



# Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 07:41 PM EDT

PDB ID : 7JT2  
EMDB ID : EMD-22469  
Title : 70S ribosome stalled on long mRNA with ArfB bound in the A site  
Authors : Carbone, C.E.; Korostelev, A.A.  
Deposited on : 2020-08-16  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

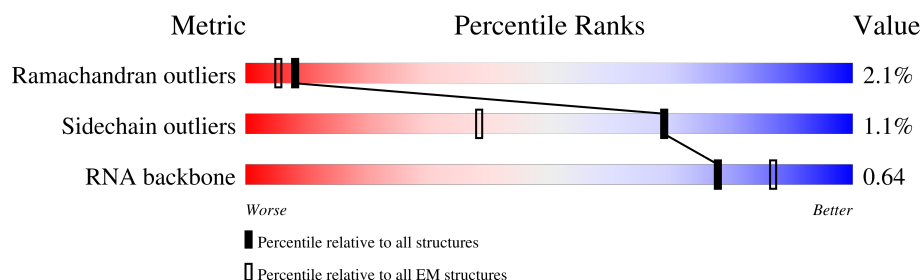
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.



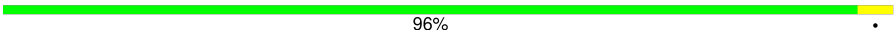

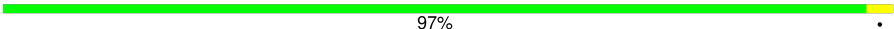
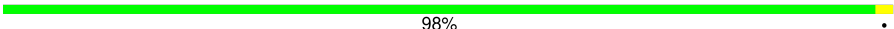
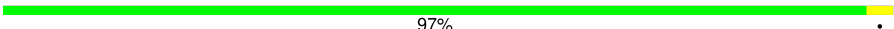

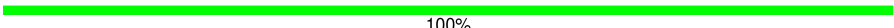
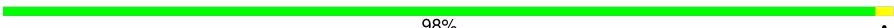
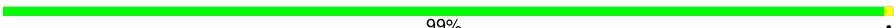
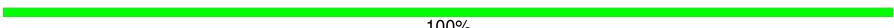
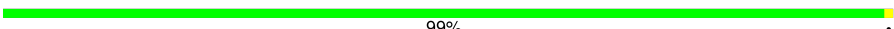

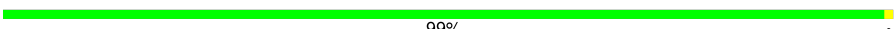
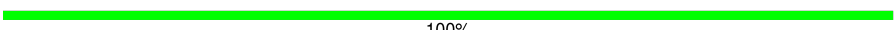
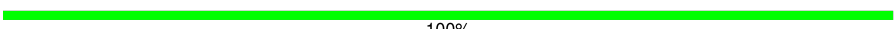
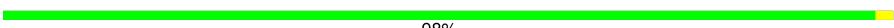
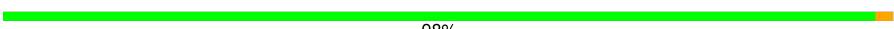
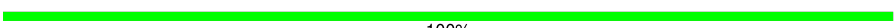
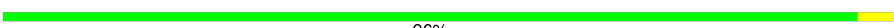
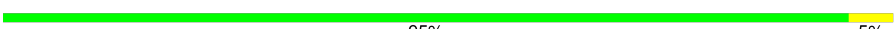
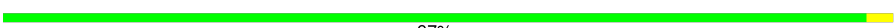

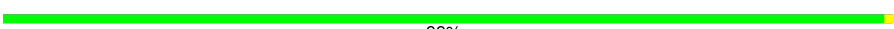


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	b	271	
2	c	209	
3	d	201	
4	e	177	
5	f	176	
6	g	149	
7	h	165	
8	j	142	


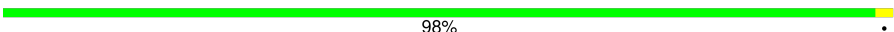
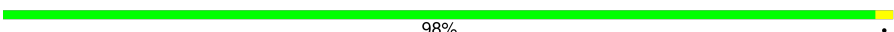

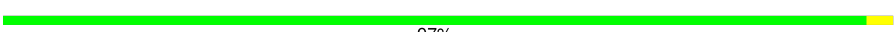







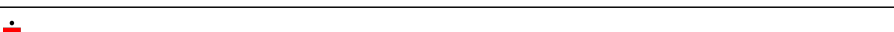

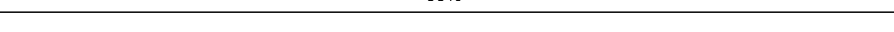
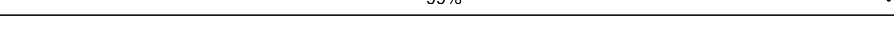
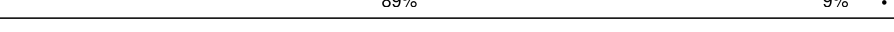





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Mol	Chain	Length	Quality of chain
9	k	122	 96% .
10	l	143	 99% .
11	m	136	 97% .
12	n	120	 98% .
13	o	116	 97% .
14	p	114	 98% .
15	q	117	 100% .
16	r	103	 98% .
17	s	110	 99% .
18	t	93	 100% .
19	u	102	 99% .
20	v	94	 98% .
21	w	75	 99% .
22	x	77	 100% .
23	y	63	 100% .
24	z	58	 98% .
25	B	56	 98% .
26	C	50	 100% .
27	D	46	 96% .
28	E	64	 95% 5% .
29	F	38	 97% .
30	G	225	 97% .
31	H	206	 99% .
32	I	205	 99% .
33	J	157	 97% .

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Mol	Chain	Length	Quality of chain
34	K	100	 92% 7% .
35	L	151	 98% .
36	M	129	 98% .
37	N	127	 98% ..
38	O	98	 97% .
39	P	116	 95% 5%
40	Q	123	 95% 5%
41	R	114	 99% .
42	S	100	 98% .
43	T	88	 97% .
44	U	82	 99% .
45	V	80	 92% 6% .
46	W	65	 91% 9%
47	X	79	 99% .
48	Y	85	 99% .
49	Z	65	 89% 9% .
50	3	1539	 90% 10%
51	1	2903	 87% 13%
52	2	120	 88% 12%
53	5	77	 90% 10%
54	4	23	 57% 35% 9%
55	8	132	 90% 8% .

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 145984 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 8 is a protein called 50S ribosomal protein L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

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

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	t	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	102	Total	C	N	O	S	0	0
			780	492	146	142			

- Molecule 20 is a protein called 50S ribosomal protein L25.

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

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 22 is a protein called 50S ribosomal protein L28.

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

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

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

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 27 is a protein called 50S ribosomal protein L34.

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

- Molecule 28 is a protein called 50S ribosomal protein L35.



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

- Molecule 29 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	225	Total	C	N	O	S	0	0
			1757	1111	315	323	8		

- Molecule 31 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 32 is a protein called 30S ribosomal protein S4.

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

- Molecule 33 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 34 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 35 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 36 is a protein called 30S ribosomal protein S8.

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

- Molecule 37 is a protein called 30S ribosomal protein S9.

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

- Molecule 38 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 39 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 40 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 41 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 42 is a protein called 30S ribosomal protein S14.

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

- Molecule 43 is a protein called 30S ribosomal protein S15.

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

- Molecule 44 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	U	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 45 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 46 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 47 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 48 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 49 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	1539	Total	C	N	O	P	0	0
			33012	14725	6053	10696	1538		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	1490	C	U	conflict	GB 1789840096

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	2903	Total	C	N	O	P	0	0
			62315	27801	11468	20144	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 53 is a RNA chain called tRNA<sup>fMet</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	21	Total 461	C 207	N 96	O 137	P 21	0	0

- Molecule 55 is a protein called Peptidyl-tRNA hydrolase ArfB.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	132	Total 1031	C 638	N 204	O 187	S 2	0	0

### 3 Residue-property plots

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

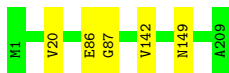
- Molecule 1: 50S ribosomal protein L2

Chain b:  97%



- Molecule 2: 50S ribosomal protein L3

Chain c:  98%



- Molecule 3: 50S ribosomal protein L4

Chain d:  99%



- Molecule 4: 50S ribosomal protein L5

Chain e:  97%



- Molecule 5: 50S ribosomal protein L6

Chain f:  98%



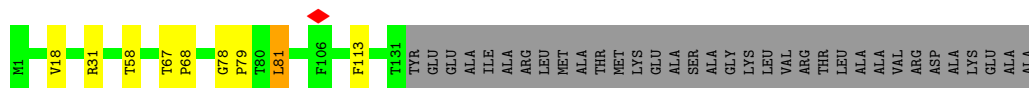
- Molecule 6: 50S ribosomal protein L9

Chain g:  94% 6%



- Molecule 7: 50S ribosomal protein L10

Chain h:  74% 5% 21%



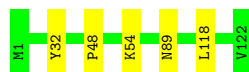
- Molecule 8: 50S ribosomal protein L13

Chain j:  98% ..



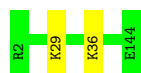
- Molecule 9: 50S ribosomal protein L14

Chain k:  96% .



- Molecule 10: 50S ribosomal protein L15

Chain l:  99% .



- Molecule 11: 50S ribosomal protein L16

Chain m:  97% .



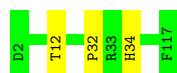
- Molecule 12: 50S ribosomal protein L17

Chain n:  98% .



- Molecule 13: 50S ribosomal protein L18

Chain o:  97% .



- Molecule 14: 50S ribosomal protein L19

Chain p:  98% .



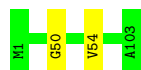
- Molecule 15: 50S ribosomal protein L20

Chain q:  100%

There are no outlier residues recorded for this chain.

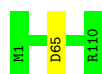
- Molecule 16: 50S ribosomal protein L21

Chain r:  98% .



- Molecule 17: 50S ribosomal protein L22

Chain s:  99% .



- Molecule 18: 50S ribosomal protein L23

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L24

Chain u:  99% .



- Molecule 20: 50S ribosomal protein L25

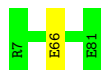
Chain v:  98% .





- Molecule 21: 50S ribosomal protein L27

Chain w:  99%



- Molecule 22: 50S ribosomal protein L28

Chain x:  100%

There are no outlier residues recorded for this chain.

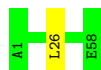
- Molecule 23: 50S ribosomal protein L29

Chain y:  100%

There are no outlier residues recorded for this chain.

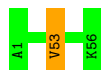
- Molecule 24: 50S ribosomal protein L30

Chain z:  98%



- Molecule 25: 50S ribosomal protein L32

Chain B:  98%



- Molecule 26: 50S ribosomal protein L33

Chain C:  100%

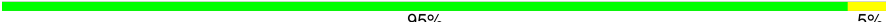
There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L34

Chain D:  96%



- Molecule 28: 50S ribosomal protein L35

Chain E:  95% 5%



- Molecule 29: 50S ribosomal protein L36

Chain F:  97% .



- Molecule 30: 30S ribosomal protein S2

Chain G:  97% .



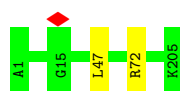
- Molecule 31: 30S ribosomal protein S3

Chain H:  99% .



- Molecule 32: 30S ribosomal protein S4

Chain I:  99% .



- Molecule 33: 30S ribosomal protein S5

Chain J:  97% .



- Molecule 34: 30S ribosomal protein S6

Chain K:  92% 7% .



- Molecule 35: 30S ribosomal protein S7

Chain L:  98% .



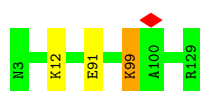
- Molecule 36: 30S ribosomal protein S8

Chain M:  98% .



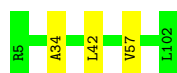
- Molecule 37: 30S ribosomal protein S9

Chain N:  98% ..



- Molecule 38: 30S ribosomal protein S10

Chain O:  97% .



- Molecule 39: 30S ribosomal protein S11

Chain P:  95% 5%



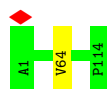
- Molecule 40: 30S ribosomal protein S12

Chain Q:  95% 5%



- Molecule 41: 30S ribosomal protein S13

Chain R:  99% .



- Molecule 42: 30S ribosomal protein S14

Chain S:  98% .



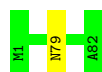
- Molecule 43: 30S ribosomal protein S15

Chain T:  97% .



- Molecule 44: 30S ribosomal protein S16

Chain U:  99% .



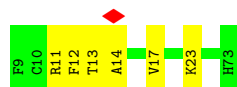
- Molecule 45: 30S ribosomal protein S17

Chain V:  92% 6% .



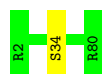
- Molecule 46: 30S ribosomal protein S18

Chain W:  91% 9% .



- Molecule 47: 30S ribosomal protein S19

Chain X:  99% .




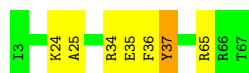
- Molecule 48: 30S ribosomal protein S20

Chain Y:  99% .




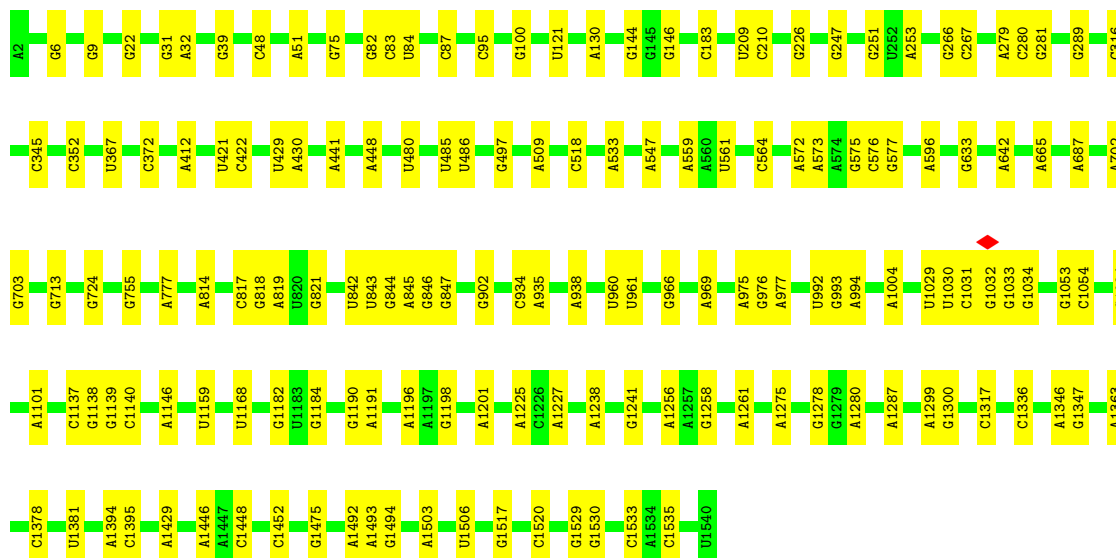
- Molecule 49: 30S ribosomal protein S21

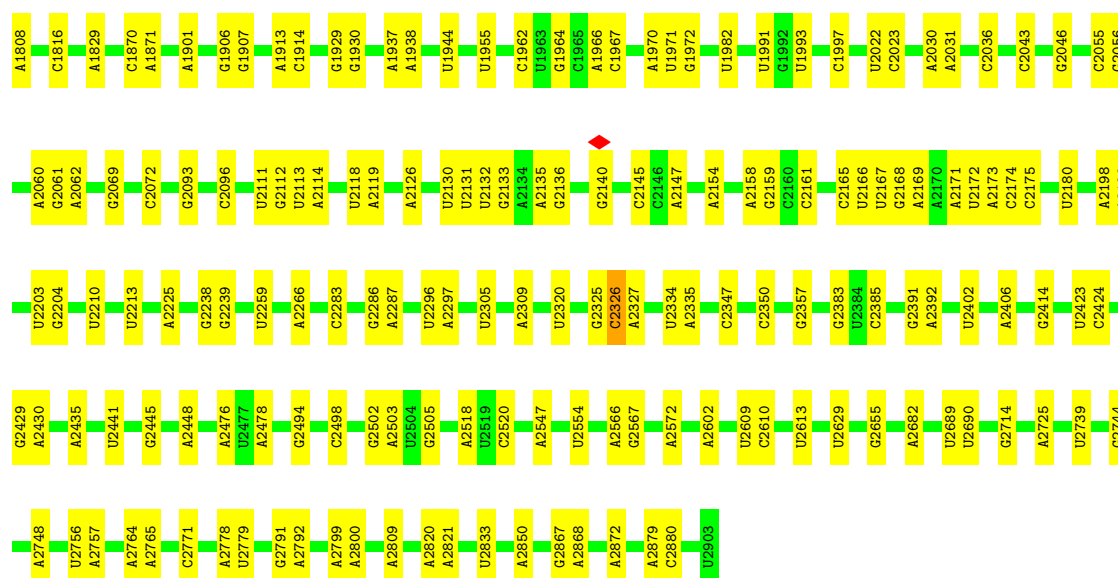
Chain Z:  89% 9% .



• Molecule 50: 16S ribosomal RNA

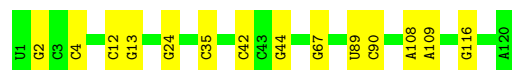
Chain 3:  90% 10%





- Molecule 52: 5S ribosomal RNA

Chain 2: 88% 12%



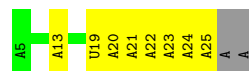
- Molecule 53: tRNAfMet

Chain 5: 90% 10%



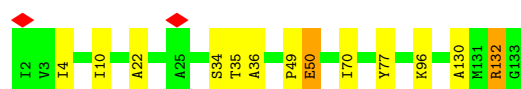
- Molecule 54: mRNA

Chain 4: 57% 35% 9%



- Molecule 55: Peptidyl-tRNA hydrolase ArfB

Chain 8: 90% 8%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.966	Depositor
Minimum map value	-5.215	Depositor
Average map value	0.097	Depositor
Map value standard deviation	0.602	Depositor
Recommended contour level	0.43	Depositor
Map size ( $\text{\AA}$ )	375.12003, 375.12003, 375.12003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.042, 1.042, 1.042	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	b	0.32	0/2122	0.60	0/2852
2	c	0.34	0/1586	0.58	0/2134
3	d	0.32	0/1571	0.55	0/2113
4	e	0.34	0/1435	0.60	0/1926
5	f	0.29	0/1343	0.55	0/1816
6	g	0.33	0/1122	0.64	0/1515
7	h	0.35	0/1001	0.69	0/1350
8	j	0.32	0/1152	0.60	0/1551
9	k	0.31	0/948	0.63	0/1268
10	l	0.32	0/1054	0.62	0/1403
11	m	0.35	0/1093	0.62	0/1460
12	n	0.33	0/974	0.56	0/1301
13	o	0.29	0/902	0.53	0/1209
14	p	0.32	0/929	0.54	0/1242
15	q	0.35	0/960	0.52	0/1278
16	r	0.34	0/829	0.66	1/1107 (0.1%)
17	s	0.30	0/864	0.61	0/1156
18	t	0.29	0/745	0.56	0/994
19	u	0.32	0/788	0.57	0/1051
20	v	0.32	0/766	0.59	0/1025
21	w	0.35	0/582	0.56	0/769
22	x	0.33	0/635	0.54	0/848
23	y	0.29	0/510	0.54	0/677
24	z	0.30	0/453	0.55	0/605
25	B	0.31	0/450	0.55	0/599
26	C	0.34	0/417	0.51	0/554
27	D	0.37	0/380	0.59	0/498
28	E	0.33	0/513	0.60	0/676
29	F	0.28	0/303	0.58	0/397
30	G	0.33	0/1788	0.56	0/2408
31	H	0.30	0/1652	0.57	0/2225
32	I	0.32	0/1665	0.61	0/2227
33	J	0.29	0/1170	0.59	0/1573
34	K	0.34	0/836	0.67	0/1128



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	L	0.30	0/1196	0.56	0/1602
36	M	0.29	0/989	0.60	0/1326
37	N	0.32	0/1034	0.62	0/1375
38	O	0.30	0/797	0.64	0/1077
39	P	0.31	0/886	0.63	0/1195
40	Q	0.29	0/969	0.64	0/1300
41	R	0.29	0/893	0.55	0/1193
42	S	0.32	0/817	0.56	0/1088
43	T	0.30	0/722	0.57	0/964
44	U	0.34	0/659	0.57	0/884
45	V	0.31	0/658	0.62	1/881 (0.1%)
46	W	0.34	0/545	0.65	0/731
47	X	0.34	0/653	0.59	0/877
48	Y	0.31	0/671	0.55	0/888
49	Z	0.36	0/551	0.62	0/728
50	3	0.33	0/36963	0.66	0/57662
51	1	0.34	0/69794	0.66	2/108883 (0.0%)
52	2	0.34	0/2872	0.66	0/4479
53	5	0.33	0/1832	0.66	0/2855
54	4	0.41	0/520	0.71	0/810
55	8	0.32	0/1043	0.74	0/1399
All	All	0.33	0/158602	0.64	4/237132 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1	2326	C	C2'-C3'-O3'	6.17	123.57	113.70
16	r	50	GLY	N-CA-C	-5.84	98.49	113.10
51	1	1178	C	N1-C1'-C2'	5.41	121.03	114.00
45	V	55	GLY	N-CA-C	5.19	126.07	113.10

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	
1	b	269/271 (99%)	236 (88%)	29 (11%)	4 (2%)	8	39
2	c	207/209 (99%)	180 (87%)	23 (11%)	4 (2%)	6	34
3	d	199/201 (99%)	181 (91%)	16 (8%)	2 (1%)	13	46
4	e	175/177 (99%)	155 (89%)	15 (9%)	5 (3%)	3	27
5	f	174/176 (99%)	161 (92%)	11 (6%)	2 (1%)	12	45
6	g	147/149 (99%)	123 (84%)	20 (14%)	4 (3%)	4	28
7	h	129/165 (78%)	99 (77%)	24 (19%)	6 (5%)	2	17
8	j	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	9	40
9	k	120/122 (98%)	103 (86%)	13 (11%)	4 (3%)	3	25
10	l	141/143 (99%)	119 (84%)	20 (14%)	2 (1%)	9	40
11	m	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	8	39
12	n	118/120 (98%)	95 (80%)	21 (18%)	2 (2%)	7	36
13	o	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	7	35
14	p	112/114 (98%)	101 (90%)	9 (8%)	2 (2%)	7	35
15	q	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
16	r	101/103 (98%)	83 (82%)	17 (17%)	1 (1%)	13	46
17	s	108/110 (98%)	93 (86%)	14 (13%)	1 (1%)	14	49
18	t	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
19	u	100/102 (98%)	86 (86%)	13 (13%)	1 (1%)	13	46
20	v	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
21	w	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
22	x	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
23	y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
24	z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
25	B	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	C	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
27	D	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	31
28	E	62/64 (97%)	49 (79%)	10 (16%)	3 (5%)	2	17
29	F	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	4	27
30	G	223/225 (99%)	192 (86%)	26 (12%)	5 (2%)	5	31
31	H	204/206 (99%)	188 (92%)	14 (7%)	2 (1%)	13	46
32	I	203/205 (99%)	173 (85%)	29 (14%)	1 (0%)	25	59
33	J	155/157 (99%)	122 (79%)	29 (19%)	4 (3%)	4	28
34	K	98/100 (98%)	77 (79%)	15 (15%)	6 (6%)	1	13
35	L	149/151 (99%)	133 (89%)	15 (10%)	1 (1%)	19	53
36	M	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	8	38
37	N	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	5	30
38	O	96/98 (98%)	78 (81%)	16 (17%)	2 (2%)	5	32
39	P	114/116 (98%)	86 (75%)	23 (20%)	5 (4%)	2	18
40	Q	121/123 (98%)	98 (81%)	20 (16%)	3 (2%)	4	29
41	R	112/114 (98%)	96 (86%)	16 (14%)	0	100	100
42	S	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	33
43	T	86/88 (98%)	78 (91%)	7 (8%)	1 (1%)	11	43
44	U	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	10	41
45	V	78/80 (98%)	63 (81%)	10 (13%)	5 (6%)	1	12
46	W	63/65 (97%)	56 (89%)	3 (5%)	4 (6%)	1	12
47	X	77/79 (98%)	66 (86%)	10 (13%)	1 (1%)	10	41
48	Y	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	11	43
49	Z	63/65 (97%)	48 (76%)	8 (13%)	7 (11%)	0	5
55	8	130/132 (98%)	99 (76%)	20 (15%)	11 (8%)	0	7
All	All	5780/5914 (98%)	5000 (86%)	661 (11%)	119 (2%)	8	32

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	e	173	ASP
5	f	47	ASN
5	f	117	PRO

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Mol	Chain	Res	Type
6	g	9	VAL
7	h	81	LEU
8	j	81	ILE
11	m	70	ASP
13	o	34	HIS
14	p	75	THR
16	r	54	VAL
25	B	53	VAL
28	E	31	ILE
29	F	37	GLN
30	G	15	PHE
33	J	93	VAL
34	K	53	LYS
34	K	54	LEU
34	K	93	LYS
37	N	91	GLU
37	N	99	LYS
39	P	125	LYS
43	T	46	LYS
44	U	79	ASN
45	V	15	LYS
46	W	14	ALA
46	W	17	VAL
55	8	4	ILE
55	8	36	ALA
55	8	49	PRO
55	8	50	GLU
55	8	70	ILE
55	8	130	ALA
55	8	132	ARG
1	b	179	GLU
2	c	86	GLU
4	e	93	GLU
6	g	49	ALA
7	h	78	GLY
9	k	32	TYR
9	k	54	LYS
11	m	15	GLY
12	n	71	ARG
17	s	65	ASP
30	G	97	GLY
30	G	101	THR

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Mol	Chain	Res	Type
32	I	47	LEU
33	J	80	LEU
34	K	40	GLU
36	M	20	ASN
39	P	54	SER
39	P	89	GLY
45	V	17	GLU
45	V	55	GLY
46	W	13	THR
49	Z	24	LYS
49	Z	34	ARG
49	Z	36	PHE
55	8	34	SER
55	8	77	TYR
2	c	149	ASN
6	g	10	ALA
6	g	113	SER
7	h	113	PHE
9	k	89	ASN
13	o	12	THR
28	E	17	GLY
30	G	192	PRO
31	H	47	ALA
34	K	92	THR
34	K	94	HIS
36	M	47	ASP
38	O	34	ALA
40	Q	35	ARG
48	Y	5	SER
55	8	22	ALA
2	c	20	VAL
3	d	20	GLY
3	d	127	GLU
10	l	29	LYS
10	l	36	LYS
33	J	49	TYR
40	Q	43	LYS
46	W	12	PHE
49	Z	25	ALA
49	Z	35	GLU
49	Z	37	TYR
1	b	108	GLY

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Mol	Chain	Res	Type
4	e	176	PHE
7	h	68	PRO
8	j	126	ALA
12	n	106	ASP
14	p	64	SER
19	u	88	ASP
28	E	16	THR
30	G	73	ARG
31	H	25	THR
33	J	97	PRO
35	L	18	GLY
37	N	12	LYS
38	O	42	LEU
39	P	88	PRO
42	S	61	ASN
45	V	49	ASN
45	V	70	LYS
47	X	34	SER
1	b	236	GLY
4	e	39	VAL
7	h	79	PRO
27	D	42	LEU
39	P	52	ARG
40	Q	87	LYS
42	S	33	VAL
49	Z	65	ARG
1	b	63	ILE
2	c	87	GLY
7	h	67	THR
9	k	48	PRO
4	e	148	VAL
55	8	10	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	213 (99%)	3 (1%)	62	79
2	c	164/164 (100%)	163 (99%)	1 (1%)	84	91
3	d	165/165 (100%)	165 (100%)	0	100	100
4	e	148/148 (100%)	147 (99%)	1 (1%)	81	89
5	f	137/137 (100%)	136 (99%)	1 (1%)	81	89
6	g	114/114 (100%)	109 (96%)	5 (4%)	24	53
7	h	100/123 (81%)	96 (96%)	4 (4%)	27	56
8	j	116/116 (100%)	114 (98%)	2 (2%)	56	75
9	k	103/103 (100%)	102 (99%)	1 (1%)	73	84
10	l	102/102 (100%)	102 (100%)	0	100	100
11	m	109/109 (100%)	107 (98%)	2 (2%)	54	74
12	n	100/100 (100%)	100 (100%)	0	100	100
13	o	86/86 (100%)	85 (99%)	1 (1%)	67	82
14	p	99/99 (100%)	99 (100%)	0	100	100
15	q	89/89 (100%)	89 (100%)	0	100	100
16	r	84/84 (100%)	84 (100%)	0	100	100
17	s	93/93 (100%)	93 (100%)	0	100	100
18	t	80/80 (100%)	80 (100%)	0	100	100
19	u	83/83 (100%)	83 (100%)	0	100	100
20	v	78/78 (100%)	76 (97%)	2 (3%)	41	66
21	w	57/57 (100%)	56 (98%)	1 (2%)	54	74
22	x	67/67 (100%)	67 (100%)	0	100	100
23	y	55/55 (100%)	55 (100%)	0	100	100
24	z	48/48 (100%)	47 (98%)	1 (2%)	48	71
25	B	47/47 (100%)	46 (98%)	1 (2%)	48	71
26	C	45/45 (100%)	45 (100%)	0	100	100
27	D	38/38 (100%)	37 (97%)	1 (3%)	41	66
28	E	51/51 (100%)	51 (100%)	0	100	100
29	F	34/34 (100%)	34 (100%)	0	100	100
30	G	186/186 (100%)	185 (100%)	1 (0%)	86	93
31	H	170/170 (100%)	170 (100%)	0	100	100
32	I	172/172 (100%)	171 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	J	119/119 (100%)	118 (99%)	1 (1%)	79	88
34	K	87/87 (100%)	84 (97%)	3 (3%)	32	60
35	L	124/124 (100%)	122 (98%)	2 (2%)	58	76
36	M	104/104 (100%)	103 (99%)	1 (1%)	73	84
37	N	105/105 (100%)	104 (99%)	1 (1%)	73	84
38	O	86/86 (100%)	85 (99%)	1 (1%)	67	82
39	P	89/89 (100%)	88 (99%)	1 (1%)	70	83
40	Q	103/103 (100%)	100 (97%)	3 (3%)	37	64
41	R	92/92 (100%)	91 (99%)	1 (1%)	70	83
42	S	83/83 (100%)	83 (100%)	0	100	100
43	T	76/76 (100%)	74 (97%)	2 (3%)	41	66
44	U	65/65 (100%)	65 (100%)	0	100	100
45	V	74/74 (100%)	73 (99%)	1 (1%)	62	79
46	W	56/56 (100%)	54 (96%)	2 (4%)	30	59
47	X	70/70 (100%)	70 (100%)	0	100	100
48	Y	65/65 (100%)	65 (100%)	0	100	100
49	Z	55/55 (100%)	54 (98%)	1 (2%)	54	74
55	8	108/108 (100%)	104 (96%)	4 (4%)	29	58
All	All	4797/4820 (100%)	4744 (99%)	53 (1%)	69	83

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	16	VAL
1	b	212	TRP
1	b	269	ARG
2	c	142	VAL
4	e	141	ASP
5	f	68	ARG
6	g	45	GLU
6	g	46	PHE
6	g	50	ARG
6	g	75	LEU
6	g	108	VAL
7	h	18	VAL
7	h	31	ARG

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Mol	Chain	Res	Type
7	h	58	THR
7	h	81	LEU
8	j	1	MET
8	j	81	ILE
9	k	118	LEU
11	m	51	ARG
11	m	64	TRP
13	o	32	PRO
20	v	65	VAL
20	v	72	VAL
21	w	66	GLU
24	z	26	LEU
25	B	53	VAL
27	D	6	GLN
30	G	46	VAL
32	I	72	ARG
33	J	137	ARG
34	K	54	LEU
34	K	78	PHE
34	K	91	ARG
35	L	6	ILE
35	L	14	ASP
36	M	60	LEU
37	N	99	LYS
38	O	57	VAL
39	P	118	ASN
40	Q	39	THR
40	Q	75	GLU
40	Q	111	GLN
41	R	64	VAL
43	T	73	ASP
43	T	88	ARG
45	V	6	THR
46	W	11	ARG
46	W	23	LYS
49	Z	37	TYR
55	8	35	THR
55	8	50	GLU
55	8	96	LYS
55	8	132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	36	ASN
1	b	45	ASN
1	b	52	HIS
1	b	69	ASN
1	b	89	ASN
1	b	114	GLN
1	b	116	GLN
1	b	152	GLN
1	b	196	ASN
1	b	225	ASN
1	b	259	ASN
2	c	67	HIS
2	c	134	HIS
2	c	148	GLN
2	c	173	GLN
3	d	62	GLN
3	d	97	ASN
4	e	20	ASN
5	f	29	ASN
5	f	142	GLN
6	g	18	GLN
6	g	43	ASN
8	j	58	ASN
9	k	3	GLN
9	k	88	ASN
9	k	89	ASN
10	l	99	ASN
12	n	23	ASN
12	n	62	ASN
13	o	34	HIS
14	p	74	GLN
14	p	114	ASN
15	q	36	GLN
15	q	51	GLN
15	q	70	GLN
15	q	71	ASN
16	r	11	GLN
16	r	91	GLN
18	t	28	ASN
18	t	59	ASN
19	u	68	ASN
19	u	73	ASN
20	v	44	HIS

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Mol	Chain	Res	Type
20	v	49	ASN
20	v	80	HIS
22	x	5	GLN
24	z	33	HIS
25	B	5	ASN
25	B	18	HIS
26	C	18	HIS
26	C	25	ASN
27	D	6	GLN
27	D	29	GLN
29	F	35	GLN
29	F	37	GLN
30	G	23	ASN
30	G	167	HIS
32	I	119	HIS
33	J	11	GLN
33	J	60	GLN
33	J	81	GLN
33	J	131	ASN
34	K	17	GLN
34	K	68	GLN
35	L	27	ASN
35	L	129	ASN
35	L	141	HIS
36	M	3	GLN
37	N	30	ASN
37	N	74	GLN
37	N	80	HIS
39	P	14	GLN
39	P	118	ASN
40	Q	74	GLN
41	R	7	ASN
41	R	13	HIS
42	S	42	ASN
42	S	61	ASN
43	T	34	GLN
44	U	9	HIS
44	U	18	GLN
45	V	30	HIS
46	W	73	HIS
48	Y	12	GLN
48	Y	60	GLN

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Mol	Chain	Res	Type
55	8	23	GLN
55	8	75	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	3	1538/1539 (99%)	157 (10%)	2 (0%)
51	1	2902/2903 (99%)	365 (12%)	9 (0%)
52	2	119/120 (99%)	14 (11%)	0
53	5	76/77 (98%)	8 (10%)	0
54	4	20/23 (86%)	6 (30%)	2 (10%)
All	All	4655/4662 (99%)	550 (11%)	13 (0%)

All (550) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	3	6	G
50	3	9	G
50	3	22	G
50	3	31	G
50	3	32	A
50	3	39	G
50	3	48	C
50	3	51	A
50	3	75	G
50	3	82	G
50	3	83	C
50	3	84	U
50	3	87	C
50	3	95	C
50	3	100	G
50	3	121	U
50	3	130	A
50	3	144	G
50	3	146	G
50	3	183	C
50	3	209	U
50	3	210	C
50	3	226	G
50	3	247	G
50	3	251	G

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Mol	Chain	Res	Type
50	3	253	A
50	3	266	G
50	3	267	C
50	3	279	A
50	3	280	C
50	3	281	G
50	3	289	G
50	3	316	C
50	3	345	C
50	3	352	C
50	3	367	U
50	3	372	C
50	3	412	A
50	3	421	U
50	3	422	C
50	3	430	A
50	3	441	A
50	3	448	A
50	3	480	U
50	3	485	U
50	3	486	U
50	3	497	G
50	3	509	A
50	3	518	C
50	3	533	A
50	3	547	A
50	3	559	A
50	3	561	U
50	3	564	C
50	3	572	A
50	3	573	A
50	3	575	G
50	3	576	C
50	3	577	G
50	3	596	A
50	3	633	G
50	3	642	A
50	3	665	A
50	3	687	A
50	3	702	A
50	3	703	G
50	3	713	G

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Mol	Chain	Res	Type
50	3	724	G
50	3	755	G
50	3	777	A
50	3	814	A
50	3	817	C
50	3	818	G
50	3	819	A
50	3	821	G
50	3	842	U
50	3	843	U
50	3	844	G
50	3	845	A
50	3	846	G
50	3	847	G
50	3	902	G
50	3	934	C
50	3	935	A
50	3	938	A
50	3	960	U
50	3	961	U
50	3	966	G
50	3	969	A
50	3	975	A
50	3	976	G
50	3	977	A
50	3	992	U
50	3	993	G
50	3	994	A
50	3	1004	A
50	3	1029	U
50	3	1030	U
50	3	1031	C
50	3	1032	G
50	3	1033	G
50	3	1034	G
50	3	1053	G
50	3	1054	C
50	3	1094	G
50	3	1101	A
50	3	1137	C
50	3	1138	G
50	3	1139	G

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Mol	Chain	Res	Type
50	3	1140	C
50	3	1146	A
50	3	1159	U
50	3	1168	U
50	3	1182	G
50	3	1184	G
50	3	1191	A
50	3	1196	A
50	3	1198	G
50	3	1201	A
50	3	1225	A
50	3	1227	A
50	3	1238	A
50	3	1241	G
50	3	1256	A
50	3	1258	G
50	3	1261	A
50	3	1275	A
50	3	1278	G
50	3	1280	A
50	3	1287	A
50	3	1299	A
50	3	1300	G
50	3	1317	C
50	3	1336	C
50	3	1346	A
50	3	1347	G
50	3	1363	A
50	3	1378	C
50	3	1381	U
50	3	1394	A
50	3	1395	C
50	3	1429	A
50	3	1446	A
50	3	1448	C
50	3	1452	C
50	3	1475	G
50	3	1492	A
50	3	1493	A
50	3	1494	G
50	3	1503	A
50	3	1506	U

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Mol	Chain	Res	Type
50	3	1517	G
50	3	1520	C
50	3	1529	G
50	3	1530	G
50	3	1533	C
50	3	1535	C
51	1	10	A
51	1	12	U
51	1	35	G
51	1	50	U
51	1	51	G
51	1	71	A
51	1	74	A
51	1	75	G
51	1	96	C
51	1	119	A
51	1	120	U
51	1	137	U
51	1	139	U
51	1	141	G
51	1	142	A
51	1	162	U
51	1	163	C
51	1	181	A
51	1	196	A
51	1	216	A
51	1	219	A
51	1	221	A
51	1	222	A
51	1	228	C
51	1	229	C
51	1	233	A
51	1	248	G
51	1	249	C
51	1	255	A
51	1	266	G
51	1	276	U
51	1	278	A
51	1	294	A
51	1	301	G
51	1	311	A
51	1	312	G

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Mol	Chain	Res	Type
51	1	323	C
51	1	324	A
51	1	329	G
51	1	330	A
51	1	362	A
51	1	363	G
51	1	371	A
51	1	372	G
51	1	386	G
51	1	387	U
51	1	404	A
51	1	405	U
51	1	406	G
51	1	411	G
51	1	424	G
51	1	481	G
51	1	491	G
51	1	504	A
51	1	505	A
51	1	529	A
51	1	530	G
51	1	531	C
51	1	532	A
51	1	543	G
51	1	548	G
51	1	549	G
51	1	563	A
51	1	572	A
51	1	573	U
51	1	575	A
51	1	588	U
51	1	603	A
51	1	615	U
51	1	627	A
51	1	637	A
51	1	646	U
51	1	654	A
51	1	686	U
51	1	687	C
51	1	730	A
51	1	747	C
51	1	752	A

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Mol	Chain	Res	Type
51	1	757	G
51	1	764	A
51	1	774	G
51	1	776	G
51	1	782	A
51	1	784	G
51	1	785	G
51	1	805	G
51	1	812	C
51	1	819	A
51	1	827	U
51	1	828	U
51	1	830	G
51	1	845	A
51	1	846	U
51	1	847	U
51	1	858	G
51	1	860	U
51	1	878	A
51	1	887	U
51	1	896	A
51	1	910	A
51	1	914	G
51	1	915	C
51	1	932	U
51	1	941	A
51	1	945	A
51	1	946	C
51	1	959	A
51	1	961	C
51	1	974	G
51	1	975	A
51	1	983	A
51	1	985	C
51	1	995	C
51	1	996	A
51	1	1012	U
51	1	1013	C
51	1	1021	A
51	1	1022	G
51	1	1033	U
51	1	1045	C

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Mol	Chain	Res	Type
51	1	1046	A
51	1	1062	G
51	1	1065	U
51	1	1066	U
51	1	1068	G
51	1	1070	A
51	1	1071	G
51	1	1075	C
51	1	1084	A
51	1	1088	A
51	1	1101	U
51	1	1104	C
51	1	1111	A
51	1	1126	A
51	1	1132	U
51	1	1135	C
51	1	1151	A
51	1	1172	C
51	1	1173	U
51	1	1174	U
51	1	1176	U
51	1	1178	C
51	1	1179	G
51	1	1180	U
51	1	1206	G
51	1	1211	C
51	1	1212	G
51	1	1247	A
51	1	1248	G
51	1	1251	C
51	1	1253	A
51	1	1256	G
51	1	1271	G
51	1	1272	A
51	1	1301	A
51	1	1302	A
51	1	1305	C
51	1	1321	A
51	1	1329	U
51	1	1332	G
51	1	1345	C
51	1	1365	A

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Mol	Chain	Res	Type
51	1	1378	A
51	1	1379	U
51	1	1383	A
51	1	1398	C
51	1	1416	G
51	1	1419	A
51	1	1420	A
51	1	1454	C
51	1	1461	C
51	1	1482	G
51	1	1490	A
51	1	1497	U
51	1	1515	A
51	1	1524	G
51	1	1535	A
51	1	1536	C
51	1	1555	G
51	1	1559	U
51	1	1560	G
51	1	1569	A
51	1	1607	C
51	1	1608	A
51	1	1611	C
51	1	1616	A
51	1	1647	U
51	1	1648	U
51	1	1654	A
51	1	1674	G
51	1	1698	A
51	1	1703	G
51	1	1713	A
51	1	1715	G
51	1	1729	U
51	1	1730	C
51	1	1738	G
51	1	1758	U
51	1	1764	C
51	1	1773	A
51	1	1782	U
51	1	1791	A
51	1	1800	C
51	1	1801	A

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Mol	Chain	Res	Type
51	1	1802	A
51	1	1808	A
51	1	1816	C
51	1	1829	A
51	1	1870	C
51	1	1871	A
51	1	1901	A
51	1	1906	G
51	1	1907	G
51	1	1913	A
51	1	1914	C
51	1	1929	G
51	1	1930	G
51	1	1937	A
51	1	1938	A
51	1	1944	U
51	1	1955	U
51	1	1962	C
51	1	1964	G
51	1	1966	A
51	1	1967	C
51	1	1970	A
51	1	1971	U
51	1	1972	G
51	1	1982	U
51	1	1991	U
51	1	1993	U
51	1	1997	C
51	1	2022	U
51	1	2023	C
51	1	2030	A
51	1	2031	A
51	1	2036	C
51	1	2043	C
51	1	2046	G
51	1	2055	C
51	1	2056	G
51	1	2060	A
51	1	2061	G
51	1	2062	A
51	1	2069	G
51	1	2072	C

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Mol	Chain	Res	Type
51	1	2093	G
51	1	2096	C
51	1	2111	U
51	1	2112	G
51	1	2113	U
51	1	2114	A
51	1	2118	U
51	1	2119	A
51	1	2126	A
51	1	2130	U
51	1	2131	U
51	1	2132	U
51	1	2133	G
51	1	2135	A
51	1	2136	G
51	1	2140	G
51	1	2145	C
51	1	2147	A
51	1	2154	A
51	1	2158	A
51	1	2159	G
51	1	2161	C
51	1	2165	C
51	1	2166	U
51	1	2167	U
51	1	2168	G
51	1	2169	A
51	1	2171	A
51	1	2172	U
51	1	2173	A
51	1	2174	C
51	1	2175	C
51	1	2180	U
51	1	2198	A
51	1	2199	A
51	1	2203	U
51	1	2204	G
51	1	2210	U
51	1	2213	U
51	1	2225	A
51	1	2238	G
51	1	2239	G

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Mol	Chain	Res	Type
51	1	2259	U
51	1	2266	A
51	1	2283	C
51	1	2287	A
51	1	2297	A
51	1	2305	U
51	1	2309	A
51	1	2320	U
51	1	2325	G
51	1	2327	A
51	1	2334	U
51	1	2335	A
51	1	2347	C
51	1	2350	C
51	1	2357	G
51	1	2383	G
51	1	2385	C
51	1	2392	A
51	1	2402	U
51	1	2406	A
51	1	2414	G
51	1	2423	U
51	1	2424	C
51	1	2429	G
51	1	2430	A
51	1	2435	A
51	1	2441	U
51	1	2445	G
51	1	2448	A
51	1	2476	A
51	1	2478	A
51	1	2494	G
51	1	2498	C
51	1	2502	G
51	1	2503	A
51	1	2505	G
51	1	2518	A
51	1	2520	C
51	1	2547	A
51	1	2554	U
51	1	2566	A
51	1	2567	G

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Mol	Chain	Res	Type
51	1	2572	A
51	1	2602	A
51	1	2609	U
51	1	2610	C
51	1	2613	U
51	1	2629	U
51	1	2655	G
51	1	2682	A
51	1	2689	U
51	1	2690	U
51	1	2714	G
51	1	2725	A
51	1	2739	U
51	1	2744	G
51	1	2748	A
51	1	2757	A
51	1	2764	A
51	1	2765	A
51	1	2771	C
51	1	2778	A
51	1	2779	U
51	1	2791	G
51	1	2792	A
51	1	2799	A
51	1	2800	A
51	1	2809	A
51	1	2820	A
51	1	2821	A
51	1	2833	U
51	1	2850	A
51	1	2867	G
51	1	2868	A
51	1	2872	A
51	1	2879	A
51	1	2880	C
52	2	2	G
52	2	4	C
52	2	12	C
52	2	13	G
52	2	24	G
52	2	35	C
52	2	42	C

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Mol	Chain	Res	Type
52	2	44	G
52	2	67	G
52	2	89	U
52	2	90	C
52	2	108	A
52	2	109	A
52	2	116	G
53	5	9	G
53	5	19	G
53	5	20	U
53	5	47	U
53	5	48	C
53	5	61	C
53	5	75	C
53	5	76	A
54	4	13	A
54	4	19	U
54	4	20	A
54	4	21	A
54	4	23	A
54	4	25	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	3	429	U
50	3	1190	G
51	1	784	G
51	1	827	U
51	1	859	G
51	1	1020	A
51	1	2286	G
51	1	2296	U
51	1	2326	C
51	1	2391	G
51	1	2756	U
54	4	22	A
54	4	24	A

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

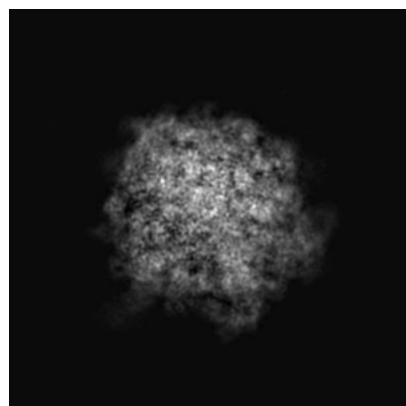
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22469. These allow visual inspection of the internal detail of the map and identification of artifacts.

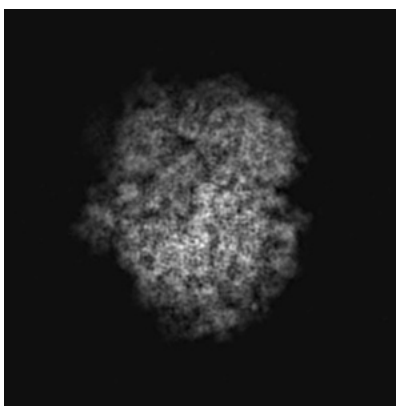
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

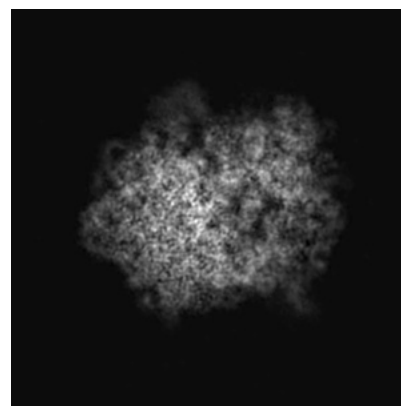
#### 6.1.1 Primary map



X

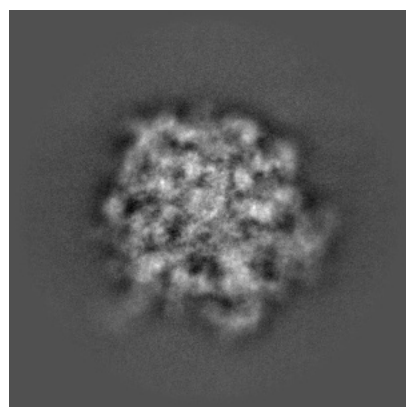


Y

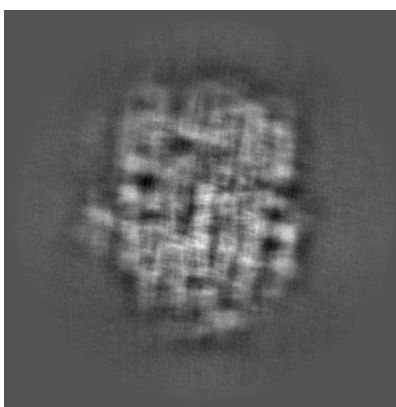


Z

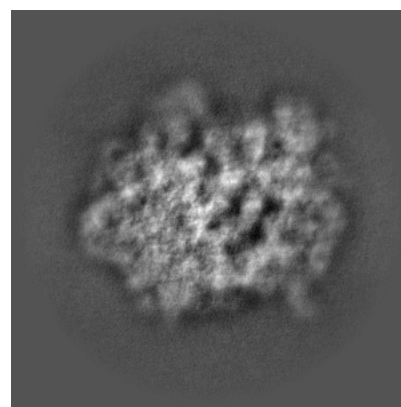
#### 6.1.2 Raw map



X



Y

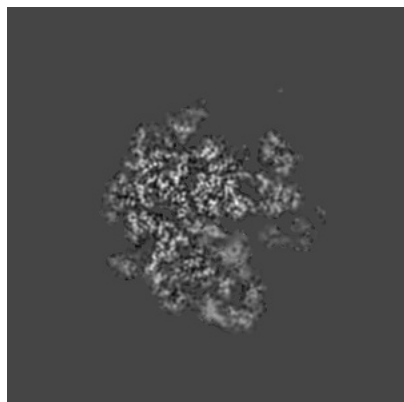


Z

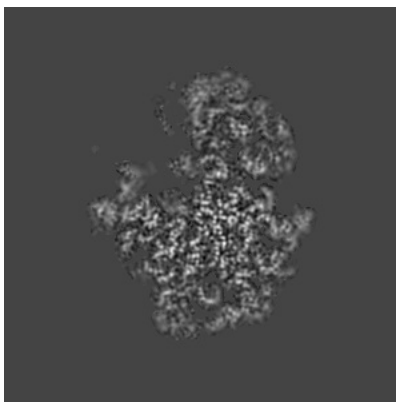
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

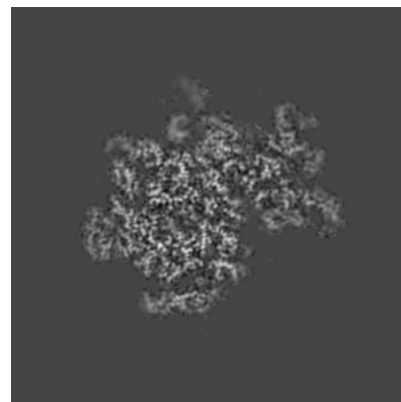
### 6.2.1 Primary map



X Index: 180

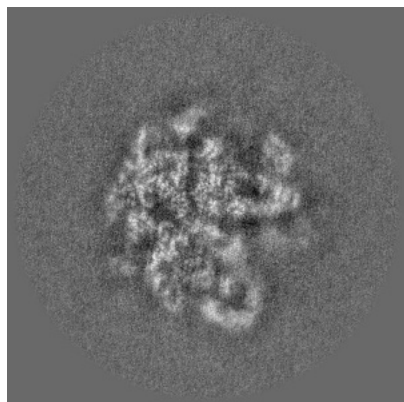


Y Index: 180

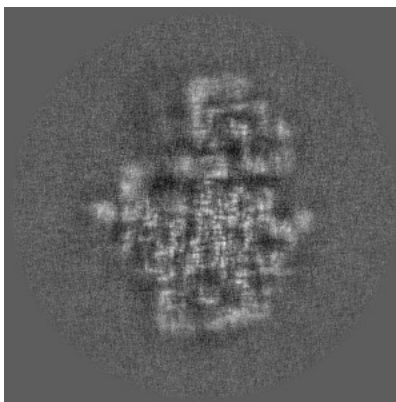


Z Index: 180

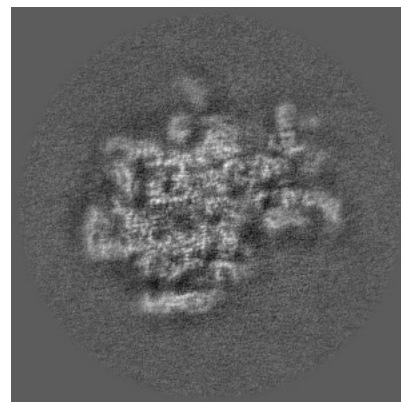
### 6.2.2 Raw map



X Index: 180



Y Index: 180

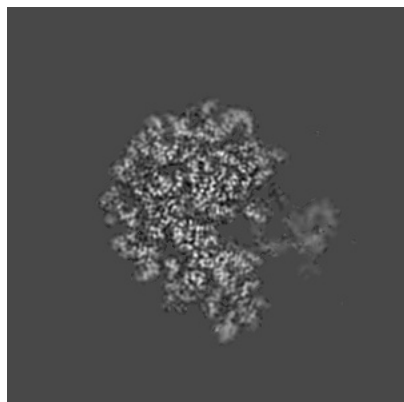


Z Index: 180

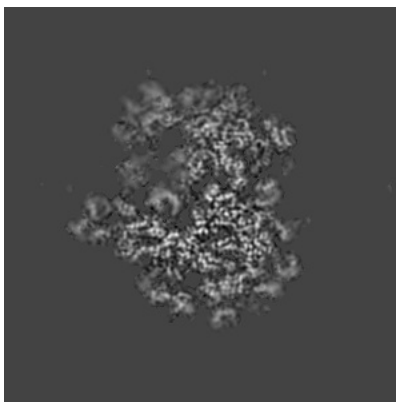
The images above show central slices of the map in three orthogonal directions.

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

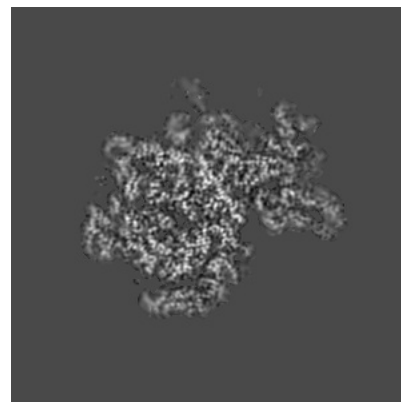
### 6.3.1 Primary map



X Index: 163

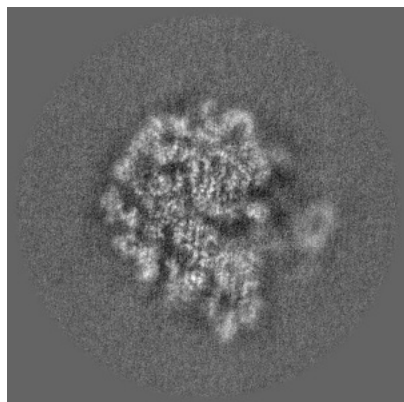


Y Index: 192

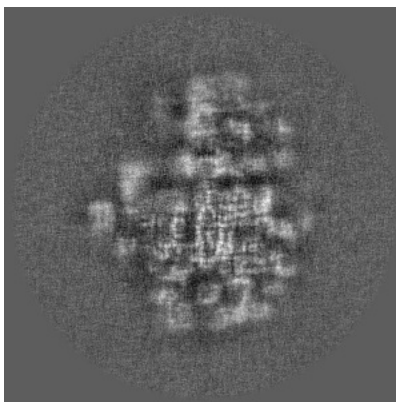


Z Index: 182

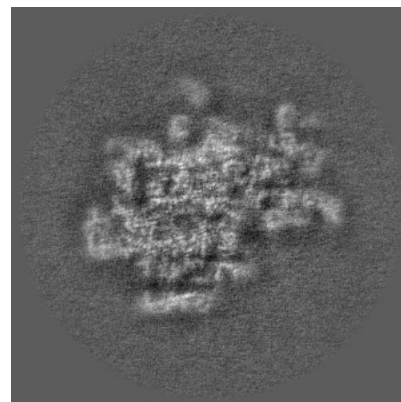
### 6.3.2 Raw map



X Index: 163



Y Index: 183

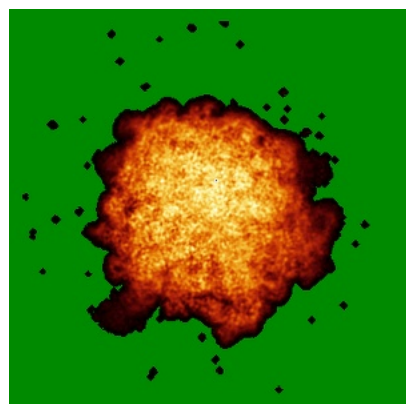


Z Index: 179

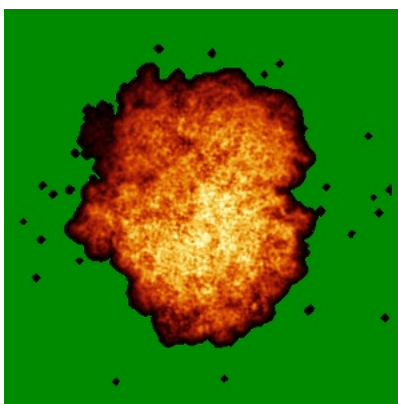
The images above show the largest variance slices of the map in three orthogonal directions.

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

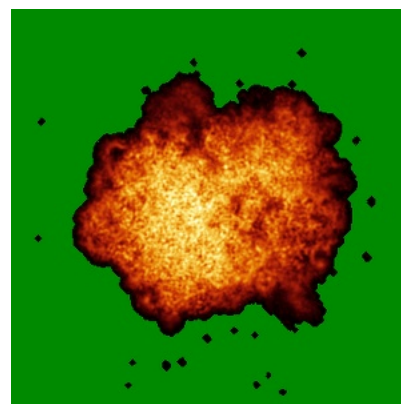
### 6.4.1 Primary map



X

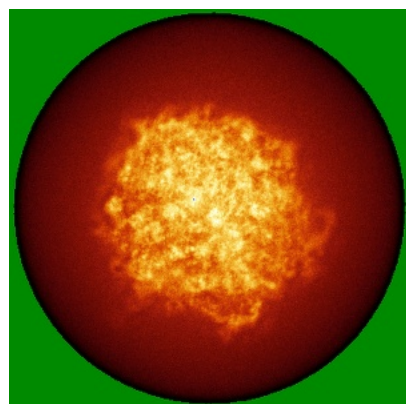


Y

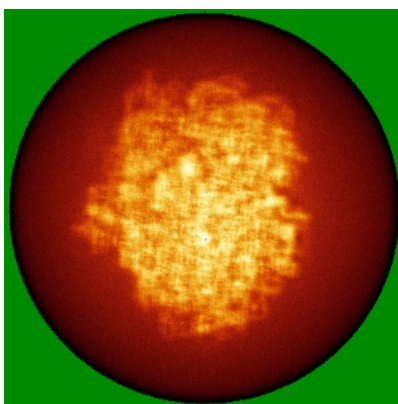


Z

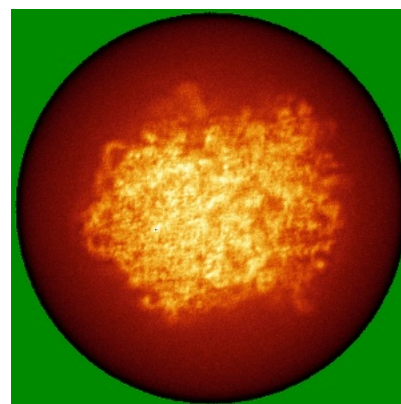
### 6.4.2 Raw map



X



Y



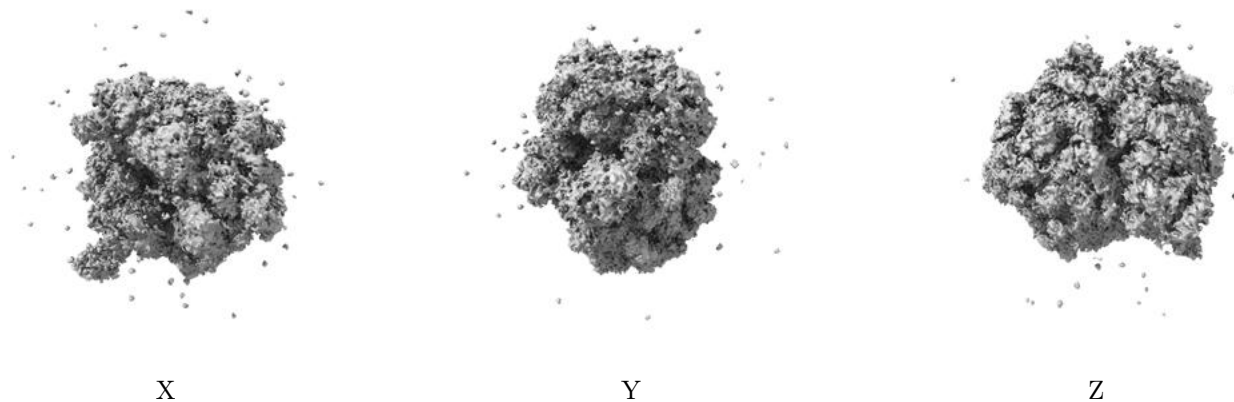
Z

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.



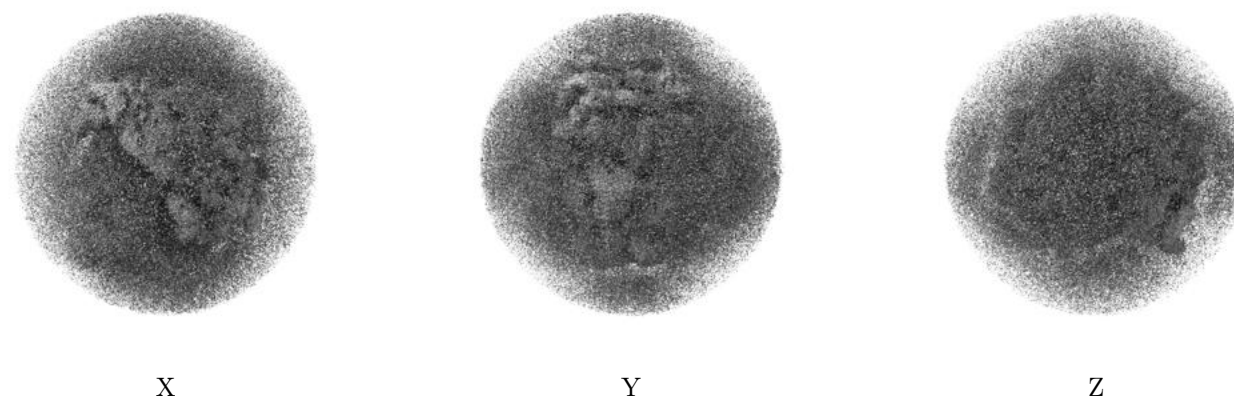
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.43. 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.

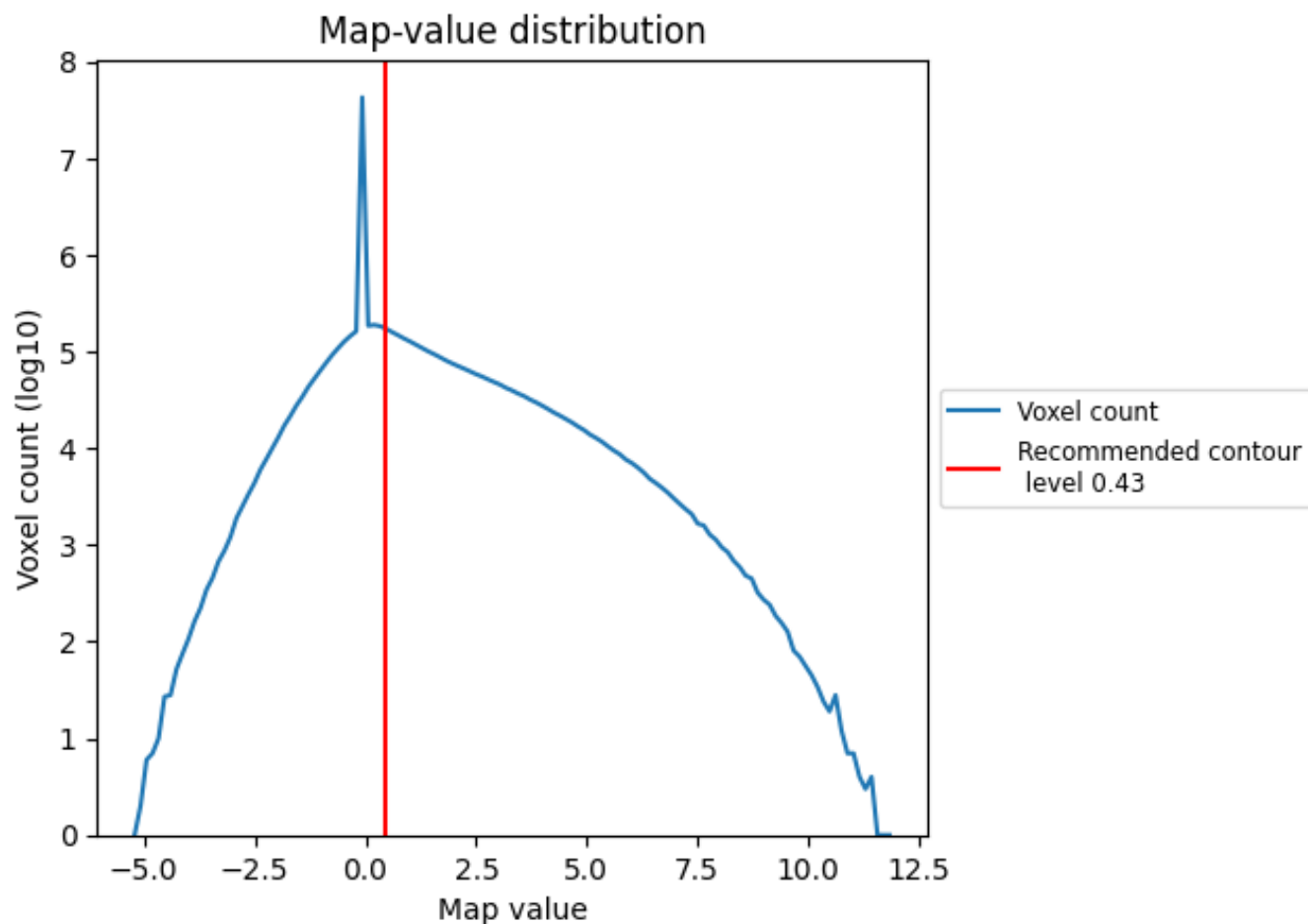
## 6.6 Mask visualisation [i](#)

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.

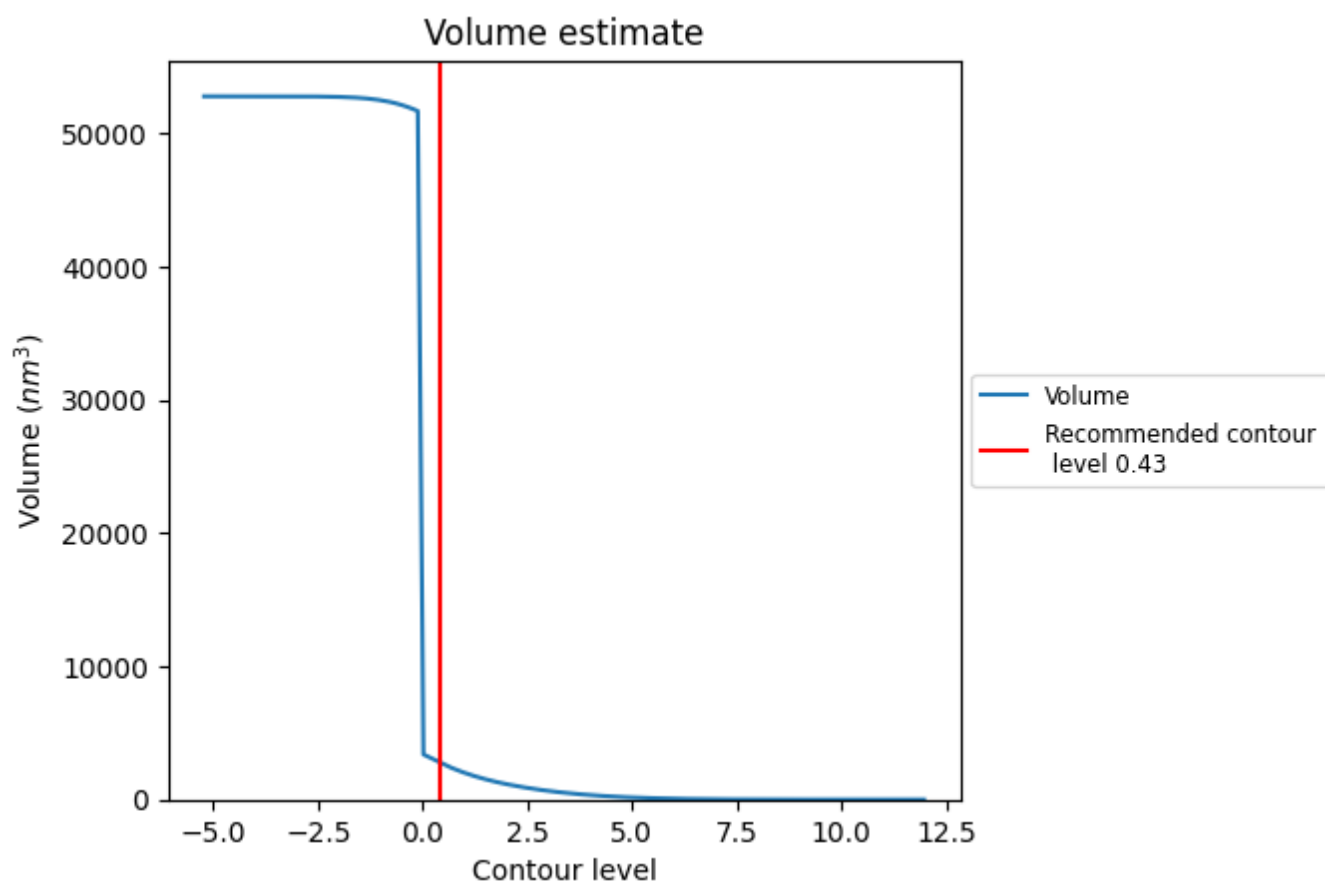
### 7.1 Map-value distribution [i](#)



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.



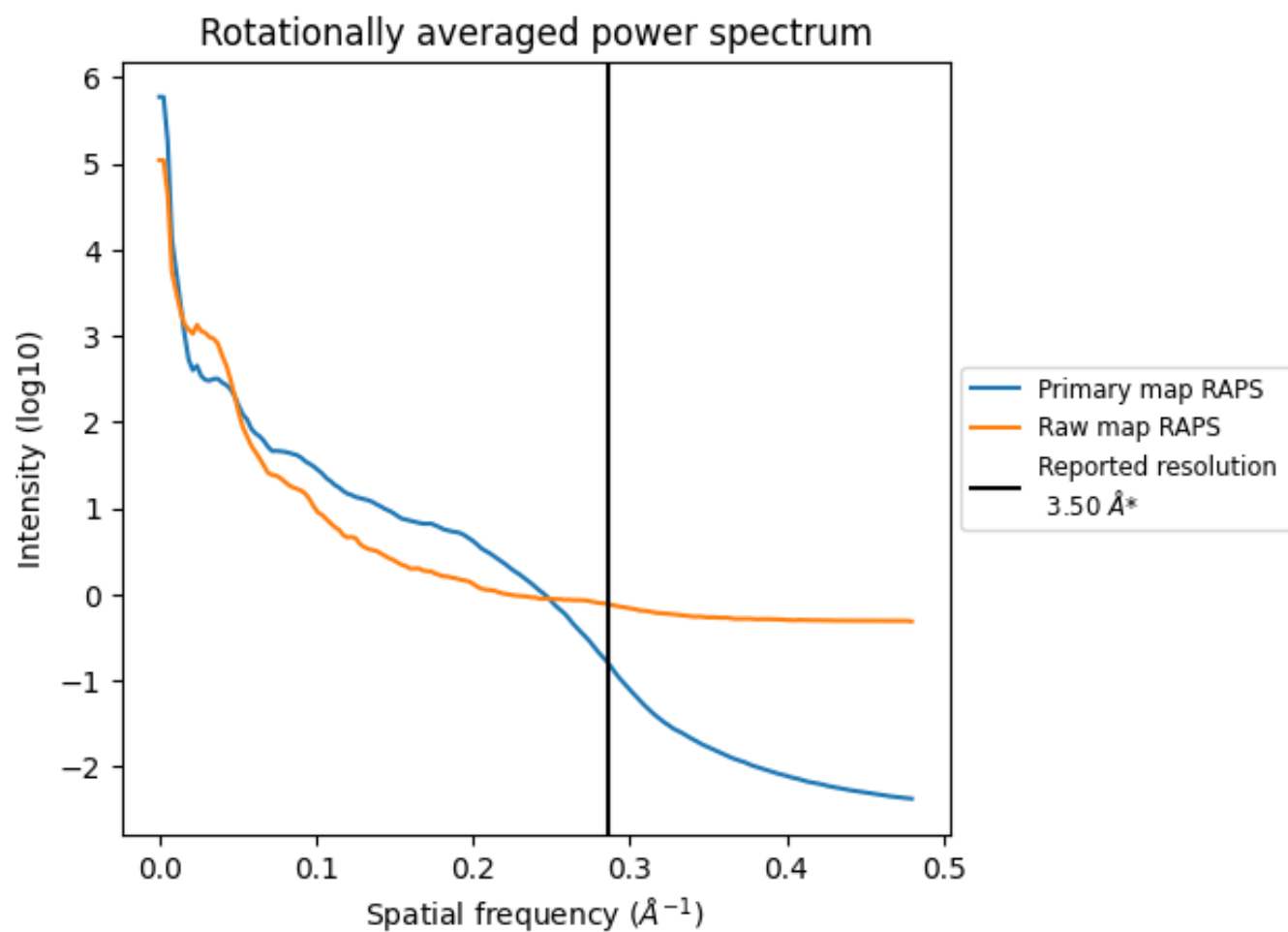
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2750 nm<sup>3</sup>; this corresponds to an approximate mass of 2484 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 ⓘ

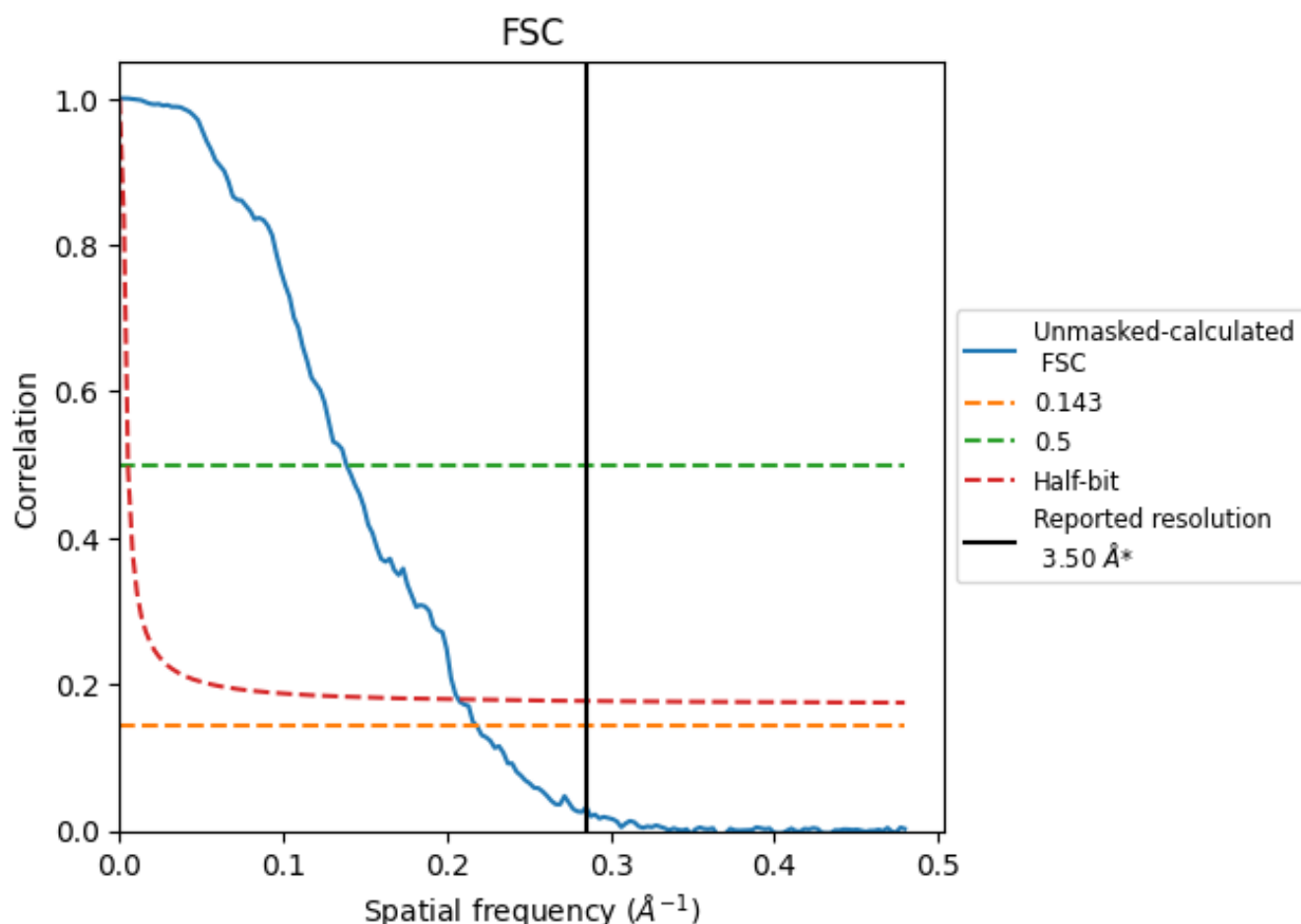


\*Reported resolution corresponds to spatial frequency of 0.286  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

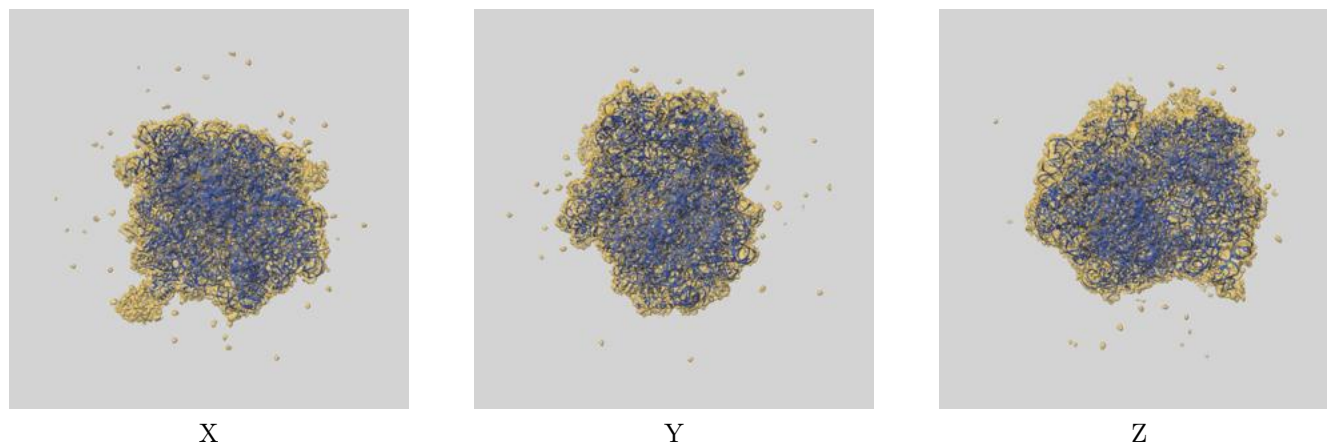
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.58	7.22	4.83

\*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 4.58 differs from the reported value 3.5 by more than 10 %

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

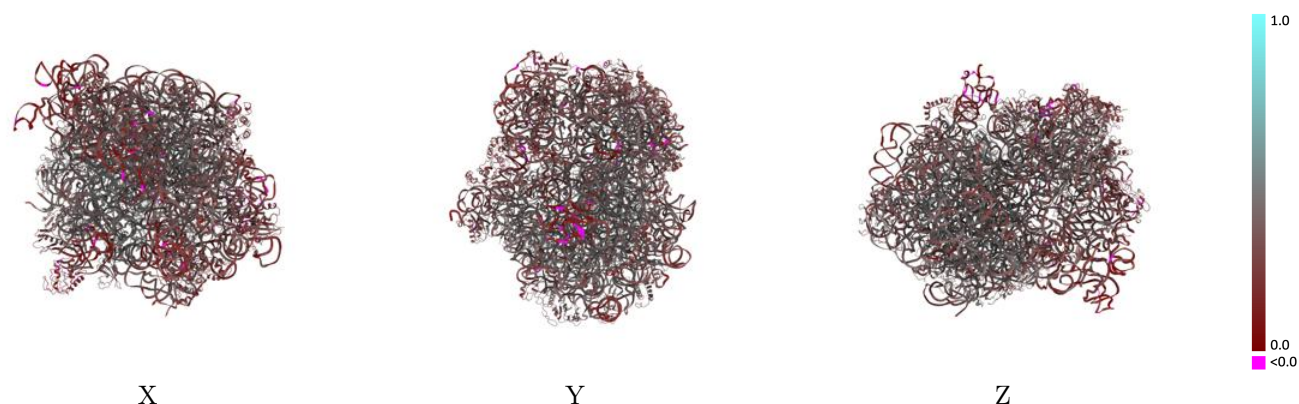
This section contains information regarding the fit between EMDB map EMD-22469 and PDB model 7JT2. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

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



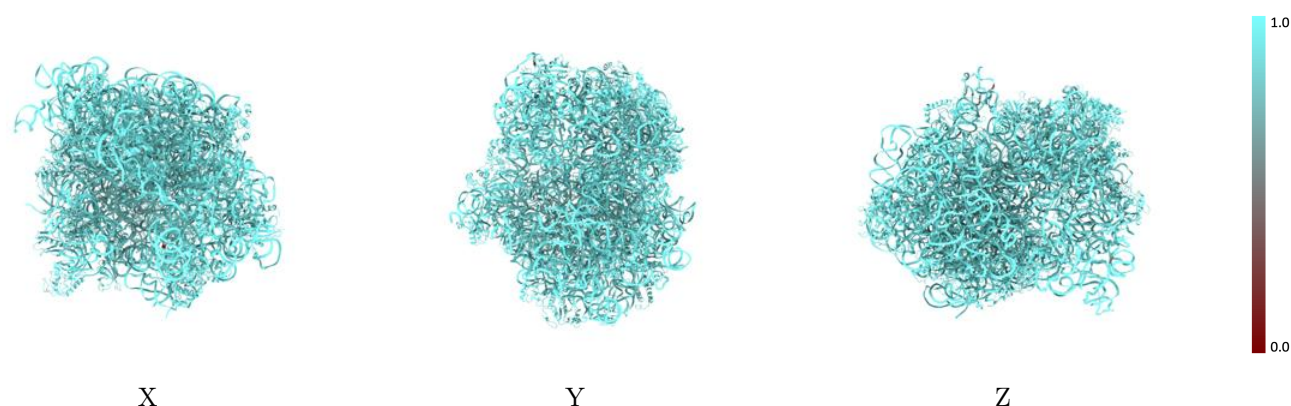
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



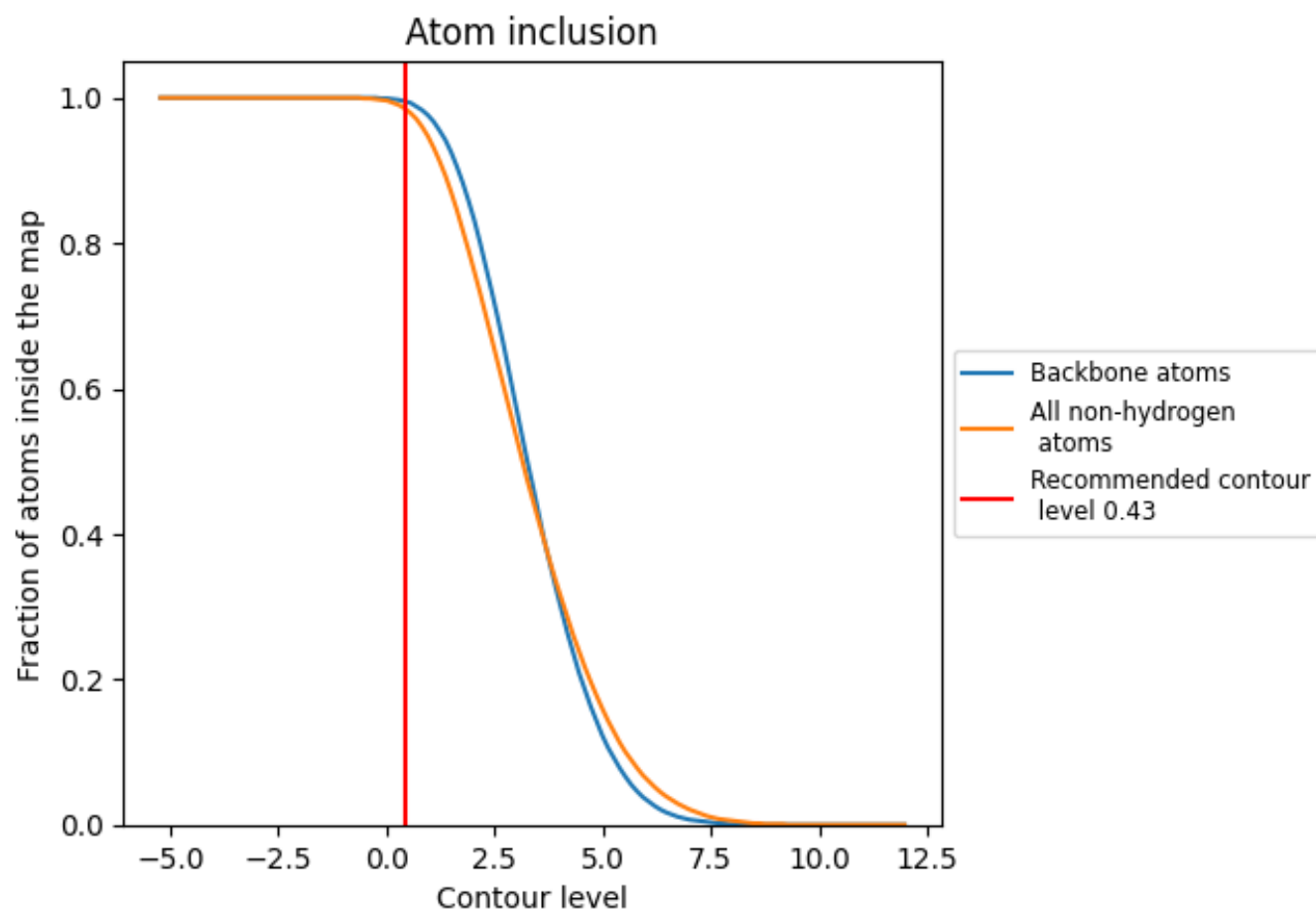
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.43).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.43) and Q-score for the entire model and for each chain.











































Chain	Atom inclusion	Q-score
All	 0.9850	 0.3660
1	 0.9930	 0.3880
2	 0.9950	 0.3270
3	 0.9910	 0.3380
4	 0.9720	 0.2130
5	 0.9870	 0.2890
8	 0.9400	 0.3190
B	 0.9700	 0.4110
C	 0.9750	 0.3730
D	 0.9750	 0.4490
E	 0.9780	 0.4270
F	 0.9760	 0.4220
G	 0.9620	 0.3140
H	 0.9680	 0.3520
I	 0.9470	 0.2780
J	 0.9740	 0.3840
K	 0.9760	 0.3470
L	 0.9750	 0.3080
M	 0.9650	 0.3540
N	 0.9610	 0.3130
O	 0.9210	 0.3180
P	 0.9800	 0.3610
Q	 0.9740	 0.3570
R	 0.9670	 0.3140
S	 0.9420	 0.3180
T	 0.9780	 0.3580
U	 0.9510	 0.3430
V	 0.9870	 0.3610
W	 0.9630	 0.3730
X	 0.9870	 0.2990
Y	 0.9540	 0.2790
Z	 0.9300	 0.3250
b	 0.9780	 0.4510
c	 0.9730	 0.4310
d	 0.9770	 0.3940



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Chain	Atom inclusion	Q-score
e	 0.9810	 0.3000
f	 0.9880	 0.3550
g	 0.9830	 0.3060
h	 0.9380	 0.1850
j	 0.9740	 0.4160
k	 0.9800	 0.4170
l	 0.9650	 0.3970
m	 0.9700	 0.4190
n	 0.9630	 0.4180
o	 0.9660	 0.3400
p	 0.9850	 0.4160
q	 0.9750	 0.4230
r	 0.9700	 0.3960
s	 0.9740	 0.4190
t	 0.9680	 0.4020
u	 0.9870	 0.3720
v	 0.9780	 0.3910
w	 0.9710	 0.4300
x	 0.9930	 0.4340
y	 0.9700	 0.3330
z	 0.9860	 0.4030