



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 11:48 PM EST

PDB ID : 7JT1
EMDB ID : EMD-22466
Title : 70S ribosome stalled on long mRNA with ArfB-1 and ArfB-2 bound (+9-III)
Authors : Carbone, C.E.; Korostelev, A.A.
Deposited on : 2020-08-16
Resolution : 3.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

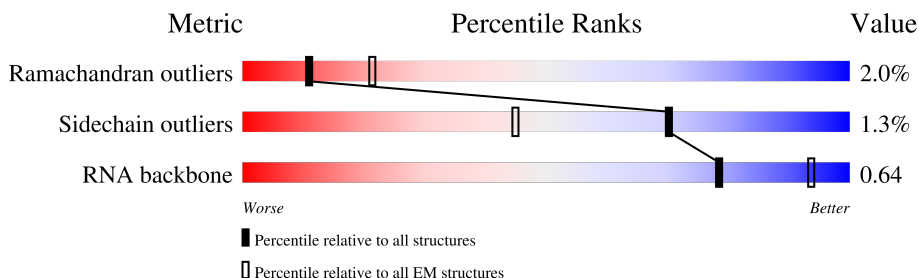
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



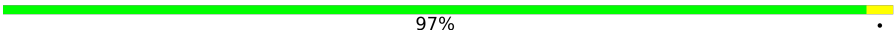
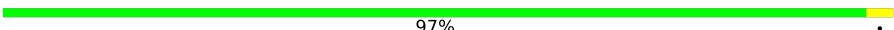
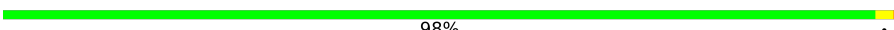
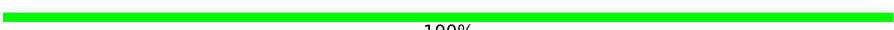
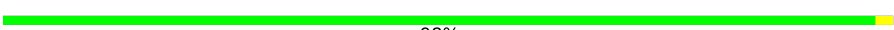





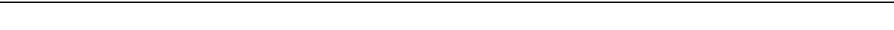

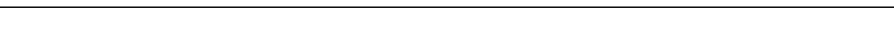
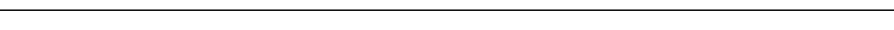
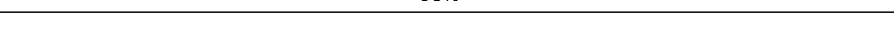
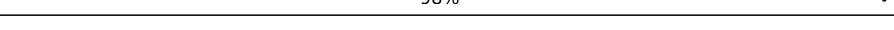
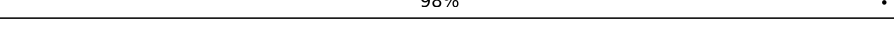
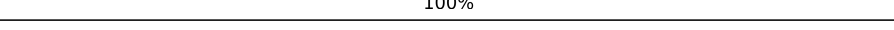
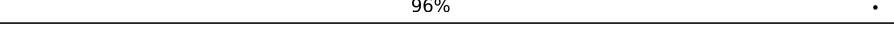
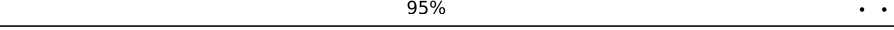
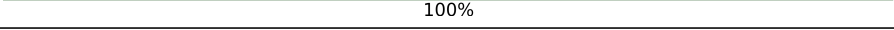
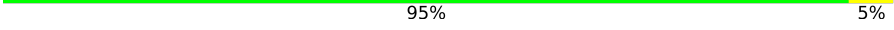
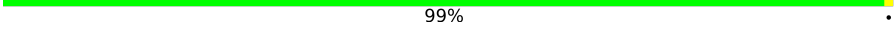
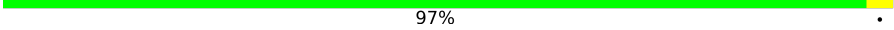
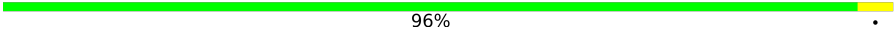
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	j	142	
8	k	122	

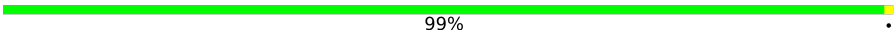
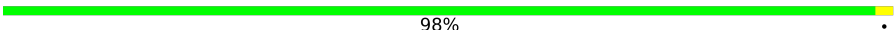
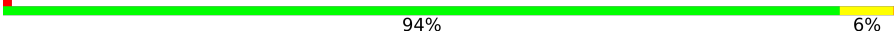

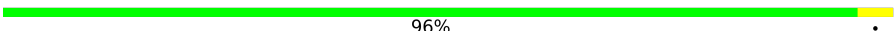
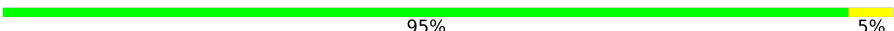

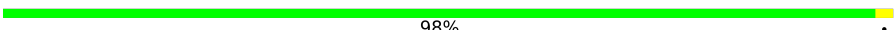
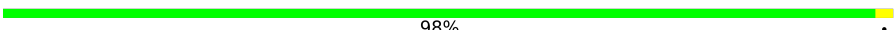
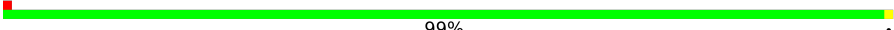


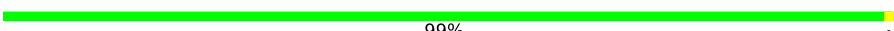
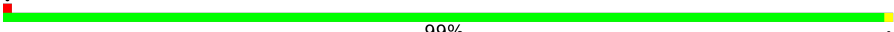








Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	L	151	 99% .
35	M	129	 98% .
36	N	127	 94% 6% .
37	O	98	 92% 8%
38	P	116	 96% .
39	Q	123	 95% 5%
40	R	114	 98% .
41	S	100	 98% .
42	T	88	 98% .
43	U	82	 99% .
44	V	80	 92% 8%
45	W	65	 94% 6%
46	X	79	 99% .
47	Y	85	 99% .
48	Z	65	 92% 8%
49	3	1539	 90% 10%
50	1	2903	 87% 13%
51	2	120	 89% 11%
52	5	77	 88% 12%
53	4	20	 80% 20%
54	8	130	 91% 9%
54	9	130	 56% 6% 38%

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 145600 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 L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

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

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

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

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

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

- Molecule 18 is a protein called 50S ribosomal protein L24.

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

- Molecule 19 is a protein called 50S ribosomal protein L25.

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

- Molecule 20 is a protein called 50S ribosomal protein L27.

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

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

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a protein called 50S ribosomal protein L36.

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

- Molecule 29 is a protein called 30S ribosomal protein S2.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S4.

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

- Molecule 32 is a protein called 30S ribosomal protein S5.

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

- Molecule 33 is a protein called 30S ribosomal protein S6.

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

- Molecule 34 is a protein called 30S ribosomal protein S7.

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

- Molecule 35 is a protein called 30S ribosomal protein S8.

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

- Molecule 36 is a protein called 30S ribosomal protein S9.

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

- Molecule 37 is a protein called 30S ribosomal protein S10.

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

- Molecule 38 is a protein called 30S ribosomal protein S11.

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

- Molecule 39 is a protein called 30S ribosomal protein S12.

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

- Molecule 40 is a protein called 30S ribosomal protein S13.

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

- Molecule 41 is a protein called 30S ribosomal protein S14.

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

- Molecule 42 is a protein called 30S ribosomal protein S15.

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

- Molecule 43 is a protein called 30S ribosomal protein S16.

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

- Molecule 44 is a protein called 30S ribosomal protein S17.

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

- Molecule 45 is a protein called 30S ribosomal protein S18.

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

- Molecule 46 is a protein called 30S ribosomal protein S19.

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

- Molecule 47 is a protein called 30S ribosomal protein S20.

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

- Molecule 48 is a protein called 30S ribosomal protein S21.

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

- Molecule 49 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	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 50 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	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 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	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 52 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	20	Total	C	N	O	P	0	0
			439	197	91	131	20		

- Molecule 54 is a protein called Peptidyl-tRNA hydrolase ArfB.

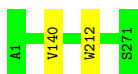
Mol	Chain	Residues	Atoms					AltConf	Trace
54	8	130	Total	C	N	O	S	0	0
			1016	627	202	185	2		
54	9	81	Total	C	N	O	S	0	0
			641	405	116	119	1		

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:  99%



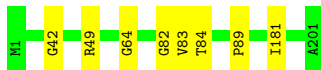
- Molecule 2: 50S ribosomal protein L3

Chain c:  98%



- Molecule 3: 50S ribosomal protein L4

Chain d:  96%



- Molecule 4: 50S ribosomal protein L5

Chain e:  96%



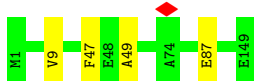
- Molecule 5: 50S ribosomal protein L6

Chain f:  98%



- Molecule 6: 50S ribosomal protein L9

Chain g:  97%



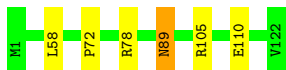
- Molecule 7: 50S ribosomal protein L13

Chain j:  98%



- Molecule 8: 50S ribosomal protein L14

Chain k:  95%



- Molecule 9: 50S ribosomal protein L15

Chain l:  97%



- Molecule 10: 50S ribosomal protein L16

Chain m:  97%



- Molecule 11: 50S ribosomal protein L17

Chain n:  98%



- Molecule 12: 50S ribosomal protein L18

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 50S ribosomal protein L19

Chain p:  98%



- Molecule 14: 50S ribosomal protein L20

Chain q:  99%



- Molecule 15: 50S ribosomal protein L21

Chain r:  96%



- Molecule 16: 50S ribosomal protein L22

Chain s:  98%



- Molecule 17: 50S ribosomal protein L23

Chain t:  99%



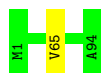
- Molecule 18: 50S ribosomal protein L24

Chain u:  97%



- Molecule 19: 50S ribosomal protein L25

Chain v:  99%



- Molecule 20: 50S ribosomal protein L27

Chain w:  99%



- Molecule 21: 50S ribosomal protein L28

Chain x: 99%



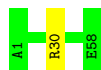
- Molecule 22: 50S ribosomal protein L29

Chain y: 98%



- Molecule 23: 50S ribosomal protein L30

Chain z: 98%



- Molecule 24: 50S ribosomal protein L32

Chain B: 98%



- Molecule 25: 50S ribosomal protein L33

Chain C: 100%

There are no outlier residues recorded for this chain.

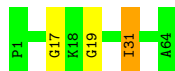
- Molecule 26: 50S ribosomal protein L34

Chain D: 96%



- Molecule 27: 50S ribosomal protein L35

Chain E: 95%



- Molecule 28: 50S ribosomal protein L36

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 30S ribosomal protein S2

Chain G:  95%  5%



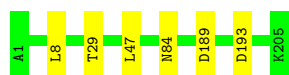
- Molecule 30: 30S ribosomal protein S3

Chain H:  99%  .



- Molecule 31: 30S ribosomal protein S4

Chain I:  97%  .



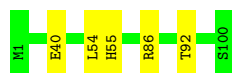
- Molecule 32: 30S ribosomal protein S5

Chain J:  96%  .



- Molecule 33: 30S ribosomal protein S6

Chain K:  95%  5%

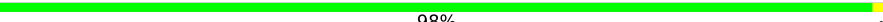


- Molecule 34: 30S ribosomal protein S7

Chain L:  99%  .



- Molecule 35: 30S ribosomal protein S8

Chain M:  98% .



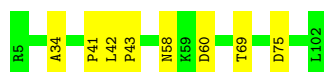
- Molecule 36: 30S ribosomal protein S9

Chain N:  94% 6% .



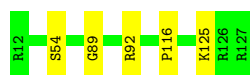
- Molecule 37: 30S ribosomal protein S10

Chain O:  92% 8% .



- Molecule 38: 30S ribosomal protein S11

Chain P:  96% .



- Molecule 39: 30S ribosomal protein S12

Chain Q:  95% 5% .



- Molecule 40: 30S ribosomal protein S13

Chain R:  98% .



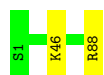
- Molecule 41: 30S ribosomal protein S14

Chain S:  98% .



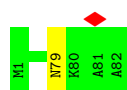
- Molecule 42: 30S ribosomal protein S15

Chain T:  98% .



- Molecule 43: 30S ribosomal protein S16

Chain U:  99% .



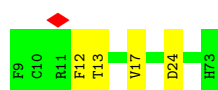
- Molecule 44: 30S ribosomal protein S17

Chain V:  92% 8%



- Molecule 45: 30S ribosomal protein S18

Chain W:  94% 6%



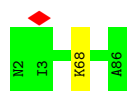
- Molecule 46: 30S ribosomal protein S19

Chain X:  99% .



- Molecule 47: 30S ribosomal protein S20

Chain Y:  99% .



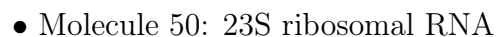
- Molecule 48: 30S ribosomal protein S21

Chain Z:  92% 8%



- Molecule 49: 16S ribosomal RNA

Frequency	Percentage
Often	90%
Rarely	10%



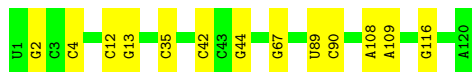
Satisfaction Level	Percentage
Very satisfied	87%
Satisfied	13%





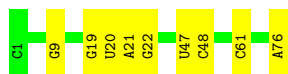
- Molecule 51: 5S ribosomal RNA

Chain 2: 89% 11%



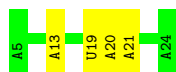
- Molecule 52: tRNAfMet

Chain 5: 88% 12%



- Molecule 53: mRNA

Chain 4: 80% 20%



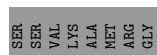
- Molecule 54: Peptidyl-tRNA hydrolase ArfB

Chain 8: 91% 9%



- Molecule 54: Peptidyl-tRNA hydrolase ArfB

Chain 9: 56% 6% 38%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14367	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	12.124	Depositor
Minimum map value	-4.894	Depositor
Average map value	0.097	Depositor
Map value standard deviation	0.600	Depositor
Recommended contour level	0.6	Depositor
Map size (\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 (\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	0.36	0/2122	0.60	0/2852
2	c	0.38	0/1586	0.62	0/2134
3	d	0.33	0/1571	0.59	1/2113 (0.0%)
4	e	0.36	0/1435	0.59	0/1926
5	f	0.30	0/1343	0.59	0/1816
6	g	0.34	0/1122	0.64	0/1515
7	j	0.36	0/1152	0.58	0/1551
8	k	0.37	0/948	0.62	0/1268
9	l	0.36	0/1054	0.61	0/1403
10	m	0.40	0/1093	0.58	0/1460
11	n	0.38	0/974	0.58	0/1301
12	o	0.30	0/902	0.56	0/1209
13	p	0.36	0/929	0.57	0/1242
14	q	0.40	0/960	0.54	0/1278
15	r	0.39	0/829	0.66	1/1107 (0.1%)
16	s	0.34	0/864	0.64	0/1156
17	t	0.32	0/745	0.54	0/994
18	u	0.33	0/788	0.56	0/1051
19	v	0.34	0/766	0.56	0/1025
20	w	0.39	0/582	0.54	0/769
21	x	0.36	0/635	0.56	0/848
22	y	0.30	0/510	0.54	0/677
23	z	0.31	0/453	0.52	0/605
24	B	0.34	0/450	0.58	0/599
25	C	0.38	0/417	0.54	0/554
26	D	0.42	0/380	0.65	0/498
27	E	0.40	0/513	0.57	0/676
28	F	0.31	0/303	0.57	0/397
29	G	0.34	0/1788	0.64	2/2408 (0.1%)
30	H	0.32	0/1652	0.56	0/2225
31	I	0.32	0/1665	0.62	0/2227
32	J	0.34	0/1170	0.61	0/1573
33	K	0.34	0/836	0.63	0/1128
34	L	0.31	0/1196	0.52	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	M	0.31	0/989	0.59	0/1326
36	N	0.32	0/1034	0.64	0/1375
37	O	0.32	0/797	0.62	0/1077
38	P	0.35	0/886	0.60	0/1195
39	Q	0.30	0/969	0.68	0/1300
40	R	0.29	0/893	0.62	0/1193
41	S	0.31	0/817	0.55	0/1088
42	T	0.32	0/722	0.59	0/964
43	U	0.34	0/659	0.60	0/884
44	V	0.33	0/658	0.65	0/881
45	W	0.36	0/545	0.58	0/731
46	X	0.34	0/653	0.57	0/877
47	Y	0.31	0/671	0.55	0/888
48	Z	0.38	0/551	0.66	0/728
49	3	0.33	0/36963	0.66	0/57662
50	1	0.36	0/69794	0.66	2/108883 (0.0%)
51	2	0.33	0/2872	0.65	0/4479
52	5	0.33	0/1832	0.65	0/2855
53	4	0.41	0/495	0.68	0/771
54	8	0.28	0/1028	0.51	0/1378
54	9	0.32	0/649	0.74	0/875
All	All	0.35	0/158210	0.64	6/236597 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
50	1	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	32	GLY	N-CA-C	7.76	132.49	113.10
29	G	33	ALA	N-CA-C	6.51	128.57	111.00
50	1	974	G	N9-C1'-C2'	5.99	121.79	114.00
3	d	82	GLY	N-CA-C	5.81	127.64	113.10
15	r	50	GLY	N-CA-C	-5.81	98.58	113.10
50	1	1178	C	N1-C1'-C2'	5.67	121.37	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	1	512	G	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	244 (91%)	25 (9%)	0	100	100
2	c	207/209 (99%)	192 (93%)	12 (6%)	3 (1%)	11	38
3	d	199/201 (99%)	182 (92%)	11 (6%)	6 (3%)	4	24
4	e	175/177 (99%)	156 (89%)	15 (9%)	4 (2%)	6	29
5	f	174/176 (99%)	160 (92%)	12 (7%)	2 (1%)	14	45
6	g	147/149 (99%)	119 (81%)	24 (16%)	4 (3%)	5	26
7	j	140/142 (99%)	126 (90%)	12 (9%)	2 (1%)	11	38
8	k	120/122 (98%)	104 (87%)	13 (11%)	3 (2%)	5	27
9	l	141/143 (99%)	120 (85%)	18 (13%)	3 (2%)	7	31
10	m	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	10	38
11	n	118/120 (98%)	103 (87%)	14 (12%)	1 (1%)	19	51
12	o	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
13	p	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
14	q	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	17	48
15	r	101/103 (98%)	84 (83%)	15 (15%)	2 (2%)	7	32
16	s	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	17	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	t	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
18	u	100/102 (98%)	88 (88%)	9 (9%)	3 (3%)	4	24
19	v	92/94 (98%)	80 (87%)	12 (13%)	0	100	100
20	w	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	11	38
21	x	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	12	40
22	y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
23	z	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
24	B	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	8	34
25	C	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
26	D	44/46 (96%)	38 (86%)	6 (14%)	0	100	100
27	E	62/64 (97%)	52 (84%)	7 (11%)	3 (5%)	2	14
28	F	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
29	G	223/225 (99%)	190 (85%)	27 (12%)	6 (3%)	5	26
30	H	204/206 (99%)	188 (92%)	14 (7%)	2 (1%)	15	46
31	I	203/205 (99%)	175 (86%)	24 (12%)	4 (2%)	7	32
32	J	155/157 (99%)	132 (85%)	18 (12%)	5 (3%)	4	22
33	K	98/100 (98%)	75 (76%)	19 (19%)	4 (4%)	3	17
34	L	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	22	54
35	M	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	51
36	N	125/127 (98%)	101 (81%)	18 (14%)	6 (5%)	2	14
37	O	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	2	13
38	P	114/116 (98%)	92 (81%)	17 (15%)	5 (4%)	2	16
39	Q	121/123 (98%)	98 (81%)	18 (15%)	5 (4%)	3	17
40	R	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	8	35
41	S	98/100 (98%)	84 (86%)	13 (13%)	1 (1%)	15	46
42	T	86/88 (98%)	76 (88%)	9 (10%)	1 (1%)	13	42
43	U	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	12	40
44	V	78/80 (98%)	56 (72%)	18 (23%)	4 (5%)	2	13
45	W	63/65 (97%)	56 (89%)	4 (6%)	3 (5%)	2	14
46	X	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
47	Y	83/85 (98%)	79 (95%)	3 (4%)	1 (1%)	13	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	Z	63/65 (97%)	42 (67%)	16 (25%)	5 (8%)	1	6
54	8	128/130 (98%)	103 (80%)	18 (14%)	7 (6%)	2	11
54	9	77/130 (59%)	55 (71%)	17 (22%)	5 (6%)	1	9
All	All	5726/5877 (97%)	4989 (87%)	620 (11%)	117 (2%)	11	32

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	49	ARG
3	d	84	THR
6	g	9	VAL
9	l	31	GLY
10	m	28	PHE
24	B	25	THR
29	G	15	PHE
29	G	193	ASP
32	J	11	GLN
32	J	93	VAL
36	N	57	VAL
36	N	99	LYS
37	O	58	ASN
39	Q	3	VAL
39	Q	87	LYS
42	T	46	LYS
43	U	79	ASN
44	V	15	LYS
44	V	17	GLU
45	W	13	THR
48	Z	25	ALA
54	9	47	SER
54	9	70	ILE
54	9	78	ARG
2	c	86	GLU
2	c	138	LEU
2	c	174	SER
3	d	64	GLY
3	d	83	VAL
4	e	135	ILE
5	f	39	ALA
5	f	117	PRO
6	g	87	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	k	110	GLU
11	n	116	VAL
15	r	26	ASP
16	s	66	ILE
18	u	6	ARG
20	w	9	GLY
27	E	31	ILE
29	G	73	ARG
31	I	47	LEU
33	K	40	GLU
33	K	54	LEU
35	M	47	ASP
36	N	12	LYS
36	N	90	ASP
36	N	100	ALA
37	O	34	ALA
38	P	54	SER
38	P	92	ARG
39	Q	77	SER
40	R	14	ALA
44	V	78	VAL
48	Z	24	LYS
54	8	47	SER
54	8	100	THR
4	e	173	ASP
6	g	49	ALA
7	j	126	ALA
9	l	29	LYS
10	m	69	PRO
27	E	19	GLY
29	G	192	PRO
32	J	80	LEU
33	K	86	ARG
33	K	92	THR
37	O	43	PRO
38	P	125	LYS
39	Q	33	CYS
48	Z	34	ARG
54	8	131	MET
54	9	6	ARG
6	g	47	PHE
9	l	94	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	G	101	THR
30	H	47	ALA
45	W	12	PHE
47	Y	68	LYS
48	Z	8	ASN
48	Z	15	LEU
54	8	26	GLY
54	8	70	ILE
54	9	48	LEU
3	d	89	PRO
4	e	93	GLU
4	e	138	PRO
8	k	72	PRO
8	k	89	ASN
18	u	30	SER
31	I	29	THR
31	I	84	ASN
32	J	50	GLY
32	J	122	VAL
37	O	42	LEU
54	8	105	ARG
7	j	110	PRO
14	q	27	ARG
27	E	17	GLY
31	I	193	ASP
34	L	18	GLY
39	Q	35	ARG
41	S	69	PRO
15	r	58	VAL
21	x	6	VAL
29	G	194	GLY
38	P	89	GLY
40	R	9	PRO
45	W	17	VAL
54	8	11	PRO
3	d	42	GLY
44	V	31	PRO
30	H	59	PRO
36	N	71	ILE
37	O	41	PRO
18	u	54	PRO
38	P	116	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	214 (99%)	2 (1%)	78	87
2	c	164/164 (100%)	162 (99%)	2 (1%)	71	83
3	d	165/165 (100%)	164 (99%)	1 (1%)	86	91
4	e	148/148 (100%)	145 (98%)	3 (2%)	55	76
5	f	137/137 (100%)	136 (99%)	1 (1%)	84	90
6	g	114/114 (100%)	114 (100%)	0	100	100
7	j	116/116 (100%)	115 (99%)	1 (1%)	78	87
8	k	103/103 (100%)	99 (96%)	4 (4%)	32	62
9	l	102/102 (100%)	100 (98%)	2 (2%)	55	76
10	m	109/109 (100%)	107 (98%)	2 (2%)	59	78
11	n	100/100 (100%)	97 (97%)	3 (3%)	41	68
12	o	86/86 (100%)	86 (100%)	0	100	100
13	p	99/99 (100%)	97 (98%)	2 (2%)	55	76
14	q	89/89 (100%)	89 (100%)	0	100	100
15	r	84/84 (100%)	83 (99%)	1 (1%)	71	83
16	s	93/93 (100%)	92 (99%)	1 (1%)	73	85
17	t	80/80 (100%)	79 (99%)	1 (1%)	69	82
18	u	83/83 (100%)	83 (100%)	0	100	100
19	v	78/78 (100%)	77 (99%)	1 (1%)	69	82
20	w	57/57 (100%)	57 (100%)	0	100	100
21	x	67/67 (100%)	67 (100%)	0	100	100
22	y	55/55 (100%)	54 (98%)	1 (2%)	59	78
23	z	48/48 (100%)	47 (98%)	1 (2%)	53	75
24	B	47/47 (100%)	47 (100%)	0	100	100
25	C	45/45 (100%)	45 (100%)	0	100	100
26	D	38/38 (100%)	36 (95%)	2 (5%)	22	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	E	51/51 (100%)	50 (98%)	1 (2%)	55	76
28	F	34/34 (100%)	34 (100%)	0	100	100
29	G	186/186 (100%)	182 (98%)	4 (2%)	52	74
30	H	170/170 (100%)	170 (100%)	0	100	100
31	I	172/172 (100%)	170 (99%)	2 (1%)	71	83
32	J	119/119 (100%)	117 (98%)	2 (2%)	60	78
33	K	87/87 (100%)	86 (99%)	1 (1%)	73	85
34	L	124/124 (100%)	124 (100%)	0	100	100
35	M	104/104 (100%)	103 (99%)	1 (1%)	76	86
36	N	105/105 (100%)	102 (97%)	3 (3%)	42	69
37	O	86/86 (100%)	83 (96%)	3 (4%)	36	64
38	P	89/89 (100%)	89 (100%)	0	100	100
39	Q	103/103 (100%)	102 (99%)	1 (1%)	76	86
40	R	92/92 (100%)	92 (100%)	0	100	100
41	S	83/83 (100%)	82 (99%)	1 (1%)	71	83
42	T	76/76 (100%)	75 (99%)	1 (1%)	69	82
43	U	65/65 (100%)	65 (100%)	0	100	100
44	V	74/74 (100%)	72 (97%)	2 (3%)	44	71
45	W	56/56 (100%)	55 (98%)	1 (2%)	59	78
46	X	70/70 (100%)	69 (99%)	1 (1%)	67	82
47	Y	65/65 (100%)	65 (100%)	0	100	100
48	Z	55/55 (100%)	55 (100%)	0	100	100
54	8	106/106 (100%)	101 (95%)	5 (5%)	26	57
54	9	68/106 (64%)	65 (96%)	3 (4%)	28	59
All	All	4763/4801 (99%)	4700 (99%)	63 (1%)	70	82

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	140	VAL
1	b	212	TRP
2	c	33	ARG
2	c	149	ASN
3	d	181	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	e	19	PHE
4	e	112	ASP
4	e	156	THR
5	f	68	ARG
7	j	57	LEU
8	k	58	LEU
8	k	78	ARG
8	k	89	ASN
8	k	105	ARG
9	l	6	LEU
9	l	81	ASP
10	m	64	TRP
10	m	91	TYR
11	n	2	ARG
11	n	8	ARG
11	n	116	VAL
13	p	65	ASN
13	p	102	ARG
15	r	78	ARG
16	s	97	LEU
17	t	73	ARG
19	v	65	VAL
22	y	2	LYS
23	z	30	ARG
26	D	9	VAL
26	D	42	LEU
27	E	31	ILE
29	G	91	VAL
29	G	94	ARG
29	G	150	ILE
29	G	202	ASN
31	I	8	LEU
31	I	189	ASP
32	J	55	VAL
32	J	95	MET
33	K	55	HIS
35	M	95	MET
36	N	60	LEU
36	N	99	LYS
36	N	122	ARG
37	O	60	ASP
37	O	69	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	O	75	ASP
39	Q	73	LEU
41	S	32	ASP
42	T	88	ARG
44	V	73	THR
44	V	77	VAL
45	W	24	ASP
46	X	11	ASP
54	8	50	GLU
54	8	52	TYR
54	8	53	LYS
54	8	54	GLU
54	8	108	THR
54	9	7	HIS
54	9	8	VAL
54	9	64	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	44	ASN
1	b	45	ASN
1	b	57	HIS
1	b	89	ASN
1	b	250	GLN
1	b	259	ASN
2	c	150	GLN
3	d	41	GLN
3	d	97	ASN
4	e	51	ASN
4	e	126	ASN
5	f	115	GLN
7	j	40	HIS
7	j	67	ASN
7	j	80	HIS
7	j	130	HIS
7	j	135	GLN
7	j	136	GLN
8	k	5	GLN
8	k	89	ASN
8	k	93	GLN
9	l	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	l	93	ASN
9	l	104	GLN
11	n	3	HIS
11	n	9	GLN
11	n	13	ASN
11	n	23	ASN
11	n	62	ASN
12	o	100	HIS
13	p	6	GLN
14	q	36	GLN
14	q	58	GLN
15	r	66	HIS
15	r	82	HIS
16	s	61	ASN
17	t	15	HIS
18	u	73	ASN
19	v	44	HIS
19	v	49	ASN
20	w	36	GLN
21	x	15	ASN
21	x	16	ASN
21	x	22	ASN
21	x	33	HIS
22	y	15	ASN
22	y	20	ASN
22	y	38	GLN
24	B	41	HIS
27	E	27	ASN
28	F	13	ASN
29	G	202	ASN
30	H	31	ASN
30	H	139	ASN
30	H	184	ASN
30	H	189	HIS
31	I	84	ASN
31	I	88	ASN
31	I	119	HIS
31	I	125	ASN
31	I	130	ASN
32	J	96	GLN
33	K	63	ASN
34	L	129	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	M	17	GLN
36	N	74	GLN
36	N	125	GLN
38	P	63	GLN
39	Q	4	ASN
42	T	27	GLN
42	T	61	GLN
42	T	79	GLN
43	U	18	GLN
44	V	30	HIS
45	W	30	ASN
45	W	51	GLN
47	Y	2	ASN
47	Y	67	HIS
47	Y	83	ASN
54	8	7	HIS
54	8	23	GLN
54	8	38	HIS
54	8	61	HIS
54	8	62	HIS
54	8	75	GLN
54	8	83	ASN
54	8	124	GLN
54	9	80	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	3	1538/1539 (99%)	155 (10%)	1 (0%)
50	1	2902/2903 (99%)	378 (13%)	10 (0%)
51	2	119/120 (99%)	13 (10%)	0
52	5	76/77 (98%)	9 (11%)	0
53	4	19/20 (95%)	4 (21%)	0
All	All	4654/4659 (99%)	559 (12%)	11 (0%)

All (559) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
49	3	6	G
49	3	9	G
49	3	22	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	3	31	G
49	3	32	A
49	3	39	G
49	3	48	C
49	3	49	U
49	3	51	A
49	3	71	A
49	3	82	G
49	3	83	C
49	3	87	C
49	3	100	G
49	3	144	G
49	3	146	G
49	3	183	C
49	3	210	C
49	3	212	G
49	3	226	G
49	3	247	G
49	3	251	G
49	3	266	G
49	3	267	C
49	3	280	C
49	3	281	G
49	3	289	G
49	3	316	C
49	3	345	C
49	3	351	G
49	3	352	C
49	3	367	U
49	3	372	C
49	3	412	A
49	3	422	C
49	3	423	G
49	3	429	U
49	3	441	A
49	3	448	A
49	3	480	U
49	3	486	U
49	3	518	C
49	3	524	G
49	3	533	A
49	3	547	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	3	559	A
49	3	561	U
49	3	566	G
49	3	572	A
49	3	573	A
49	3	575	G
49	3	576	C
49	3	577	G
49	3	633	G
49	3	642	A
49	3	665	A
49	3	687	A
49	3	688	G
49	3	703	G
49	3	713	G
49	3	724	G
49	3	755	G
49	3	777	A
49	3	814	A
49	3	817	C
49	3	818	G
49	3	819	A
49	3	821	G
49	3	842	U
49	3	843	U
49	3	844	G
49	3	845	A
49	3	846	G
49	3	847	G
49	3	890	G
49	3	902	G
49	3	926	G
49	3	934	C
49	3	935	A
49	3	960	U
49	3	961	U
49	3	966	G
49	3	969	A
49	3	971	G
49	3	975	A
49	3	976	G
49	3	977	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	3	992	U
49	3	993	G
49	3	994	A
49	3	1004	A
49	3	1029	U
49	3	1030	U
49	3	1031	C
49	3	1032	G
49	3	1033	G
49	3	1034	G
49	3	1053	G
49	3	1054	C
49	3	1094	G
49	3	1101	A
49	3	1108	G
49	3	1130	A
49	3	1136	C
49	3	1137	C
49	3	1138	G
49	3	1139	G
49	3	1159	U
49	3	1168	U
49	3	1182	G
49	3	1184	G
49	3	1191	A
49	3	1196	A
49	3	1198	G
49	3	1201	A
49	3	1202	U
49	3	1212	U
49	3	1213	A
49	3	1225	A
49	3	1227	A
49	3	1238	A
49	3	1241	G
49	3	1256	A
49	3	1258	G
49	3	1261	A
49	3	1275	A
49	3	1278	G
49	3	1280	A
49	3	1287	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	3	1299	A
49	3	1300	G
49	3	1317	C
49	3	1320	C
49	3	1336	C
49	3	1346	A
49	3	1347	G
49	3	1363	A
49	3	1378	C
49	3	1381	U
49	3	1394	A
49	3	1395	C
49	3	1398	A
49	3	1446	A
49	3	1448	C
49	3	1452	C
49	3	1492	A
49	3	1493	A
49	3	1503	A
49	3	1505	G
49	3	1506	U
49	3	1517	G
49	3	1529	G
49	3	1530	G
49	3	1533	C
49	3	1535	C
50	1	10	A
50	1	12	U
50	1	15	G
50	1	34	U
50	1	35	G
50	1	46	G
50	1	49	A
50	1	51	G
50	1	71	A
50	1	74	A
50	1	75	G
50	1	96	C
50	1	102	U
50	1	118	A
50	1	120	U
50	1	137	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	139	U
50	1	141	G
50	1	142	A
50	1	162	U
50	1	163	C
50	1	181	A
50	1	196	A
50	1	216	A
50	1	218	A
50	1	221	A
50	1	222	A
50	1	224	U
50	1	228	C
50	1	229	C
50	1	248	G
50	1	249	C
50	1	255	A
50	1	266	G
50	1	276	U
50	1	278	A
50	1	294	A
50	1	301	G
50	1	311	A
50	1	323	C
50	1	324	A
50	1	329	G
50	1	330	A
50	1	361	G
50	1	362	A
50	1	363	G
50	1	371	A
50	1	372	G
50	1	386	G
50	1	387	U
50	1	395	U
50	1	404	A
50	1	405	U
50	1	406	G
50	1	411	G
50	1	412	A
50	1	424	G
50	1	455	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	481	G
50	1	491	G
50	1	504	A
50	1	505	A
50	1	518	G
50	1	529	A
50	1	531	C
50	1	532	A
50	1	543	G
50	1	547	A
50	1	548	G
50	1	549	G
50	1	563	A
50	1	573	U
50	1	575	A
50	1	588	U
50	1	603	A
50	1	615	U
50	1	627	A
50	1	637	A
50	1	646	U
50	1	654	A
50	1	669	G
50	1	686	U
50	1	687	C
50	1	730	A
50	1	747	C
50	1	752	A
50	1	757	G
50	1	764	A
50	1	776	G
50	1	782	A
50	1	784	G
50	1	785	G
50	1	800	A
50	1	805	G
50	1	812	C
50	1	819	A
50	1	827	U
50	1	828	U
50	1	830	G
50	1	845	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	846	U
50	1	847	U
50	1	858	G
50	1	860	U
50	1	878	A
50	1	887	U
50	1	889	C
50	1	896	A
50	1	910	A
50	1	915	C
50	1	932	U
50	1	941	A
50	1	946	C
50	1	953	G
50	1	961	C
50	1	962	G
50	1	974	G
50	1	983	A
50	1	985	C
50	1	995	C
50	1	996	A
50	1	1009	A
50	1	1012	U
50	1	1013	C
50	1	1021	A
50	1	1022	G
50	1	1026	G
50	1	1033	U
50	1	1045	C
50	1	1046	A
50	1	1047	G
50	1	1060	U
50	1	1062	G
50	1	1066	U
50	1	1068	G
50	1	1070	A
50	1	1071	G
50	1	1072	C
50	1	1075	C
50	1	1076	C
50	1	1084	A
50	1	1088	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1101	U
50	1	1104	C
50	1	1111	A
50	1	1126	A
50	1	1130	U
50	1	1132	U
50	1	1135	C
50	1	1136	G
50	1	1156	A
50	1	1172	C
50	1	1173	U
50	1	1174	U
50	1	1176	U
50	1	1178	C
50	1	1179	G
50	1	1180	U
50	1	1181	U
50	1	1211	C
50	1	1212	G
50	1	1247	A
50	1	1248	G
50	1	1251	C
50	1	1253	A
50	1	1256	G
50	1	1271	G
50	1	1272	A
50	1	1301	A
50	1	1302	A
50	1	1305	C
50	1	1321	A
50	1	1329	U
50	1	1330	C
50	1	1332	G
50	1	1345	C
50	1	1365	A
50	1	1378	A
50	1	1379	U
50	1	1383	A
50	1	1416	G
50	1	1419	A
50	1	1420	A
50	1	1421	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1454	C
50	1	1461	C
50	1	1476	U
50	1	1482	G
50	1	1490	A
50	1	1498	C
50	1	1515	A
50	1	1524	G
50	1	1535	A
50	1	1536	C
50	1	1537	G
50	1	1555	G
50	1	1559	U
50	1	1560	G
50	1	1569	A
50	1	1608	A
50	1	1611	C
50	1	1616	A
50	1	1617	C
50	1	1647	U
50	1	1648	U
50	1	1660	G
50	1	1674	G
50	1	1695	G
50	1	1713	A
50	1	1715	G
50	1	1729	U
50	1	1730	C
50	1	1738	G
50	1	1758	U
50	1	1764	C
50	1	1773	A
50	1	1780	A
50	1	1782	U
50	1	1791	A
50	1	1800	C
50	1	1801	A
50	1	1808	A
50	1	1816	C
50	1	1829	A
50	1	1847	A
50	1	1871	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1901	A
50	1	1906	G
50	1	1907	G
50	1	1913	A
50	1	1929	G
50	1	1930	G
50	1	1931	U
50	1	1936	A
50	1	1937	A
50	1	1938	A
50	1	1944	U
50	1	1955	U
50	1	1966	A
50	1	1967	C
50	1	1970	A
50	1	1971	U
50	1	1972	G
50	1	1991	U
50	1	1992	G
50	1	1997	C
50	1	2022	U
50	1	2023	C
50	1	2030	A
50	1	2031	A
50	1	2036	C
50	1	2043	C
50	1	2049	G
50	1	2055	C
50	1	2056	G
50	1	2060	A
50	1	2061	G
50	1	2062	A
50	1	2069	G
50	1	2072	C
50	1	2093	G
50	1	2096	C
50	1	2104	C
50	1	2110	G
50	1	2111	U
50	1	2112	G
50	1	2113	U
50	1	2114	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2118	U
50	1	2119	A
50	1	2126	A
50	1	2130	U
50	1	2131	U
50	1	2132	U
50	1	2133	G
50	1	2135	A
50	1	2136	G
50	1	2140	G
50	1	2145	C
50	1	2147	A
50	1	2154	A
50	1	2159	G
50	1	2161	C
50	1	2163	A
50	1	2165	C
50	1	2166	U
50	1	2167	U
50	1	2168	G
50	1	2171	A
50	1	2172	U
50	1	2173	A
50	1	2174	C
50	1	2175	C
50	1	2180	U
50	1	2198	A
50	1	2203	U
50	1	2204	G
50	1	2210	U
50	1	2211	A
50	1	2213	U
50	1	2223	G
50	1	2225	A
50	1	2238	G
50	1	2279	G
50	1	2283	C
50	1	2287	A
50	1	2297	A
50	1	2305	U
50	1	2309	A
50	1	2325	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2327	A
50	1	2334	U
50	1	2335	A
50	1	2345	G
50	1	2350	C
50	1	2357	G
50	1	2383	G
50	1	2385	C
50	1	2392	A
50	1	2402	U
50	1	2406	A
50	1	2423	U
50	1	2424	C
50	1	2429	G
50	1	2430	A
50	1	2431	U
50	1	2434	A
50	1	2435	A
50	1	2441	U
50	1	2447	G
50	1	2448	A
50	1	2476	A
50	1	2498	C
50	1	2502	G
50	1	2503	A
50	1	2505	G
50	1	2518	A
50	1	2520	C
50	1	2529	G
50	1	2547	A
50	1	2554	U
50	1	2566	A
50	1	2567	G
50	1	2572	A
50	1	2602	A
50	1	2609	U
50	1	2613	U
50	1	2621	G
50	1	2655	G
50	1	2682	A
50	1	2689	U
50	1	2690	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2714	G
50	1	2718	G
50	1	2722	G
50	1	2733	A
50	1	2744	G
50	1	2748	A
50	1	2757	A
50	1	2764	A
50	1	2765	A
50	1	2778	A
50	1	2779	U
50	1	2791	G
50	1	2792	A
50	1	2797	U
50	1	2799	A
50	1	2800	A
50	1	2809	A
50	1	2820	A
50	1	2821	A
50	1	2833	U
50	1	2849	U
50	1	2867	G
50	1	2868	A
50	1	2872	A
50	1	2879	A
50	1	2880	C
51	2	2	G
51	2	4	C
51	2	12	C
51	2	13	G
51	2	35	C
51	2	42	C
51	2	44	G
51	2	67	G
51	2	89	U
51	2	90	C
51	2	108	A
51	2	109	A
51	2	116	G
52	5	9	G
52	5	19	G
52	5	20	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	5	21	A
52	5	22	G
52	5	47	U
52	5	48	C
52	5	61	C
52	5	76	A
53	4	13	A
53	4	19	U
53	4	20	A
53	4	21	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	3	1190	G
50	1	784	G
50	1	859	G
50	1	1020	A
50	1	1475	G
50	1	1930	G
50	1	2286	G
50	1	2296	U
50	1	2326	C
50	1	2391	G
50	1	2756	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

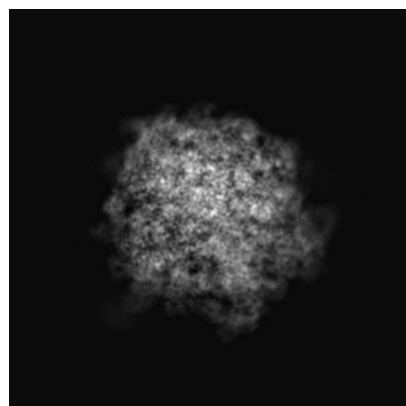
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22466. These allow visual inspection of the internal detail of the map and identification of artifacts.

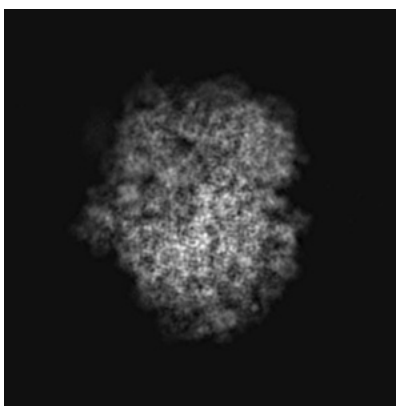
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

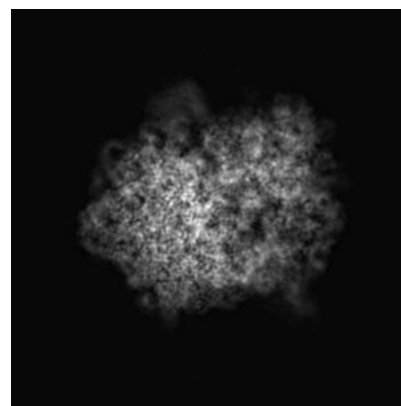
6.1.1 Primary map



X

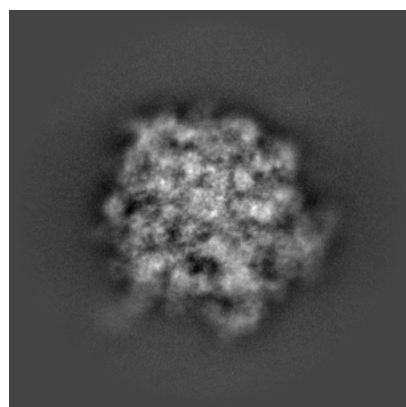


Y

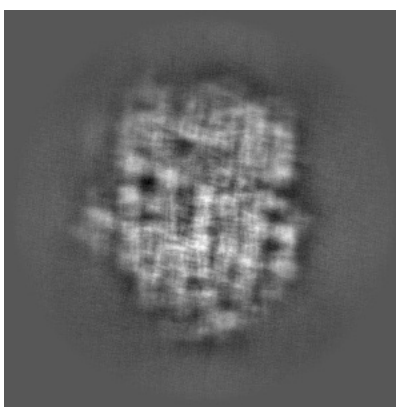


Z

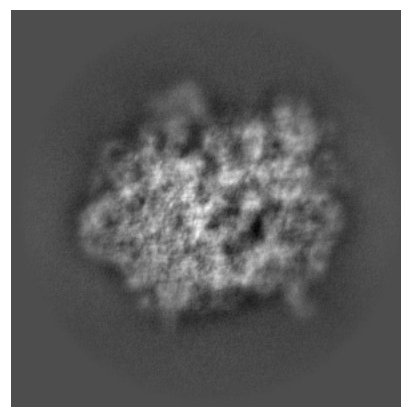
6.1.2 Raw map



X



Y

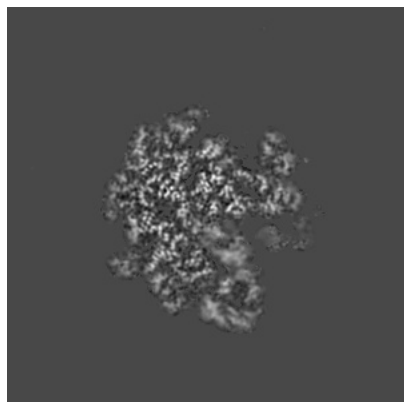


Z

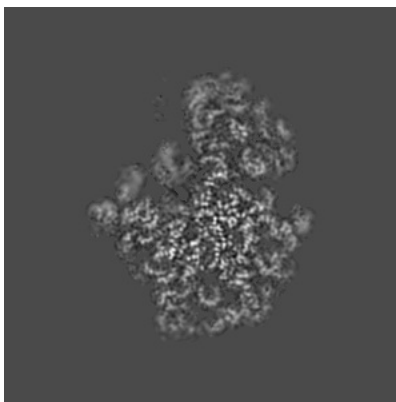
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

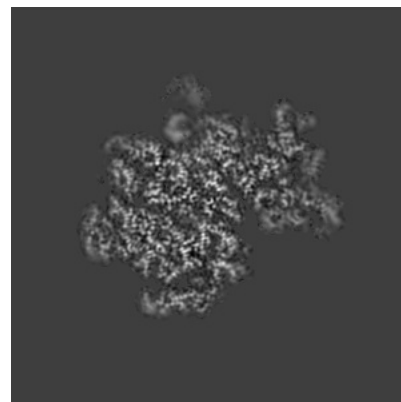
6.2.1 Primary map



X Index: 180

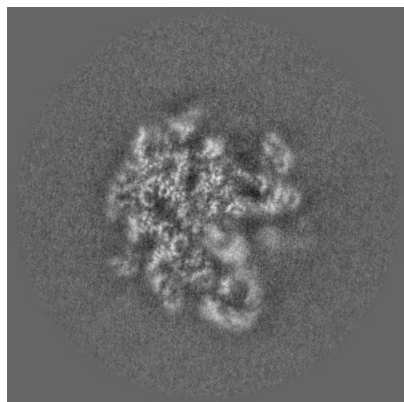


Y Index: 180

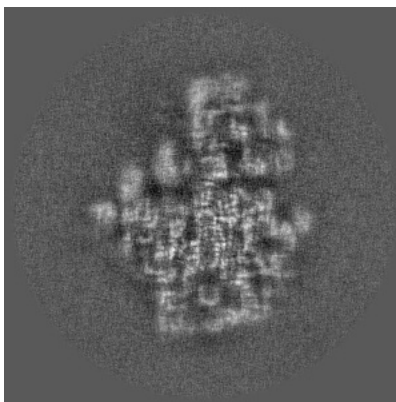


Z Index: 180

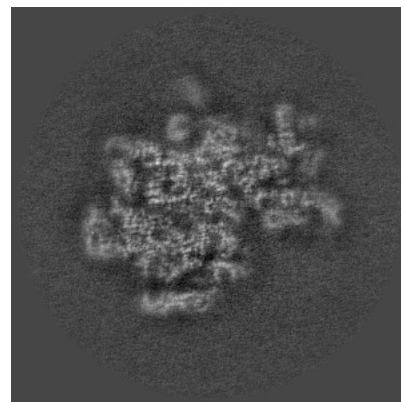
6.2.2 Raw map



X Index: 180



Y Index: 180

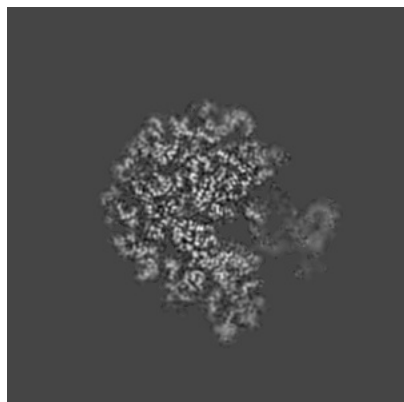


Z Index: 180

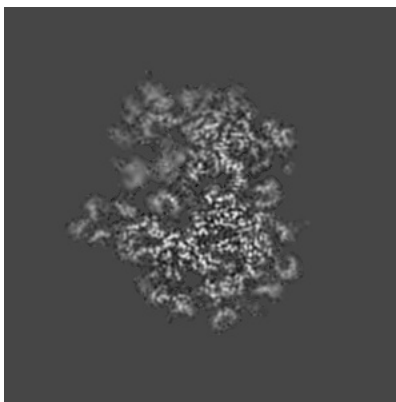
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

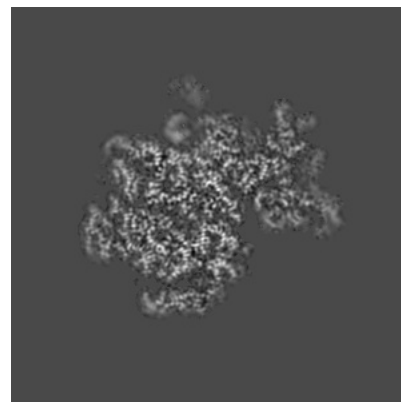
6.3.1 Primary map



X Index: 162

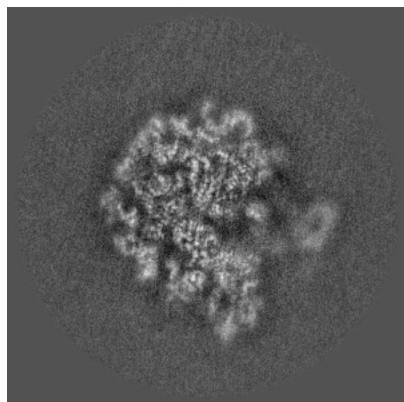


Y Index: 192

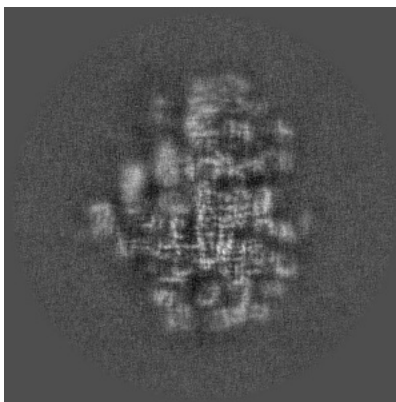


Z Index: 181

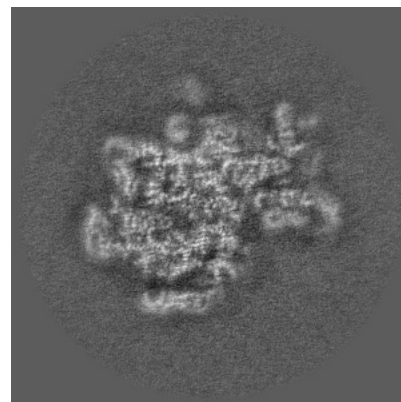
6.3.2 Raw map



X Index: 162



Y Index: 184

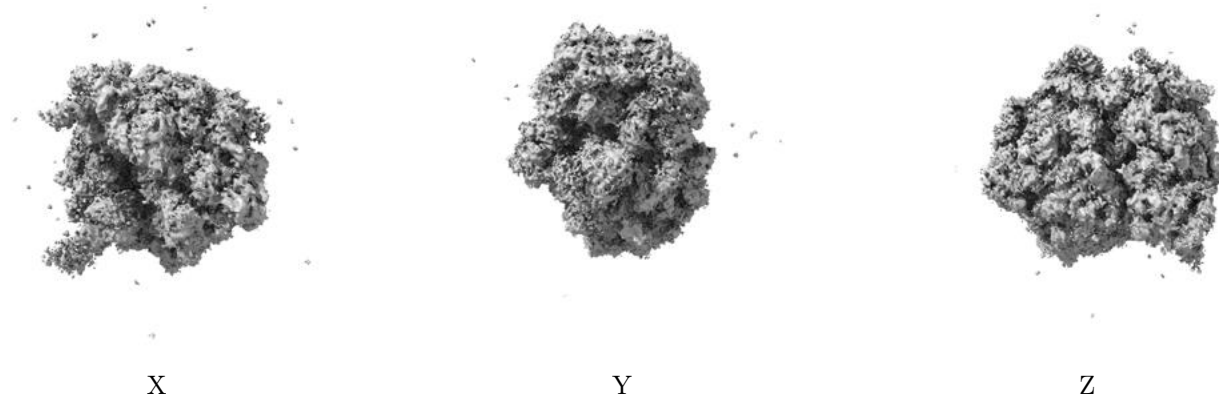


Z Index: 181

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

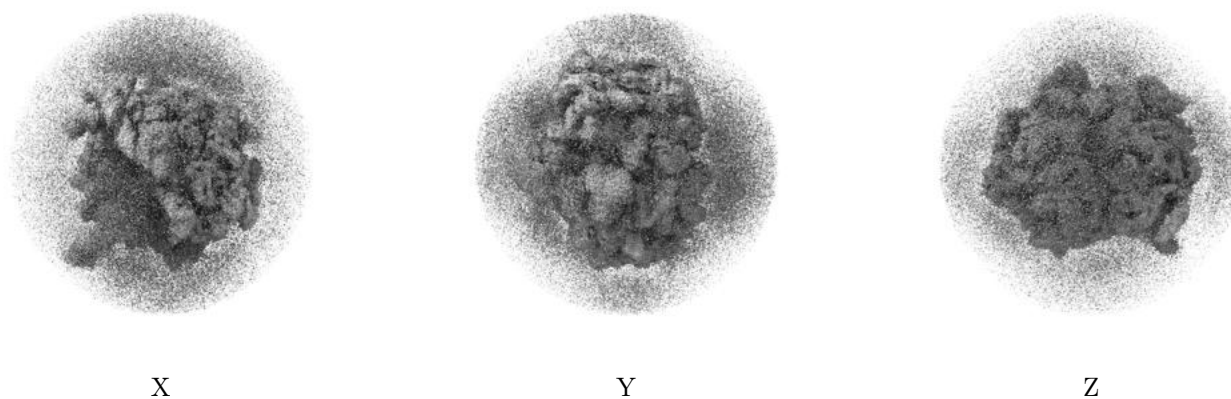
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

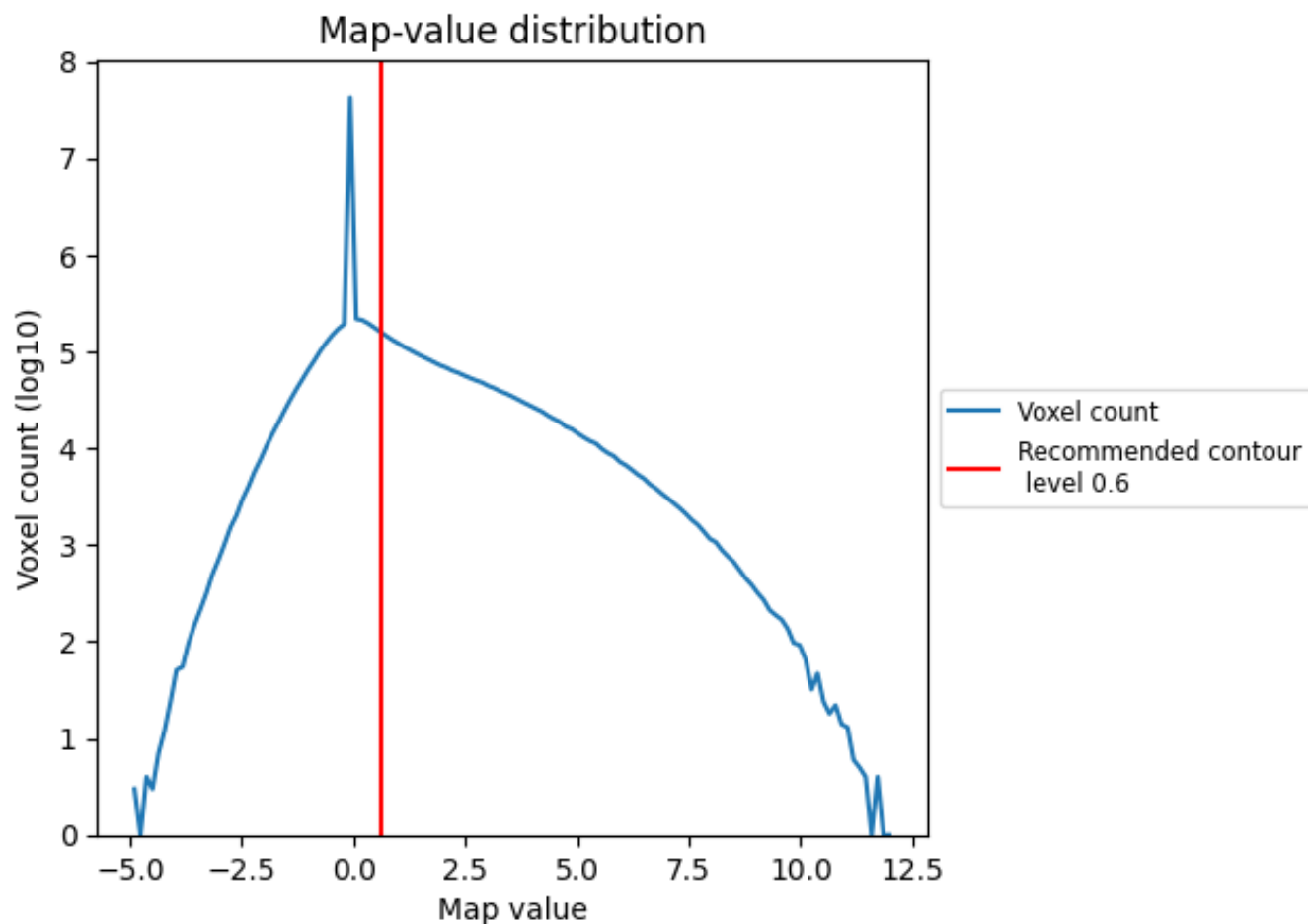
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

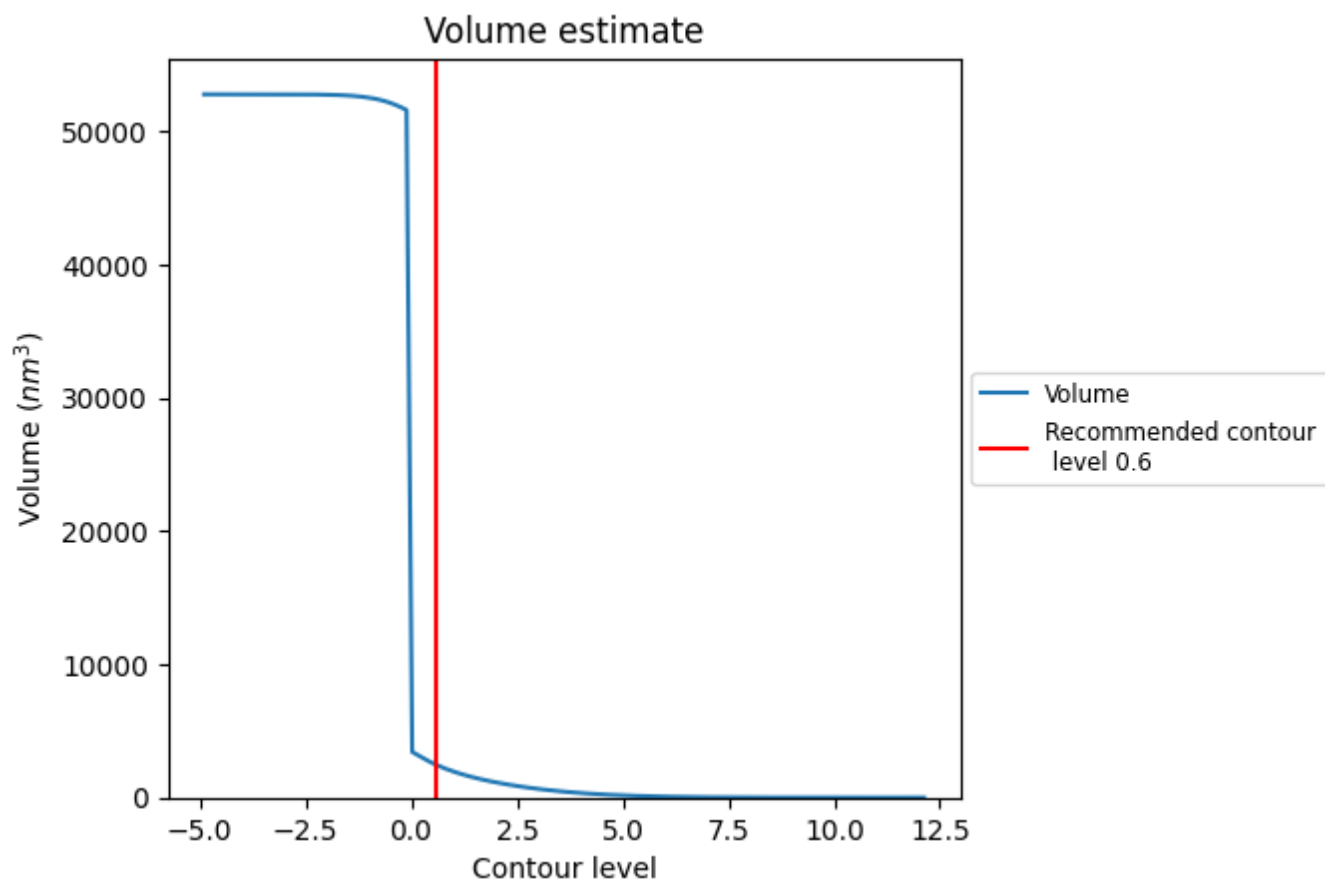
This section contains the results of statistical analysis of the map.

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.

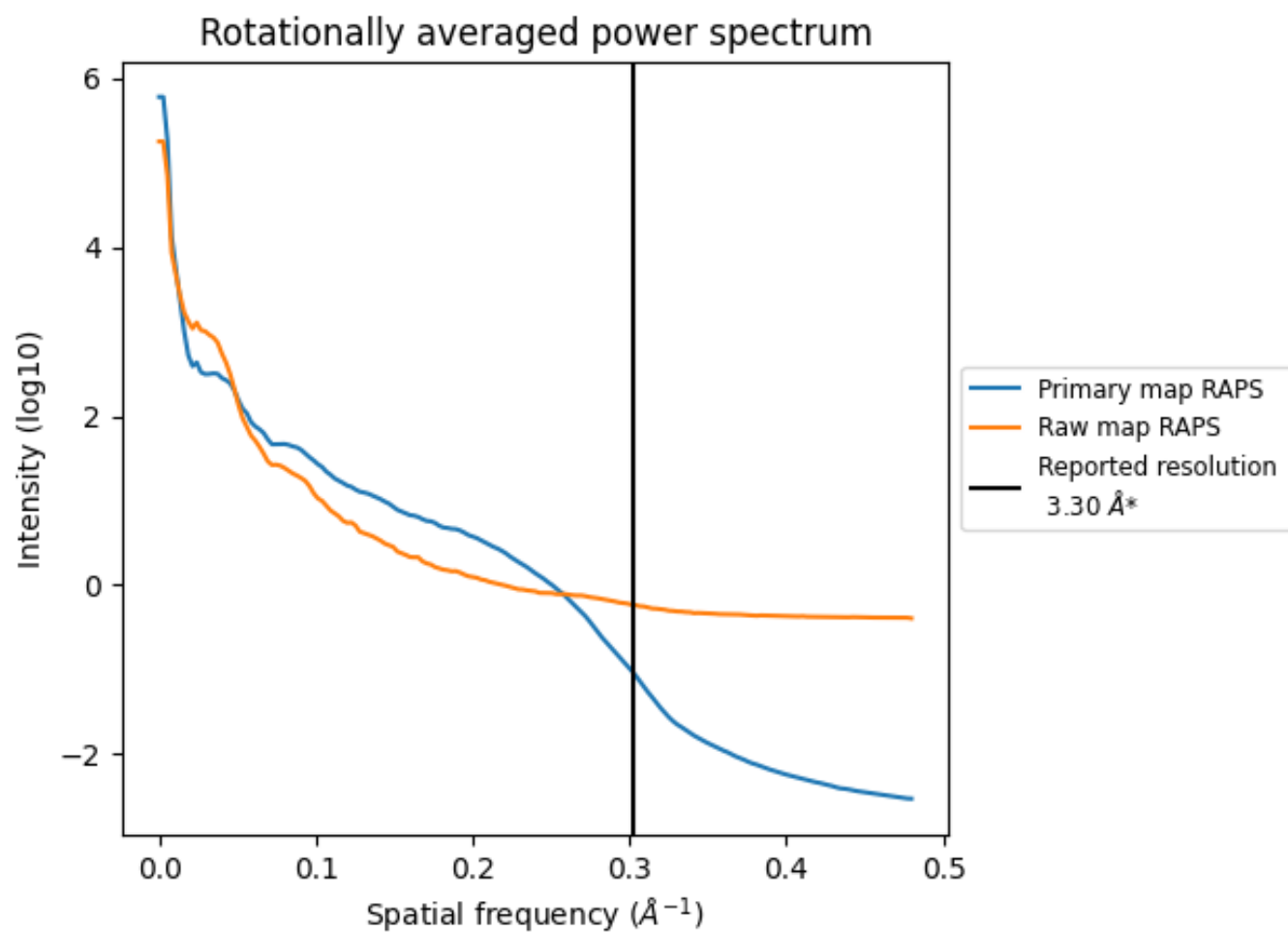
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2449 nm³; this corresponds to an approximate mass of 2212 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 ⓘ

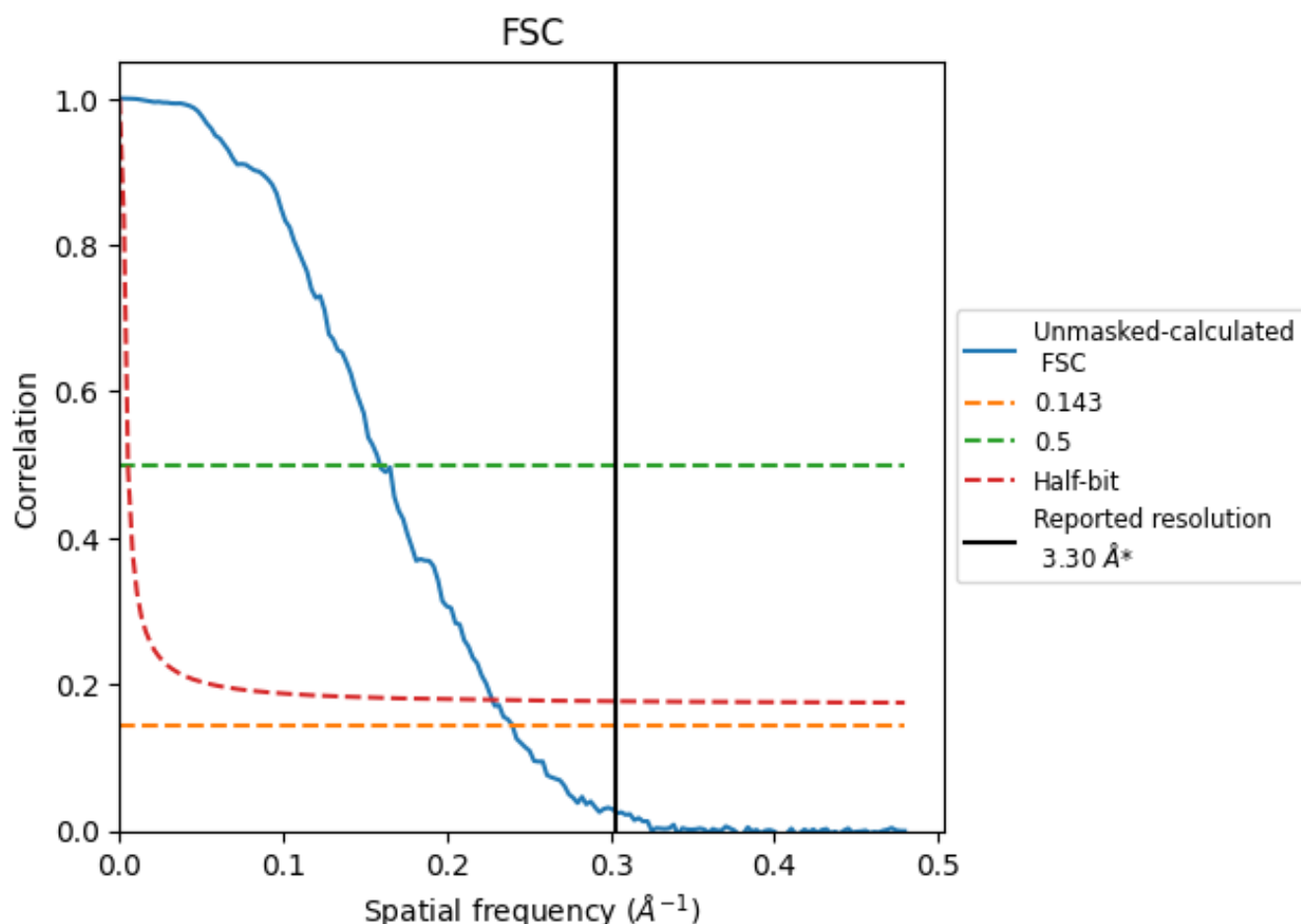


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

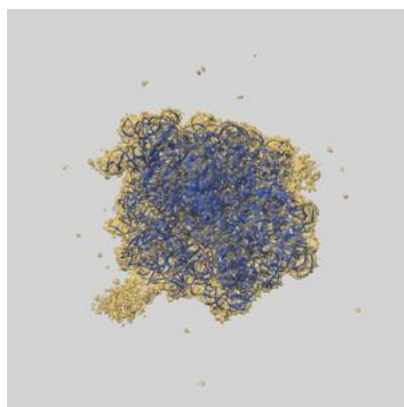
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	6.28	4.39

*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 4.16 differs from the reported value 3.3 by more than 10 %

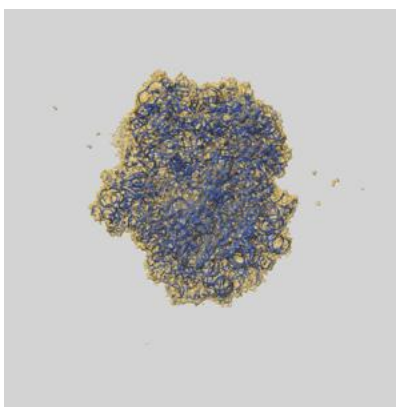
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22466 and PDB model 7JT1. Per-residue inclusion information can be found in section [3](#) on page [14](#).

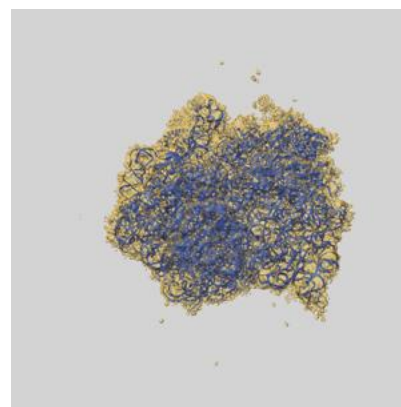
9.1 Map-model overlay [i](#)



X



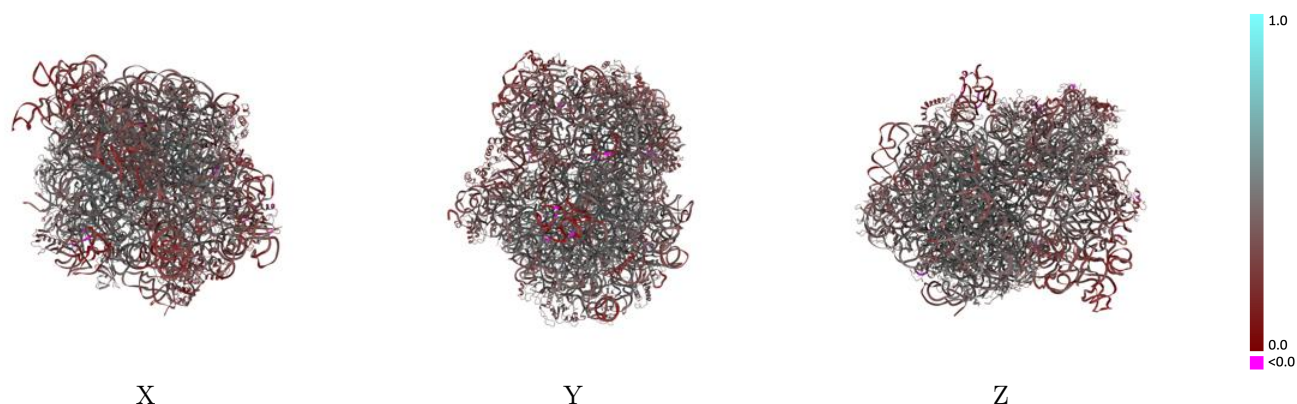
Y



Z

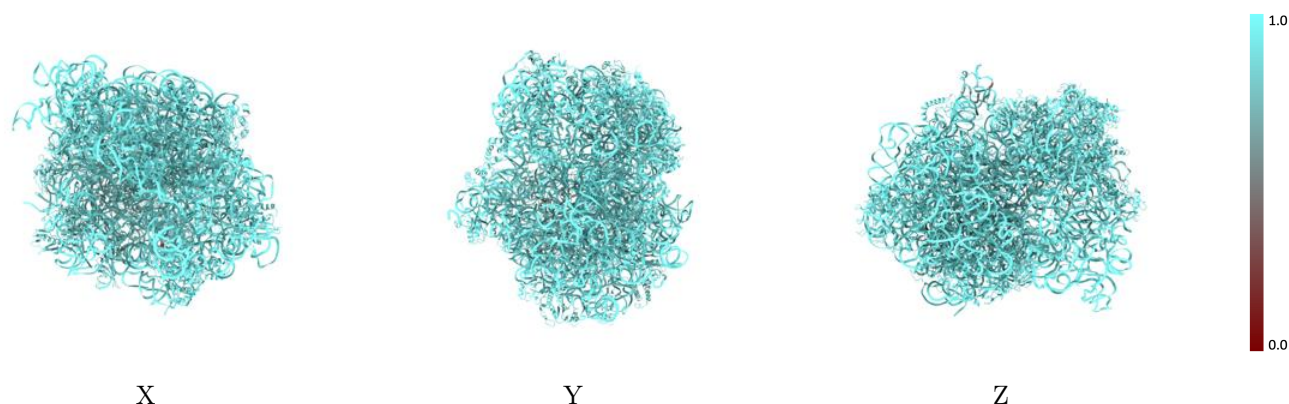
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



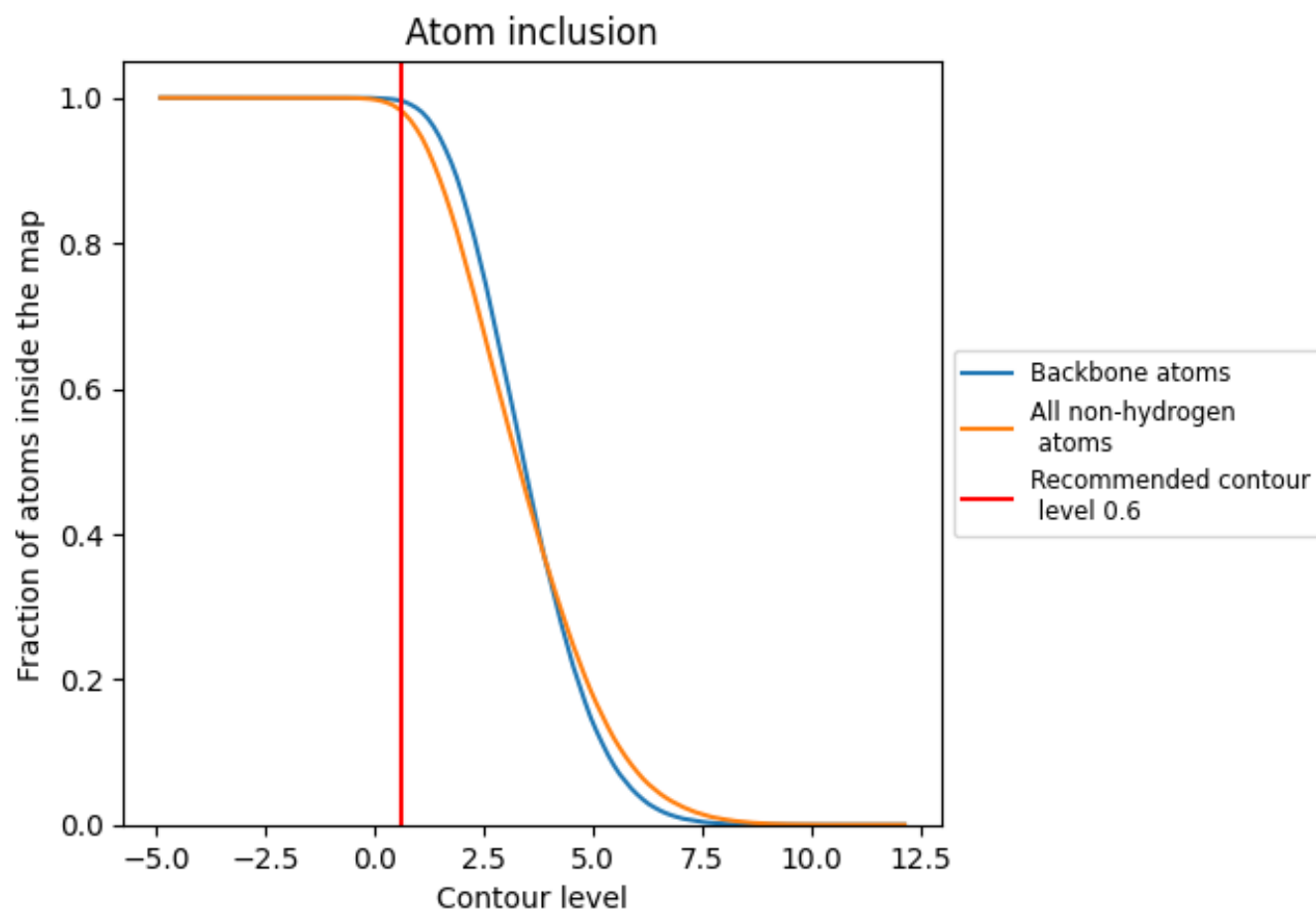
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).







































































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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9827	 0.3960
1	 0.9935	 0.4180
2	 0.9903	 0.3500
3	 0.9904	 0.3710
4	 0.9795	 0.2550
5	 0.9860	 0.3370
8	 0.9379	 0.3490
9	 0.9872	 0.2550
B	 0.9673	 0.4460
C	 0.9701	 0.4240
D	 0.9718	 0.4720
E	 0.9613	 0.4730
F	 0.9452	 0.4360
G	 0.9502	 0.3450
H	 0.9525	 0.3850
I	 0.9528	 0.3130
J	 0.9630	 0.4060
K	 0.9674	 0.3810
L	 0.9729	 0.3280
M	 0.9656	 0.4100
N	 0.9326	 0.3420
O	 0.9003	 0.3360
P	 0.9645	 0.3960
Q	 0.9761	 0.3980
R	 0.9636	 0.3070
S	 0.9587	 0.3540
T	 0.9609	 0.3760
U	 0.9522	 0.3440
V	 0.9763	 0.3750
W	 0.9223	 0.3540
X	 0.9582	 0.3300
Y	 0.9246	 0.3030
Z	 0.9247	 0.3090
b	 0.9747	 0.4730
c	 0.9584	 0.4520



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.9651	 0.4070
e	 0.9687	 0.3080
f	 0.9738	 0.3720
g	 0.9681	 0.3230
j	 0.9591	 0.4370
k	 0.9748	 0.4590
l	 0.9695	 0.4370
m	 0.9559	 0.4410
n	 0.9653	 0.4500
o	 0.9652	 0.3740
p	 0.9809	 0.4290
q	 0.9604	 0.4450
r	 0.9737	 0.4260
s	 0.9689	 0.4550
t	 0.9571	 0.4290
u	 0.9753	 0.4060
v	 0.9702	 0.4030
w	 0.9624	 0.4490
x	 0.9817	 0.4530
y	 0.9598	 0.3630
z	 0.9703	 0.4440