



Full wwPDB EM Validation Report ⓘ

Sep 29, 2024 – 03:40 AM EDT

PDB ID : 7ST2
EMDB ID : EMD-25418
Title : Post translocation, non-rotated 70S ribosome with EF-G dissociated (Structure VII)
Authors : Carbone, C.E.; Korostelev, A.A.
Deposited on : 2021-11-11
Resolution : 2.90 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.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

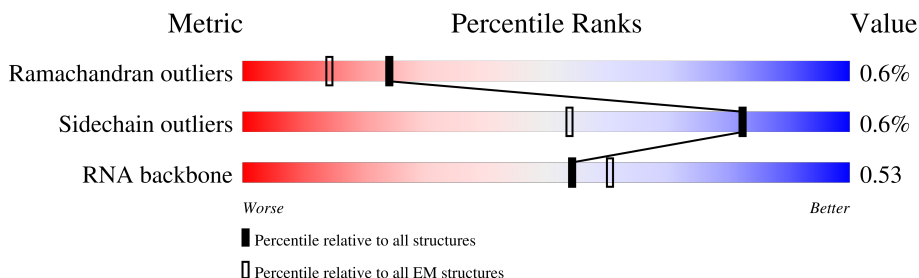
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	3	1539	
2	1	2903	
3	2	120	
4	6	77	
5	b	271	
6	c	209	
7	d	201	
8	e	177	

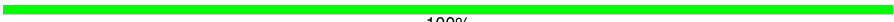













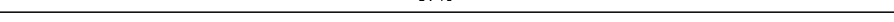
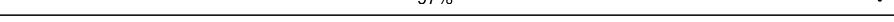
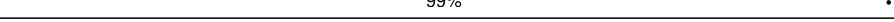
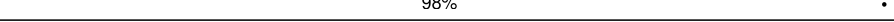
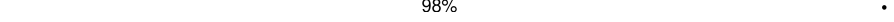
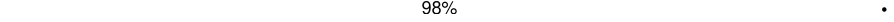
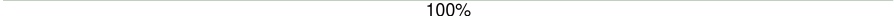
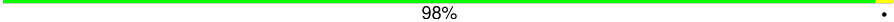
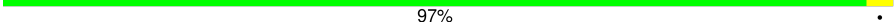


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Mol	Chain	Length	Quality of chain
9	f	176	100%
10	g	149	44% 98% ..
11	a	234	29% 57% 43%
12	h	131	63% 95% .
13	i	142	32% 96% ..
14	j	142	100%
15	k	122	97% .
16	l	143	99% ..
17	m	136	99% ..
18	n	120	98% .
19	o	116	99% .
20	p	114	99% .
21	q	117	100%
22	r	103	98% .
23	s	110	95% 5%
24	t	93	100%
25	u	102	99% .
26	v	94	99% .
27	w	75	99% .
28	x	77	100%
29	y	63	95% ..
30	z	58	100%
31	A	66	98% .
32	B	56	96% .
33	C	50	100%

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Mol	Chain	Length	Quality of chain
34	D	46	 100%
35	E	64	 97%
36	F	38	 97%
37	4	35	 31% 17% 6% 46%
38	5	77	 71% 27%
39	G	225	 93%
40	H	206	 100%
41	I	205	 98%
42	J	157	 97%
43	K	100	 99%
44	L	151	 100%
45	M	129	 100%
46	N	127	 100%
47	O	98	 97%
48	P	116	 97%
49	Q	123	 99%
50	R	114	 98%
51	S	100	 98%
52	T	88	 98%
53	U	82	 100%
54	V	80	 98%
55	W	65	 97%
56	X	79	 100%
57	Y	85	 100%
58	Z	65	 88% 9%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 149087 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	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 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	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 4 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

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

- Molecule 16 is a protein called 50S ribosomal protein L15.

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

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

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

- Molecule 19 is a protein called 50S ribosomal protein L18.

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

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

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

- Molecule 25 is a protein called 50S ribosomal protein L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

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

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L34.

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

- Molecule 35 is a protein called 50S ribosomal protein L35.

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

- Molecule 36 is a protein called 50S ribosomal protein L36.

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

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	19	Total	C	N	O	P	0	0
			416	186	85	126	19		

- Molecule 38 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	77	Total	C	N	O	P	0	0
			1647	733	295	542	77		

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 40 is a protein called 30S ribosomal protein S3.

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

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

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

- Molecule 43 is a protein called 30S ribosomal protein S6.

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

- Molecule 44 is a protein called 30S ribosomal protein S7.

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

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

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

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

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

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

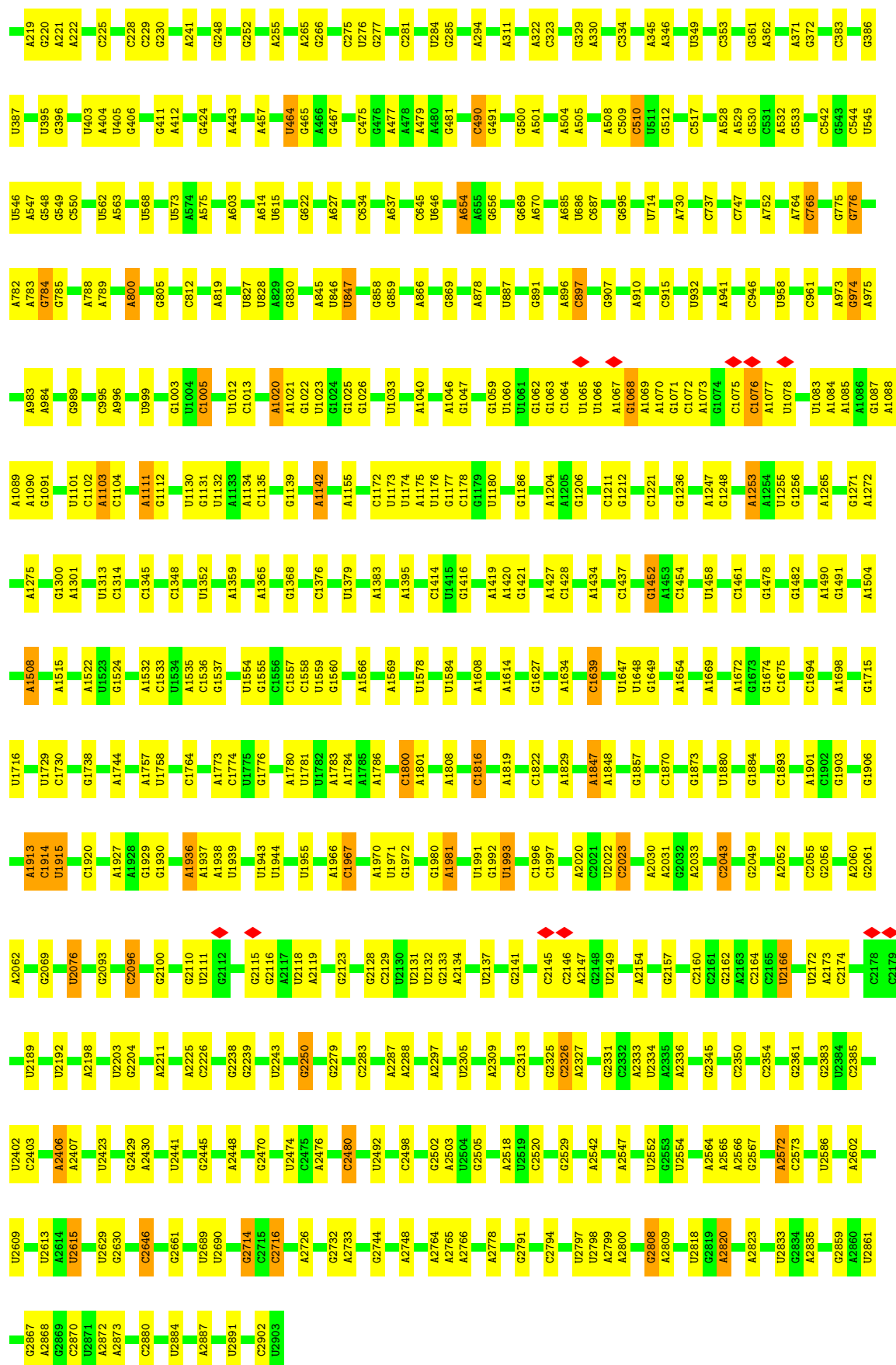
Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 57 is a protein called 30S ribosomal protein S20.


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

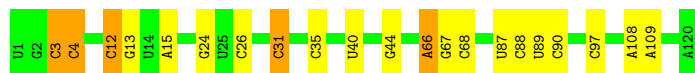
- Molecule 58 is a protein called 30S ribosomal protein S21.

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




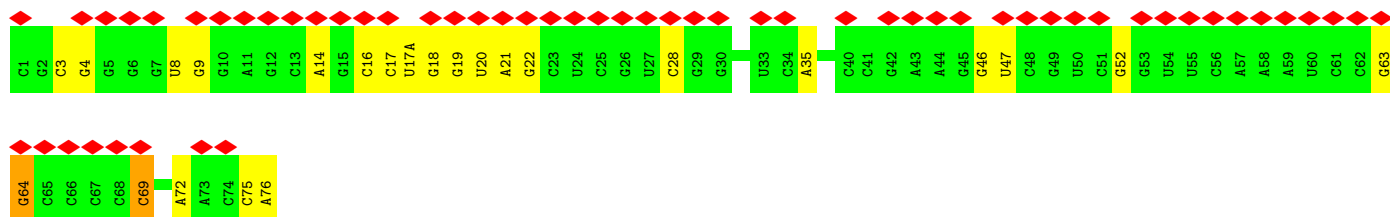
- Molecule 3: 5S rRNA

Chain 2:  82% 13% .



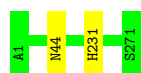
- Molecule 4: tRNA fMet

Chain 6:  75% 69% 29% .



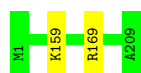
- Molecule 5: 50S ribosomal protein L2

Chain b:  99% .



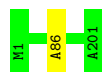
- Molecule 6: 50S ribosomal protein L3

Chain c:  99% .



- Molecule 7: 50S ribosomal protein L4

Chain d:  100% .



- Molecule 8: 50S ribosomal protein L5

Chain e:  98% ..



- Molecule 9: 50S ribosomal protein L6

Chain f:  100% .

- Molecule 10: 50S ribosomal protein L9

[illegible]

Chain a: 


[illegible]

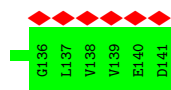
Chain h:

63%

95%

M1
A2
L3
F6
N4
L5
T11
V12
S16
E17
V18
K20
G21
A22
L23
S24
A25
V26
V27
A44
G45
R46
E47
A48
G49
V50
Y51
M52
R53
R61
T67
P68
F69
E70
C71
L72
K73
D74
A75
F76
V77
G78
P79
T80
Y84
S85
M86
E87
H88
P89
G90
A91
A92
A93

Chain i: 



- Molecule 14: 50S ribosomal protein L13

Chain j: 100%

There are no outlier residues recorded for this chain.

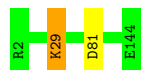
- Molecule 15: 50S ribosomal protein L14

Chain k: 97%



- Molecule 16: 50S ribosomal protein L15

Chain l: 99%



- Molecule 17: 50S ribosomal protein L16

Chain m: 99%



- Molecule 18: 50S ribosomal protein L17

Chain n: 98%



- Molecule 19: 50S ribosomal protein L18

Chain o: 99%



- Molecule 20: 50S ribosomal protein L19

Chain p: 99%



- Molecule 21: 50S ribosomal protein L20

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: 50S ribosomal protein L21

Chain r:  98%



- Molecule 23: 50S ribosomal protein L22

Chain s:  95%



- Molecule 24: 50S ribosomal protein L23

Chain t:  100%



- Molecule 25: 50S ribosomal protein L24

Chain u:  99%



- Molecule 26: 50S ribosomal protein L25

Chain v:  99%



- Molecule 27: 50S ribosomal protein L27

Chain w:  99%



- Molecule 28: 50S ribosomal protein L28

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L29

Chain y:  95%



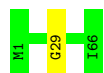
- Molecule 30: 50S ribosomal protein L30

Chain z:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L31

Chain A:  98%



- Molecule 32: 50S ribosomal protein L32

Chain B:  96%



- Molecule 33: 50S ribosomal protein L33

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 50S ribosomal protein L34

Chain D:  100%

There are no outlier residues recorded for this chain.

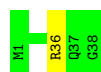
- Molecule 35: 50S ribosomal protein L35

Chain E:  97%

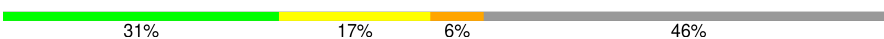


- Molecule 36: 50S ribosomal protein L36

Chain F:  97%



- Molecule 37: mRNA

Chain 4:  31% 17% 6% 46%



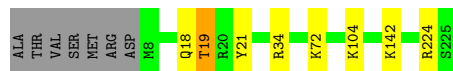
- Molecule 38: tRNA Pro

Chain 5:  71% 27%



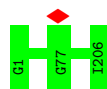
- Molecule 39: 30S ribosomal protein S2

Chain G:  93%



- Molecule 40: 30S ribosomal protein S3

Chain H:  100%



- Molecule 41: 30S ribosomal protein S4

Chain I:  98%



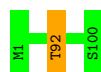
- Molecule 42: 30S ribosomal protein S5

Chain J:  97%



- Molecule 43: 30S ribosomal protein S6

Chain K: 99%



- Molecule 44: 30S ribosomal protein S7

Chain L: 100%

There are no outlier residues recorded for this chain.

- Molecule 45: 30S ribosomal protein S8

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 46: 30S ribosomal protein S9

Chain N: 100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S10

Chain O: 97%



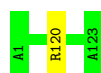
- Molecule 48: 30S ribosomal protein S11

Chain P: 97%



- Molecule 49: 30S ribosomal protein S12

Chain Q: 99%



- Molecule 50: 30S ribosomal protein S13

Chain R:  98% .



- Molecule 51: 30S ribosomal protein S14

Chain S:  98% .



- Molecule 52: 30S ribosomal protein S15

Chain T:  98% .



- Molecule 53: 30S ribosomal protein S16

Chain U:  100% .



- Molecule 54: 30S ribosomal protein S17

Chain V:  98% .



- Molecule 55: 30S ribosomal protein S18

Chain W:  97% .



- Molecule 56: 30S ribosomal protein S19

Chain X:  100% .


There are no outlier residues recorded for this chain.

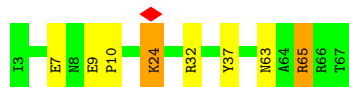
- Molecule 57: 30S ribosomal protein S20

Chain Y:  100% .

There are no outlier residues recorded for this chain.

- Molecule 58: 30S ribosomal protein S21

Chain Z:  88% 9% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.855	Depositor
Minimum map value	-7.489	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.005	Depositor
Recommended contour level	1.35	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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	3	1.23	1/36963 (0.0%)	0.99	51/57662 (0.1%)
2	1	1.34	19/69796 (0.0%)	1.02	141/108888 (0.1%)
3	2	0.99	0/2872	1.02	11/4479 (0.2%)
4	6	0.41	0/1832	0.93	3/2855 (0.1%)
5	b	0.66	0/2122	0.63	1/2852 (0.0%)
6	c	0.61	0/1586	0.59	0/2134
7	d	0.47	0/1571	0.58	0/2113
8	e	0.45	0/1435	0.59	0/1926
9	f	0.41	0/1343	0.53	0/1816
10	g	0.35	0/1122	0.67	0/1515
11	a	0.29	0/1033	0.62	0/1387
12	h	0.34	0/1002	0.76	1/1350 (0.1%)
13	i	0.31	0/1046	0.63	1/1410 (0.1%)
14	j	0.55	0/1152	0.53	0/1551
15	k	0.61	0/948	0.66	0/1268
16	l	0.54	0/1054	0.63	1/1403 (0.1%)
17	m	0.59	0/1093	0.59	1/1460 (0.1%)
18	n	0.55	0/974	0.62	0/1301
19	o	0.44	0/902	0.50	0/1209
20	p	0.61	0/929	0.62	1/1242 (0.1%)
21	q	0.64	0/960	0.53	0/1278
22	r	0.53	0/829	0.59	0/1107
23	s	0.53	0/864	0.62	1/1156 (0.1%)
24	t	0.48	0/745	0.54	0/994
25	u	0.45	0/788	0.62	0/1051
26	v	0.49	0/766	0.53	0/1025
27	w	0.60	0/582	0.56	0/769
28	x	0.56	0/635	0.56	0/848
29	y	0.37	0/510	0.63	1/677 (0.1%)
30	z	0.48	0/453	0.53	0/605
31	A	0.37	0/532	0.58	0/709
32	B	0.53	0/450	0.59	0/599
33	C	0.37	0/417	0.52	0/554
34	D	0.59	0/380	0.58	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	E	0.58	0/513	0.59	0/676
36	F	0.56	0/303	0.59	0/397
37	4	0.81	0/468	1.47	8/729 (1.1%)
38	5	0.96	0/1840	1.06	7/2868 (0.2%)
39	G	0.42	0/1736	0.63	0/2338
40	H	0.46	0/1652	0.55	0/2225
41	I	0.46	0/1665	0.63	2/2227 (0.1%)
42	J	0.55	0/1170	0.62	0/1573
43	K	0.44	0/836	0.62	1/1128 (0.1%)
44	L	0.41	0/1196	0.58	0/1602
45	M	0.52	0/989	0.60	0/1326
46	N	0.44	0/1034	0.59	0/1375
47	O	0.45	0/797	0.67	0/1077
48	P	0.52	0/886	0.61	0/1195
49	Q	0.63	0/969	0.69	0/1300
50	R	0.45	0/893	0.62	1/1193 (0.1%)
51	S	0.46	0/817	0.54	0/1088
52	T	0.46	0/722	0.57	0/964
53	U	0.51	0/659	0.59	0/884
54	V	0.51	0/658	0.57	0/881
55	W	0.51	0/545	0.63	0/731
56	X	0.44	0/653	0.59	0/877
57	Y	0.40	0/671	0.49	0/888
58	Z	0.43	0/551	0.87	1/728 (0.1%)
All	All	1.10	20/161909 (0.0%)	0.92	234/241961 (0.1%)

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
2	l	0	1
6	c	0	1
8	e	0	2
10	g	0	2
12	h	0	4
15	k	0	2
18	n	0	1
22	r	0	1
23	s	0	1
29	y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	A	0	1
35	E	0	1
36	F	0	1
39	G	0	2
41	I	0	2
42	J	0	2
47	O	0	1
48	P	0	2
50	R	0	1
51	S	0	1
54	V	0	2
55	W	0	1
58	Z	0	1
All	All	0	34

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	1936	A	N9-C4	-7.70	1.33	1.37
2	1	528	A	N9-C4	-7.28	1.33	1.37
2	1	984	A	N9-C4	-7.08	1.33	1.37
2	1	783	A	N9-C4	-6.98	1.33	1.37
2	1	1784	A	N7-C5	-6.10	1.35	1.39
2	1	1142	A	N9-C4	-6.01	1.34	1.37
2	1	1783	A	N9-C4	-5.98	1.34	1.37
2	1	788	A	N9-C4	-5.82	1.34	1.37
2	1	783	A	N7-C5	-5.77	1.35	1.39
2	1	2542	A	N9-C4	-5.67	1.34	1.37
2	1	800	A	N9-C4	-5.48	1.34	1.37
2	1	687	C	N3-C4	-5.36	1.30	1.33
2	1	1614	A	N9-C4	-5.21	1.34	1.37
1	3	1518	A	N7-C5	-5.19	1.36	1.39
2	1	528	A	N7-C5	-5.19	1.36	1.39
2	1	783	A	C5-C6	-5.08	1.36	1.41
2	1	1800	C	N1-C6	-5.05	1.34	1.37
2	1	1253	A	N9-C4	-5.04	1.34	1.37
2	1	1936	A	N3-C4	-5.01	1.31	1.34
2	1	1981	A	N9-C4	-5.01	1.34	1.37

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	13	A	O4'-C1'-N9	15.19	120.35	108.20
1	3	1301	U	C2-N1-C1'	10.97	130.86	117.70
1	3	1301	U	N1-C2-O2	10.82	130.37	122.80
2	1	62	U	N1-C2-O2	10.43	130.10	122.80
2	1	62	U	C2-N1-C1'	10.22	129.96	117.70
1	3	1301	U	N3-C2-O2	-9.42	115.61	122.20
2	1	1313	U	C2-N1-C1'	9.41	128.99	117.70
2	1	62	U	N3-C2-O2	-9.36	115.65	122.20
2	1	687	C	N3-C2-O2	-9.22	115.44	121.90
2	1	783	A	C5-N7-C8	-9.21	99.30	103.90
2	1	1313	U	N3-C2-O2	-9.18	115.78	122.20
2	1	1915	U	N3-C2-O2	-9.09	115.84	122.20
2	1	1313	U	N1-C2-O2	8.94	129.06	122.80
37	4	13	A	C5'-C4'-O4'	8.73	119.58	109.10
1	3	1158	C	C2-N1-C1'	8.33	127.96	118.80
2	1	783	A	N7-C8-N9	8.18	117.89	113.80
1	3	1158	C	N1-C2-O2	8.05	123.73	118.90
2	1	687	C	C2-N1-C1'	8.01	127.61	118.80
2	1	2572	A	P-O3'-C3'	7.98	129.27	119.70
1	3	1518	A	O4'-C1'-N9	7.97	114.58	108.20
37	4	13	A	C4-N9-C1'	-7.97	111.94	126.30
1	3	1301	U	C6-N1-C1'	-7.85	110.21	121.20
1	3	983	A	C2-N3-C4	7.84	114.52	110.60
2	1	687	C	N1-C2-O2	7.83	123.59	118.90
2	1	669	G	C4-N9-C1'	7.79	136.63	126.50
2	1	1915	U	N1-C2-O2	7.70	128.19	122.80
2	1	1915	U	C2-N1-C1'	7.40	126.58	117.70
2	1	669	G	C8-N9-C1'	-7.38	117.41	127.00
37	4	13	A	C8-N9-C1'	7.26	140.76	127.70
2	1	1005	C	N1-C2-O2	7.21	123.22	118.90
2	1	897	C	N1-C2-O2	7.06	123.14	118.90
1	3	1138	G	C4-N9-C1'	7.04	135.66	126.50
2	1	783	A	C8-N9-C4	-7.02	102.99	105.80
1	3	1383	C	C6-N1-C2	-6.94	117.52	120.30
2	1	1914	C	C2-N1-C1'	6.92	126.41	118.80
1	3	1398	A	O4'-C1'-N9	6.85	113.68	108.20
3	2	4	C	C6-N1-C2	-6.83	117.57	120.30
2	1	783	A	C4-C5-N7	6.83	114.11	110.70
2	1	12	U	N3-C2-O2	-6.78	117.45	122.20
20	p	113	LEU	CA-CB-CG	6.77	130.88	115.30
1	3	438	U	N3-C2-O2	-6.74	117.48	122.20
1	3	754	C	C2-N1-C1'	6.72	126.19	118.80
3	2	4	C	C5-C6-N1	6.71	124.36	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	512	G	O4'-C1'-N9	6.70	113.56	108.20
2	1	2646	C	C6-N1-C2	-6.67	117.63	120.30
1	3	1138	G	N3-C4-N9	6.63	129.98	126.00
1	3	813	U	N3-C2-O2	-6.63	117.56	122.20
2	1	2250	G	C5-N7-C8	-6.59	101.00	104.30
2	1	62	U	C6-N1-C1'	-6.58	111.99	121.20
2	1	542	C	N1-C2-O2	6.56	122.83	118.90
2	1	1936	A	C2-N3-C4	-6.53	107.33	110.60
2	1	528	A	C2-N3-C4	-6.53	107.33	110.60
38	5	62	C	N1-C2-O2	6.53	122.82	118.90
37	4	13	A	C1'-O4'-C4'	-6.53	104.68	109.90
1	3	1382	C	C2-N1-C1'	6.50	125.95	118.80
1	3	1138	G	N3-C4-C5	-6.46	125.37	128.60
2	1	2250	G	C2-N3-C4	-6.45	108.68	111.90
2	1	2552	U	N3-C2-O2	-6.43	117.70	122.20
1	3	1158	C	N3-C2-O2	-6.42	117.41	121.90
2	1	1508	A	O4'-C1'-N9	6.40	113.32	108.20
2	1	143	C	N1-C2-O2	6.40	122.74	118.90
1	3	1382	C	N3-C2-O2	-6.39	117.43	121.90
2	1	1993	U	N3-C2-O2	-6.38	117.74	122.20
2	1	528	A	C5-N7-C8	-6.36	100.72	103.90
2	1	974	G	C4-C5-N7	6.35	113.34	110.80
2	1	2646	C	C5-C6-N1	6.34	124.17	121.00
2	1	1313	U	C6-N1-C1'	-6.34	112.33	121.20
2	1	974	G	C4-N9-C1'	6.33	134.73	126.50
2	1	1914	C	N1-C2-O2	6.32	122.69	118.90
38	5	55	U	C2-N1-C1'	6.30	125.26	117.70
2	1	12	U	N1-C2-O2	6.27	127.19	122.80
2	1	1020	A	P-O3'-C3'	6.25	127.19	119.70
2	1	974	G	C6-C5-N7	-6.22	126.67	130.40
3	2	3	C	P-O3'-C3'	6.22	127.17	119.70
58	Z	7	GLU	C-N-CA	6.22	137.25	121.70
38	5	55	U	N3-C2-O2	-6.21	117.86	122.20
2	1	2820	A	OP1-P-O3'	6.19	118.82	105.20
2	1	510	C	N1-C2-O2	6.18	122.61	118.90
1	3	1158	C	C6-N1-C1'	-6.17	113.39	120.80
2	1	2808	G	P-O3'-C3'	6.16	127.09	119.70
2	1	687	C	C6-N1-C2	-6.15	117.84	120.30
1	3	1256	A	P-O3'-C3'	6.12	127.05	119.70
1	3	1383	C	N3-C2-O2	-6.08	117.64	121.90
2	1	2096	C	N1-C2-O2	6.08	122.55	118.90
2	1	528	A	C8-N9-C4	-6.07	103.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	776	G	C4-N9-C1'	6.01	134.32	126.50
1	3	1138	G	C8-N9-C1'	-6.01	119.19	127.00
1	3	439	U	N3-C2-O2	-6.00	118.00	122.20
41	I	8	LEU	CA-CB-CG	5.99	129.07	115.30
2	1	2076	U	N3-C2-O2	-5.99	118.01	122.20
2	1	62	U	C5-C6-N1	5.98	125.69	122.70
2	1	1920	C	C6-N1-C2	-5.97	117.91	120.30
2	1	2313	C	N1-C2-O2	5.97	122.48	118.90
1	3	1301	U	C5-C6-N1	5.94	125.67	122.70
2	1	2096	C	N3-C2-O2	-5.94	117.74	121.90
38	5	62	C	N3-C2-O2	-5.93	117.75	121.90
2	1	1103	A	OP1-P-O3'	5.92	118.22	105.20
2	1	1005	C	N3-C2-O2	-5.92	117.76	121.90
2	1	1774	C	C6-N1-C2	-5.90	117.94	120.30
1	3	1382	C	N1-C2-O2	5.89	122.43	118.90
2	1	2250	G	C4-C5-N7	5.87	113.15	110.80
1	3	54	C	N1-C2-O2	5.85	122.41	118.90
2	1	1221	C	N1-C2-O2	5.84	122.40	118.90
1	3	438	U	N1-C2-O2	5.83	126.88	122.80
2	1	1102	C	N1-C2-O2	5.83	122.39	118.90
2	1	490	C	OP2-P-O3'	5.81	117.99	105.20
2	1	1111	A	C2-N3-C4	5.81	113.51	110.60
2	1	2480	C	C6-N1-C2	-5.81	117.97	120.30
2	1	847	U	N3-C2-O2	-5.76	118.17	122.20
2	1	784	G	P-O3'-C3'	5.76	126.61	119.70
23	s	65	ASP	CB-CG-OD2	5.75	123.48	118.30
43	K	92	THR	C-N-CA	5.73	136.03	121.70
41	I	97	LEU	CA-CB-CG	5.73	128.48	115.30
2	1	2023	C	N1-C2-O2	5.72	122.33	118.90
2	1	12	U	C2-N1-C1'	5.72	124.56	117.70
37	4	12	A	OP2-P-O3'	5.72	117.78	105.20
2	1	897	C	N3-C2-O2	-5.71	117.91	121.90
2	1	974	G	N7-C8-N9	5.71	115.95	113.10
1	3	1402	C	C6-N1-C2	-5.70	118.02	120.30
2	1	1005	C	C6-N1-C2	-5.70	118.02	120.30
2	1	765	C	N1-C2-O2	5.70	122.32	118.90
2	1	140	C	N1-C2-O2	5.69	122.31	118.90
1	3	439	U	N1-C2-O2	5.68	126.78	122.80
12	h	118	ILE	CG1-CB-CG2	-5.65	98.96	111.40
2	1	2313	C	N3-C2-O2	-5.64	117.95	121.90
38	5	13	C	N1-C2-O2	5.64	122.29	118.90
1	3	531	U	N1-C2-O2	5.64	126.75	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	1518	A	N7-C8-N9	5.62	116.61	113.80
4	6	69	C	N1-C2-O2	5.62	122.27	118.90
2	1	974	G	C5-N7-C8	-5.62	101.49	104.30
2	1	776	G	C8-N9-C1'	-5.61	119.71	127.00
2	1	984	A	C2-N3-C4	-5.59	107.81	110.60
3	2	31	C	N1-C2-O2	5.59	122.25	118.90
2	1	2572	A	OP2-P-O3'	5.58	117.47	105.20
2	1	528	A	N3-C4-N9	-5.56	122.95	127.40
2	1	143	C	N3-C2-O2	-5.56	118.01	121.90
2	1	1314	C	C6-N1-C2	-5.56	118.08	120.30
2	1	1993	U	N1-C2-O2	5.54	126.68	122.80
2	1	544	C	N1-C2-O2	5.52	122.21	118.90
4	6	3	C	C6-N1-C2	-5.52	118.09	120.30
1	3	754	C	N1-C2-O2	5.51	122.21	118.90
1	3	983	A	N3-C4-N9	5.51	131.81	127.40
2	1	2714	G	C8-N9-C4	-5.48	104.21	106.40
2	1	915	C	N1-C2-O2	5.47	122.18	118.90
2	1	737	C	C6-N1-C2	-5.46	118.12	120.30
37	4	13	A	N7-C8-N9	-5.45	111.07	113.80
2	1	654	A	C2-N3-C4	5.44	113.32	110.60
2	1	2615	U	N1-C2-O2	5.44	126.61	122.80
2	1	2615	U	N3-C2-O2	-5.44	118.39	122.20
1	3	1398	A	C2-N3-C4	5.43	113.32	110.60
2	1	1314	C	C5-C6-N1	5.43	123.72	121.00
2	1	2870	C	C6-N1-C2	-5.42	118.13	120.30
2	1	528	A	N7-C8-N9	5.42	116.51	113.80
1	3	54	C	N3-C2-O2	-5.41	118.12	121.90
2	1	141	G	C2-N3-C4	5.41	114.60	111.90
1	3	813	U	N1-C2-O2	5.39	126.58	122.80
2	1	1068	G	C8-N9-C4	-5.39	104.24	106.40
29	y	19	LEU	CA-CB-CG	5.39	127.70	115.30
3	2	4	C	O5'-P-OP2	-5.39	100.85	105.70
1	3	1382	C	C6-N1-C2	-5.38	118.15	120.30
2	1	2498	C	N3-C2-O2	-5.38	118.14	121.90
2	1	1005	C	C2-N1-C1'	5.37	124.71	118.80
3	2	68	C	N1-C2-O2	5.36	122.11	118.90
2	1	464	U	P-O3'-C3'	5.35	126.12	119.70
2	1	1005	C	C5-C6-N1	5.35	123.67	121.00
2	1	2326	C	C6-N1-C2	-5.35	118.16	120.30
2	1	2250	G	N7-C8-N9	5.35	115.77	113.10
2	1	1816	C	N1-C2-O2	5.32	122.09	118.90
2	1	1920	C	C5-C6-N1	5.32	123.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	m	69	PRO	C-N-CA	5.31	134.97	121.70
3	2	66	A	P-O3'-C3'	5.30	126.06	119.70
2	1	752	A	C5-N7-C8	-5.28	101.26	103.90
2	1	1452	G	N3-C4-C5	5.28	131.24	128.60
2	1	158	U	N1-C2-O2	5.27	126.49	122.80
2	1	2714	G	N7-C8-N9	5.27	115.73	113.10
50	R	113	LYS	C-N-CD	5.27	139.46	128.40
1	3	983	A	N3-C4-C5	-5.27	123.11	126.80
1	3	990	C	N1-C2-O2	5.26	122.06	118.90
4	6	64	G	C4-N9-C1'	5.26	133.34	126.50
13	i	52	LEU	CA-CB-CG	5.24	127.34	115.30
2	1	1348	C	N3-C2-O2	-5.23	118.24	121.90
38	5	40	C	N1-C2-O2	5.23	122.04	118.90
2	1	1076	C	C6-N1-C2	-5.23	118.21	120.30
1	3	972	C	C6-N1-C2	-5.22	118.21	120.30
1	3	792	A	O4'-C1'-N9	5.21	112.37	108.20
2	1	687	C	C6-N1-C1'	-5.21	114.55	120.80
2	1	1914	C	N3-C2-O2	-5.21	118.25	121.90
2	1	2480	C	N1-C2-O2	5.20	122.02	118.90
38	5	55	U	N1-C2-O2	5.20	126.44	122.80
1	3	531	U	N3-C2-O2	-5.20	118.56	122.20
3	2	3	C	OP1-P-O3'	5.20	116.63	105.20
3	2	12	C	C2-N1-C1'	5.20	124.51	118.80
2	1	2552	U	C2-N1-C1'	5.19	123.93	117.70
2	1	1639	C	N1-C2-O2	5.18	122.01	118.90
2	1	198	C	C6-N1-C2	-5.17	118.23	120.30
2	1	2096	C	C6-N1-C2	-5.17	118.23	120.30
2	1	2354	C	C6-N1-C2	-5.15	118.24	120.30
2	1	479	A	OP1-P-O3'	5.14	116.51	105.20
2	1	1880	U	N1-C2-O2	5.13	126.39	122.80
2	1	1639	C	N3-C2-O2	-5.13	118.31	121.90
37	4	12	A	O5'-P-OP1	5.13	116.86	110.70
1	3	58	C	C6-N1-C2	-5.12	118.25	120.30
2	1	915	C	N3-C2-O2	-5.11	118.32	121.90
2	1	1847	A	P-O3'-C3'	5.11	125.83	119.70
2	1	2076	U	C2-N1-C1'	5.11	123.83	117.70
3	2	97	C	N3-C2-O2	-5.11	118.33	121.90
2	1	2043	C	N1-C2-O2	5.11	121.96	118.90
1	3	397	A	C2-N3-C4	5.10	113.15	110.60
2	1	225	C	N1-C2-O2	5.10	121.96	118.90
2	1	510	C	N3-C2-O2	-5.10	118.33	121.90
2	1	2250	G	N3-C4-C5	5.09	131.15	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	1398	A	N7-C8-N9	5.08	116.34	113.80
3	2	31	C	N3-C2-O2	-5.08	118.34	121.90
16	1	29	LYS	N-CA-C	-5.08	97.28	111.00
1	3	754	C	C6-N1-C1'	-5.08	114.71	120.80
2	1	2406	A	P-O3'-C3'	5.07	125.78	119.70
5	b	231	HIS	C-N-CA	-5.07	111.66	122.30
2	1	1913	A	C2-N3-C4	5.06	113.13	110.60
2	1	1102	C	C6-N1-C2	-5.06	118.28	120.30
2	1	1913	A	C4-N9-C1'	5.06	135.40	126.30
1	3	439	U	C5-C6-N1	5.04	125.22	122.70
2	1	2716	C	C6-N1-C2	-5.04	118.28	120.30
2	1	1893	C	N1-C2-O2	5.04	121.92	118.90
1	3	779	C	C6-N1-C2	-5.03	118.29	120.30
2	1	275	C	C6-N1-C2	-5.03	118.29	120.30
2	1	542	C	N3-C2-O2	-5.03	118.38	121.90
1	3	311	C	C6-N1-C2	-5.03	118.29	120.30
2	1	349	U	N1-C2-O2	5.03	126.32	122.80
2	1	1557	C	OP1-P-O3'	5.02	116.25	105.20
2	1	1967	C	N1-C2-O2	5.02	121.91	118.90
2	1	1920	C	N1-C2-O2	5.02	121.91	118.90
2	1	1822	C	C6-N1-C2	-5.02	118.29	120.30
2	1	765	C	N3-C2-O2	-5.01	118.39	121.90
1	3	990	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	2166	U	Sidechain
31	A	29	GLY	Peptide
35	E	30	HIS	Peptide
36	F	36	ARG	Peptide
39	G	18	GLN	Peptide
39	G	21	TYR	Peptide
41	I	151	GLN	Peptide
41	I	190	LEU	Peptide
42	J	101	GLY	Peptide
42	J	158	LYS	Peptide
47	O	34	ALA	Peptide
48	P	118	ASN	Peptide
48	P	124	LYS	Peptide
50	R	8	ILE	Peptide

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Mol	Chain	Res	Type	Group
51	S	33	VAL	Peptide
54	V	16	MET	Peptide
54	V	49	ASN	Peptide
55	W	19	GLU	Peptide
58	Z	63	ASN	Peptide
6	c	159	LYS	Peptide
8	e	174	PHE	Peptide
8	e	175	PRO	Peptide
10	g	51	ARG	Peptide
10	g	8	LYS	Peptide
12	h	105	LYS	Peptide
12	h	118	ILE	Peptide
12	h	122	GLN	Peptide
12	h	80	THR	Peptide
15	k	91	SER	Peptide
15	k	93	GLN	Peptide
18	n	10	LEU	Peptide
22	r	53	PHE	Peptide
23	s	8	ARG	Peptide
29	y	23	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	269/271 (99%)	251 (93%)	18 (7%)	0	100	100
6	c	207/209 (99%)	190 (92%)	16 (8%)	1 (0%)	25	56
7	d	199/201 (99%)	181 (91%)	17 (8%)	1 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	e	175/177 (99%)	158 (90%)	15 (9%)	2 (1%)	12	37
9	f	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
10	g	147/149 (99%)	125 (85%)	20 (14%)	2 (1%)	9	31
11	a	130/234 (56%)	115 (88%)	15 (12%)	0	100	100
12	h	129/131 (98%)	95 (74%)	31 (24%)	3 (2%)	5	20
13	i	139/142 (98%)	119 (86%)	19 (14%)	1 (1%)	19	49
14	j	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
15	k	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	16	45
16	l	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	19	49
17	m	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	8	29
18	n	118/120 (98%)	101 (86%)	15 (13%)	2 (2%)	7	27
19	o	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
20	p	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
21	q	115/117 (98%)	115 (100%)	0	0	100	100
22	r	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	13	40
23	s	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
24	t	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
25	u	100/102 (98%)	87 (87%)	12 (12%)	1 (1%)	13	40
26	v	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
27	w	73/75 (97%)	63 (86%)	10 (14%)	0	100	100
28	x	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
29	y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	8	28
30	z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
31	A	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
32	B	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	2	11
33	C	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
34	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
35	E	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	8	28
36	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
39	G	216/225 (96%)	193 (89%)	21 (10%)	2 (1%)	14	43
40	H	204/206 (99%)	190 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	I	203/205 (99%)	177 (87%)	26 (13%)	0	100	100
42	J	155/157 (99%)	136 (88%)	19 (12%)	0	100	100
43	K	98/100 (98%)	84 (86%)	13 (13%)	1 (1%)	13	40
44	L	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
45	M	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
46	N	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
47	O	96/98 (98%)	81 (84%)	14 (15%)	1 (1%)	13	40
48	P	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
49	Q	121/123 (98%)	100 (83%)	20 (16%)	1 (1%)	16	45
50	R	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
51	S	98/100 (98%)	81 (83%)	17 (17%)	0	100	100
52	T	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	5	20
53	U	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
54	V	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
55	W	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
56	X	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
57	Y	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
58	Z	63/65 (97%)	39 (62%)	19 (30%)	5 (8%)	1	2
All	All	5976/6190 (96%)	5372 (90%)	570 (10%)	34 (1%)	24	52

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	n	70	THR
8	e	175	PRO
8	e	176	PHE
10	g	9	VAL
16	l	29	LYS
17	m	70	ASP
29	y	24	GLU
35	E	31	ILE
39	G	19	THR
52	T	45	HIS
58	Z	24	LYS
58	Z	65	ARG
15	k	108	ARG

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Mol	Chain	Res	Type
25	u	98	ASN
32	B	23	ALA
7	d	86	ALA
17	m	69	PRO
18	n	69	ARG
22	r	54	VAL
39	G	72	LYS
43	K	92	THR
52	T	44	GLU
58	Z	37	TYR
12	h	80	THR
58	Z	9	GLU
6	c	169	ARG
10	g	8	LYS
47	O	57	VAL
58	Z	10	PRO
12	h	79	PRO
12	h	123	ILE
49	Q	120	ARG
32	B	24	VAL
13	i	90	GLY

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	
5	b	216/216 (100%)	215 (100%)	1 (0%)	86	96
6	c	164/164 (100%)	164 (100%)	0	100	100
7	d	165/165 (100%)	165 (100%)	0	100	100
8	e	148/148 (100%)	147 (99%)	1 (1%)	81	94
9	f	137/137 (100%)	137 (100%)	0	100	100
10	g	114/114 (100%)	114 (100%)	0	100	100
11	a	110/181 (61%)	109 (99%)	1 (1%)	75	92
12	h	100/100 (100%)	99 (99%)	1 (1%)	73	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	i	109/110 (99%)	106 (97%)	3 (3%)	38	73
14	j	116/116 (100%)	116 (100%)	0	100	100
15	k	103/103 (100%)	102 (99%)	1 (1%)	73	91
16	l	102/102 (100%)	101 (99%)	1 (1%)	73	91
17	m	109/109 (100%)	109 (100%)	0	100	100
18	n	100/100 (100%)	100 (100%)	0	100	100
19	o	86/86 (100%)	85 (99%)	1 (1%)	67	89
20	p	99/99 (100%)	99 (100%)	0	100	100
21	q	89/89 (100%)	89 (100%)	0	100	100
22	r	84/84 (100%)	84 (100%)	0	100	100
23	s	93/93 (100%)	90 (97%)	3 (3%)	34	69
24	t	80/80 (100%)	80 (100%)	0	100	100
25	u	83/83 (100%)	83 (100%)	0	100	100
26	v	78/78 (100%)	77 (99%)	1 (1%)	65	88
27	w	57/57 (100%)	56 (98%)	1 (2%)	54	82
28	x	67/67 (100%)	67 (100%)	0	100	100
29	y	55/55 (100%)	54 (98%)	1 (2%)	54	82
30	z	48/48 (100%)	48 (100%)	0	100	100
31	A	59/59 (100%)	59 (100%)	0	100	100
32	B	47/47 (100%)	47 (100%)	0	100	100
33	C	45/45 (100%)	45 (100%)	0	100	100
34	D	38/38 (100%)	38 (100%)	0	100	100
35	E	51/51 (100%)	51 (100%)	0	100	100
36	F	34/34 (100%)	34 (100%)	0	100	100
39	G	180/186 (97%)	175 (97%)	5 (3%)	38	73
40	H	170/170 (100%)	170 (100%)	0	100	100
41	I	172/172 (100%)	171 (99%)	1 (1%)	84	95
42	J	119/119 (100%)	117 (98%)	2 (2%)	56	83
43	K	87/87 (100%)	87 (100%)	0	100	100
44	L	124/124 (100%)	124 (100%)	0	100	100
45	M	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	N	105/105 (100%)	105 (100%)	0	100	100
47	O	86/86 (100%)	85 (99%)	1 (1%)	67	89
48	P	89/89 (100%)	88 (99%)	1 (1%)	70	90
49	Q	103/103 (100%)	103 (100%)	0	100	100
50	R	92/92 (100%)	92 (100%)	0	100	100
51	S	83/83 (100%)	82 (99%)	1 (1%)	67	89
52	T	76/76 (100%)	76 (100%)	0	100	100
53	U	65/65 (100%)	65 (100%)	0	100	100
54	V	74/74 (100%)	74 (100%)	0	100	100
55	W	56/56 (100%)	55 (98%)	1 (2%)	54	82
56	X	70/70 (100%)	70 (100%)	0	100	100
57	Y	65/65 (100%)	65 (100%)	0	100	100
58	Z	55/55 (100%)	52 (94%)	3 (6%)	18	48
All	All	4961/5039 (98%)	4930 (99%)	31 (1%)	82	95

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	b	44	ASN
8	e	154	THR
11	a	164	ARG
12	h	109	LYS
13	i	99	LYS
13	i	112	LYS
13	i	133	ARG
15	k	49	ARG
16	l	81	ASP
19	o	10	ARG
23	s	1	MET
23	s	11	ARG
23	s	106	VAL
26	v	79	ARG
27	w	51	ARG
29	y	19	LEU
39	G	19	THR
39	G	34	ARG
39	G	104	LYS

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Mol	Chain	Res	Type
39	G	142	LYS
39	G	224	ARG
41	I	153	ARG
42	J	122	VAL
42	J	156	ARG
47	O	30	LYS
48	P	12	ARG
51	S	22	LYS
55	W	11	ARG
58	Z	24	LYS
58	Z	32	ARG
58	Z	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
5	b	116	GLN
5	b	152	GLN
5	b	238	ASN
6	c	32	ASN
6	c	150	GLN
7	d	46	GLN
7	d	94	GLN
8	e	26	GLN
8	e	134	GLN
9	f	47	ASN
9	f	103	ASN
10	g	28	ASN
11	a	165	ASN
13	i	110	GLN
14	j	40	HIS
14	j	58	ASN
14	j	135	GLN
16	l	4	ASN
18	n	11	ASN
19	o	38	GLN
19	o	43	ASN
21	q	19	GLN
21	q	71	ASN
22	r	43	ASN
24	t	48	GLN
25	u	68	ASN

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Mol	Chain	Res	Type
25	u	73	ASN
26	v	80	HIS
27	w	8	ASN
27	w	72	ASN
28	x	5	GLN
29	y	27	ASN
31	A	65	ASN
32	B	5	ASN
34	D	13	ASN
36	F	37	GLN
39	G	14	HIS
39	G	169	HIS
40	H	139	ASN
41	I	73	ASN
41	I	88	ASN
41	I	151	GLN
42	J	121	ASN
42	J	134	ASN
42	J	145	ASN
43	K	3	HIS
44	L	147	ASN
45	M	3	GLN
45	M	17	GLN
46	N	30	ASN
46	N	31	GLN
47	O	70	HIS
48	P	39	ASN
49	Q	4	ASN
49	Q	45	ASN
50	R	99	GLN
51	S	42	ASN
52	T	34	GLN
53	U	9	HIS
54	V	30	HIS
55	W	51	GLN
56	X	68	HIS
57	Y	51	ASN
57	Y	69	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	1538/1539 (99%)	234 (15%)	1 (0%)
2	1	2902/2903 (99%)	508 (17%)	11 (0%)
3	2	119/120 (99%)	17 (14%)	3 (2%)
37	4	18/35 (51%)	8 (44%)	2 (11%)
38	5	76/77 (98%)	19 (25%)	0
4	6	76/77 (98%)	23 (30%)	0
All	All	4729/4751 (99%)	809 (17%)	17 (0%)

All (809) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	4	U
1	3	5	U
1	3	6	G
1	3	7	A
1	3	9	G
1	3	22	G
1	3	32	A
1	3	39	G
1	3	47	C
1	3	48	C
1	3	51	A
1	3	54	C
1	3	71	A
1	3	81	A
1	3	82	G
1	3	85	U
1	3	87	C
1	3	91	U
1	3	94	G
1	3	95	C
1	3	100	G
1	3	116	A
1	3	121	U
1	3	128	G
1	3	130	A
1	3	141	G
1	3	144	G
1	3	149	A
1	3	154	U
1	3	163	C
1	3	183	C
1	3	184	G

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Mol	Chain	Res	Type
1	3	191	G
1	3	197	A
1	3	208	U
1	3	209	U
1	3	210	C
1	3	211	G
1	3	212	G
1	3	226	G
1	3	245	U
1	3	247	G
1	3	251	G
1	3	266	G
1	3	267	C
1	3	279	A
1	3	280	C
1	3	281	G
1	3	289	G
1	3	298	A
1	3	306	A
1	3	309	A
1	3	321	A
1	3	328	C
1	3	347	G
1	3	351	G
1	3	352	C
1	3	354	G
1	3	367	U
1	3	372	C
1	3	392	C
1	3	397	A
1	3	406	G
1	3	411	A
1	3	413	G
1	3	414	A
1	3	424	G
1	3	429	U
1	3	436	C
1	3	437	U
1	3	451	A
1	3	467	U
1	3	479	U
1	3	484	G

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Mol	Chain	Res	Type
1	3	485	U
1	3	486	U
1	3	494	G
1	3	495	A
1	3	497	G
1	3	511	C
1	3	518	C
1	3	519	C
1	3	521	G
1	3	524	G
1	3	527	G
1	3	529	G
1	3	533	A
1	3	536	C
1	3	547	A
1	3	559	A
1	3	560	A
1	3	561	U
1	3	562	U
1	3	564	C
1	3	572	A
1	3	573	A
1	3	576	C
1	3	577	G
1	3	615	G
1	3	620	C
1	3	633	G
1	3	642	A
1	3	650	G
1	3	653	U
1	3	665	A
1	3	688	G
1	3	702	A
1	3	703	G
1	3	720	C
1	3	721	G
1	3	723	U
1	3	724	G
1	3	733	G
1	3	734	G
1	3	753	A
1	3	754	C

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Mol	Chain	Res	Type
1	3	755	G
1	3	777	A
1	3	781	A
1	3	793	U
1	3	794	A
1	3	815	A
1	3	817	C
1	3	818	G
1	3	819	A
1	3	821	G
1	3	832	G
1	3	843	U
1	3	844	G
1	3	845	A
1	3	846	G
1	3	849	G
1	3	851	G
1	3	864	A
1	3	884	U
1	3	889	A
1	3	902	G
1	3	914	A
1	3	926	G
1	3	934	C
1	3	935	A
1	3	960	U
1	3	961	U
1	3	966	G
1	3	969	A
1	3	971	G
1	3	975	A
1	3	976	G
1	3	977	A
1	3	983	A
1	3	991	U
1	3	992	U
1	3	993	G
1	3	1004	A
1	3	1020	G
1	3	1028	C
1	3	1031	C
1	3	1032	G

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Mol	Chain	Res	Type
1	3	1033	G
1	3	1034	G
1	3	1053	G
1	3	1080	A
1	3	1081	A
1	3	1085	U
1	3	1094	G
1	3	1095	U
1	3	1099	G
1	3	1101	A
1	3	1130	A
1	3	1132	C
1	3	1133	G
1	3	1137	C
1	3	1138	G
1	3	1139	G
1	3	1140	C
1	3	1159	U
1	3	1160	G
1	3	1168	U
1	3	1171	A
1	3	1182	G
1	3	1184	G
1	3	1196	A
1	3	1199	U
1	3	1212	U
1	3	1213	A
1	3	1214	C
1	3	1227	A
1	3	1228	C
1	3	1238	A
1	3	1257	A
1	3	1260	G
1	3	1261	A
1	3	1274	A
1	3	1275	A
1	3	1280	A
1	3	1282	C
1	3	1286	U
1	3	1287	A
1	3	1290	G
1	3	1300	G

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Mol	Chain	Res	Type
1	3	1301	U
1	3	1305	G
1	3	1317	C
1	3	1331	G
1	3	1346	A
1	3	1353	G
1	3	1363	A
1	3	1370	G
1	3	1379	G
1	3	1381	U
1	3	1395	C
1	3	1398	A
1	3	1399	C
1	3	1419	G
1	3	1429	A
1	3	1432	G
1	3	1441	A
1	3	1446	A
1	3	1448	C
1	3	1452	C
1	3	1453	G
1	3	1487	G
1	3	1497	G
1	3	1499	A
1	3	1502	A
1	3	1503	A
1	3	1506	U
1	3	1507	A
1	3	1517	G
1	3	1519	A
1	3	1529	G
1	3	1530	G
1	3	1534	A
1	3	1535	C
2	1	10	A
2	1	12	U
2	1	30	G
2	1	35	G
2	1	46	G
2	1	50	U
2	1	51	G
2	1	58	G

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Mol	Chain	Res	Type
2	1	71	A
2	1	74	A
2	1	75	G
2	1	84	A
2	1	96	C
2	1	100	U
2	1	110	G
2	1	118	A
2	1	119	A
2	1	120	U
2	1	125	A
2	1	139	U
2	1	140	C
2	1	141	G
2	1	142	A
2	1	149	A
2	1	158	U
2	1	162	U
2	1	163	C
2	1	196	A
2	1	199	A
2	1	204	A
2	1	215	G
2	1	216	A
2	1	219	A
2	1	220	G
2	1	221	A
2	1	222	A
2	1	228	C
2	1	229	C
2	1	230	G
2	1	241	A
2	1	248	G
2	1	252	G
2	1	255	A
2	1	265	A
2	1	266	G
2	1	276	U
2	1	277	G
2	1	281	C
2	1	284	U
2	1	285	G

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Mol	Chain	Res	Type
2	1	294	A
2	1	311	A
2	1	322	A
2	1	323	C
2	1	329	G
2	1	330	A
2	1	334	C
2	1	345	A
2	1	346	A
2	1	353	C
2	1	361	G
2	1	362	A
2	1	371	A
2	1	372	G
2	1	383	C
2	1	386	G
2	1	387	U
2	1	395	U
2	1	396	G
2	1	403	U
2	1	404	A
2	1	405	U
2	1	406	G
2	1	411	G
2	1	412	A
2	1	424	G
2	1	443	A
2	1	457	A
2	1	465	G
2	1	467	G
2	1	475	C
2	1	477	A
2	1	481	G
2	1	491	G
2	1	500	G
2	1	501	A
2	1	504	A
2	1	505	A
2	1	508	A
2	1	509	C
2	1	510	C
2	1	517	C

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Mol	Chain	Res	Type
2	1	529	A
2	1	530	G
2	1	532	A
2	1	533	G
2	1	545	U
2	1	546	U
2	1	547	A
2	1	548	G
2	1	549	G
2	1	550	C
2	1	562	U
2	1	563	A
2	1	568	U
2	1	573	U
2	1	575	A
2	1	603	A
2	1	614	A
2	1	615	U
2	1	622	G
2	1	627	A
2	1	634	C
2	1	637	A
2	1	645	C
2	1	646	U
2	1	654	A
2	1	656	G
2	1	670	A
2	1	685	A
2	1	686	U
2	1	695	G
2	1	714	U
2	1	730	A
2	1	747	C
2	1	764	A
2	1	765	C
2	1	775	G
2	1	776	G
2	1	782	A
2	1	784	G
2	1	785	G
2	1	789	A
2	1	800	A

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Mol	Chain	Res	Type
2	1	805	G
2	1	812	C
2	1	819	A
2	1	827	U
2	1	828	U
2	1	830	G
2	1	845	A
2	1	846	U
2	1	847	U
2	1	858	G
2	1	859	G
2	1	866	A
2	1	869	G
2	1	878	A
2	1	887	U
2	1	891	G
2	1	896	A
2	1	897	C
2	1	907	G
2	1	910	A
2	1	932	U
2	1	941	A
2	1	946	C
2	1	958	U
2	1	961	C
2	1	973	A
2	1	974	G
2	1	975	A
2	1	983	A
2	1	989	G
2	1	995	C
2	1	996	A
2	1	999	U
2	1	1003	G
2	1	1005	C
2	1	1012	U
2	1	1013	C
2	1	1021	A
2	1	1022	G
2	1	1023	U
2	1	1025	G
2	1	1026	G

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Mol	Chain	Res	Type
2	1	1033	U
2	1	1040	A
2	1	1046	A
2	1	1047	G
2	1	1059	G
2	1	1060	U
2	1	1062	G
2	1	1063	G
2	1	1064	C
2	1	1065	U
2	1	1066	U
2	1	1067	A
2	1	1068	G
2	1	1069	A
2	1	1070	A
2	1	1071	G
2	1	1072	C
2	1	1073	A
2	1	1075	C
2	1	1076	C
2	1	1077	A
2	1	1078	U
2	1	1083	U
2	1	1084	A
2	1	1085	A
2	1	1087	G
2	1	1088	A
2	1	1089	A
2	1	1090	A
2	1	1091	G
2	1	1101	U
2	1	1103	A
2	1	1104	C
2	1	1111	A
2	1	1112	G
2	1	1130	U
2	1	1131	G
2	1	1132	U
2	1	1134	A
2	1	1135	C
2	1	1139	G
2	1	1142	A

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Mol	Chain	Res	Type
2	1	1155	A
2	1	1172	C
2	1	1173	U
2	1	1174	U
2	1	1175	A
2	1	1176	U
2	1	1177	G
2	1	1178	C
2	1	1180	U
2	1	1186	G
2	1	1204	A
2	1	1206	G
2	1	1211	C
2	1	1212	G
2	1	1236	G
2	1	1247	A
2	1	1248	G
2	1	1253	A
2	1	1255	U
2	1	1256	G
2	1	1265	A
2	1	1271	G
2	1	1272	A
2	1	1275	A
2	1	1300	G
2	1	1301	A
2	1	1345	C
2	1	1352	U
2	1	1359	A
2	1	1365	A
2	1	1368	G
2	1	1376	C
2	1	1379	U
2	1	1383	A
2	1	1395	A
2	1	1414	C
2	1	1416	G
2	1	1419	A
2	1	1420	A
2	1	1421	G
2	1	1427	A
2	1	1428	C

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Mol	Chain	Res	Type
2	1	1434	A
2	1	1437	C
2	1	1452	G
2	1	1454	C
2	1	1458	U
2	1	1461	C
2	1	1478	G
2	1	1482	G
2	1	1490	A
2	1	1491	G
2	1	1504	A
2	1	1508	A
2	1	1515	A
2	1	1522	A
2	1	1524	G
2	1	1532	A
2	1	1533	C
2	1	1535	A
2	1	1536	C
2	1	1537	G
2	1	1554	U
2	1	1555	G
2	1	1558	C
2	1	1559	U
2	1	1560	G
2	1	1566	A
2	1	1569	A
2	1	1578	U
2	1	1584	U
2	1	1608	A
2	1	1627	G
2	1	1634	A
2	1	1639	C
2	1	1647	U
2	1	1648	U
2	1	1649	G
2	1	1654	A
2	1	1669	A
2	1	1672	A
2	1	1674	G
2	1	1675	C
2	1	1694	C

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Mol	Chain	Res	Type
2	1	1698	A
2	1	1715	G
2	1	1716	U
2	1	1729	U
2	1	1730	C
2	1	1738	G
2	1	1744	A
2	1	1757	A
2	1	1758	U
2	1	1764	C
2	1	1773	A
2	1	1776	G
2	1	1780	A
2	1	1781	U
2	1	1786	A
2	1	1800	C
2	1	1801	A
2	1	1808	A
2	1	1816	C
2	1	1819	A
2	1	1829	A
2	1	1848	A
2	1	1857	G
2	1	1870	C
2	1	1873	G
2	1	1884	G
2	1	1901	A
2	1	1903	G
2	1	1906	G
2	1	1913	A
2	1	1914	C
2	1	1915	U
2	1	1927	A
2	1	1929	G
2	1	1930	G
2	1	1936	A
2	1	1937	A
2	1	1938	A
2	1	1939	U
2	1	1943	U
2	1	1944	U
2	1	1955	U

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Mol	Chain	Res	Type
2	1	1966	A
2	1	1967	C
2	1	1970	A
2	1	1971	U
2	1	1972	G
2	1	1980	G
2	1	1981	A
2	1	1991	U
2	1	1992	G
2	1	1993	U
2	1	1996	C
2	1	1997	C
2	1	2020	A
2	1	2022	U
2	1	2023	C
2	1	2030	A
2	1	2031	A
2	1	2033	A
2	1	2043	C
2	1	2049	G
2	1	2052	A
2	1	2055	C
2	1	2056	G
2	1	2060	A
2	1	2061	G
2	1	2062	A
2	1	2069	G
2	1	2076	U
2	1	2093	G
2	1	2096	C
2	1	2100	G
2	1	2110	G
2	1	2111	U
2	1	2115	G
2	1	2116	G
2	1	2118	U
2	1	2119	A
2	1	2123	G
2	1	2128	G
2	1	2129	C
2	1	2131	U
2	1	2132	U

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Mol	Chain	Res	Type
2	1	2133	G
2	1	2134	A
2	1	2137	U
2	1	2141	G
2	1	2145	C
2	1	2146	C
2	1	2147	A
2	1	2149	U
2	1	2154	A
2	1	2157	G
2	1	2160	C
2	1	2162	G
2	1	2164	C
2	1	2166	U
2	1	2172	U
2	1	2173	A
2	1	2174	C
2	1	2189	U
2	1	2192	U
2	1	2198	A
2	1	2203	U
2	1	2204	G
2	1	2211	A
2	1	2225	A
2	1	2226	C
2	1	2238	G
2	1	2239	G
2	1	2243	U
2	1	2250	G
2	1	2279	G
2	1	2283	C
2	1	2287	A
2	1	2288	A
2	1	2297	A
2	1	2305	U
2	1	2309	A
2	1	2325	G
2	1	2327	A
2	1	2331	G
2	1	2333	A
2	1	2334	U
2	1	2336	A

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Mol	Chain	Res	Type
2	1	2345	G
2	1	2350	C
2	1	2361	G
2	1	2383	G
2	1	2385	C
2	1	2402	U
2	1	2403	C
2	1	2406	A
2	1	2407	A
2	1	2423	U
2	1	2429	G
2	1	2430	A
2	1	2441	U
2	1	2445	G
2	1	2448	A
2	1	2470	G
2	1	2474	U
2	1	2476	A
2	1	2480	C
2	1	2492	U
2	1	2502	G
2	1	2503	A
2	1	2505	G
2	1	2518	A
2	1	2520	C
2	1	2529	G
2	1	2547	A
2	1	2554	U
2	1	2564	A
2	1	2565	A
2	1	2566	A
2	1	2567	G
2	1	2572	A
2	1	2573	C
2	1	2586	U
2	1	2602	A
2	1	2609	U
2	1	2613	U
2	1	2615	U
2	1	2629	U
2	1	2630	G
2	1	2646	C

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Mol	Chain	Res	Type
2	1	2661	G
2	1	2689	U
2	1	2690	U
2	1	2714	G
2	1	2716	C
2	1	2726	A
2	1	2732	G
2	1	2733	A
2	1	2744	G
2	1	2748	A
2	1	2764	A
2	1	2765	A
2	1	2766	A
2	1	2778	A
2	1	2791	G
2	1	2794	C
2	1	2797	U
2	1	2798	U
2	1	2799	A
2	1	2800	A
2	1	2808	G
2	1	2809	A
2	1	2818	U
2	1	2820	A
2	1	2823	A
2	1	2833	U
2	1	2835	A
2	1	2859	G
2	1	2861	U
2	1	2867	G
2	1	2868	A
2	1	2872	A
2	1	2873	A
2	1	2880	C
2	1	2884	U
2	1	2887	A
2	1	2891	U
2	1	2902	C
3	2	4	C
3	2	12	C
3	2	13	G
3	2	15	A

Continued on next page...

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Mol	Chain	Res	Type
3	2	24	G
3	2	26	C
3	2	31	C
3	2	35	C
3	2	40	U
3	2	44	G
3	2	67	G
3	2	87	U
3	2	88	C
3	2	89	U
3	2	90	C
3	2	108	A
3	2	109	A
4	6	4	G
4	6	8	U
4	6	9	G
4	6	14	A
4	6	16	C
4	6	17	C
4	6	17(A)	U
4	6	18	G
4	6	19	G
4	6	20	U
4	6	21	A
4	6	22	G
4	6	28	C
4	6	35	A
4	6	46	G
4	6	47	U
4	6	52	G
4	6	63	G
4	6	64	G
4	6	69	C
4	6	72	A
4	6	75	C
4	6	76	A
37	4	9	G
37	4	10	G
37	4	11	U
37	4	12	A
37	4	13	A
37	4	14	A

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Mol	Chain	Res	Type
37	4	15	A
37	4	16	A
38	5	3	G
38	5	4	C
38	5	5	G
38	5	10	G
38	5	17	U
38	5	19	G
38	5	20	U
38	5	21	A
38	5	22	G
38	5	41	A
38	5	42	G
38	5	46	G
38	5	47	U
38	5	48	C
38	5	49	G
38	5	62	C
38	5	65	U
38	5	73	A
38	5	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	1256	A
2	1	464	U
2	1	490	C
2	1	784	G
2	1	858	G
2	1	1020	A
2	1	1715	G
2	1	1847	A
2	1	2326	C
2	1	2406	A
2	1	2572	A
2	1	2808	G
3	2	3	C
3	2	66	A
3	2	88	C
37	4	12	A
37	4	13	A

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 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.

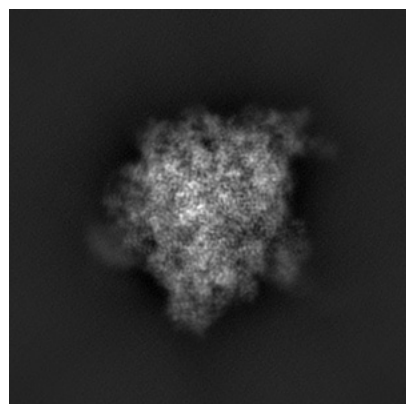
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25418. These allow visual inspection of the internal detail of the map and identification of artifacts.

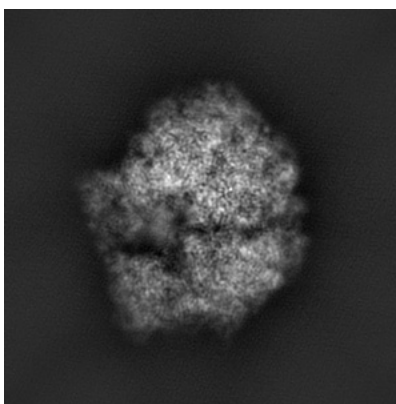
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

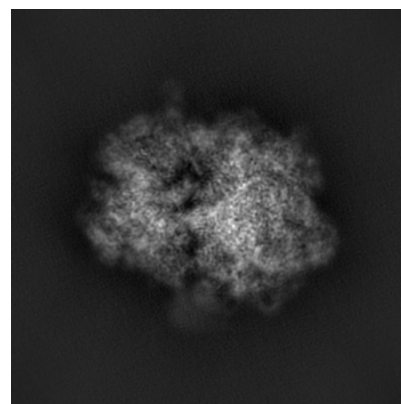
6.1.1 Primary map



X

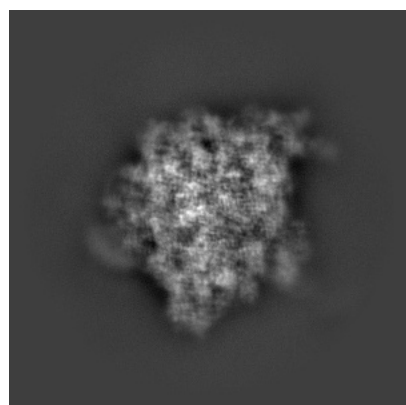


Y

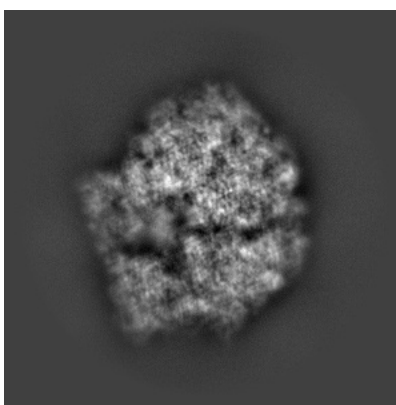


Z

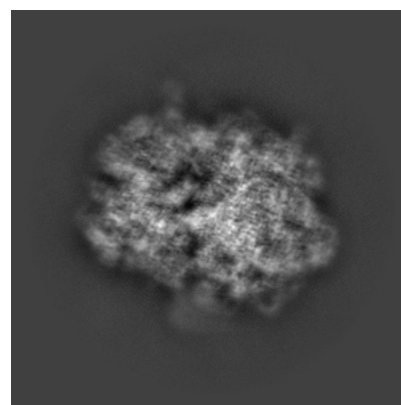
6.1.2 Raw map



X



Y

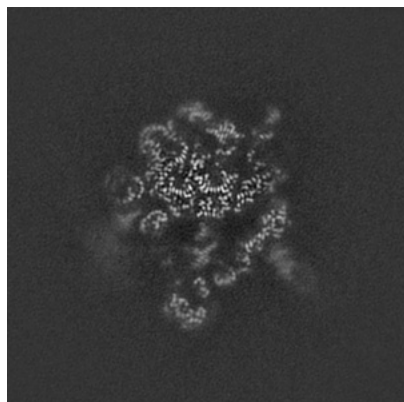


Z

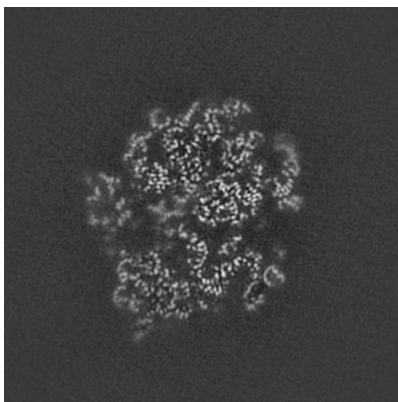
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

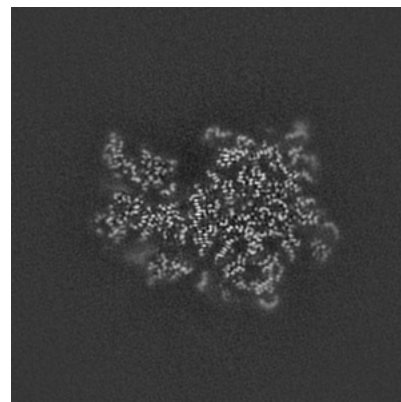
6.2.1 Primary map



X Index: 224

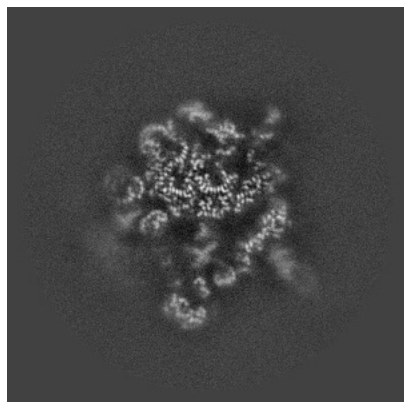


Y Index: 224

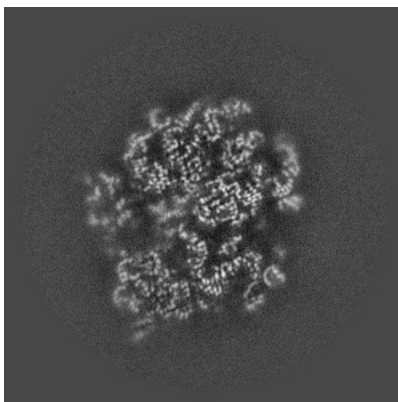


Z Index: 224

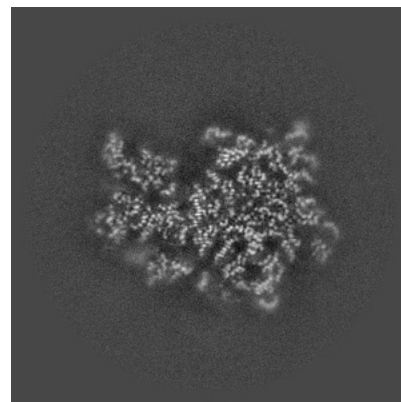
6.2.2 Raw map



X Index: 224



Y Index: 224

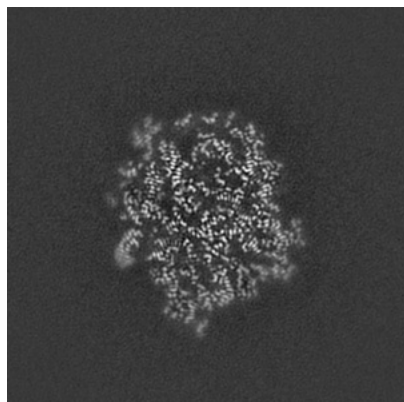


Z Index: 224

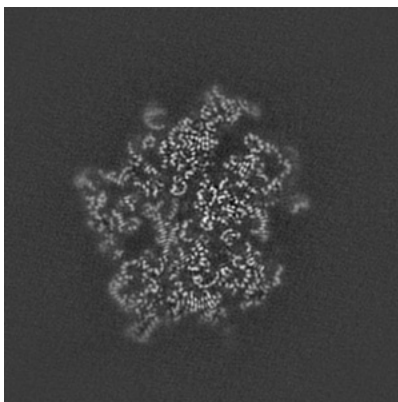
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

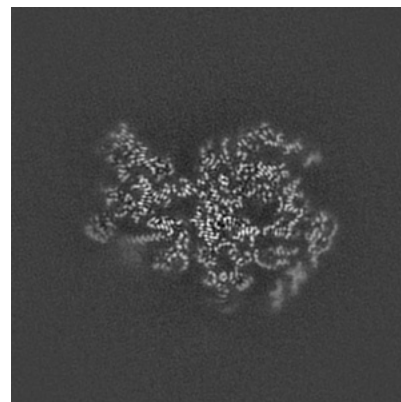
6.3.1 Primary map



X Index: 254

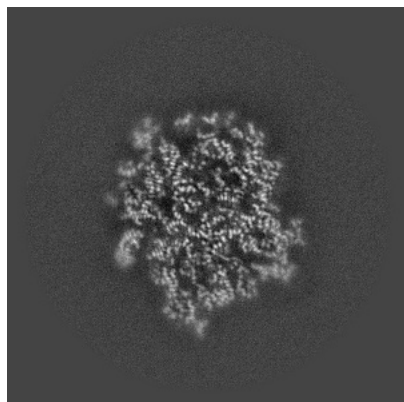


Y Index: 215

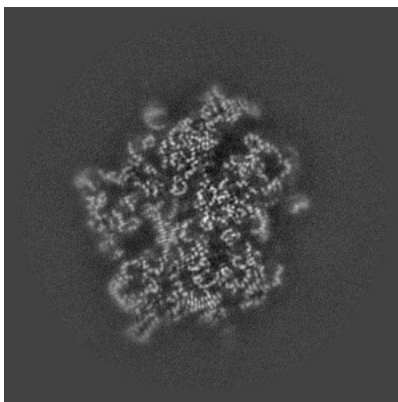


Z Index: 240

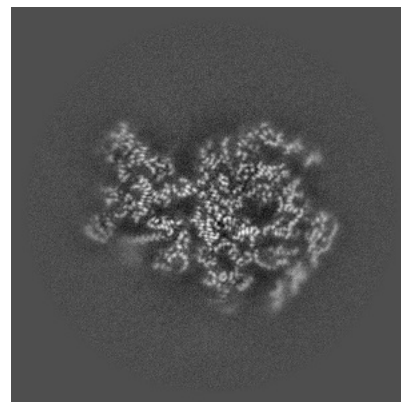
6.3.2 Raw map



X Index: 253



Y Index: 215

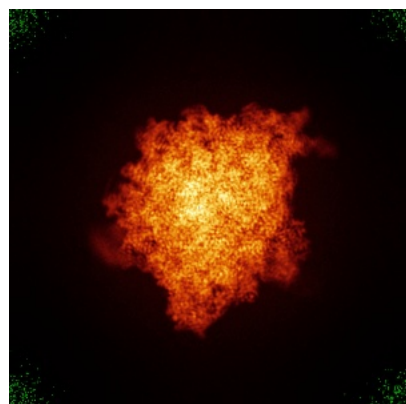


Z Index: 240

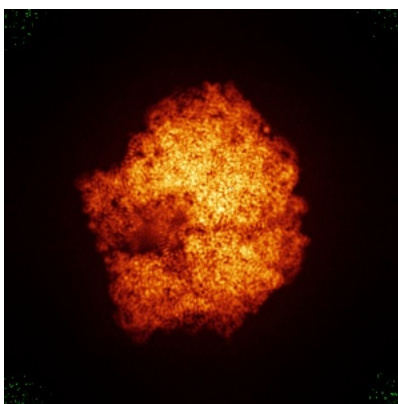
The images above show the largest variance slices of the map in three orthogonal directions.

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

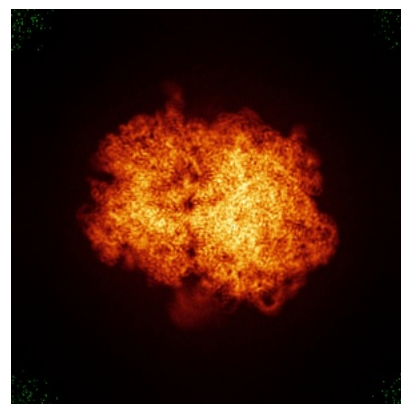
6.4.1 Primary map



X

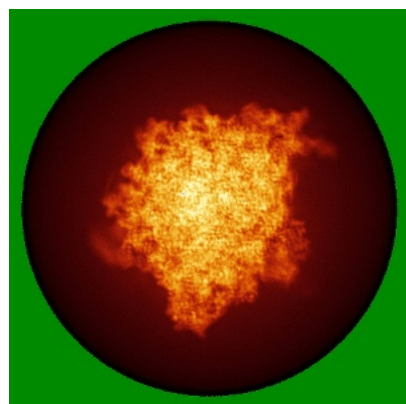


Y

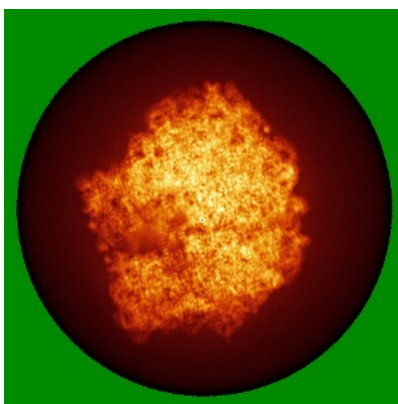


Z

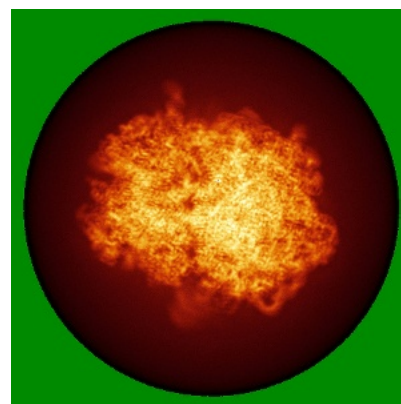
6.4.2 Raw map



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



X



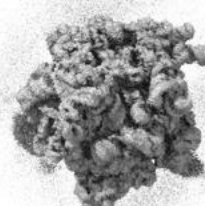
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

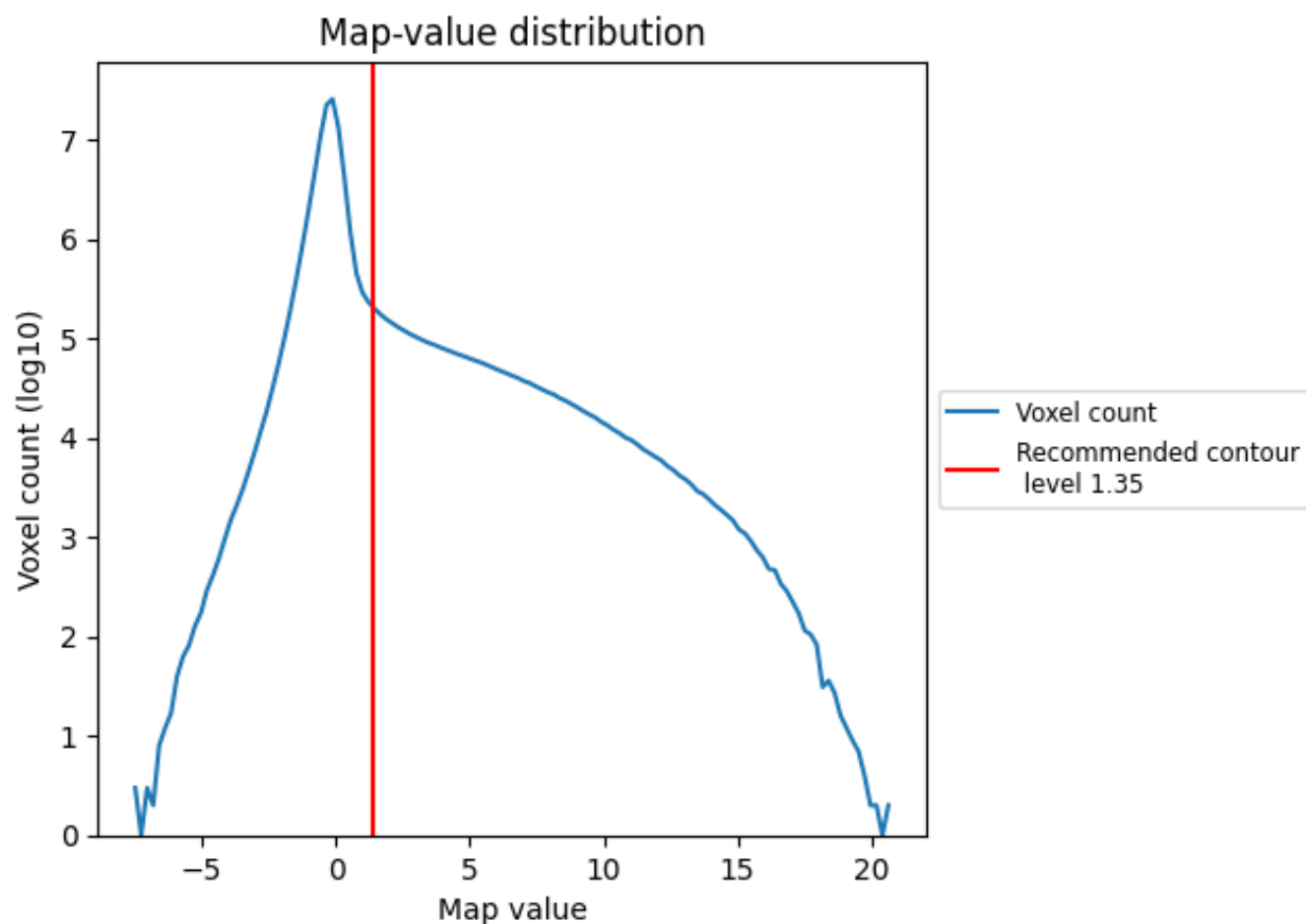
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

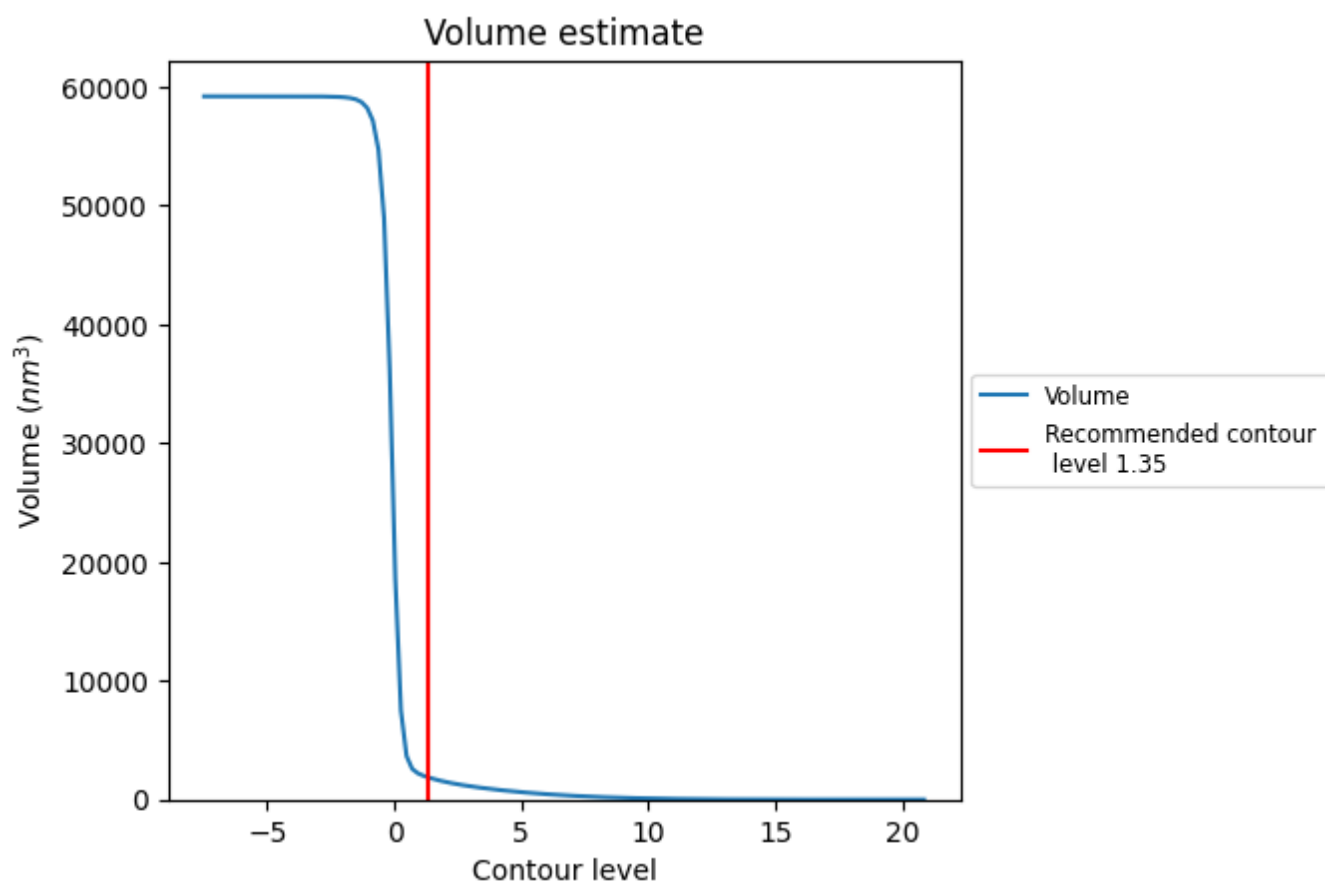
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

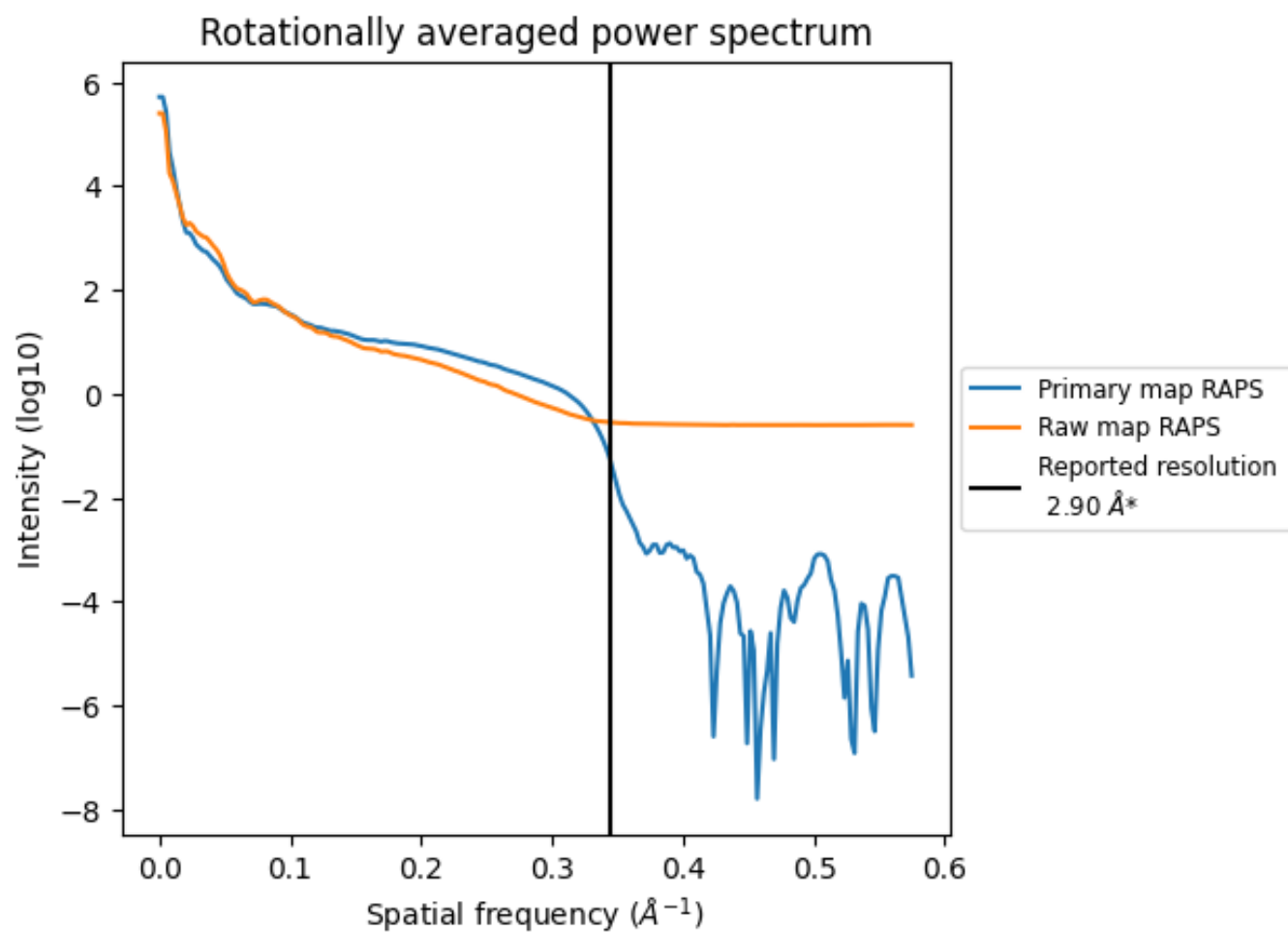
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1857 nm^3 ; this corresponds to an approximate mass of 1677 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

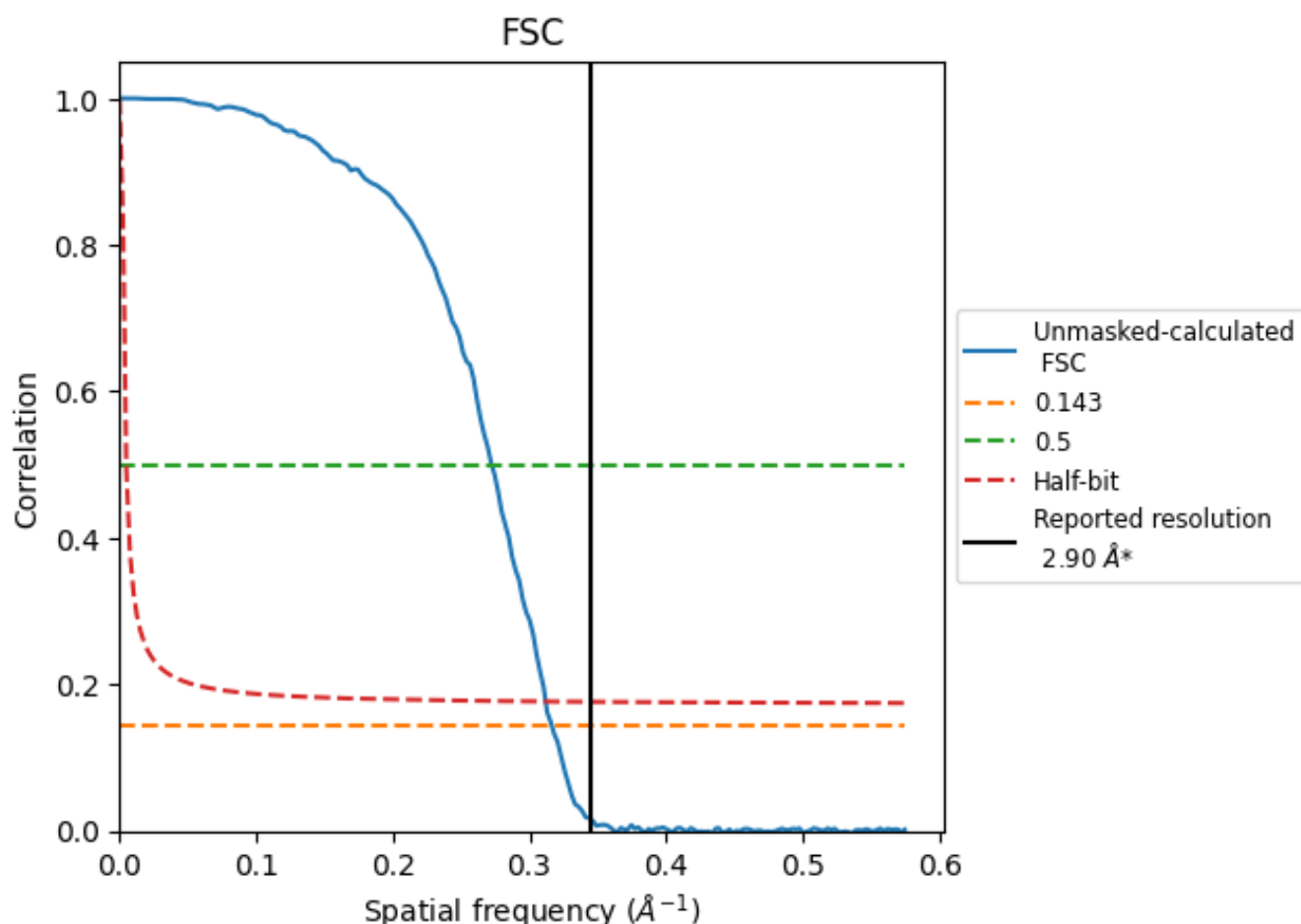


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

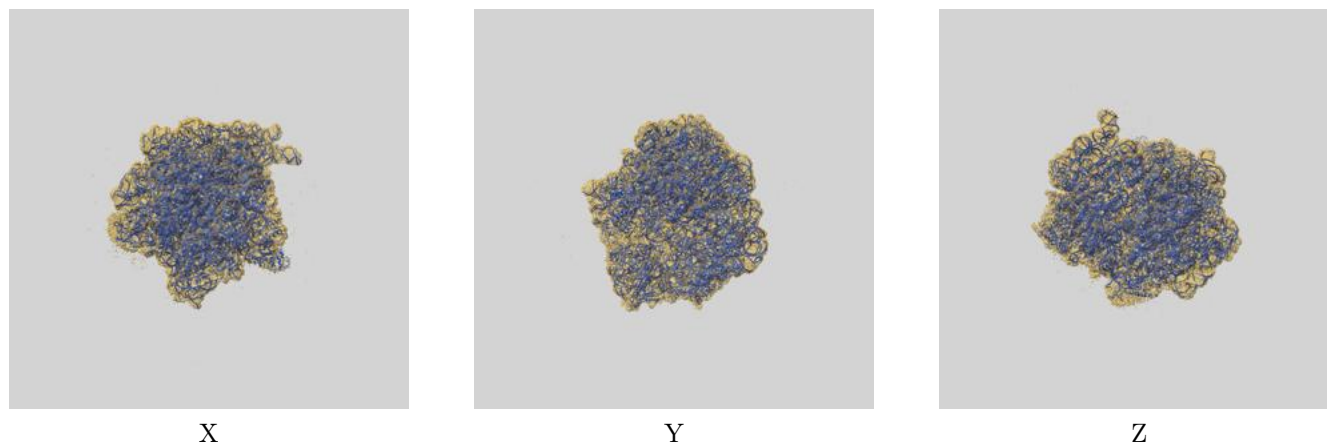
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.67	3.21

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

9 Map-model fit [i](#)

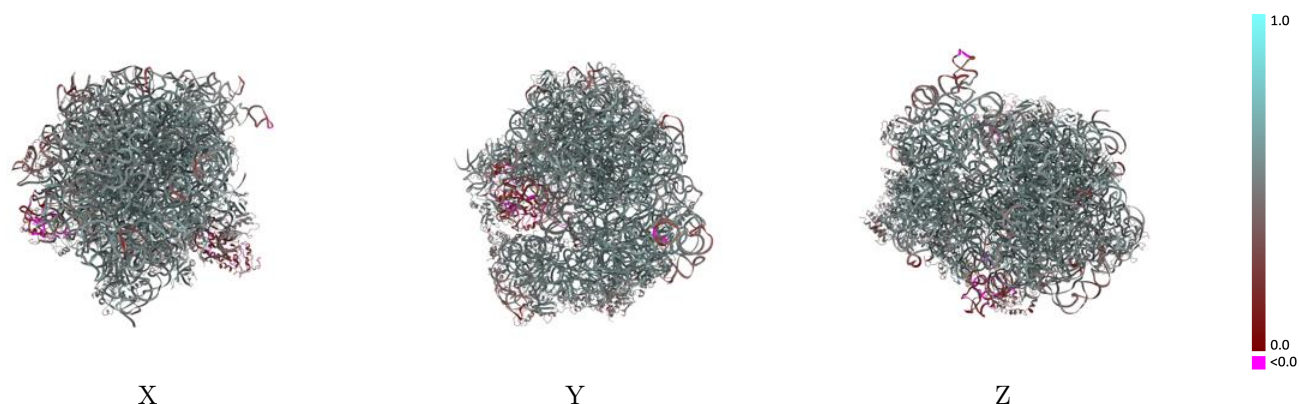
This section contains information regarding the fit between EMDB map EMD-25418 and PDB model 7ST2. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



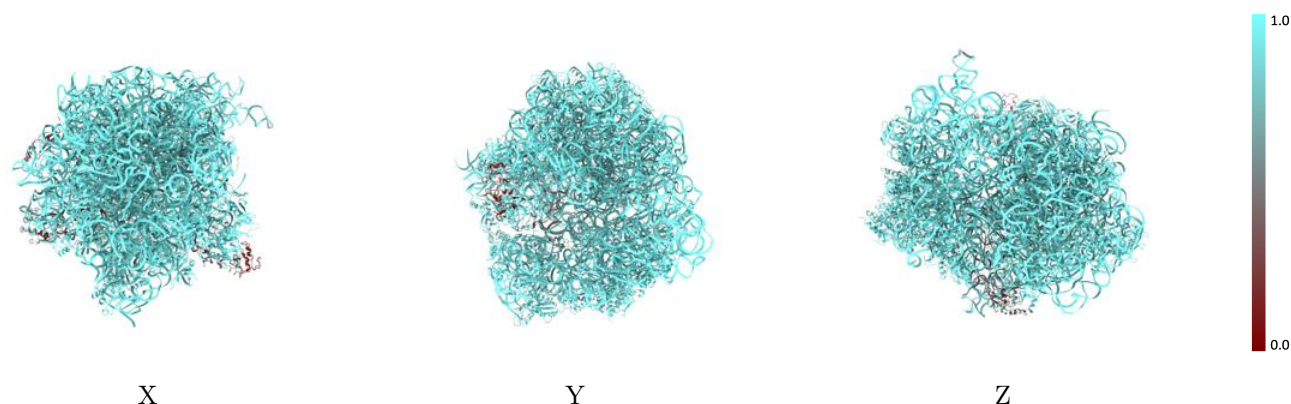
The images above show the 3D surface view of the map at the recommended contour level 1.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



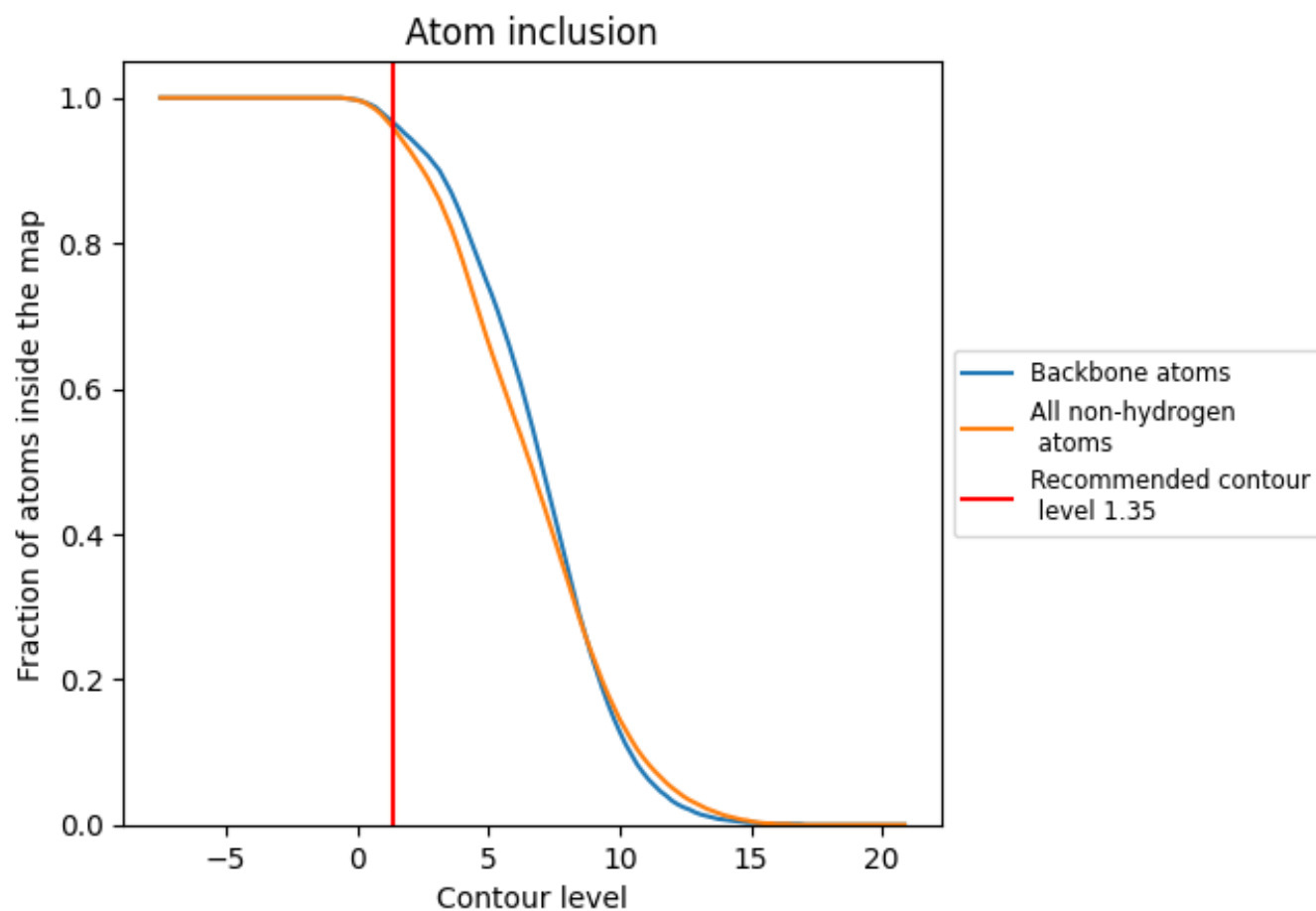
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.35).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.5090
1	 0.9890	 0.5190
2	 0.9980	 0.5200
3	 0.9960	 0.5350
4	 0.9180	 0.3070
5	 0.9950	 0.5100
6	 0.2760	 0.3070
A	 0.9350	 0.4240
B	 0.9720	 0.5370
C	 0.8460	 0.5230
D	 0.9660	 0.5560
E	 0.9780	 0.5670
F	 0.9760	 0.5480
G	 0.9060	 0.4560
H	 0.9510	 0.5190
I	 0.9400	 0.4730
J	 0.9630	 0.5320
K	 0.9670	 0.4820
L	 0.9350	 0.4770
M	 0.9570	 0.5330
N	 0.9510	 0.4870
O	 0.8960	 0.4650
P	 0.9700	 0.5140
Q	 0.9610	 0.5400
R	 0.9450	 0.4810
S	 0.9610	 0.5030
T	 0.9780	 0.5110
U	 0.9590	 0.5080
V	 0.9510	 0.5190
W	 0.9710	 0.4950
X	 0.9610	 0.4840
Y	 0.9460	 0.4990
Z	 0.8570	 0.3510
a	 0.4660	 0.1910
b	 0.9780	 0.5630



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Chain	Atom inclusion	Q-score
c	 0.9810	 0.5460
d	 0.9460	 0.5040
e	 0.9630	 0.4860
f	 0.9750	 0.4860
g	 0.5350	 0.3510
h	 0.3520	 0.1820
i	 0.6260	 0.1690
j	 0.9660	 0.5350
k	 0.9640	 0.5480
l	 0.9660	 0.5270
m	 0.9760	 0.5510
n	 0.9740	 0.5410
o	 0.9770	 0.5040
p	 0.9640	 0.5470
q	 0.9790	 0.5390
r	 0.9650	 0.5250
s	 0.9590	 0.5240
t	 0.9520	 0.5040
u	 0.9670	 0.4890
v	 0.9590	 0.5190
w	 0.9710	 0.5540
x	 0.9670	 0.5340
y	 0.9480	 0.4370
z	 0.9540	 0.5270