



## wwPDB EM Validation Summary Report ⓘ

Mar 10, 2025 – 02:51 PM JST

PDB ID : 8ZTU  
EMDB ID : EMD-60473  
Title : 70S ribosome arrested by PepNL  
Authors : Ando, Y.; Kobo, A.; Nureki, O.; Taguchi, H.; Itoh, Y.; Chadani, Y.  
Deposited on : 2024-06-07  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

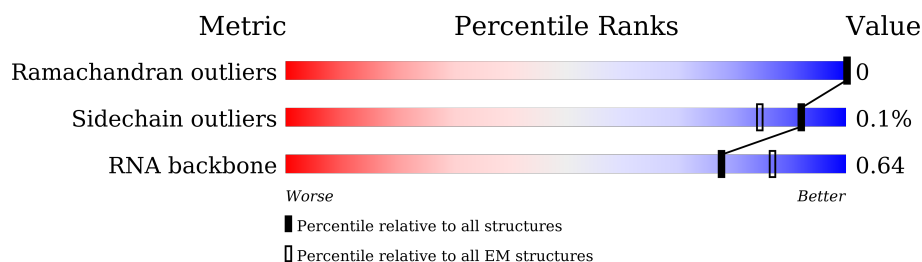
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.



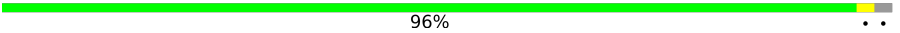
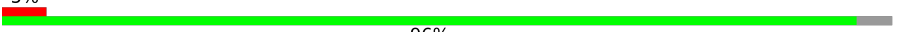

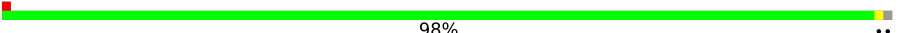
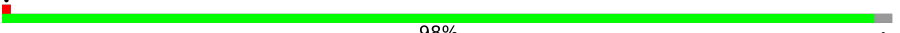
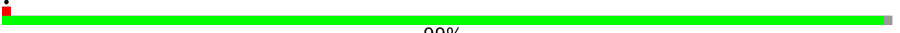










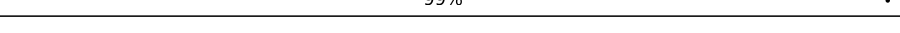
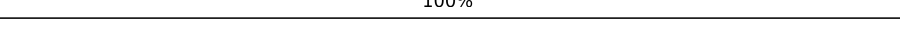
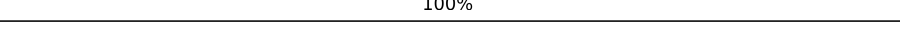
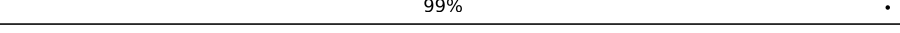
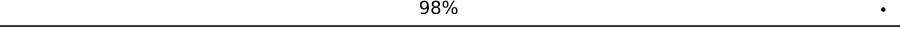

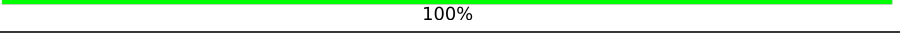
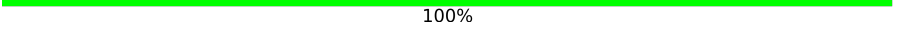
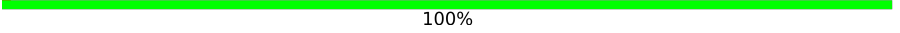
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	


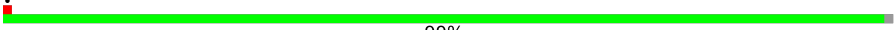
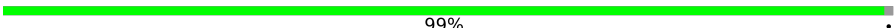
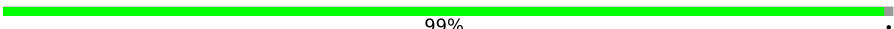
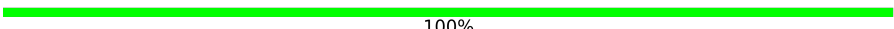
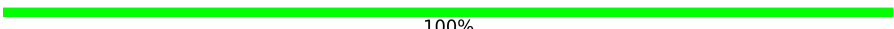

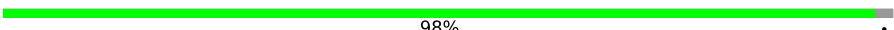
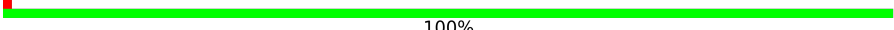

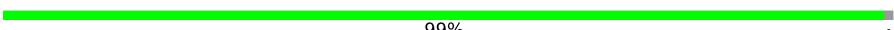
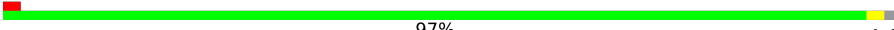
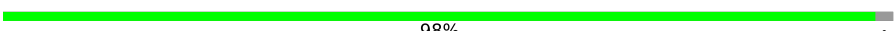


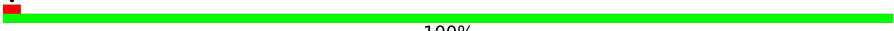
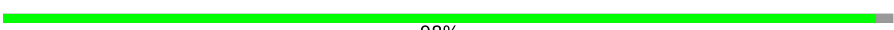
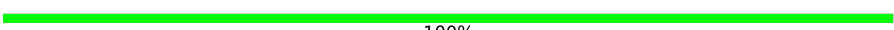

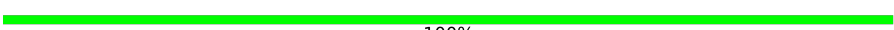



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Mol	Chain	Length	Quality of chain
9	I	130	 96%
10	J	103	 96%
11	K	129	 91% 9%
12	L	124	 98%
13	M	118	 98%
14	N	101	 99%
15	O	89	 99%
16	P	82	 99%
17	Q	84	 95% 5%
18	R	75	 88% 12%
19	S	92	 91% 9%
20	T	87	 99%
21	U	71	 99%
22	a	2904	 83% 12% 5%
23	b	120	 89% 10%
24	c	273	 99%
25	d	209	 100%
26	e	201	 100%
27	f	179	 99%
28	g	177	 98%
29	h	149	 45% 55%
30	i	142	 100%
31	j	123	 100%
32	k	144	 100%
33	l	136	 99%

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Mol	Chain	Length	Quality of chain
34	m	127	 93% 7%
35	n	117	 99%
36	o	115	 99%
37	p	118	 99%
38	q	103	 100%
39	r	110	 100%
40	s	100	 92% 7%
41	t	104	 98%
42	u	94	 100%
43	v	85	 92% 8%
44	w	78	 99%
45	x	63	 97%
46	y	59	 98%
47	z	57	 98%
48	0	55	 93% 7%
49	1	46	 100%
50	2	65	 98%
51	3	38	 100%
52	4	70	 67% 33%
53	W	14	 100%
54	X	9	 33% 89% 11%
55	Y	77	 79% 16% 5%
56	Z	3	 67% 33%

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 140242 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0
			32360	14439	5944	10470	1507		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	225	Total	C	N	O	S	0	0
			1758	1112	316	322	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	67	Total	C	N	O	S	0	0
			505	322	90	92	1		

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 50 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 53 is a protein called PepNL.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	W	14	Total	C	N	O	S	0	0
			108	70	17	20	1		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	X	9	Total	C	N	O	P	0	0
			194	87	37	61	9		

- Molecule 55 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Y	73	Total	C	N	O	P	0	0
			1563	695	281	514	73		

- Molecule 56 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Z	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

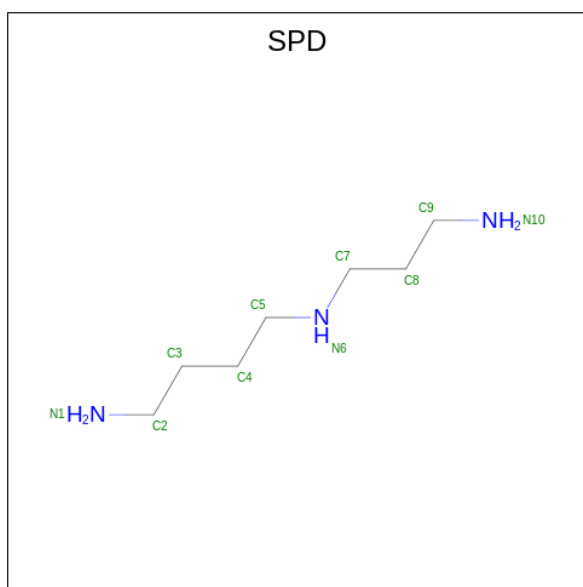
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	83	Total	Mg	0
			83	83	
57	a	209	Total	Mg	0
			209	209	
57	b	5	Total	Mg	0
			5	5	
57	p	2	Total	Mg	0
			2	2	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

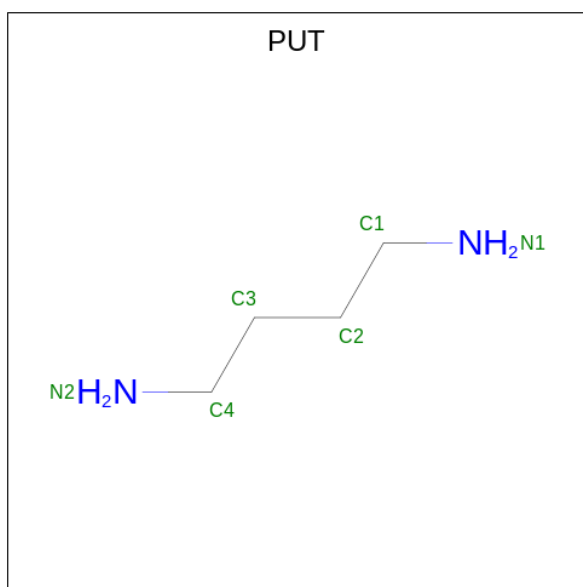
Mol	Chain	Residues	Atoms		AltConf
58	A	4	Total	K	0
			4	4	
58	D	1	Total	K	0
			1	1	
58	a	40	Total	K	0
			40	40	
58	c	2	Total	K	0
			2	2	

- Molecule 59 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
59	a	1	Total	C	N	0
			10	7	3	
59	a	1	Total	C	N	0
			10	7	3	
59	a	1	Total	C	N	0
			10	7	3	
59	a	1	Total	C	N	0
			10	7	3	
59	a	1	Total	C	N	0
			10	7	3	
59	a	1	Total	C	N	0
			10	7	3	

- Molecule 60 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
60	a	1	Total	C	N	0
			6	4	2	

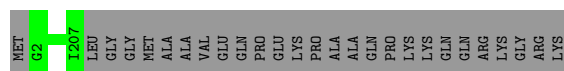
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	3	1	Total	Zn	0
			1	1	
61	4	1	Total	Zn	0
			1	1	





Chain C:  88% 12%



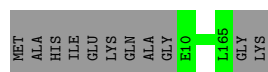
- Molecule 4: 30S ribosomal protein S4

Chain D:  100%



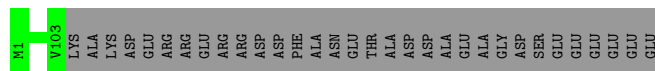
- Molecule 5: 30S ribosomal protein S5

Chain E:  93% 7%



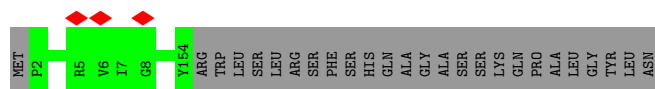
- Molecule 6: 30S ribosomal protein S6, fully modified isoform

Chain F:  76% 24%



- Molecule 7: 30S ribosomal protein S7

Chain G:  85% 15%



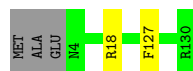
- Molecule 8: 30S ribosomal protein S8

Chain H:  99%

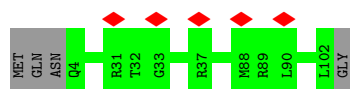


- Molecule 9: 30S ribosomal protein S9

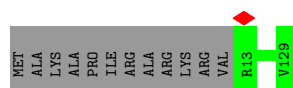
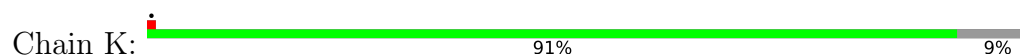
Chain I:  96%



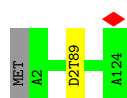
- Molecule 10: 30S ribosomal protein S10



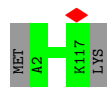
- Molecule 11: 30S ribosomal protein S11



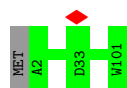
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

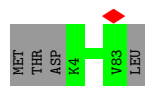


- Molecule 16: 30S ribosomal protein S16




- Molecule 17: 30S ribosomal protein S17

Chain Q:  95% 5%



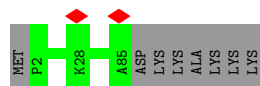
- Molecule 18: 30S ribosomal protein S18

Chain R:  88% 12%



- Molecule 19: 30S ribosomal protein S19

Chain S:  91% 9%



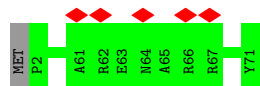
- Molecule 20: 30S ribosomal protein S20

Chain T:  99%




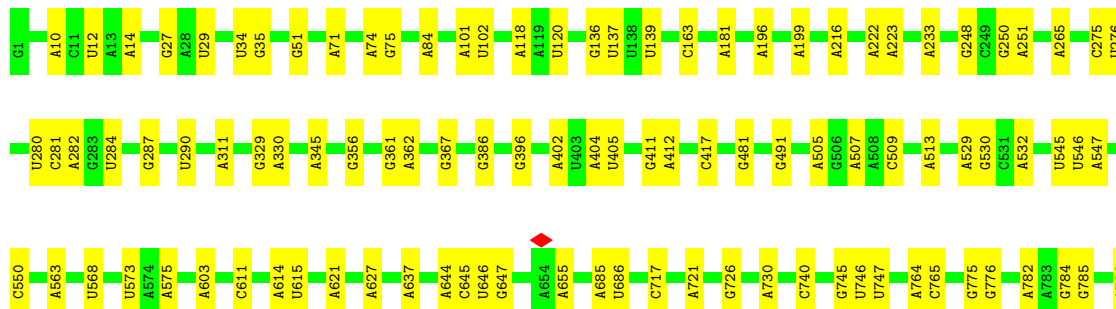
- Molecule 21: 30S ribosomal protein S21

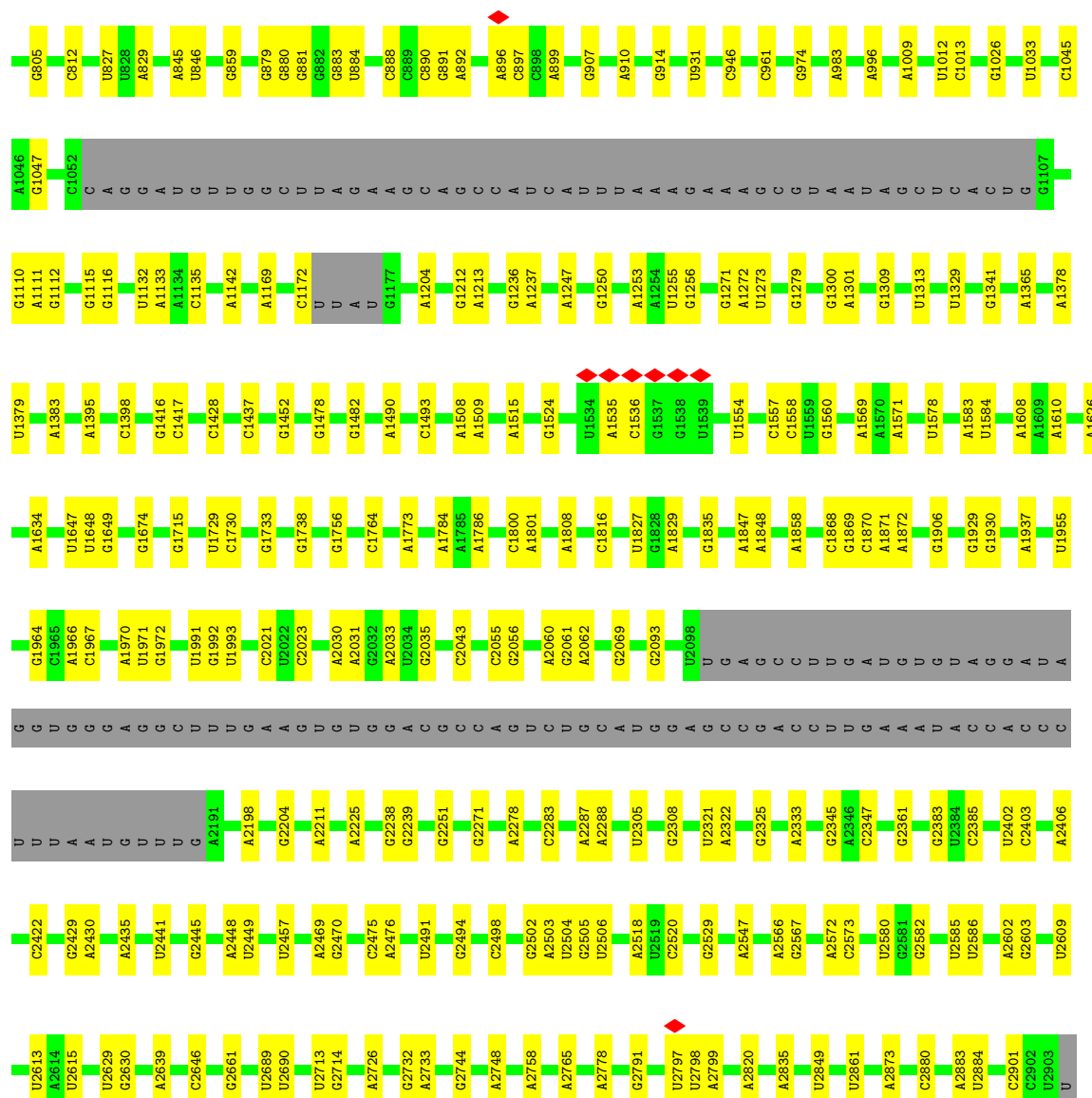
Chain U:  7% 99%



- Molecule 22: 23S rRNA

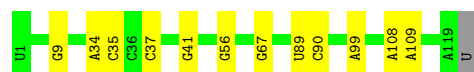
Chain a:  83% 12% 5%





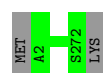
### • Molecule 23: 5S rRNA

Chain b: 89% 10%



### • Molecule 24: 50S ribosomal protein L2

Chain c: 99%



### • Molecule 25: 50S ribosomal protein L3

Chain d:  100%

There are no outlier residues recorded for this chain.

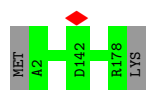
- Molecule 26: 50S ribosomal protein L4

Chain e:  100%



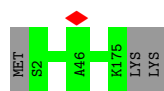
- Molecule 27: 50S ribosomal protein L5

Chain f:  99%



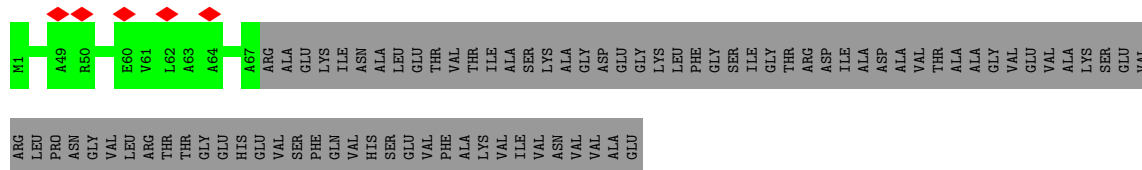
- Molecule 28: 50S ribosomal protein L6

Chain g:  98%



- Molecule 29: 50S ribosomal protein L9

Chain h:  45% 55%



- Molecule 30: 50S ribosomal protein L13

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L14

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L15

Chain k:  100%



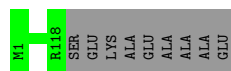
- Molecule 33: 50S ribosomal protein L16

Chain l:  99%



- Molecule 34: 50S ribosomal protein L17

Chain m:  93%



- Molecule 35: 50S ribosomal protein L18

Chain n:  99%



- Molecule 36: 50S ribosomal protein L19

Chain o:  99%



- Molecule 37: 50S ribosomal protein L20

Chain p:  99%



- Molecule 38: 50S ribosomal protein L21

Chain q:  100%

There are no outlier residues recorded for this chain.

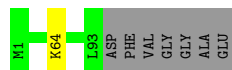
- Molecule 39: 50S ribosomal protein L22

Chain r:  100%

There are no outlier residues recorded for this chain.

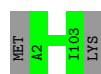
- Molecule 40: 50S ribosomal protein L23

Chain s:  92% • 7%



- Molecule 41: 50S ribosomal protein L24

Chain t:  98% .




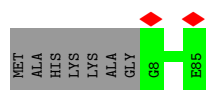
- Molecule 42: 50S ribosomal protein L25

Chain u:  100%



- Molecule 43: 50S ribosomal protein L27

Chain v:  92% 8%



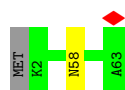
- Molecule 44: 50S ribosomal protein L28

Chain w:  99% .



- Molecule 45: 50S ribosomal protein L29

Chain x:  97% . .



- Molecule 46: 50S ribosomal protein L30

Chain y:  98% .



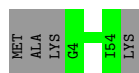
- Molecule 47: 50S ribosomal protein L32

Chain z:  98% .



- Molecule 48: 50S ribosomal protein L33

Chain 0:  93% 7%



- Molecule 49: 50S ribosomal protein L34

Chain 1:  100%



- Molecule 50: 50S ribosomal protein L35

Chain 2:  98% .



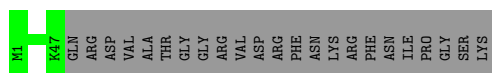
- Molecule 51: 50S ribosomal protein L36

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 50S ribosomal protein L31

Chain 4:  67% 33%



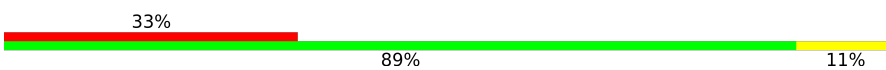
- Molecule 53: PepNL

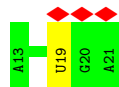
Chain W:  100%




There are no outlier residues recorded for this chain.

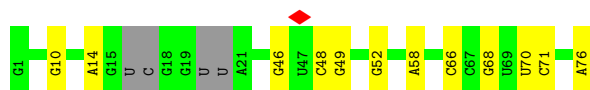
- Molecule 54: mRNA

Chain X: 



- Molecule 55: P-tRNA

Chain Y: 



- Molecule 56: E-tRNA

Chain Z: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87514	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.050	Depositor
Minimum map value	-0.688	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	358.56, 358.56, 358.56	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 4D4, ZN, IAS, MG, D2T, 2MG, 1MG, OMC, K, MS6, PUT, 2MA, SPD, H2U, MA6, 6MZ, PSU, 5MC, MEQ, 3TD, G7M, FME, 4OC, OMG, UR3, OMU

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	A	0.20	1/35954 (0.0%)	0.75	1/56077 (0.0%)
2	B	0.24	0/1789	0.45	0/2410
3	C	0.24	0/1651	0.50	0/2225
4	D	0.24	0/1665	0.49	0/2227
5	E	0.25	0/1165	0.50	0/1568
6	F	0.24	0/858	0.48	0/1160
7	G	0.25	0/1219	0.51	0/1635
8	H	0.24	0/989	0.48	0/1326
9	I	0.24	0/1034	0.55	0/1375
10	J	0.24	0/805	0.55	0/1089
11	K	0.25	0/884	0.53	0/1191
12	L	0.24	0/960	0.56	0/1286
13	M	0.23	0/909	0.53	0/1215
14	N	0.23	0/817	0.52	0/1088
15	O	0.23	0/722	0.50	0/964
16	P	0.24	0/653	0.54	0/877
17	Q	0.24	0/657	0.51	0/881
18	R	0.25	0/553	0.51	0/742
19	S	0.24	0/685	0.49	0/922
20	T	0.24	0/676	0.44	0/895
21	U	0.24	0/597	0.56	0/792
22	a	0.21	0/65651	0.75	5/102413 (0.0%)
23	b	0.18	0/2850	0.75	0/4444
24	c	0.25	0/2121	0.54	0/2852
25	d	0.24	0/1576	0.51	0/2119
26	e	0.24	0/1571	0.48	0/2113
27	f	0.24	0/1434	0.48	0/1926
28	g	0.24	0/1324	0.49	0/1794
29	h	0.26	0/510	0.47	0/687
30	i	0.24	0/1152	0.49	0/1551
31	j	0.24	0/955	0.54	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	k	0.24	0/1062	0.54	0/1413
33	l	0.25	0/1073	0.52	0/1433
34	m	0.24	0/958	0.56	0/1281
35	n	0.24	0/902	0.52	0/1209
36	o	0.24	0/929	0.51	0/1242
37	p	0.25	0/960	0.51	0/1278
38	q	0.25	0/829	0.52	0/1107
39	r	0.23	0/864	0.52	0/1156
40	s	0.23	0/744	0.48	0/994
41	t	0.24	0/787	0.49	0/1051
42	u	0.24	0/766	0.47	0/1025
43	v	0.25	0/599	0.52	0/792
44	w	0.23	0/635	0.54	0/848
45	x	0.23	0/502	0.45	0/667
46	y	0.23	0/453	0.51	0/605
47	z	0.24	0/450	0.55	0/599
48	0	0.24	0/424	0.48	0/565
49	1	0.24	0/380	0.62	0/498
50	2	0.23	0/513	0.52	0/676
51	3	0.23	0/303	0.54	0/397
52	4	0.23	0/371	0.43	0/496
53	W	0.28	0/99	0.56	0/133
54	X	0.15	0/217	0.68	0/336
55	Y	0.24	0/1744	0.82	0/2714
56	Z	0.15	0/46	0.63	0/69
All	All	0.22	1/150996 (0.0%)	0.70	6/225707 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	A	OP3-P	-10.64	1.48	1.61

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	1313	U	C2-N1-C1'	7.17	126.30	117.70
22	a	2321	U	C2-N1-C1'	6.01	124.91	117.70
22	a	1313	U	N1-C2-O2	5.73	126.81	122.80
22	a	1313	U	N3-C2-O2	-5.30	118.49	122.20
22	a	2321	U	N1-C2-O2	5.08	126.36	122.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 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	
2	B	223/241 (92%)	220 (99%)	3 (1%)	0	100	100
3	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
4	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	E	154/167 (92%)	153 (99%)	1 (1%)	0	100	100
6	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
7	G	151/179 (84%)	149 (99%)	2 (1%)	0	100	100
8	H	127/130 (98%)	127 (100%)	0	0	100	100
9	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	J	97/103 (94%)	96 (99%)	1 (1%)	0	100	100
11	K	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
12	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	M	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
14	N	98/101 (97%)	98 (100%)	0	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	R	64/75 (85%)	64 (100%)	0	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
25	d	206/209 (99%)	203 (98%)	3 (2%)	0	100	100
26	e	199/201 (99%)	199 (100%)	0	0	100	100
27	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
28	g	172/177 (97%)	168 (98%)	4 (2%)	0	100	100
29	h	65/149 (44%)	61 (94%)	4 (6%)	0	100	100
30	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
31	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
32	k	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
33	l	132/136 (97%)	132 (100%)	0	0	100	100
34	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
35	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
36	o	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
37	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
38	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	s	91/100 (91%)	91 (100%)	0	0	100	100
41	t	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
42	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	v	76/85 (89%)	76 (100%)	0	0	100	100
44	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	x	60/63 (95%)	60 (100%)	0	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
51	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
52	4	45/70 (64%)	45 (100%)	0	0	100	100
53	W	12/14 (86%)	11 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5510/5927 (93%)	5421 (98%)	89 (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	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	103 (98%)	2 (2%)	52	81
10	J	87/90 (97%)	87 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	94/96 (98%)	94 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	74/78 (95%)	74 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	135/138 (98%)	135 (100%)	0	100	100
29	h	50/114 (44%)	50 (100%)	0	100	100
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	79 (99%)	1 (1%)	65	88
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	59/63 (94%)	59 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	53 (98%)	1 (2%)	52	81
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	43/62 (69%)	43 (100%)	0	100	100
53	W	10/10 (100%)	10 (100%)	0	100	100
All	All	4590/4835 (95%)	4586 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
9	I	18	ARG
9	I	127	PHE
40	s	64	LYS
45	x	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
24	c	86	ASN
28	g	115	HIS
24	c	163	GLN
26	e	136	GLN
30	i	136	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1500/1542 (97%)	194 (12%)	1 (0%)
22	a	2745/2904 (94%)	341 (12%)	0
23	b	118/120 (98%)	12 (10%)	0
54	X	8/9 (88%)	1 (12%)	0
55	Y	70/77 (90%)	12 (17%)	0
56	Z	1/3 (33%)	0	0
All	All	4442/4655 (95%)	560 (12%)	1 (0%)

5 of 560 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	7	A
1	A	9	G
1	A	22	G
1	A	31	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	264	C

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

40 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$
22	PSU	a	1917	22	18,21,22	0.50	0	22,30,33	0.56	0
1	G7M	A	527	1	20,26,27	0.56	0	17,39,42	0.43	0
22	5MC	a	1962	58,22	18,22,23	0.30	0	26,32,35	0.46	0
22	PSU	a	2605	22	18,21,22	0.52	0	22,30,33	0.62	0
22	OMG	a	2251	58,55,22	18,26,27	0.93	2 (11%)	19,38,41	0.61	0
25	MEQ	d	150	25	8,9,10	0.87	0	5,10,12	0.46	0
11	IAS	K	119	11	6,7,8	0.74	0	6,8,10	0.96	0
1	5MC	A	1407	1	18,22,23	0.31	0	26,32,35	0.45	0
22	OMU	a	2552	22	19,22,23	0.28	0	26,31,34	0.43	0
1	2MG	A	1516	1	18,26,27	0.91	1 (5%)	16,38,41	0.71	0
22	PSU	a	746	57,22	18,21,22	0.58	1 (5%)	22,30,33	0.67	1 (4%)
22	6MZ	a	1618	22	18,25,26	0.74	0	16,36,39	0.80	0
22	2MG	a	1835	22	18,26,27	0.92	1 (5%)	16,38,41	0.67	0
22	2MG	a	2445	22	18,26,27	0.96	2 (11%)	16,38,41	0.67	0
22	PSU	a	2580	22	18,21,22	0.58	1 (5%)	22,30,33	0.67	1 (4%)
1	5MC	A	967	1	18,22,23	0.29	0	26,32,35	0.44	0
53	FME	W	1	53	8,9,10	0.50	0	7,9,11	0.47	0
22	5MU	a	747	22	19,22,23	0.28	0	28,32,35	0.33	0
22	H2U	a	2449	22	18,21,22	0.46	0	21,30,33	1.03	1 (4%)
22	2MA	a	2503	57,22	19,25,26	1.02	2 (10%)	21,37,40	3.05	5 (23%)
1	2MG	A	966	1	18,26,27	0.92	1 (5%)	16,38,41	0.77	0
1	MA6	A	1518	1	18,26,27	0.74	0	19,38,41	0.69	0
12	D2T	L	89	12	7,9,10	0.88	0	6,11,13	1.70	2 (33%)
22	G7M	a	2069	58,22	20,26,27	0.55	0	17,39,42	0.46	0
1	2MG	A	1207	1	18,26,27	0.91	1 (5%)	16,38,41	0.69	0
1	MA6	A	1519	1	18,26,27	0.74	0	19,38,41	0.65	0
1	PSU	A	516	1	18,21,22	0.50	0	22,30,33	0.61	1 (4%)
22	6MZ	a	2030	22	18,25,26	0.73	0	16,36,39	0.78	1 (6%)
22	PSU	a	2457	22	18,21,22	0.50	0	22,30,33	0.60	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	3TD	a	1915	22	18,22,23	0.47	0	22,32,35	0.59	0
1	4OC	A	1402	1	20,23,24	0.32	0	26,32,35	0.46	0
22	OMC	a	2498	57,22	19,22,23	0.32	0	26,31,34	0.39	0
22	PSU	a	2504	22	18,21,22	0.49	0	22,30,33	0.59	0
22	5MU	a	1939	58,22	19,22,23	0.28	0	28,32,35	0.38	0
22	PSU	a	2604	22	18,21,22	0.54	0	22,30,33	0.58	0
1	UR3	A	1498	1	19,22,23	0.30	0	26,32,35	0.37	0
33	4D4	l	81	33	9,11,12	0.84	0	8,13,15	1.93	3 (37%)
22	PSU	a	955	58,22	18,21,22	0.48	0	22,30,33	0.58	0
22	1MG	a	745	22	18,26,27	0.86	2 (11%)	19,39,42	0.46	0
22	PSU	a	1911	22	18,21,22	0.47	0	22,30,33	0.58	0

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
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3
22	5MC	a	1962	58,22	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	58,55,22	-	1/5/27/28	0/3/3/3
25	MEQ	d	150	25	-	5/8/9/11	-
11	IAS	K	119	11	-	2/7/7/8	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
22	PSU	a	746	57,22	-	2/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/5/27/28	0/3/3/3
22	2MG	a	1835	22	-	0/5/27/28	0/3/3/3
22	2MG	a	2445	22	-	0/5/27/28	0/3/3/3
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
53	FME	W	1	53	-	3/7/9/11	-
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	1/7/38/39	0/2/2/2
22	2MA	a	2503	57,22	-	1/3/25/26	0/3/3/3
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	1/7/29/30	0/3/3/3
12	D2T	L	89	12	-	2/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	G7M	a	2069	58,22	-	1/3/25/26	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/5/27/28	0/3/3/3
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
22	OMC	a	2498	57,22	-	0/9/27/28	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
22	5MU	a	1939	58,22	-	0/7/25/26	0/2/2/2
22	PSU	a	2604	22	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
33	4D4	l	81	33	-	5/11/12/14	-
22	PSU	a	955	58,22	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/3/25/26	0/3/3/3
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2445	2MG	C5-C6	-2.41	1.42	1.47
22	a	1835	2MG	C5-C6	-2.35	1.42	1.47
22	a	745	1MG	C5-C4	-2.33	1.37	1.43
1	A	966	2MG	C5-C6	-2.33	1.42	1.47
22	a	2251	OMG	C5-C6	-2.24	1.42	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2503	2MA	C5-C6-N1	-12.28	112.94	121.01
33	l	81	4D4	NE-CZ-NH2	3.90	127.56	120.70
22	a	2503	2MA	C2-N1-C6	3.80	124.00	118.08
22	a	2503	2MA	C2-N3-C4	-3.75	112.47	115.52
22	a	2449	H2U	C5-C4-N3	-3.12	113.15	116.65

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	C5-C6-N6-C10
12	L	89	D2T	CG-CB-SB-CB1
33	l	81	4D4	N-CA-CB-CG
33	l	81	4D4	NH2-CZ-NE-CD
22	a	2251	OMG	C1'-C2'-O2'-CM2

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 357 ligands modelled in this entry, 349 are monoatomic - leaving 8 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	$\# Z  > 2$
59	SPD	a	6199	-	9,9,9	0.19	0	8,8,8	0.78	0
59	SPD	a	6195	-	9,9,9	0.27	0	8,8,8	0.85	0
59	SPD	a	6193	-	9,9,9	0.30	0	8,8,8	0.89	0
60	PUT	a	6200	-	5,5,5	0.12	0	4,4,4	0.16	0
59	SPD	a	6196	-	9,9,9	0.29	0	8,8,8	0.82	0
59	SPD	a	6198	-	9,9,9	0.23	0	8,8,8	0.87	0
59	SPD	a	6194	-	9,9,9	0.25	0	8,8,8	0.88	0
59	SPD	a	6197	-	9,9,9	0.22	0	8,8,8	0.89	0

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
59	SPD	a	6199	-	-	0/7/7/7	-
59	SPD	a	6195	-	-	0/7/7/7	-
59	SPD	a	6193	-	-	0/7/7/7	-
60	PUT	a	6200	-	-	0/3/3/3	-
59	SPD	a	6196	-	-	1/7/7/7	-
59	SPD	a	6198	-	-	0/7/7/7	-
59	SPD	a	6194	-	-	0/7/7/7	-
59	SPD	a	6197	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	a	6197	SPD	C3-C4-C5-N6
59	a	6197	SPD	N6-C7-C8-C9
59	a	6197	SPD	C4-C5-N6-C7
59	a	6196	SPD	N6-C7-C8-C9

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.

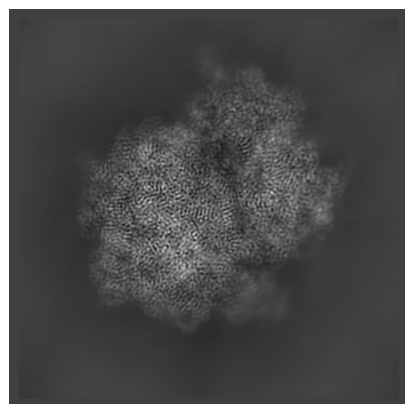
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60473. These allow visual inspection of the internal detail of the map and identification of artifacts.

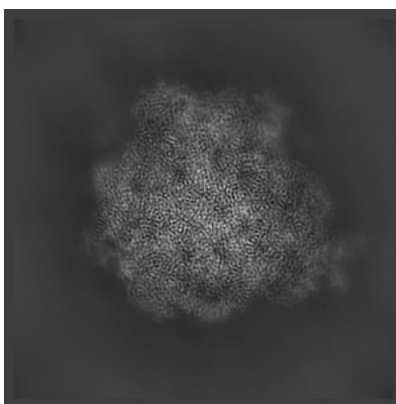
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

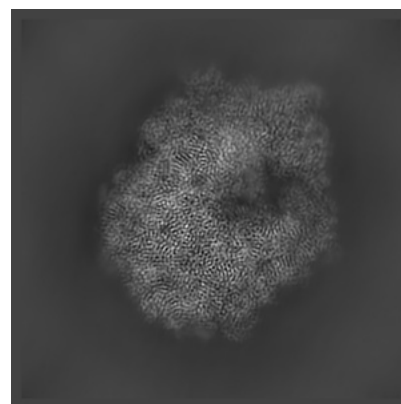
#### 6.1.1 Primary map



X

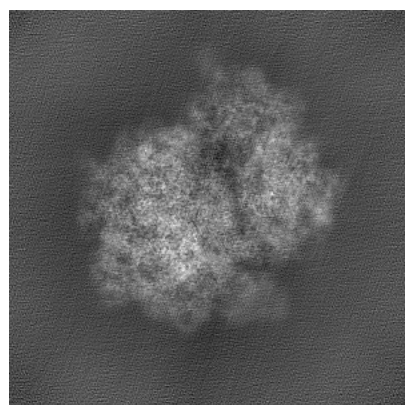


Y

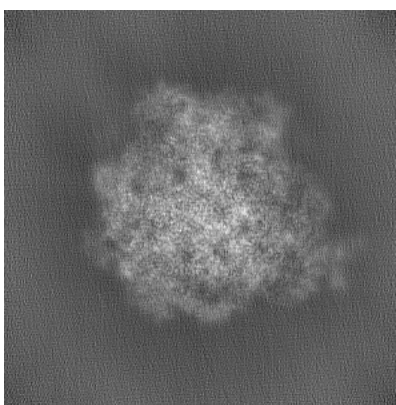


Z

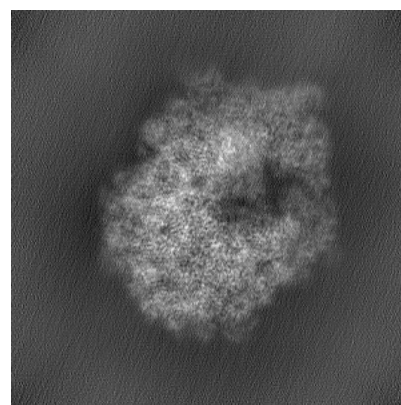
#### 6.1.2 Raw map



X



Y



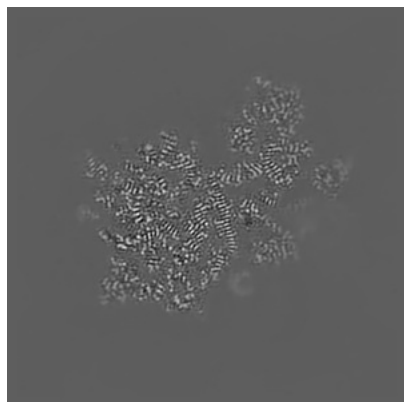
Z

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

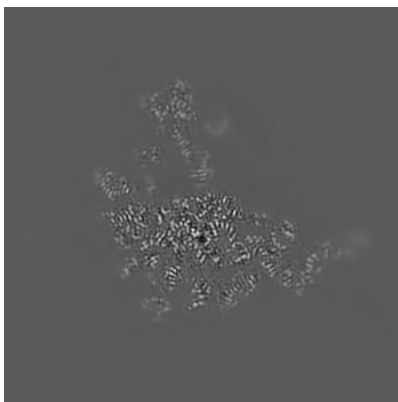


## 6.2 Central slices [i](#)

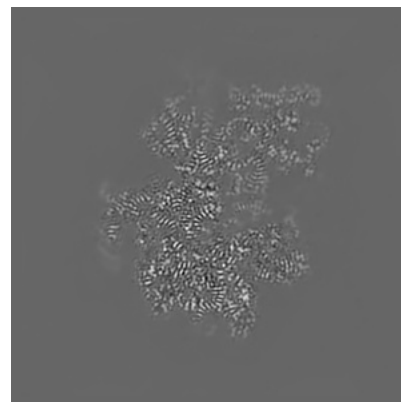
### 6.2.1 Primary map



X Index: 216

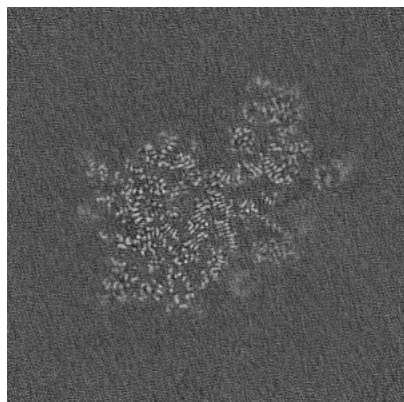


Y Index: 216

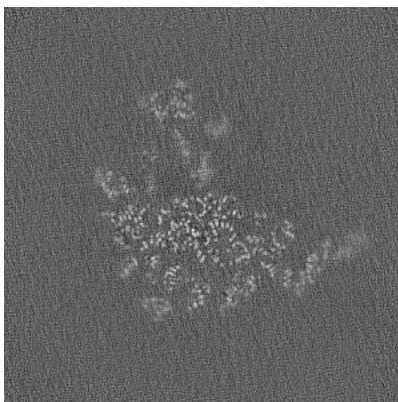


Z Index: 216

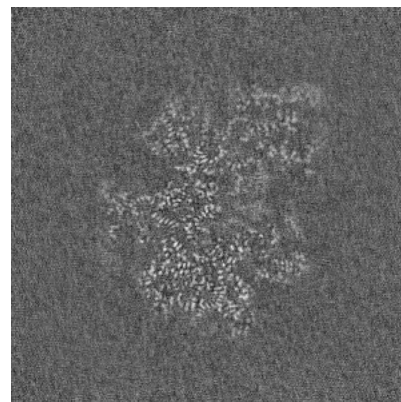
### 6.2.2 Raw map



X Index: 216



Y Index: 216



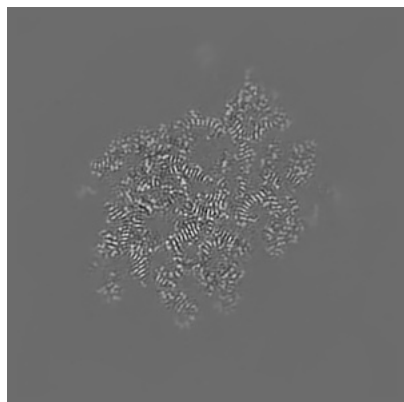
Z Index: 216

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

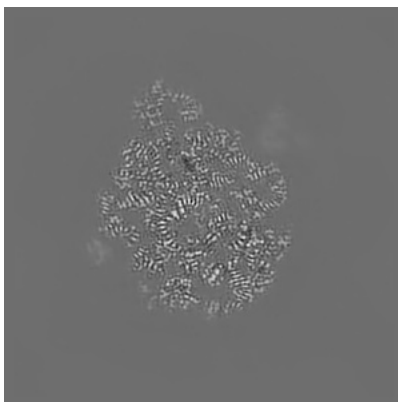


## 6.3 Largest variance slices [i](#)

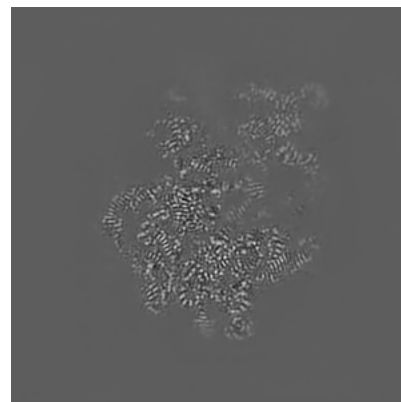
### 6.3.1 Primary map



X Index: 186

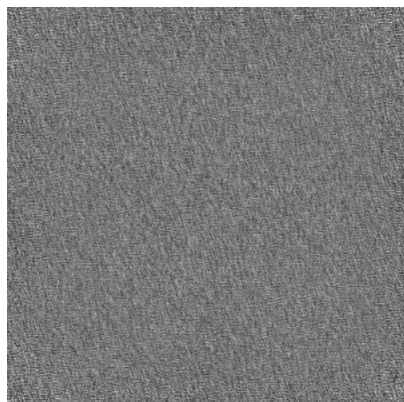


Y Index: 178

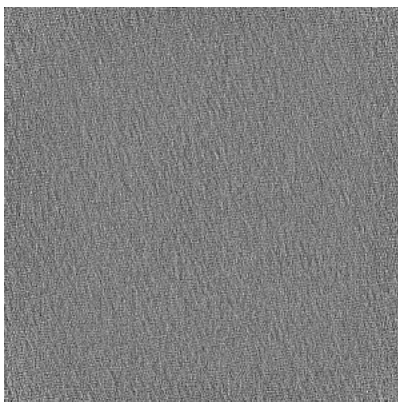


Z Index: 208

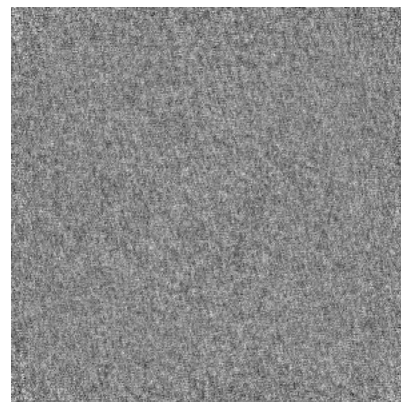
### 6.3.2 Raw map



X Index: 0



Y Index: 0

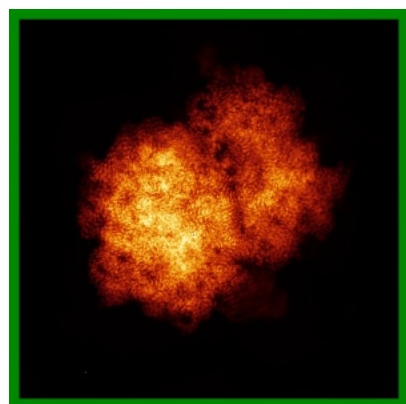


Z Index: 0

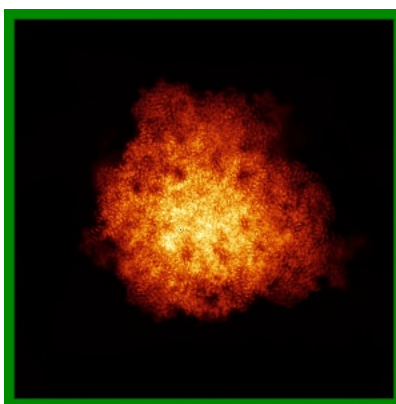
The images above show the largest variance slices of the map in three orthogonal directions.

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

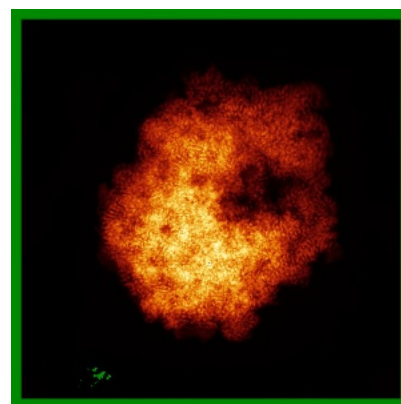
### 6.4.1 Primary map



X

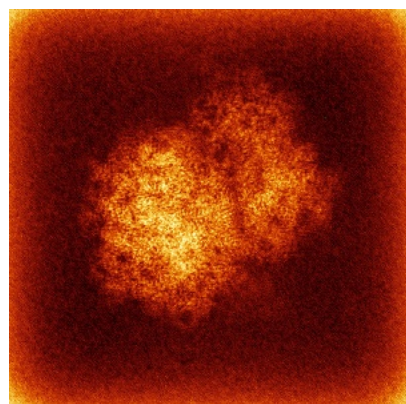


Y

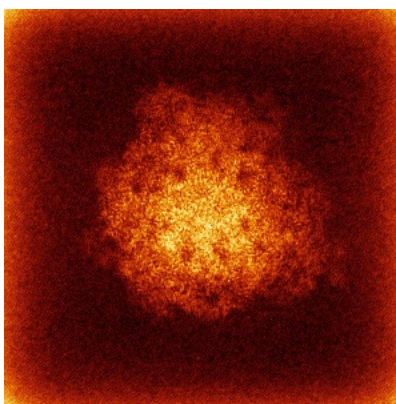


Z

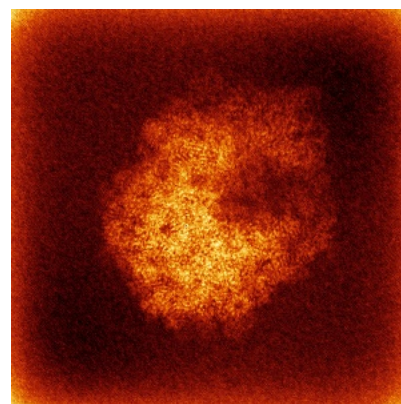
### 6.4.2 Raw map



X



Y

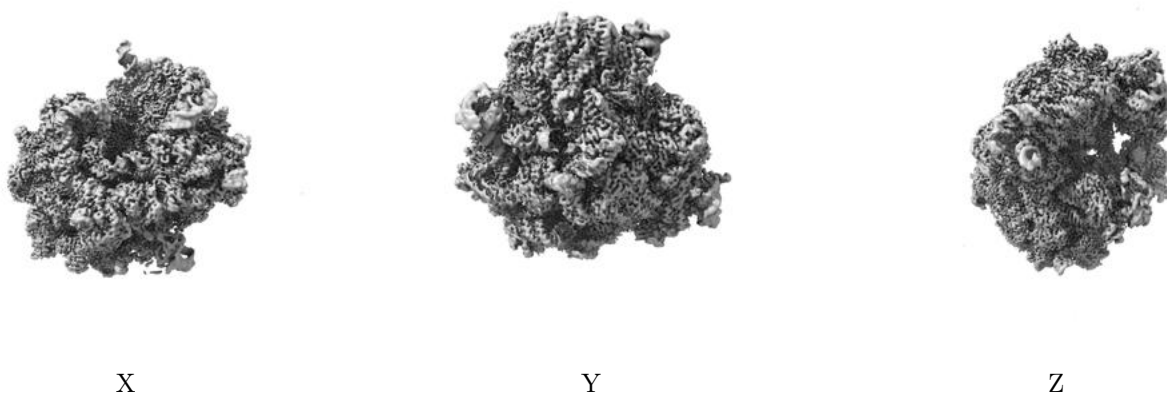


Z

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

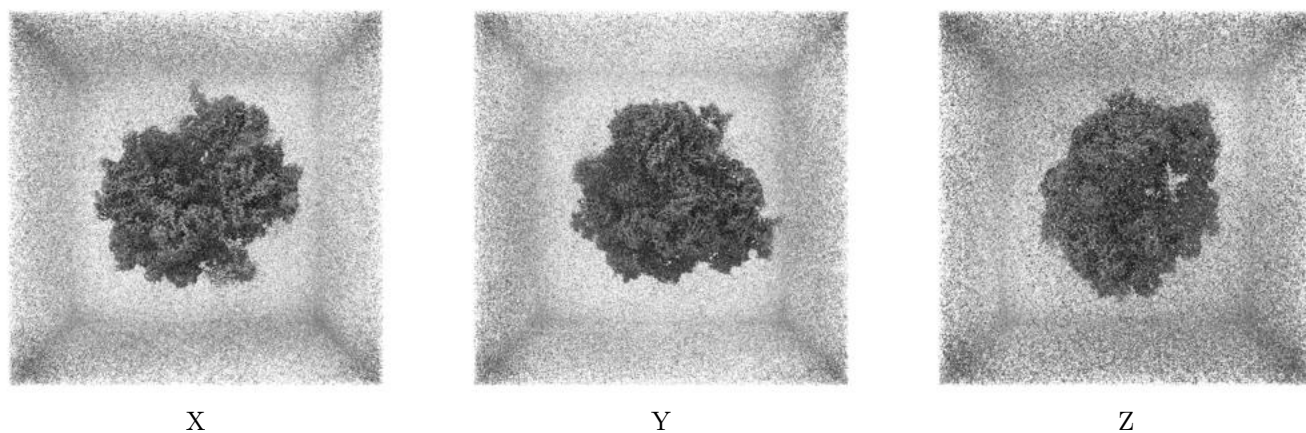
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

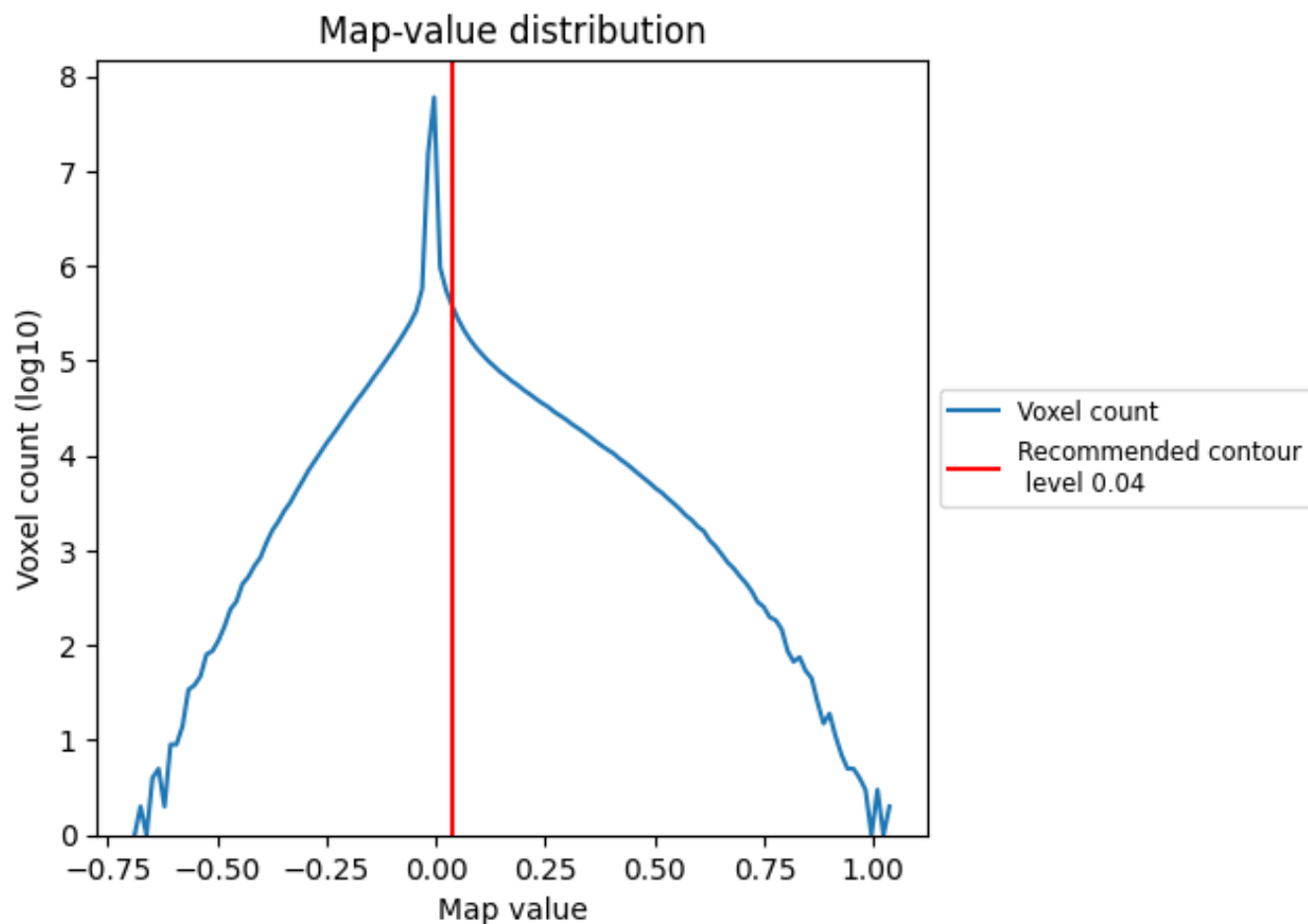
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

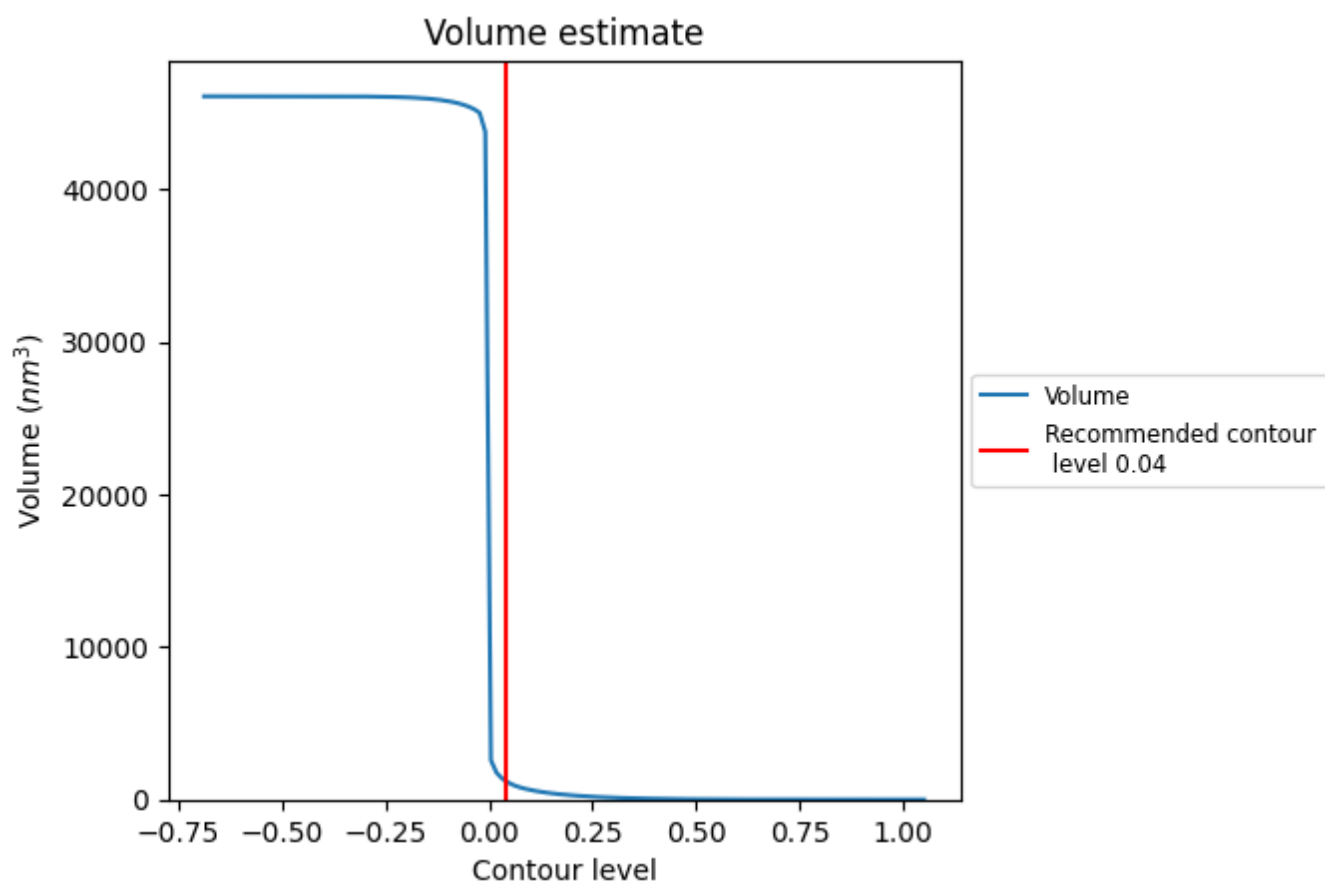
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

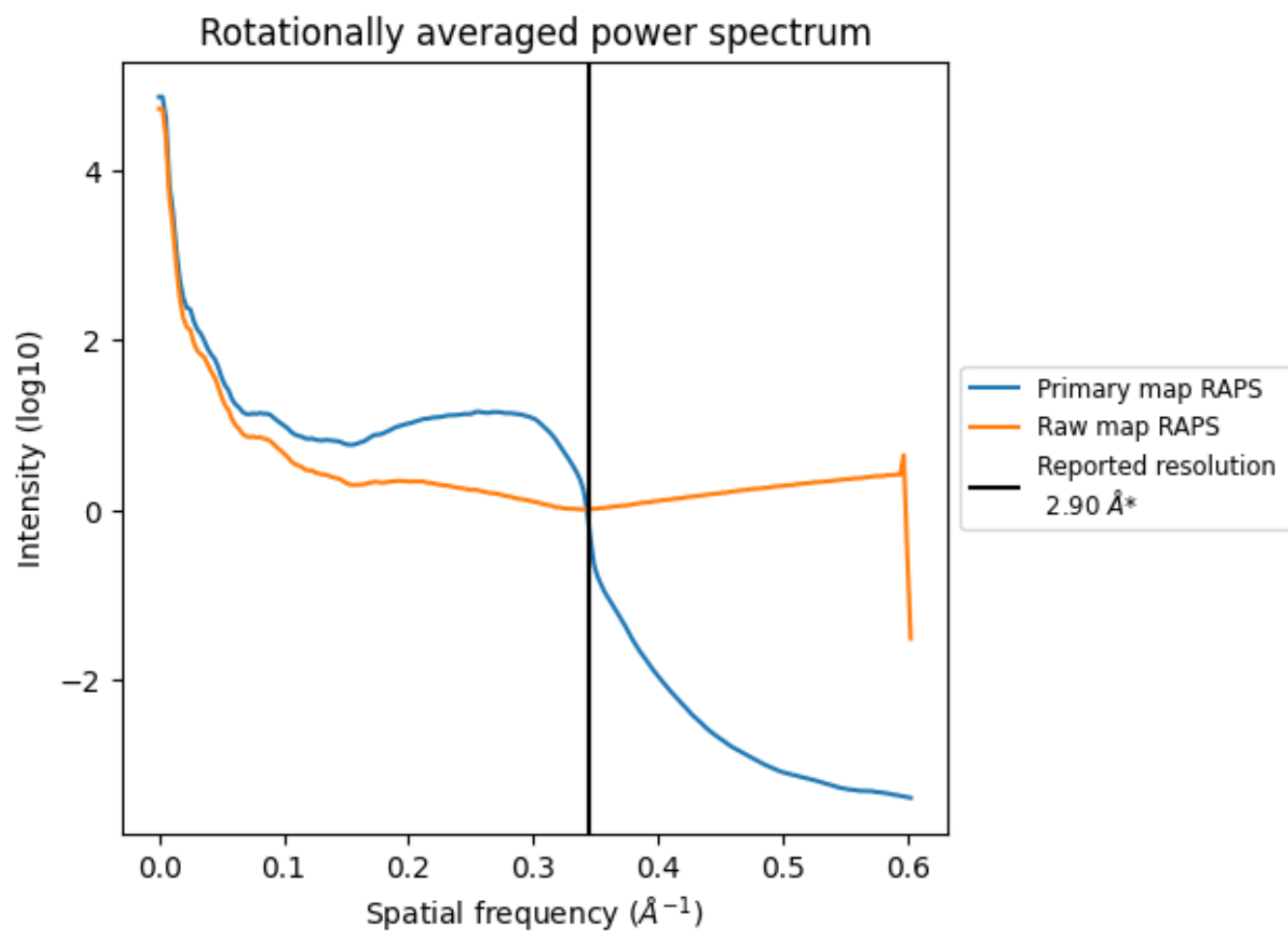
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1224 nm<sup>3</sup>; this corresponds to an approximate mass of 1106 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 ⓘ



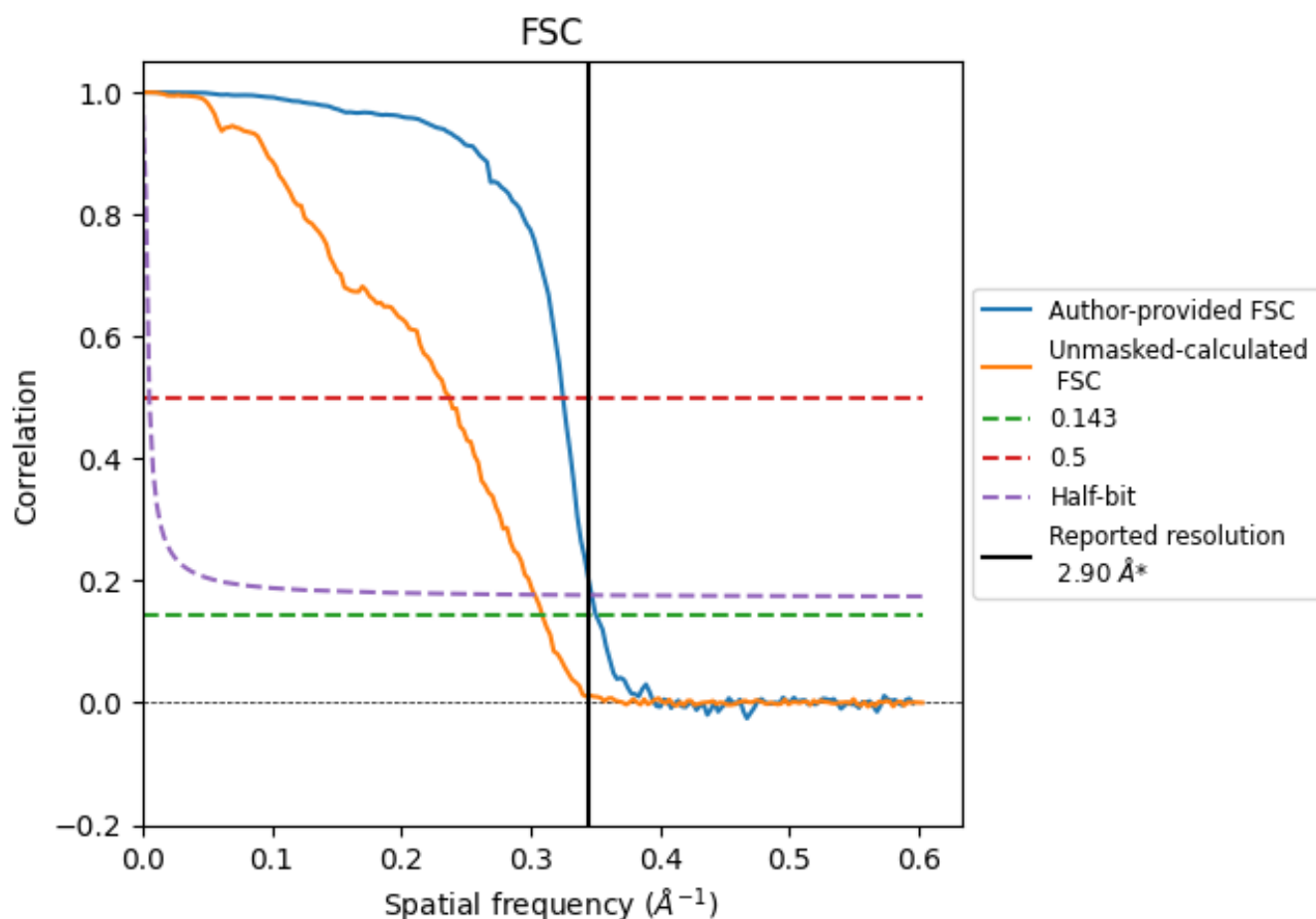
\*Reported resolution corresponds to spatial frequency of  $0.345 \text{ \AA}^{-1}$



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.345 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.85	3.08	2.88
Unmasked-calculated*	3.24	4.21	3.30

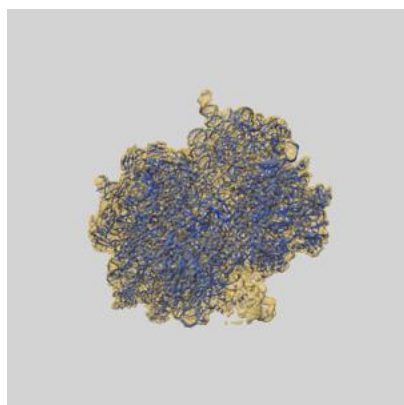
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.24 differs from the reported value 2.9 by more than 10 %



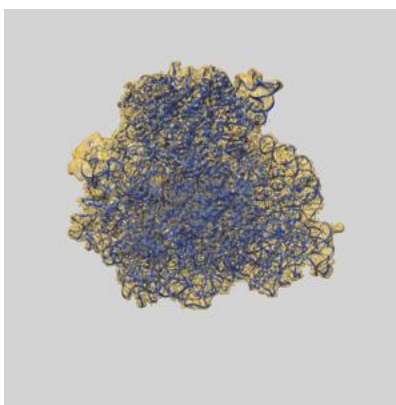
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60473 and PDB model 8ZTU. Per-residue inclusion information can be found in section 3 on page 16.

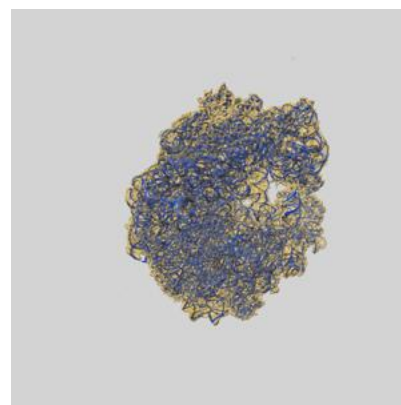
### 9.1 Map-model overlay [i](#)



X



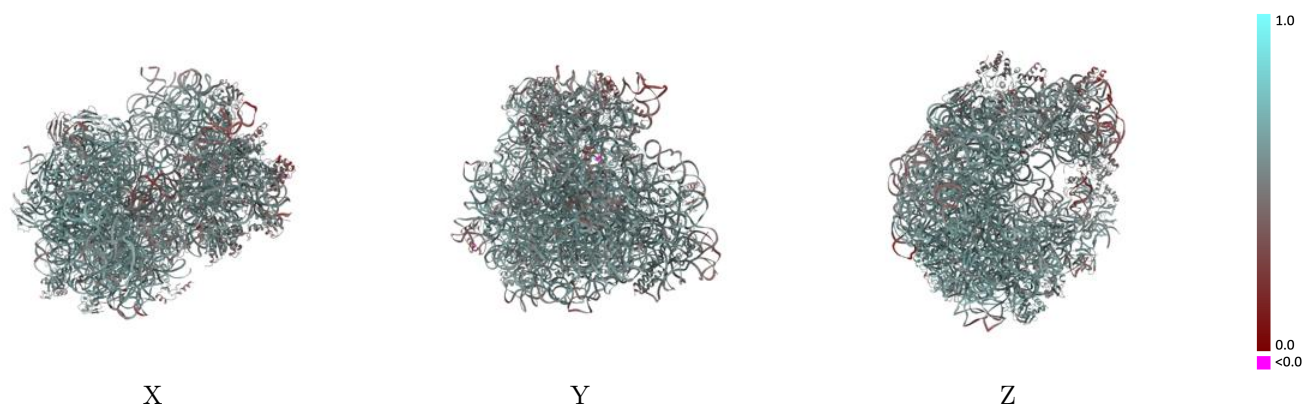
Y



Z

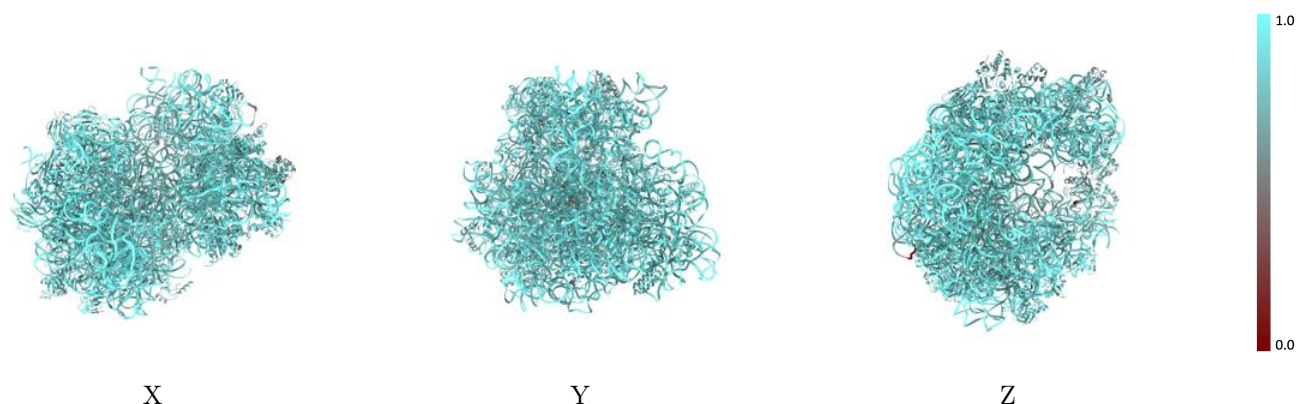
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



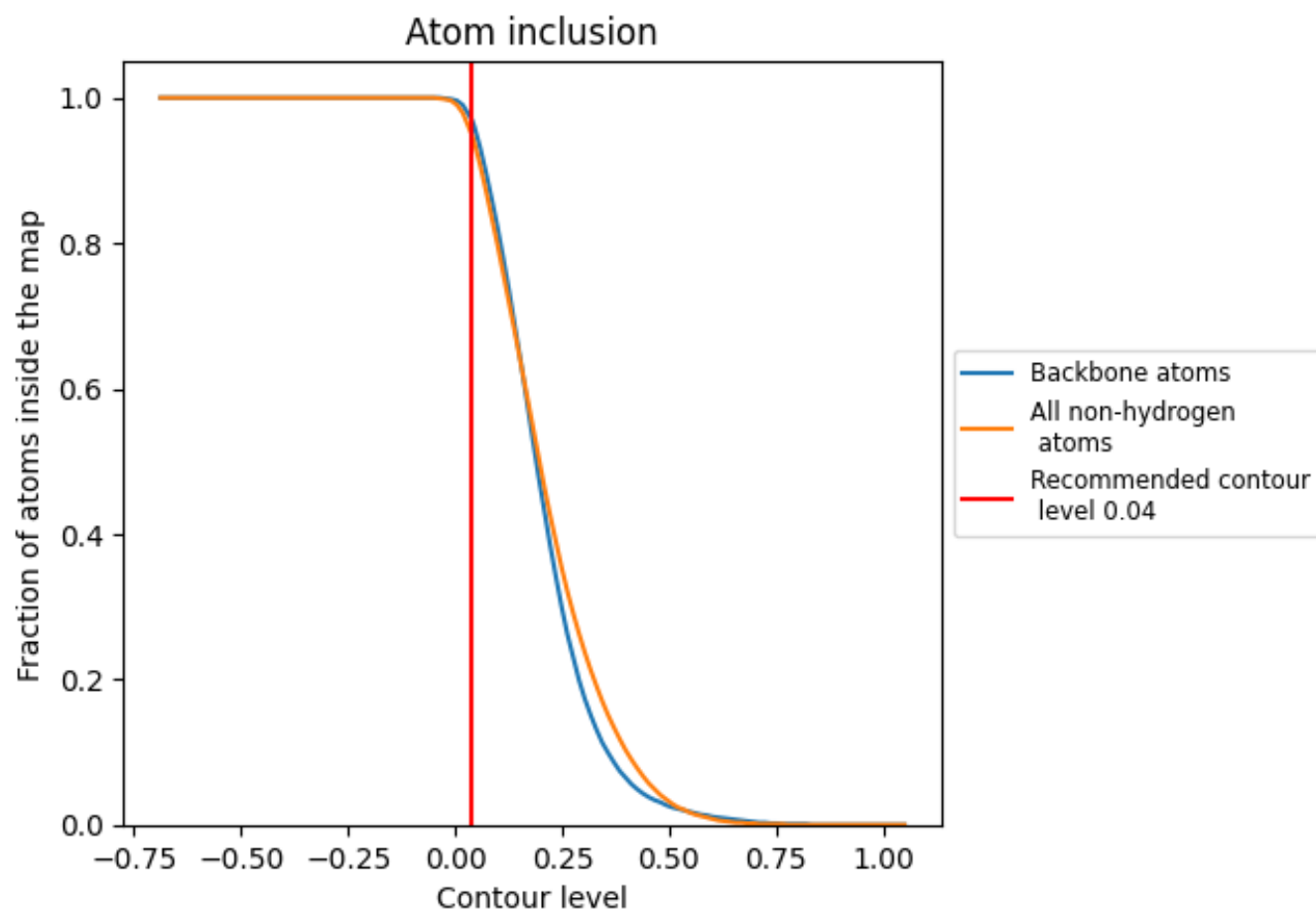
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.5710
0	 0.9050	 0.5580
1	 0.9660	 0.6250
2	 0.9550	 0.6130
3	 0.9420	 0.5840
4	 0.8070	 0.4660
A	 0.9680	 0.5620
B	 0.7970	 0.4690
C	 0.8800	 0.5300
D	 0.8640	 0.5160
E	 0.9110	 0.5640
F	 0.8470	 0.5120
G	 0.8400	 0.4850
H	 0.8900	 0.5490
I	 0.8530	 0.4880
J	 0.7620	 0.4360
K	 0.9030	 0.5510
L	 0.9100	 0.5560
M	 0.8240	 0.4940
N	 0.8610	 0.5060
O	 0.9010	 0.5510
P	 0.8950	 0.5440
Q	 0.8800	 0.5310
R	 0.8740	 0.5400
S	 0.8220	 0.5010
T	 0.8840	 0.5260
U	 0.7480	 0.4570
W	 0.8780	 0.5120
X	 0.7270	 0.4410
Y	 0.8870	 0.5050
Z	 0.9290	 0.5800
a	 0.9790	 0.5980
b	 0.9710	 0.5680
c	 0.9620	 0.6060
d	 0.9490	 0.5930



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Chain	Atom inclusion	Q-score
e	 0.8930	 0.5560
f	 0.8380	 0.4970
g	 0.8440	 0.4930
h	 0.7490	 0.4250
i	 0.9530	 0.6000
j	 0.9470	 0.5900
k	 0.9380	 0.5870
l	 0.9500	 0.5920
m	 0.9710	 0.6140
n	 0.9030	 0.5410
o	 0.9350	 0.5890
p	 0.9660	 0.6130
q	 0.9280	 0.5810
r	 0.9330	 0.5850
s	 0.9040	 0.5660
t	 0.8940	 0.5430
u	 0.8770	 0.5350
v	 0.9240	 0.5840
w	 0.9430	 0.5910
x	 0.8730	 0.5330
y	 0.9130	 0.5880
z	 0.9440	 0.5970