



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 09:39 am GMT

PDB ID : 7NHM
EMDB ID : EMD-12333
Title : 70S ribosome from Staphylococcus aureus
Authors : Crowe-McAuliffe, C.; Murina, V.; Hauryliuk, V.; Wilson, D.N.
Deposited on : 2021-02-10
Resolution : 3.10 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:

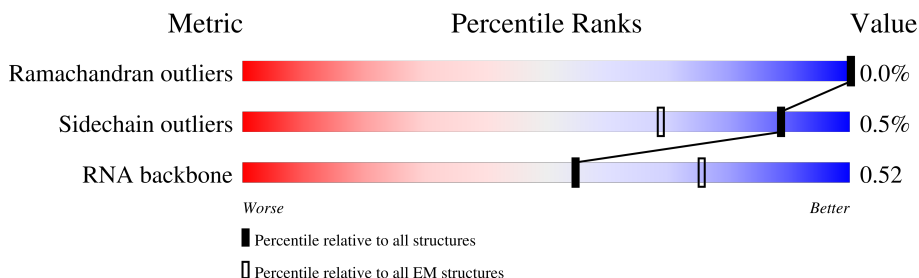
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.10 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	Z	94	
2	P	144	
3	A	2923	
4	a	1551	
5	B	115	
6	G	277	
7	H	220	
8	I	207	

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Mol	Chain	Length	Quality of chain
9	J	179	6% 98%
10	K	178	7% 91% 8%
11	M	145	98%
12	N	122	100%
13	O	146	98%
14	Q	122	98%
15	R	119	98%
16	S	116	97%
17	T	118	96%
18	U	102	99%
19	V	117	92% 5%
20	W	91	97%
21	X	105	10% 93% 6%
22	Y	217	43% 57%
23	1	62	6% 94% 5%
24	2	69	91% 7%
25	3	59	95% 5%
26	5	58	10% 91% 7%
27	6	49	96%
28	8	66	95%
29	7	45	91% 7%
30	d	217	14% 95% 5%
31	e	200	25% 98%
32	h	156	8% 93% 5%
33	k	102	20% 100%

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Mol	Chain	Length	Quality of chain
34	l	129	9% 91% 9%
35	o	60	98% .
36	p	89	. 97% .
37	q	91	20% 98% ..
38	u	83	13% 95% ..
39	g	37	. 97% .
40	t	92	8% 86% 14%
41	n	121	9% 93% . 7%
42	j	132	10% 95% . .
43	f	166	. 94% 6%
44	i	132	5% 98% ..
45	s	80	5% 76% . 21%
46	g	98	9% 94% . 5%
47	b	15	27% 40% 20% 40%
48	m	137	18% 97% ..
49	r	87	5% 91% 9%
50	c	255	18% 86% 13%
51	D	77	16% 83% 17%
52	4	84	6% 69% . 30%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 140248 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 L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	Z	82	626	386	122	118	0	0

- Molecule 2 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	135	1081	693	205	180	3	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2824	60551	27035	11081	19611	2824	0	0

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	a	1531	32794	14642	5986	10635	1531	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	B	113	2408	1076	431	788	113	0	0

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	273	2085	1297	413	370	5	0	0

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	216	1637	1024	301	307	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	204	1564	981	286	295	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	175	1381	876	237	261	7	0	0

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	164	1284	799	232	250	3	0	0

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	142	1127	704	205	216	2	0	0

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	122	920	572	174	170	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	145	1090	674	214	201	1	0	0

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	120	952	584	182	185	1	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	118	914	569	173	172		0	0

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	114	922	580	185	157		0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	116	943	593	189	157	4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	U	101	793	503	141	148	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	V	111	853	532	163	155	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	W	89	725	457	130	134	4	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	99	Total	C	N	O	S	0	0
			761	480	140	139	2		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace	
24	2	64	Total	C	N	O		0	0
			527	324	99	104			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace	
25	3	56	Total	C	N	O		0	0
			436	271	82	83			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	54	Total	C	N	O	S	0	0
			433	262	90	76	5		

- Molecule 27 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	6	47	Total	C	N	O	S	0	0
			389	232	79	74	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	42	Total	C	N	O	S	0	0
			360	220	88	51	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	207	Total	C	N	O	S	0	0
			1634	1030	305	297	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 32 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	148	Total	C	N	O	S	0	0
			1180	734	226	216	4		

- Molecule 33 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	102	Total	C	N	O	S	0	0
			814	513	149	150	2		

- Molecule 34 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 35 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	o	59	Total	C	N	O	S	0	0
			496	314	99	78	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	?	-	ALA	deletion	UNP Q2FW19

- Molecule 36 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 37 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 38 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 39 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	9	36	Total	C	N	O	S	0	0
			292	184	59	44	5		

- Molecule 40 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	t	79	Total	C	N	O	S	0	0
			646	416	116	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	127	Total	C	N	O	S	0	0
			1008	624	201	182	1		

- Molecule 43 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 46 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 47 is a RNA chain called RNA (5'-R(P*GP*GP*AP*GP*GP*UP*NP*NP*NP*N P*NP*NP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
47	b	9	Total	C	N	O	P	0	0
			199	88	39	63	9		

- Molecule 48 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	79	Total	C	N	O	S	0	0
			651	413	116	121	1		

- Molecule 50 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 51 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D	77	Total	C	N	O	P	0	0
			1644	733	298	536	77		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	59	Total	C	N	O	S	0	0
			486	310	88	87	1		

- Molecule 53 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
53	A	9	Total	K	0
			9	9	
53	a	2	Total	K	0
			2	2	

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	114	Total	Mg	0
			114	114	
54	a	25	Total	Mg	0
			25	25	

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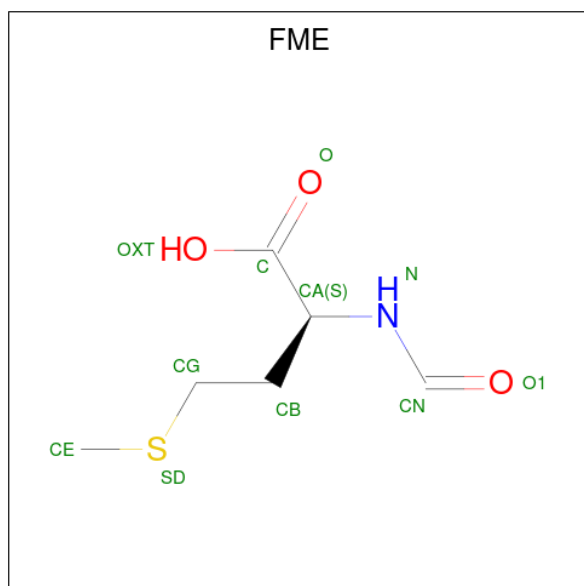
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Mol	Chain	Residues	Atoms		AltConf
54	U	1	Total	Mg	0
			1	1	
54	D	1	Total	Mg	0
			1	1	

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5	1	Total	Zn	0
			1	1	
55	6	1	Total	Zn	0
			1	1	
55	o	1	Total	Zn	0
			1	1	
55	9	1	Total	Zn	0
			1	1	

- Molecule 56 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).

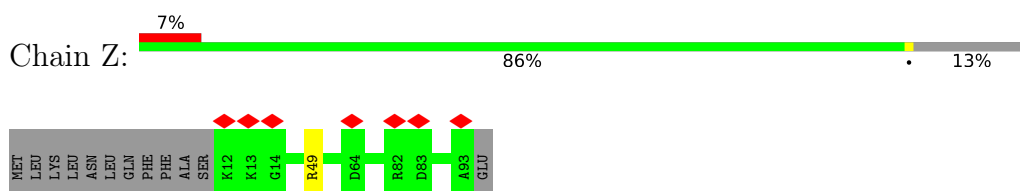


Mol	Chain	Residues	Atoms					AltConf
56	D	1	Total	C	N	O	S	0
			10	6	1	2	1	

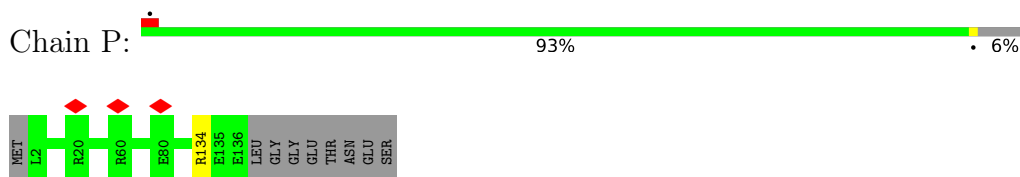
3 Residue-property plots

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.

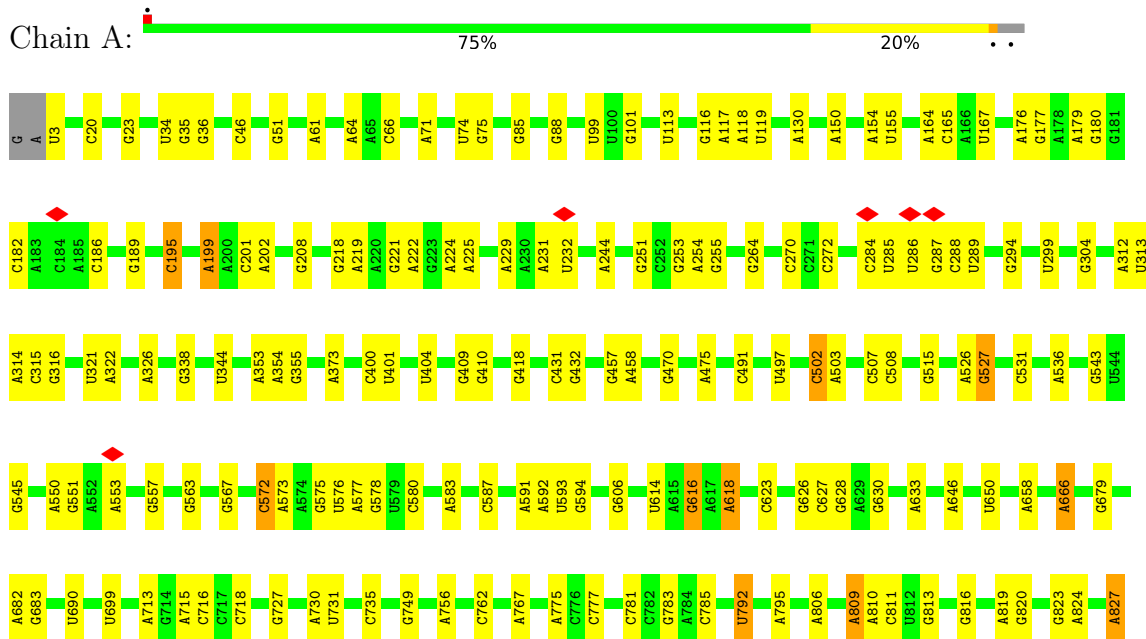
- Molecule 1: 50S ribosomal protein L27

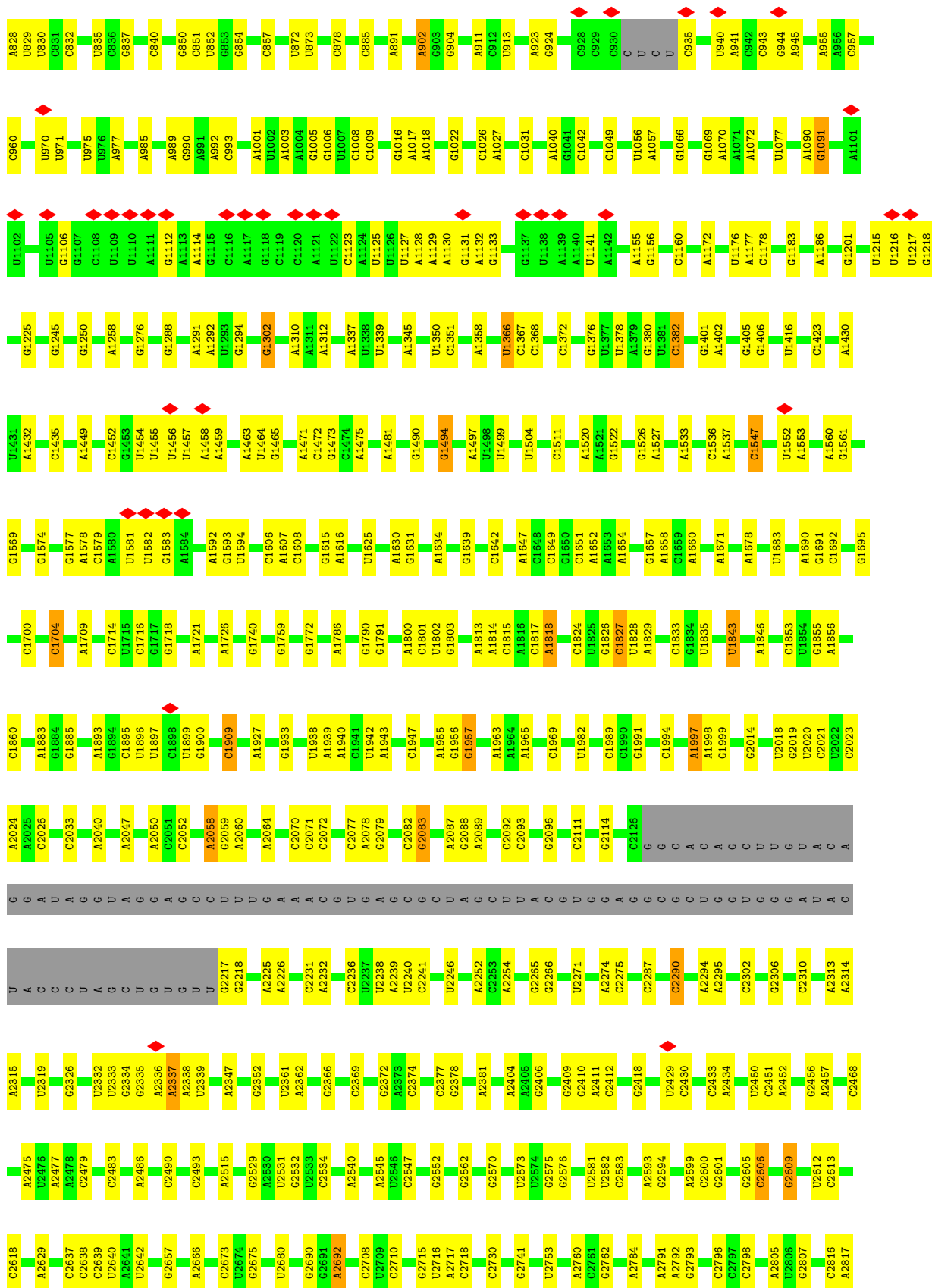


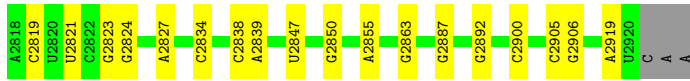
- Molecule 2: 50S ribosomal protein L16



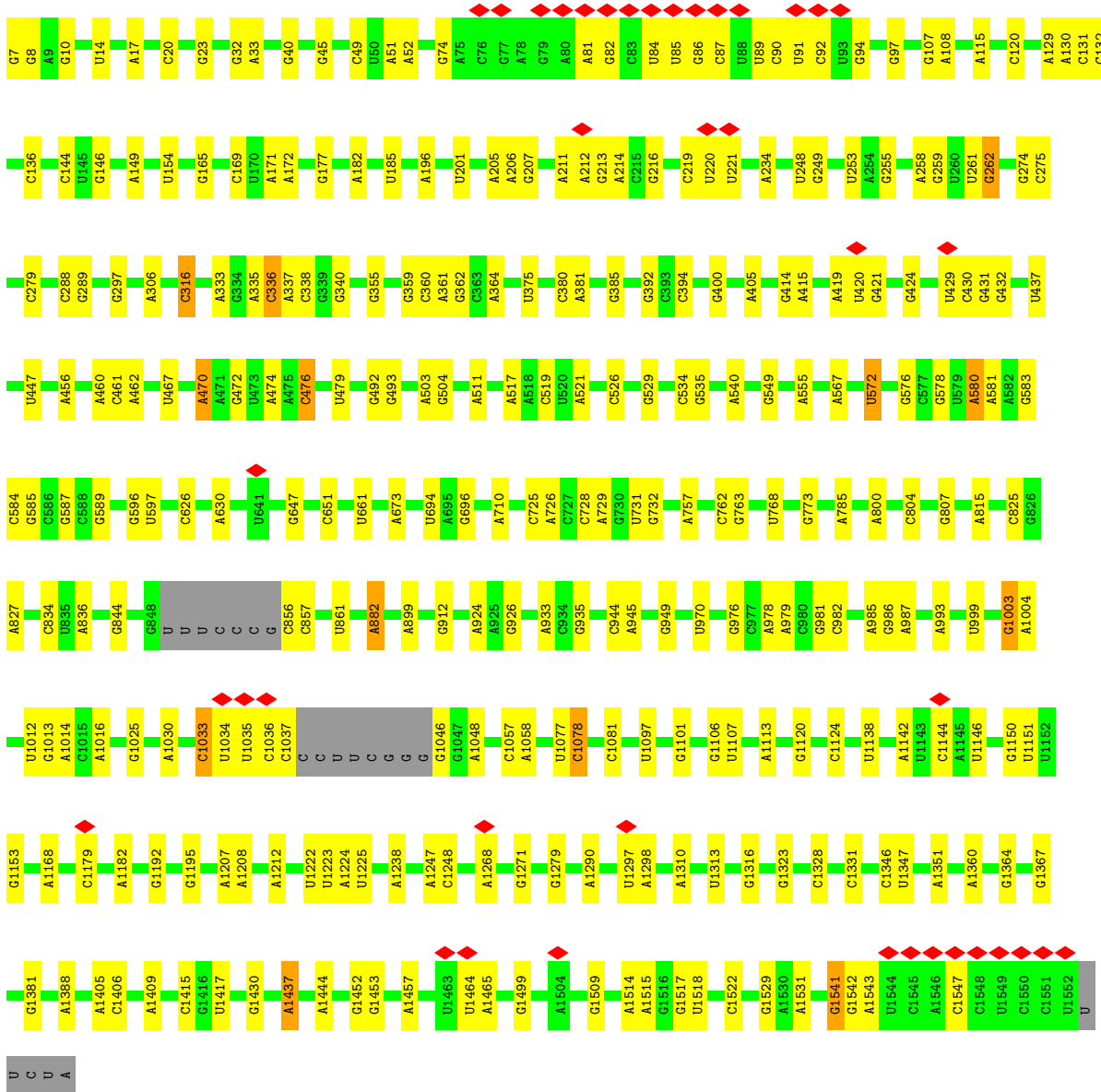
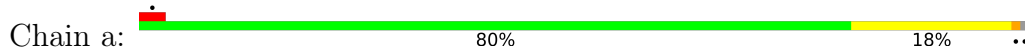
- Molecule 3: 23S rRNA



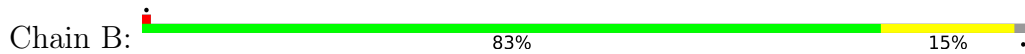




• Molecule 4: 16S rRNA

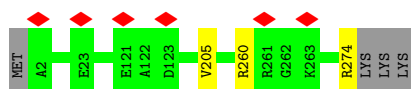


• Molecule 5: 5S rRNA



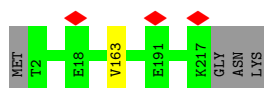
• Molecule 6: 50S ribosomal protein L2

Chain G:  97%



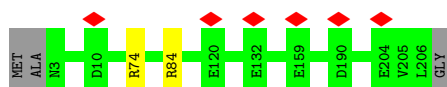
- Molecule 7: 50S ribosomal protein L3

Chain H:  98%



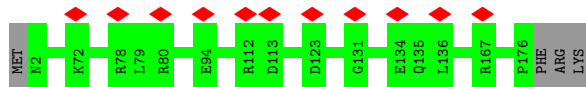
- Molecule 8: 50S ribosomal protein L4

Chain I:  98%

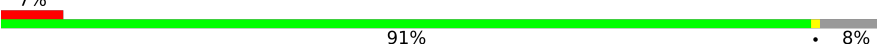


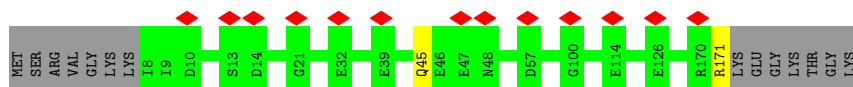
- Molecule 9: 50S ribosomal protein L5

Chain J:  6% 98%



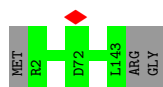
- Molecule 10: 50S ribosomal protein L6

Chain K:  7% 91% 8%



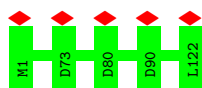
- Molecule 11: 50S ribosomal protein L13

Chain M:  98%



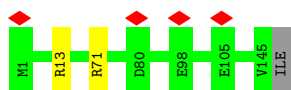
- Molecule 12: 50S ribosomal protein L14

Chain N:  100%



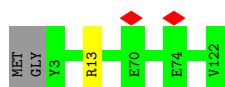
- Molecule 13: 50S ribosomal protein L15

Chain O:  98%



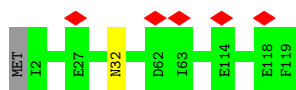
- Molecule 14: 50S ribosomal protein L17

Chain Q:  98%



- Molecule 15: 50S ribosomal protein L18

Chain R:  98%



- Molecule 16: 50S ribosomal protein L19

Chain S:  97%



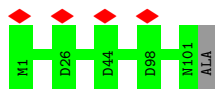
- Molecule 17: 50S ribosomal protein L20

Chain T:  96%

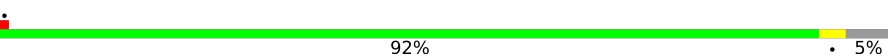


- Molecule 18: 50S ribosomal protein L21

Chain U:  99%

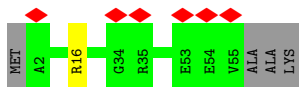


- Molecule 19: 50S ribosomal protein L22

Chain V:  92% 5%



- Molecule 26: 50S ribosomal protein L32



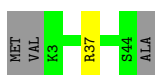
- Molecule 27: 50S ribosomal protein L33 2



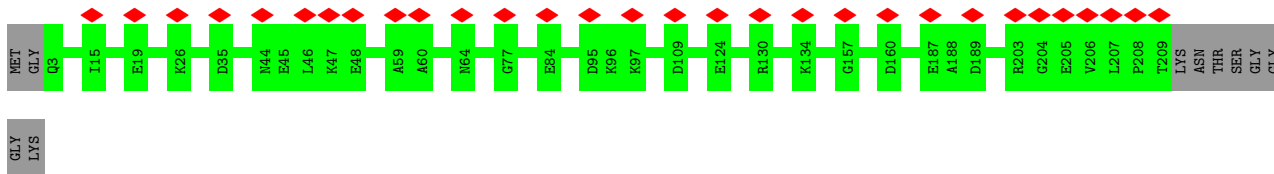
- Molecule 28: 50S ribosomal protein L35



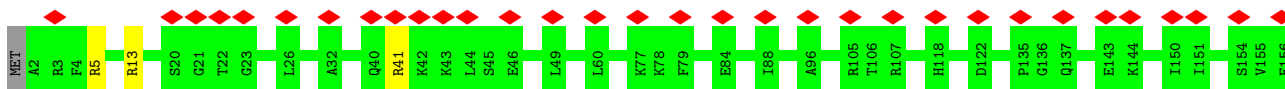
- Molecule 29: 50S ribosomal protein L34

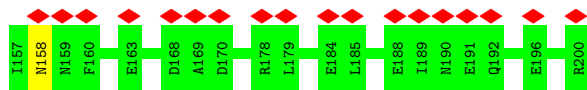


- Molecule 30: 30S ribosomal protein S3

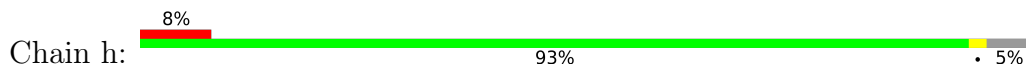


- Molecule 31: 30S ribosomal protein S4

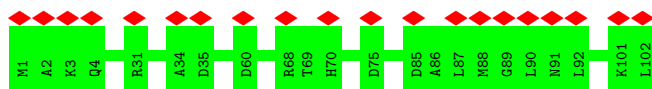




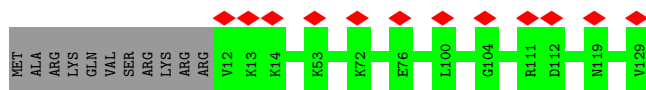
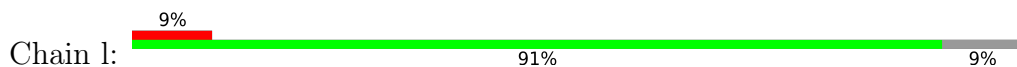
- Molecule 32: 30S ribosomal protein S7



- Molecule 33: 30S ribosomal protein S10



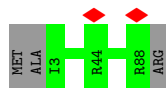
- Molecule 34: 30S ribosomal protein S11



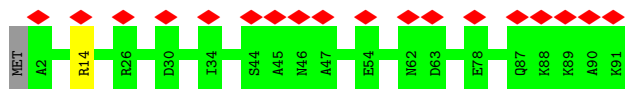
- Molecule 35: 30S ribosomal protein S14 type Z



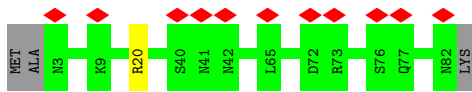
- Molecule 36: 30S ribosomal protein S15



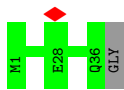
- Molecule 37: 30S ribosomal protein S16



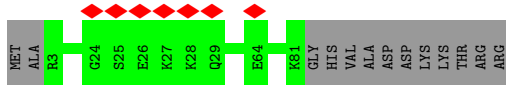
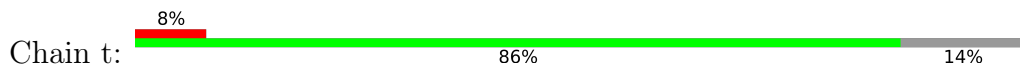
- Molecule 38: 30S ribosomal protein S20



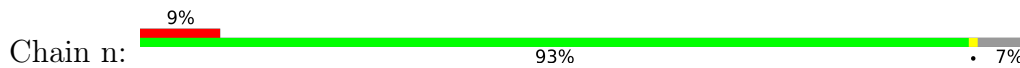
- Molecule 39: 50S ribosomal protein L36



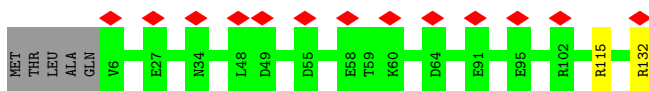
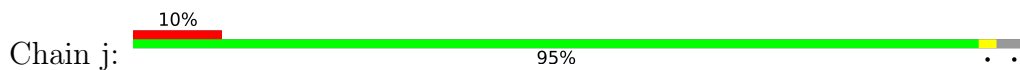
- Molecule 40: 30S ribosomal protein S19



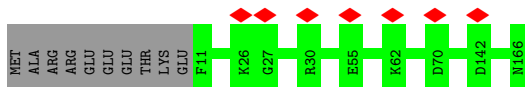
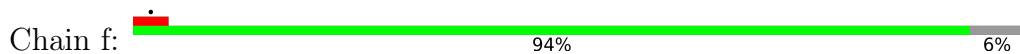
- Molecule 41: 30S ribosomal protein S13



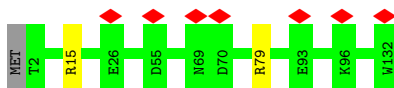
- Molecule 42: 30S ribosomal protein S9



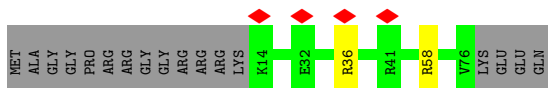
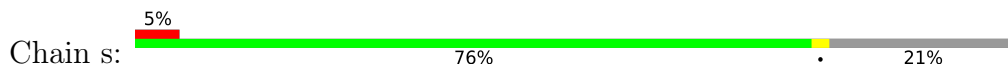
- Molecule 43: 30S ribosomal protein S5



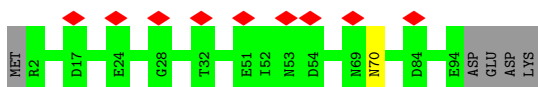
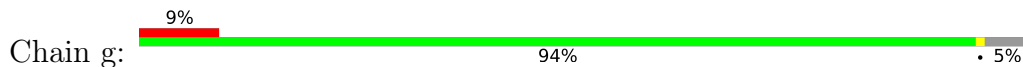
- Molecule 44: 30S ribosomal protein S8



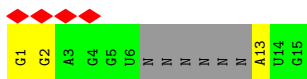
- Molecule 45: 30S ribosomal protein S18



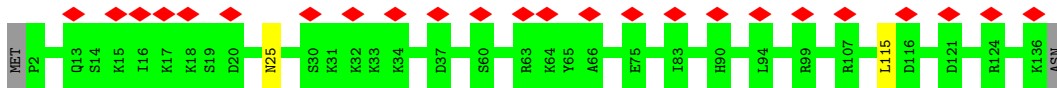
- Molecule 46: 30S ribosomal protein S6



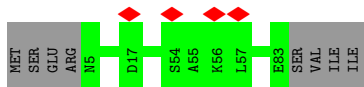
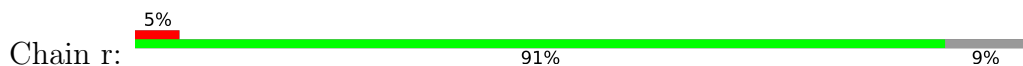
- Molecule 47: RNA (5'-R(P*GP*GP*AP*GP*GP*UP*NP*NP*NP*NP*NP*NP*AP*UP*G)-3')



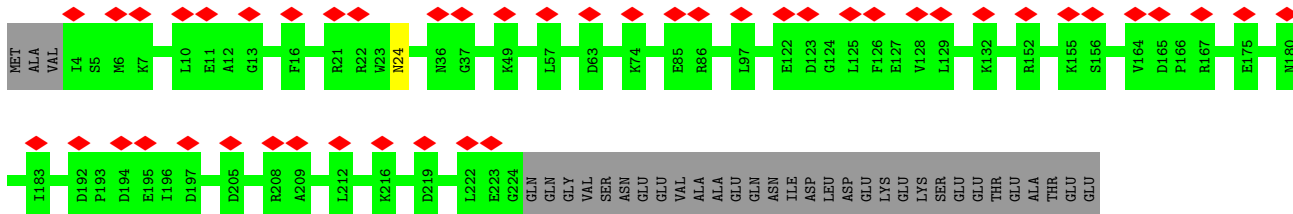
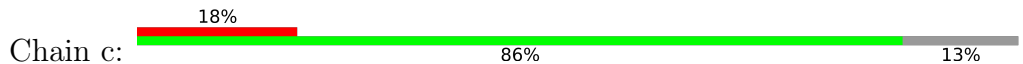
- Molecule 48: 30S ribosomal protein S12



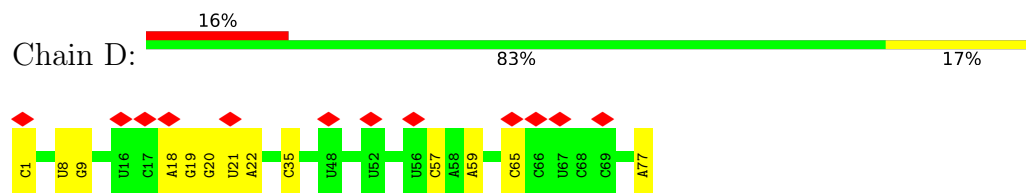
- Molecule 49: 30S ribosomal protein S17



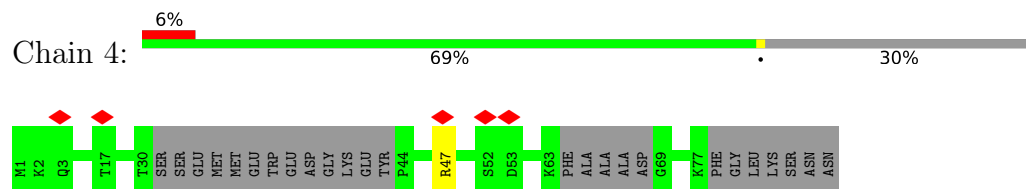
- Molecule 50: 30S ribosomal protein S2



- Molecule 51: tRNA-fMet



- Molecule 52: 50S ribosomal protein L31 type B



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26.3	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-1900	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	366.432, 366.432, 366.432	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, K, FME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Z	0.86	0/632	0.89	1/838 (0.1%)
2	P	0.80	0/1105	0.72	1/1483 (0.1%)
3	A	1.35	49/67815 (0.1%)	1.24	246/105765 (0.2%)
4	a	1.01	2/36716 (0.0%)	1.14	75/57253 (0.1%)
5	B	0.96	0/2692	1.10	3/4193 (0.1%)
6	G	0.83	1/2120 (0.0%)	0.77	1/2847 (0.0%)
7	H	0.85	1/1661 (0.1%)	0.71	0/2227
8	I	0.80	0/1587	0.71	1/2143 (0.0%)
9	J	0.60	0/1398	0.68	0/1877
10	K	0.51	0/1302	0.68	1/1757 (0.1%)
11	M	0.76	0/1149	0.69	0/1549
12	N	0.83	0/927	0.80	0/1243
13	O	0.80	0/1104	0.78	1/1471 (0.1%)
14	Q	0.74	0/956	0.73	1/1277 (0.1%)
15	R	0.63	0/923	0.71	0/1234
16	S	0.77	0/934	0.79	0/1249
17	T	0.89	0/955	0.82	5/1265 (0.4%)
18	U	0.80	0/803	0.71	0/1073
19	V	0.79	0/861	0.75	0/1159
20	W	0.77	0/733	0.76	0/978
21	X	0.61	0/770	0.69	2/1029 (0.2%)
22	Y	0.56	0/746	0.69	1/1000 (0.1%)
23	1	0.67	0/469	0.79	0/625
24	2	0.56	0/528	0.74	1/703 (0.1%)
25	3	0.71	0/438	0.71	0/590
26	5	0.84	0/440	0.77	1/585 (0.2%)
27	6	0.67	0/392	0.76	0/523
28	8	0.85	0/526	0.89	2/690 (0.3%)
29	7	0.98	0/364	0.85	1/474 (0.2%)
30	d	0.56	0/1657	0.71	0/2228
31	e	0.53	0/1647	0.73	1/2211 (0.0%)
32	h	0.52	0/1195	0.70	0/1605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	k	0.53	0/826	0.71	0/1111
34	l	0.52	0/891	0.65	0/1203
35	o	0.69	0/506	0.77	0/671
36	p	0.58	0/730	0.72	0/975
37	q	0.50	0/723	0.68	1/971 (0.1%)
38	u	0.43	0/606	0.63	1/810 (0.1%)
39	9	0.76	0/295	0.75	0/388
40	t	0.52	0/663	0.66	0/889
41	n	0.53	0/909	0.68	0/1218
42	j	0.57	0/1024	0.74	1/1374 (0.1%)
43	f	0.68	0/1174	0.69	0/1583
44	i	0.61	0/1044	0.70	2/1401 (0.1%)
45	s	0.62	0/525	0.75	2/704 (0.3%)
46	g	0.59	0/784	0.67	0/1052
47	b	0.71	0/222	1.37	3/343 (0.9%)
48	m	0.57	0/1075	0.73	0/1439
49	r	0.59	0/659	0.68	0/881
50	c	0.47	0/1808	0.64	0/2426
51	D	0.73	0/1837	1.02	3/2862 (0.1%)
52	4	0.51	0/496	0.64	0/661
All	All	1.10	53/152342 (0.0%)	1.10	358/228106 (0.2%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	623	C	C4-C5	-6.08	1.38	1.43
3	A	627	C	N1-C6	-5.99	1.33	1.37
3	A	811	C	N1-C6	-5.95	1.33	1.37
3	A	580	C	N1-C6	-5.94	1.33	1.37
3	A	1008	C	N1-C6	-5.91	1.33	1.37
3	A	2483	C	C4-C5	-5.90	1.38	1.43
3	A	2606	C	C4-C5	-5.89	1.38	1.43
3	A	832	C	N1-C6	-5.86	1.33	1.37
3	A	2708	C	N1-C6	-5.80	1.33	1.37
3	A	716	C	N1-C6	-5.65	1.33	1.37
3	A	201	C	C4-C5	-5.64	1.38	1.43
3	A	1817	C	N1-C6	-5.62	1.33	1.37
3	A	2072	C	C4-C5	-5.61	1.38	1.43
3	A	1351	C	C4-C5	-5.59	1.38	1.43
3	A	1818	A	N9-C4	-5.56	1.34	1.37
3	A	1700	C	C4-C5	-5.48	1.38	1.43
3	A	781	C	C4-C5	-5.48	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2093	C	C4-C5	-5.45	1.38	1.43
3	A	2092	C	C4-C5	-5.44	1.38	1.43
3	A	1368	C	N1-C6	-5.43	1.33	1.37
3	A	1714	C	C4-C5	-5.41	1.38	1.43
3	A	2477	A	N9-C4	-5.27	1.34	1.37
3	A	2026	C	N1-C6	-5.26	1.33	1.37
3	A	1292	A	N9-C4	-5.26	1.34	1.37
3	A	1704	C	C4-C5	-5.26	1.38	1.43
3	A	2093	C	N1-C6	-5.25	1.34	1.37
3	A	2618	C	C4-C5	-5.22	1.38	1.43
3	A	735	C	N1-C6	-5.22	1.34	1.37
3	A	508	C	N1-C6	-5.21	1.34	1.37
3	A	2570	G	N9-C8	-5.21	1.34	1.37
3	A	254	A	N9-C4	-5.21	1.34	1.37
3	A	1382	C	C4-C5	-5.20	1.38	1.43
3	A	244	A	N9-C4	-5.17	1.34	1.37
4	a	20	C	C4-C5	-5.16	1.38	1.43
3	A	1649	C	C4-C5	-5.16	1.38	1.43
3	A	2077	C	N1-C6	-5.15	1.34	1.37
6	G	205	VAL	CB-CG1	-5.15	1.42	1.52
3	A	628	G	N9-C4	-5.15	1.33	1.38
3	A	1824	C	C4-C5	-5.15	1.38	1.43
3	A	650	U	C2-N3	-5.11	1.34	1.37
4	a	834	C	C4-C5	-5.11	1.38	1.43
3	A	840	C	C4-C5	-5.11	1.38	1.43
3	A	572	C	N1-C6	-5.08	1.34	1.37
7	H	163	VAL	CB-CG2	-5.07	1.42	1.52
3	A	827	A	N9-C4	-5.06	1.34	1.37
3	A	2021	C	C4-C5	-5.05	1.39	1.43
3	A	1927	A	N9-C4	-5.04	1.34	1.37
3	A	1814	A	N7-C5	-5.04	1.36	1.39
3	A	878	C	N1-C6	-5.04	1.34	1.37
3	A	1372	C	C4-C5	-5.04	1.39	1.43
3	A	713	A	N9-C4	-5.03	1.34	1.37
3	A	1833	C	N1-C6	-5.03	1.34	1.37
3	A	777	C	N1-C6	-5.02	1.34	1.37

All (358) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2023	C	C2-N3-C4	-11.17	114.32	119.90
3	A	666	A	N1-C6-N6	9.75	124.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2433	C	O4'-C1'-N1	8.94	115.35	108.20
3	A	2609	G	C4-C5-N7	8.71	114.28	110.80
4	a	1033	C	C2-N1-C1'	8.28	127.90	118.80
3	A	2609	G	C6-C5-N7	-8.23	125.46	130.40
3	A	1989	C	C5-C4-N4	-8.17	114.48	120.20
3	A	1608	C	N1-C2-O2	8.12	123.77	118.90
3	A	592	A	N1-C6-N6	-8.01	113.79	118.60
3	A	2271	U	N3-C4-O4	8.01	125.01	119.40
4	a	580	A	N1-C6-N6	-7.82	113.91	118.60
3	A	1351	C	C2-N1-C1'	7.80	127.38	118.80
3	A	222	A	OP1-P-OP2	-7.62	108.17	119.60
4	a	316	C	N1-C2-O2	7.50	123.40	118.90
28	8	57	ARG	NE-CZ-NH1	7.45	124.02	120.30
3	A	2609	G	N9-C4-C5	-7.41	102.44	105.40
3	A	809	A	C8-N9-C4	-7.41	102.84	105.80
3	A	1351	C	C6-N1-C2	-7.39	117.34	120.30
8	I	74	ARG	NE-CZ-NH2	-7.38	116.61	120.30
3	A	2798	C	N1-C2-O2	7.29	123.28	118.90
4	a	762	C	C2-N1-C1'	7.27	126.79	118.80
3	A	1350	U	C2-N1-C1'	7.25	126.41	117.70
3	A	2606	C	C6-N1-C2	-7.23	117.41	120.30
3	A	2609	G	N3-C4-N9	7.22	130.33	126.00
4	a	279	C	N1-C2-O2	7.21	123.23	118.90
3	A	1855	G	N1-C2-N2	-7.20	109.72	116.20
3	A	1714	C	C5-C4-N4	-7.17	115.18	120.20
3	A	616	G	C2-N3-C4	-7.15	108.33	111.90
3	A	2271	U	C5-C4-O4	-7.10	121.64	125.90
4	a	1367	G	C6-C5-N7	-7.10	126.14	130.40
3	A	2290	C	C6-N1-C2	-7.09	117.47	120.30
4	a	534	C	N1-C2-O2	7.07	123.14	118.90
4	a	7	G	OP1-P-OP2	-7.05	109.03	119.60
3	A	2033	C	N1-C2-O2	7.04	123.12	118.90
3	A	2023	C	N3-C4-C5	7.02	124.71	121.90
3	A	2217	G	OP1-P-OP2	-7.01	109.08	119.60
3	A	221	G	OP1-P-O3'	7.00	120.60	105.20
3	A	527	G	O4'-C1'-N9	6.97	113.78	108.20
3	A	491	C	N1-C2-O2	6.96	123.07	118.90
3	A	1716	C	C5-C4-N4	-6.93	115.35	120.20
3	A	2023	C	C5-C4-N4	-6.92	115.35	120.20
3	A	1475	A	C4-C5-N7	6.89	114.14	110.70
3	A	1351	C	N1-C2-O2	6.88	123.03	118.90
47	b	13	A	OP1-P-OP2	-6.87	109.30	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	X	80	ARG	NE-CZ-NH2	-6.83	116.89	120.30
47	b	1	G	OP1-P-OP2	-6.81	109.38	119.60
4	a	1367	G	N7-C8-N9	6.80	116.50	113.10
4	a	1046	G	OP1-P-OP2	-6.79	109.42	119.60
51	D	1	C	OP1-P-OP2	-6.78	109.42	119.60
3	A	851	C	N1-C2-O2	6.75	122.95	118.90
3	A	3	U	OP1-P-OP2	-6.75	109.48	119.60
3	A	2433	C	OP1-P-OP2	-6.73	109.51	119.60
4	a	856	C	OP1-P-OP2	-6.72	109.52	119.60
3	A	827	A	N1-C6-N6	6.66	122.59	118.60
3	A	935	C	OP1-P-OP2	-6.65	109.62	119.60
3	A	2369	C	N1-C2-O2	6.62	122.87	118.90
3	A	502	C	N3-C4-C5	6.59	124.53	121.90
3	A	827	A	C5-C6-N6	-6.56	118.45	123.70
3	A	1475	A	C5-C6-N6	-6.55	118.46	123.70
3	A	2798	C	N3-C2-O2	-6.55	117.31	121.90
3	A	2302	C	N1-C2-O2	6.54	122.82	118.90
3	A	1072	A	C5-C6-N6	-6.52	118.48	123.70
5	B	2	C	OP1-P-OP2	-6.49	109.86	119.60
47	b	1	G	O4'-C1'-N9	-6.49	103.01	108.20
3	A	2919	A	C5-C6-N6	-6.48	118.52	123.70
4	a	182	A	N1-C6-N6	-6.44	114.74	118.60
3	A	1091	G	O4'-C1'-N9	6.43	113.35	108.20
3	A	1657	G	N3-C4-N9	-6.42	122.15	126.00
3	A	2606	C	C5-C6-N1	6.39	124.20	121.00
3	A	2847	U	C5-C4-O4	-6.39	122.07	125.90
3	A	1473	G	C4-C5-N7	6.39	113.36	110.80
4	a	14	U	N3-C4-O4	6.37	123.86	119.40
3	A	2816	C	O4'-C1'-N1	6.36	113.29	108.20
3	A	2275	C	N1-C2-O2	6.34	122.70	118.90
17	T	92	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	A	840	C	N1-C2-O2	6.33	122.70	118.90
3	A	355	G	C6-C5-N7	-6.32	126.61	130.40
3	A	1700	C	N1-C2-O2	6.32	122.69	118.90
4	a	1013	G	C4-N9-C1'	6.31	134.71	126.50
3	A	809	A	N7-C8-N9	6.31	116.96	113.80
3	A	1475	A	N9-C4-C5	-6.28	103.29	105.80
4	a	827	A	N1-C6-N6	6.25	122.35	118.60
3	A	2275	C	C6-N1-C2	-6.24	117.80	120.30
3	A	1026	C	C5-C4-N4	-6.24	115.83	120.20
3	A	1802	U	C5-C4-O4	-6.23	122.16	125.90
3	A	1016	G	N1-C2-N2	-6.21	110.61	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1700	C	C5-C4-N4	-6.21	115.85	120.20
17	T	53	ARG	NE-CZ-NH1	6.21	123.40	120.30
4	a	1367	G	C4-N9-C1'	6.20	134.55	126.50
3	A	851	C	C2-N1-C1'	6.18	125.59	118.80
17	T	92	ARG	NE-CZ-NH2	-6.17	117.21	120.30
3	A	2618	C	C5-C4-N4	-6.16	115.89	120.20
17	T	58	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	A	1006	G	N1-C2-N2	-6.15	110.67	116.20
3	A	1579	C	C6-N1-C2	-6.15	117.84	120.30
3	A	1814	A	C4-C5-N7	6.15	113.77	110.70
4	a	316	C	N3-C2-O2	-6.15	117.60	121.90
3	A	253	G	N3-C4-N9	-6.14	122.32	126.00
3	A	1855	G	N3-C2-N2	6.11	124.18	119.90
3	A	1615	G	N3-C2-N2	-6.11	115.63	119.90
4	a	1033	C	N1-C2-O2	6.10	122.56	118.90
3	A	902	A	N1-C6-N6	6.07	122.24	118.60
3	A	2369	C	C2-N1-C1'	6.07	125.47	118.80
1	Z	49	ARG	NE-CZ-NH1	6.06	123.33	120.30
3	A	623	C	C5-C4-N4	-6.06	115.96	120.20
3	A	1957	G	N3-C4-N9	-6.06	122.36	126.00
3	A	1351	C	N3-C4-N4	6.05	122.24	118.00
3	A	1006	G	N3-C2-N2	6.03	124.12	119.90
3	A	2609	G	N3-C2-N2	6.01	124.11	119.90
3	A	1520	A	N1-C6-N6	-6.00	115.00	118.60
4	a	1003	G	C8-N9-C1'	-6.00	119.21	127.00
4	a	476	C	N1-C2-O2	5.99	122.50	118.90
4	a	804	C	N1-C2-O2	5.97	122.48	118.90
3	A	1547	C	N1-C2-O2	5.96	122.47	118.90
4	a	647	G	N3-C4-N9	5.95	129.57	126.00
3	A	1475	A	C5-N7-C8	-5.94	100.93	103.90
3	A	902	A	N7-C8-N9	5.93	116.76	113.80
4	a	834	C	C5-C4-N4	-5.92	116.06	120.20
3	A	1367	C	C6-N1-C2	-5.91	117.94	120.30
3	A	1817	C	C5-C4-N4	-5.90	116.07	120.20
3	A	718	C	C5-C4-N4	-5.88	116.08	120.20
3	A	666	A	C5-N7-C8	-5.86	100.97	103.90
3	A	1997	A	O5'-P-OP1	-5.86	100.43	105.70
3	A	1957	G	N3-C2-N2	-5.85	115.81	119.90
4	a	1033	C	C6-N1-C1'	-5.83	113.80	120.80
3	A	1376	G	N3-C4-N9	-5.82	122.51	126.00
3	A	1853	C	N1-C2-O2	5.82	122.39	118.90
3	A	355	G	C4-C5-N7	5.82	113.13	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1473	G	N9-C4-C5	-5.79	103.08	105.40
3	A	2606	C	C2-N1-C1'	5.79	125.17	118.80
3	A	2609	G	C8-N9-C1'	-5.79	119.48	127.00
3	A	2023	C	N1-C2-N3	5.78	123.25	119.20
3	A	1435	C	N1-C2-O2	5.78	122.37	118.90
3	A	2369	C	C5-C4-N4	-5.78	116.16	120.20
3	A	666	A	C5-C6-N6	-5.78	119.08	123.70
3	A	2451	C	C5-C4-N4	-5.77	116.16	120.20
4	a	827	A	C5-C6-N6	-5.77	119.08	123.70
3	A	1615	G	N3-C4-N9	-5.75	122.55	126.00
3	A	221	G	N3-C4-N9	-5.75	122.55	126.00
3	A	2083	G	N7-C8-N9	5.75	115.98	113.10
3	A	1016	G	N3-C2-N2	5.74	123.92	119.90
3	A	2274	A	C4-C5-N7	5.74	113.57	110.70
4	a	316	C	C6-N1-C2	-5.74	118.00	120.30
3	A	179	A	N1-C6-N6	5.73	122.04	118.60
3	A	993	C	N1-C2-O2	5.73	122.34	118.90
3	A	633	A	N7-C8-N9	5.72	116.66	113.80
3	A	1608	C	N3-C2-O2	-5.72	117.90	121.90
4	a	172	A	N1-C6-N6	-5.72	115.17	118.60
3	A	2609	G	C4-N9-C1'	5.72	133.93	126.50
3	A	2246	U	C5-C4-O4	-5.71	122.48	125.90
3	A	113	U	C5-C6-N1	5.70	125.55	122.70
3	A	2710	C	C5-C4-N4	-5.70	116.21	120.20
4	a	182	A	N9-C4-C5	5.70	108.08	105.80
3	A	781	C	C5-C4-N4	-5.68	116.22	120.20
3	A	2232	A	N9-C4-C5	-5.67	103.53	105.80
3	A	545	G	C2-N3-C4	-5.67	109.07	111.90
3	A	2919	A	N1-C6-N6	5.66	122.00	118.60
4	a	694	U	O4'-C1'-N1	5.65	112.72	108.20
44	i	79	ARG	NE-CZ-NH1	5.65	123.13	120.30
3	A	557	G	O4'-C1'-N9	5.65	112.72	108.20
4	a	336	C	C6-N1-C2	-5.64	118.04	120.30
4	a	1003	G	C4-N9-C1'	5.64	133.84	126.50
4	a	725	C	N1-C2-O2	5.64	122.28	118.90
3	A	1814	A	C6-C5-N7	-5.63	128.36	132.30
4	a	572	U	C2-N1-C1'	5.63	124.45	117.70
4	a	1367	G	N3-C4-N9	5.62	129.38	126.00
3	A	272	C	C6-N1-C2	-5.61	118.06	120.30
4	a	154	U	C5-C4-O4	-5.61	122.53	125.90
3	A	1826	G	C2-N3-C4	-5.60	109.10	111.90
5	B	61	C	N1-C2-O2	5.60	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2606	C	N1-C2-O2	5.59	122.26	118.90
22	Y	22	ARG	NE-CZ-NH1	5.59	123.10	120.30
3	A	1802	U	N3-C4-O4	5.58	123.31	119.40
3	A	2274	A	N9-C4-C5	-5.58	103.57	105.80
31	e	13	ARG	NE-CZ-NH2	-5.58	117.51	120.30
4	a	1415	C	N1-C2-O2	5.58	122.25	118.90
3	A	179	A	C4-C5-N7	5.57	113.49	110.70
3	A	2847	U	N3-C4-O4	5.57	123.30	119.40
3	A	1957	G	N9-C4-C5	5.57	107.63	105.40
21	X	80	ARG	NE-CZ-NH1	5.57	123.08	120.30
4	a	1522	C	N1-C2-O2	5.56	122.24	118.90
3	A	1473	G	N3-C4-N9	5.56	129.34	126.00
3	A	902	A	C5-C6-N6	-5.56	119.25	123.70
3	A	1827	C	N3-C4-C5	5.55	124.12	121.90
4	a	1003	G	C6-C5-N7	-5.54	127.08	130.40
3	A	2275	C	N3-C2-O2	-5.54	118.02	121.90
3	A	614	U	C5-C6-N1	5.53	125.47	122.70
4	a	1003	G	N9-C4-C5	-5.53	103.19	105.40
3	A	2319	U	C5-C6-N1	5.53	125.46	122.70
3	A	1009	C	N1-C2-O2	5.53	122.22	118.90
3	A	400	C	N1-C2-O2	5.52	122.21	118.90
3	A	1475	A	N1-C6-N6	5.52	121.91	118.60
3	A	2274	A	C5-N7-C8	-5.52	101.14	103.90
3	A	2483	C	C5-C4-N4	-5.52	116.34	120.20
3	A	1351	C	C5-C6-N1	5.50	123.75	121.00
3	A	2715	G	C2-N3-C4	-5.50	109.15	111.90
4	a	1517	G	N3-C4-N9	-5.50	122.70	126.00
3	A	1473	G	C6-C5-N7	-5.49	127.10	130.40
4	a	762	C	C6-N1-C1'	-5.48	114.22	120.80
3	A	2083	G	C5-N7-C8	-5.48	101.56	104.30
3	A	2692	A	O4'-C1'-N9	5.48	112.58	108.20
3	A	792	U	C5'-C4'-O4'	5.47	115.67	109.10
3	A	491	C	C2-N1-C1'	5.47	124.82	118.80
3	A	2730	C	N1-C2-O2	5.47	122.18	118.90
3	A	1909	C	C5-C4-N4	-5.46	116.37	120.20
4	a	1452	G	C2-N3-C4	-5.46	109.17	111.90
51	D	65	C	N1-C2-O2	5.46	122.18	118.90
3	A	1947	C	C5-C4-N4	-5.46	116.38	120.20
3	A	1072	A	N1-C6-N6	5.46	121.88	118.60
3	A	633	A	C5-N7-C8	-5.43	101.18	103.90
3	A	2111	C	N1-C2-O2	5.43	122.16	118.90
14	Q	13	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1658	A	C5-C6-N6	-5.41	119.37	123.70
4	a	1388	A	N1-C6-N6	5.41	121.84	118.60
3	A	2019	G	O4'-C1'-N9	-5.41	103.88	108.20
28	8	57	ARG	NE-CZ-NH2	-5.41	117.60	120.30
3	A	1465	G	C4-N9-C1'	5.40	133.53	126.50
10	K	171	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	A	1593	G	N3-C2-N2	-5.40	116.12	119.90
17	T	58	ARG	NE-CZ-NH2	-5.39	117.60	120.30
3	A	1547	C	N3-C2-O2	-5.39	118.13	121.90
3	A	2302	C	C5-C6-N1	5.39	123.69	121.00
6	G	260	ARG	NE-CZ-NH2	-5.38	117.61	120.30
3	A	1989	C	N3-C4-N4	5.38	121.76	118.00
3	A	2064	A	C5-C6-N1	5.37	120.39	117.70
42	j	132	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	A	2483	C	C2-N1-C1'	5.37	124.70	118.80
4	a	933	A	N9-C4-C5	-5.36	103.65	105.80
3	A	1947	C	N3-C4-N4	5.36	121.75	118.00
3	A	2534	C	N1-C2-O2	5.36	122.12	118.90
3	A	418	G	O4'-C1'-N9	5.36	112.49	108.20
3	A	507	C	N1-C2-O2	5.36	122.12	118.90
3	A	2290	C	C5-C4-N4	-5.35	116.45	120.20
37	q	14	ARG	NE-CZ-NH1	5.35	122.97	120.30
4	a	476	C	C2-N1-C1'	5.34	124.67	118.80
3	A	208	G	O4'-C1'-N9	5.33	112.46	108.20
3	A	2606	C	C5-C4-N4	-5.33	116.47	120.20
3	A	1042	C	N1-C2-O2	5.32	122.09	118.90
3	A	885	C	N1-C2-O2	5.32	122.09	118.90
3	A	1843	U	N1-C2-O2	5.32	126.52	122.80
3	A	2639	C	C5-C4-N4	-5.32	116.48	120.20
3	A	2515	A	C4-C5-N7	5.31	113.36	110.70
3	A	2287	C	N1-C2-O2	5.31	122.09	118.90
3	A	2378	G	C2-N3-C4	-5.31	109.25	111.90
3	A	2601	G	N7-C8-N9	5.31	115.75	113.10
4	a	815	A	C4-C5-N7	5.31	113.35	110.70
4	a	815	A	C5-C6-N6	-5.31	119.46	123.70
45	s	58	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	A	186	C	C6-N1-C2	-5.30	118.18	120.30
26	5	16	ARG	NE-CZ-NH1	5.30	122.95	120.30
4	a	476	C	N3-C2-O2	-5.29	118.19	121.90
5	B	58	C	C5-C4-N4	-5.29	116.50	120.20
38	u	20	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	A	20	C	C5-C4-N4	-5.28	116.50	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	834	C	N1-C2-O2	5.28	122.07	118.90
3	A	1826	G	N3-C4-N9	-5.27	122.84	126.00
3	A	199	A	O4'-C1'-N9	5.27	112.42	108.20
3	A	2254	A	N1-C6-N6	-5.26	115.45	118.60
3	A	1814	A	C5-N7-C8	-5.25	101.27	103.90
3	A	1843	U	N3-C2-O2	-5.25	118.52	122.20
3	A	491	C	N3-C2-O2	-5.25	118.22	121.90
3	A	749	G	O4'-C1'-N9	5.25	112.40	108.20
3	A	2290	C	N3-C4-N4	5.24	121.67	118.00
3	A	810	A	C5-C6-N6	-5.24	119.51	123.70
3	A	1350	U	C6-N1-C1'	-5.24	113.86	121.20
4	a	1081	C	C5-C4-N4	-5.24	116.53	120.20
3	A	2236	C	C5-C4-N4	-5.24	116.53	120.20
3	A	2834	C	C6-N1-C2	-5.24	118.21	120.30
3	A	515	G	C2-N3-C4	-5.23	109.28	111.90
3	A	2019	G	N1-C2-N3	5.23	127.04	123.90
3	A	2071	C	N1-C2-O2	5.23	122.04	118.90
4	a	279	C	N3-C2-O2	-5.23	118.24	121.90
4	a	1078	C	C5-C4-N4	-5.23	116.54	120.20
3	A	824	A	C5-C6-N1	5.23	120.31	117.70
3	A	618	A	N9-C4-C5	-5.22	103.71	105.80
3	A	1801	C	C6-N1-C2	-5.22	118.21	120.30
3	A	1704	C	C5-C6-N1	5.22	123.61	121.00
4	a	20	C	C5-C4-N4	-5.22	116.55	120.20
3	A	113	U	N3-C4-O4	5.21	123.05	119.40
3	A	2337	A	N1-C6-N6	-5.21	115.47	118.60
4	a	800	A	O4'-C1'-N9	5.21	112.37	108.20
2	P	134	ARG	NE-CZ-NH1	5.21	122.90	120.30
3	A	960	C	C5-C4-N4	-5.21	116.55	120.20
4	a	470	A	N3-C4-N9	5.21	131.57	127.40
4	a	262	G	N3-C4-N9	5.21	129.12	126.00
3	A	2058	A	N1-C6-N6	5.20	121.72	118.60
3	A	2072	C	C5-C4-N4	-5.20	116.56	120.20
4	a	578	G	C4-N9-C1'	5.20	133.26	126.50
3	A	2606	C	O5'-P-OP2	-5.19	101.03	105.70
3	A	623	C	N1-C2-O2	5.19	122.01	118.90
4	a	1003	G	N3-C4-N9	5.19	129.11	126.00
4	a	394	C	N1-C2-O2	5.18	122.01	118.90
4	a	1033	C	N3-C2-O2	-5.18	118.27	121.90
4	a	1437	A	C5-C6-N1	5.18	120.29	117.70
4	a	549	G	N3-C4-N9	-5.17	122.90	126.00
4	a	882	A	O4'-C1'-N9	5.17	112.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	861	U	C5-C4-O4	-5.17	122.80	125.90
3	A	2493	C	C5-C4-N4	-5.16	116.59	120.20
3	A	1657	G	N3-C4-C5	5.15	131.17	128.60
3	A	2540	A	C5-C6-N1	5.15	120.27	117.70
3	A	1826	G	C5-C6-O6	5.14	131.69	128.60
4	a	804	C	N3-C2-O2	-5.14	118.30	121.90
3	A	1031	C	C5-C4-N4	-5.14	116.60	120.20
3	A	2582	U	C5-C6-N1	5.14	125.27	122.70
3	A	1366	U	C5-C6-N1	5.14	125.27	122.70
3	A	2409	G	C2-N3-C4	-5.14	109.33	111.90
29	7	37	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	A	1642	C	N1-C2-O2	5.13	121.98	118.90
3	A	2601	G	C5-N7-C8	-5.13	101.73	104.30
3	A	264	G	N3-C4-N9	-5.13	122.92	126.00
3	A	913	U	N3-C4-O4	5.12	122.99	119.40
3	A	1302	G	C2-N3-C4	-5.12	109.34	111.90
3	A	992	A	N7-C8-N9	5.12	116.36	113.80
4	a	647	G	C4-N9-C1'	5.11	133.15	126.50
3	A	1815	C	N1-C2-O2	5.11	121.97	118.90
3	A	2033	C	N3-C2-O2	-5.11	118.32	121.90
45	s	36	ARG	NE-CZ-NH1	5.11	122.85	120.30
3	A	1814	A	N9-C4-C5	-5.10	103.76	105.80
3	A	1700	C	N3-C4-N4	5.10	121.57	118.00
4	a	1541	G	C8-N9-C4	-5.10	104.36	106.40
3	A	2369	C	C6-N1-C2	-5.09	118.26	120.30
3	A	1814	A	C5-C6-N6	-5.09	119.63	123.70
3	A	179	A	C5-C6-N6	-5.09	119.63	123.70
3	A	902	A	C6-C5-N7	-5.09	128.74	132.30
4	a	651	C	N1-C2-O2	5.08	121.95	118.90
3	A	355	G	N3-C4-N9	5.08	129.05	126.00
4	a	1033	C	C6-N1-C2	-5.08	118.27	120.30
3	A	195	C	C5-C4-N4	-5.08	116.64	120.20
3	A	1380	G	C4-N9-C1'	5.08	133.10	126.50
3	A	1435	C	C6-N1-C2	-5.08	118.27	120.30
3	A	1647	A	C5-N7-C8	-5.08	101.36	103.90
3	A	2058	A	C5-C6-N6	-5.08	119.64	123.70
4	a	1013	G	C8-N9-C1'	-5.08	120.40	127.00
24	2	52	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	A	1494	G	C4-C5-N7	5.07	112.83	110.80
13	O	13	ARG	NE-CZ-NH2	-5.07	117.77	120.30
3	A	1201	G	C4-C5-N7	5.06	112.83	110.80
4	a	1367	G	C8-N9-C4	-5.06	104.38	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2490	C	N1-C2-O2	5.06	121.94	118.90
4	a	827	A	C4-C5-N7	5.05	113.23	110.70
3	A	1843	U	C2-N1-C1'	5.04	123.75	117.70
3	A	628	G	C5-N7-C8	-5.04	101.78	104.30
3	A	531	C	C5-C4-N4	-5.04	116.67	120.20
3	A	1465	G	C8-N9-C1'	-5.04	120.45	127.00
3	A	616	G	N3-C4-C5	5.04	131.12	128.60
3	A	2052	C	C2-N1-C1'	5.04	124.34	118.80
3	A	2483	C	N3-C4-N4	5.03	121.52	118.00
3	A	253	G	N9-C4-C5	5.03	107.41	105.40
3	A	355	G	N9-C4-C5	-5.03	103.39	105.40
44	i	15	ARG	NE-CZ-NH1	5.03	122.81	120.30
4	a	651	C	N3-C2-O2	-5.02	118.38	121.90
51	D	57	C	C6-N1-C2	-5.02	118.29	120.30
3	A	66	C	N1-C2-O2	5.02	121.91	118.90
4	a	1013	G	C2-N3-C4	5.02	114.41	111.90
3	A	1351	C	C5-C4-N4	-5.01	116.69	120.20
4	a	479	U	C5-C4-O4	-5.01	122.89	125.90
3	A	116	G	C2-N3-C4	-5.00	109.40	111.90
3	A	1695	G	C4-C5-N7	5.00	112.80	110.80

There are no chirality outliers.

There are no planarity outliers.

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	Z	80/94 (85%)	72 (90%)	8 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	133/144 (92%)	125 (94%)	8 (6%)	0	100	100
6	G	271/277 (98%)	251 (93%)	20 (7%)	0	100	100
7	H	214/220 (97%)	192 (90%)	22 (10%)	0	100	100
8	I	202/207 (98%)	186 (92%)	16 (8%)	0	100	100
9	J	173/179 (97%)	165 (95%)	8 (5%)	0	100	100
10	K	162/178 (91%)	147 (91%)	15 (9%)	0	100	100
11	M	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
12	N	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
13	O	143/146 (98%)	135 (94%)	8 (6%)	0	100	100
14	Q	118/122 (97%)	115 (98%)	3 (2%)	0	100	100
15	R	116/119 (98%)	101 (87%)	15 (13%)	0	100	100
16	S	112/116 (97%)	100 (89%)	12 (11%)	0	100	100
17	T	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
18	U	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
19	V	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
20	W	87/91 (96%)	77 (88%)	10 (12%)	0	100	100
21	X	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
22	Y	92/217 (42%)	77 (84%)	15 (16%)	0	100	100
23	1	57/62 (92%)	49 (86%)	8 (14%)	0	100	100
24	2	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
25	3	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
26	5	52/58 (90%)	43 (83%)	9 (17%)	0	100	100
27	6	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
28	8	62/66 (94%)	54 (87%)	8 (13%)	0	100	100
29	7	40/45 (89%)	39 (98%)	1 (2%)	0	100	100
30	d	205/217 (94%)	187 (91%)	18 (9%)	0	100	100
31	e	197/200 (98%)	175 (89%)	22 (11%)	0	100	100
32	h	144/156 (92%)	133 (92%)	10 (7%)	1 (1%)	22	57
33	k	100/102 (98%)	87 (87%)	13 (13%)	0	100	100
34	l	116/129 (90%)	108 (93%)	8 (7%)	0	100	100
35	o	57/60 (95%)	57 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	p	84/89 (94%)	80 (95%)	4 (5%)	0	100	100
37	q	88/91 (97%)	78 (89%)	10 (11%)	0	100	100
38	u	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
39	9	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
40	t	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
41	n	111/121 (92%)	100 (90%)	11 (10%)	0	100	100
42	j	125/132 (95%)	114 (91%)	11 (9%)	0	100	100
43	f	154/166 (93%)	147 (96%)	7 (4%)	0	100	100
44	i	129/132 (98%)	118 (92%)	11 (8%)	0	100	100
45	s	61/80 (76%)	56 (92%)	5 (8%)	0	100	100
46	g	91/98 (93%)	83 (91%)	8 (9%)	0	100	100
48	m	133/137 (97%)	116 (87%)	17 (13%)	0	100	100
49	r	77/87 (88%)	67 (87%)	10 (13%)	0	100	100
50	c	219/255 (86%)	202 (92%)	17 (8%)	0	100	100
52	4	53/84 (63%)	51 (96%)	2 (4%)	0	100	100
All	All	5287/5775 (92%)	4856 (92%)	430 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	h	53	ARG

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	64/75 (85%)	64 (100%)	0	100	100
2	P	112/119 (94%)	112 (100%)	0	100	100
6	G	220/224 (98%)	219 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	174/177 (98%)	174 (100%)	0	100	100
8	I	168/169 (99%)	167 (99%)	1 (1%)	86	94
9	J	154/158 (98%)	154 (100%)	0	100	100
10	K	144/155 (93%)	143 (99%)	1 (1%)	84	93
11	M	121/123 (98%)	121 (100%)	0	100	100
12	N	100/100 (100%)	100 (100%)	0	100	100
13	O	111/112 (99%)	110 (99%)	1 (1%)	78	91
14	Q	101/102 (99%)	101 (100%)	0	100	100
15	R	94/95 (99%)	93 (99%)	1 (1%)	73	89
16	S	100/102 (98%)	98 (98%)	2 (2%)	55	80
17	T	96/98 (98%)	96 (100%)	0	100	100
18	U	86/86 (100%)	86 (100%)	0	100	100
19	V	90/94 (96%)	87 (97%)	3 (3%)	38	69
20	W	80/82 (98%)	79 (99%)	1 (1%)	69	87
21	X	84/90 (93%)	84 (100%)	0	100	100
22	Y	83/190 (44%)	83 (100%)	0	100	100
23	1	49/52 (94%)	48 (98%)	1 (2%)	55	80
24	2	58/62 (94%)	58 (100%)	0	100	100
25	3	51/53 (96%)	51 (100%)	0	100	100
26	5	49/51 (96%)	49 (100%)	0	100	100
27	6	45/47 (96%)	45 (100%)	0	100	100
28	8	55/57 (96%)	55 (100%)	0	100	100
29	7	38/40 (95%)	38 (100%)	0	100	100
30	d	169/175 (97%)	169 (100%)	0	100	100
31	e	174/175 (99%)	171 (98%)	3 (2%)	60	83
32	h	126/132 (96%)	124 (98%)	2 (2%)	62	84
33	k	91/91 (100%)	91 (100%)	0	100	100
34	l	94/104 (90%)	94 (100%)	0	100	100
35	o	52/53 (98%)	52 (100%)	0	100	100
36	p	79/81 (98%)	79 (100%)	0	100	100
37	q	76/77 (99%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	u	67/69 (97%)	67 (100%)	0	100	100
39	9	35/35 (100%)	35 (100%)	0	100	100
40	t	70/80 (88%)	70 (100%)	0	100	100
41	n	98/104 (94%)	97 (99%)	1 (1%)	76	90
42	j	105/109 (96%)	104 (99%)	1 (1%)	76	90
43	f	122/131 (93%)	122 (100%)	0	100	100
44	i	112/113 (99%)	112 (100%)	0	100	100
45	s	56/68 (82%)	56 (100%)	0	100	100
46	g	81/86 (94%)	80 (99%)	1 (1%)	71	88
48	m	117/119 (98%)	115 (98%)	2 (2%)	60	83
49	r	74/82 (90%)	74 (100%)	0	100	100
50	c	192/221 (87%)	191 (100%)	1 (0%)	88	94
52	4	55/75 (73%)	54 (98%)	1 (2%)	59	82
All	All	4572/4893 (93%)	4548 (100%)	24 (0%)	89	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	G	274	ARG
8	I	84	ARG
10	K	45	GLN
13	O	71	ARG
15	R	32	ASN
16	S	53	ARG
16	S	96	ARG
19	V	10	ILE
19	V	11	ARG
19	V	12	ILE
20	W	67	ARG
23	l	27	ARG
31	e	5	ARG
31	e	41	ARG
31	e	158	ASN
32	h	54	SER
32	h	78	ARG
41	n	65	VAL
42	j	115	ARG

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Mol	Chain	Res	Type
46	g	70	ASN
48	m	25	ASN
48	m	115	LEU
50	c	24	ASN
52	4	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	2821/2923 (96%)	470 (16%)	9 (0%)
4	a	1528/1551 (98%)	262 (17%)	0
47	b	7/15 (46%)	1 (14%)	0
5	B	112/115 (97%)	13 (11%)	1 (0%)
51	D	76/77 (98%)	10 (13%)	0
All	All	4544/4681 (97%)	756 (16%)	10 (0%)

All (756) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	23	G
3	A	34	U
3	A	35	G
3	A	36	G
3	A	46	C
3	A	51	G
3	A	61	A
3	A	64	A
3	A	71	A
3	A	74	U
3	A	75	G
3	A	85	G
3	A	88	G
3	A	99	U
3	A	101	G
3	A	117	A
3	A	118	A
3	A	119	U
3	A	130	A

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Mol	Chain	Res	Type
3	A	150	A
3	A	154	A
3	A	155	U
3	A	164	A
3	A	165	C
3	A	167	U
3	A	176	A
3	A	177	G
3	A	180	G
3	A	182	C
3	A	189	G
3	A	199	A
3	A	202	A
3	A	218	G
3	A	219	A
3	A	224	A
3	A	225	A
3	A	229	A
3	A	231	A
3	A	232	U
3	A	251	G
3	A	255	G
3	A	270	C
3	A	284	C
3	A	285	U
3	A	286	U
3	A	287	G
3	A	288	C
3	A	289	U
3	A	294	G
3	A	299	U
3	A	304	G
3	A	312	A
3	A	313	U
3	A	314	A
3	A	315	C
3	A	316	G
3	A	321	U
3	A	322	A
3	A	326	A
3	A	338	G
3	A	344	U

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Mol	Chain	Res	Type
3	A	353	A
3	A	354	A
3	A	373	A
3	A	401	U
3	A	404	U
3	A	409	G
3	A	410	G
3	A	431	C
3	A	432	G
3	A	457	G
3	A	458	A
3	A	470	G
3	A	497	U
3	A	502	C
3	A	503	A
3	A	526	A
3	A	527	G
3	A	536	A
3	A	543	G
3	A	550	A
3	A	551	G
3	A	553	A
3	A	563	G
3	A	567	G
3	A	572	C
3	A	573	A
3	A	575	G
3	A	576	U
3	A	577	A
3	A	578	G
3	A	583	A
3	A	587	C
3	A	591	A
3	A	593	U
3	A	594	G
3	A	606	G
3	A	616	G
3	A	618	A
3	A	626	G
3	A	630	G
3	A	646	A
3	A	658	A

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Mol	Chain	Res	Type
3	A	666	A
3	A	679	G
3	A	682	A
3	A	683	G
3	A	690	U
3	A	699	U
3	A	715	A
3	A	727	G
3	A	730	A
3	A	731	U
3	A	762	C
3	A	767	A
3	A	775	A
3	A	783	G
3	A	785	C
3	A	792	U
3	A	795	A
3	A	806	A
3	A	809	A
3	A	813	G
3	A	816	G
3	A	819	A
3	A	820	G
3	A	823	G
3	A	827	A
3	A	828	A
3	A	829	U
3	A	830	U
3	A	835	U
3	A	837	G
3	A	850	G
3	A	852	U
3	A	854	G
3	A	857	C
3	A	872	U
3	A	873	U
3	A	891	A
3	A	902	A
3	A	904	G
3	A	911	A
3	A	923	A
3	A	924	G

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Mol	Chain	Res	Type
3	A	940	U
3	A	941	A
3	A	943	C
3	A	944	G
3	A	945	A
3	A	955	A
3	A	957	C
3	A	970	U
3	A	971	U
3	A	975	U
3	A	977	A
3	A	985	A
3	A	989	A
3	A	990	G
3	A	1001	A
3	A	1003	A
3	A	1005	G
3	A	1017	A
3	A	1018	A
3	A	1022	G
3	A	1027	A
3	A	1040	A
3	A	1049	C
3	A	1056	U
3	A	1057	A
3	A	1066	G
3	A	1069	G
3	A	1070	A
3	A	1077	U
3	A	1090	A
3	A	1091	G
3	A	1106	G
3	A	1112	G
3	A	1114	A
3	A	1123	C
3	A	1125	U
3	A	1127	U
3	A	1128	A
3	A	1129	A
3	A	1130	A
3	A	1131	G
3	A	1132	A

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Mol	Chain	Res	Type
3	A	1133	G
3	A	1141	U
3	A	1155	A
3	A	1156	G
3	A	1160	C
3	A	1172	A
3	A	1176	U
3	A	1177	A
3	A	1178	C
3	A	1183	G
3	A	1186	A
3	A	1215	U
3	A	1216	U
3	A	1217	U
3	A	1218	G
3	A	1225	G
3	A	1245	G
3	A	1250	G
3	A	1258	A
3	A	1276	G
3	A	1288	G
3	A	1291	A
3	A	1294	G
3	A	1302	G
3	A	1310	A
3	A	1312	A
3	A	1337	A
3	A	1339	U
3	A	1345	A
3	A	1358	A
3	A	1366	U
3	A	1378	U
3	A	1382	C
3	A	1401	G
3	A	1402	A
3	A	1405	G
3	A	1406	G
3	A	1416	U
3	A	1423	C
3	A	1430	A
3	A	1432	A
3	A	1449	A

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Mol	Chain	Res	Type
3	A	1452	C
3	A	1454	U
3	A	1455	U
3	A	1456	U
3	A	1457	U
3	A	1458	A
3	A	1459	A
3	A	1463	A
3	A	1464	U
3	A	1471	A
3	A	1472	C
3	A	1481	A
3	A	1490	G
3	A	1494	G
3	A	1497	A
3	A	1499	U
3	A	1504	U
3	A	1511	C
3	A	1522	G
3	A	1526	G
3	A	1527	A
3	A	1533	A
3	A	1536	C
3	A	1537	A
3	A	1547	C
3	A	1552	U
3	A	1553	A
3	A	1560	A
3	A	1561	G
3	A	1569	G
3	A	1574	G
3	A	1578	A
3	A	1581	U
3	A	1582	U
3	A	1583	G
3	A	1592	A
3	A	1594	U
3	A	1606	C
3	A	1607	A
3	A	1616	A
3	A	1625	U
3	A	1630	A

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Mol	Chain	Res	Type
3	A	1631	G
3	A	1634	A
3	A	1639	G
3	A	1651	C
3	A	1652	A
3	A	1654	A
3	A	1660	A
3	A	1671	A
3	A	1678	A
3	A	1683	U
3	A	1690	A
3	A	1691	G
3	A	1692	C
3	A	1704	C
3	A	1709	A
3	A	1718	G
3	A	1721	A
3	A	1726	A
3	A	1740	G
3	A	1759	G
3	A	1772	G
3	A	1786	A
3	A	1790	G
3	A	1791	G
3	A	1800	A
3	A	1803	G
3	A	1813	A
3	A	1818	A
3	A	1827	C
3	A	1828	U
3	A	1829	A
3	A	1835	U
3	A	1843	U
3	A	1846	A
3	A	1856	A
3	A	1860	C
3	A	1883	A
3	A	1885	G
3	A	1893	A
3	A	1895	C
3	A	1896	U
3	A	1897	U

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Mol	Chain	Res	Type
3	A	1899	U
3	A	1900	G
3	A	1909	C
3	A	1933	G
3	A	1939	A
3	A	1940	A
3	A	1942	U
3	A	1943	A
3	A	1955	A
3	A	1956	G
3	A	1957	G
3	A	1963	A
3	A	1965	A
3	A	1969	C
3	A	1982	U
3	A	1991	G
3	A	1994	C
3	A	1997	A
3	A	1998	A
3	A	1999	G
3	A	2014	G
3	A	2018	U
3	A	2020	U
3	A	2024	A
3	A	2040	A
3	A	2047	A
3	A	2050	A
3	A	2058	A
3	A	2059	G
3	A	2060	A
3	A	2070	C
3	A	2078	A
3	A	2079	G
3	A	2082	C
3	A	2083	G
3	A	2087	A
3	A	2088	G
3	A	2089	A
3	A	2096	G
3	A	2114	G
3	A	2218	G
3	A	2225	A

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Mol	Chain	Res	Type
3	A	2226	A
3	A	2231	C
3	A	2238	U
3	A	2239	A
3	A	2240	U
3	A	2241	C
3	A	2252	A
3	A	2265	G
3	A	2266	G
3	A	2290	C
3	A	2294	A
3	A	2295	A
3	A	2306	G
3	A	2310	C
3	A	2313	A
3	A	2314	A
3	A	2315	A
3	A	2326	G
3	A	2332	U
3	A	2333	U
3	A	2334	G
3	A	2335	G
3	A	2336	A
3	A	2337	A
3	A	2338	A
3	A	2339	U
3	A	2347	A
3	A	2352	G
3	A	2361	U
3	A	2362	A
3	A	2366	G
3	A	2372	G
3	A	2374	C
3	A	2377	C
3	A	2381	A
3	A	2404	A
3	A	2406	G
3	A	2410	G
3	A	2411	A
3	A	2412	C
3	A	2418	G
3	A	2429	U

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Mol	Chain	Res	Type
3	A	2430	C
3	A	2434	A
3	A	2450	U
3	A	2452	A
3	A	2456	G
3	A	2457	A
3	A	2468	C
3	A	2475	A
3	A	2479	C
3	A	2486	A
3	A	2529	G
3	A	2531	U
3	A	2532	G
3	A	2545	A
3	A	2547	C
3	A	2552	G
3	A	2562	G
3	A	2573	U
3	A	2575	G
3	A	2576	G
3	A	2581	U
3	A	2583	C
3	A	2593	A
3	A	2594	G
3	A	2599	A
3	A	2600	C
3	A	2605	G
3	A	2606	C
3	A	2609	G
3	A	2612	U
3	A	2613	C
3	A	2629	A
3	A	2637	C
3	A	2638	C
3	A	2640	U
3	A	2642	U
3	A	2657	G
3	A	2666	A
3	A	2673	C
3	A	2675	G
3	A	2680	U
3	A	2690	G

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Mol	Chain	Res	Type
3	A	2692	A
3	A	2716	U
3	A	2717	A
3	A	2718	C
3	A	2741	G
3	A	2753	U
3	A	2760	A
3	A	2762	G
3	A	2784	A
3	A	2791	A
3	A	2792	A
3	A	2793	G
3	A	2796	C
3	A	2805	A
3	A	2807	G
3	A	2817	A
3	A	2819	C
3	A	2821	U
3	A	2823	G
3	A	2824	G
3	A	2827	A
3	A	2838	C
3	A	2839	A
3	A	2850	G
3	A	2855	A
3	A	2863	G
3	A	2887	G
3	A	2892	G
3	A	2900	C
3	A	2905	C
3	A	2906	G
4	a	8	G
4	a	10	G
4	a	17	A
4	a	23	G
4	a	32	G
4	a	33	A
4	a	40	G
4	a	45	G
4	a	49	C
4	a	51	A
4	a	52	A

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Mol	Chain	Res	Type
4	a	74	G
4	a	81	A
4	a	82	G
4	a	84	U
4	a	85	U
4	a	86	G
4	a	87	C
4	a	89	U
4	a	90	C
4	a	91	U
4	a	92	C
4	a	94	G
4	a	97	G
4	a	107	G
4	a	108	A
4	a	115	A
4	a	120	C
4	a	129	A
4	a	130	A
4	a	131	C
4	a	132	C
4	a	136	C
4	a	144	C
4	a	146	G
4	a	149	A
4	a	165	G
4	a	169	C
4	a	171	A
4	a	177	G
4	a	185	U
4	a	196	A
4	a	201	U
4	a	205	A
4	a	206	A
4	a	207	G
4	a	211	A
4	a	212	A
4	a	213	G
4	a	214	A
4	a	216	G
4	a	219	C
4	a	220	U

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Mol	Chain	Res	Type
4	a	221	U
4	a	234	A
4	a	248	U
4	a	249	G
4	a	253	U
4	a	255	G
4	a	258	A
4	a	259	G
4	a	261	U
4	a	262	G
4	a	274	G
4	a	275	C
4	a	288	C
4	a	289	G
4	a	297	G
4	a	306	A
4	a	316	C
4	a	333	A
4	a	335	A
4	a	336	C
4	a	337	A
4	a	338	C
4	a	340	G
4	a	355	G
4	a	359	G
4	a	360	C
4	a	361	A
4	a	362	G
4	a	364	A
4	a	375	U
4	a	380	C
4	a	381	A
4	a	385	G
4	a	392	G
4	a	400	G
4	a	405	A
4	a	414	G
4	a	415	A
4	a	419	A
4	a	420	U
4	a	421	G
4	a	424	G

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Mol	Chain	Res	Type
4	a	429	U
4	a	430	C
4	a	431	G
4	a	432	G
4	a	437	U
4	a	447	U
4	a	456	A
4	a	460	A
4	a	461	C
4	a	462	A
4	a	467	U
4	a	470	A
4	a	472	G
4	a	474	A
4	a	476	C
4	a	492	G
4	a	493	G
4	a	503	A
4	a	504	G
4	a	511	A
4	a	517	A
4	a	519	C
4	a	521	A
4	a	526	C
4	a	529	G
4	a	535	G
4	a	540	A
4	a	555	A
4	a	567	A
4	a	572	U
4	a	576	G
4	a	580	A
4	a	581	A
4	a	583	G
4	a	584	C
4	a	585	G
4	a	587	G
4	a	589	G
4	a	596	G
4	a	597	U
4	a	626	C
4	a	630	A

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Mol	Chain	Res	Type
4	a	661	U
4	a	673	A
4	a	696	G
4	a	710	A
4	a	726	A
4	a	728	C
4	a	729	A
4	a	731	U
4	a	732	G
4	a	757	A
4	a	763	G
4	a	768	U
4	a	773	G
4	a	785	A
4	a	807	G
4	a	825	C
4	a	836	A
4	a	844	G
4	a	857	C
4	a	882	A
4	a	899	A
4	a	912	G
4	a	924	A
4	a	926	G
4	a	935	G
4	a	944	C
4	a	945	A
4	a	949	G
4	a	970	U
4	a	976	G
4	a	978	A
4	a	979	A
4	a	981	G
4	a	982	C
4	a	985	A
4	a	986	G
4	a	987	A
4	a	993	A
4	a	999	U
4	a	1003	G
4	a	1004	A
4	a	1012	U

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Mol	Chain	Res	Type
4	a	1014	A
4	a	1016	A
4	a	1025	G
4	a	1030	A
4	a	1033	C
4	a	1034	U
4	a	1035	U
4	a	1036	C
4	a	1037	C
4	a	1048	A
4	a	1057	C
4	a	1058	A
4	a	1077	U
4	a	1078	C
4	a	1097	U
4	a	1101	G
4	a	1106	G
4	a	1107	U
4	a	1113	A
4	a	1120	G
4	a	1124	C
4	a	1138	U
4	a	1142	A
4	a	1144	C
4	a	1146	U
4	a	1150	G
4	a	1151	U
4	a	1153	G
4	a	1168	A
4	a	1179	C
4	a	1182	A
4	a	1192	G
4	a	1195	G
4	a	1207	A
4	a	1208	A
4	a	1212	A
4	a	1222	U
4	a	1223	U
4	a	1224	A
4	a	1225	U
4	a	1238	A
4	a	1247	A

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Mol	Chain	Res	Type
4	a	1248	C
4	a	1268	A
4	a	1271	G
4	a	1279	G
4	a	1290	A
4	a	1297	U
4	a	1298	A
4	a	1310	A
4	a	1313	U
4	a	1316	G
4	a	1323	G
4	a	1328	C
4	a	1331	C
4	a	1346	C
4	a	1347	U
4	a	1351	A
4	a	1360	A
4	a	1364	G
4	a	1381	G
4	a	1405	A
4	a	1406	C
4	a	1409	A
4	a	1417	U
4	a	1430	G
4	a	1437	A
4	a	1444	A
4	a	1453	G
4	a	1457	A
4	a	1464	U
4	a	1465	A
4	a	1499	G
4	a	1509	G
4	a	1514	A
4	a	1515	A
4	a	1518	U
4	a	1529	G
4	a	1531	A
4	a	1541	G
4	a	1542	G
4	a	1543	A
4	a	1547	C
5	B	10	U

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Mol	Chain	Res	Type
5	B	27	A
5	B	30	U
5	B	39	G
5	B	40	C
5	B	42	G
5	B	43	A
5	B	51	A
5	B	55	A
5	B	85	U
5	B	87	C
5	B	88	G
5	B	106	G
47	b	2	G
51	D	8	U
51	D	9	G
51	D	18	A
51	D	19	G
51	D	20	G
51	D	21	U
51	D	22	A
51	D	35	C
51	D	59	A
51	D	77	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	195	C
3	A	475	A
3	A	756	A
3	A	943	C
3	A	1128	A
3	A	1577	G
3	A	1938	U
3	A	1939	A
3	A	2337	A
5	B	9	C

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](#)

Of 157 ligands modelled in this entry, 156 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	FME	D	102	51	8,9,10	0.95	0	7,9,11	1.26	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	FME	D	102	51	-	3/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D	102	FME	C-CA-N	2.36	113.98	109.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	D	102	FME	CB-CA-N-CN
56	D	102	FME	O-C-CA-CB
56	D	102	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

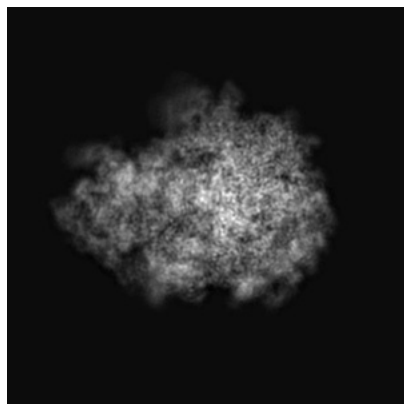
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12333. These allow visual inspection of the internal detail of the map and identification of artifacts.

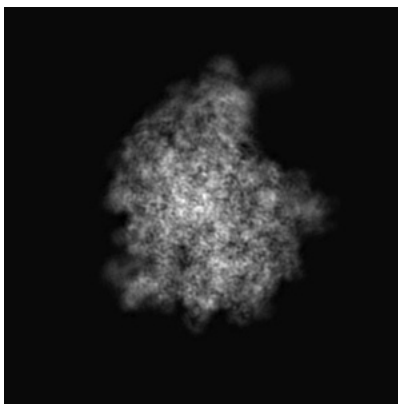
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

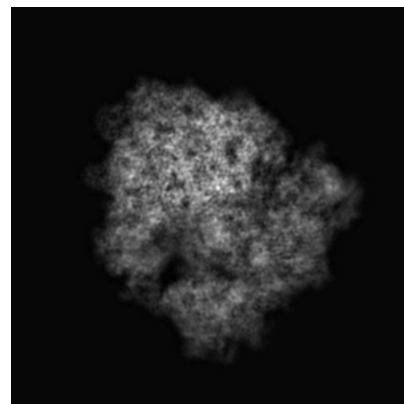
6.1.1 Primary map



X

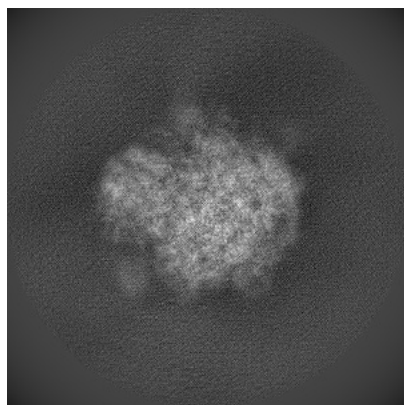


Y

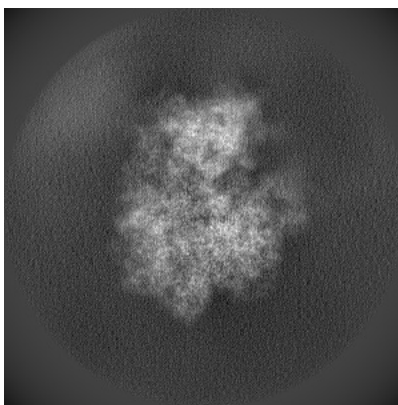


Z

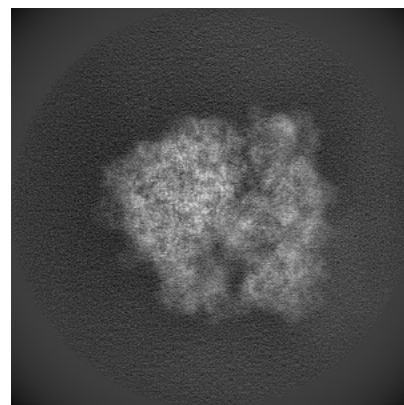
6.1.2 Raw map



X



Y

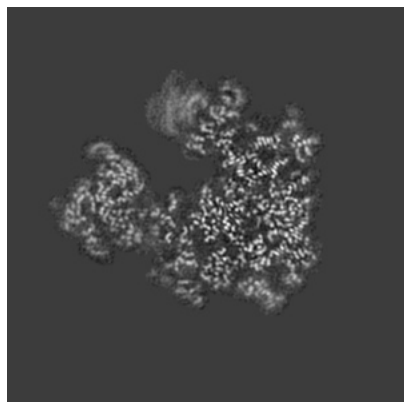


Z

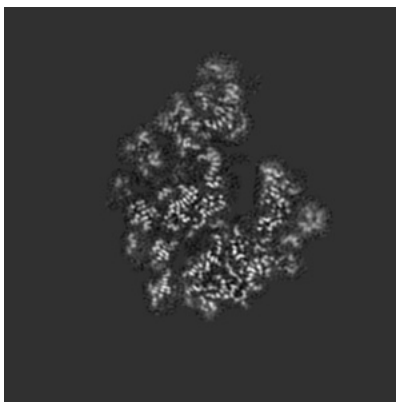
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

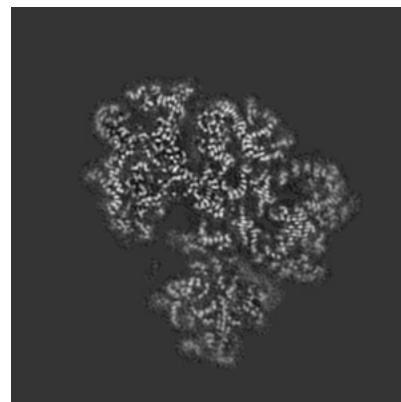
6.2.1 Primary map



X Index: 176

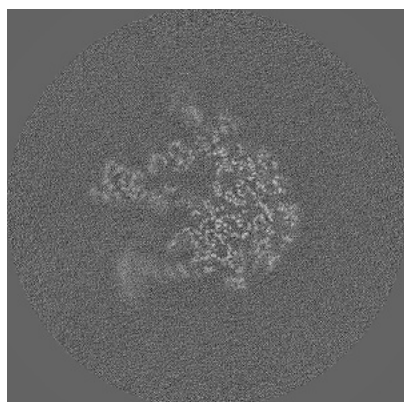


Y Index: 176

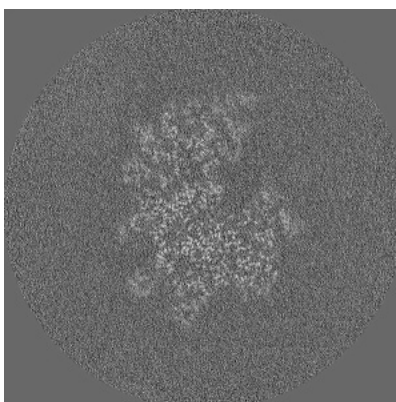


Z Index: 176

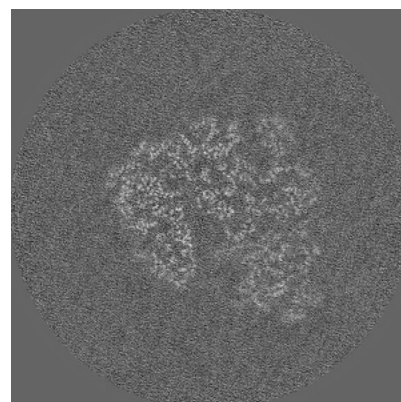
6.2.2 Raw map



X Index: 255



Y Index: 255

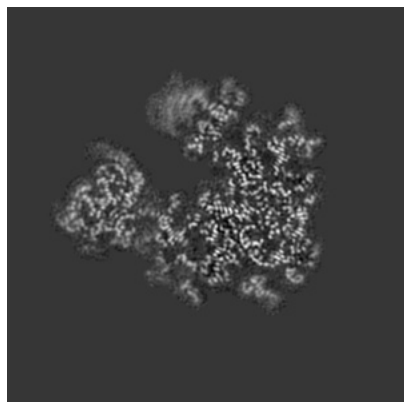


Z Index: 255

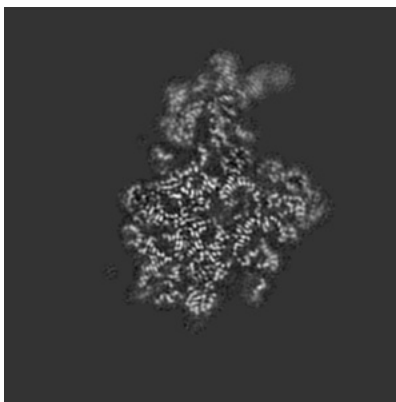
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

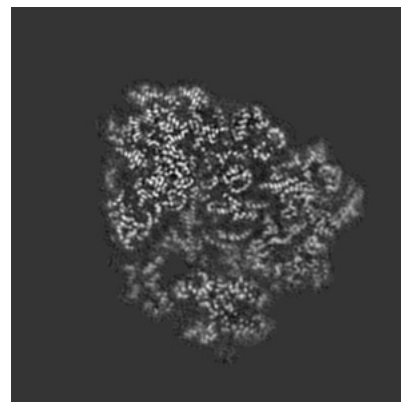
6.3.1 Primary map



X Index: 173

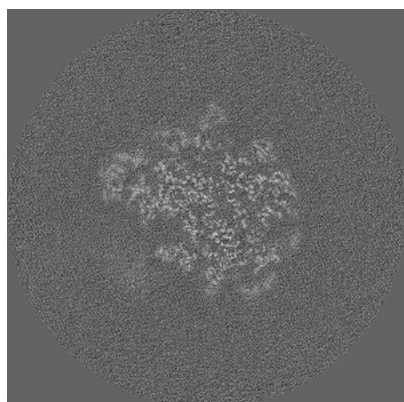


Y Index: 189

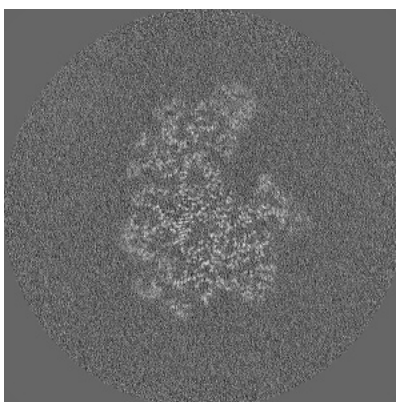


Z Index: 186

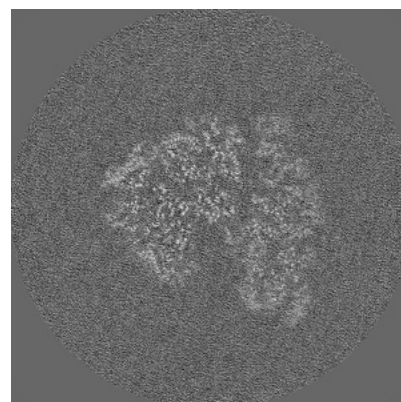
6.3.2 Raw map



X Index: 228



Y Index: 268

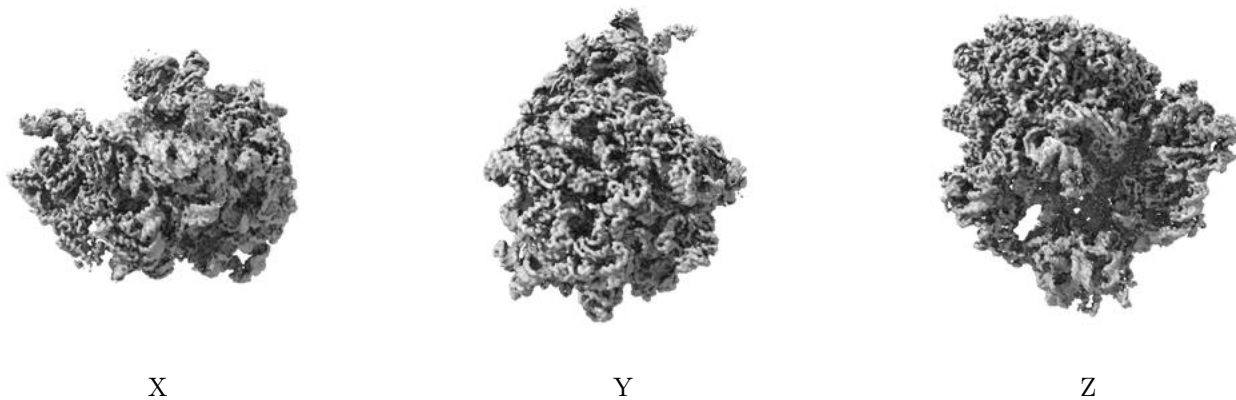


Z Index: 250

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

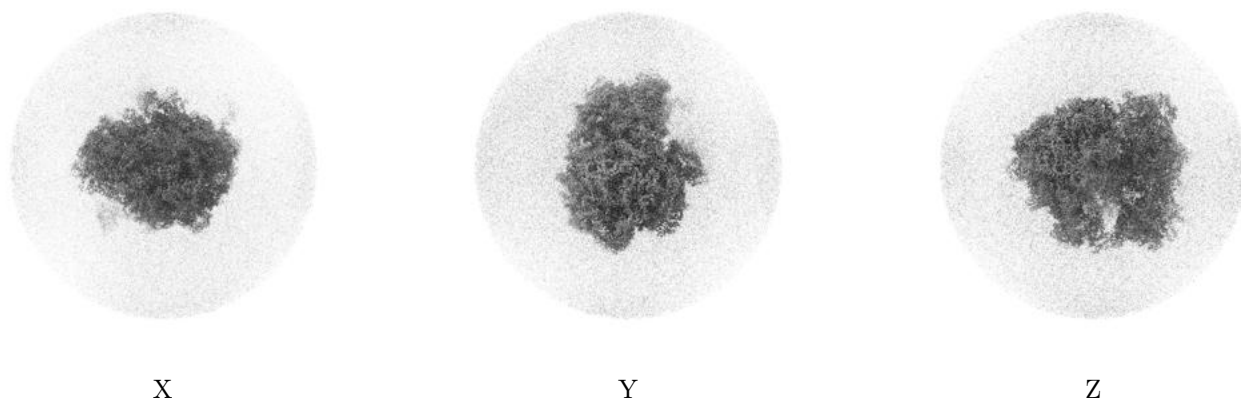
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

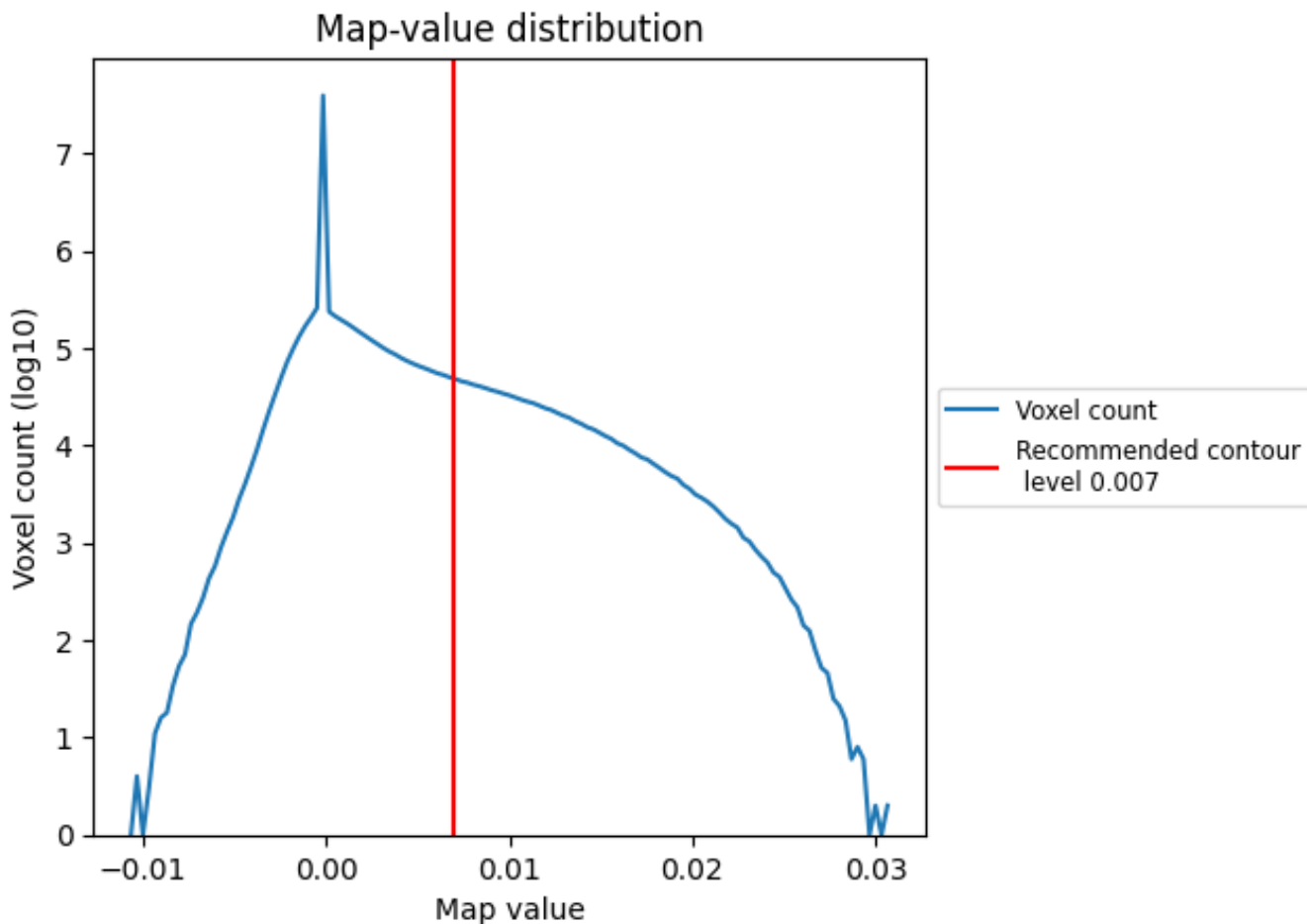
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

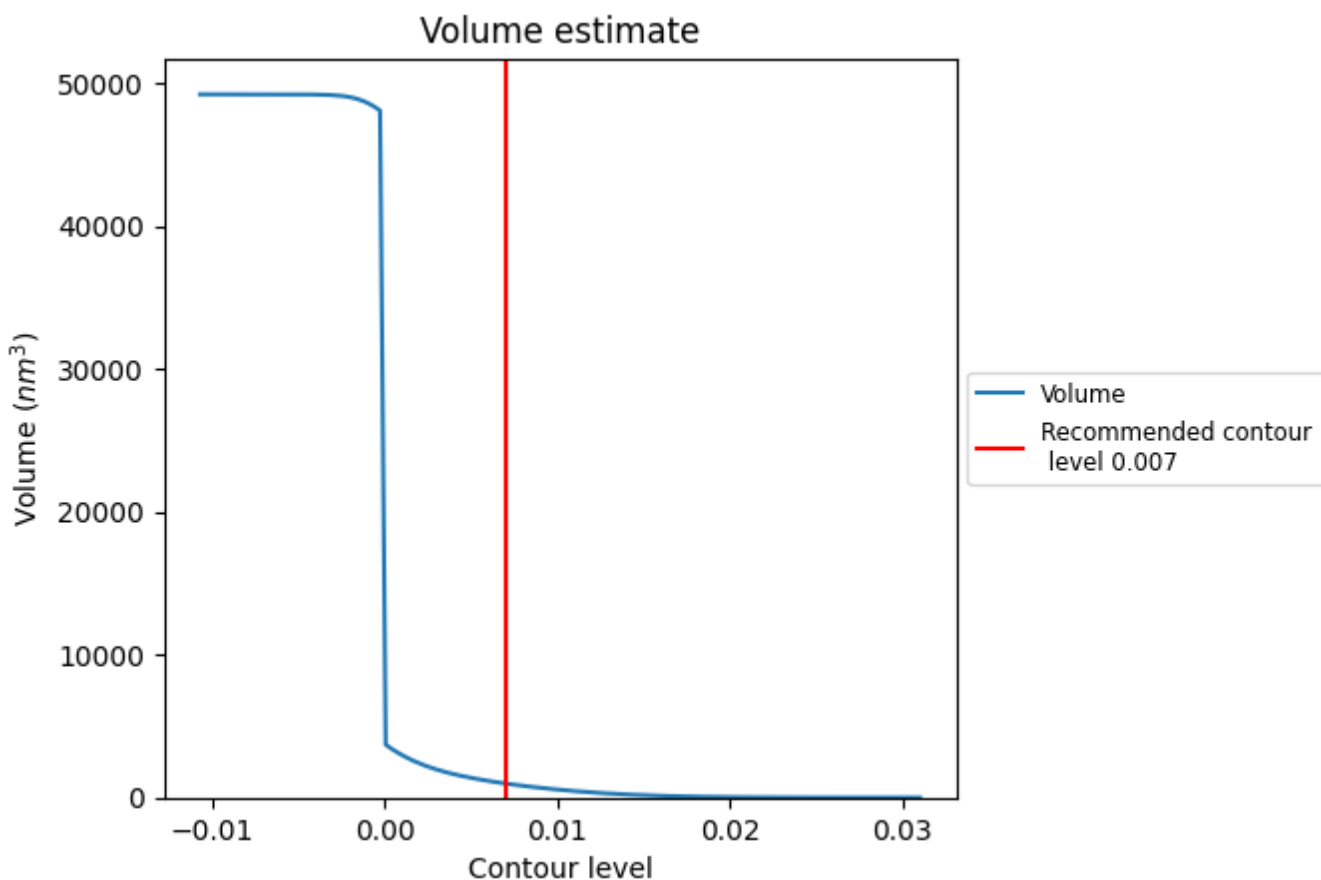
This section contains the results of statistical analysis of the map.

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.

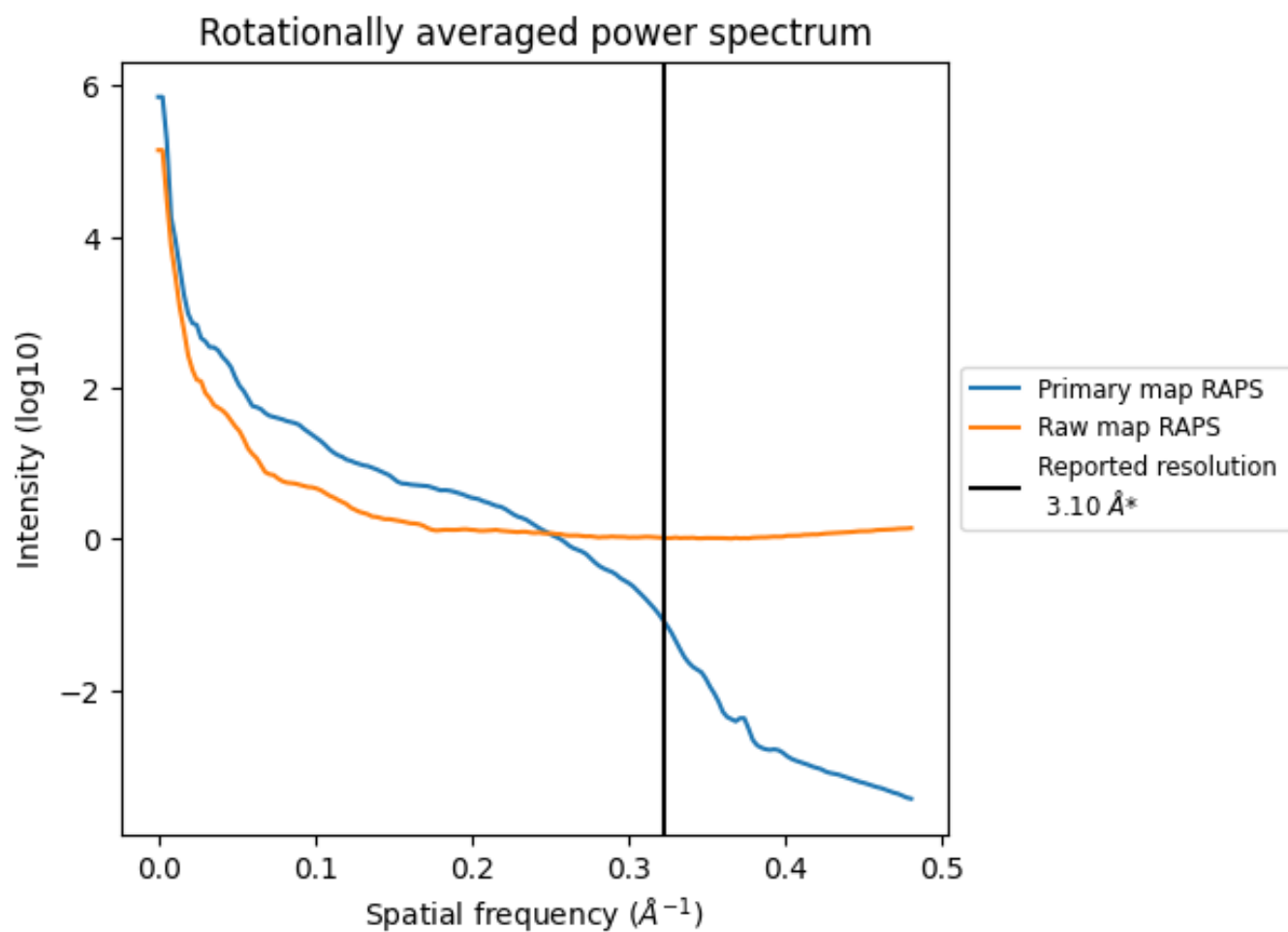
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 982 nm³; this corresponds to an approximate mass of 887 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 i

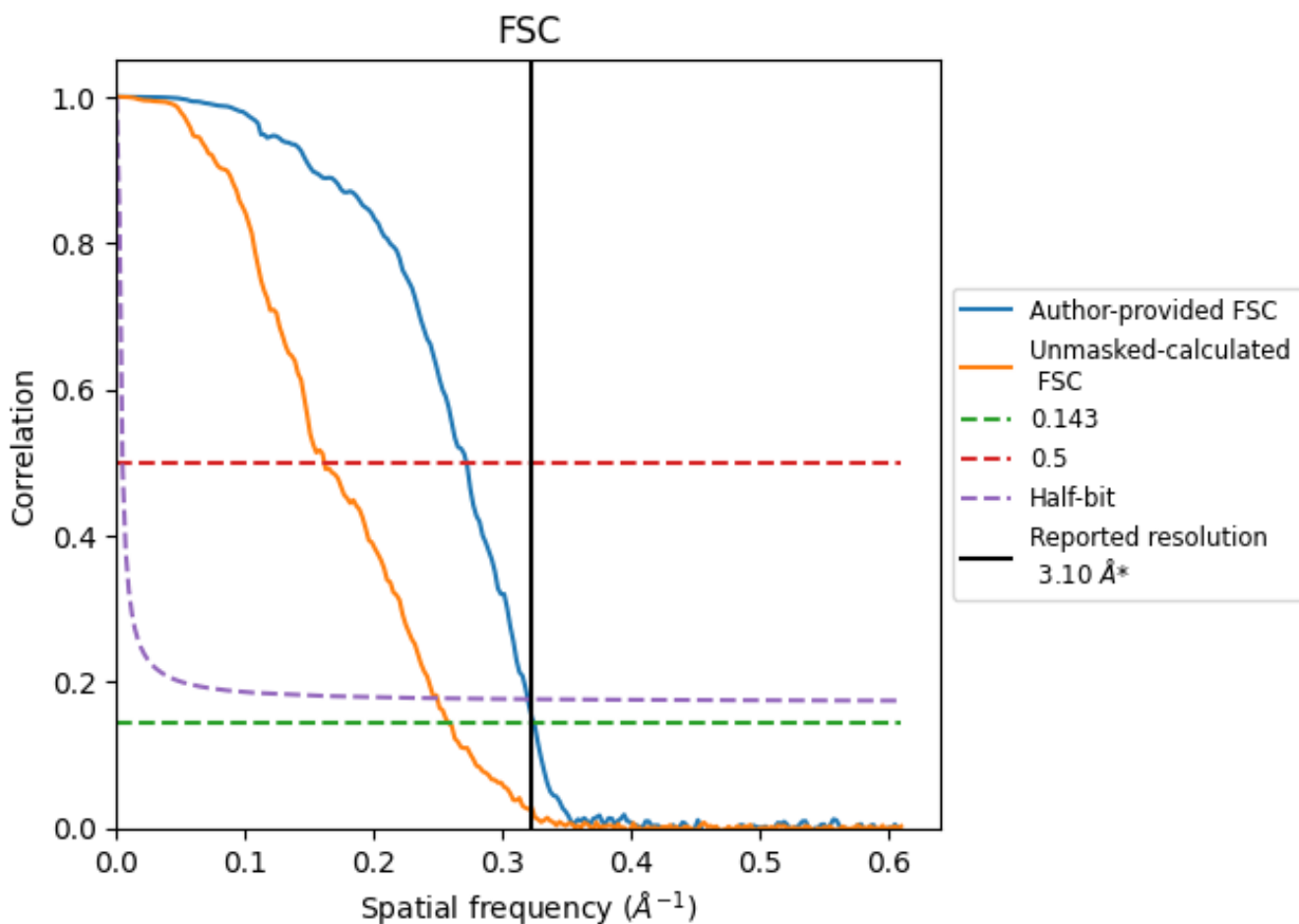


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323\AA^{-1}

8.2 Resolution estimates [i](#)

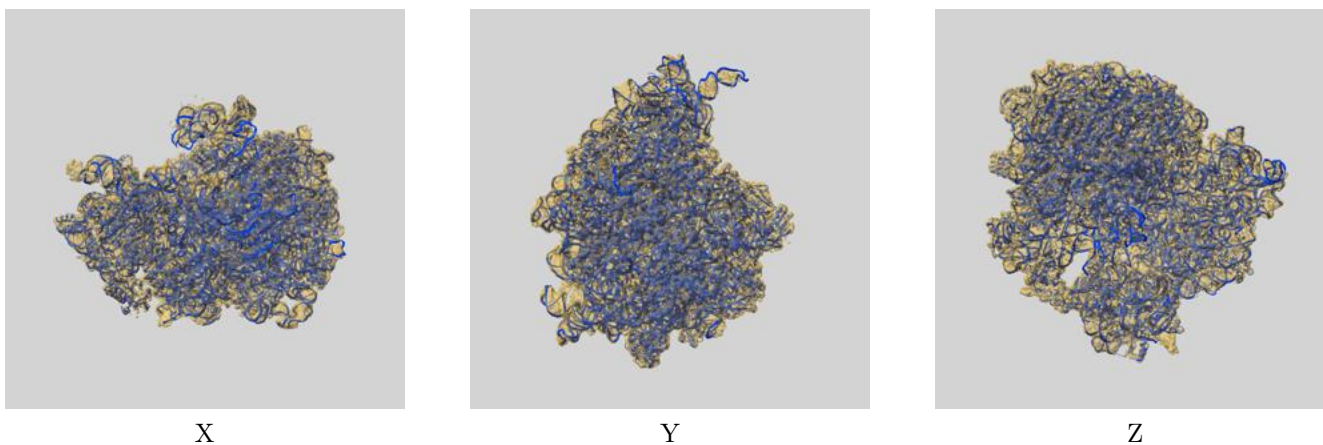
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.68	3.13
Unmasked-calculated*	3.87	6.19	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

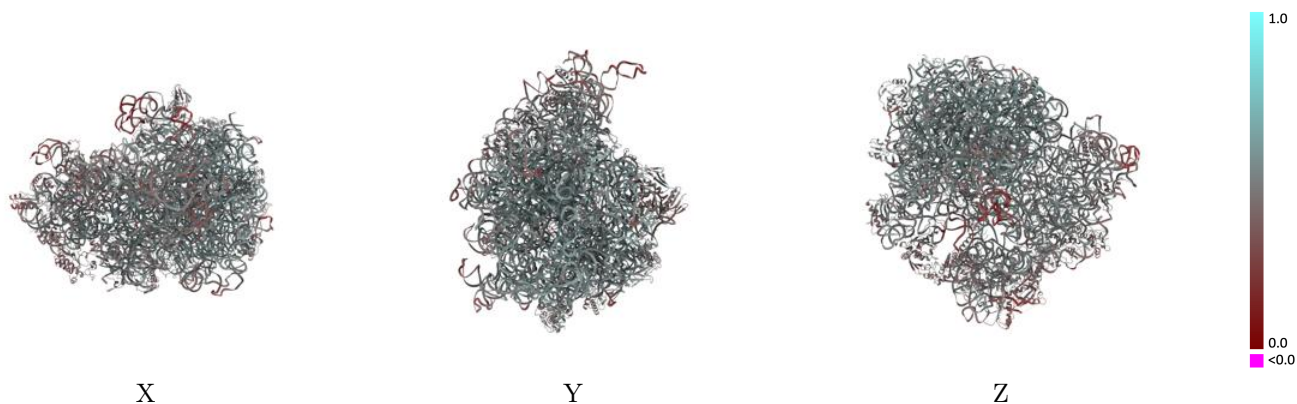
This section contains information regarding the fit between EMDB map EMD-12333 and PDB model 7NHM. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



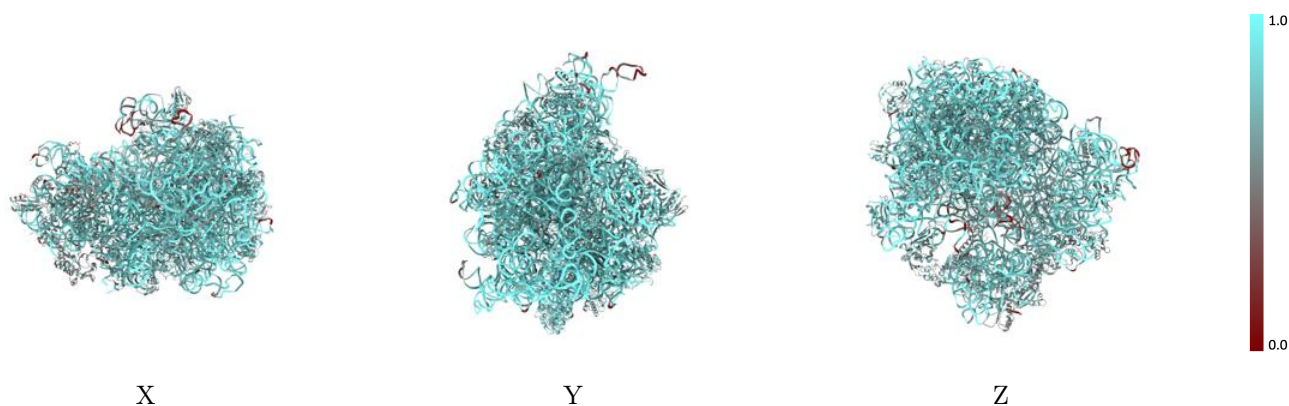
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



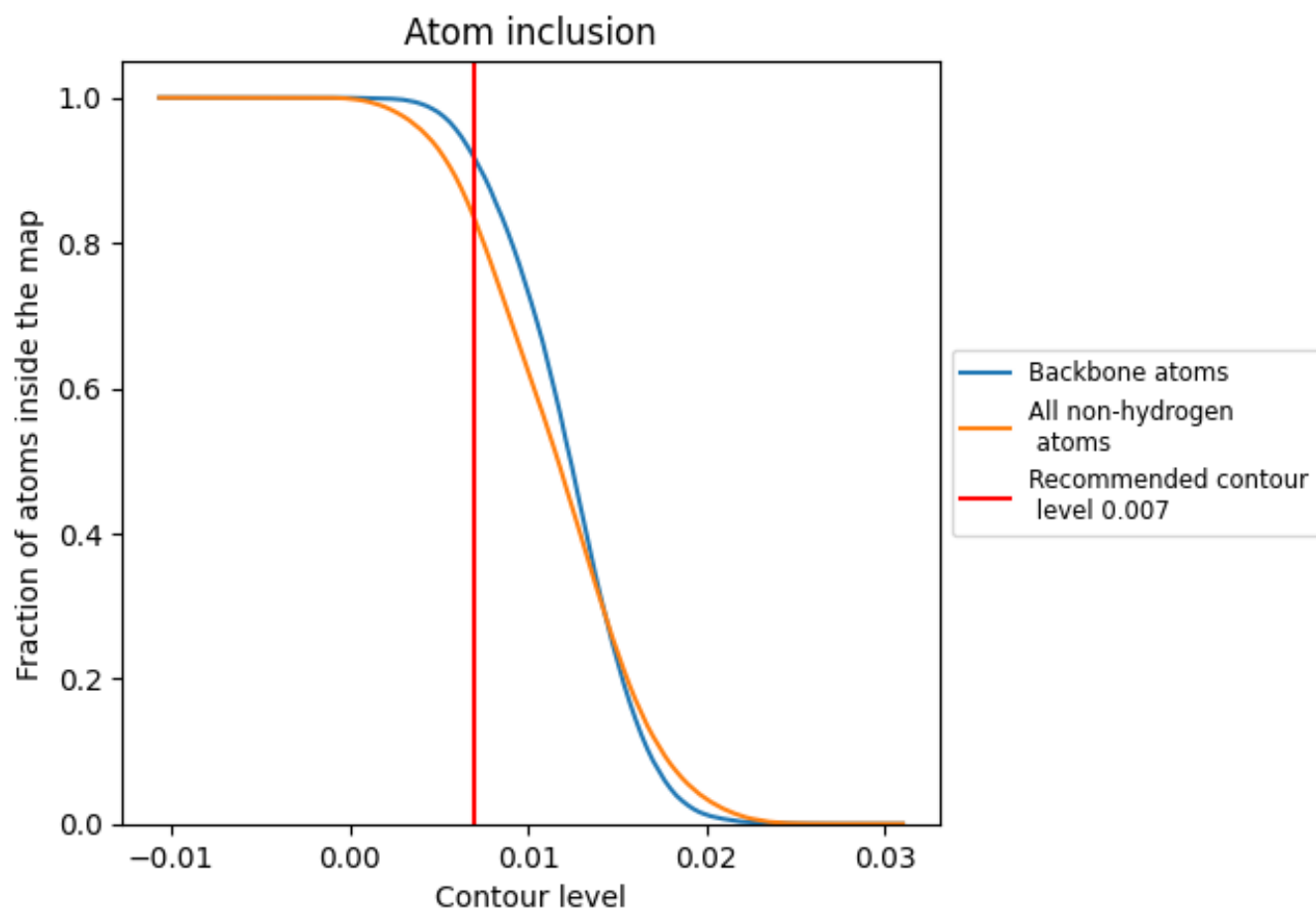
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8324	 0.4940
1	 0.6801	 0.5010
2	 0.7241	 0.4500
3	 0.7243	 0.4990
4	 0.6366	 0.4010
5	 0.7297	 0.5120
6	 0.7825	 0.4780
7	 0.7788	 0.5460
8	 0.7729	 0.5370
9	 0.7282	 0.5210
A	 0.9171	 0.5200
B	 0.9269	 0.4840
D	 0.6211	 0.4700
G	 0.7393	 0.5310
H	 0.7564	 0.5230
I	 0.7312	 0.4900
J	 0.6382	 0.4240
K	 0.6648	 0.4340
M	 0.7266	 0.5050
N	 0.6756	 0.5150
O	 0.7366	 0.5080
P	 0.7247	 0.5090
Q	 0.7399	 0.4980
R	 0.6984	 0.4480
S	 0.7133	 0.4990
T	 0.7593	 0.5000
U	 0.7455	 0.5110
V	 0.7425	 0.5200
W	 0.7199	 0.4860
X	 0.6605	 0.4730
Y	 0.6510	 0.4520
Z	 0.7166	 0.5240
a	 0.8793	 0.4820
b	 0.4322	 0.3770
c	 0.5395	 0.4130



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Chain	Atom inclusion	Q-score
d	 0.6142	 0.4330
e	 0.5635	 0.4110
f	 0.6787	 0.4870
g	 0.6555	 0.4530
h	 0.6294	 0.4160
i	 0.6878	 0.4690
j	 0.6515	 0.4560
k	 0.5572	 0.4010
l	 0.5984	 0.4400
m	 0.5984	 0.4580
n	 0.6339	 0.4280
o	 0.7080	 0.4690
p	 0.7161	 0.4410
q	 0.5683	 0.4380
r	 0.6462	 0.4600
s	 0.6908	 0.4750
t	 0.6382	 0.4300
u	 0.6137	 0.4070