	2	853	C	C6-N1-C2	-5.63	118.05	120.30
1	2	824	C	C2-N1-C1'	5.62	124.99	118.80
1	2	659	G	C8-N9-C1'	-5.62	119.69	127.00
1	2	666	U	C2-N1-C1'	5.61	124.44	117.70
1	2	407	G	C4-N9-C1'	5.59	133.77	126.50
1	2	749	U	C2-N1-C1'	5.58	124.40	117.70
1	2	119	U	N1-C2-O2	5.55	126.69	122.80
1	2	1306	U	C6-N1-C1'	-5.55	113.44	121.20
1	2	1774	C	C6-N1-C2	-5.54	118.08	120.30
1	2	102	A	O4'-C1'-N9	5.54	112.63	108.20
1	2	1234	C	C2-N1-C1'	5.53	124.89	118.80
1	2	1693	G	P-O3'-C3'	5.52	126.33	119.70
1	2	570	C	N3-C2-O2	-5.52	118.03	121.90
1	2	321	C	C2-N1-C1'	5.52	124.87	118.80
1	2	1311	C	N1-C2-O2	5.51	122.21	118.90
1	2	1123	C	C6-N1-C2	-5.50	118.10	120.30
1	2	1453	C	C6-N1-C2	-5.50	118.10	120.30
1	2	1683	C	N1-C2-O2	5.50	122.20	118.90
1	2	958	G	C4-N9-C1'	5.49	133.63	126.50
23	O	131	ASP	CB-CG-OD1	5.47	123.22	118.30
1	2	958	G	O4'-C1'-N9	5.47	112.57	108.20
1	2	1292	C	N3-C2-O2	-5.45	118.08	121.90
17	u	773	VAL	C-N-CA	5.45	135.33	121.70
1	2	178	C	N3-C2-O2	-5.44	118.09	121.90
1	2	1218	C	C6-N1-C2	-5.44	118.12	120.30
1	2	409	C	C6-N1-C2	-5.43	118.13	120.30
1	2	1865	C	C6-N1-C1'	-5.42	114.29	120.80
1	2	472	C	N3-C2-O2	-5.41	118.11	121.90
1	2	1311	C	N3-C2-O2	-5.41	118.11	121.90
1	2	570	C	N1-C2-O2	5.40	122.14	118.90
1	2	1865	C	C6-N1-C2	-5.40	118.14	120.30
1	2	1139	C	N1-C2-O2	5.38	122.13	118.90
1	2	1314	U	C2-N1-C1'	5.36	124.13	117.70
1	2	314	U	P-O3'-C3'	5.35	126.12	119.70
1	2	1366	G	C5-C6-O6	5.35	131.81	128.60
1	2	466	G	N9-C4-C5	-5.33	103.27	105.40
1	2	369	C	N1-C2-O2	5.33	122.10	118.90
1	2	856	C	C2-N1-C1'	5.33	124.66	118.80
1	2	4	C	C5-C6-N1	5.30	123.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1785	C	N3-C2-O2	-5.30	118.19	121.90
1	2	532	C	C5-C6-N1	5.29	123.65	121.00
1	2	636	C	P-O3'-C3'	5.29	126.05	119.70
1	2	814	U	N1-C2-O2	5.29	126.50	122.80
1	2	1304	U	P-O3'-C3'	5.28	126.04	119.70
1	2	824	C	N3-C2-O2	-5.28	118.20	121.90
1	2	1292	C	N1-C2-O2	5.28	122.07	118.90
1	2	293	C	C5-C6-N1	5.27	123.64	121.00
1	2	1689	C	N1-C2-O2	5.26	122.06	118.90
1	2	168	C	N3-C2-O2	-5.25	118.22	121.90
1	2	96	C	N1-C2-O2	5.21	122.03	118.90
1	2	943	U	C5-C4-O4	-5.21	122.77	125.90
1	2	168	C	C2-N1-C1'	5.21	124.53	118.80
1	2	410	G	O5'-P-OP2	-5.21	101.01	105.70
1	2	1534	C	P-O3'-C3'	5.21	125.95	119.70
1	2	369	C	C2-N1-C1'	5.20	124.52	118.80
22	P	56	LEU	CA-CB-CG	5.20	127.26	115.30
1	2	1683	C	C6-N1-C2	-5.19	118.22	120.30
1	2	4	C	N1-C2-O2	5.19	122.01	118.90
1	2	180	G	P-O3'-C3'	5.18	125.91	119.70
1	2	1485	U	N3-C2-O2	-5.17	118.58	122.20
1	2	45	A	O4'-C1'-N9	-5.16	104.07	108.20
1	2	1501	C	N1-C2-O2	5.16	122.00	118.90
1	2	1759	G	C5-C6-O6	5.16	131.70	128.60
1	2	102	A	OP2-P-O3'	5.16	116.54	105.20
1	2	1323	U	C6-N1-C2	-5.15	117.91	121.00
1	2	853	C	O4'-C1'-N1	5.12	112.30	108.20
1	2	1022	U	C6-N1-C1'	-5.12	114.03	121.20
1	2	1591	C	N3-C2-O2	-5.12	118.31	121.90
1	2	1109	C	C2-N1-C1'	5.12	124.43	118.80
1	2	1664	A	P-O3'-C3'	5.12	125.84	119.70
1	2	310	C	C6-N1-C2	-5.10	118.26	120.30
15	w	365	LEU	CA-CB-CG	5.10	127.03	115.30
1	2	130	G	N3-C4-C5	-5.08	126.06	128.60
1	2	1501	C	N3-C2-O2	-5.07	118.35	121.90
1	2	1568	C	C6-N1-C2	-5.07	118.27	120.30
1	2	178	C	C2-N1-C1'	5.06	124.37	118.80
1	2	1078	C	N1-C2-O2	5.06	121.94	118.90
1	2	1123	C	C2-N1-C1'	5.06	124.36	118.80
1	2	750	C	P-O3'-C3'	5.05	125.75	119.70
1	2	600	G	C4-N9-C1'	5.04	133.05	126.50
1	2	441	C	C6-N1-C2	-5.03	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	321	C	N1-C2-O2	5.02	121.91	118.90
1	2	1039	C	C2-N1-C1'	5.02	124.32	118.80
1	2	1503	C	C2-N1-C1'	5.01	124.31	118.80
1	2	309	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	K	378	VAL	Peptide
18	t	255	GLN	Peptide

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	79/135 (58%)	78 (99%)	1 (1%)	0	100	100
3	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
4	B	211/264 (80%)	201 (95%)	10 (5%)	0	100	100
5	c	59/69 (86%)	57 (97%)	2 (3%)	0	100	100
6	E	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
7	e	18/59 (30%)	18 (100%)	0	0	100	100
8	F	187/204 (92%)	174 (93%)	12 (6%)	1 (0%)	29	64
9	H	184/194 (95%)	178 (97%)	6 (3%)	0	100	100
10	G	228/249 (92%)	221 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Z	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
12	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
13	x	173/252 (69%)	166 (96%)	7 (4%)	0	100	100
14	X	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
15	w	321/437 (74%)	309 (96%)	12 (4%)	0	100	100
16	W	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
17	u	630/804 (78%)	602 (96%)	27 (4%)	1 (0%)	47	79
18	t	53/475 (11%)	44 (83%)	9 (17%)	0	100	100
19	T	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
20	S	125/152 (82%)	120 (96%)	5 (4%)	0	100	100
21	Q	123/146 (84%)	120 (98%)	3 (2%)	0	100	100
22	P	117/145 (81%)	117 (100%)	0	0	100	100
23	O	133/151 (88%)	124 (93%)	9 (7%)	0	100	100
24	N	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
25	L	149/158 (94%)	140 (94%)	9 (6%)	0	100	100
26	J	178/194 (92%)	173 (97%)	5 (3%)	0	100	100
27	I	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
28	r	116/125 (93%)	109 (94%)	7 (6%)	0	100	100
29	q	231/281 (82%)	222 (96%)	8 (4%)	1 (0%)	34	69
30	K	1000/1297 (77%)	954 (95%)	46 (5%)	0	100	100
31	M	102/132 (77%)	100 (98%)	2 (2%)	0	100	100
32	f	53/156 (34%)	48 (91%)	5 (9%)	0	100	100
33	a	296/337 (88%)	285 (96%)	11 (4%)	0	100	100
34	z	78/230 (34%)	75 (96%)	3 (4%)	0	100	100
All	All	6134/8028 (76%)	5886 (96%)	245 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	163	PHE
17	u	351	ARG
29	q	63	GLY

### 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	
2	R	72/122 (59%)	72 (100%)	0	100	100
3	b	74/76 (97%)	74 (100%)	0	100	100
4	B	194/231 (84%)	194 (100%)	0	100	100
5	c	52/62 (84%)	52 (100%)	0	100	100
6	E	224/225 (100%)	223 (100%)	1 (0%)	91	96
7	e	18/48 (38%)	18 (100%)	0	100	100
8	F	159/170 (94%)	159 (100%)	0	100	100
9	H	167/174 (96%)	167 (100%)	0	100	100
10	G	200/218 (92%)	200 (100%)	0	100	100
11	Z	64/103 (62%)	64 (100%)	0	100	100
12	Y	108/115 (94%)	108 (100%)	0	100	100
13	x	148/208 (71%)	147 (99%)	1 (1%)	84	93
14	X	113/115 (98%)	113 (100%)	0	100	100
15	w	262/370 (71%)	259 (99%)	3 (1%)	73	89
16	W	112/113 (99%)	112 (100%)	0	100	100
17	u	561/705 (80%)	546 (97%)	15 (3%)	44	74
18	t	59/434 (14%)	58 (98%)	1 (2%)	60	83
19	T	114/115 (99%)	113 (99%)	1 (1%)	78	91
20	S	111/132 (84%)	111 (100%)	0	100	100
21	Q	106/121 (88%)	106 (100%)	0	100	100
22	P	111/130 (85%)	111 (100%)	0	100	100
23	O	105/119 (88%)	104 (99%)	1 (1%)	76	90
24	N	130/131 (99%)	130 (100%)	0	100	100
25	L	135/142 (95%)	133 (98%)	2 (2%)	65	85
26	J	160/168 (95%)	155 (97%)	5 (3%)	40	70
27	I	178/180 (99%)	176 (99%)	2 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	r	105/112 (94%)	105 (100%)	0	100	100
29	q	198/240 (82%)	195 (98%)	3 (2%)	65	85
30	K	871/1094 (80%)	868 (100%)	3 (0%)	92	96
31	M	91/108 (84%)	91 (100%)	0	100	100
32	f	51/140 (36%)	51 (100%)	0	100	100
33	a	262/291 (90%)	260 (99%)	2 (1%)	81	92
34	z	72/185 (39%)	72 (100%)	0	100	100
All	All	5387/6897 (78%)	5347 (99%)	40 (1%)	84	93

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	E	233	LYS
13	x	110	ASN
15	w	88	ARG
15	w	244	ARG
15	w	418	ARG
17	u	296	ASP
17	u	298	GLN
17	u	300	LYS
17	u	343	VAL
17	u	344	LEU
17	u	345	MET
17	u	346	LYS
17	u	348	ASP
17	u	351	ARG
17	u	352	GLN
17	u	355	LEU
17	u	358	GLU
17	u	598	VAL
17	u	599	ARG
17	u	679	ILE
18	t	262	ARG
19	T	24	LYS
23	O	84	ARG
25	L	30	LYS
25	L	69	ARG
26	J	138	ARG
26	J	139	LYS
26	J	158	ASP

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Mol	Chain	Res	Type
26	J	159	PHE
26	J	179	LYS
27	I	67	TRP
27	I	73	THR
29	q	7	ARG
29	q	82	ASP
29	q	123	SER
30	K	186	LYS
30	K	819	LYS
30	K	935	MET
33	a	65	LYS
33	a	278	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
13	x	110	ASN
15	w	410	HIS
20	S	73	ASN
22	P	32	GLN
30	K	527	HIS
33	a	128	HIS
33	a	134	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1557/1873 (83%)	340 (21%)	28 (1%)

All (340) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	26	U
1	2	33	G
1	2	37	C
1	2	41	G
1	2	46	A
1	2	56	G
1	2	59	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	71	G
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	100	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	128	U
1	2	130	G
1	2	143	U
1	2	144	U
1	2	149	A
1	2	155	G
1	2	160	U
1	2	168	C
1	2	172	U
1	2	181	A
1	2	182	C
1	2	184	G
1	2	188	C
1	2	291	G
1	2	292	A
1	2	295	C
1	2	302	A
1	2	310	C
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	332	G
1	2	333	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	335	G
1	2	338	G
1	2	339	A
1	2	340	C
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	370	G
1	2	377	G
1	2	385	G
1	2	386	C
1	2	400	C
1	2	409	C
1	2	413	G
1	2	418	A
1	2	429	C
1	2	438	G
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	466	G
1	2	470	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	487	U
1	2	492	C
1	2	493	A
1	2	516	A
1	2	525	A
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	554	A
1	2	555	A
1	2	556	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	559	G
1	2	560	A
1	2	563	G
1	2	570	C
1	2	574	A
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	595	U
1	2	600	G
1	2	601	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	606	G
1	2	613	G
1	2	631	U
1	2	637	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	658	U
1	2	660	C
1	2	662	G
1	2	664	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	673	G
1	2	678	U
1	2	683	G
1	2	684	G
1	2	687	C
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	794	A
1	2	797	C
1	2	799	U
1	2	800	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	823	U
1	2	824	C
1	2	827	A
1	2	830	A
1	2	844	U
1	2	847	A
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G
1	2	881	G
1	2	886	A
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	896	U
1	2	898	U
1	2	903	A
1	2	908	A
1	2	913	A
1	2	914	U
1	2	920	A
1	2	922	A
1	2	930	C
1	2	933	G
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	981	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	985	G
1	2	990	A
1	2	991	G
1	2	992	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1034	A
1	2	1041	G
1	2	1044	G
1	2	1045	U
1	2	1049	A
1	2	1050	A
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1089	G
1	2	1096	G
1	2	1099	G
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1121	G
1	2	1130	G
1	2	1138	C
1	2	1139	C
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1183	A
1	2	1200	A
1	2	1203	G
1	2	1204	A
1	2	1206	G
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1227	G
1	2	1232	U
1	2	1235	G
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1265	A
1	2	1273	C
1	2	1274	G
1	2	1275	G
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1296	U
1	2	1298	G
1	2	1299	A
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1305	C
1	2	1307	U
1	2	1308	U
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1315	U
1	2	1317	C
1	2	1322	G
1	2	1323	U
1	2	1325	G
1	2	1327	G
1	2	1335	G
1	2	1364	U
1	2	1371	U
1	2	1372	U
1	2	1376	A
1	2	1383	A
1	2	1387	G
1	2	1388	A
1	2	1389	C
1	2	1396	A
1	2	1397	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1398	G
1	2	1444	U
1	2	1445	U
1	2	1446	A
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1465	A
1	2	1476	A
1	2	1477	U
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1498	A
1	2	1512	C
1	2	1519	U
1	2	1528	G
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1548	G
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1569	A
1	2	1570	G
1	2	1580	A
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1588	A
1	2	1601	A
1	2	1606	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1639	G7M

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1640	A
1	2	1648	G
1	2	1654	G
1	2	1660	C
1	2	1661	A
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1669	G
1	2	1675	A
1	2	1686	G
1	2	1689	C
1	2	1694	U
1	2	1704	C
1	2	1705	C
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1729	U
1	2	1744	G
1	2	1756	C
1	2	1761	U
1	2	1772	C
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1800	A
1	2	1801	A
1	2	1805	G
1	2	1806	A
1	2	1826	G
1	2	1829	G
1	2	1839	U
1	2	1841	C
1	2	1861	G
1	2	1864	U
1	2	1872	G

All (28) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	417	C
1	2	440	G
1	2	465	A
1	2	604	A
1	2	636	C
1	2	750	C
1	2	958	G
1	2	980	A
1	2	1231	C
1	2	1264	C
1	2	1295	A
1	2	1304	U
1	2	1386	A
1	2	1494	U
1	2	1497	G
1	2	1511	U
1	2	1534	C
1	2	1565	C
1	2	1640	A
1	2	1693	G
1	2	1726	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	G7M	2	1639	1	20,26,27	5.86	13 (65%)	17,39,42	1.40	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	2	1639	1	-	2/3/25/26	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	G7M	C2'-C1'	-16.57	1.28	1.53
1	2	1639	G7M	C3'-C4'	-10.46	1.26	1.53
1	2	1639	G7M	O4'-C1'	9.79	1.54	1.41
1	2	1639	G7M	C2-N2	6.50	1.49	1.34
1	2	1639	G7M	C2-N3	5.66	1.47	1.33
1	2	1639	G7M	O4'-C4'	5.34	1.56	1.45
1	2	1639	G7M	C4-N3	5.05	1.49	1.37
1	2	1639	G7M	C2'-C3'	4.94	1.66	1.53
1	2	1639	G7M	C6-N1	4.20	1.44	1.37
1	2	1639	G7M	C5-C6	3.67	1.54	1.45
1	2	1639	G7M	C2-N1	2.84	1.44	1.37
1	2	1639	G7M	O6-C6	-2.13	1.19	1.23
1	2	1639	G7M	O3'-C3'	2.03	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1639	G7M	C2-N1-C6	-2.82	119.90	125.10
1	2	1639	G7M	C3'-C2'-C1'	2.59	104.87	100.98
1	2	1639	G7M	O6-C6-N1	-2.10	118.17	120.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1639	G7M	C3'-C4'-C5'-O5'
1	2	1639	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	SAH	q	301	-	24,28,28	0.69	0	25,40,40	0.89	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	SAH	q	301	-	-	3/11/31/31	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	q	301	SAH	C5-C6-N6	2.17	123.65	120.35

There are no chirality outliers.

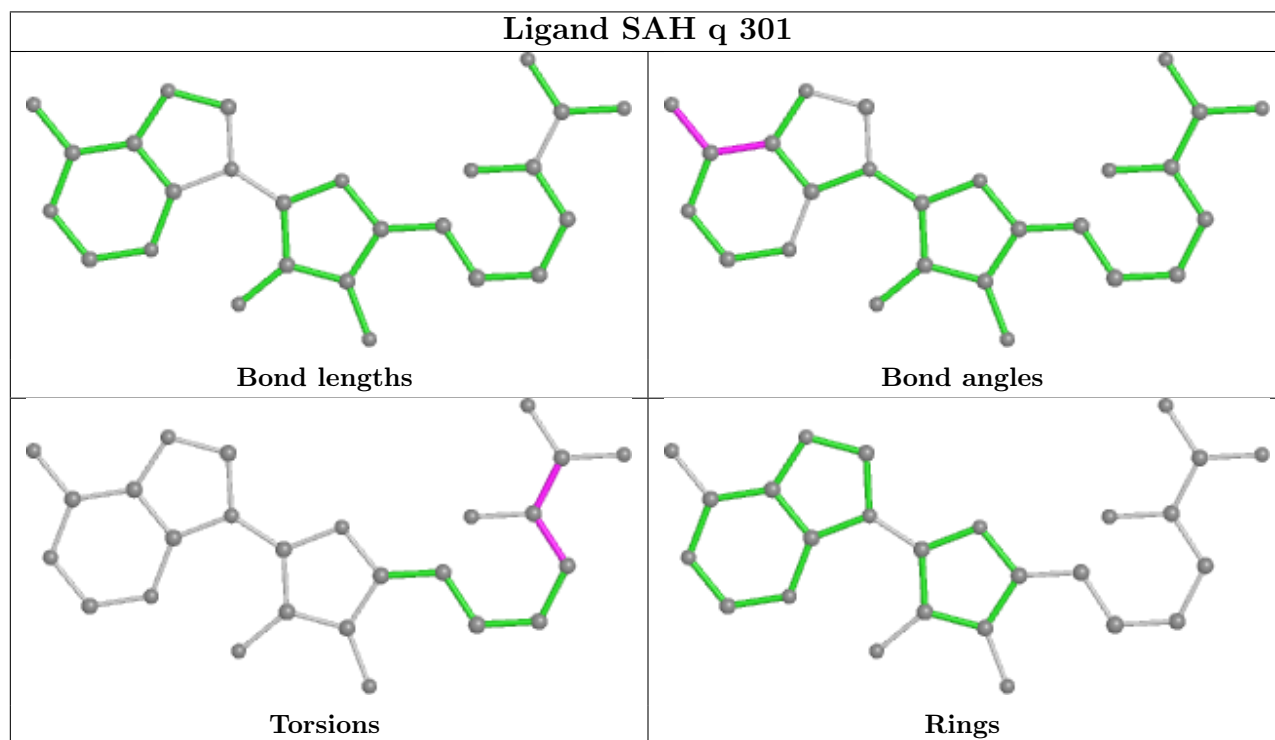
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	q	301	SAH	OXT-C-CA-N
35	q	301	SAH	O-C-CA-N
35	q	301	SAH	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

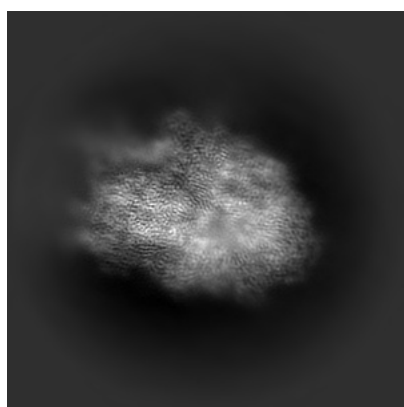
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32800. These allow visual inspection of the internal detail of the map and identification of artifacts.

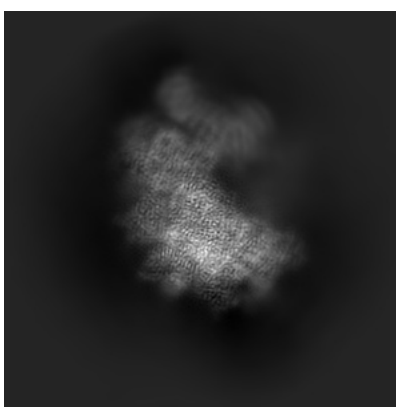
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

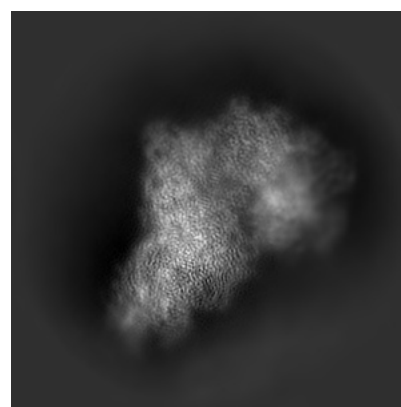
#### 6.1.1 Primary map



X



Y

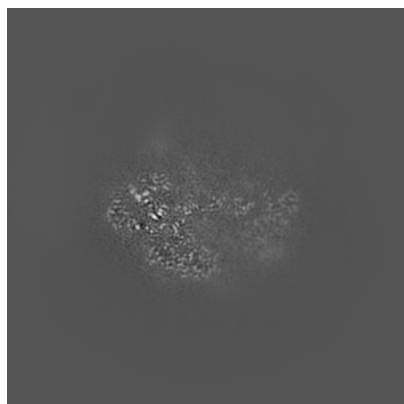


Z

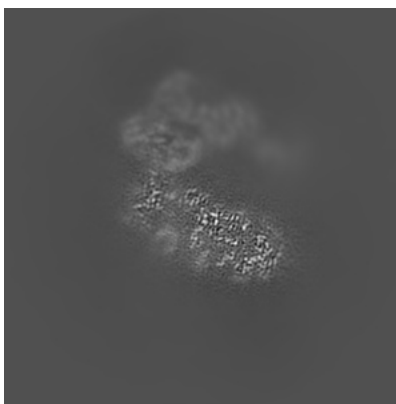
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

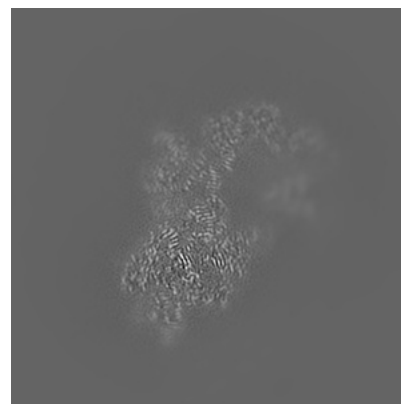
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

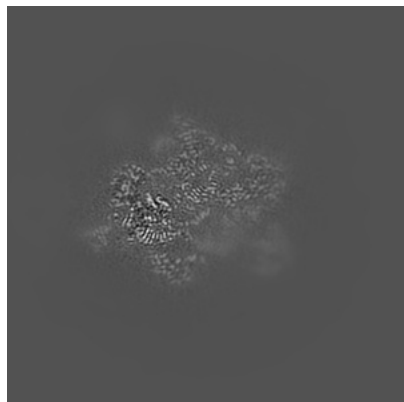


Z Index: 180

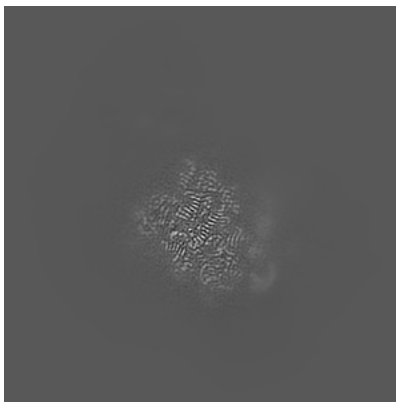
The images above show central slices of the map in three orthogonal directions.

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

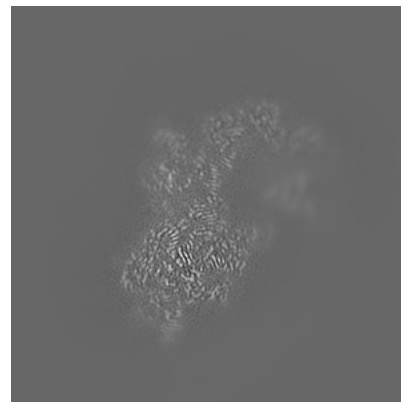
### 6.3.1 Primary map



X Index: 159



Y Index: 133

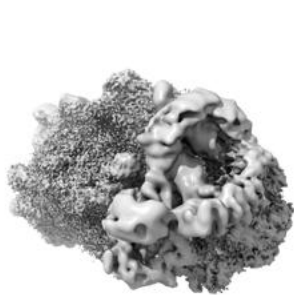


Z Index: 181

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

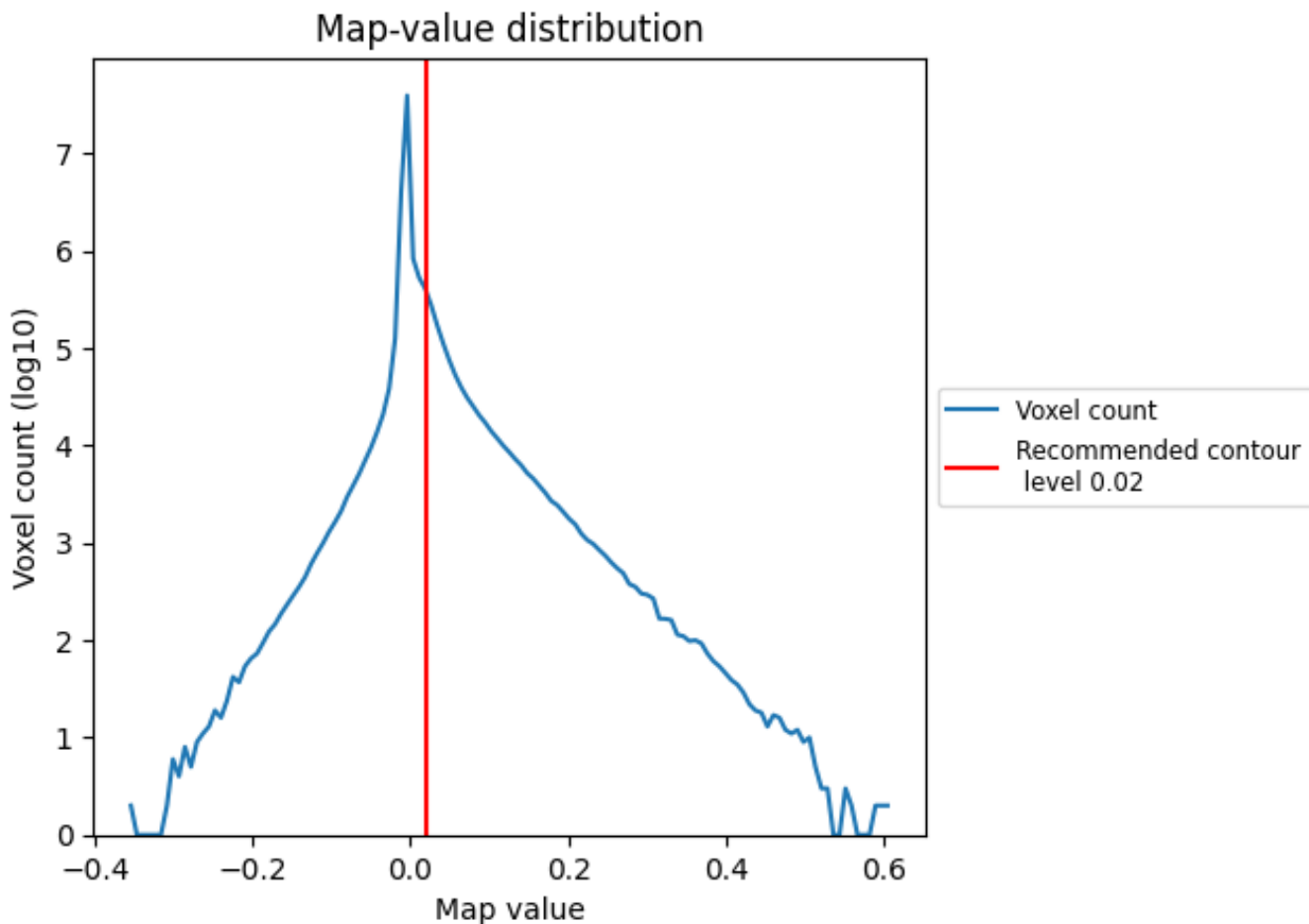
## 6.5 Mask visualisation

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.

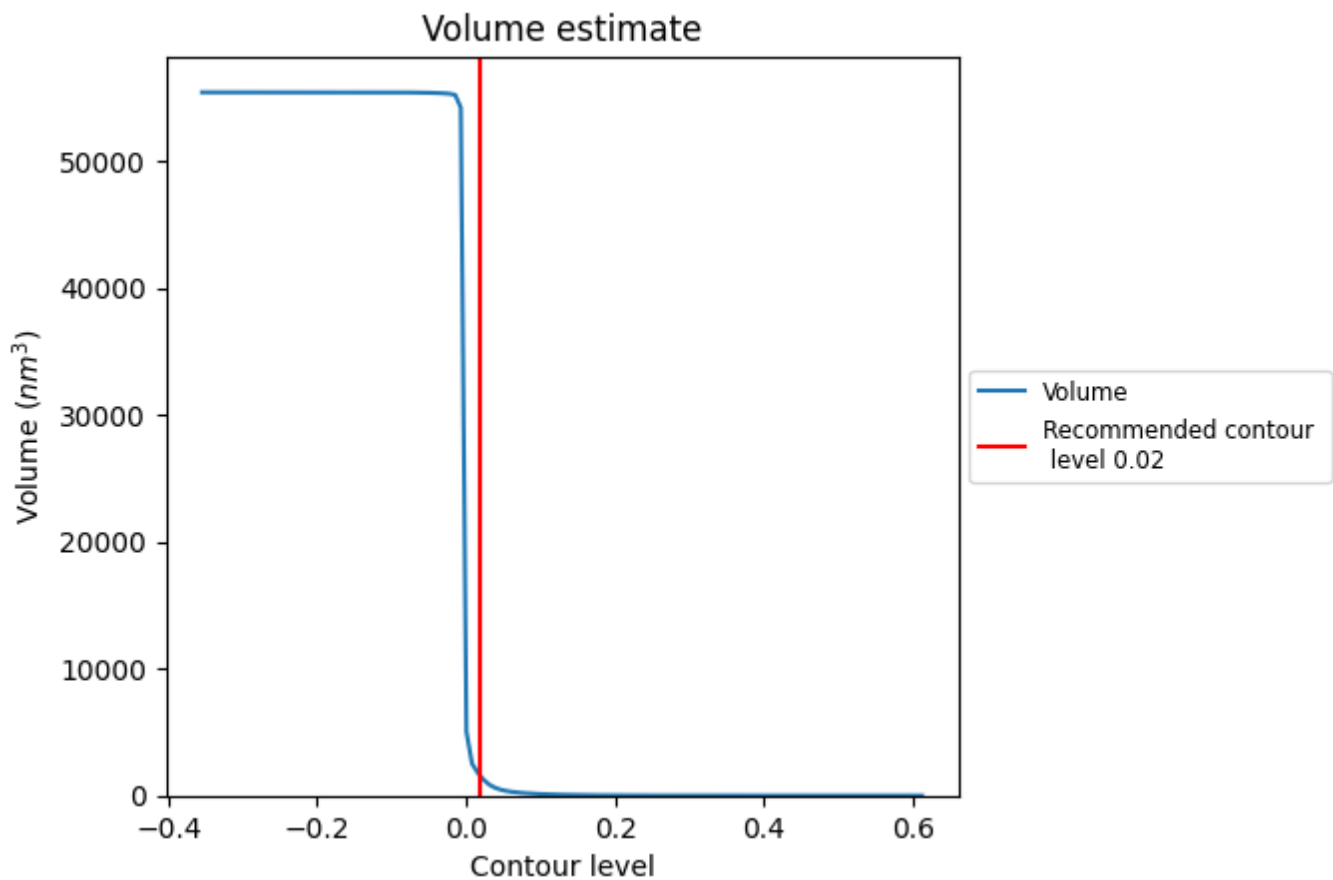
### 7.1 Map-value distribution [i](#)



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.



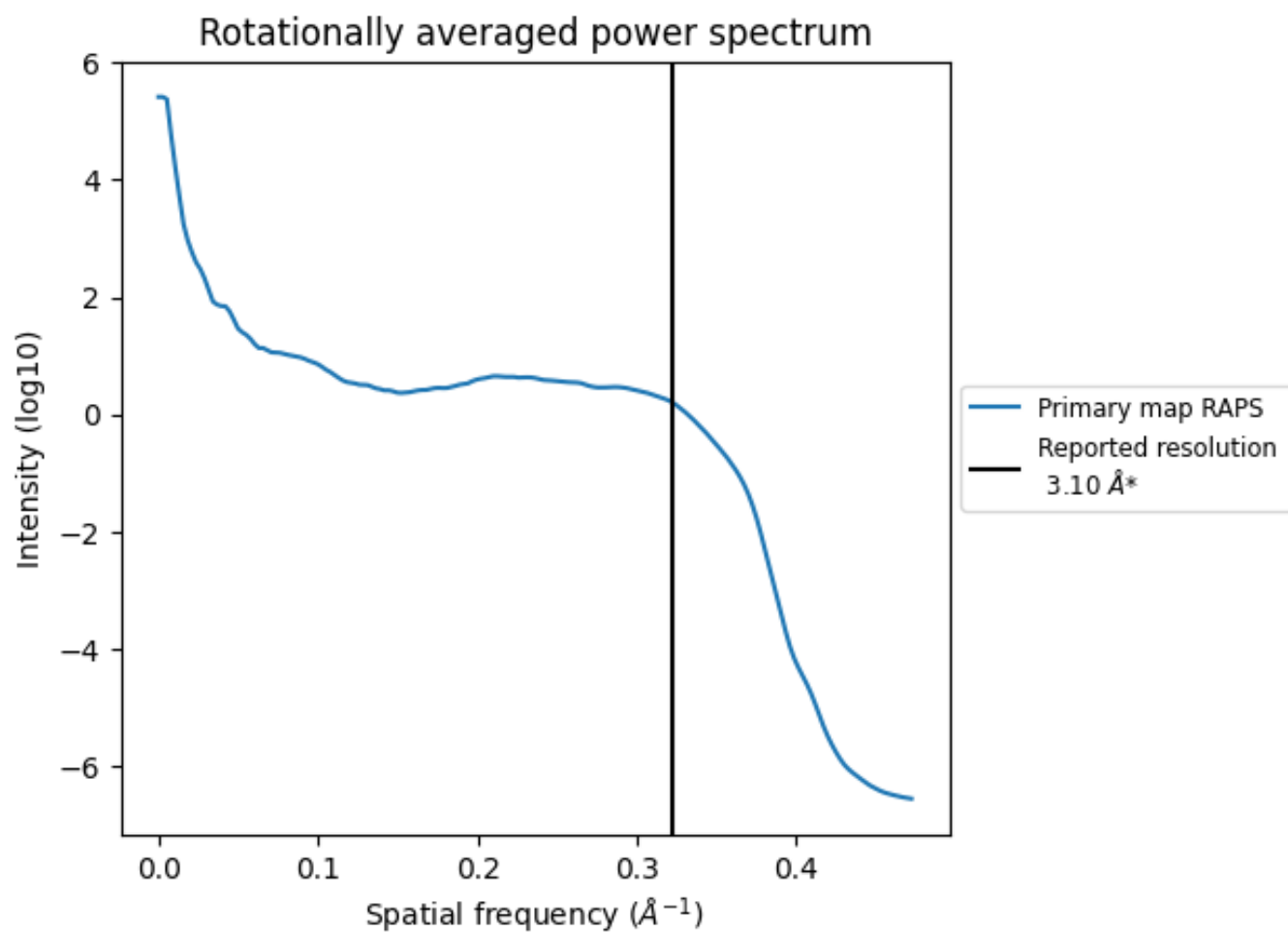
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1502 nm<sup>3</sup>; this corresponds to an approximate mass of 1357 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

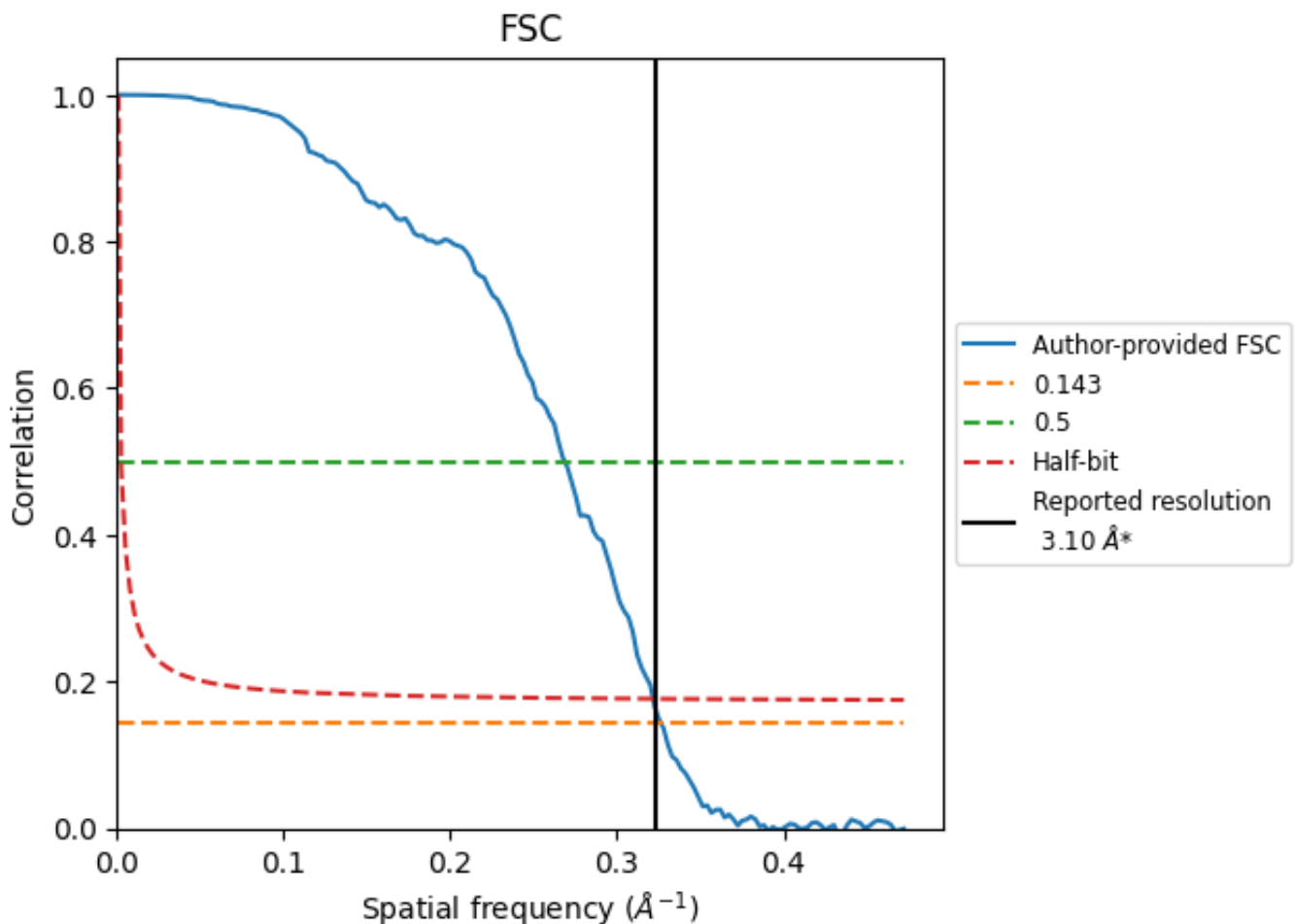


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [\(i\)](#)



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

## 8.2 Resolution estimates [i](#)

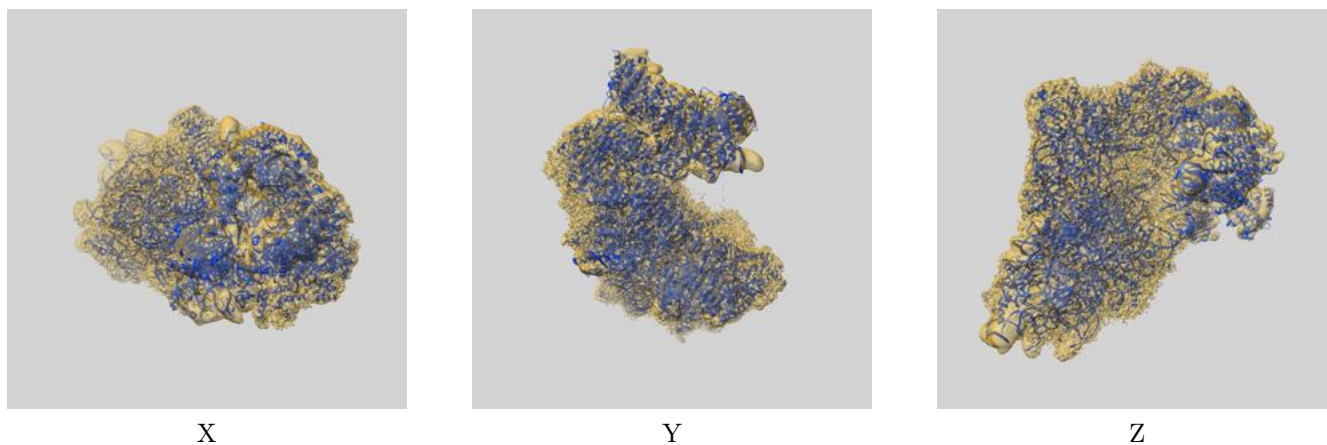
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.72	3.11
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

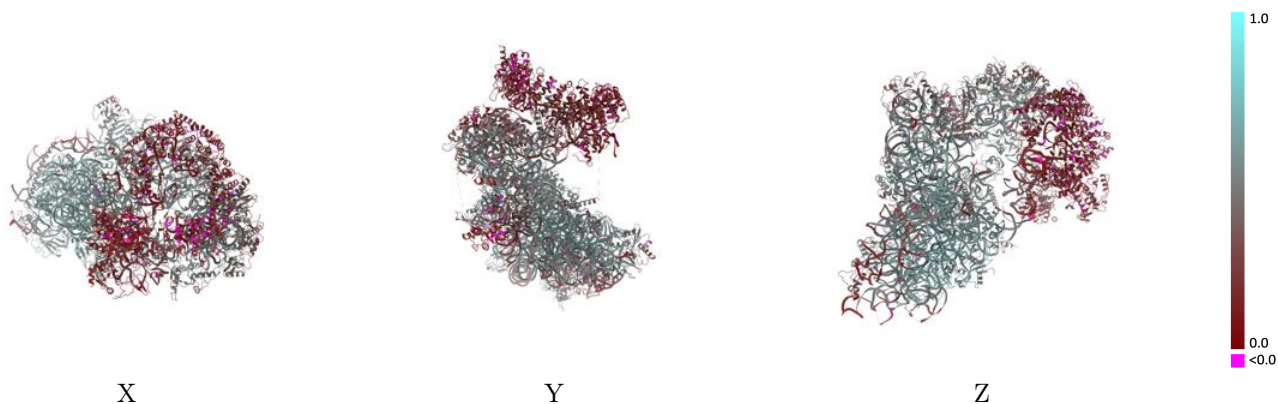
This section contains information regarding the fit between EMDB map EMD-32800 and PDB model 7WTT. Per-residue inclusion information can be found in section 3 on page 11.

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



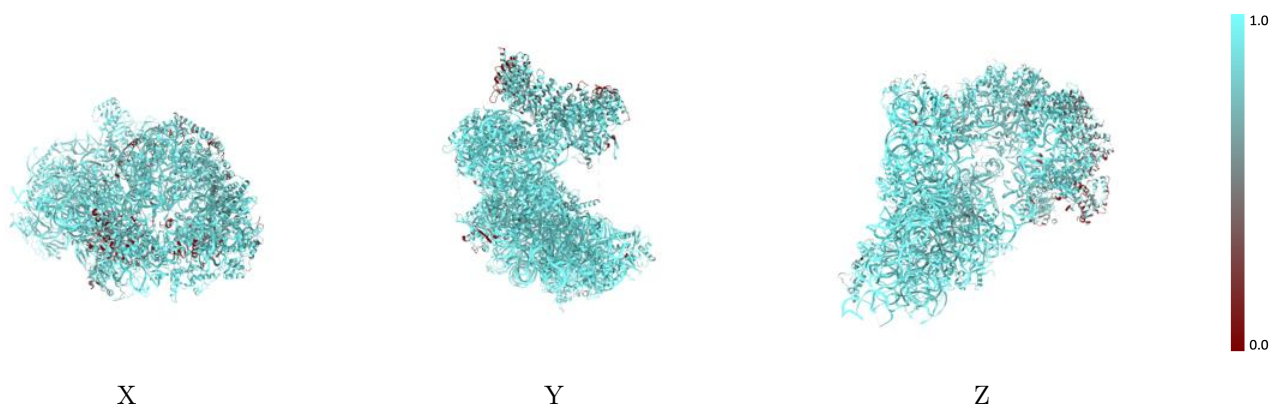
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



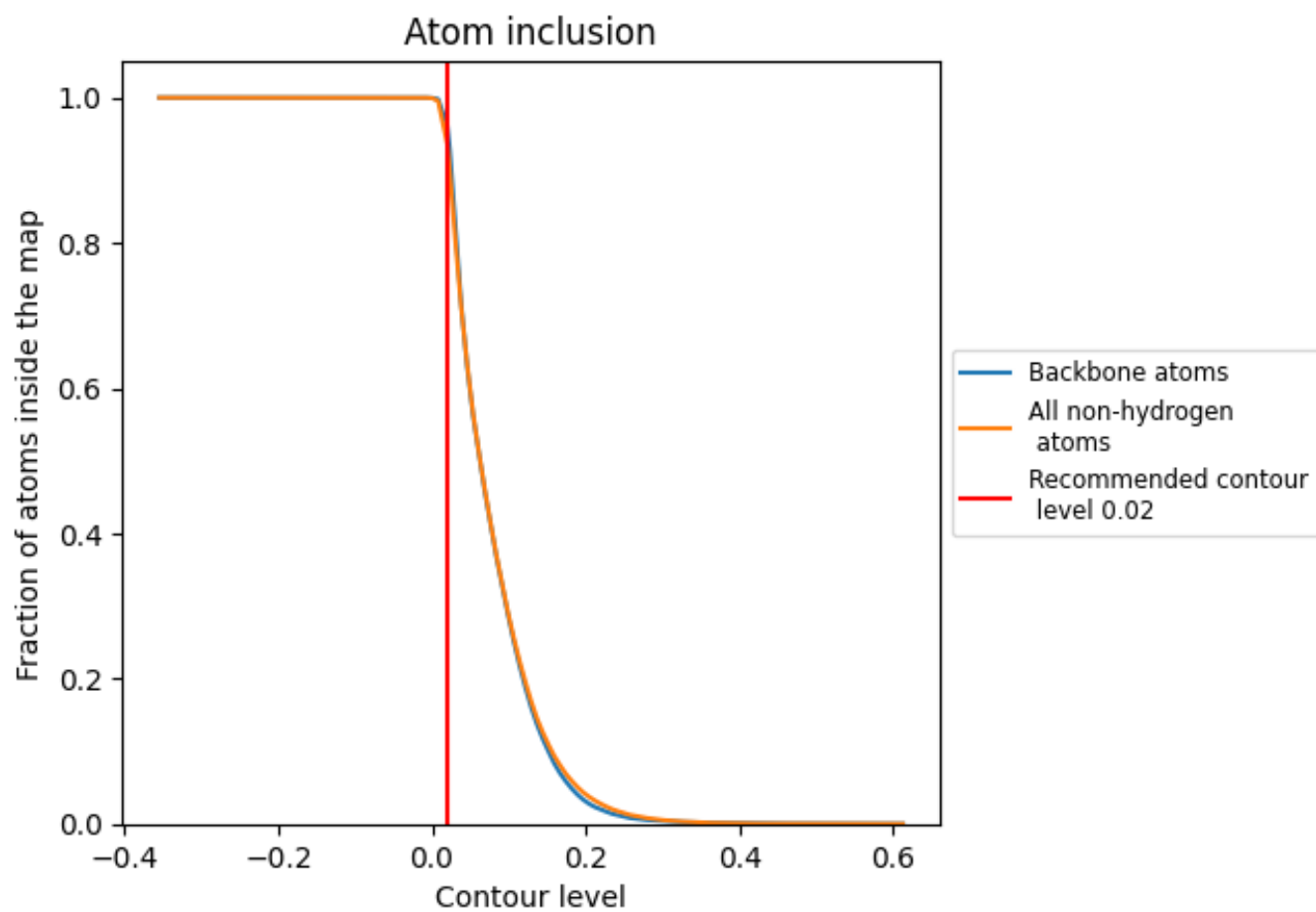
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9361	 0.4260
2	 0.9874	 0.4790
B	 0.9364	 0.4610
E	 0.9911	 0.6050
F	 0.9532	 0.4580
G	 0.9700	 0.4920
H	 0.9477	 0.4320
I	 0.9445	 0.5080
J	 0.9861	 0.5720
K	 0.8105	 0.1840
L	 0.9548	 0.5670
M	 0.7345	 0.1650
N	 0.9828	 0.5060
O	 0.9316	 0.4460
P	 0.9631	 0.4630
Q	 0.9227	 0.4350
R	 0.9211	 0.1730
S	 0.9401	 0.4310
T	 0.9020	 0.4540
W	 0.9931	 0.5660
X	 0.9720	 0.5300
Y	 0.9909	 0.5860
Z	 0.8681	 0.3450
a	 0.6033	 0.1150
b	 0.9745	 0.5180
c	 0.9316	 0.4570
e	 0.9821	 0.5350
f	 0.8916	 0.1620
q	 0.9321	 0.3280
r	 0.7141	 0.1530
t	 0.8730	 0.3040
u	 0.9828	 0.5350
w	 0.8795	 0.2580
x	 0.9792	 0.5000
z	 0.7002	 0.2310

