



## Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 10:43 am BST

PDB ID : 9TZ9 / pdb\_00009tz9  
EMDB ID : EMD-56461  
Title : Empty 50S Subunit of the Coxiella burnetii Ribosome  
Authors : Stuart, W.S.; Isupov, M.N.; Harmer, N.J.  
Deposited on : 2026-01-22  
Resolution : 2.19 Å(reported)  
Based on initial model : .

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.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

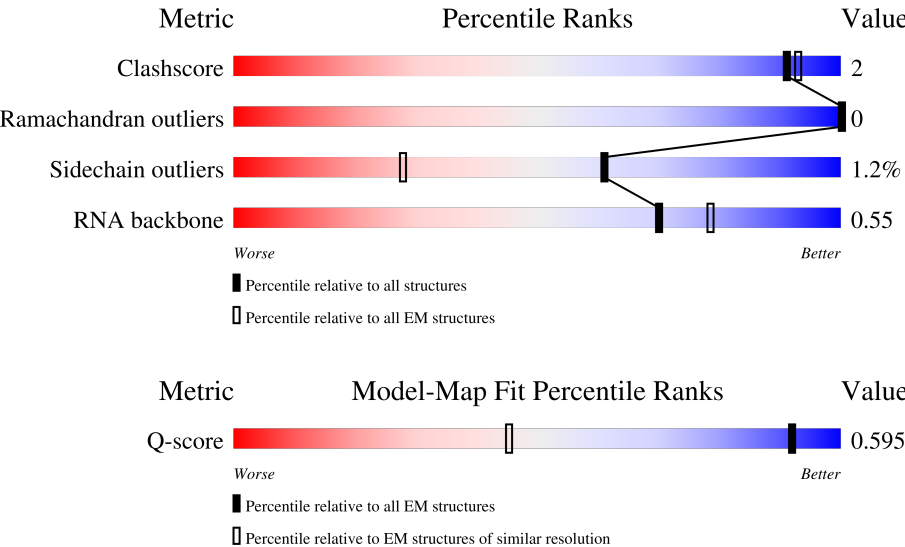
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.19 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.




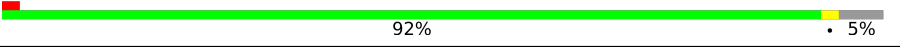

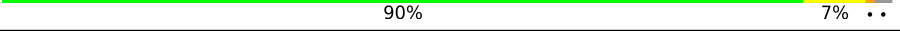
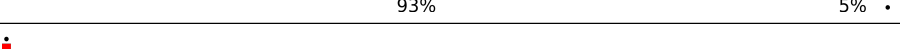

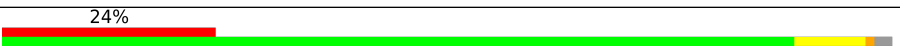

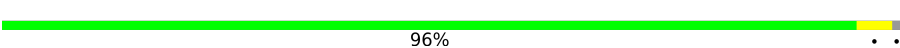

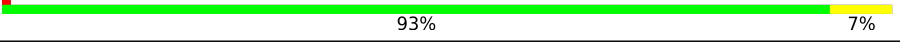
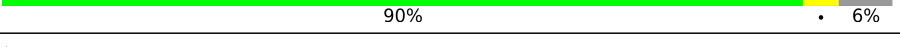
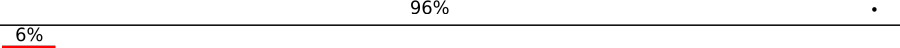





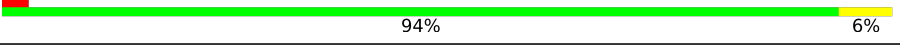
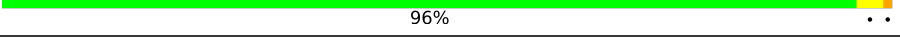
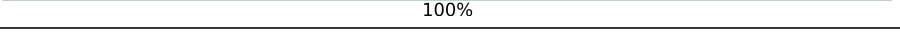
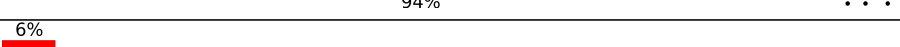



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2745 ( 1.70 - 2.69 )

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	Z	21	76% 24%
2	0	70	91% 6% .
3	1	107	8% 93% 5% ..

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Mol	Chain	Length	Quality of chain
4	2	117	 91% 7% ..
5	3	40	 92% 5%
6	b	117	 87% 12% .
7	c	115	 9% 90% 7% ..
8	d	217	 93% 5% .
9	e	119	 97% ..
10	f	182	 76% 93% 7% .
11	g	178	 24% 89% 8% ..
12	h	115	 89% 10%
13	i	142	 96% ..
14	j	115	 88% 8% .
15	k	143	 93% 7%
16	m	126	 90% 6%
17	o	275	 96% .
18	q	152	 6% 28% 70%
19	r	65	 89% 8% .
20	s	137	 95% 5%
21	t	63	 86% 11%
22	u	244	 25% 75% 22%
23	v	64	 75% 9% 16%
24	w	205	 94% 6%
25	x	122	 96% ..
26	y	44	 100%
27	z	64	 94% ...
28	a	2925	 6% 79% 17% ..

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Mol	Chain	Length	Quality of chain
29	8	90	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>79%7%14%</div></div>
30	7	95	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>89%6%</div></div>
31	9	79	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>89%9%</div></div>

## 2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 89972 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 protein called Coxiellaceae Large Subunit Peptide (CLaSP).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Z	16	Total	C	N	O	0	0
			133	82	34	17		

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	68	Total	C	N	O	S	0	0
			550	349	99	99	3		

- Molecule 3 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1	105	Total	C	N	O	0	0
			813	512	153	148		

- Molecule 4 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	116	Total	C	N	O	S	0	0
			913	566	188	157	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	38	Total	C	N	O	S	0	0
			307	183	73	46	5		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	117	Total	C	N	O	P	0	0
			2488	1112	445	815	116		

- Molecule 7 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	c	113	Total	C	N	O	0	0
			919	573	184	162		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	211	Total	C	N	O	S	0	0
			1596	995	298	298	5		

- Molecule 9 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	118	Total	C	N	O	S	0	0
			941	595	194	151	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	182	Total	C	N	O	S	0	0
			1457	930	258	261	8		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	174	Total	C	N	O	S	0	0
			1310	818	245	243	4		

- Molecule 12 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	104	Total	C	N	O	S	0	0
			813	511	150	148	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	141	Total	C	N	O	S	0	0
			1108	707	206	193	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	j	110	Total	C	N	O	S	0	0
			839	516	165	154	4		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	143	Total	C	N	O	S	0	0
			1076	672	217	185	2		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	m	119	Total	C	N	O	S	0	0
			967	605	195	162	5		

- Molecule 17 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	274	Total	C	N	O	S	0	0
			2131	1314	443	368	6		

- Molecule 18 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	q	45	Total	C	N	O	S	0	0
			339	221	59	58	1		

- Molecule 19 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	63	Total	C	N	O	S	0	0
			522	324	106	91	1		

- Molecule 20 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	137	Total	C	N	O	S	0	0
			1090	688	215	182	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	t	56	Total	C	N	O	S	0	0
			449	281	86	78	4		

- Molecule 22 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	u	191	Total	C	N	O	S	0	0
			1486	940	260	281	5		

- Molecule 23 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	54	Total	C	N	O	S	0	0
			436	263	95	76	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	205	Total	C	N	O	S	0	0
			1571	974	296	296	5		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	122	Total	C	N	O	S	0	0
			948	594	184	165	5		

- Molecule 26 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	44	Total	C	N	O	S	0	0
			374	224	91	57	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	z	62	Total	C	N	O	S	0	0
			500	308	110	80	2		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2873	Total	C	N	O	P	0	0
			61614	27502	11282	19957	2873		

- Molecule 29 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	8	77	Total	C	N	O	S	0	0
			613	381	124	105	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	91	Total	C	N	O	S	0	0
			732	464	135	130	3		

- Molecule 31 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	77	Total	C	N	O	S	0	0
			631	395	128	106	2		

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	3	1	Total	Zn	0
			1	1	

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	b	1	Total	Mg	0
			1	1	
33	d	1	Total	Mg	0
			1	1	
33	o	1	Total	Mg	0
			1	1	
33	a	159	Total	Mg	0
			159	159	

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	b	1	Total 1	K 1	0
34	d	1	Total 1	K 1	0
34	o	2	Total 2	K 2	0
34	s	1	Total 1	K 1	0
34	v	2	Total 2	K 2	0
34	w	1	Total 1	K 1	0
34	a	127	Total 127	K 127	0
34	8	1	Total 1	K 1	0


- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	a	7	Total 7	O 7	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: Coxiellaceae Large Subunit Peptide (CLaSP)

Chain Z:  76% 24%

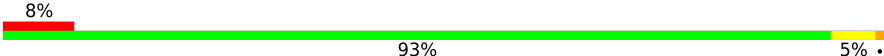


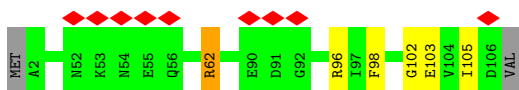
- Molecule 2: Large ribosomal subunit protein bL33

Chain 0:  91% 6% .




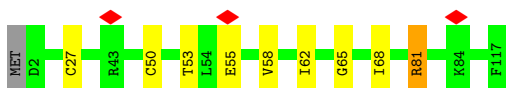
- Molecule 3: Large ribosomal subunit protein uL24

Chain 1:  8% 93% 5% ..




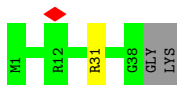
- Molecule 4: Large ribosomal subunit protein uL18

Chain 2:  91% 7% ..




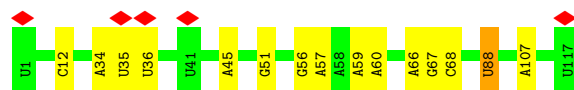
- Molecule 5: Large ribosomal subunit protein bL36

Chain 3:  92% . 5%




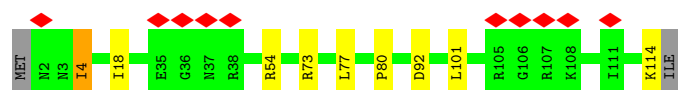
- Molecule 6: 5S ribosomal RNA

Chain b:  87% 12%



- Molecule 7: Large ribosomal subunit protein bL19

Chain c:  9% 90% 7%



- Molecule 8: Large ribosomal subunit protein uL3

Chain d:  93% 5%

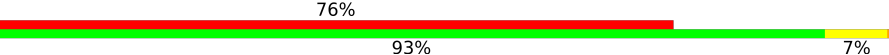


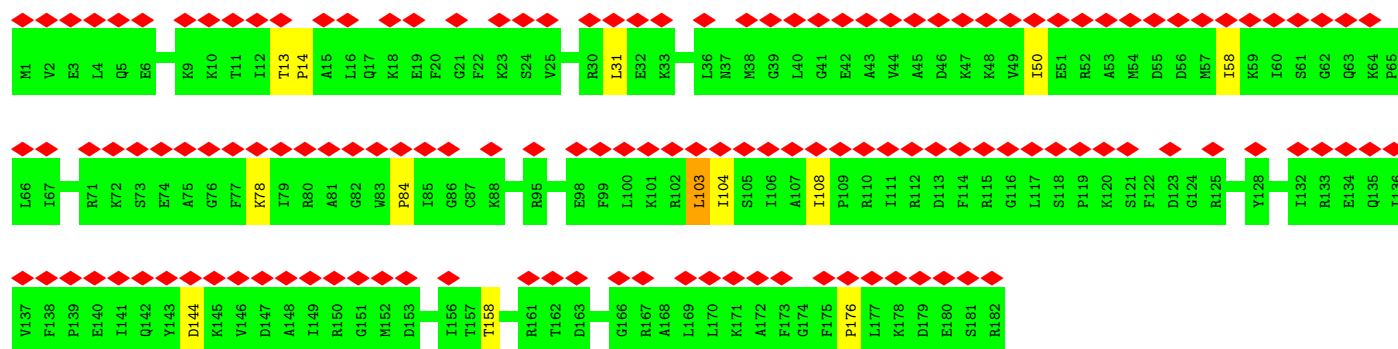
- Molecule 9: Large ribosomal subunit protein bL20

Chain e:  97%




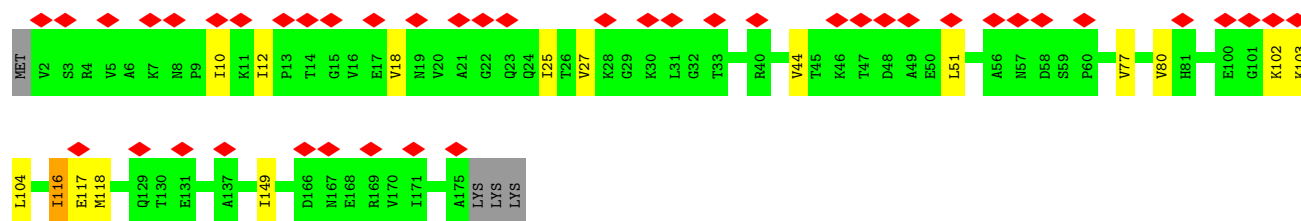
- Molecule 10: Large ribosomal subunit protein uL5

Chain f:  76% 93% 7%

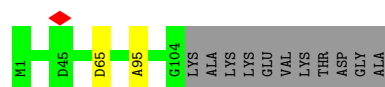


- Molecule 11: Large ribosomal subunit protein uL6

Chain g:  24% 89% 8%



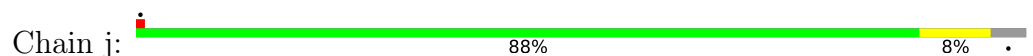
- Molecule 12: Large ribosomal subunit protein bL21



- Molecule 13: Large ribosomal subunit protein uL13



- Molecule 14: Large ribosomal subunit protein uL22



- Molecule 15: Large ribosomal subunit protein uL15



- Molecule 16: Large ribosomal subunit protein bL17



- Molecule 17: Large ribosomal subunit protein uL2





ALA  
SER  
GLU  
ALA  
GLU  
SER  
GLY  
ALA  
GLU  
GLN  
ALA  
ASP  
THR  
ASP  
LYS  
LYS  
GLU

- Molecule 23: Large ribosomal subunit protein bL32

Chain v:  75% 9% 16%

MET  
A2  
T9  
R16  
M26  
L27  
Q52  
I53  
I54  
T55  
PRO  
LYS  
GLU  
SER  
TYR  
GLU  
ASP  
GLU  
GLU

- Molecule 24: Large ribosomal subunit protein uL4

Chain w:  94% 6%

H1  
F8  
D9  
K10  
K11  
E12  
A13  
Y27  
R73  
K92  
K99  
L113  
L116  
I161  
N167  
V173  
V179  
I190  
R199  
L204  
S205

- Molecule 25: Large ribosomal subunit protein uL14

Chain x:  96%

H1  
R49  
Q50  
K51  
R64  
I77  
D80  
F99  
G109  
L119  
L122

- Molecule 26: Large ribosomal subunit protein bL34

Chain y:  100%


There are no outlier residues recorded for this chain.

- Molecule 27: Large ribosomal subunit protein bL35

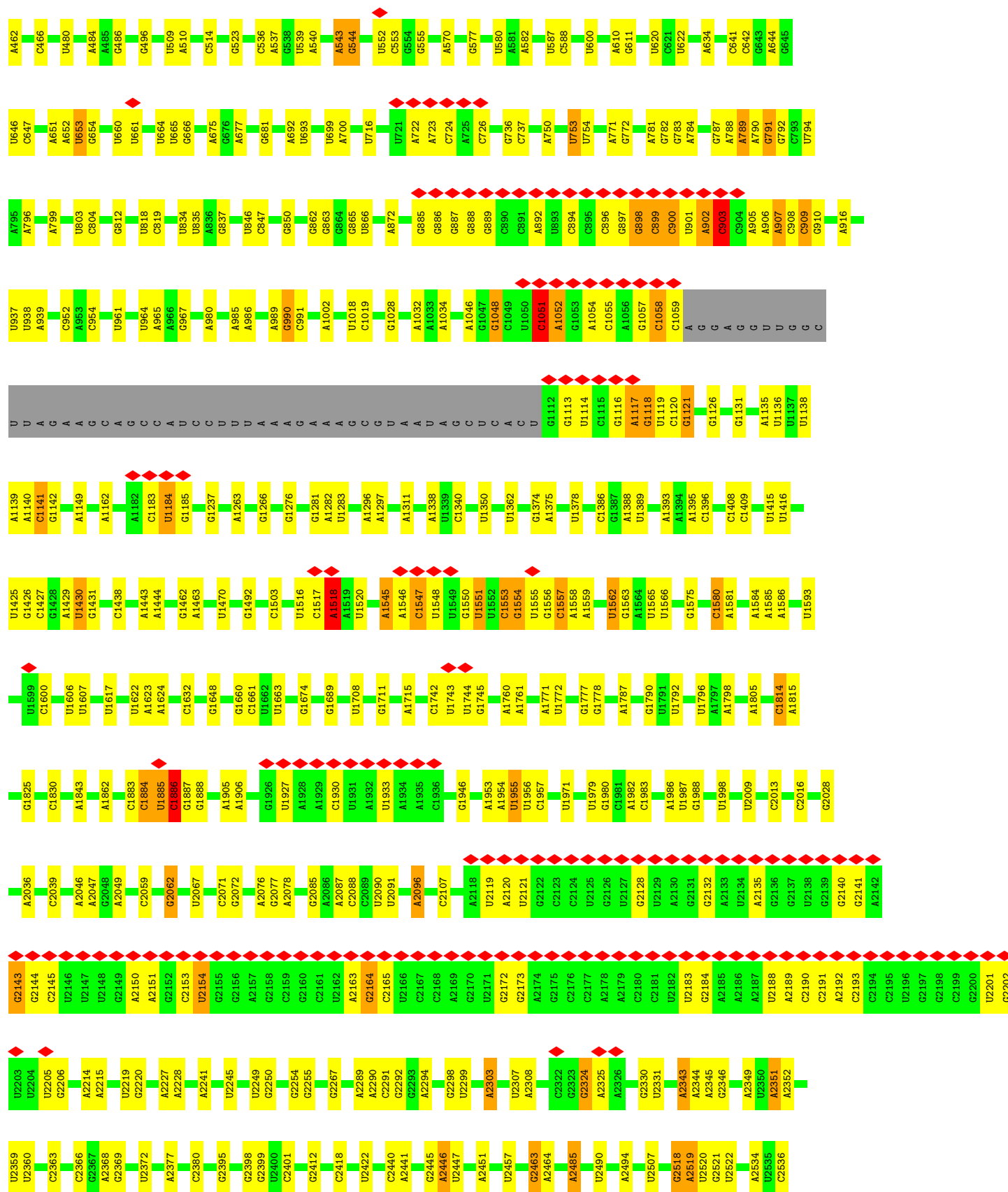
Chain z:  94%

MET  
P2  
T6  
R63  
ASP

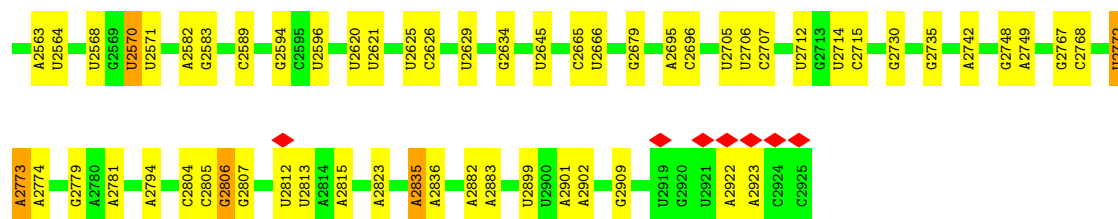
- Molecule 28: 23S ribosomal RNA

Chain a:  6% 79% 17%

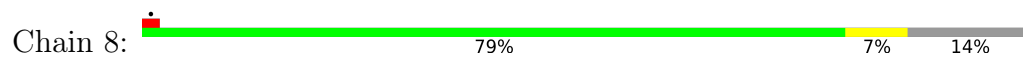
G1  
G2  
U3  
U4  
G5  
C6  
A7  
U8  
U20  
G23  
C26  
U42  
A57  
A79  
A82  
G83  
G93  
A126  
A127  
U128  
A133  
A134  
U145  
C146  
G147  
A148  
G149  
U167  
A185  
A194  
A200  
A201  
C202  
A203  
A208  
A211  
C212  
G219  
A220  
A225  
A226  
A237  
G249  
G252  
G256  
G270  
G275  
U294  
U295  
G299  
C300  
A301  
U305  
G311  
G312  
A313  
A314  
A315  
A326  
G327  
C328  
A334  
U364  
G365  
G372  
G391  
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C419  
A420  
C426  
A427  
U453  
A458  
C461



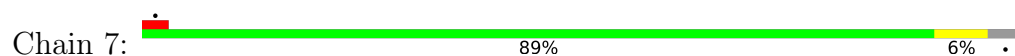




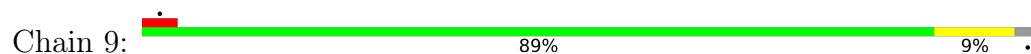
- Molecule 29: Large ribosomal subunit protein bL27



- Molecule 30: Large ribosomal subunit protein uL23



- Molecule 31: Large ribosomal subunit protein bL28



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129328	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.535	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: PSU, OMU, K, OMG, ZN, 2MA, MG

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	Z	0.46	0/137	0.95	0/178
2	0	0.42	0/561	0.87	0/747
3	1	0.44	0/820	0.92	0/1098
4	2	0.45	0/922	1.07	0/1227
5	3	0.43	0/307	0.90	0/402
6	b	0.38	0/2780	0.74	2/4331 (0.0%)
7	c	0.41	0/929	0.89	0/1241
8	d	0.44	0/1617	0.94	0/2173
9	e	0.42	0/954	1.09	0/1268
10	f	0.46	0/1480	1.06	0/1980
11	g	0.46	0/1325	0.98	0/1791
12	h	0.42	0/822	0.84	0/1098
13	i	0.46	0/1132	0.97	0/1526
14	j	0.45	0/845	0.99	0/1131
15	k	0.46	0/1088	0.99	0/1443
16	m	0.45	0/983	1.03	0/1316
17	o	0.48	0/2170	0.97	0/2909
18	q	0.48	0/345	0.97	0/468
19	r	0.39	0/526	1.19	0/697
20	s	0.43	0/1107	1.00	0/1475
21	t	0.45	0/454	0.96	0/605
22	u	0.46	0/1512	0.92	0/2041
23	v	0.47	0/443	1.00	0/589
24	w	0.43	0/1589	1.02	0/2136
25	x	0.41	0/954	0.91	0/1277
26	y	0.41	0/377	1.11	0/493
27	z	0.43	0/505	1.03	0/665
28	a	0.37	1/68792 (0.0%)	0.76	60/107300 (0.1%)
29	8	0.45	0/623	0.90	0/829
30	7	0.44	0/744	0.98	0/999
31	9	0.43	0/640	1.00	0/853
All	All	0.39	1/97483 (0.0%)	0.81	62/146286 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2568	OMU	O3'-P	5.11	1.61	1.56

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	395	U	C4'-C3'-O3'	13.01	128.92	109.40
28	a	1184	U	C2'-C3'-O3'	11.74	127.11	109.50
28	a	426	C	C2'-C3'-O3'	10.82	125.72	109.50
6	b	34	A	C2'-C3'-O3'	-10.59	97.81	113.70
28	a	1374	G	P-O3'-C3'	-9.27	106.30	120.20
28	a	2835	A	C4'-C3'-O3'	-9.16	99.26	113.00
28	a	1051	C	C2'-C3'-O3'	8.80	122.70	109.50
28	a	1430	U	C2'-C3'-O3'	8.33	122.00	109.50
28	a	1771	A	C4'-C3'-O3'	-7.54	101.68	113.00
28	a	1744	U	C2'-C3'-O3'	7.51	120.76	109.50
28	a	1388	A	C2'-C3'-O3'	7.44	120.67	109.50
28	a	1617	U	C4'-C3'-O3'	7.37	120.46	109.40
28	a	903	C	N1-C1'-C2'	7.14	122.71	112.00
28	a	909	C	C2'-C3'-O3'	7.11	124.36	113.70
28	a	2806	G	C2'-C3'-O3'	6.97	119.96	109.50
28	a	1562	U	C2'-C3'-O3'	6.89	119.84	109.50
28	a	1580	C	C2'-C3'-O3'	6.87	119.80	109.50
28	a	1884	C	C4'-C3'-O3'	6.79	123.18	113.00
28	a	1956	U	C2'-C3'-O3'	6.78	119.67	109.50
28	a	964	U	C2'-C3'-O3'	-6.68	103.67	113.70
28	a	1886	C	C2'-C3'-O3'	-6.64	99.54	109.50
28	a	791	G	C2'-C3'-O3'	-6.57	103.85	113.70
28	a	906	A	C2'-C3'-O3'	6.49	119.24	109.50
28	a	938	U	C4'-C3'-O3'	6.34	118.91	109.40
28	a	834	U	C2'-C3'-O3'	-6.32	104.22	113.70
28	a	653	U	C2'-C3'-O3'	6.17	118.76	109.50
28	a	364	U	C2'-C3'-O3'	6.17	118.75	109.50
28	a	2779	G	C4'-C3'-O3'	-6.08	103.87	113.00
28	a	2172	G	C4'-C3'-O3'	6.07	118.51	109.40
28	a	1141	C	C4'-C3'-O3'	-5.99	104.02	113.00
28	a	788	A	C4'-C3'-O3'	-5.96	104.06	113.00
28	a	208	A	C2'-C3'-O3'	-5.95	100.58	109.50
28	a	2625	U	C2'-C3'-O3'	5.93	118.40	109.50
28	a	2303	A	C2'-C3'-O3'	-5.93	100.61	109.50
28	a	753	U	C2'-C3'-O3'	5.92	118.38	109.50
28	a	395	U	C2'-C3'-O3'	-5.92	100.63	109.50
28	a	552	U	C4'-C3'-O3'	5.82	118.14	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	1955	U	C1'-C2'-O2'	-5.77	103.15	111.80
28	a	2463	G	C4'-C3'-O3'	5.70	117.94	109.40
28	a	2806	G	C4'-C3'-O3'	5.54	117.71	109.40
28	a	2772	U	C4'-C3'-O3'	5.46	117.59	109.40
28	a	909	C	C4'-C3'-O3'	5.43	121.14	113.00
6	b	88	U	C4'-C3'-O3'	-5.39	104.91	113.00
28	a	2324	G	C2'-C3'-O3'	5.34	117.51	109.50
28	a	484	A	C2'-C3'-O3'	-5.34	101.50	109.50
28	a	2518	G	C4'-C3'-O3'	5.33	120.99	113.00
28	a	1982	A	C4'-C3'-O3'	5.32	117.38	109.40
28	a	426	C	C4'-C3'-O3'	5.30	117.35	109.40
28	a	1116	G	C2'-C3'-O3'	5.29	121.64	113.70
28	a	1518	A	C4'-C3'-O3'	-5.26	105.11	113.00
28	a	2351	A	C4'-C3'-O3'	-5.26	105.12	113.00
28	a	2735	G	C4'-C3'-O3'	-5.25	105.12	113.00
28	a	458	A	C4'-C3'-O3'	-5.24	105.14	113.00
28	a	1744	U	C3'-C2'-O2'	5.20	122.39	114.60
28	a	2748	G	C4'-C3'-O3'	5.17	117.15	109.40
28	a	2368	A	P-O3'-C3'	-5.17	112.45	120.20
28	a	900	C	C4'-C3'-O3'	-5.16	105.26	113.00
28	a	1648	G	C4'-C3'-O3'	-5.15	105.27	113.00
28	a	818	U	C2'-C3'-O3'	5.14	117.21	109.50
28	a	600	U	C4'-C3'-O3'	-5.11	105.33	113.00
28	a	203	A	C2'-C3'-O3'	5.09	117.14	109.50
28	a	1051	C	C4'-C3'-O3'	5.05	116.97	109.40

There are no chirality outliers.

There are no planarity outliers.

## 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	Z	133	0	143	0	0
2	0	550	0	580	2	0
3	1	813	0	884	4	0
4	2	913	0	974	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	3	307	0	342	0	0
6	b	2488	0	1265	2	0
7	c	919	0	966	7	0
8	d	1596	0	1647	8	0
9	e	941	0	1015	2	0
10	f	1457	0	1530	5	0
11	g	1310	0	1389	10	0
12	h	813	0	849	1	0
13	i	1108	0	1150	2	0
14	j	839	0	881	4	0
15	k	1076	0	1162	5	0
16	m	967	0	1018	4	0
17	o	2131	0	2231	8	0
18	q	339	0	367	1	0
19	r	522	0	559	3	0
20	s	1090	0	1163	5	0
21	t	449	0	481	1	0
22	u	1486	0	1523	4	0
23	v	436	0	446	7	0
24	w	1571	0	1631	7	0
25	x	948	0	1033	4	0
26	y	374	0	412	0	0
27	z	500	0	557	2	0
28	a	61614	0	30965	158	0
29	8	613	0	635	5	0
30	7	732	0	764	8	0
31	9	631	0	677	8	0
32	3	1	0	0	0	0
33	a	159	0	0	0	0
33	b	1	0	0	0	0
33	d	1	0	0	0	0
33	o	1	0	0	0	0
34	8	1	0	0	0	0
34	a	127	0	0	0	0
34	b	1	0	0	0	0
34	d	1	0	0	0	0
34	o	2	0	0	0	0
34	s	1	0	0	0	0
34	v	2	0	0	0	0
34	w	1	0	0	0	0
35	a	7	0	0	0	0
All	All	89972	0	59239	233	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 2.

All (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:12:C:O2'	29:8:74:PRO:HA	1.65	0.94
13:i:59:VAL:HG21	13:i:124:ILE:HG23	1.52	0.91
28:a:1048:G:H1	28:a:1119:U:H3	1.23	0.86
7:c:92:ASP:HB2	7:c:114:LYS:HB3	1.60	0.82
7:c:4:ILE:HD11	8:d:27:VAL:HG11	1.64	0.79
23:v:16:ARG:HA	28:a:2062:G:H5'	1.68	0.75
28:a:20:U:H2'	28:a:20:U:O2	1.86	0.75
28:a:466:C:P	30:7:70:ARG:HH12	2.09	0.75
17:o:130:LEU:HD12	17:o:192:ILE:HD11	1.67	0.74
22:u:78:ILE:HG23	22:u:99:ILE:HD11	1.70	0.74
4:2:53:THR:HG21	4:2:65:GLY:HA3	1.71	0.73
28:a:790:A:H2'	28:a:791:G:C5'	2.19	0.73
28:a:194:A:OP1	31:9:26:ASN:ND2	2.20	0.69
28:a:1547:C:O2	28:a:1547:C:H2'	1.92	0.69
11:g:27:VAL:HG12	11:g:80:VAL:HG21	1.74	0.69
28:a:2245:U:O2	31:9:34:LYS:NZ	2.29	0.66
28:a:790:A:H2'	28:a:791:G:H5'	1.80	0.64
17:o:119:GLY:O	17:o:130:LEU:HD23	1.98	0.64
25:x:64:ARG:NH1	25:x:99:PHE:O	2.31	0.64
28:a:790:A:H2'	28:a:791:G:H5''	1.80	0.63
28:a:466:C:P	30:7:70:ARG:NH1	2.73	0.61
28:a:2096:A:OP1	31:9:19:SER:HB2	2.00	0.61
11:g:25:ILE:HD11	11:g:44:VAL:HG21	1.83	0.60
15:k:116:LEU:HD21	15:k:120:VAL:HG22	1.84	0.59
28:a:1046:A:H2	28:a:1121:G:H22	1.49	0.59
24:w:113:LEU:HD12	24:w:204:LEU:HD11	1.85	0.59
28:a:784:A:N1	28:a:794:U:H5	2.00	0.58
15:k:108:VAL:HB	15:k:125:LEU:HD22	1.84	0.58
28:a:148:A:N3	28:a:148:A:C5'	2.67	0.58
10:f:103:LEU:HD23	10:f:104:ILE:HG13	1.86	0.58
19:r:45:ARG:NH2	19:r:49:ASP:OD2	2.37	0.57
28:a:790:A:C2'	28:a:791:G:H5''	2.35	0.57
28:a:2380:C:H4'	29:8:56:ASP:OD1	2.05	0.57
16:m:112:ILE:HD11	23:v:54:LEU:HD11	1.87	0.57
3:1:62:ARG:HH21	3:1:62:ARG:HB2	1.70	0.56
28:a:1034:A:N6	28:a:1131:G:H2'	2.20	0.56
28:a:1350:U:OP2	30:7:78:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2201:U:H2'	28:a:2202:G:C8	2.40	0.56
25:x:119:LEU:HD23	25:x:119:LEU:H	1.69	0.56
28:a:2307:U:H2'	28:a:2308:A:C8	2.41	0.56
23:v:9:THR:CG2	28:a:2036:A:H5'	2.36	0.56
7:c:73:ARG:HD2	25:x:77:ILE:CD1	2.36	0.56
28:a:148:A:N3	28:a:148:A:H5'	2.22	0.55
7:c:4:ILE:CD1	8:d:27:VAL:HG11	2.35	0.55
4:2:53:THR:HG21	4:2:65:GLY:CA	2.37	0.55
28:a:311:G:H22	28:a:314:A:H5'	1.72	0.55
20:s:34:LEU:HD13	20:s:118:PHE:HB3	1.88	0.54
24:w:161:ILE:HG22	24:w:173:VAL:HG21	1.88	0.54
17:o:207:LYS:HB2	28:a:736:G:C6	2.42	0.54
28:a:466:C:OP1	30:7:70:ARG:NH1	2.40	0.54
17:o:16:VAL:HG22	17:o:206:GLY:HA3	1.89	0.54
28:a:1350:U:OP1	30:7:18:LYS:NZ	2.39	0.54
28:a:2922:A:N6	28:a:2923:A:C6	2.75	0.54
7:c:73:ARG:HD2	25:x:77:ILE:HD13	1.89	0.53
28:a:2143:G:H2'	28:a:2144:G:C8	2.43	0.53
21:t:49:MET:O	21:t:53:VAL:HG22	2.08	0.53
28:a:148:A:H2'	28:a:149:G:O4'	2.08	0.53
28:a:2191:C:H2'	28:a:2192:A:O4'	2.09	0.53
28:a:2191:C:N4	28:a:2192:A:C2	2.77	0.53
8:d:184:ASP:HB3	8:d:189:LEU:HB2	1.91	0.53
28:a:2107:C:H1'	31:9:34:LYS:HE3	1.91	0.53
28:a:2164:G:H2'	28:a:2165:C:C6	2.44	0.53
28:a:1052:A:C2	28:a:1119:U:H1'	2.44	0.53
28:a:790:A:C2'	28:a:791:G:C5'	2.87	0.52
28:a:641:C:H2'	28:a:642:C:C6	2.44	0.52
14:j:24:VAL:HG23	14:j:32:ALA:HB1	1.91	0.52
28:a:2369:G:O2'	29:8:35:ASN:ND2	2.43	0.52
6:b:59:A:H2'	6:b:60:A:C8	2.45	0.52
11:g:118:MET:HE1	11:g:149:ILE:HD11	1.90	0.52
17:o:124:ILE:HA	17:o:192:ILE:HD13	1.91	0.52
27:z:63:ARG:HG2	27:z:63:ARG:HH21	1.75	0.52
28:a:396:A:H1'	28:a:416:G:O4'	2.09	0.52
28:a:543:A:C2'	28:a:544:G:H5'	2.39	0.52
28:a:1052:A:N1	28:a:1119:U:H1'	2.25	0.51
28:a:1547:C:O2	28:a:1547:C:C2'	2.56	0.51
28:a:1120:C:H2'	28:a:1121:G:C8	2.45	0.51
11:g:27:VAL:CG1	11:g:80:VAL:HG21	2.40	0.51
28:a:7:A:H2'	28:a:8:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:s:56:ARG:CD	28:a:2485:A:H4'	2.41	0.51
28:a:2215:A:O2'	31:9:36:ARG:NH2	2.43	0.50
24:w:73:ARG:HD3	28:a:681:G:H1'	1.93	0.50
28:a:2190:C:H2'	28:a:2191:C:C6	2.46	0.50
28:a:2346:G:O2'	29:8:41:ARG:O	2.28	0.49
11:g:10:ILE:CG2	11:g:77:VAL:HG21	2.42	0.49
20:s:35:LYS:HE2	20:s:130:LEU:HD23	1.94	0.49
28:a:2344:A:H2'	28:a:2345:A:C8	2.47	0.49
11:g:103:LYS:NZ	11:g:117:GLU:OE1	2.46	0.49
28:a:2289:A:H2'	28:a:2290:A:C8	2.48	0.49
8:d:149:ILE:HG12	28:a:2067:U:H4'	1.93	0.49
28:a:1760:A:H2'	28:a:1761:A:C8	2.48	0.49
28:a:646:U:H2'	28:a:647:C:C6	2.48	0.49
28:a:1883:C:H2'	28:a:1884:C:O4'	2.12	0.49
24:w:116:LEU:HD13	24:w:190:ILE:HD12	1.94	0.49
28:a:2144:G:H2'	28:a:2145:C:C6	2.48	0.49
14:j:11:ARG:HH11	14:j:98:LYS:HE3	1.78	0.49
16:m:112:ILE:CD1	23:v:54:LEU:HD11	2.43	0.48
28:a:587:U:H2'	28:a:588:C:C6	2.48	0.48
28:a:803:U:H2'	28:a:804:C:C6	2.48	0.48
28:a:20:U:O2	28:a:20:U:C2'	2.59	0.48
28:a:2372:U:O3'	29:8:20:MET:SD	2.71	0.48
28:a:1051:C:H1'	28:a:1052:A:OP2	2.12	0.48
28:a:651:A:H2'	28:a:652:A:C8	2.49	0.48
28:a:539:U:H2'	28:a:540:A:C8	2.49	0.48
28:a:201:A:N6	28:a:2446:A:H2'	2.29	0.47
28:a:781:A:H2	28:a:794:U:O2'	1.97	0.47
28:a:1117:A:H1'	28:a:1118:G:H4'	1.96	0.47
2:0:50:TRP:CZ2	2:0:55:SER:HA	2.49	0.47
4:2:58:VAL:O	4:2:62:ILE:HG22	2.13	0.47
23:v:26:MET:HE3	23:v:27:LEU:H	1.79	0.47
28:a:866:U:O2	28:a:866:U:O4'	2.31	0.47
28:a:907:A:H2'	28:a:908:C:O4'	2.14	0.47
28:a:1545:A:N6	28:a:1551:U:C4	2.83	0.47
10:f:13:THR:HB	10:f:14:PRO:HD3	1.96	0.47
28:a:402:A:H5''	31:9:32:ASN:HB2	1.96	0.47
28:a:1117:A:H1'	28:a:1118:G:C4'	2.45	0.47
2:0:40:LEU:HD22	2:0:42:ILE:HD11	1.96	0.47
4:2:50:CYS:O	4:2:81:ARG:NH1	2.48	0.47
11:g:102:LYS:HB3	11:g:117:GLU:OE1	2.15	0.47
16:m:5:LYS:NZ	28:a:2016:C:OP1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:675:A:H2'	28:a:677:A:H62	1.81	0.46
8:d:28:VAL:HG11	8:d:206:ILE:HD11	1.96	0.46
19:r:33:GLY:HA3	30:7:13:PRO:HG2	1.96	0.46
22:u:163:LEU:HD23	22:u:186:ILE:HD11	1.96	0.46
28:a:898:G:H3'	28:a:899:C:H5''	1.98	0.46
28:a:664:U:H2'	28:a:665:U:C6	2.50	0.46
28:a:2563:A:H2'	28:a:2564:U:C6	2.51	0.45
23:v:52:GLN:NE2	23:v:54:LEU:O	2.50	0.45
28:a:790:A:N3	28:a:791:G:H5'	2.31	0.45
7:c:18:ILE:HD13	7:c:77:LEU:HD21	1.98	0.45
28:a:902:A:C8	28:a:903:C:C6	3.05	0.45
18:q:7:GLU:HA	18:q:15:ILE:HG12	1.98	0.45
28:a:148:A:H2'	28:a:149:G:C8	2.51	0.45
22:u:193:ARG:HH12	28:a:903:C:H5''	1.82	0.45
24:w:99:LYS:HG2	28:a:666:G:H4'	1.98	0.45
28:a:2183:U:H2'	28:a:2184:G:O4'	2.17	0.45
17:o:207:LYS:HB2	28:a:736:G:C5	2.52	0.45
28:a:1276:G:O2'	28:a:2028:G:O6	2.34	0.45
14:j:55:ILE:HG21	14:j:66:ILE:HD12	1.99	0.45
28:a:2090:U:H2'	28:a:2091:U:C6	2.52	0.44
28:a:2153:C:H2'	28:a:2154:U:C1'	2.46	0.44
20:s:56:ARG:HD2	28:a:2485:A:H4'	1.99	0.44
28:a:211:A:H2'	28:a:212:C:O4'	2.17	0.44
28:a:1660:G:H5''	28:a:1661:C:H5'	1.99	0.44
7:c:80:PRO:HG2	8:d:20:GLY:HA2	2.00	0.44
8:d:158:VAL:HG21	28:a:2634:G:H21	1.82	0.44
28:a:146:C:O2	28:a:146:C:O4'	2.34	0.44
28:a:2804:C:H2'	28:a:2805:C:C6	2.52	0.44
11:g:104:LEU:HD23	11:g:116:ILE:HD12	1.99	0.44
28:a:312:G:H2'	28:a:313:A:C8	2.53	0.44
28:a:699:U:H2'	28:a:700:A:C8	2.52	0.44
28:a:1516:U:H2'	28:a:1517:C:C6	2.53	0.44
28:a:1742:C:H2'	28:a:1743:U:O4'	2.17	0.44
28:a:1905:A:H2'	28:a:1906:A:C8	2.53	0.44
10:f:108:ILE:HG21	10:f:176:PRO:HG3	1.99	0.44
14:j:75:MET:HE3	28:a:523:G:H21	1.83	0.44
16:m:103:ARG:O	16:m:107:SER:HA	2.18	0.44
28:a:1443:A:H2'	28:a:1444:A:C8	2.52	0.44
28:a:2343:A:H2'	28:a:2344:A:C8	2.53	0.44
28:a:2087:A:H2'	28:a:2088:C:C6	2.53	0.44
15:k:78:ARG:HG2	15:k:113:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2205:U:H2'	28:a:2206:G:C8	2.53	0.43
28:a:2695:A:H2'	28:a:2696:C:O4'	2.18	0.43
24:w:167:ASN:HB2	28:a:326:A:OP2	2.18	0.43
28:a:985:A:H5'	28:a:986:A:H5''	2.00	0.43
28:a:2772:U:H1'	28:a:2773:A:H5''	2.00	0.43
28:a:1338:A:H2'	28:a:1340:C:C4	2.54	0.43
28:a:2144:G:H2'	28:a:2145:C:H6	1.83	0.43
13:i:89:PHE:CE2	13:i:100:ILE:HD13	2.53	0.43
28:a:313:A:H2'	28:a:314:A:H5''	2.01	0.43
28:a:1553:C:H4'	28:a:1554:G:O5'	2.18	0.43
28:a:1408:C:OP1	30:7:55:ARG:NH2	2.42	0.43
28:a:419:C:H2'	28:a:420:A:C8	2.54	0.43
28:a:543:A:H2'	28:a:544:G:H5'	2.01	0.43
28:a:862:G:H2'	28:a:863:G:C8	2.54	0.43
28:a:1585:A:H2'	28:a:1586:A:C8	2.54	0.43
4:2:55:GLU:HB2	4:2:58:VAL:HG22	2.00	0.42
19:r:48:ARG:NH1	28:a:83:G:H4'	2.35	0.42
28:a:294:U:H2'	28:a:295:U:C6	2.54	0.42
28:a:784:A:N1	28:a:794:U:C5	2.84	0.42
28:a:1955:U:OP1	28:a:2620:U:O2'	2.38	0.42
28:a:1058:C:O2	28:a:1058:C:H2'	2.19	0.42
28:a:1557:C:N4	28:a:1558:A:C6	2.87	0.42
28:a:2119:U:H2'	28:a:2120:A:O4'	2.19	0.42
28:a:2249:U:H2'	28:a:2250:G:C8	2.54	0.42
3:1:103:GLU:OE1	3:1:103:GLU:N	2.53	0.42
28:a:787:G:H2'	28:a:789:A:N7	2.35	0.42
28:a:1517:C:H2'	28:a:1518:A:H4'	2.02	0.42
9:e:31:VAL:HG13	28:a:587:U:O3'	2.19	0.42
28:a:846:U:H2'	28:a:847:C:C6	2.55	0.42
28:a:2714:U:H2'	28:a:2715:C:C6	2.54	0.42
10:f:50:ILE:HD13	10:f:84:PRO:HB2	2.01	0.42
28:a:577:G:H2'	28:a:2046:A:N7	2.35	0.42
9:e:30:ARG:NH1	28:a:26:C:OP1	2.53	0.42
10:f:31:LEU:HD23	10:f:158:THR:HG22	2.02	0.41
23:v:9:THR:HG21	28:a:2036:A:H5'	2.02	0.41
28:a:750:A:O2'	28:a:1674:G:OP1	2.35	0.41
28:a:2107:C:O3'	31:9:56:MET:HE1	2.20	0.41
28:a:2120:A:H1'	28:a:2202:G:N2	2.34	0.41
28:a:1415:U:H2'	28:a:1416:U:C6	2.54	0.41
28:a:2901:A:H2'	28:a:2902:A:C8	2.55	0.41
28:a:1051:C:C6	28:a:1117:A:N1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:g:12:ILE:HG12	11:g:18:VAL:HG21	2.03	0.41
22:u:174:LEU:HD13	22:u:178:VAL:HG21	2.02	0.41
28:a:1606:U:H2'	28:a:1607:U:C6	2.55	0.41
28:a:2120:A:H2'	28:a:2121:U:O4'	2.19	0.41
8:d:109:VAL:CG1	8:d:177:SER:HA	2.50	0.41
28:a:300:C:H2'	28:a:301:A:C8	2.56	0.41
28:a:1884:C:H2'	28:a:1885:U:O2	2.21	0.41
28:a:1885:U:C2	28:a:1886:C:N3	2.89	0.41
28:a:2192:A:C2	28:a:2193:C:C5	3.08	0.41
28:a:954:C:H1'	28:a:990:G:C8	2.56	0.41
28:a:1052:A:N7	28:a:1117:A:N1	2.69	0.41
28:a:1772:U:C5	28:a:2712:U:H5'	2.56	0.41
3:l:98:PHE:O	3:l:102:GLY:N	2.53	0.41
28:a:1792:U:H2'	28:a:1798:A:N6	2.36	0.41
28:a:2665:C:H2'	28:a:2666:U:C6	2.55	0.41
11:g:10:ILE:HB	11:g:51:LEU:HB2	2.03	0.40
15:k:1:MET:HE3	24:w:27:TYR:CE1	2.57	0.40
20:s:43:THR:HG22	20:s:94:VAL:HG12	2.03	0.40
3:l:96:ARG:HB3	3:l:105:ILE:HD12	2.03	0.40
28:a:401:G:H1'	31:9:29:PHE:HB3	2.03	0.40
28:a:2143:G:H2'	28:a:2144:G:H8	1.85	0.40
28:a:2359:U:H2'	28:a:2360:U:C6	2.57	0.40
28:a:790:A:C2'	28:a:791:G:H5'	2.50	0.40
28:a:1565:U:H2'	28:a:1566:U:C6	2.57	0.40
28:a:2330:G:H2'	28:a:2331:U:C6	2.56	0.40
28:a:2570:U:H2'	28:a:2571:U:C6	2.56	0.40
17:o:14:ARG:NH1	28:a:1708:U:O2'	2.55	0.40
27:z:63:ARG:HH21	27:z:63:ARG:CG	2.34	0.40
28:a:1409:C:OP1	30:7:82:MET:HE3	2.22	0.40
12:h:65:ASP:HB3	12:h:95:ALA:HB3	2.03	0.40
15:k:123:ARG:NH2	15:k:143:GLU:OE2	2.55	0.40
17:o:146:LEU:CD2	28:a:1814:C:H3'	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	14/21 (67%)	14 (100%)	0	0	100	100
2	0	66/70 (94%)	66 (100%)	0	0	100	100
3	1	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
4	2	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
5	3	36/40 (90%)	36 (100%)	0	0	100	100
7	c	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
8	d	209/217 (96%)	203 (97%)	6 (3%)	0	100	100
9	e	116/119 (98%)	116 (100%)	0	0	100	100
10	f	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
11	g	172/178 (97%)	167 (97%)	5 (3%)	0	100	100
12	h	102/115 (89%)	102 (100%)	0	0	100	100
13	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
14	j	108/115 (94%)	107 (99%)	1 (1%)	0	100	100
15	k	141/143 (99%)	134 (95%)	7 (5%)	0	100	100
16	m	117/126 (93%)	111 (95%)	6 (5%)	0	100	100
17	o	272/275 (99%)	265 (97%)	7 (3%)	0	100	100
18	q	43/152 (28%)	41 (95%)	2 (5%)	0	100	100
19	r	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
20	s	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
21	t	54/63 (86%)	52 (96%)	2 (4%)	0	100	100
22	u	189/244 (78%)	182 (96%)	7 (4%)	0	100	100
23	v	52/64 (81%)	51 (98%)	1 (2%)	0	100	100
24	w	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
25	x	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
26	y	42/44 (96%)	42 (100%)	0	0	100	100
27	z	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
29	8	75/90 (83%)	73 (97%)	2 (3%)	0	100	100
30	7	89/95 (94%)	88 (99%)	1 (1%)	0	100	100
31	9	75/79 (95%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3198/3506 (91%)	3123 (98%)	75 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	Z	13/18 (72%)	13 (100%)	0	100	100
2	0	62/63 (98%)	62 (100%)	0	100	100
3	1	91/93 (98%)	90 (99%)	1 (1%)	65	79
4	2	92/93 (99%)	89 (97%)	3 (3%)	33	45
5	3	34/35 (97%)	33 (97%)	1 (3%)	37	51
7	c	98/100 (98%)	95 (97%)	3 (3%)	35	48
8	d	169/175 (97%)	169 (100%)	0	100	100
9	e	88/89 (99%)	87 (99%)	1 (1%)	65	79
10	f	155/155 (100%)	151 (97%)	4 (3%)	40	55
11	g	142/146 (97%)	141 (99%)	1 (1%)	76	87
12	h	85/93 (91%)	85 (100%)	0	100	100
13	i	115/116 (99%)	114 (99%)	1 (1%)	70	84
14	j	86/91 (94%)	84 (98%)	2 (2%)	44	59
15	k	107/107 (100%)	106 (99%)	1 (1%)	70	84
16	m	102/109 (94%)	101 (99%)	1 (1%)	68	81
17	o	223/224 (100%)	221 (99%)	2 (1%)	70	84
18	q	36/123 (29%)	36 (100%)	0	100	100
19	r	56/58 (97%)	55 (98%)	1 (2%)	51	68
20	s	111/111 (100%)	111 (100%)	0	100	100
21	t	50/57 (88%)	50 (100%)	0	100	100
22	u	167/201 (83%)	165 (99%)	2 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	v	46/56 (82%)	46 (100%)	0	100	100
24	w	169/169 (100%)	166 (98%)	3 (2%)	51	68
25	x	105/105 (100%)	103 (98%)	2 (2%)	50	66
26	y	38/38 (100%)	38 (100%)	0	100	100
27	z	54/56 (96%)	52 (96%)	2 (4%)	30	41
29	8	64/73 (88%)	63 (98%)	1 (2%)	55	71
30	7	79/81 (98%)	79 (100%)	0	100	100
31	9	70/72 (97%)	70 (100%)	0	100	100
All	All	2707/2907 (93%)	2675 (99%)	32 (1%)	61	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1	62	ARG
4	2	27	CYS
4	2	68	ILE
4	2	81	ARG
5	3	31	ARG
7	c	4	ILE
7	c	54	ARG
7	c	101	LEU
9	e	112	LYS
10	f	58	ILE
10	f	78	LYS
10	f	103	LEU
10	f	144	ASP
11	g	116	ILE
13	i	31	ARG
14	j	70	LYS
14	j	85	PHE
15	k	68	SER
16	m	35	LYS
17	o	13	ARG
17	o	168	GLU
19	r	9	LYS
22	u	118	ASP
22	u	194	VAL
24	w	92	LYS
24	w	179	VAL

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Mol	Chain	Res	Type
24	w	199	ARG
25	x	77	ILE
25	x	80	ASP
27	z	6	THR
27	z	63	ARG
29	8	80	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
3	1	32	ASN
4	2	64	HIS
7	c	88	ASN
8	d	37	GLN
8	d	128	HIS
8	d	188	ASN
10	f	5	GLN
11	g	115	ASN
13	i	133	GLN
14	j	94	ASN
16	m	2	HIS
16	m	9	HIS
17	o	111	HIS
17	o	134	ASN
17	o	143	ASN
18	q	14	ASN
22	u	97	GLN
22	u	190	HIS
24	w	98	GLN
24	w	149	ASN
24	w	162	ASN
24	w	167	ASN
25	x	3	GLN
25	x	92	GLN
27	z	28	ASN
29	8	35	ASN
29	8	44	HIS
29	8	78	ASN
31	9	22	ASN

### 5.3.3 RNA



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2871/2925 (98%)	355 (12%)	0
6	b	116/117 (99%)	11 (9%)	0
All	All	2987/3042 (98%)	366 (12%)	0

All (366) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	b	35	U
6	b	36	U
6	b	45	A
6	b	51	G
6	b	56	G
6	b	57	A
6	b	66	A
6	b	67	G
6	b	68	C
6	b	88	U
6	b	107	A
28	a	2	G
28	a	23	G
28	a	42	U
28	a	57	A
28	a	79	A
28	a	82	A
28	a	83	G
28	a	93	G
28	a	126	A
28	a	127	A
28	a	128	U
28	a	133	A
28	a	134	A
28	a	145	U
28	a	146	C
28	a	147	G
28	a	148	A
28	a	167	U
28	a	185	A
28	a	194	A
28	a	200	A
28	a	201	A
28	a	203	A
28	a	219	G
28	a	220	A

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Mol	Chain	Res	Type
28	a	225	A
28	a	226	A
28	a	237	A
28	a	249	G
28	a	252	G
28	a	256	G
28	a	270	G
28	a	275	G
28	a	299	G
28	a	305	U
28	a	315	A
28	a	328	C
28	a	334	A
28	a	364	U
28	a	365	G
28	a	372	G
28	a	391	G
28	a	427	A
28	a	453	U
28	a	461	C
28	a	462	A
28	a	480	U
28	a	486	G
28	a	496	G
28	a	509	U
28	a	510	A
28	a	514	C
28	a	536	C
28	a	537	A
28	a	543	A
28	a	544	G
28	a	553	C
28	a	555	G
28	a	570	A
28	a	580	U
28	a	582	A
28	a	610	A
28	a	611	G
28	a	620	U
28	a	622	U
28	a	634	A
28	a	644	A

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Mol	Chain	Res	Type
28	a	653	U
28	a	654	G
28	a	660	U
28	a	661	U
28	a	692	A
28	a	693	U
28	a	716	U
28	a	722	A
28	a	723	A
28	a	724	C
28	a	726	C
28	a	737	C
28	a	753	U
28	a	754	U
28	a	771	A
28	a	772	G
28	a	782	G
28	a	783	G
28	a	789	A
28	a	792	G
28	a	796	A
28	a	799	A
28	a	812	G
28	a	819	C
28	a	835	U
28	a	837	G
28	a	850	G
28	a	865	G
28	a	872	A
28	a	885	G
28	a	886	G
28	a	887	G
28	a	888	G
28	a	889	G
28	a	892	A
28	a	894	C
28	a	896	C
28	a	897	G
28	a	898	G
28	a	899	C
28	a	900	C
28	a	901	U

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Mol	Chain	Res	Type
28	a	902	A
28	a	903	C
28	a	905	A
28	a	907	A
28	a	909	C
28	a	910	G
28	a	916	A
28	a	937	U
28	a	939	A
28	a	952	C
28	a	965	A
28	a	967	G
28	a	980	A
28	a	989	A
28	a	990	G
28	a	991	C
28	a	1002	A
28	a	1018	U
28	a	1019	C
28	a	1028	G
28	a	1032	A
28	a	1048	G
28	a	1051	C
28	a	1052	A
28	a	1054	A
28	a	1055	C
28	a	1057	G
28	a	1058	C
28	a	1059	C
28	a	1113	G
28	a	1114	U
28	a	1117	A
28	a	1118	G
28	a	1121	G
28	a	1126	G
28	a	1135	A
28	a	1136	U
28	a	1138	U
28	a	1139	A
28	a	1140	A
28	a	1141	C
28	a	1142	G

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Mol	Chain	Res	Type
28	a	1149	A
28	a	1162	A
28	a	1183	C
28	a	1184	U
28	a	1185	G
28	a	1237	G
28	a	1263	A
28	a	1266	G
28	a	1281	G
28	a	1282	A
28	a	1283	U
28	a	1296	A
28	a	1297	A
28	a	1311	A
28	a	1362	U
28	a	1375	A
28	a	1378	U
28	a	1386	C
28	a	1389	U
28	a	1393	A
28	a	1395	A
28	a	1396	C
28	a	1425	U
28	a	1426	G
28	a	1427	C
28	a	1429	A
28	a	1430	U
28	a	1431	G
28	a	1438	C
28	a	1462	G
28	a	1463	A
28	a	1470	U
28	a	1492	G
28	a	1503	C
28	a	1518	A
28	a	1520	U
28	a	1545	A
28	a	1546	A
28	a	1547	C
28	a	1548	U
28	a	1550	G
28	a	1551	U

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Mol	Chain	Res	Type
28	a	1553	C
28	a	1554	G
28	a	1555	U
28	a	1556	G
28	a	1557	C
28	a	1559	A
28	a	1562	U
28	a	1563	G
28	a	1575	G
28	a	1580	C
28	a	1581	A
28	a	1584	A
28	a	1593	U
28	a	1600	C
28	a	1622	U
28	a	1623	A
28	a	1624	A
28	a	1632	C
28	a	1663	U
28	a	1689	G
28	a	1711	G
28	a	1715	A
28	a	1745	G
28	a	1777	G
28	a	1778	G
28	a	1787	A
28	a	1790	G
28	a	1796	U
28	a	1805	A
28	a	1814	C
28	a	1815	A
28	a	1825	G
28	a	1830	C
28	a	1843	A
28	a	1862	A
28	a	1885	U
28	a	1886	C
28	a	1887	G
28	a	1888	G
28	a	1930	C
28	a	1946	G
28	a	1953	A

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Mol	Chain	Res	Type
28	a	1954	A
28	a	1957	C
28	a	1971	U
28	a	1979	U
28	a	1980	G
28	a	1983	C
28	a	1986	A
28	a	1987	U
28	a	1988	G
28	a	1998	U
28	a	2009	U
28	a	2013	C
28	a	2039	C
28	a	2047	A
28	a	2049	A
28	a	2059	C
28	a	2062	G
28	a	2071	C
28	a	2072	G
28	a	2076	A
28	a	2077	G
28	a	2078	A
28	a	2085	G
28	a	2096	A
28	a	2128	G
28	a	2132	G
28	a	2135	A
28	a	2140	G
28	a	2141	G
28	a	2143	G
28	a	2150	A
28	a	2151	A
28	a	2154	U
28	a	2163	A
28	a	2164	G
28	a	2173	G
28	a	2188	U
28	a	2189	A
28	a	2214	A
28	a	2219	U
28	a	2220	G
28	a	2227	A

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Mol	Chain	Res	Type
28	a	2228	A
28	a	2241	A
28	a	2254	G
28	a	2255	G
28	a	2291	C
28	a	2292	G
28	a	2294	A
28	a	2298	G
28	a	2299	U
28	a	2303	A
28	a	2324	G
28	a	2325	A
28	a	2343	A
28	a	2349	A
28	a	2351	A
28	a	2352	A
28	a	2363	C
28	a	2366	C
28	a	2377	A
28	a	2395	G
28	a	2398	G
28	a	2399	G
28	a	2401	C
28	a	2412	G
28	a	2418	C
28	a	2422	U
28	a	2440	C
28	a	2441	A
28	a	2445	G
28	a	2446	A
28	a	2447	U
28	a	2451	A
28	a	2457	U
28	a	2463	G
28	a	2464	A
28	a	2485	A
28	a	2490	U
28	a	2494	A
28	a	2507	U
28	a	2518	G
28	a	2519	2MA
28	a	2521	G

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Mol	Chain	Res	Type
28	a	2522	U
28	a	2534	A
28	a	2536	C
28	a	2570	U
28	a	2582	A
28	a	2583	G
28	a	2589	C
28	a	2594	G
28	a	2626	C
28	a	2629	U
28	a	2645	U
28	a	2679	G
28	a	2705	U
28	a	2706	U
28	a	2707	C
28	a	2730	G
28	a	2742	A
28	a	2749	A
28	a	2767	G
28	a	2768	C
28	a	2773	A
28	a	2774	A
28	a	2781	A
28	a	2794	A
28	a	2806	G
28	a	2807	G
28	a	2812	U
28	a	2813	U
28	a	2815	A
28	a	2823	A
28	a	2835	A
28	a	2836	A
28	a	2882	A
28	a	2883	A
28	a	2899	U
28	a	2909	G

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

9 non-standard protein/DNA/RNA residues are 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
28	PSU	a	2596	28,34	18,21,22	1.49	2 (11%)	22,30,33	1.81	5 (22%)
28	2MA	a	2519	28,33	22,25,26	1.56	4 (18%)	33,37,40	2.14	8 (24%)
28	PSU	a	1933	28	18,21,22	1.43	3 (16%)	22,30,33	1.88	5 (22%)
28	PSU	a	961	28	18,21,22	1.42	3 (16%)	22,30,33	1.89	4 (18%)
28	PSU	a	1927	28	18,21,22	1.42	3 (16%)	22,30,33	1.84	4 (18%)
28	PSU	a	2621	28	18,21,22	1.40	3 (16%)	22,30,33	1.89	4 (18%)
28	PSU	a	2520	28,34	18,21,22	1.59	3 (16%)	22,30,33	2.63	4 (18%)
28	OMU	a	2568	28,33	19,22,23	1.21	3 (15%)	26,31,34	1.83	6 (23%)
28	OMG	a	2267	28,33,34	23,26,27	1.22	3 (13%)	33,38,41	2.07	8 (24%)

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
28	PSU	a	2596	28,34	-	0/7/25/26	0/2/2/2
28	2MA	a	2519	28,33	-	2/7/25/26	0/3/3/3
28	PSU	a	1933	28	-	0/7/25/26	0/2/2/2
28	PSU	a	961	28	-	0/7/25/26	0/2/2/2
28	PSU	a	1927	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2621	28	-	2/7/25/26	0/2/2/2
28	PSU	a	2520	28,34	-	0/7/25/26	0/2/2/2
28	OMU	a	2568	28,33	-	0/9/27/28	0/2/2/2
28	OMG	a	2267	28,33,34	-	1/9/27/28	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2519	2MA	C5-C4	4.63	1.47	1.39
28	a	2596	PSU	C6-C5	4.54	1.40	1.35
28	a	1927	PSU	C6-C5	4.51	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1933	PSU	C6-C5	4.35	1.40	1.35
28	a	961	PSU	C6-C5	4.26	1.40	1.35
28	a	2621	PSU	C6-C5	4.19	1.40	1.35
28	a	2520	PSU	O2-C2	4.07	1.31	1.23
28	a	2520	PSU	C6-C5	3.66	1.39	1.35
28	a	2267	OMG	C5-C4	3.24	1.47	1.38
28	a	2568	OMU	C2-N1	2.86	1.43	1.38
28	a	2519	2MA	C5-C6	2.84	1.49	1.41
28	a	2596	PSU	C4-N3	-2.69	1.33	1.38
28	a	2519	2MA	C8-N7	2.43	1.36	1.31
28	a	2520	PSU	C4-C5	2.31	1.50	1.44
28	a	961	PSU	C4-N3	-2.30	1.34	1.38
28	a	1933	PSU	C4-C5	2.27	1.50	1.44
28	a	2621	PSU	C4-N3	-2.21	1.34	1.38
28	a	1927	PSU	C4-C5	2.21	1.50	1.44
28	a	2519	2MA	C5-N7	-2.17	1.34	1.39
28	a	2267	OMG	C5-N7	-2.17	1.34	1.39
28	a	2568	OMU	C4-N3	-2.16	1.34	1.38
28	a	2621	PSU	C4-C5	2.14	1.50	1.44
28	a	2267	OMG	C6-N1	-2.12	1.34	1.38
28	a	1933	PSU	C4-N3	-2.11	1.34	1.38
28	a	1927	PSU	C4-N3	-2.08	1.35	1.38
28	a	2568	OMU	C6-C5	2.07	1.39	1.35
28	a	961	PSU	C4-C5	2.05	1.50	1.44

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2520	PSU	O2-C2-N1	-8.66	113.26	122.79
28	a	2519	2MA	C5-C4-N3	-7.31	118.96	127.19
28	a	2267	OMG	C5-C4-N3	-6.19	118.41	128.46
28	a	2520	PSU	C6-C5-C4	-5.80	114.14	118.20
28	a	2519	2MA	N3-C4-N9	5.79	135.02	126.99
28	a	961	PSU	N1-C2-N3	5.78	121.68	115.13
28	a	1933	PSU	N1-C2-N3	5.69	121.57	115.13
28	a	2621	PSU	N1-C2-N3	5.67	121.56	115.13
28	a	1927	PSU	N1-C2-N3	5.60	121.48	115.13
28	a	2596	PSU	N1-C2-N3	5.22	121.04	115.13
28	a	2267	OMG	C2-N3-C4	5.18	121.54	112.30
28	a	2267	OMG	N9-C4-N3	4.54	135.05	125.94
28	a	2520	PSU	O2-C2-N3	4.28	129.88	121.82
28	a	2568	OMU	C4-N3-C2	-4.11	121.16	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2568	OMU	N3-C2-N1	4.05	120.27	114.89
28	a	961	PSU	C4-N3-C2	-3.82	120.83	126.34
28	a	2568	OMU	C5-C4-N3	3.79	120.51	114.84
28	a	2621	PSU	C4-N3-C2	-3.69	121.02	126.34
28	a	1927	PSU	C4-N3-C2	-3.65	121.07	126.34
28	a	1933	PSU	C4-N3-C2	-3.65	121.08	126.34
28	a	2267	OMG	C6-C5-N7	3.40	136.57	130.25
28	a	961	PSU	O2-C2-N1	-3.16	119.31	122.79
28	a	1933	PSU	O2-C2-N1	-3.13	119.35	122.79
28	a	2519	2MA	C4-C5-N7	-3.12	106.82	110.62
28	a	2621	PSU	O2-C2-N1	-3.11	119.36	122.79
28	a	1927	PSU	O2-C2-N1	-3.08	119.40	122.79
28	a	2596	PSU	C3'-C2'-C1'	3.05	105.19	101.64
28	a	2568	OMU	C2'-C1'-N1	-3.02	108.36	114.22
28	a	2568	OMU	O4-C4-C5	-3.02	119.85	125.16
28	a	2596	PSU	C4-N3-C2	-2.97	122.07	126.34
28	a	2621	PSU	C6-C5-C4	-2.85	116.20	118.20
28	a	2519	2MA	C2-N1-C6	2.73	122.33	118.08
28	a	2519	2MA	C4-N9-C8	2.70	108.65	105.73
28	a	1927	PSU	C6-C5-C4	-2.69	116.32	118.20
28	a	2519	2MA	C5-N7-C8	2.68	107.32	103.51
28	a	2267	OMG	C4-C5-N7	-2.68	106.48	110.72
28	a	2568	OMU	O4'-C1'-N1	2.60	114.31	108.36
28	a	1933	PSU	C3'-C2'-C1'	2.55	104.61	101.64
28	a	2519	2MA	C6-C5-N7	2.52	136.72	132.02
28	a	2596	PSU	C6-C5-C4	-2.46	116.48	118.20
28	a	961	PSU	C6-C5-C4	-2.45	116.49	118.20
28	a	2267	OMG	O2'-C2'-C1'	2.40	113.76	109.08
28	a	2519	2MA	N6-C6-N1	2.33	120.33	117.03
28	a	2596	PSU	O2-C2-N3	-2.31	117.46	121.82
28	a	2267	OMG	O6-C6-C5	-2.22	120.72	126.60
28	a	2520	PSU	C4-N3-C2	-2.17	123.21	126.34
28	a	1933	PSU	C6-C5-C4	-2.16	116.69	118.20
28	a	2267	OMG	C5-C6-N1	2.06	118.41	113.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	a	2267	OMG	C1'-C2'-O2'-CM2
28	a	2621	PSU	O4'-C1'-C5-C4
28	a	2621	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
28	a	2519	2MA	O4'-C4'-C5'-O5'
28	a	2519	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 299 ligands modelled in this entry, 299 are monoatomic - 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.

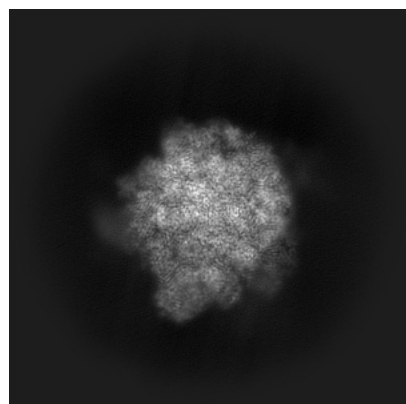
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56461. These allow visual inspection of the internal detail of the map and identification of artifacts.

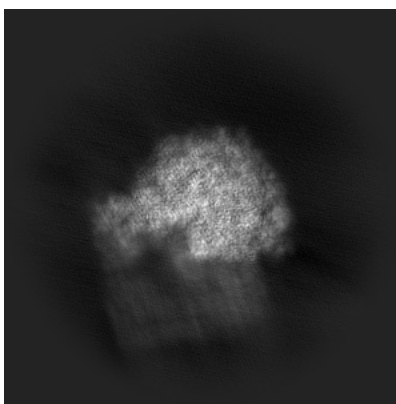
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

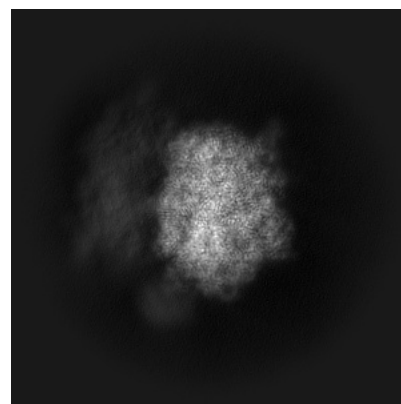
#### 6.1.1 Primary map



X

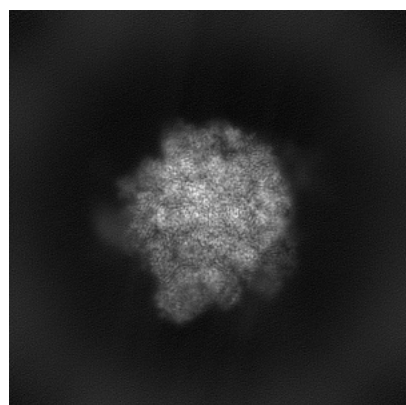


Y

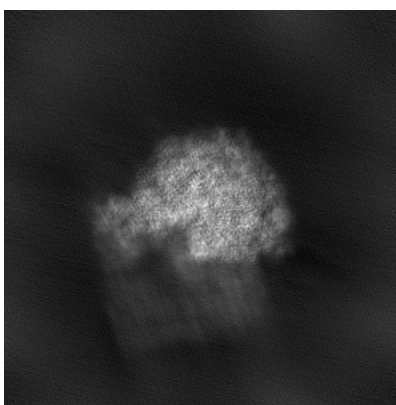


Z

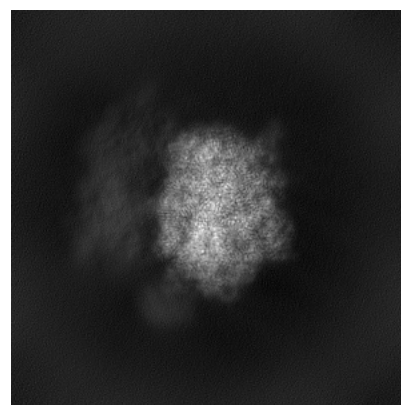
#### 6.1.2 Raw map



X



Y

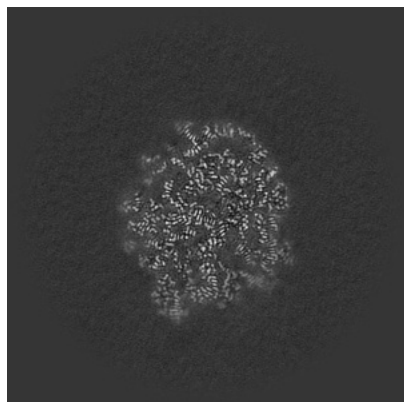


Z

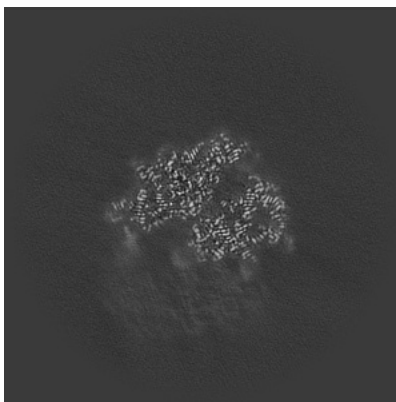
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

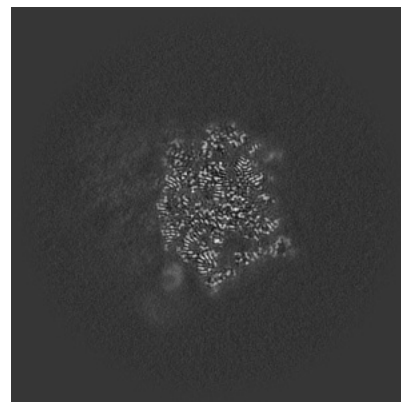
### 6.2.1 Primary map



X Index: 200

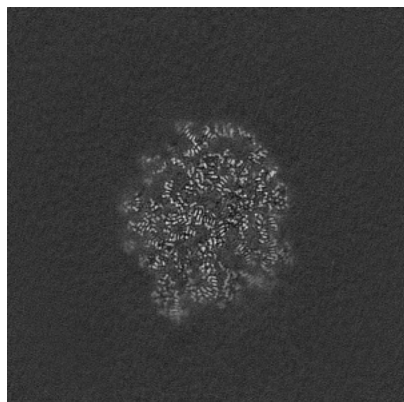


Y Index: 200

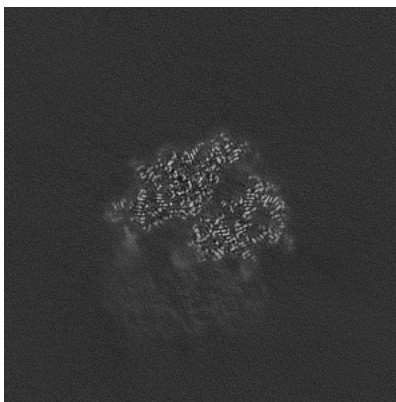


Z Index: 200

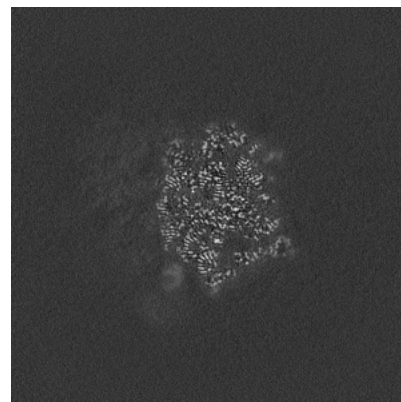
### 6.2.2 Raw map



X Index: 200



Y Index: 200



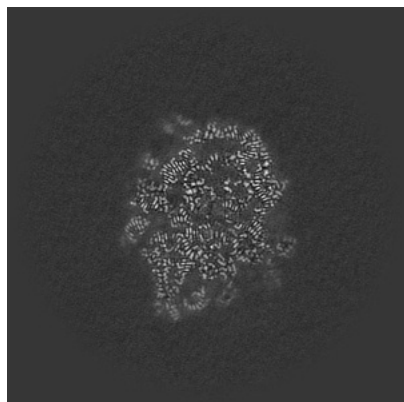
Z Index: 200

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

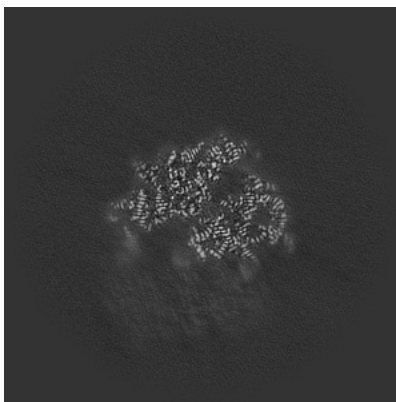


## 6.3 Largest variance slices [i](#)

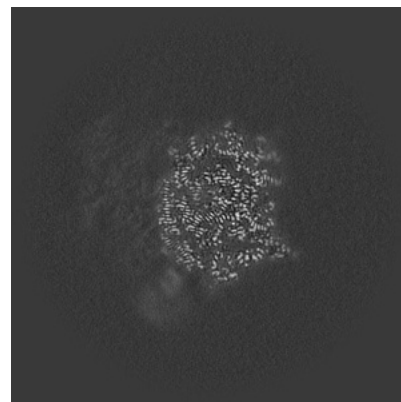
### 6.3.1 Primary map



X Index: 191

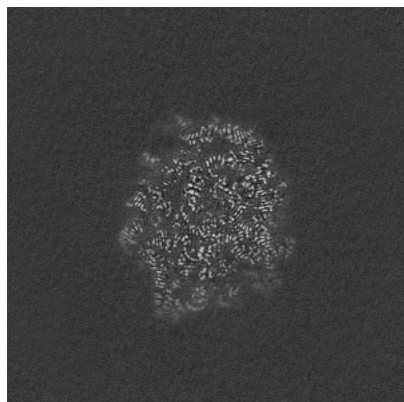


Y Index: 201

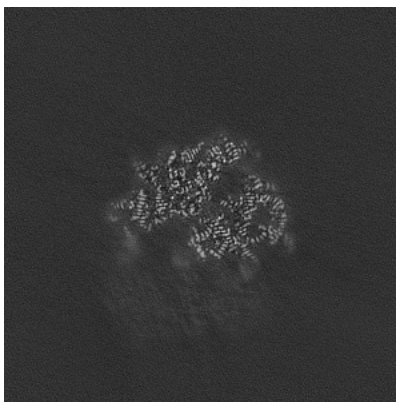


Z Index: 194

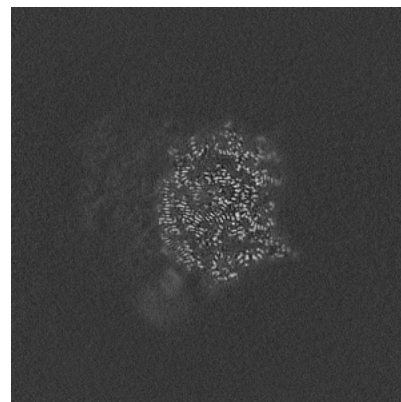
### 6.3.2 Raw map



X Index: 194



Y Index: 201



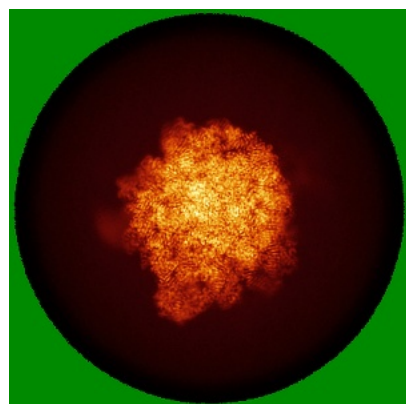
Z Index: 194

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

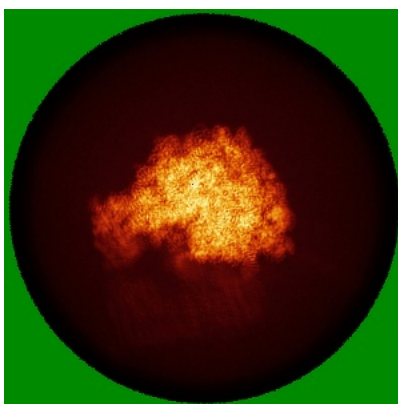


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

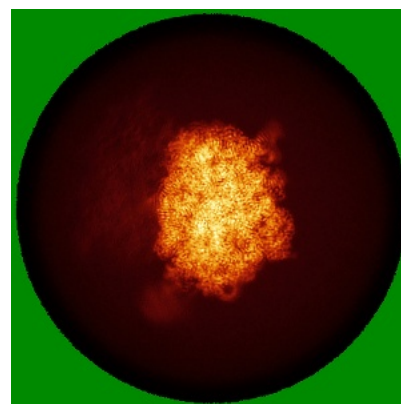
### 6.4.1 Primary map



X

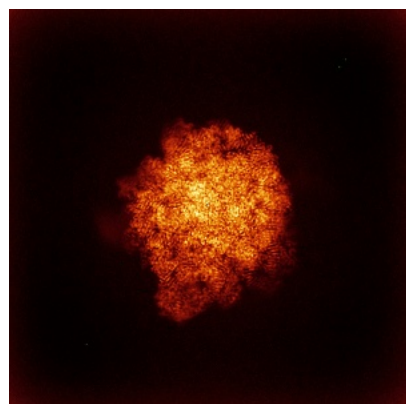


Y

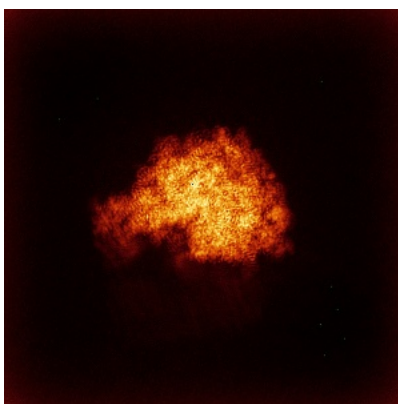


Z

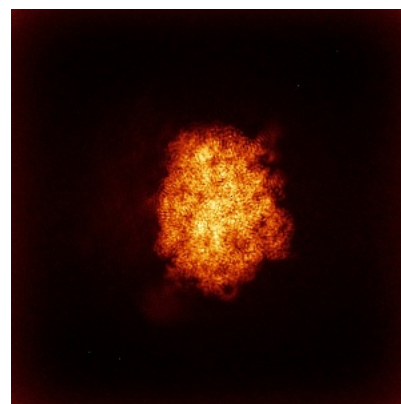
### 6.4.2 Raw map



X



Y

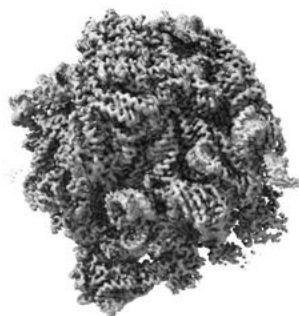


Z

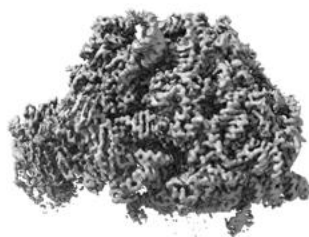
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

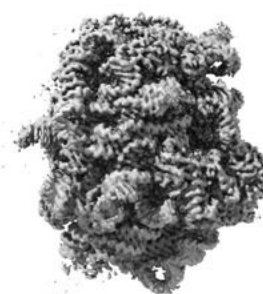
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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



X



Y



Z

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.

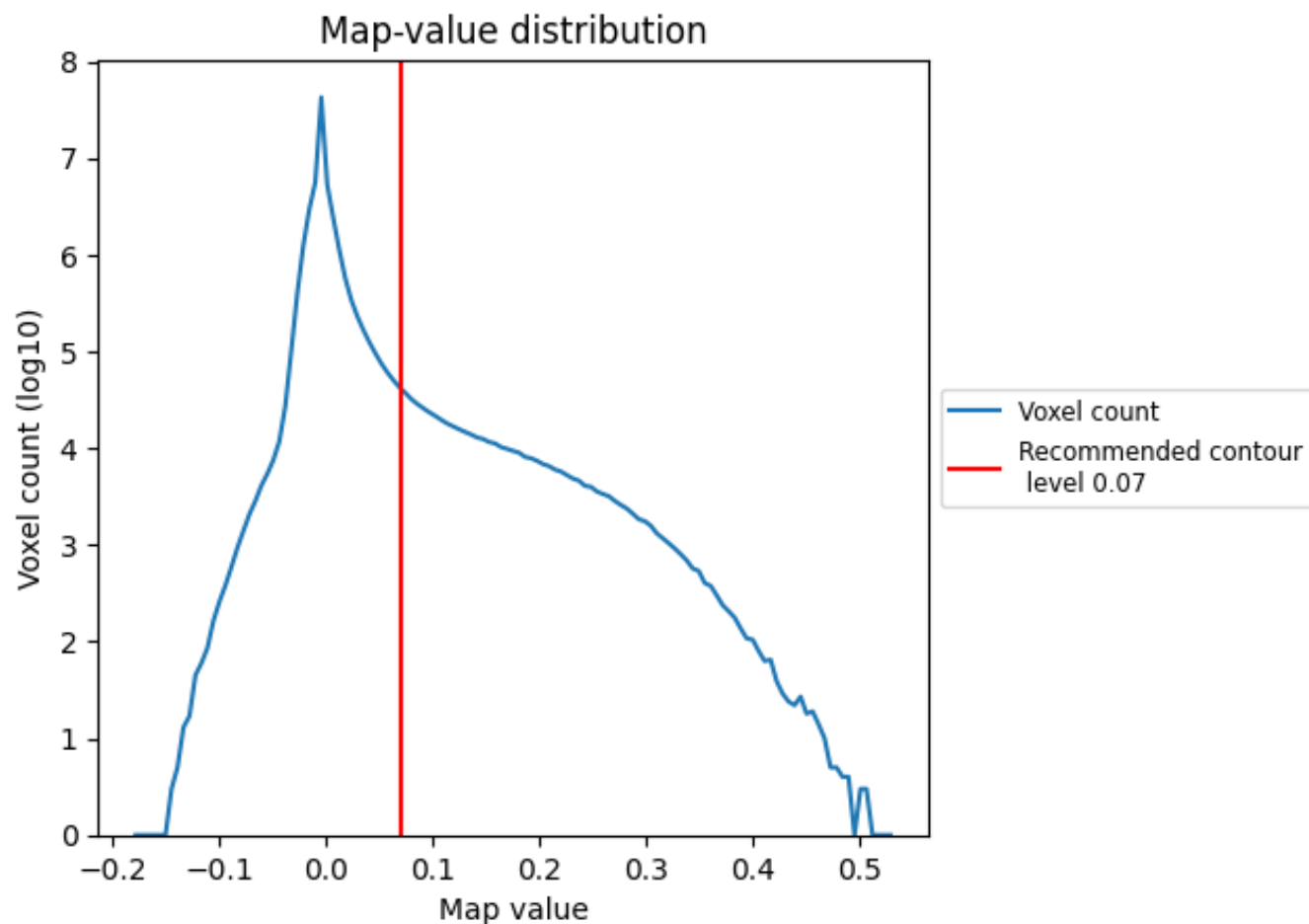
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

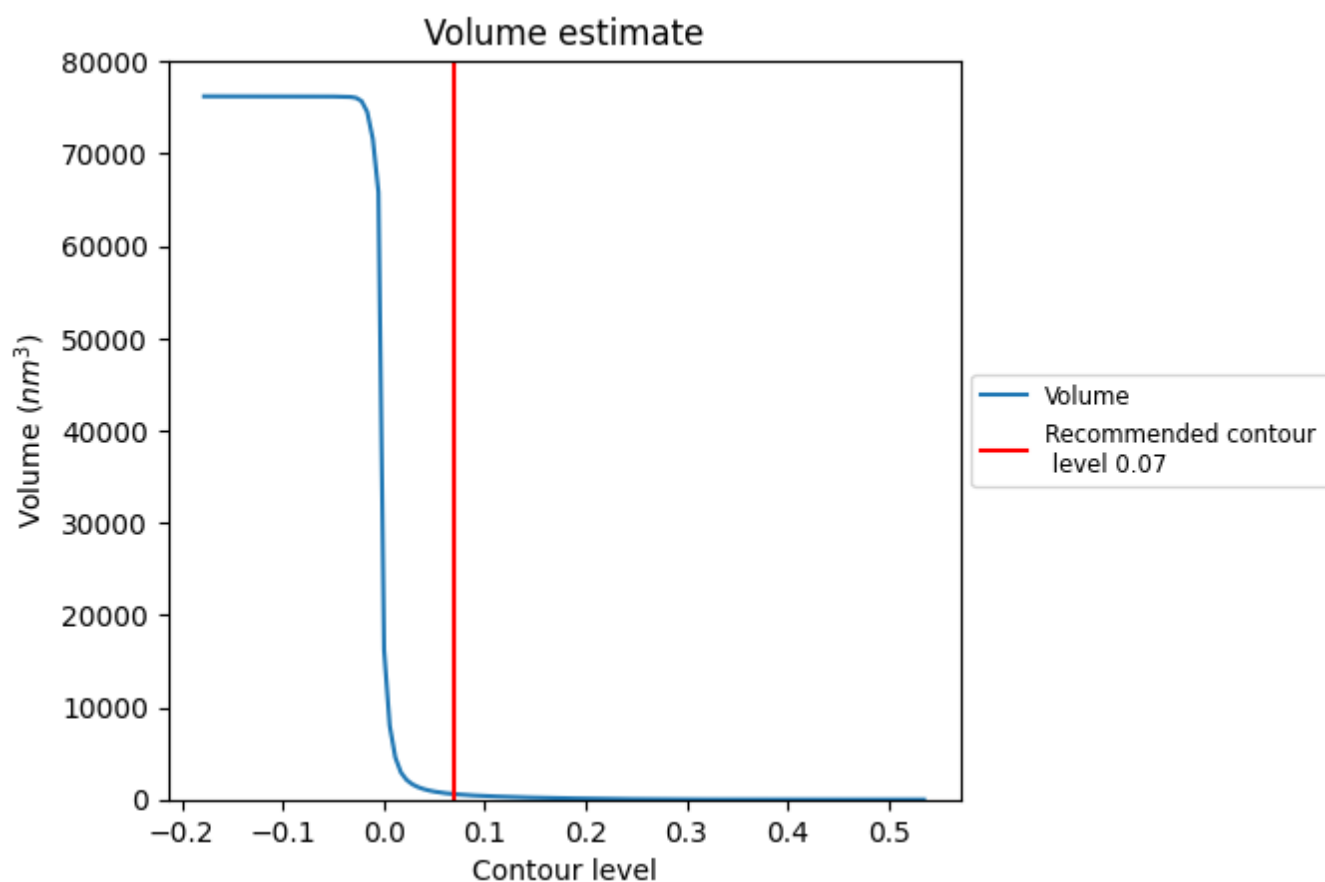
This section contains the results of statistical analysis of the map.

### 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.

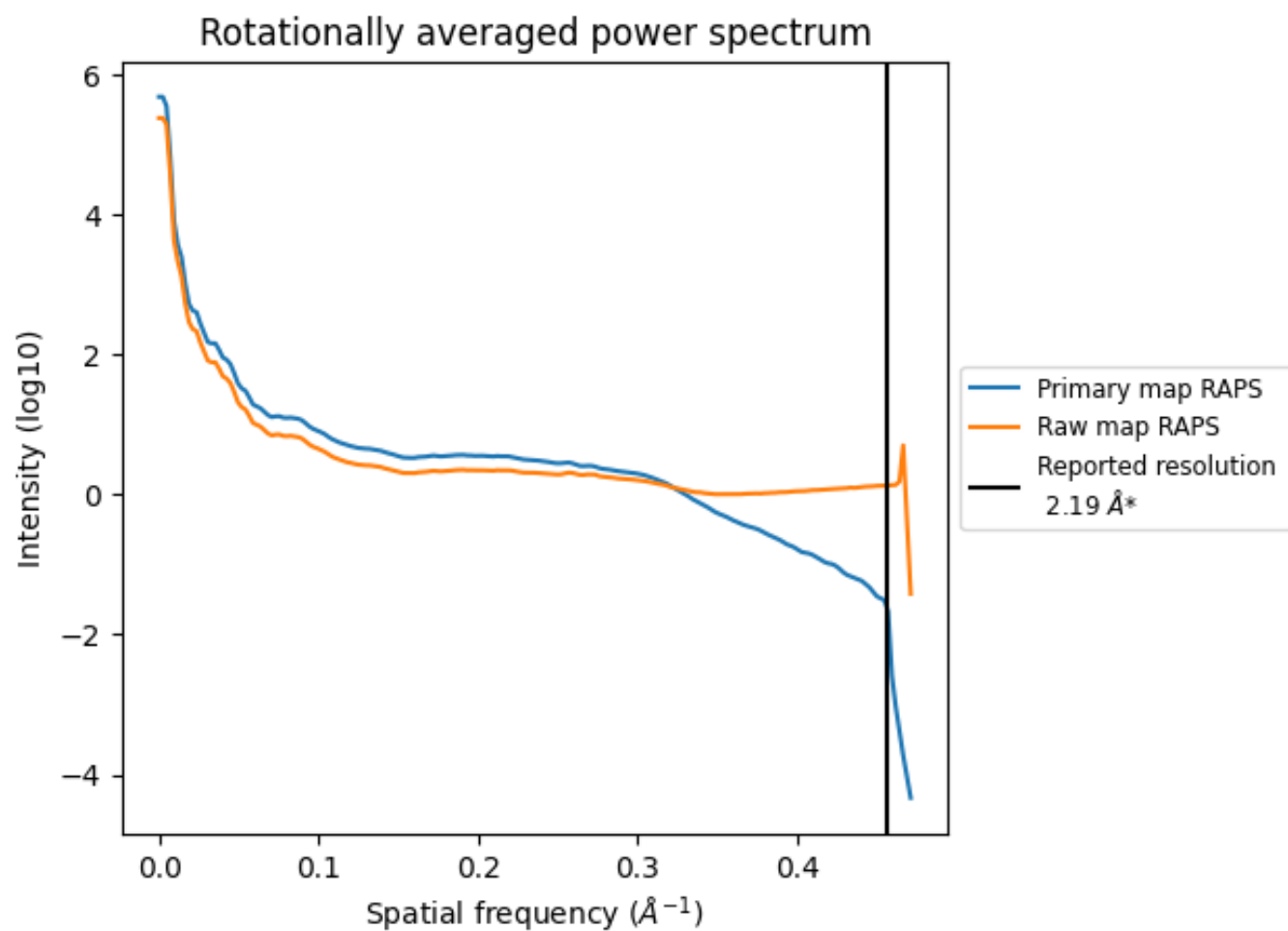
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 594 nm<sup>3</sup>; this corresponds to an approximate mass of 536 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 ⓘ

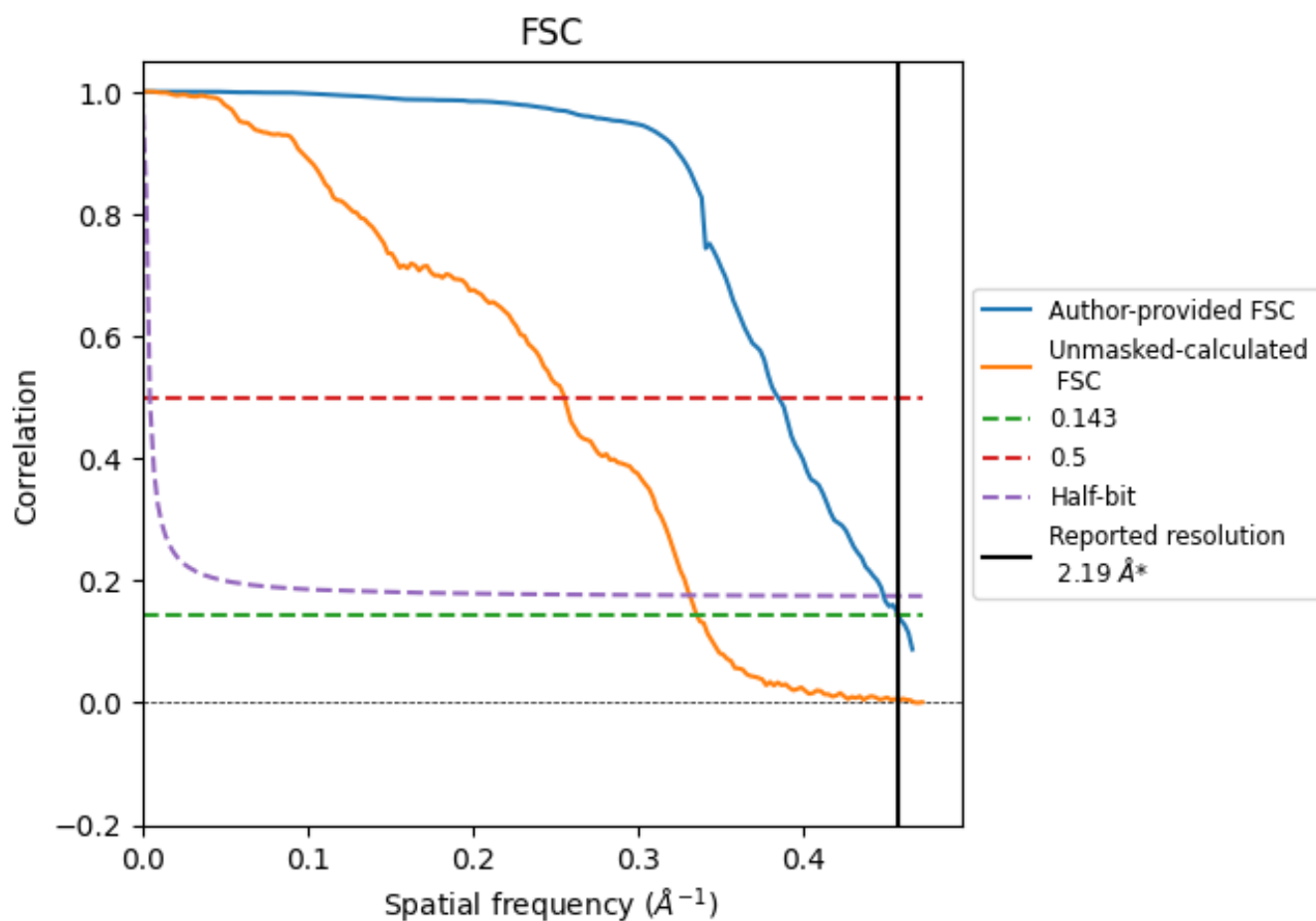


\*Reported resolution corresponds to spatial frequency of 0.457 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

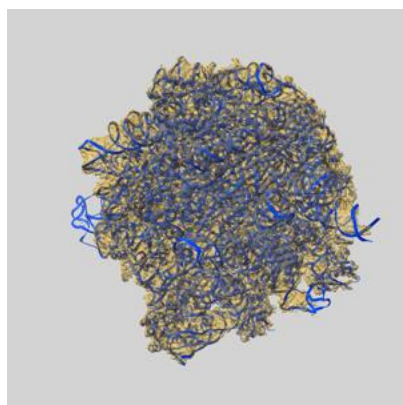
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.60	2.23
Unmasked-calculated*	2.98	3.92	3.02

\*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 2.98 differs from the reported value 2.19 by more than 10 %

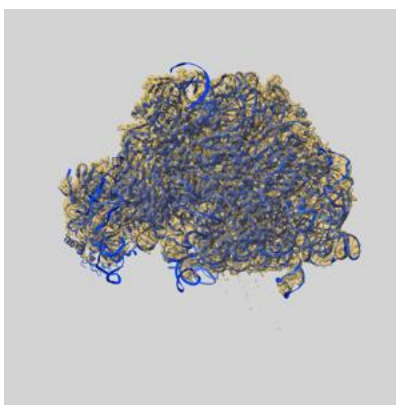
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56461 and PDB model 9TZ9. Per-residue inclusion information can be found in section 3 on page 11.

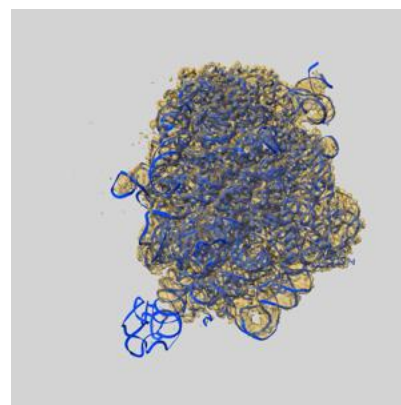
### 9.1 Map-model overlay [i](#)



X



Y

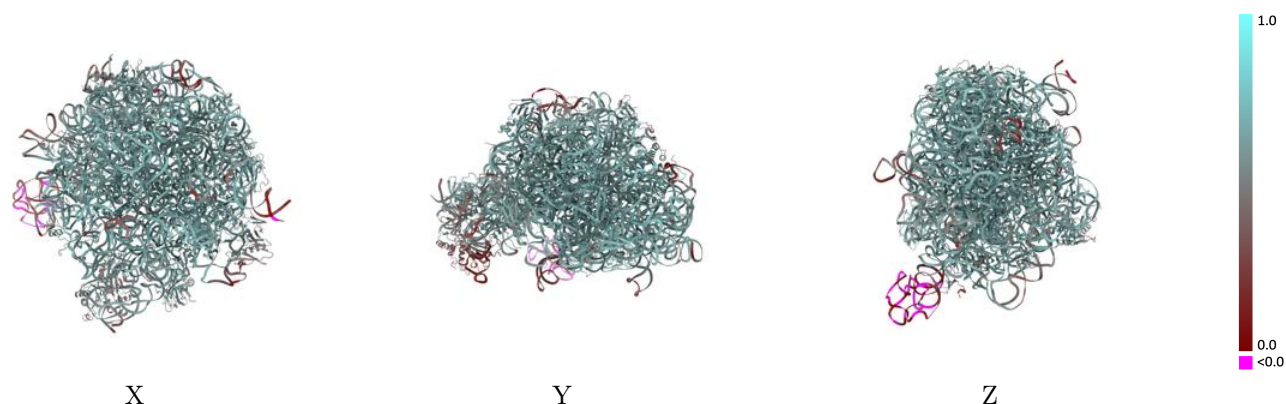


Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

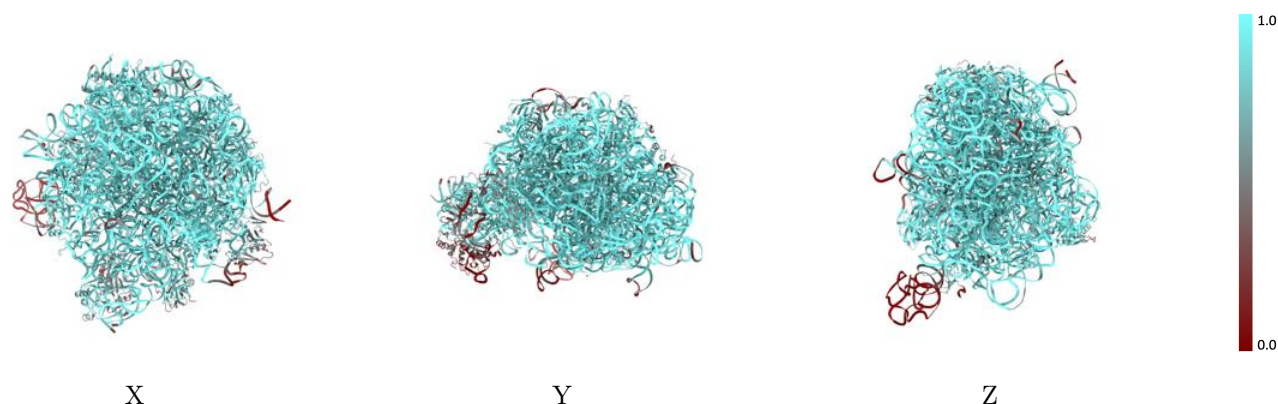


## 9.2 Q-score mapped to coordinate model [i](#)



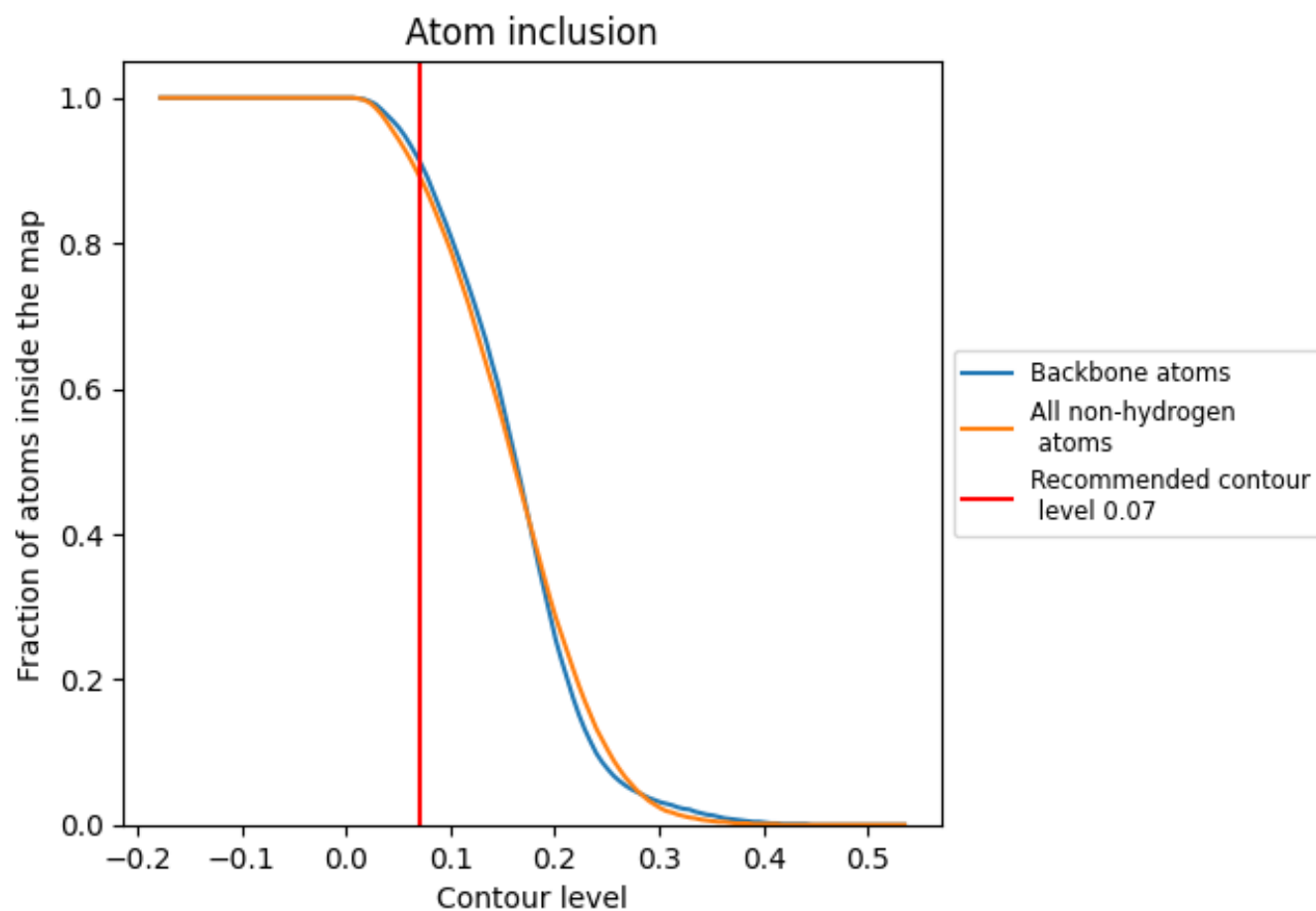
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.5950
0	 0.8600	 0.6000
1	 0.7850	 0.5420
2	 0.8120	 0.5430
3	 0.9040	 0.6270
7	 0.8750	 0.5970
8	 0.9040	 0.6220
9	 0.8640	 0.5970
Z	 0.9520	 0.6260
a	 0.9220	 0.6010
b	 0.9260	 0.5660
c	 0.8300	 0.5870
d	 0.9300	 0.6370
e	 0.9560	 0.6570
f	 0.2420	 0.3190
g	 0.5590	 0.4850
h	 0.8860	 0.6200
i	 0.9470	 0.6380
j	 0.9200	 0.6270
k	 0.8990	 0.6190
m	 0.9450	 0.6420
o	 0.9270	 0.6400
q	 0.5980	 0.4900
r	 0.8140	 0.5510
s	 0.8930	 0.6250
t	 0.9060	 0.6310
u	 0.5820	 0.5090
v	 0.9400	 0.6330
w	 0.8710	 0.6050
x	 0.8690	 0.6040
y	 0.9630	 0.6620
z	 0.9560	 0.6470

