



## Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 01:22 am GMT

PDB ID : 7PIS  
EMDB ID : EMD-13449  
Title : 70S ribosome with EF-G, A\*- and P/E-site tRNAs in pseudouridimycin-treated Mycoplasma pneumoniae cells  
Authors : Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.  
Deposited on : 2021-08-23  
Resolution : 15.00 Å (reported)  
Based on initial models : 4V7C, 4V7D, 7OOD, 7OOC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

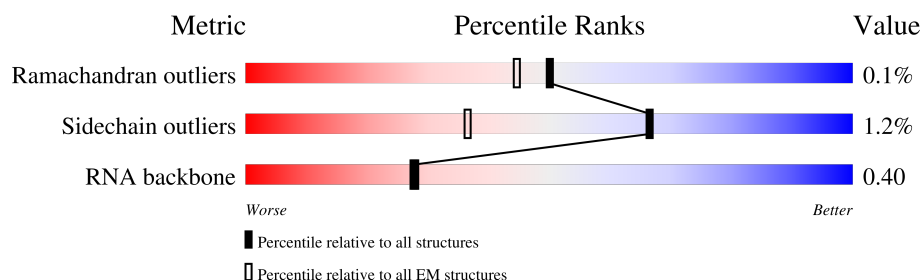
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 15.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	48	
2	1	59	
3	2	37	
4	9	688	
5	A	294	
6	B	273	
7	C	205	
8	D	219	

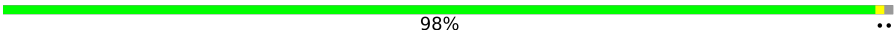
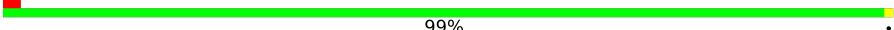
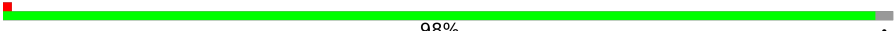
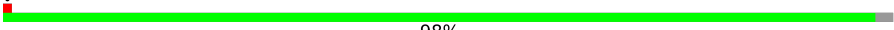
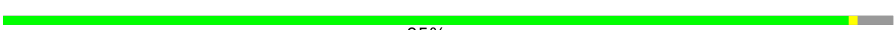





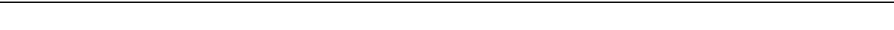

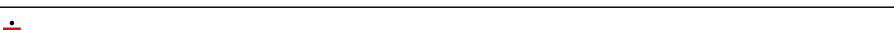
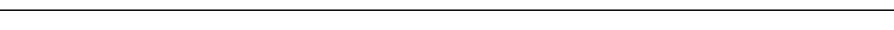
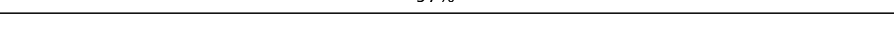


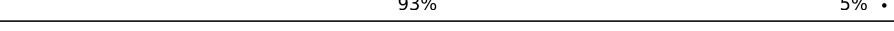
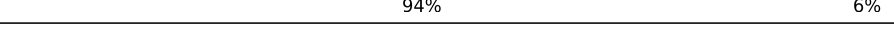




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Mol	Chain	Length	Quality of chain
9	E	215	
10	F	155	
11	G	142	
12	H	132	
13	I	108	
14	J	121	
15	K	139	
16	L	124	
17	M	61	
18	N	86	
19	O	94	
20	P	85	
21	Q	104	
22	R	87	
23	S	87	
24	T	60	
25	W	122	
26	a	287	
27	b	287	
28	c	212	
29	d	180	
30	e	184	
31	f	149	
32	g	161	
33	h	137	

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Mol	Chain	Length	Quality of chain
34	i	146	 98% ..
35	j	122	 99% .
36	k	151	 98% .
37	l	139	 98% .
38	m	124	 95% . .
39	n	116	 97% .
40	o	119	 97% .
41	p	127	 89% . 10%
42	q	100	 96% . .
43	r	159	 87% . 13%
44	s	237	 39% 61%
45	t	111	 100%
46	u	104	 82% . 17%
47	v	65	 97% .
48	w	111	 89% . 10%
49	x	97	 45% 55%
50	y	57	 93% 5% .
51	z	53	 94% 6%
52	3	2907	 63% 35% ..
53	4	108	 56% 40% . .
54	5	1520	 65% 33% .
55	6	76	 43% 54% .
55	8	76	 43% 54% .

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 151980 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	47	Total	C	N	O	S	0	0
			380	236	81	61	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	682	Total	C	N	O	S	0	0
			5326	3369	911	1021	25		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	240	Total	C	N	O	S	0	0
			1921	1226	334	352	9		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	215	Total	C	N	O	S	0	0
			1698	1073	313	307	5		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	203	Total	C	N	O	S	0	0
			1660	1051	314	290	5		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	153	Total	C	N	O	S	0	0
			1173	742	226	202	3		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	167	Total	C	N	O	S	0	0
			1362	857	240	263	2		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	154	Total	C	N	O	S	0	0
			1246	785	239	216	6		

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	128	Total	C	N	O	S	0	0
			1028	655	191	181	1		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	101	Total	C	N	O	S	0	0
			809	523	142	143	1		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	136	Total	C	N	O	S	0	0
			1076	680	213	181	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	118	Total	C	N	O	S	0	0
			951	594	191	166			

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	83	Total	C	N	O	S	0	0
			673	428	125	120			

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	80	Total	C	N	O	S	0	0
			646	414	119	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	83	Total	C	N	O	S	0	0
			675	425	135	115			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	65	Total	C	N	O	S	0	0
			535	342	103	86	4		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	84	Total	C	N	O	S	0	0
			682	435	127	118	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	77	Total	C	N	O		0	0
			629	383	135	111			

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	53	Total	C	N	O	S	0	0
			471	295	103	72	1		

- Molecule 25 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	69	Total	C	N	O	S	0	0
			534	342	87	103	2		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	229	Total	C	N	O	S	0	0
			1762	1119	318	318	7		

- Molecule 28 is a protein called 50S ribosomal protein L4.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	210	Total	C	N	O	S	0	0
			1644	1047	297	297	3		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	175	Total	C	N	O	S	0	0
			1388	893	245	246	4		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	176	Total	C	N	O	S	0	0
			1396	899	247	250			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	145	Total	C	N	O	S	0	0
			1160	746	204	207	3		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	126	Total	C	N	O	S	0	0
			960	612	167	178	3		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	148	Total	C	N	O		0	0
			1153	731	226	196			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	112	Total	C	N	O	S	0	0
			889	557	175	155	2		

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	115	Total	C	N	O	S	0	0
			938	592	180	165	1		

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	114	Total	C	N	O	S	0	0
			947	603	188	154	2		

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	139	Total	C	N	O	S	0	0
			1068	663	207	191	7		

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	92	Total	C	N	O	S	0	0
			720	475	122	122	1		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	111	Total	C	N	O	S	0	0
			872	550	166	153	3		

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	86	Total	C	N	O	S	0	0
			657	409	130	117	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	63	Total	C	N	O	S	0	0
			513	317	108	87	1		

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	100	Total	C	N	O		0	0
			818	517	153	148			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	44	Total	C	N	O	S	0	0
			344	221	55	64	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 51 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 52 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	2878	Total	C	N	O	P	0	0
			61664	27558	11236	19995	2875		

- Molecule 53 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	105	Total	C	N	O	P	0	0
			2239	1003	409	724	103		

- Molecule 54 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	5	1493	Total	C	N	O	P	0	0
			31943	14279	5792	10382	1490		

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

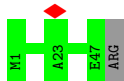
Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		
55	8	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		

### 3 Residue-property plots [i](#)

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 L34

Chain 0:  98%



- Molecule 2: 50S ribosomal protein L35

Chain 1:  98%



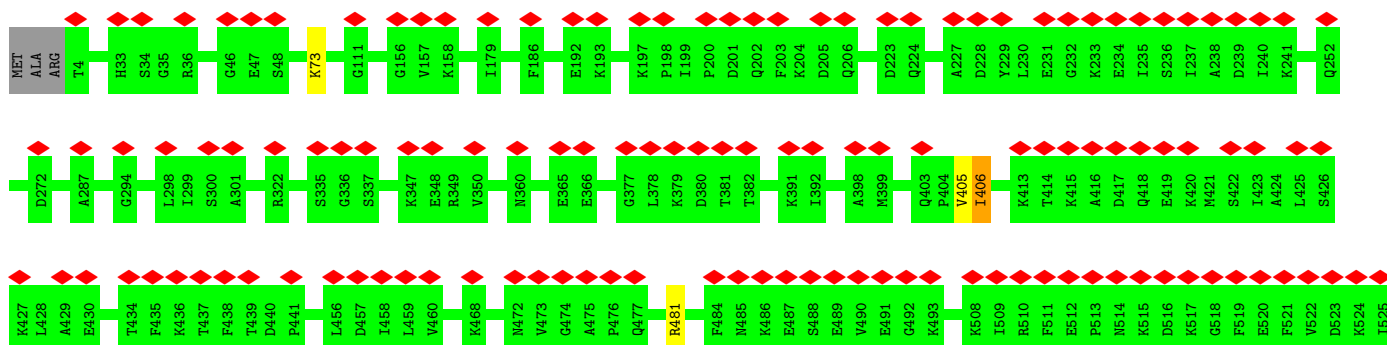
- Molecule 3: 50S ribosomal protein L36

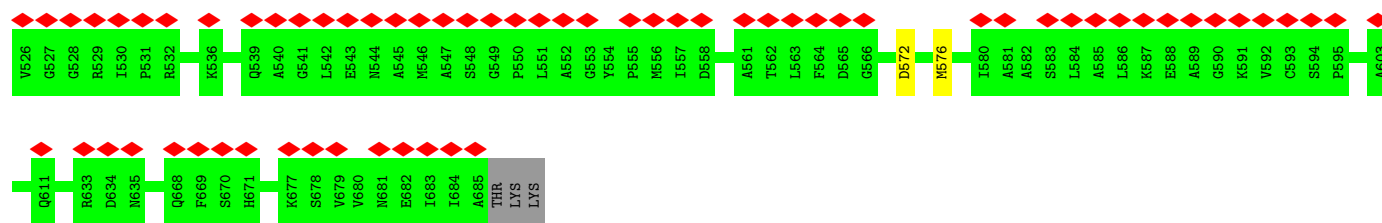
Chain 2:  100%

There are no outlier residues recorded for this chain.

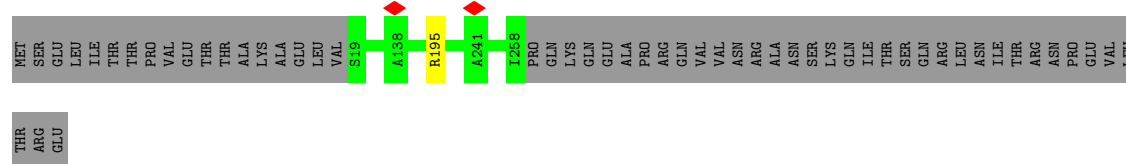
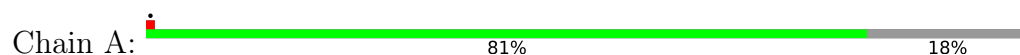
- Molecule 4: Elongation factor G

Chain 9:  28% 98%

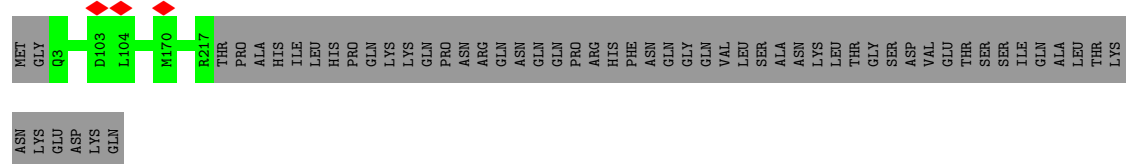
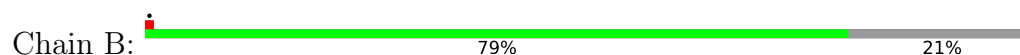




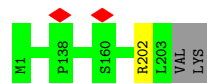
• Molecule 5: 30S ribosomal protein S2



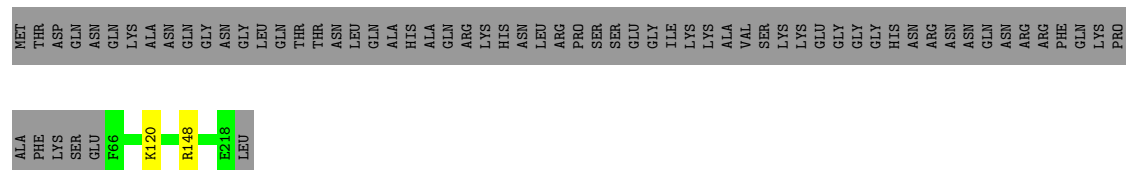
• Molecule 6: 30S ribosomal protein S3



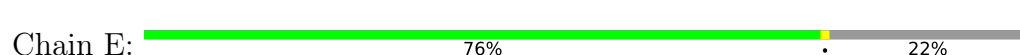
• Molecule 7: 30S ribosomal protein S4

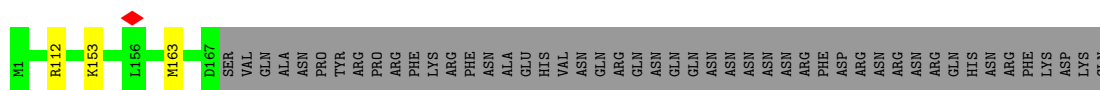


• Molecule 8: 30S ribosomal protein S5

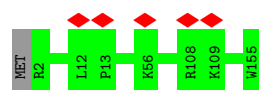


• Molecule 9: 30S ribosomal protein S6





- Molecule 10: 30S ribosomal protein S7



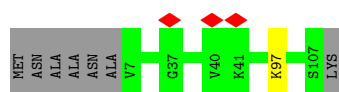
- Molecule 11: 30S ribosomal protein S8



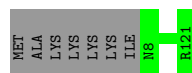
- Molecule 12: 30S ribosomal protein S9



- Molecule 13: 30S ribosomal protein S10



- Molecule 14: 30S ribosomal protein S11

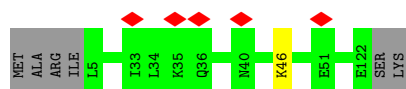


- Molecule 15: 30S ribosomal protein S12



- Molecule 16: 30S ribosomal protein S13

Chain L:  94% 5%



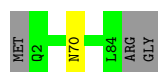
- Molecule 17: 30S ribosomal protein S14 type Z

Chain M:  97%



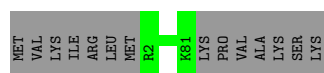
- Molecule 18: 30S ribosomal protein S15

Chain N:  95%



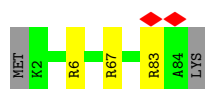
- Molecule 19: 30S ribosomal protein S16

Chain O:  85% 15%



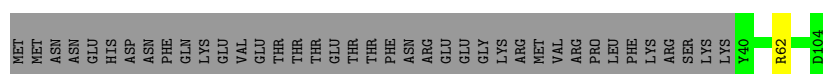
- Molecule 20: 30S ribosomal protein S17

Chain P:  94%



- Molecule 21: 30S ribosomal protein S18

Chain Q:  62% 38%




- Molecule 22: 30S ribosomal protein S19

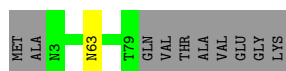
Chain R:  95%



- Molecule 23: 30S ribosomal protein S20



Chain S:  87% 11%




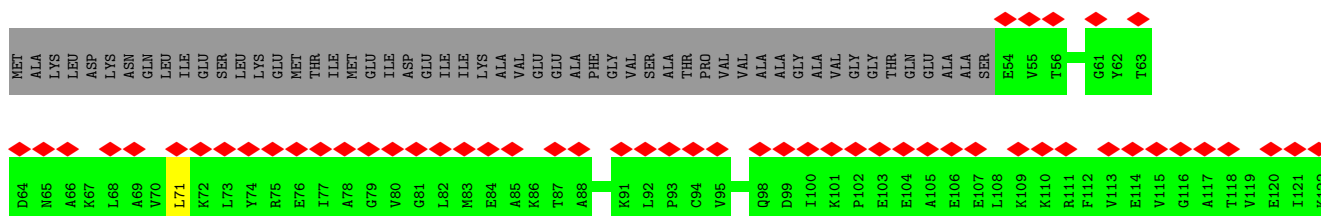
- Molecule 24: 30S ribosomal protein S21

Chain T:  88% 12%



- Molecule 25: 50S ribosomal protein L7/L12

Chain W:  44% 56% 43%




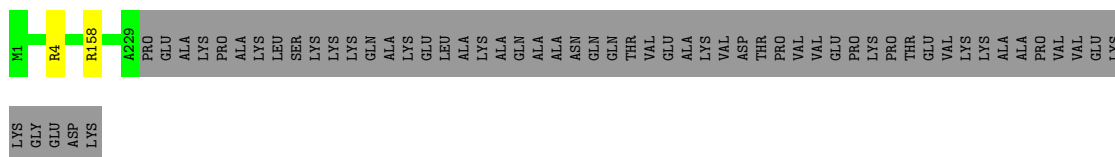
- Molecule 26: 50S ribosomal protein L2

Chain a:  99%



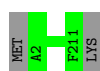
- Molecule 27: 50S ribosomal protein L3

Chain b:  79% 20%



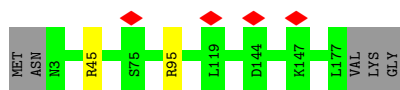
- Molecule 28: 50S ribosomal protein L4

Chain c:  99%

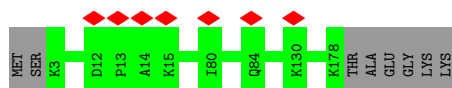


- Molecule 29: 50S ribosomal protein L5

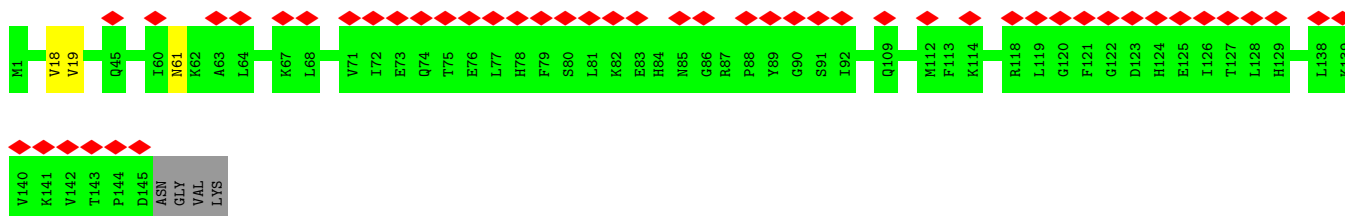
Chain d:  96%



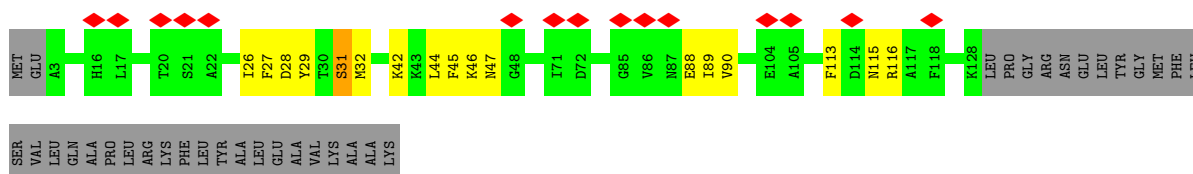
- Molecule 30: 50S ribosomal protein L6



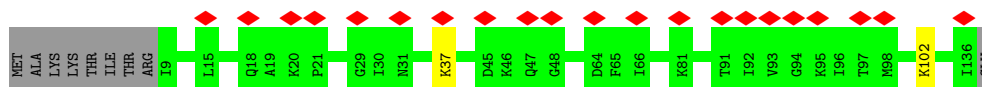
- Molecule 31: 50S ribosomal protein L9



- Molecule 32: 50S ribosomal protein L10



- Molecule 33: 50S ribosomal protein L11

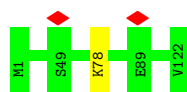


- Molecule 34: 50S ribosomal protein L13

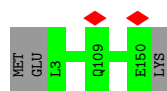


- Molecule 35: 50S ribosomal protein L14

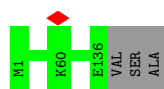




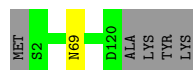
- Molecule 36: 50S ribosomal protein L15



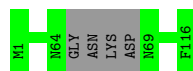
- Molecule 37: 50S ribosomal protein L16



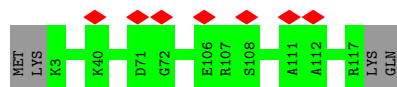
- Molecule 38: 50S ribosomal protein L17



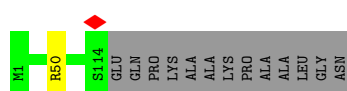
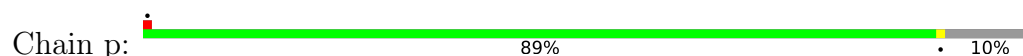
- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21

- Chain r:  87% . 13%

M1		N60	R139	Gln	Lys	Ala	Val	Thr	Ser	Val	Val	Lys	Ala	Pro	Ser	Lys	Thr	Gln	Gly	Gly	Val	Gln	Lys
----	--	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain s:  39% 61%

MET	D2	V93	THR
		GLY	
		GLU	
		ALA	
		PRO	
		GLU	
		LYS	
		THR	
		ASP	
		PRO	
		ALA	
		ASP	
		LYS	
		THR	
		THR	
		LEU	
		LYS	
		GLU	
		THR	
		VAL	
		LYS	
		ILE	
		LYS	
		ASP	
		THR	
		LYS	
		ASN	
		SER	
		PRO	
		GLU	
		ALA	
		VAL	
		VAL	
		LYS	
		THR	
		ALA	
		GLU	
		ALA	
		LEU	
		GLN	
		ILE	
		LYS	
		PRO	
		THR	
		ALA	
		ALA	
		PRO	
		VAL	
		THR	
		THR	
		ALA	

[illegible]

LYS THR GLU LYS SER ALA LYS THR THR LYS THR THR ALA THR LYS THR THR LYS THR LYS THR THR THR LYS LYS GLU VAL LYS LYS

- Chain t: 

The diagram shows a 12-lead ECG system with leads M1, A30, R31, T52, A56, Q84, K96, T97, and L111. Red diamonds are placed above the following leads: A30, R31, T52, A56, Q84, K96, and T97. These leads are not used in the 12-lead system.

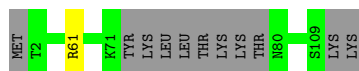
- Chain u:  82% 17%

MET ASN ASN LYS TYR PHE LEU THR LYS ILE ASP LEU GLN PHE PHE ALA S17 R58 K101 L102 ASP ALA

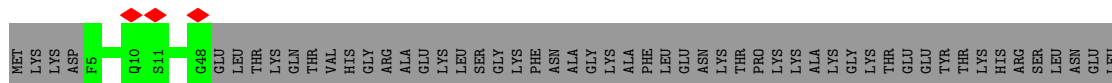
- Chain v:  97%

MET A2 L64 SER

- Chain w:  89% • 10%



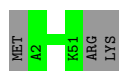
- Molecule 49: 50S ribosomal protein L31



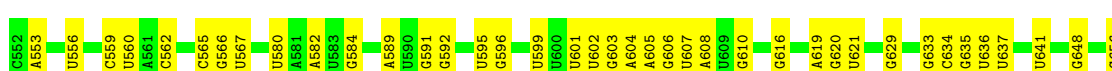
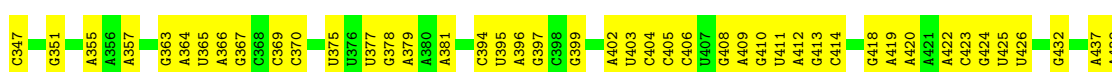
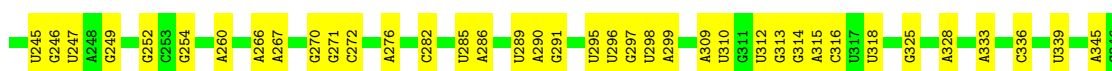
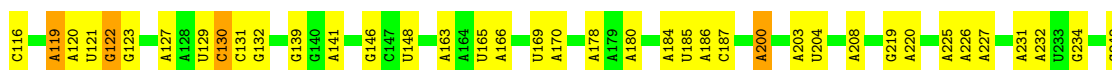
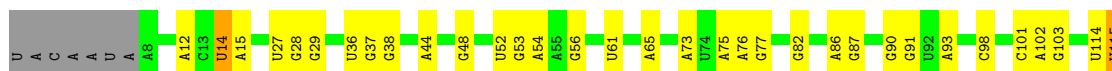
- Molecule 50: 50S ribosomal protein L32



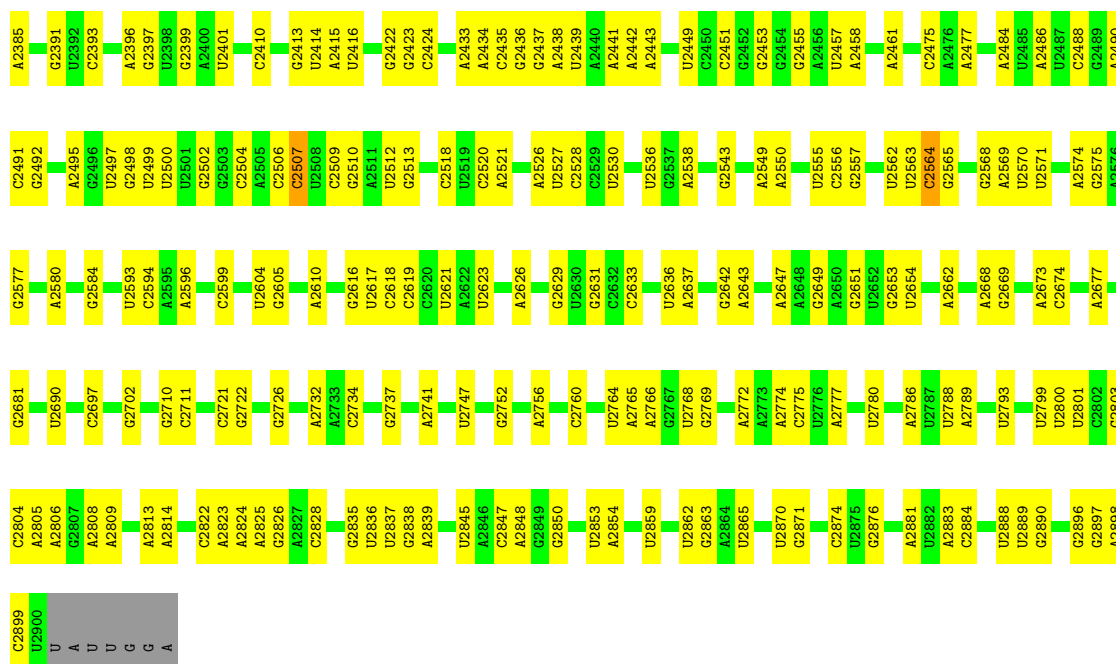
- Molecule 51: 50S ribosomal protein L33 1



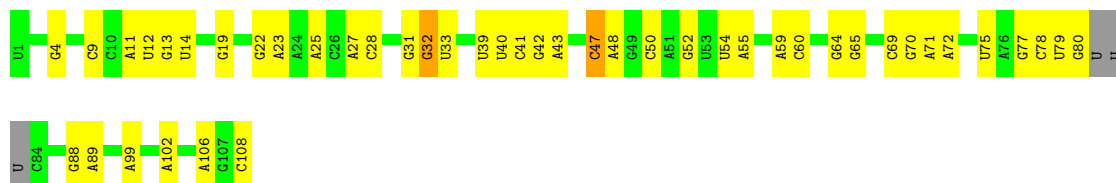
- Molecule 52: 23S ribosomal RNA



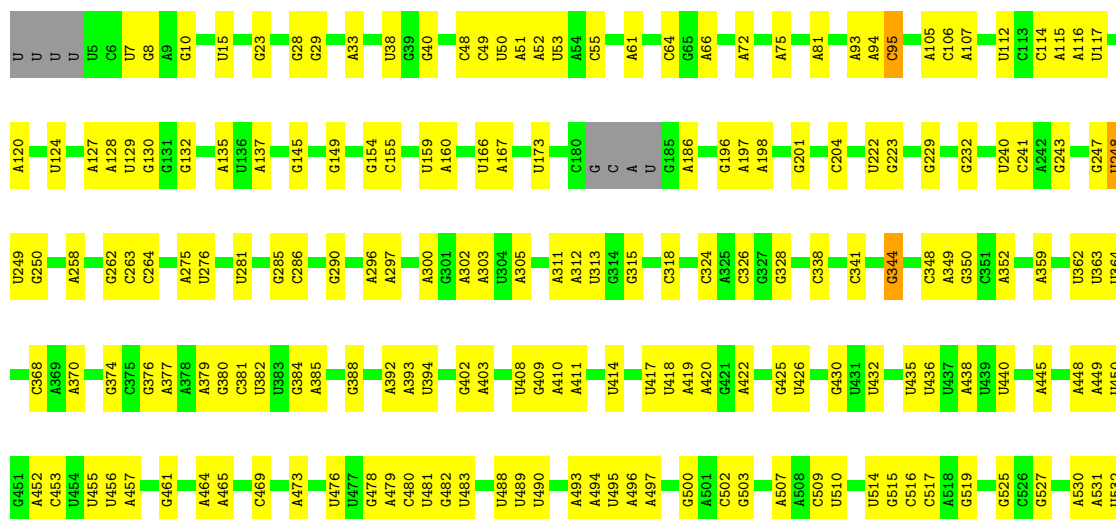


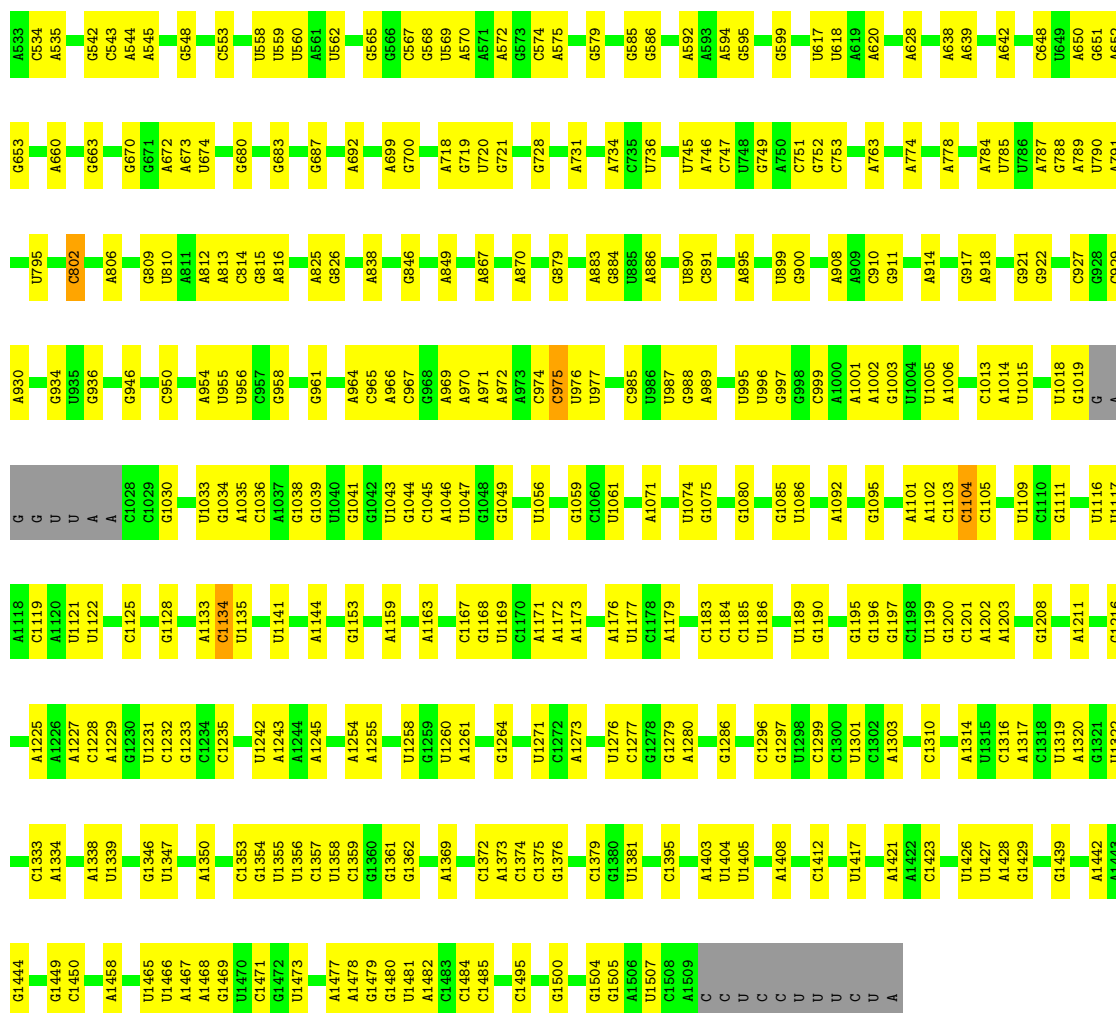


• Molecule 53: 5S ribosomal RNA



• Molecule 54: 16S ribosomal RNA





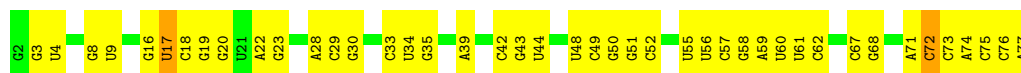
- Molecule 55: tRNA-Phe

Chain 6: 43% 54%



- Molecule 55: tRNA-Phe

Chain 8: 43% 54%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	627	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 ( $e^-/\text{\AA}^2$ )	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.988	Depositor
Minimum map value	-0.372	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	435.328, 435.328, 435.328	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7005, 1.7005, 1.7005	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0	0.34	0/383	0.54	0/504
2	1	0.23	0/484	0.44	0/637
3	2	0.22	0/306	0.45	0/401
4	9	0.27	0/5419	0.51	1/7307 (0.0%)
5	A	0.26	0/1954	0.47	0/2642
6	B	0.24	0/1721	0.45	0/2323
7	C	0.27	0/1691	0.46	0/2267
8	D	0.24	0/1188	0.47	0/1593
9	E	0.26	0/1384	0.51	1/1867 (0.1%)
10	F	0.25	0/1266	0.46	0/1700
11	G	0.26	0/1126	0.46	0/1517
12	H	0.25	0/1044	0.47	0/1395
13	I	0.24	0/820	0.47	0/1103
14	J	0.26	0/844	0.49	0/1136
15	K	0.31	0/1094	0.55	0/1468
16	L	0.23	0/962	0.46	0/1289
17	M	0.26	0/483	0.45	0/643
18	N	0.23	0/679	0.42	0/907
19	O	0.24	0/659	0.48	0/885
20	P	0.23	0/684	0.47	0/913
21	Q	0.31	0/545	0.61	0/730
22	R	0.26	0/698	0.52	0/936
23	S	0.24	0/631	0.41	0/838
24	T	0.30	0/475	0.45	0/621
25	W	0.27	0/538	0.58	1/722 (0.1%)
26	a	0.23	0/2267	0.47	0/3044
27	b	0.25	0/1795	0.50	0/2412
28	c	0.26	0/1671	0.50	0/2246
29	d	0.25	0/1409	0.48	0/1894
30	e	0.25	0/1420	0.50	0/1912
31	f	0.30	0/1183	0.54	0/1587
32	g	0.39	0/969	0.61	0/1295
33	h	0.26	0/968	0.50	0/1298
34	i	0.24	0/1186	0.45	0/1592

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	j	0.25	0/953	0.50	0/1275
36	k	0.24	0/1170	0.45	0/1559
37	l	0.29	0/1104	0.50	0/1481
38	m	0.24	0/973	0.47	0/1309
39	n	0.28	0/897	0.51	0/1198
40	o	0.29	0/948	0.53	0/1262
41	p	0.24	0/961	0.43	0/1278
42	q	0.26	0/828	0.54	0/1111
43	r	0.26	0/1077	0.47	0/1441
44	s	0.25	0/732	0.50	0/988
45	t	0.24	0/879	0.51	0/1165
46	u	0.25	0/665	0.44	0/884
47	v	0.23	0/519	0.48	0/695
48	w	0.23	0/826	0.43	0/1104
49	x	0.26	0/353	0.47	0/474
50	y	0.31	0/457	0.49	0/601
51	z	0.30	0/412	0.52	0/547
52	3	0.24	0/69073	0.88	75/107710 (0.1%)
53	4	0.23	0/2505	0.91	5/3902 (0.1%)
54	5	0.24	0/35768	0.87	25/55764 (0.0%)
55	6	0.31	0/1808	1.08	9/2817 (0.3%)
55	8	0.31	0/1808	1.08	9/2817 (0.3%)
All	All	0.25	0/164662	0.79	126/245006 (0.1%)

There are no bond length outliers.

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	3	131	C	N3-C2-O2	-10.59	114.48	121.90
52	3	1111	C	N3-C2-O2	-10.39	114.63	121.90
52	3	131	C	N1-C2-O2	9.73	124.74	118.90
52	3	1672	C	N3-C2-O2	-9.27	115.41	121.90
52	3	1111	C	N1-C2-O2	9.21	124.43	118.90
52	3	370	C	N3-C2-O2	-9.06	115.56	121.90
52	3	1207	U	C5-C4-O4	8.83	131.20	125.90
52	3	1997	C	N3-C2-O2	-8.63	115.86	121.90
52	3	1207	U	N3-C4-O4	-8.20	113.66	119.40
52	3	1359	C	N3-C2-O2	-8.15	116.19	121.90
53	4	47	C	N3-C2-O2	-7.95	116.33	121.90
54	5	1125	C	N1-C2-O2	7.76	123.56	118.90
54	5	1134	C	N1-C2-O2	7.76	123.56	118.90
54	5	1105	C	N3-C2-O2	-7.69	116.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	8	17	U	C2-N1-C1'	7.65	126.88	117.70
55	6	17	U	C2-N1-C1'	7.64	126.87	117.70
52	3	2199	C	N3-C2-O2	-7.56	116.61	121.90
54	5	338	C	N3-C2-O2	-7.55	116.61	121.90
54	5	802	C	N3-C2-O2	-7.50	116.65	121.90
55	6	72	C	N1-C2-O2	7.47	123.38	118.90
54	5	1183	C	N3-C2-O2	-7.46	116.68	121.90
55	8	72	C	N1-C2-O2	7.46	123.37	118.90
52	3	1110	C	N1-C2-O2	7.32	123.29	118.90
52	3	131	C	C6-N1-C2	-7.32	117.37	120.30
52	3	517	G	O4'-C1'-N9	7.23	113.98	108.20
52	3	772	C	N3-C2-O2	-7.22	116.84	121.90
52	3	115	U	C2-N1-C1'	7.21	126.36	117.70
52	3	14	U	C2-N1-C1'	7.21	126.35	117.70
52	3	1518	C	C2-N1-C1'	6.81	126.29	118.80
54	5	1134	C	N3-C2-O2	-6.69	117.22	121.90
52	3	2199	C	N1-C2-O2	6.62	122.87	118.90
52	3	2507	C	N1-C2-O2	6.62	122.87	118.90
54	5	1125	C	C2-N1-C1'	6.60	126.06	118.80
52	3	1518	C	N1-C2-O2	6.60	122.86	118.90
52	3	370	C	N1-C2-O2	6.59	122.86	118.90
55	6	72	C	C2-N1-C1'	6.59	126.05	118.80
55	8	72	C	C2-N1-C1'	6.59	126.05	118.80
54	5	1134	C	C2-N1-C1'	6.56	126.01	118.80
52	3	2564	C	C2-N1-C1'	6.41	125.85	118.80
54	5	534	C	N1-C2-O2	6.41	122.74	118.90
52	3	130	C	N1-C2-O2	6.36	122.72	118.90
9	E	163	MET	CA-CB-CG	6.34	124.08	113.30
52	3	370	C	C6-N1-C2	-6.31	117.77	120.30
25	W	71	LEU	CA-CB-CG	6.31	129.82	115.30
52	3	1672	C	N1-C2-O2	6.30	122.68	118.90
55	8	17	U	N1-C2-O2	6.27	127.19	122.80
52	3	2507	C	N3-C2-O2	-6.23	117.54	121.90
52	3	1507	G	O4'-C1'-N9	6.21	113.17	108.20
55	6	17	U	N1-C2-O2	6.20	127.14	122.80
52	3	1098	G	N1-C2-N2	-6.11	110.70	116.20
52	3	2070	C	N1-C2-O2	6.11	122.56	118.90
52	3	2564	C	N1-C2-O2	6.09	122.56	118.90
52	3	2070	C	C2-N1-C1'	6.02	125.42	118.80
54	5	975	C	C2-N1-C1'	6.00	125.40	118.80
52	3	27	U	N1-C2-O2	5.92	126.94	122.80
52	3	559	C	N3-C2-O2	-5.91	117.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	5	751	C	C2-N1-C1'	5.91	125.30	118.80
52	3	2272	C	N3-C2-O2	-5.90	117.77	121.90
52	3	394	C	N3-C2-O2	-5.88	117.78	121.90
53	4	32	G	C5-C6-O6	5.86	132.12	128.60
52	3	440	C	N1-C2-O2	5.85	122.41	118.90
54	5	1105	C	C6-N1-C2	-5.82	117.97	120.30
52	3	556	U	C2-N1-C1'	5.79	124.64	117.70
52	3	2272	C	C6-N1-C2	-5.78	117.99	120.30
54	5	1119	C	C2-N1-C1'	5.72	125.10	118.80
54	5	974	C	N1-C2-O2	5.72	122.33	118.90
55	6	29	C	C6-N1-C1'	5.69	127.63	120.80
55	8	29	C	C6-N1-C1'	5.66	127.59	120.80
52	3	1110	C	N3-C2-O2	-5.66	117.94	121.90
52	3	14	U	N3-C2-O2	-5.64	118.25	122.20
52	3	14	U	N1-C2-O2	5.63	126.74	122.80
54	5	1104	C	N1-C2-O2	5.61	122.27	118.90
52	3	200	A	O4'-C1'-N9	5.59	112.67	108.20
54	5	248	U	C2-N1-C1'	5.58	124.39	117.70
52	3	1027	U	C2-N1-C1'	5.56	124.37	117.70
52	3	1786	U	C2-N1-C1'	5.54	124.35	117.70
55	6	72	C	N3-C2-O2	-5.53	118.03	121.90
52	3	1010	G	O4'-C1'-N9	5.53	112.62	108.20
52	3	115	U	C6-N1-C1'	-5.52	113.47	121.20
52	3	1425	U	C2-N1-C1'	5.52	124.33	117.70
52	3	556	U	N1-C2-O2	5.50	126.65	122.80
52	3	2271	C	N1-C2-O2	5.49	122.20	118.90
55	8	72	C	N3-C2-O2	-5.49	118.06	121.90
52	3	1583	G	P-O3'-C3'	5.49	126.28	119.70
52	3	122	G	N3-C4-N9	5.48	129.29	126.00
52	3	1518	C	N3-C2-O2	-5.48	118.06	121.90
52	3	115	U	N1-C2-O2	5.47	126.63	122.80
52	3	1997	C	N1-C2-O2	5.47	122.18	118.90
52	3	1546	U	C2-N1-C1'	5.47	124.26	117.70
52	3	661	G	C5-C6-O6	-5.46	125.32	128.60
52	3	27	U	N3-C2-O2	-5.45	118.39	122.20
52	3	1839	C	N1-C2-O2	5.44	122.16	118.90
54	5	1125	C	N3-C2-O2	-5.43	118.10	121.90
52	3	1672	C	C6-N1-C2	-5.42	118.13	120.30
53	4	47	C	C6-N1-C1'	5.41	127.29	120.80
55	8	17	U	N3-C2-O2	-5.39	118.42	122.20
54	5	891	C	N1-C2-O2	5.39	122.14	118.90
52	3	1359	C	N1-C2-O2	5.36	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	5	974	C	C2-N1-C1'	5.35	124.68	118.80
55	6	4	U	C2-N1-C1'	5.34	124.11	117.70
55	8	4	U	C2-N1-C1'	5.34	124.11	117.70
55	6	17	U	N3-C2-O2	-5.33	118.47	122.20
52	3	123	G	N1-C2-N2	-5.28	111.45	116.20
55	8	17	U	C6-N1-C1'	-5.27	113.82	121.20
55	6	17	U	C6-N1-C1'	-5.25	113.85	121.20
52	3	119	A	O4'-C1'-N9	5.24	112.39	108.20
54	5	95	C	C2-N1-C1'	5.23	124.55	118.80
4	9	576	MET	CG-SD-CE	5.22	108.55	100.20
53	4	32	G	N1-C6-O6	-5.20	116.78	119.90
54	5	1125	C	C5-C6-N1	5.18	123.59	121.00
52	3	1098	G	N3-C2-N2	5.18	123.53	119.90
52	3	27	U	C2-N1-C1'	5.15	123.88	117.70
52	3	1837	C	C2-N1-C1'	5.14	124.45	118.80
52	3	440	C	N3-C2-O2	-5.12	118.32	121.90
52	3	1997	C	C6-N1-C2	-5.11	118.25	120.30
54	5	651	G	C4-N9-C1'	5.08	133.10	126.50
54	5	344	G	N1-C2-N2	-5.07	111.64	116.20
53	4	52	G	N1-C6-O6	-5.07	116.86	119.90
52	3	313	G	N3-C4-N9	5.07	129.04	126.00
52	3	1097	G	N3-C4-N9	5.07	129.04	126.00
54	5	344	G	N3-C2-N2	5.05	123.44	119.90
52	3	1425	U	N1-C2-O2	5.05	126.34	122.80
52	3	394	C	N1-C2-O2	5.02	121.91	118.90
52	3	2085	C	N1-C2-O2	5.01	121.91	118.90
52	3	515	A	P-O3'-C3'	5.01	125.71	119.70
52	3	440	C	C2-N1-C1'	5.00	124.30	118.80

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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	45/48 (94%)	45 (100%)	0	0	100	100
2	1	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
3	2	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
4	9	680/688 (99%)	620 (91%)	58 (8%)	2 (0%)	37	73
5	A	238/294 (81%)	221 (93%)	17 (7%)	0	100	100
6	B	213/273 (78%)	205 (96%)	8 (4%)	0	100	100
7	C	201/205 (98%)	185 (92%)	16 (8%)	0	100	100
8	D	151/219 (69%)	138 (91%)	13 (9%)	0	100	100
9	E	165/215 (77%)	139 (84%)	26 (16%)	0	100	100
10	F	152/155 (98%)	137 (90%)	15 (10%)	0	100	100
11	G	139/142 (98%)	124 (89%)	15 (11%)	0	100	100
12	H	126/132 (96%)	121 (96%)	5 (4%)	0	100	100
13	I	99/108 (92%)	93 (94%)	6 (6%)	0	100	100
14	J	112/121 (93%)	108 (96%)	4 (4%)	0	100	100
15	K	134/139 (96%)	109 (81%)	25 (19%)	0	100	100
16	L	116/124 (94%)	103 (89%)	13 (11%)	0	100	100
17	M	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
18	N	81/86 (94%)	78 (96%)	3 (4%)	0	100	100
19	O	78/94 (83%)	67 (86%)	11 (14%)	0	100	100
20	P	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
21	Q	63/104 (61%)	56 (89%)	7 (11%)	0	100	100
22	R	82/87 (94%)	63 (77%)	19 (23%)	0	100	100
23	S	75/87 (86%)	75 (100%)	0	0	100	100
24	T	51/60 (85%)	50 (98%)	1 (2%)	0	100	100
25	W	67/122 (55%)	61 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	a	283/287 (99%)	257 (91%)	26 (9%)	0	100	100
27	b	227/287 (79%)	199 (88%)	28 (12%)	0	100	100
28	c	208/212 (98%)	193 (93%)	15 (7%)	0	100	100
29	d	173/180 (96%)	154 (89%)	19 (11%)	0	100	100
30	e	174/184 (95%)	166 (95%)	8 (5%)	0	100	100
31	f	143/149 (96%)	133 (93%)	8 (6%)	2 (1%)	9	41
32	g	124/161 (77%)	109 (88%)	13 (10%)	2 (2%)	8	38
33	h	126/137 (92%)	113 (90%)	13 (10%)	0	100	100
34	i	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
35	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
36	k	146/151 (97%)	131 (90%)	15 (10%)	0	100	100
37	l	134/139 (96%)	127 (95%)	7 (5%)	0	100	100
38	m	117/124 (94%)	103 (88%)	14 (12%)	0	100	100
39	n	108/116 (93%)	99 (92%)	9 (8%)	0	100	100
40	o	113/119 (95%)	100 (88%)	13 (12%)	0	100	100
41	p	112/127 (88%)	106 (95%)	6 (5%)	0	100	100
42	q	97/100 (97%)	88 (91%)	8 (8%)	1 (1%)	13	49
43	r	137/159 (86%)	126 (92%)	11 (8%)	0	100	100
44	s	90/237 (38%)	86 (96%)	4 (4%)	0	100	100
45	t	109/111 (98%)	98 (90%)	11 (10%)	0	100	100
46	u	84/104 (81%)	79 (94%)	5 (6%)	0	100	100
47	v	61/65 (94%)	52 (85%)	9 (15%)	0	100	100
48	w	96/111 (86%)	84 (88%)	12 (12%)	0	100	100
49	x	42/97 (43%)	39 (93%)	3 (7%)	0	100	100
50	y	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
51	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	6567/7480 (88%)	6003 (91%)	557 (8%)	7 (0%)	50	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	9	406	ILE
4	9	572	ASP

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Mol	Chain	Res	Type
32	g	31	SER
31	f	18	VAL
32	g	116	ARG
31	f	19	VAL
42	q	48	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	40/41 (98%)	40 (100%)	0	100	100
2	1	51/51 (100%)	50 (98%)	1 (2%)	50	68
3	2	35/35 (100%)	35 (100%)	0	100	100
4	9	579/584 (99%)	575 (99%)	4 (1%)	81	87
5	A	212/262 (81%)	211 (100%)	1 (0%)	86	89
6	B	180/232 (78%)	180 (100%)	0	100	100
7	C	181/183 (99%)	180 (99%)	1 (1%)	84	88
8	D	123/178 (69%)	121 (98%)	2 (2%)	58	73
9	E	150/196 (76%)	148 (99%)	2 (1%)	65	77
10	F	131/132 (99%)	131 (100%)	0	100	100
11	G	123/124 (99%)	121 (98%)	2 (2%)	58	73
12	H	111/115 (96%)	110 (99%)	1 (1%)	75	83
13	I	95/99 (96%)	94 (99%)	1 (1%)	70	80
14	J	91/97 (94%)	91 (100%)	0	100	100
15	K	117/120 (98%)	111 (95%)	6 (5%)	20	41
16	L	100/105 (95%)	99 (99%)	1 (1%)	73	82
17	M	47/48 (98%)	46 (98%)	1 (2%)	48	66
18	N	76/78 (97%)	75 (99%)	1 (1%)	65	77
19	O	69/82 (84%)	69 (100%)	0	100	100
20	P	73/75 (97%)	70 (96%)	3 (4%)	26	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	Q	56/94 (60%)	55 (98%)	1 (2%)	54	71
22	R	74/77 (96%)	73 (99%)	1 (1%)	62	75
23	S	70/77 (91%)	69 (99%)	1 (1%)	62	75
24	T	49/56 (88%)	49 (100%)	0	100	100
25	W	58/98 (59%)	58 (100%)	0	100	100
26	a	241/243 (99%)	240 (100%)	1 (0%)	89	91
27	b	186/233 (80%)	184 (99%)	2 (1%)	70	80
28	c	182/184 (99%)	182 (100%)	0	100	100
29	d	150/154 (97%)	148 (99%)	2 (1%)	65	77
30	e	153/159 (96%)	153 (100%)	0	100	100
31	f	123/134 (92%)	122 (99%)	1 (1%)	79	85
32	g	101/129 (78%)	85 (84%)	16 (16%)	2	10
33	h	102/110 (93%)	100 (98%)	2 (2%)	50	68
34	i	126/128 (98%)	125 (99%)	1 (1%)	79	85
35	j	103/103 (100%)	102 (99%)	1 (1%)	73	82
36	k	123/126 (98%)	123 (100%)	0	100	100
37	l	113/115 (98%)	113 (100%)	0	100	100
38	m	105/109 (96%)	104 (99%)	1 (1%)	73	82
39	n	96/99 (97%)	96 (100%)	0	100	100
40	o	101/105 (96%)	101 (100%)	0	100	100
41	p	100/108 (93%)	99 (99%)	1 (1%)	73	82
42	q	90/91 (99%)	88 (98%)	2 (2%)	47	65
43	r	116/132 (88%)	115 (99%)	1 (1%)	75	83
44	s	82/208 (39%)	82 (100%)	0	100	100
45	t	96/96 (100%)	96 (100%)	0	100	100
46	u	69/85 (81%)	68 (99%)	1 (1%)	62	75
47	v	58/60 (97%)	58 (100%)	0	100	100
48	w	87/98 (89%)	86 (99%)	1 (1%)	70	80
49	x	41/86 (48%)	41 (100%)	0	100	100
50	y	48/49 (98%)	45 (94%)	3 (6%)	15	36
51	z	47/50 (94%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5730/6433 (89%)	5664 (99%)	66 (1%)	66	78

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	8	LYS
4	9	73	LYS
4	9	405	VAL
4	9	406	ILE
4	9	481	ARG
5	A	195	ARG
7	C	202	ARG
8	D	120	LYS
8	D	148	ARG
9	E	112	ARG
9	E	153	LYS
11	G	80	ARG
11	G	107	VAL
12	H	27	LYS
13	I	97	LYS
15	K	16	LYS
15	K	32	ASN
15	K	117	THR
15	K	118	VAL
15	K	121	GLU
15	K	122	LYS
16	L	46	LYS
17	M	41	ARG
18	N	70	ASN
20	P	6	ARG
20	P	67	ARG
20	P	83	ARG
21	Q	62	ARG
22	R	26	GLU
23	S	63	ASN
26	a	282	ARG
27	b	4	ARG
27	b	158	ARG
29	d	45	ARG
29	d	95	ARG
31	f	61	ASN
32	g	26	ILE

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Mol	Chain	Res	Type
32	g	27	PHE
32	g	28	ASP
32	g	29	TYR
32	g	31	SER
32	g	32	MET
32	g	42	LYS
32	g	44	LEU
32	g	45	PHE
32	g	46	LYS
32	g	47	ASN
32	g	88	GLU
32	g	89	ILE
32	g	90	VAL
32	g	113	PHE
32	g	115	ASN
33	h	37	LYS
33	h	102	LYS
34	i	15	ARG
35	j	78	LYS
38	m	69	ASN
41	p	50	ARG
42	q	24	LYS
42	q	37	LYS
43	r	60	ASN
46	u	58	ARG
48	w	61	ARG
50	y	47	MET
50	y	51	LEU
50	y	52	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	16	HIS
4	9	12	ASN
4	9	152	GLN
4	9	362	ASN
4	9	445	GLN
5	A	29	HIS
5	A	52	ASN
5	A	140	ASN
6	B	193	GLN

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Mol	Chain	Res	Type
7	C	115	GLN
7	C	118	ASN
8	D	202	GLN
9	E	22	ASN
9	E	25	GLN
9	E	110	GLN
10	F	83	ASN
11	G	23	ASN
11	G	58	GLN
11	G	109	ASN
12	H	33	ASN
12	H	62	ASN
15	K	32	ASN
16	L	76	ASN
18	N	70	ASN
20	P	18	ASN
22	R	23	ASN
22	R	52	HIS
23	S	63	ASN
26	a	269	ASN
27	b	35	GLN
29	d	161	ASN
32	g	10	GLN
32	g	47	ASN
33	h	47	GLN
34	i	74	ASN
36	k	36	GLN
38	m	117	GLN
39	n	88	ASN
39	n	99	HIS
41	p	90	ASN
42	q	11	GLN
42	q	76	GLN
43	r	34	ASN
46	u	43	GLN
48	w	35	HIS
50	y	4	GLN

### 5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	2875/2907 (98%)	1011 (35%)	30 (1%)
53	4	103/108 (95%)	41 (39%)	4 (3%)
54	5	1490/1520 (98%)	492 (33%)	10 (0%)
55	6	75/76 (98%)	40 (53%)	4 (5%)
55	8	75/76 (98%)	40 (53%)	4 (5%)
All	All	4618/4687 (98%)	1624 (35%)	52 (1%)

All (1624) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	12	A
52	3	14	U
52	3	15	A
52	3	28	G
52	3	29	G
52	3	36	U
52	3	37	G
52	3	38	G
52	3	44	A
52	3	48	G
52	3	52	U
52	3	53	G
52	3	54	A
52	3	56	G
52	3	61	U
52	3	65	A
52	3	73	A
52	3	75	A
52	3	76	A
52	3	77	G
52	3	82	G
52	3	86	A
52	3	87	G
52	3	90	G
52	3	91	G
52	3	93	A
52	3	98	C
52	3	101	C
52	3	102	A
52	3	103	G
52	3	114	U

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Mol	Chain	Res	Type
52	3	115	U
52	3	116	C
52	3	119	A
52	3	120	A
52	3	121	U
52	3	122	G
52	3	127	A
52	3	129	U
52	3	130	C
52	3	132	G
52	3	139	G
52	3	141	A
52	3	146	G
52	3	148	U
52	3	163	A
52	3	165	U
52	3	166	A
52	3	169	U
52	3	170	A
52	3	178	A
52	3	180	A
52	3	184	A
52	3	185	U
52	3	186	A
52	3	187	C
52	3	200	A
52	3	203	A
52	3	204	U
52	3	208	A
52	3	219	G
52	3	220	A
52	3	225	A
52	3	226	A
52	3	227	A
52	3	231	A
52	3	232	A
52	3	234	G
52	3	242	G
52	3	245	U
52	3	246	G
52	3	247	U
52	3	249	G

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Mol	Chain	Res	Type
52	3	252	G
52	3	254	G
52	3	260	A
52	3	266	A
52	3	267	A
52	3	270	G
52	3	271	G
52	3	272	C
52	3	276	A
52	3	282	C
52	3	285	U
52	3	286	A
52	3	289	U
52	3	290	A
52	3	291	G
52	3	295	U
52	3	296	U
52	3	297	G
52	3	298	U
52	3	299	A
52	3	309	A
52	3	310	U
52	3	312	U
52	3	314	G
52	3	315	A
52	3	316	C
52	3	318	U
52	3	325	G
52	3	328	A
52	3	333	A
52	3	336	C
52	3	339	U
52	3	345	A
52	3	347	C
52	3	351	G
52	3	355	A
52	3	357	A
52	3	363	G
52	3	364	A
52	3	365	U
52	3	366	A
52	3	367	G

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Mol	Chain	Res	Type
52	3	369	C
52	3	375	U
52	3	377	U
52	3	378	G
52	3	379	A
52	3	381	A
52	3	395	U
52	3	396	A
52	3	397	G
52	3	399	G
52	3	402	A
52	3	403	U
52	3	404	C
52	3	405	C
52	3	406	C
52	3	408	G
52	3	409	A
52	3	410	G
52	3	411	U
52	3	412	A
52	3	413	G
52	3	414	C
52	3	418	G
52	3	419	A
52	3	420	A
52	3	422	A
52	3	423	C
52	3	424	G
52	3	425	U
52	3	426	U
52	3	432	G
52	3	437	A
52	3	438	A
52	3	439	U
52	3	440	C
52	3	441	U
52	3	446	A
52	3	447	G
52	3	448	A
52	3	455	G
52	3	457	U
52	3	459	A

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Mol	Chain	Res	Type
52	3	460	G
52	3	466	A
52	3	467	U
52	3	472	A
52	3	479	A
52	3	483	A
52	3	485	A
52	3	486	G
52	3	487	C
52	3	490	A
52	3	491	A
52	3	493	A
52	3	494	G
52	3	495	U
52	3	500	U
52	3	501	G
52	3	506	A
52	3	509	G
52	3	515	A
52	3	516	A
52	3	517	G
52	3	527	A
52	3	531	G
52	3	532	A
52	3	539	U
52	3	540	A
52	3	542	A
52	3	543	U
52	3	544	U
52	3	545	C
52	3	551	C
52	3	553	A
52	3	560	U
52	3	562	C
52	3	565	C
52	3	566	G
52	3	567	U
52	3	580	U
52	3	582	A
52	3	584	G
52	3	589	A
52	3	591	G

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Mol	Chain	Res	Type
52	3	592	G
52	3	595	U
52	3	596	G
52	3	599	U
52	3	601	U
52	3	602	U
52	3	603	G
52	3	604	A
52	3	605	A
52	3	606	G
52	3	607	U
52	3	608	A
52	3	610	G
52	3	616	G
52	3	619	A
52	3	620	G
52	3	621	U
52	3	629	G
52	3	633	G
52	3	634	C
52	3	635	G
52	3	636	U
52	3	637	U
52	3	641	U
52	3	648	G
52	3	656	G
52	3	659	C
52	3	661	G
52	3	663	A
52	3	664	G
52	3	670	G
52	3	673	A
52	3	682	A
52	3	683	G
52	3	687	G
52	3	689	U
52	3	690	U
52	3	691	G
52	3	701	A
52	3	703	A
52	3	704	G
52	3	706	C

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Mol	Chain	Res	Type
52	3	707	C
52	3	709	G
52	3	712	A
52	3	721	G
52	3	725	G
52	3	730	G
52	3	737	U
52	3	739	G
52	3	740	A
52	3	750	A
52	3	751	A
52	3	752	C
52	3	760	G
52	3	761	G
52	3	762	A
52	3	764	G
52	3	765	A
52	3	766	C
52	3	774	A
52	3	775	C
52	3	780	G
52	3	782	U
52	3	783	G
52	3	787	C
52	3	792	G
52	3	797	U
52	3	799	A
52	3	809	A
52	3	810	G
52	3	811	G
52	3	817	A
52	3	818	A
52	3	819	U
52	3	823	A
52	3	824	A
52	3	827	G
52	3	828	A
52	3	829	A
52	3	832	C
52	3	840	G
52	3	841	C
52	3	844	G

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Mol	Chain	Res	Type
52	3	847	C
52	3	854	A
52	3	862	U
52	3	863	U
52	3	865	A
52	3	880	C
52	3	881	A
52	3	882	C
52	3	884	A
52	3	885	A
52	3	896	U
52	3	902	U
52	3	904	C
52	3	906	G
52	3	914	G
52	3	917	G
52	3	920	G
52	3	922	C
52	3	931	G
52	3	932	U
52	3	933	A
52	3	936	G
52	3	938	A
52	3	940	A
52	3	943	A
52	3	944	U
52	3	945	U
52	3	947	A
52	3	949	C
52	3	951	C
52	3	952	U
52	3	953	G
52	3	964	A
52	3	968	U
52	3	970	U
52	3	977	A
52	3	981	A
52	3	982	G
52	3	983	A
52	3	989	G
52	3	990	G
52	3	994	U

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Mol	Chain	Res	Type
52	3	995	A
52	3	997	G
52	3	998	C
52	3	1001	C
52	3	1008	A
52	3	1009	A
52	3	1010	G
52	3	1016	A
52	3	1019	A
52	3	1025	G
52	3	1026	A
52	3	1027	U
52	3	1031	U
52	3	1032	A
52	3	1039	G
52	3	1041	C
52	3	1046	A
52	3	1047	A
52	3	1048	A
52	3	1049	U
52	3	1055	A
52	3	1057	G
52	3	1058	U
52	3	1059	G
52	3	1061	A
52	3	1068	U
52	3	1069	G
52	3	1074	A
52	3	1075	G
52	3	1080	A
52	3	1081	A
52	3	1082	A
52	3	1088	A
52	3	1089	A
52	3	1094	G
52	3	1095	U
52	3	1096	U
52	3	1097	G
52	3	1099	C
52	3	1102	A
52	3	1103	G
52	3	1104	A

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Mol	Chain	Res	Type
52	3	1105	A
52	3	1106	G
52	3	1107	C
52	3	1109	G
52	3	1112	A
52	3	1113	U
52	3	1118	U
52	3	1119	A
52	3	1120	A
52	3	1122	G
52	3	1123	A
52	3	1124	G
52	3	1125	U
52	3	1126	G
52	3	1129	U
52	3	1131	A
52	3	1132	C
52	3	1144	C
52	3	1147	G
52	3	1149	G
52	3	1151	U
52	3	1162	A
52	3	1163	G
52	3	1165	U
52	3	1166	G
52	3	1167	U
52	3	1168	A
52	3	1170	C
52	3	1171	G
52	3	1176	U
52	3	1177	A
52	3	1178	A
52	3	1179	G
52	3	1186	A
52	3	1192	U
52	3	1193	U
52	3	1199	A
52	3	1200	U
52	3	1204	A
52	3	1208	A
52	3	1210	A
52	3	1212	C

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Mol	Chain	Res	Type
52	3	1213	U
52	3	1215	G
52	3	1216	U
52	3	1217	G
52	3	1226	G
52	3	1227	C
52	3	1234	U
52	3	1235	U
52	3	1236	G
52	3	1240	U
52	3	1241	U
52	3	1242	G
52	3	1246	U
52	3	1250	A
52	3	1251	G
52	3	1253	G
52	3	1254	U
52	3	1256	A
52	3	1257	G
52	3	1259	A
52	3	1265	G
52	3	1266	G
52	3	1267	A
52	3	1268	U
52	3	1272	A
52	3	1273	U
52	3	1274	A
52	3	1276	A
52	3	1278	G
52	3	1279	U
52	3	1280	G
52	3	1281	A
52	3	1283	A
52	3	1285	U
52	3	1286	G
52	3	1289	G
52	3	1297	U
52	3	1298	A
52	3	1299	A
52	3	1300	C
52	3	1301	G
52	3	1302	C

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Mol	Chain	Res	Type
52	3	1303	U
52	3	1316	U
52	3	1317	C
52	3	1325	C
52	3	1328	A
52	3	1329	U
52	3	1331	G
52	3	1338	G
52	3	1341	U
52	3	1342	C
52	3	1343	C
52	3	1347	A
52	3	1353	G
52	3	1355	C
52	3	1356	G
52	3	1358	C
52	3	1360	U
52	3	1361	U
52	3	1364	A
52	3	1366	G
52	3	1369	U
52	3	1370	A
52	3	1371	G
52	3	1373	C
52	3	1375	G
52	3	1378	C
52	3	1388	G
52	3	1393	A
52	3	1400	U
52	3	1404	C
52	3	1406	A
52	3	1407	U
52	3	1410	A
52	3	1413	A
52	3	1414	C
52	3	1415	A
52	3	1419	U
52	3	1421	A
52	3	1424	U
52	3	1425	U
52	3	1426	C
52	3	1428	U

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Mol	Chain	Res	Type
52	3	1430	U
52	3	1435	A
52	3	1437	A
52	3	1439	U
52	3	1444	C
52	3	1445	U
52	3	1447	A
52	3	1448	U
52	3	1449	G
52	3	1453	U
52	3	1456	C
52	3	1457	A
52	3	1466	U
52	3	1467	U
52	3	1478	U
52	3	1479	A
52	3	1480	A
52	3	1481	U
52	3	1483	G
52	3	1484	G
52	3	1486	U
52	3	1489	G
52	3	1494	U
52	3	1495	A
52	3	1502	A
52	3	1508	G
52	3	1514	U
52	3	1522	U
52	3	1523	C
52	3	1530	G
52	3	1532	A
52	3	1534	A
52	3	1535	A
52	3	1541	A
52	3	1542	G
52	3	1546	U
52	3	1548	A
52	3	1549	U
52	3	1571	G
52	3	1582	G
52	3	1584	U
52	3	1585	A

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Mol	Chain	Res	Type
52	3	1586	U
52	3	1587	U
52	3	1588	A
52	3	1589	A
52	3	1592	A
52	3	1594	G
52	3	1599	C
52	3	1600	A
52	3	1603	A
52	3	1615	G
52	3	1618	U
52	3	1619	A
52	3	1632	C
52	3	1633	C
52	3	1637	A
52	3	1640	G
52	3	1641	A
52	3	1642	G
52	3	1643	A
52	3	1644	A
52	3	1645	C
52	3	1648	A
52	3	1660	A
52	3	1661	A
52	3	1665	G
52	3	1670	U
52	3	1673	U
52	3	1674	A
52	3	1679	U
52	3	1680	A
52	3	1681	G
52	3	1682	C
52	3	1683	G
52	3	1686	U
52	3	1687	G
52	3	1694	A
52	3	1695	G
52	3	1702	A
52	3	1703	A
52	3	1706	C
52	3	1707	U
52	3	1708	G

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Mol	Chain	Res	Type
52	3	1709	C
52	3	1710	A
52	3	1714	U
52	3	1715	A
52	3	1716	A
52	3	1727	U
52	3	1728	A
52	3	1730	C
52	3	1732	A
52	3	1733	G
52	3	1734	A
52	3	1735	A
52	3	1741	G
52	3	1748	U
52	3	1749	A
52	3	1750	A
52	3	1751	A
52	3	1752	A
52	3	1753	G
52	3	1761	C
52	3	1762	A
52	3	1763	G
52	3	1764	U
52	3	1765	G
52	3	1766	A
52	3	1767	A
52	3	1769	A
52	3	1770	A
52	3	1771	C
52	3	1780	A
52	3	1781	C
52	3	1782	U
52	3	1786	U
52	3	1787	A
52	3	1788	A
52	3	1791	A
52	3	1806	G
52	3	1807	C
52	3	1808	C
52	3	1809	A
52	3	1811	A
52	3	1815	U

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Mol	Chain	Res	Type
52	3	1816	A
52	3	1821	G
52	3	1822	A
52	3	1823	U
52	3	1826	A
52	3	1828	A
52	3	1836	A
52	3	1842	G
52	3	1843	C
52	3	1855	A
52	3	1860	A
52	3	1864	A
52	3	1865	A
52	3	1866	G
52	3	1867	G
52	3	1871	U
52	3	1872	U
52	3	1873	A
52	3	1874	G
52	3	1885	G
52	3	1890	U
52	3	1891	A
52	3	1892	A
52	3	1896	A
52	3	1903	A
52	3	1906	G
52	3	1907	A
52	3	1910	G
52	3	1913	G
52	3	1914	G
52	3	1915	C
52	3	1919	A
52	3	1921	C
52	3	1927	C
52	3	1934	A
52	3	1936	G
52	3	1937	G
52	3	1938	U
52	3	1943	A
52	3	1944	A
52	3	1945	A
52	3	1946	U

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Mol	Chain	Res	Type
52	3	1951	A
52	3	1956	G
52	3	1958	U
52	3	1959	A
52	3	1961	A
52	3	1962	U
52	3	1963	U
52	3	1964	C
52	3	1966	G
52	3	1967	U
52	3	1970	C
52	3	1972	C
52	3	1973	U
52	3	1974	U
52	3	1976	A
52	3	1977	A
52	3	1979	G
52	3	1982	G
52	3	1993	U
52	3	1997	C
52	3	1998	U
52	3	1999	G
52	3	2000	U
52	3	2003	C
52	3	2004	G
52	3	2010	A
52	3	2012	A
52	3	2020	A
52	3	2027	G
52	3	2028	G
52	3	2030	A
52	3	2031	C
52	3	2038	A
52	3	2039	G
52	3	2040	A
52	3	2041	C
52	3	2043	C
52	3	2044	C
52	3	2050	G
52	3	2058	G
52	3	2059	G
52	3	2062	C

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Mol	Chain	Res	Type
52	3	2063	G
52	3	2066	A
52	3	2067	A
52	3	2068	G
52	3	2076	G
52	3	2084	A
52	3	2087	G
52	3	2090	G
52	3	2091	C
52	3	2098	U
52	3	2099	U
52	3	2100	G
52	3	2106	G
52	3	2107	A
52	3	2110	U
52	3	2111	U
52	3	2112	A
52	3	2115	A
52	3	2117	G
52	3	2123	A
52	3	2124	A
52	3	2125	U
52	3	2126	A
52	3	2127	G
52	3	2132	G
52	3	2133	A
52	3	2134	G
52	3	2137	A
52	3	2138	U
52	3	2139	C
52	3	2140	G
52	3	2141	A
52	3	2143	G
52	3	2145	A
52	3	2152	C
52	3	2155	G
52	3	2163	U
52	3	2170	A
52	3	2171	A
52	3	2174	G
52	3	2176	G
52	3	2178	A

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Mol	Chain	Res	Type
52	3	2180	U
52	3	2184	A
52	3	2187	C
52	3	2190	G
52	3	2193	U
52	3	2194	G
52	3	2195	U
52	3	2197	U
52	3	2199	C
52	3	2200	U
52	3	2202	U
52	3	2203	U
52	3	2204	C
52	3	2205	U
52	3	2206	A
52	3	2208	U
52	3	2211	G
52	3	2212	U
52	3	2219	U
52	3	2220	A
52	3	2221	U
52	3	2222	C
52	3	2223	C
52	3	2227	U
52	3	2229	C
52	3	2231	A
52	3	2233	A
52	3	2234	C
52	3	2246	G
52	3	2247	G
52	3	2251	U
52	3	2257	U
52	3	2260	G
52	3	2261	G
52	3	2262	C
52	3	2267	G
52	3	2274	A
52	3	2276	A
52	3	2278	G
52	3	2281	A
52	3	2283	C
52	3	2285	G

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Mol	Chain	Res	Type
52	3	2291	U
52	3	2293	C
52	3	2295	A
52	3	2300	A
52	3	2304	U
52	3	2305	C
52	3	2308	U
52	3	2311	G
52	3	2313	U
52	3	2315	G
52	3	2316	G
52	3	2317	A
52	3	2319	A
52	3	2320	U
52	3	2323	U
52	3	2327	U
52	3	2331	G
52	3	2333	G
52	3	2334	U
52	3	2341	G
52	3	2342	U
52	3	2343	A
52	3	2345	G
52	3	2348	U
52	3	2352	U
52	3	2353	G
52	3	2354	A
52	3	2355	C
52	3	2356	U
52	3	2358	U
52	3	2362	A
52	3	2369	G
52	3	2370	G
52	3	2380	U
52	3	2381	G
52	3	2385	A
52	3	2391	G
52	3	2393	C
52	3	2396	A
52	3	2397	G
52	3	2399	G
52	3	2401	U

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Mol	Chain	Res	Type
52	3	2410	C
52	3	2413	G
52	3	2414	U
52	3	2415	A
52	3	2416	U
52	3	2422	G
52	3	2423	G
52	3	2424	C
52	3	2433	A
52	3	2434	A
52	3	2435	C
52	3	2436	G
52	3	2437	G
52	3	2438	A
52	3	2439	U
52	3	2441	A
52	3	2442	A
52	3	2443	A
52	3	2449	U
52	3	2451	C
52	3	2453	G
52	3	2455	G
52	3	2457	U
52	3	2458	A
52	3	2461	A
52	3	2475	C
52	3	2477	A
52	3	2484	A
52	3	2486	A
52	3	2488	C
52	3	2490	A
52	3	2491	C
52	3	2492	G
52	3	2495	A
52	3	2497	U
52	3	2498	G
52	3	2499	U
52	3	2500	U
52	3	2502	G
52	3	2504	C
52	3	2507	C
52	3	2509	C

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Mol	Chain	Res	Type
52	3	2510	G
52	3	2512	U
52	3	2513	G
52	3	2518	C
52	3	2520	C
52	3	2521	A
52	3	2526	A
52	3	2527	U
52	3	2528	C
52	3	2530	U
52	3	2536	U
52	3	2538	A
52	3	2543	G
52	3	2549	A
52	3	2550	A
52	3	2555	U
52	3	2556	C
52	3	2557	G
52	3	2562	U
52	3	2563	U
52	3	2564	C
52	3	2565	G
52	3	2568	G
52	3	2569	A
52	3	2570	U
52	3	2571	U
52	3	2574	A
52	3	2575	G
52	3	2577	G
52	3	2580	A
52	3	2584	G
52	3	2593	U
52	3	2594	C
52	3	2596	A
52	3	2599	C
52	3	2604	U
52	3	2605	G
52	3	2610	A
52	3	2616	G
52	3	2617	U
52	3	2618	C
52	3	2619	C

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Mol	Chain	Res	Type
52	3	2621	U
52	3	2623	U
52	3	2626	A
52	3	2629	G
52	3	2631	G
52	3	2633	C
52	3	2636	U
52	3	2637	A
52	3	2642	G
52	3	2643	A
52	3	2647	A
52	3	2649	G
52	3	2651	G
52	3	2653	G
52	3	2654	U
52	3	2662	A
52	3	2668	A
52	3	2669	G
52	3	2673	A
52	3	2674	C
52	3	2677	A
52	3	2681	G
52	3	2690	U
52	3	2697	C
52	3	2702	G
52	3	2710	G
52	3	2711	C
52	3	2721	C
52	3	2722	G
52	3	2726	G
52	3	2732	A
52	3	2734	C
52	3	2737	G
52	3	2741	A
52	3	2747	U
52	3	2752	G
52	3	2756	A
52	3	2760	C
52	3	2764	U
52	3	2765	A
52	3	2766	A
52	3	2768	U

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Mol	Chain	Res	Type
52	3	2769	G
52	3	2772	A
52	3	2774	A
52	3	2775	C
52	3	2777	A
52	3	2780	U
52	3	2786	A
52	3	2788	U
52	3	2789	A
52	3	2793	U
52	3	2799	U
52	3	2800	U
52	3	2801	U
52	3	2803	G
52	3	2804	C
52	3	2805	A
52	3	2806	A
52	3	2808	A
52	3	2809	A
52	3	2813	A
52	3	2814	A
52	3	2822	C
52	3	2823	A
52	3	2824	A
52	3	2825	A
52	3	2826	G
52	3	2828	C
52	3	2835	G
52	3	2836	U
52	3	2837	U
52	3	2838	G
52	3	2839	A
52	3	2845	U
52	3	2847	C
52	3	2848	A
52	3	2850	G
52	3	2853	U
52	3	2854	A
52	3	2859	U
52	3	2862	U
52	3	2863	G
52	3	2865	U

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Mol	Chain	Res	Type
52	3	2870	U
52	3	2871	G
52	3	2874	C
52	3	2876	G
52	3	2881	A
52	3	2883	A
52	3	2884	C
52	3	2888	U
52	3	2889	U
52	3	2890	G
52	3	2896	G
52	3	2897	G
52	3	2898	A
52	3	2899	C
53	4	4	G
53	4	9	C
53	4	11	A
53	4	12	U
53	4	13	G
53	4	14	U
53	4	19	G
53	4	22	G
53	4	23	A
53	4	25	A
53	4	27	A
53	4	28	C
53	4	31	G
53	4	33	U
53	4	39	U
53	4	40	U
53	4	41	C
53	4	42	G
53	4	43	A
53	4	47	C
53	4	48	A
53	4	50	C
53	4	54	U
53	4	55	A
53	4	60	C
53	4	64	G
53	4	65	G
53	4	69	C

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Mol	Chain	Res	Type
53	4	71	A
53	4	72	A
53	4	75	U
53	4	77	G
53	4	78	C
53	4	79	U
53	4	80	G
53	4	88	G
53	4	89	A
53	4	99	A
53	4	102	A
53	4	106	A
53	4	108	C
54	5	7	U
54	5	8	G
54	5	10	G
54	5	15	U
54	5	23	G
54	5	28	G
54	5	29	G
54	5	33	A
54	5	38	U
54	5	40	G
54	5	48	C
54	5	49	C
54	5	50	U
54	5	51	A
54	5	52	A
54	5	53	U
54	5	55	C
54	5	61	A
54	5	64	C
54	5	66	A
54	5	72	A
54	5	75	A
54	5	81	A
54	5	93	A
54	5	94	A
54	5	95	C
54	5	105	A
54	5	106	C
54	5	107	A

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Mol	Chain	Res	Type
54	5	112	U
54	5	114	C
54	5	115	A
54	5	116	A
54	5	117	U
54	5	120	A
54	5	124	U
54	5	127	A
54	5	128	A
54	5	129	U
54	5	130	G
54	5	132	G
54	5	135	A
54	5	137	A
54	5	145	G
54	5	149	G
54	5	154	G
54	5	155	C
54	5	160	A
54	5	167	A
54	5	173	U
54	5	186	A
54	5	196	G
54	5	197	A
54	5	198	A
54	5	201	G
54	5	204	C
54	5	222	U
54	5	223	G
54	5	229	G
54	5	232	G
54	5	240	U
54	5	241	C
54	5	243	G
54	5	247	G
54	5	248	U
54	5	249	U
54	5	250	G
54	5	258	A
54	5	262	G
54	5	263	C
54	5	264	C

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Mol	Chain	Res	Type
54	5	275	A
54	5	276	U
54	5	281	U
54	5	285	G
54	5	286	C
54	5	290	G
54	5	296	A
54	5	297	A
54	5	300	A
54	5	302	A
54	5	303	A
54	5	305	A
54	5	311	A
54	5	312	A
54	5	313	U
54	5	315	G
54	5	318	C
54	5	324	C
54	5	326	C
54	5	328	G
54	5	341	C
54	5	344	G
54	5	348	C
54	5	349	A
54	5	350	G
54	5	352	A
54	5	359	A
54	5	362	U
54	5	363	U
54	5	364	U
54	5	368	C
54	5	370	A
54	5	374	G
54	5	376	G
54	5	377	A
54	5	379	A
54	5	380	G
54	5	381	C
54	5	382	U
54	5	384	G
54	5	385	A
54	5	388	G

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Mol	Chain	Res	Type
54	5	392	A
54	5	393	A
54	5	394	U
54	5	402	G
54	5	403	A
54	5	408	U
54	5	409	G
54	5	410	A
54	5	411	A
54	5	414	U
54	5	417	U
54	5	418	U
54	5	419	A
54	5	420	A
54	5	422	A
54	5	425	G
54	5	426	U
54	5	430	G
54	5	432	U
54	5	435	U
54	5	436	U
54	5	438	A
54	5	440	U
54	5	445	A
54	5	448	A
54	5	449	A
54	5	450	U
54	5	452	A
54	5	453	C
54	5	455	U
54	5	456	U
54	5	457	A
54	5	461	G
54	5	464	A
54	5	465	A
54	5	469	C
54	5	473	A
54	5	476	U
54	5	478	G
54	5	479	A
54	5	480	C
54	5	481	U

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Mol	Chain	Res	Type
54	5	482	G
54	5	483	U
54	5	488	U
54	5	489	U
54	5	490	U
54	5	493	A
54	5	494	A
54	5	495	U
54	5	496	A
54	5	497	A
54	5	500	G
54	5	502	C
54	5	503	G
54	5	507	A
54	5	509	C
54	5	510	U
54	5	514	U
54	5	515	G
54	5	516	C
54	5	517	C
54	5	519	G
54	5	525	G
54	5	527	G
54	5	530	A
54	5	531	A
54	5	532	U
54	5	535	A
54	5	542	G
54	5	543	C
54	5	544	A
54	5	545	A
54	5	548	G
54	5	553	C
54	5	558	U
54	5	559	U
54	5	560	U
54	5	562	U
54	5	565	G
54	5	567	C
54	5	568	G
54	5	569	U
54	5	570	A

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Mol	Chain	Res	Type
54	5	572	A
54	5	574	C
54	5	575	A
54	5	579	G
54	5	585	G
54	5	586	G
54	5	592	A
54	5	594	A
54	5	595	G
54	5	599	G
54	5	617	U
54	5	618	U
54	5	620	A
54	5	628	A
54	5	638	A
54	5	639	A
54	5	642	A
54	5	648	C
54	5	650	A
54	5	652	A
54	5	653	G
54	5	660	A
54	5	663	G
54	5	670	G
54	5	672	A
54	5	673	A
54	5	674	U
54	5	680	G
54	5	683	G
54	5	687	G
54	5	692	A
54	5	699	A
54	5	700	G
54	5	718	A
54	5	719	G
54	5	720	U
54	5	721	G
54	5	728	G
54	5	731	A
54	5	734	A
54	5	736	U
54	5	745	U

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Mol	Chain	Res	Type
54	5	746	A
54	5	747	C
54	5	749	G
54	5	752	G
54	5	753	C
54	5	763	A
54	5	774	A
54	5	778	A
54	5	784	A
54	5	785	U
54	5	787	A
54	5	788	G
54	5	789	A
54	5	790	U
54	5	791	A
54	5	795	U
54	5	802	C
54	5	806	A
54	5	809	G
54	5	810	U
54	5	812	A
54	5	813	A
54	5	814	C
54	5	815	G
54	5	816	A
54	5	825	A
54	5	826	G
54	5	838	A
54	5	846	G
54	5	849	A
54	5	867	A
54	5	870	A
54	5	879	G
54	5	884	G
54	5	886	A
54	5	890	U
54	5	895	A
54	5	900	G
54	5	908	A
54	5	910	C
54	5	911	G
54	5	914	A

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Mol	Chain	Res	Type
54	5	917	G
54	5	918	A
54	5	921	G
54	5	922	G
54	5	927	C
54	5	929	C
54	5	930	A
54	5	934	G
54	5	936	G
54	5	946	G
54	5	950	C
54	5	954	A
54	5	955	U
54	5	956	U
54	5	958	G
54	5	961	G
54	5	964	A
54	5	965	C
54	5	966	A
54	5	967	C
54	5	969	A
54	5	970	A
54	5	971	A
54	5	972	A
54	5	976	U
54	5	977	U
54	5	985	C
54	5	987	U
54	5	988	G
54	5	989	A
54	5	995	U
54	5	996	U
54	5	997	G
54	5	999	C
54	5	1001	A
54	5	1002	A
54	5	1003	G
54	5	1005	U
54	5	1006	A
54	5	1013	C
54	5	1014	A
54	5	1015	U

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Mol	Chain	Res	Type
54	5	1018	U
54	5	1019	G
54	5	1030	G
54	5	1033	U
54	5	1034	G
54	5	1035	A
54	5	1036	C
54	5	1038	G
54	5	1039	G
54	5	1041	G
54	5	1043	U
54	5	1044	G
54	5	1045	C
54	5	1046	A
54	5	1047	U
54	5	1049	G
54	5	1056	U
54	5	1059	G
54	5	1061	U
54	5	1071	A
54	5	1074	U
54	5	1075	G
54	5	1080	G
54	5	1085	G
54	5	1086	U
54	5	1092	A
54	5	1095	G
54	5	1101	A
54	5	1102	A
54	5	1103	C
54	5	1104	C
54	5	1109	U
54	5	1111	G
54	5	1116	U
54	5	1117	U
54	5	1121	U
54	5	1122	U
54	5	1128	G
54	5	1134	C
54	5	1135	U
54	5	1141	U
54	5	1144	A

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Mol	Chain	Res	Type
54	5	1153	G
54	5	1159	A
54	5	1163	A
54	5	1167	C
54	5	1168	G
54	5	1169	U
54	5	1171	A
54	5	1172	A
54	5	1173	A
54	5	1176	A
54	5	1177	U
54	5	1179	A
54	5	1184	C
54	5	1185	C
54	5	1186	U
54	5	1189	U
54	5	1190	G
54	5	1195	G
54	5	1196	G
54	5	1197	G
54	5	1199	U
54	5	1200	G
54	5	1201	C
54	5	1202	A
54	5	1203	A
54	5	1208	G
54	5	1211	A
54	5	1216	G
54	5	1225	A
54	5	1227	A
54	5	1228	C
54	5	1229	A
54	5	1231	U
54	5	1232	C
54	5	1233	G
54	5	1235	C
54	5	1242	U
54	5	1243	A
54	5	1245	A
54	5	1254	A
54	5	1255	A
54	5	1258	U

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Mol	Chain	Res	Type
54	5	1260	U
54	5	1261	A
54	5	1264	G
54	5	1271	U
54	5	1273	A
54	5	1276	U
54	5	1277	C
54	5	1279	G
54	5	1280	A
54	5	1286	G
54	5	1296	C
54	5	1297	G
54	5	1299	C
54	5	1301	U
54	5	1303	A
54	5	1310	C
54	5	1314	A
54	5	1316	C
54	5	1317	A
54	5	1319	U
54	5	1320	A
54	5	1322	U
54	5	1333	C
54	5	1334	A
54	5	1338	A
54	5	1339	U
54	5	1346	G
54	5	1347	U
54	5	1350	A
54	5	1353	C
54	5	1354	G
54	5	1355	U
54	5	1356	U
54	5	1357	C
54	5	1358	U
54	5	1359	C
54	5	1361	G
54	5	1362	G
54	5	1369	A
54	5	1372	C
54	5	1373	A
54	5	1374	C

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Mol	Chain	Res	Type
54	5	1375	C
54	5	1376	G
54	5	1379	C
54	5	1381	U
54	5	1395	C
54	5	1403	A
54	5	1404	U
54	5	1405	U
54	5	1408	A
54	5	1412	C
54	5	1417	U
54	5	1421	A
54	5	1423	C
54	5	1426	U
54	5	1427	U
54	5	1428	A
54	5	1429	G
54	5	1439	G
54	5	1442	A
54	5	1444	G
54	5	1449	G
54	5	1450	C
54	5	1458	A
54	5	1465	U
54	5	1466	U
54	5	1467	A
54	5	1468	A
54	5	1469	G
54	5	1471	C
54	5	1473	U
54	5	1477	A
54	5	1478	A
54	5	1479	G
54	5	1480	G
54	5	1481	U
54	5	1482	A
54	5	1484	C
54	5	1485	C
54	5	1495	C
54	5	1500	G
54	5	1504	G
54	5	1505	G

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Mol	Chain	Res	Type
54	5	1507	U
55	6	3	G
55	6	8	G
55	6	9	U
55	6	17	U
55	6	18	C
55	6	19	G
55	6	20	G
55	6	22	A
55	6	23	G
55	6	28	A
55	6	30	G
55	6	33	C
55	6	34	U
55	6	35	G
55	6	39	A
55	6	42	C
55	6	43	G
55	6	44	U
55	6	48	U
55	6	49	C
55	6	50	G
55	6	51	G
55	6	52	C
55	6	55	U
55	6	56	U
55	6	57	C
55	6	58	G
55	6	59	A
55	6	60	U
55	6	61	U
55	6	62	C
55	6	67	C
55	6	68	G
55	6	71	A
55	6	72	C
55	6	73	C
55	6	74	A
55	6	75	C
55	6	76	C
55	6	77	A
55	8	3	G

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Mol	Chain	Res	Type
55	8	8	G
55	8	9	U
55	8	17	U
55	8	18	C
55	8	19	G
55	8	20	G
55	8	22	A
55	8	23	G
55	8	28	A
55	8	30	G
55	8	33	C
55	8	34	U
55	8	35	G
55	8	39	A
55	8	42	C
55	8	43	G
55	8	44	U
55	8	48	U
55	8	49	C
55	8	50	G
55	8	51	G
55	8	52	C
55	8	55	U
55	8	56	U
55	8	57	C
55	8	58	G
55	8	59	A
55	8	60	U
55	8	61	U
55	8	62	C
55	8	67	C
55	8	68	G
55	8	71	A
55	8	72	C
55	8	73	C
55	8	74	A
55	8	75	C
55	8	76	C
55	8	77	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	3	315	A
52	3	403	U
52	3	410	G
52	3	425	U
52	3	437	A
52	3	500	U
52	3	602	U
52	3	750	A
52	3	881	A
52	3	901	C
52	3	1048	A
52	3	1124	G
52	3	1209	U
52	3	1297	U
52	3	1355	C
52	3	1507	G
52	3	1583	G
52	3	1587	U
52	3	1588	A
52	3	1820	U
52	3	1872	U
52	3	2140	G
52	3	2282	A
52	3	2333	G
52	3	2342	U
52	3	2506	C
52	3	2604	U
52	3	2668	A
52	3	2721	C
52	3	2897	G
53	4	32	G
53	4	54	U
53	4	59	A
53	4	70	G
54	5	159	U
54	5	166	U
54	5	482	G
54	5	883	A
54	5	899	U
54	5	921	G
54	5	975	C
54	5	1133	A
54	5	1338	A

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Mol	Chain	Res	Type
54	5	1468	A
55	6	16	G
55	6	18	C
55	6	56	U
55	6	58	G
55	8	16	G
55	8	18	C
55	8	56	U
55	8	58	G

## 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-13449. These allow visual inspection of the internal detail of the map and identification of artifacts.

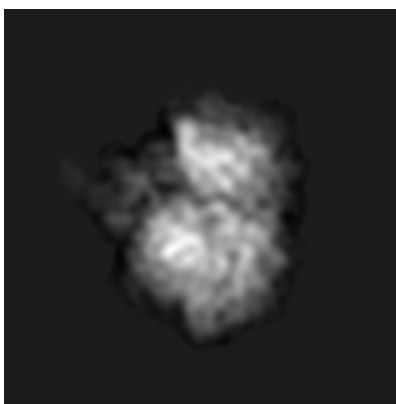
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

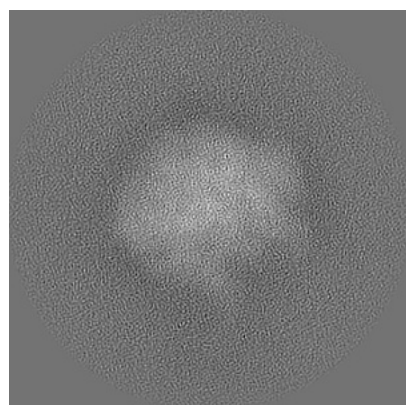


Y

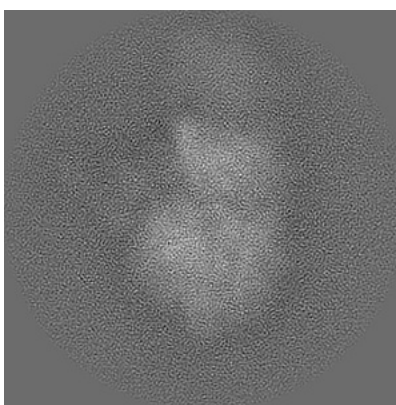


Z

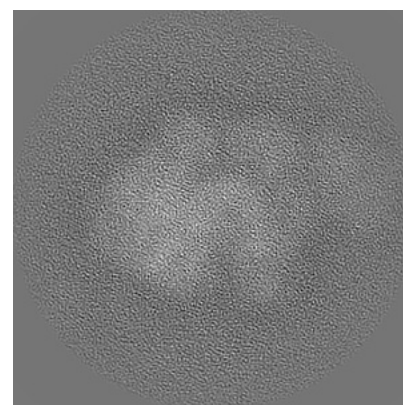
#### 6.1.2 Raw map



X



Y

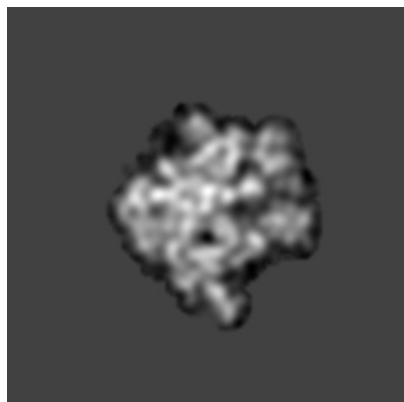


Z

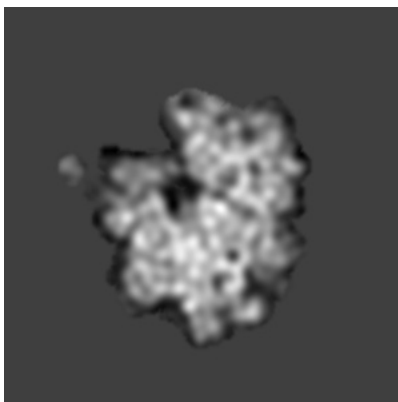
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

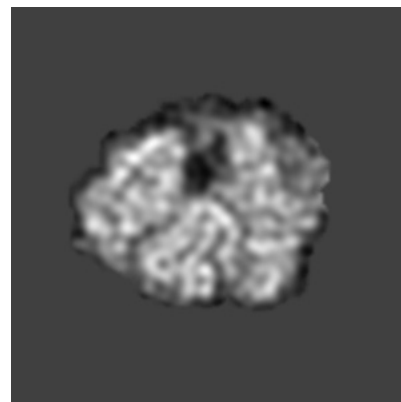
### 6.2.1 Primary map



X Index: 128

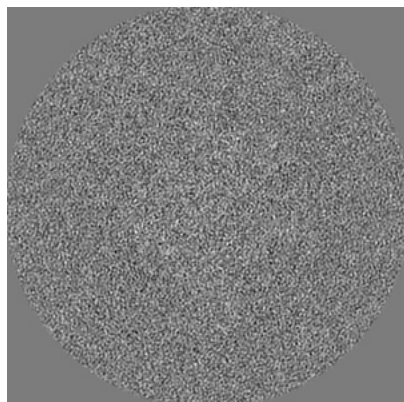


Y Index: 128

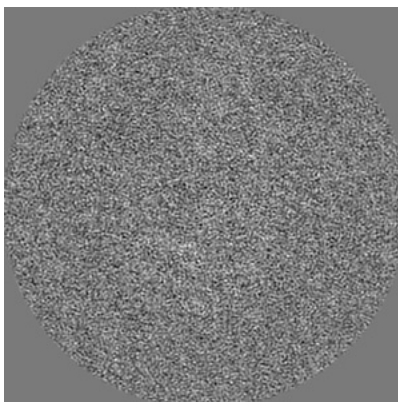


Z Index: 128

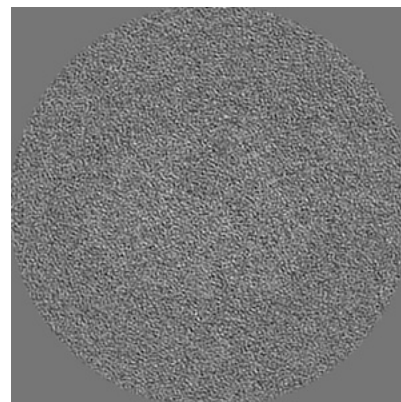
### 6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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

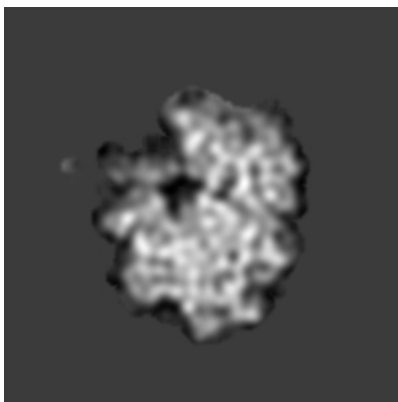


## 6.3 Largest variance slices [i](#)

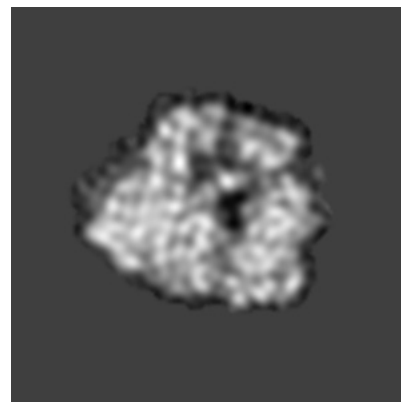
### 6.3.1 Primary map



X Index: 102

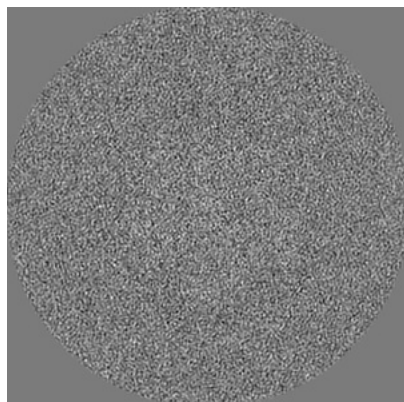


Y Index: 125

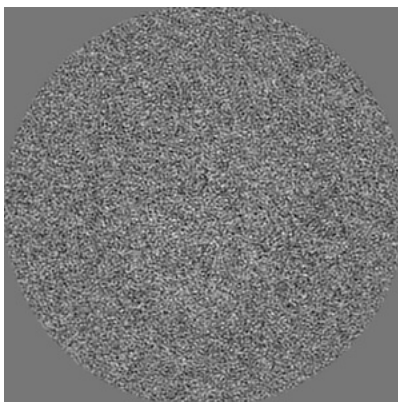


Z Index: 119

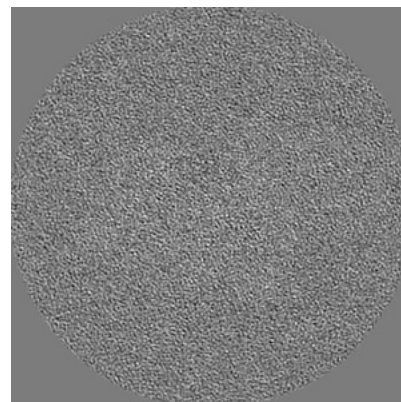
### 6.3.2 Raw map



X Index: 118



Y Index: 118



Z Index: 130

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

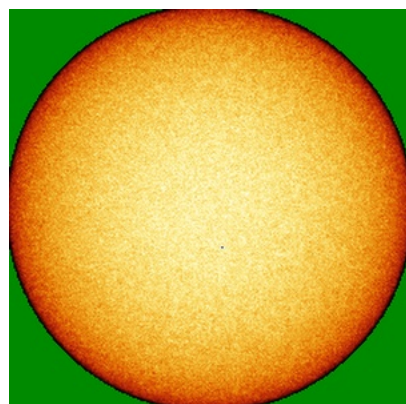


Y

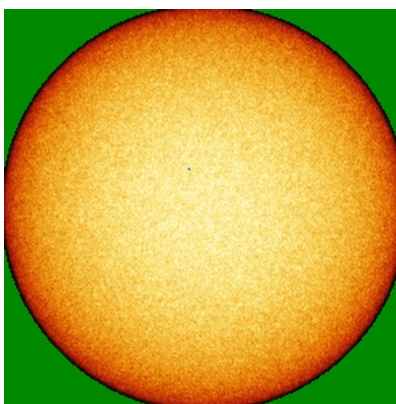


Z

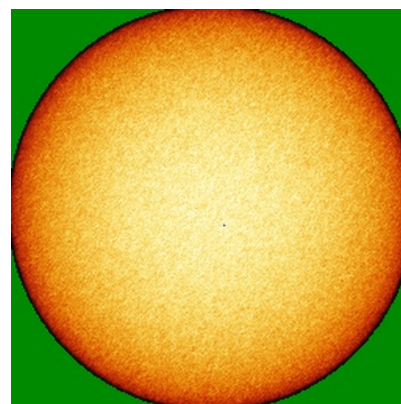
### 6.4.2 Raw map



X



Y

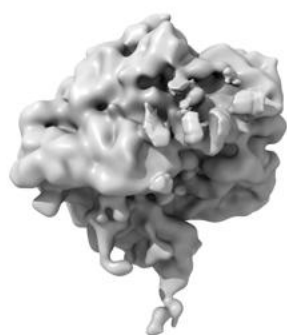


Z

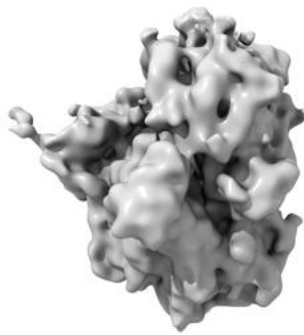
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

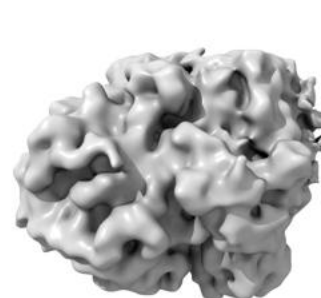
### 6.5.1 Primary map



X



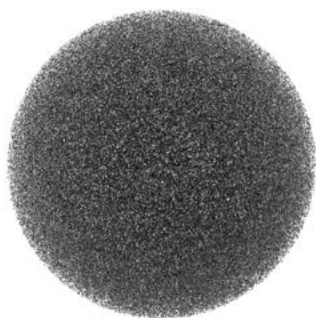
Y



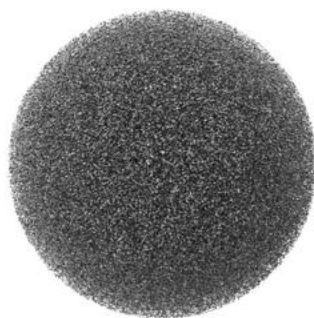
Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

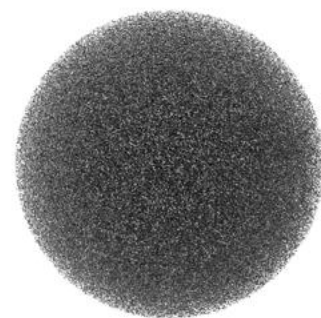
### 6.5.2 Raw map



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.

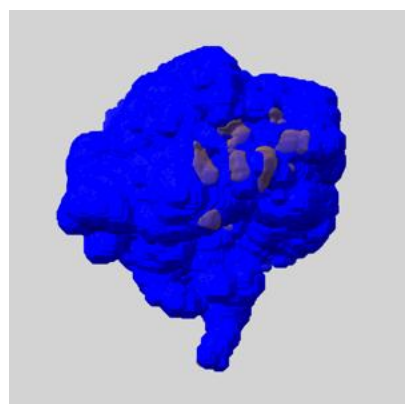
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

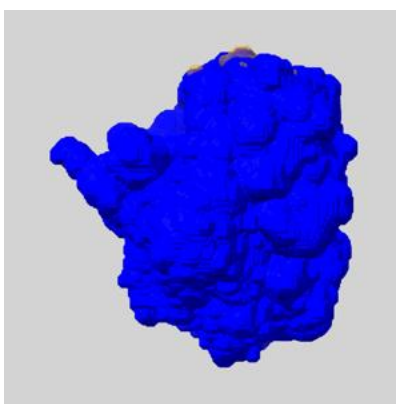
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

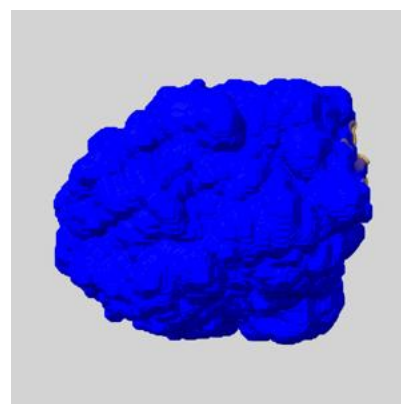
### 6.6.1 emd\_13449\_msk\_1.map [i](#)



X



Y

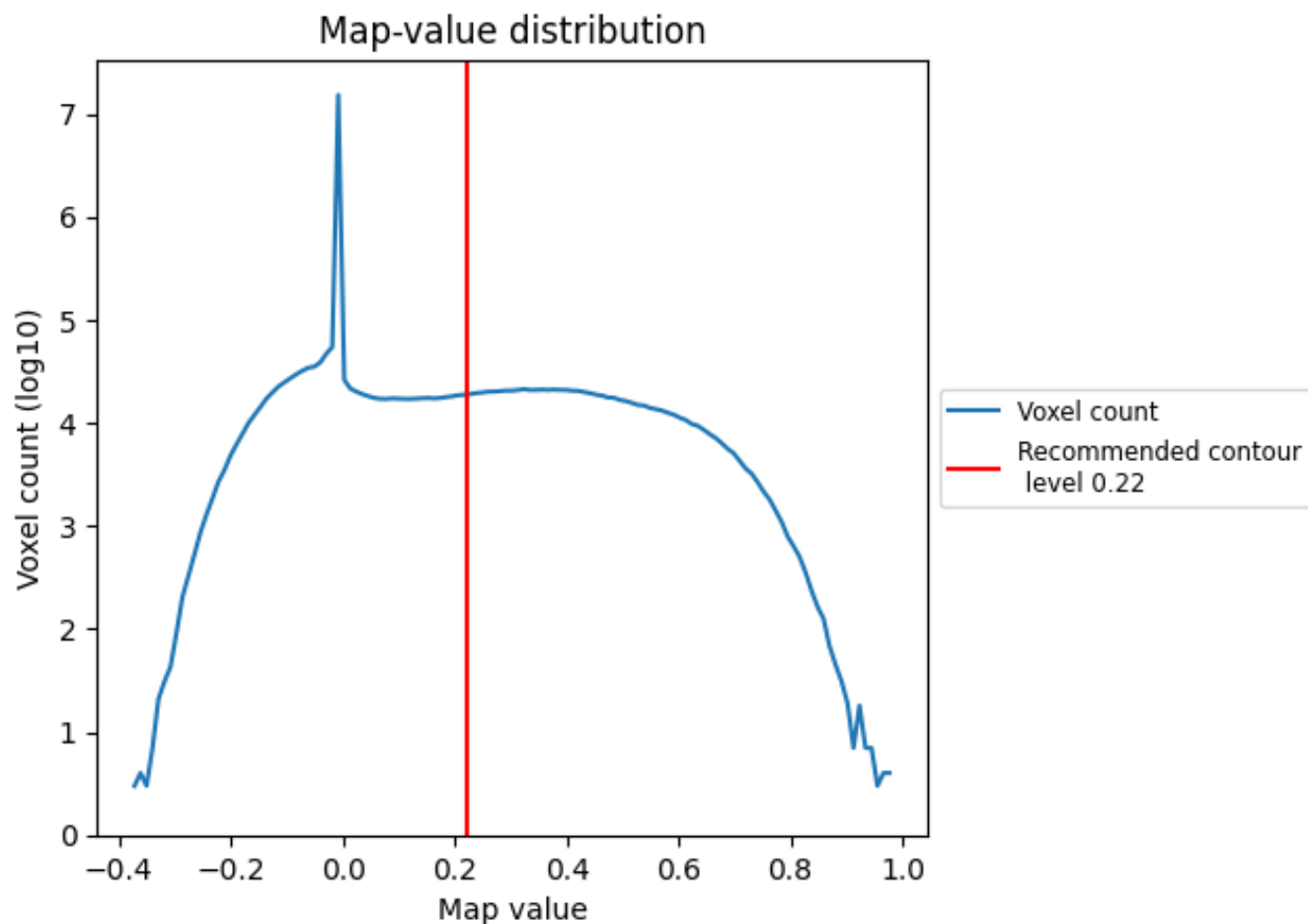


Z

## 7 Map analysis [i](#)

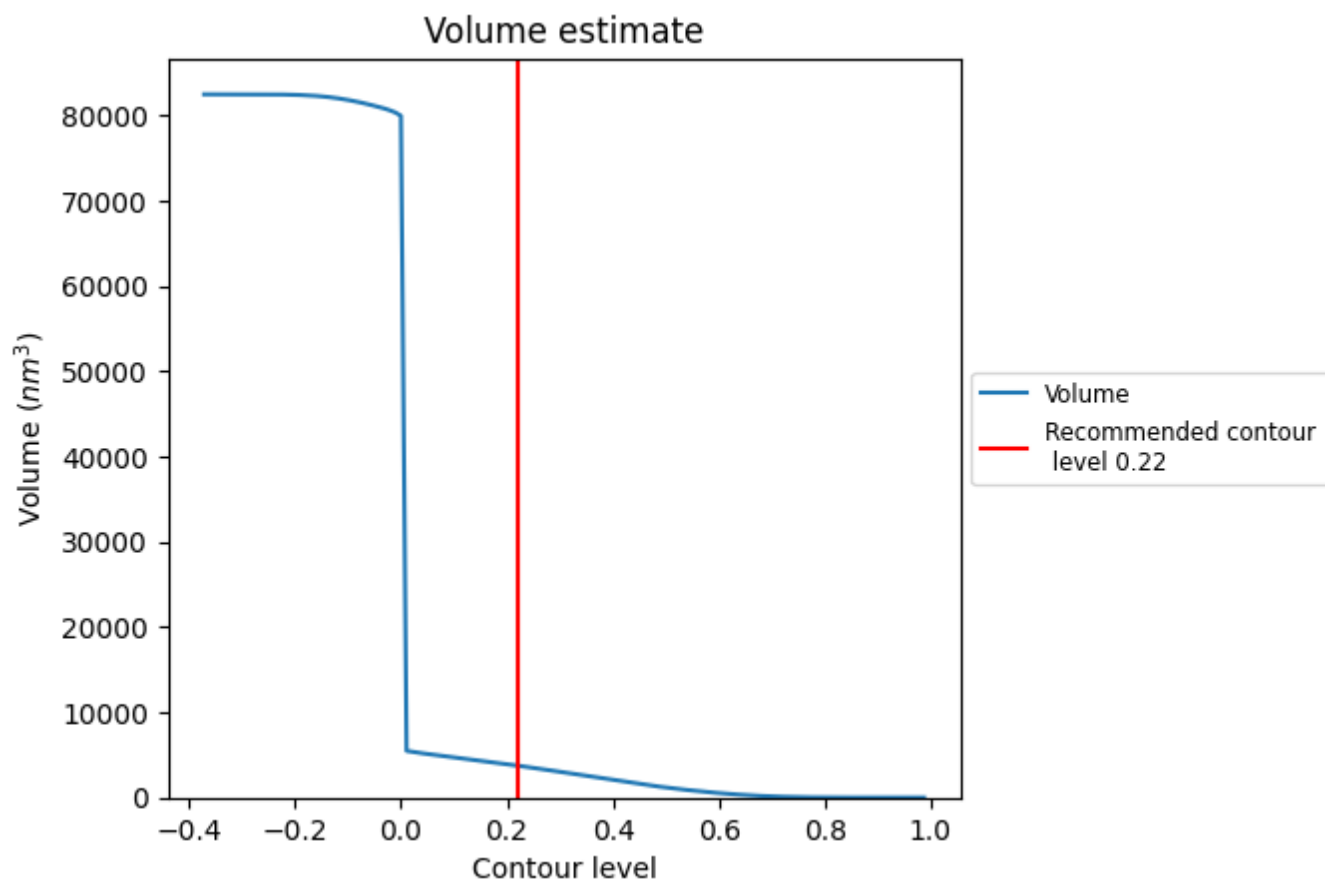
This section contains the results of statistical analysis of the map.

### 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.

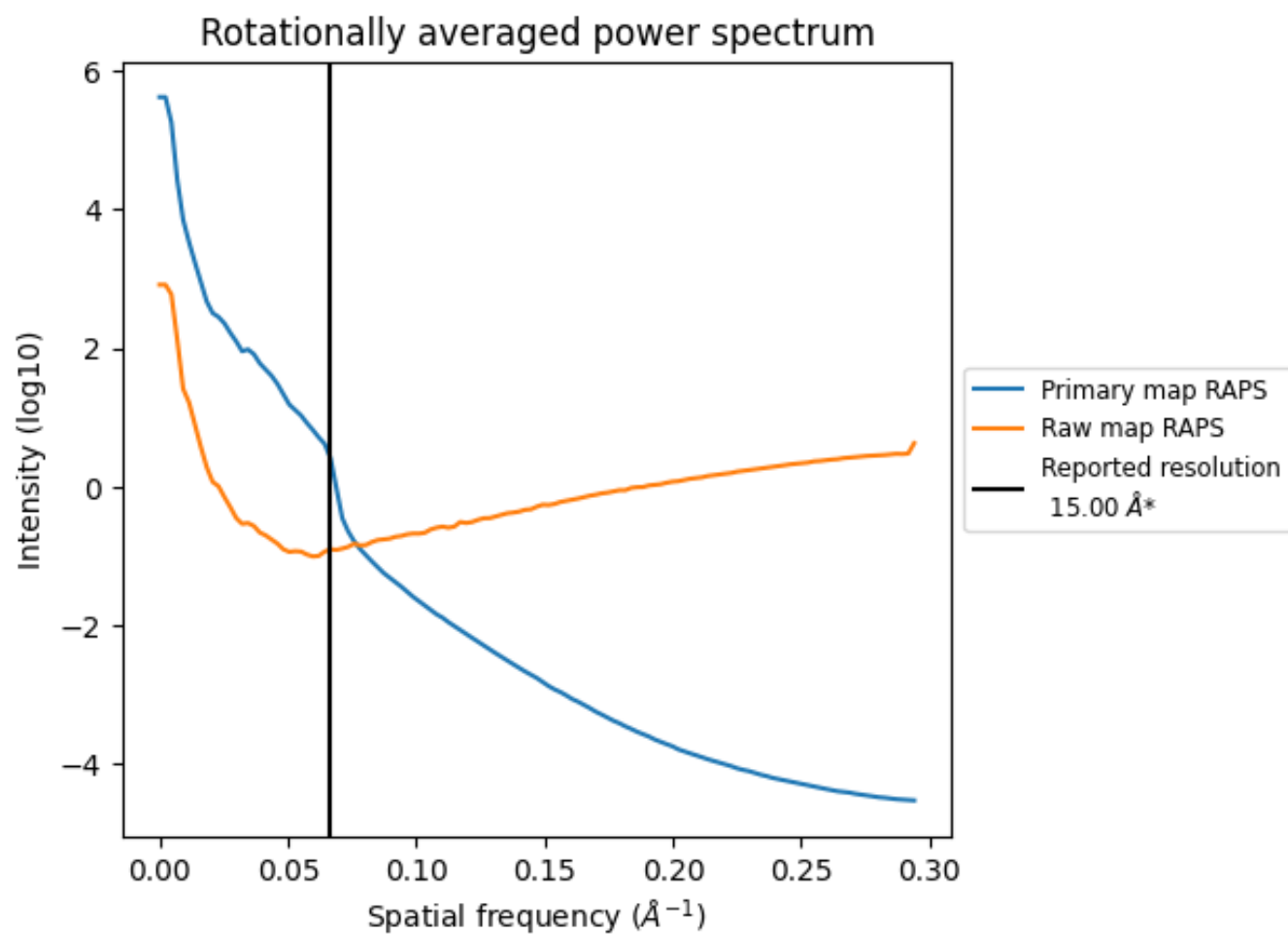
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3746 nm<sup>3</sup>; this corresponds to an approximate mass of 3384 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 ⓘ



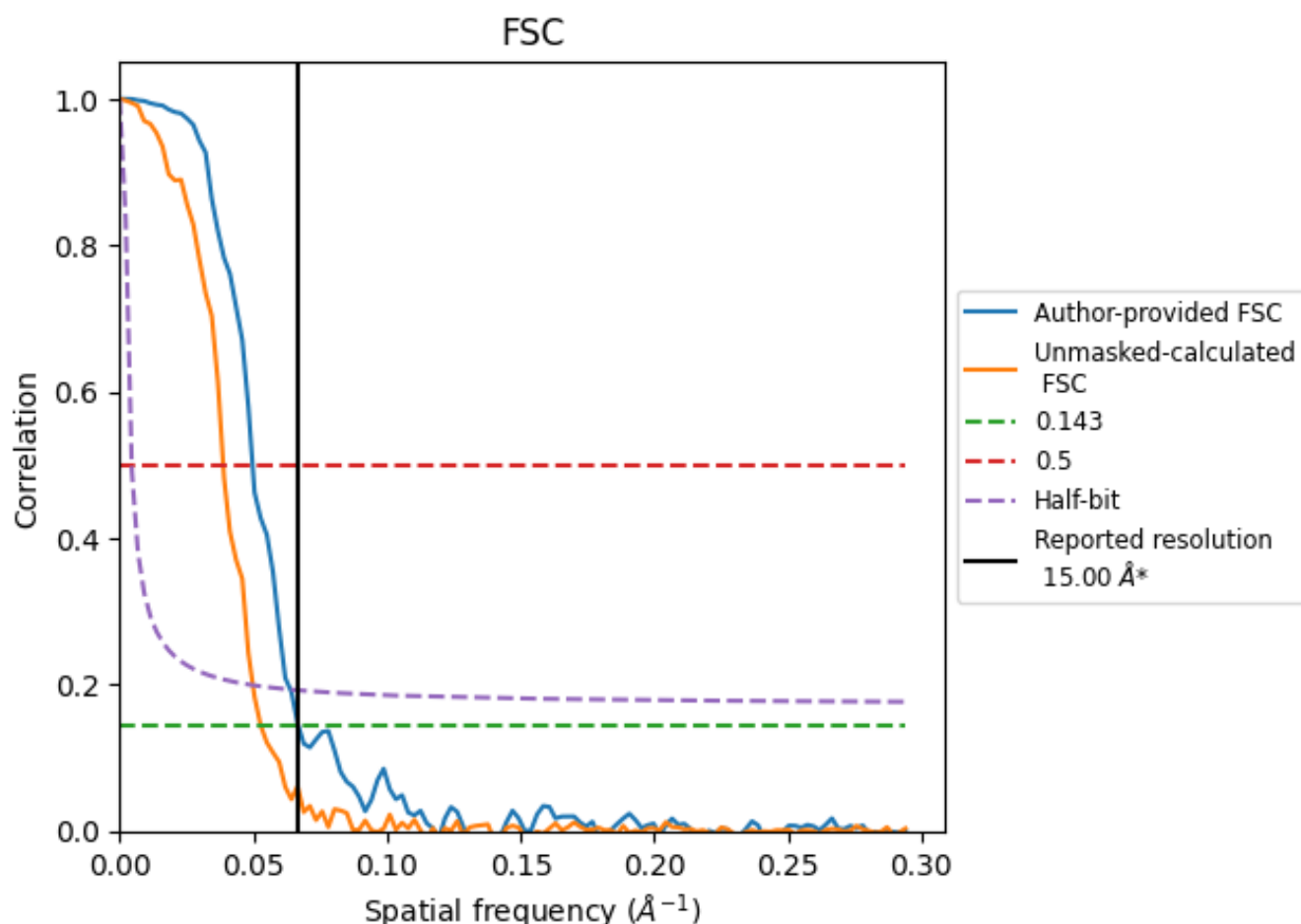
\*Reported resolution corresponds to spatial frequency of 0.067 Å<sup>-1</sup>



## 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 0.067 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

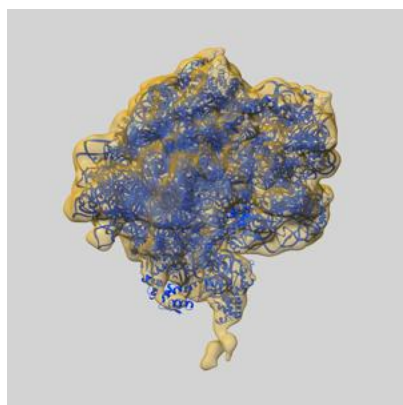
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	15.00	-	-
Author-provided FSC curve	14.95	20.08	15.62
Unmasked-calculated*	18.90	25.84	20.04

\*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 18.90 differs from the reported value 15.0 by more than 10 %

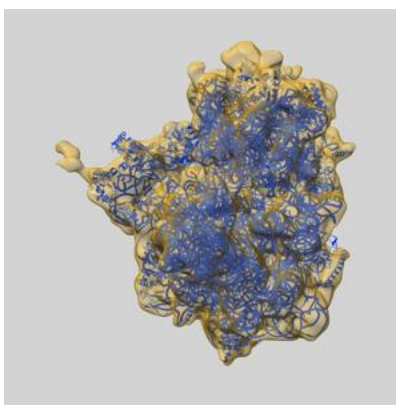
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13449 and PDB model 7PIS. Per-residue inclusion information can be found in section 3 on page 13.

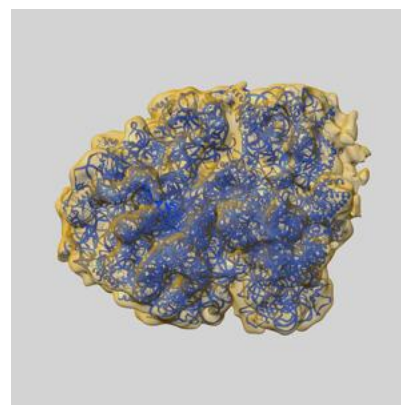
### 9.1 Map-model overlay [i](#)



X



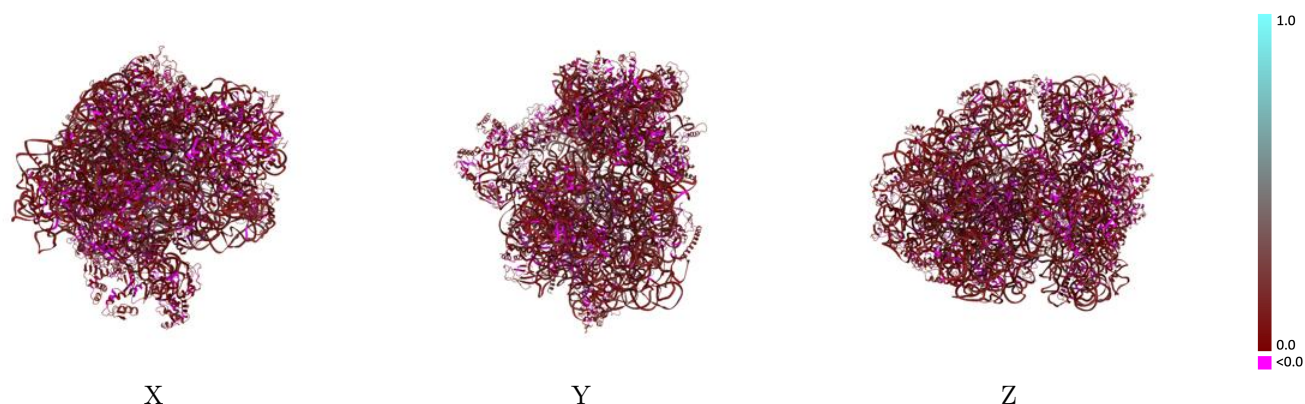
Y



Z

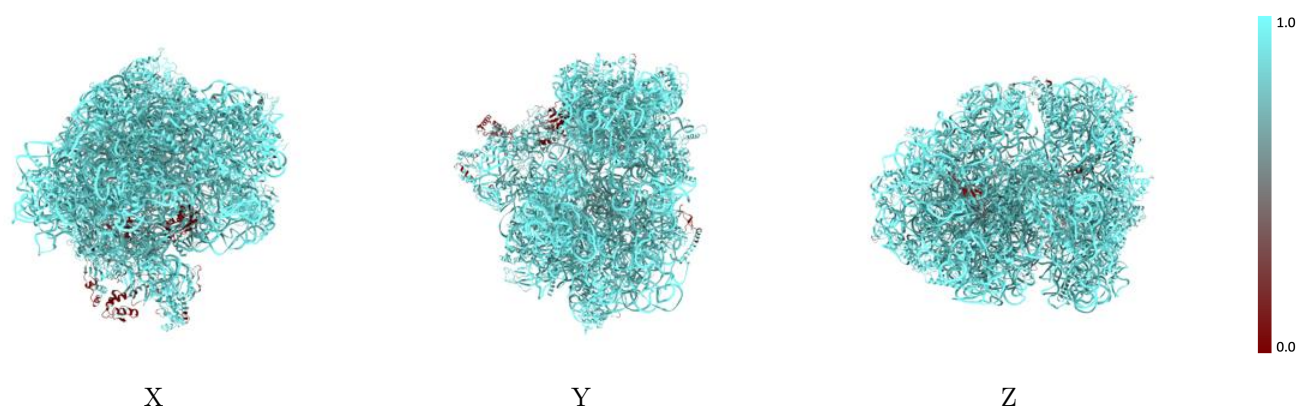
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



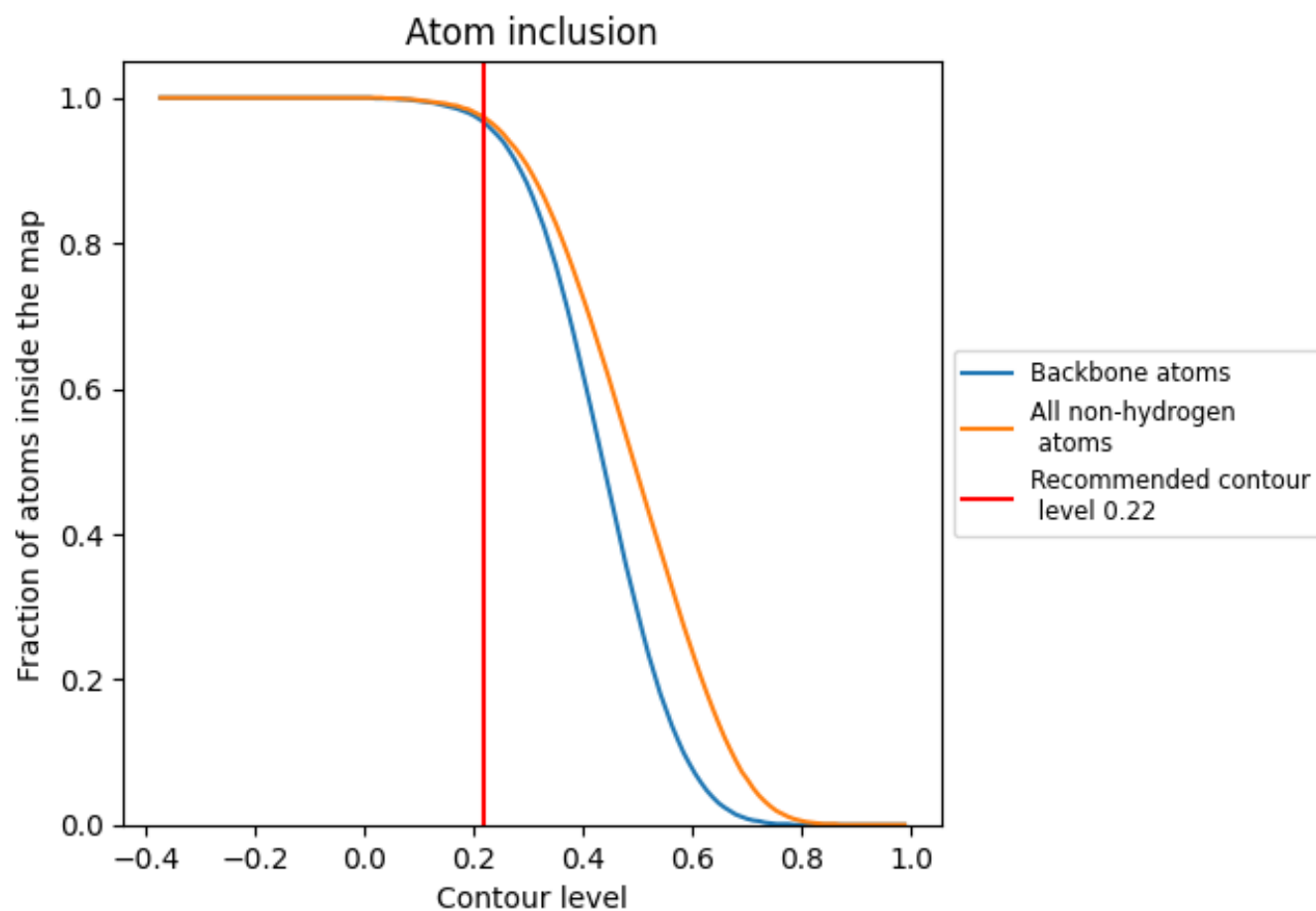
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9730	 0.0820
0	 0.9920	 0.0050
1	 1.0000	 0.0320
2	 1.0000	 0.0070
3	 0.9990	 0.0970
4	 1.0000	 0.1040
5	 0.9980	 0.1000
6	 0.9880	 0.0950
8	 0.9840	 0.0790
9	 0.6770	 0.0620
A	 0.9830	 0.0770
B	 0.9770	 0.0530
C	 0.9880	 0.0340
D	 0.9900	 0.0530
E	 0.9630	 0.0830
F	 0.9500	 0.0770
G	 0.9990	 0.0570
H	 0.9450	 0.0480
I	 0.9480	 0.0380
J	 0.9890	 0.0460
K	 0.9880	 0.0270
L	 0.9080	 0.0510
M	 1.0000	 0.0280
N	 0.9940	 0.0500
O	 1.0000	 0.0400
P	 0.9570	 0.0600
Q	 0.9850	 0.0700
R	 0.9940	 0.0610
S	 0.9950	 0.0440
T	 0.9890	 0.0700
W	 0.1690	 0.0900
a	 1.0000	 0.0280
b	 0.9930	 0.0380
c	 0.9960	 0.0580
d	 0.9630	 0.0700



*Continued on next page...*

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Chain	Atom inclusion	Q-score
e	 0.9290	 0.0580
f	 0.6120	 0.0700
g	 0.8340	 0.0780
h	 0.7950	 0.0770
i	 0.9940	 0.0450
j	 0.9760	 0.0240
k	 0.9820	 0.0370
l	 0.9900	 0.0490
m	 0.9940	 0.0260
n	 0.9860	 0.0590
o	 0.9310	 0.0400
p	 0.9800	 0.0390
q	 0.9470	 0.0690
r	 0.9980	 0.0510
s	 1.0000	 0.0370
t	 0.9170	 0.0620
u	 0.9750	 0.0320
v	 1.0000	 0.0320
w	 0.9880	 0.0950
x	 0.9010	 0.1130
y	 0.9890	 0.0720
z	 1.0000	 0.0290