



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2023 – 12:18 PM EST

PDB ID : 6PJ6
EMDB ID : EMD-20353
Title : High resolution cryo-EM structure of E.coli 50S
Authors : Stojkovic, V.; Myasnikov, A.; Frost, A.; Fujimori, D.G.
Deposited on : 2019-06-27
Resolution : 2.20 Å(reported)

This is a wwPDB EM Validation Summary 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:

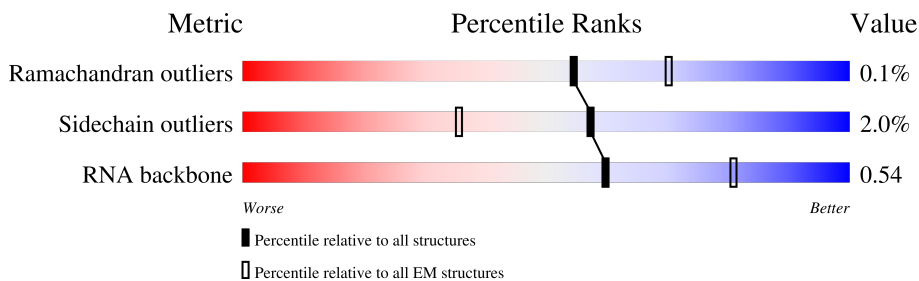
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	I	2904	
2	J	118	
3	K	271	
4	L	209	
5	M	201	
6	N	177	
7	O	176	
8	P	149	

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Mol	Chain	Length	Quality of chain
9	Q	134	100% 99%
10	R	142	97%
11	S	122	13% 97%
12	T	144	6% 98%
13	U	136	7% 96%
14	V	120	95% 5%
15	W	117	25% 98%
16	X	114	20% 100%
17	Y	117	94% 6%
18	Z	103	12% 96%
19	a	110	7% 100%
20	b	93	16% 99%
21	c	102	21% 98%
22	d	94	19% 100%
23	e	75	97%
24	f	77	13% 96%
25	g	62	29% 98%
26	h	58	7% 98%
27	i	56	9% 100%
28	j	50	20% 100%
29	k	46	96%
30	l	64	97%
31	m	38	8% 97%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 154828 atoms, of which 59910 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	I	2898	93536	27768	31307	11448	20115	2898	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	J	118	3810	1126	1281	464	821	118	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	K	271	4261	1294	2167	427	366	7	1	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	L	209	3175	979	1610	288	294	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	M	201	3171	974	1619	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	N	177	2855	899	1444	249	257	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	O	176	2694	832	1371	243	246	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	P	149	2258	699	1148	197	213	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	Q	134	2007	619	1028	169	185	6	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	R	142	2291	714	1162	212	199	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	S	122	1950	587	1012	180	165	6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	T	144	2169	654	1116	207	190	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	U	136	2229	686	1154	205	178	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	V	120	1960	593	1000	196	166	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	W	116	1815	552	923	178	162		0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	X	114	1879	574	962	179	163	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	Y	117	1967	604	1020	192	151		0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	Z	103	1582	516	766	153	145	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	a	110	1779	532	922	166	156	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	b	93	1546	466	807	139	132	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
21	c	102	1611	492	831	146	142	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	d	94	1533	479	780	137	134	3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	e	75	1156	356	581	116	102	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	f	77	1277	388	652	129	106	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	g	62	1032	308	531	98	94	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	h	58	937	281	488	87	79	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	i	56	902	269	458	94	80	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	50	Total	C	H	N	O	0	0
			849	263	440	75	71		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
29	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	l	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	m	38	Total	C	H	N	O	S	0	0
			642	185	340	65	48	4		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	I	182	Total	Mg	0
			182	182	
32	J	1	Total	Mg	0
			1	1	
32	K	1	Total	Mg	0
			1	1	
32	L	1	Total	Mg	0
			1	1	

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
33	K	1	Total	Na	0
			1	1	

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	m	1	Total 1	Zn 1	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	I	3347	Total 3347	O 3347	0
35	J	62	Total 62	O 62	0
35	K	59	Total 59	O 59	0
35	L	41	Total 41	O 41	0
35	M	42	Total 42	O 42	0
35	N	14	Total 14	O 14	0
35	O	13	Total 13	O 13	0
35	P	6	Total 6	O 6	0
35	Q	10	Total 10	O 10	0
35	R	17	Total 17	O 17	0
35	S	7	Total 7	O 7	0
35	T	33	Total 33	O 33	0
35	U	13	Total 13	O 13	0
35	V	23	Total 23	O 23	0
35	W	11	Total 11	O 11	0
35	X	14	Total 14	O 14	0
35	Y	33	Total 33	O 33	0
35	Z	16	Total 16	O 16	0
35	a	18	Total 18	O 18	0

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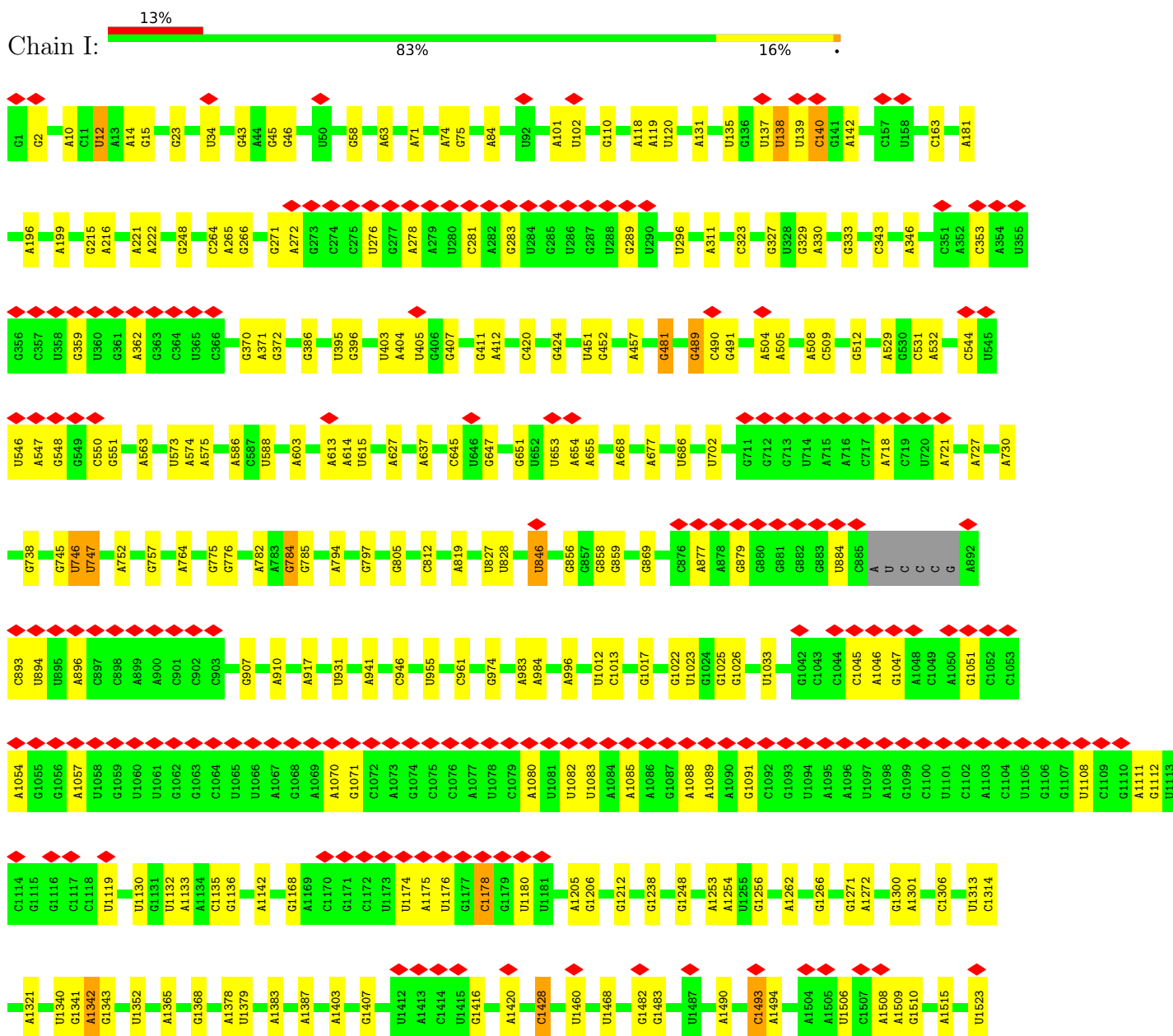
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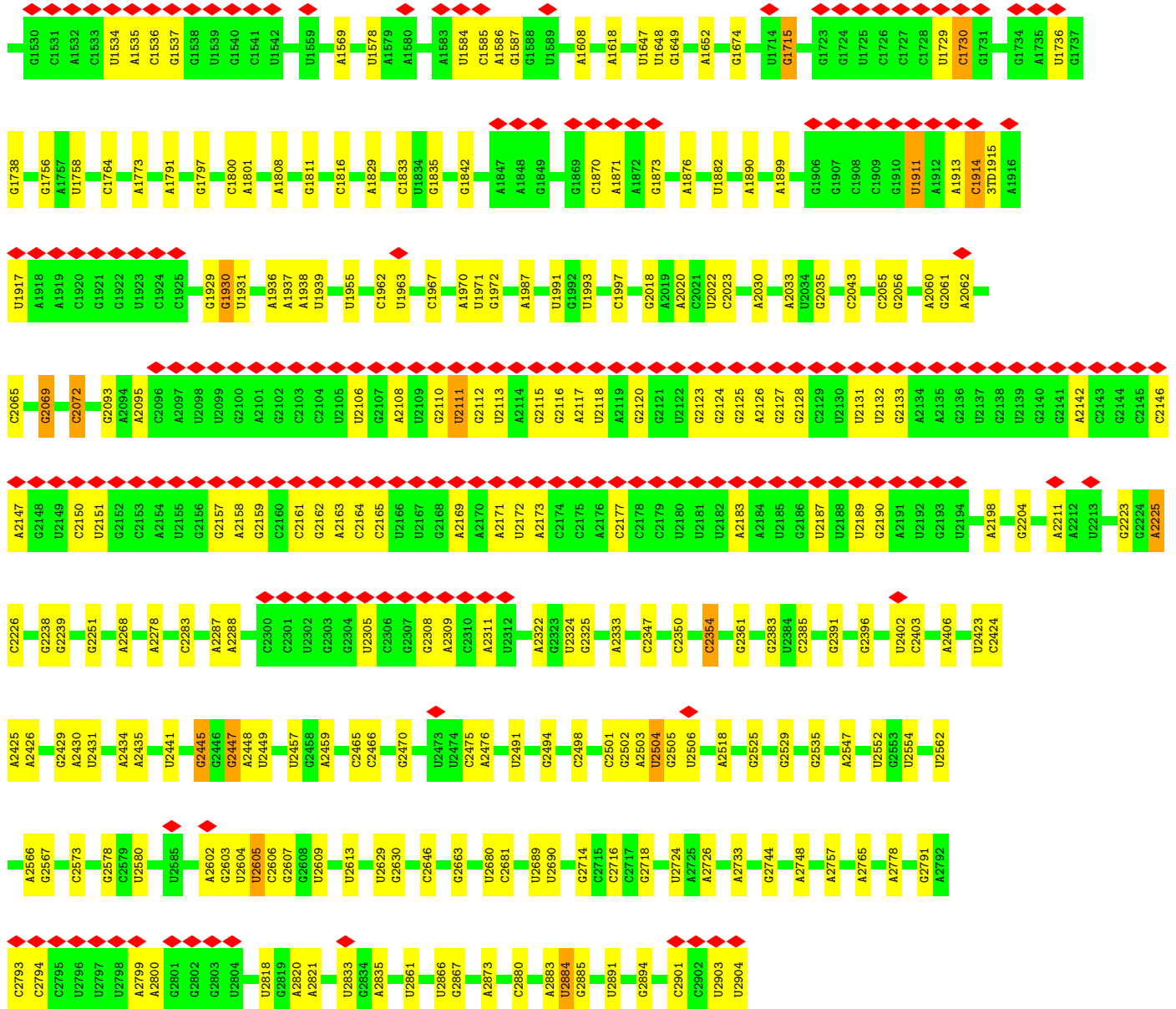
Mol	Chain	Residues	Atoms		AltConf
35	b	15	Total 15	O 15	0
35	c	7	Total 7	O 7	0
35	d	9	Total 9	O 9	0
35	e	13	Total 13	O 13	0
35	f	9	Total 9	O 9	0
35	g	6	Total 6	O 6	0
35	h	4	Total 4	O 4	0
35	i	12	Total 12	O 12	0
35	j	9	Total 9	O 9	0
35	k	11	Total 11	O 11	0
35	l	19	Total 19	O 19	0
35	m	4	Total 4	O 4	0

3 Residue-property plots [i](#)

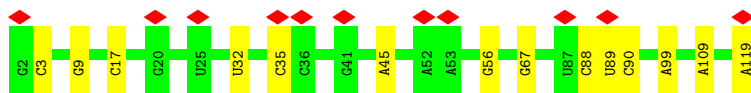
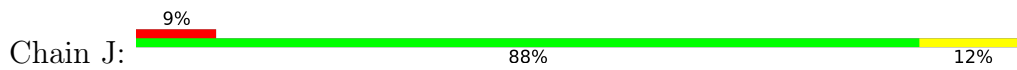
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S rRNA





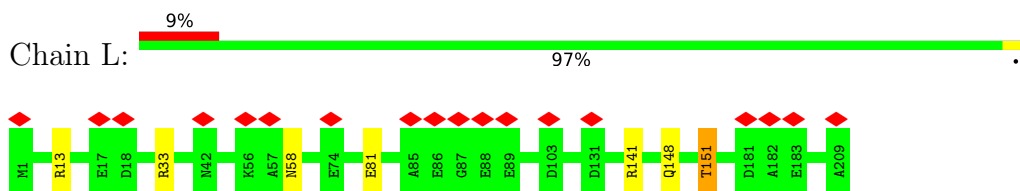
• Molecule 2: 5S rRNA



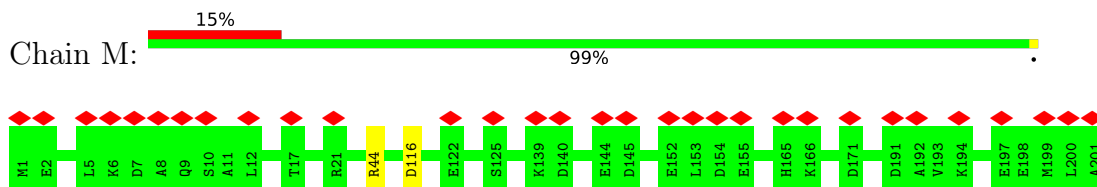
• Molecule 3: 50S ribosomal protein L2



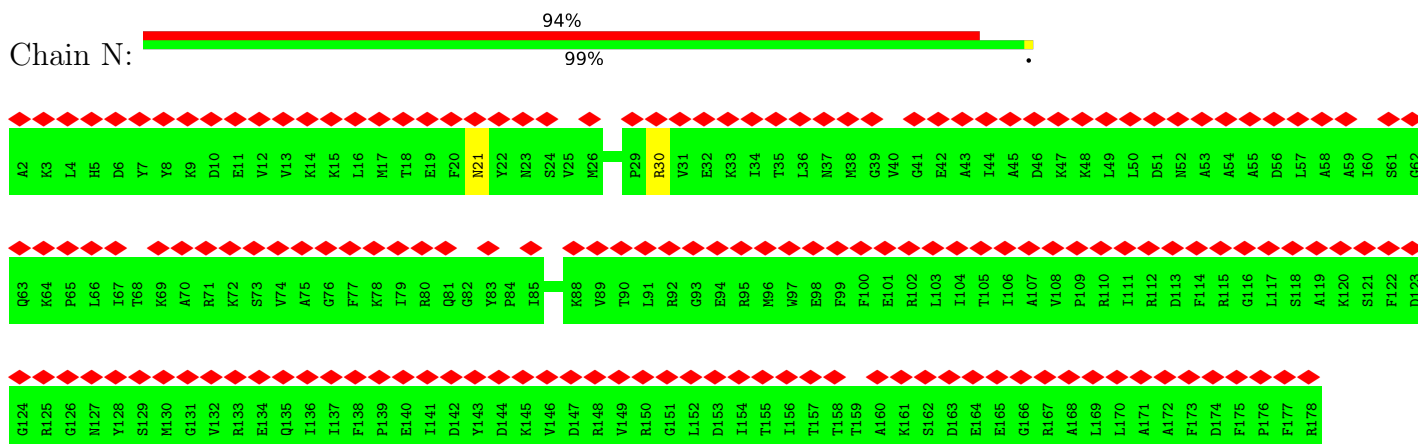
- Molecule 4: 50S ribosomal protein L3



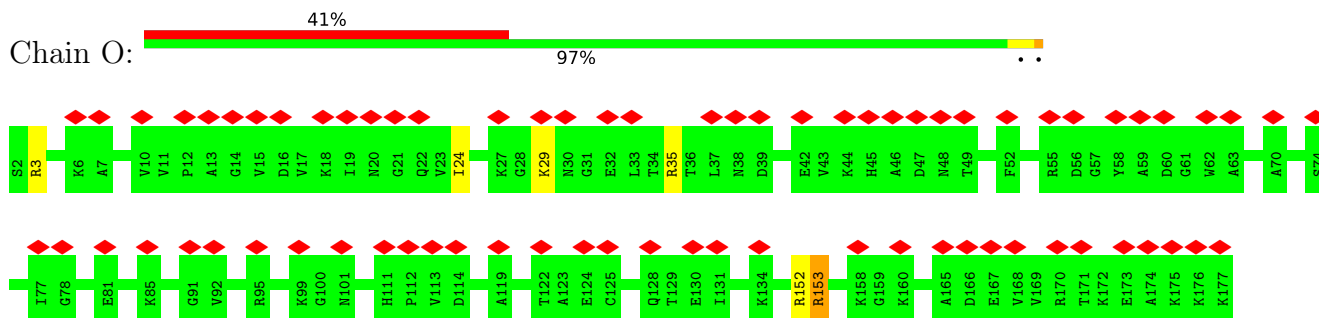
- Molecule 5: 50S ribosomal protein L4



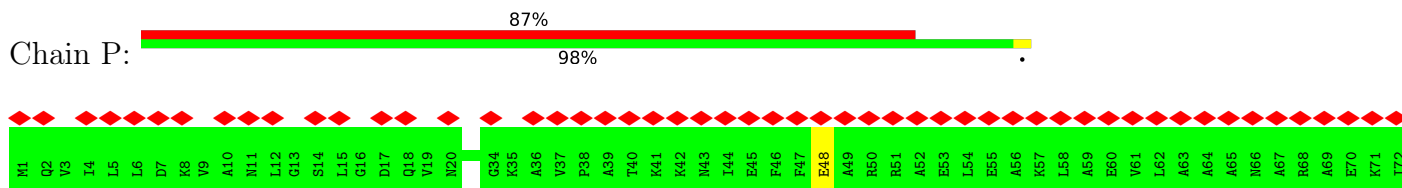
- Molecule 6: 50S ribosomal protein L5

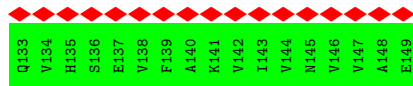
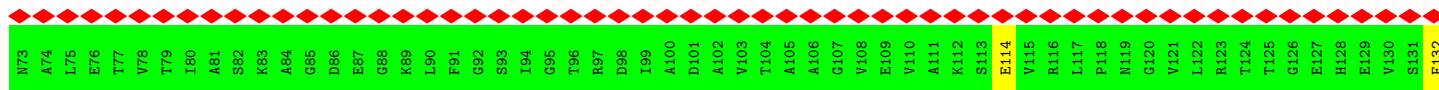


- Molecule 7: 50S ribosomal protein L6

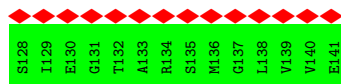
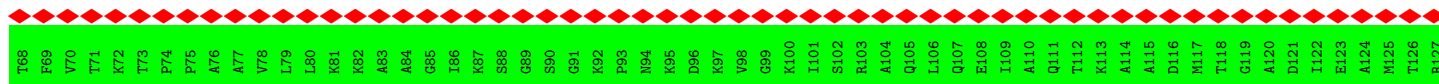
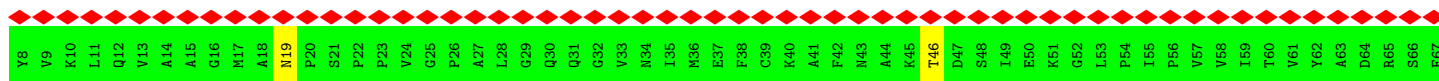


- Molecule 8: 50S ribosomal protein L9

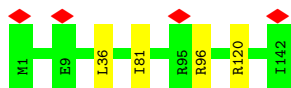




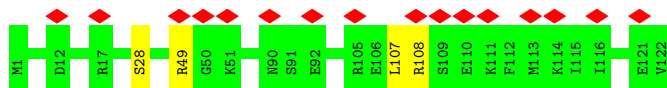
- Molecule 9: 50S ribosomal protein L11



- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14

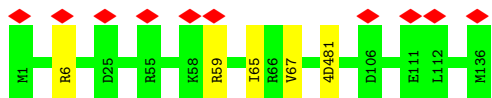


- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16

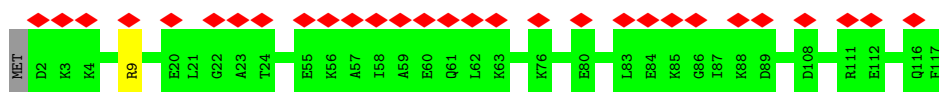




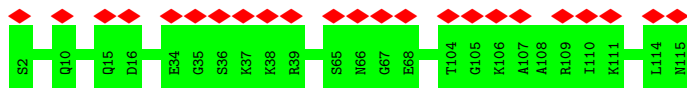
- Molecule 14: 50S ribosomal protein L17



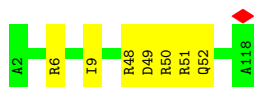
- Molecule 15: 50S ribosomal protein L18



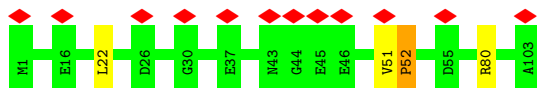
- Molecule 16: 50S ribosomal protein L19



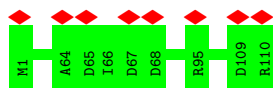
- Molecule 17: 50S ribosomal protein L20



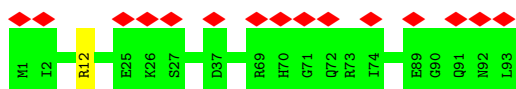
- Molecule 18: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L22



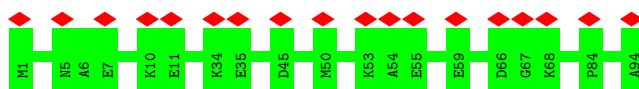
- Molecule 20: 50S ribosomal protein L23



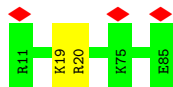
- Molecule 21: 50S ribosomal protein L24



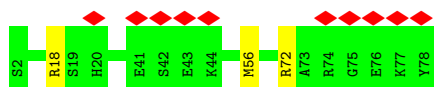
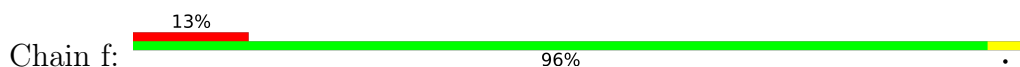
- Molecule 22: 50S ribosomal protein L25



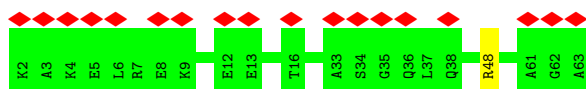
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



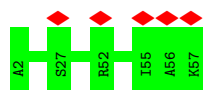
- Molecule 25: 50S ribosomal protein L29



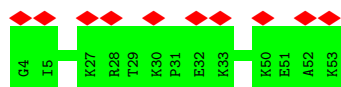
- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L32



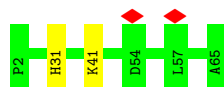
- Molecule 28: 50S ribosomal protein L33



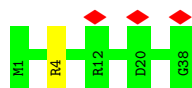
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	60827	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	66.611	Depositor
Minimum map value	-32.287	Depositor
Average map value	-0.035	Depositor
Map value standard deviation	2.434	Depositor
Recommended contour level	10.0	Depositor
Map size (\AA)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.822, 0.822, 0.822	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: H2U, 2MG, MG, 5MC, 1MG, G7M, NA, OMU, 2MA, OMG, 4D4, ZN, 6MZ, PSU, 3TD, OMC, 5MU

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	I	1.15	4/69121 (0.0%)	1.06	63/107828 (0.1%)
2	J	0.94	0/2828	0.99	0/4410
3	K	0.69	0/2133	0.81	3/2866 (0.1%)
4	L	0.70	1/1586 (0.1%)	0.80	1/2134 (0.0%)
5	M	0.64	0/1571	0.71	0/2113
6	N	0.37	0/1435	0.68	0/1926
7	O	0.49	0/1343	0.70	1/1816 (0.1%)
8	P	0.44	0/1121	0.71	0/1515
9	Q	0.36	0/993	0.67	0/1341
10	R	0.67	0/1152	0.75	1/1551 (0.1%)
11	S	0.62	0/947	0.81	0/1268
12	T	0.73	0/1062	0.86	1/1413 (0.1%)
13	U	0.67	0/1081	0.80	0/1443
14	V	0.79	0/973	0.91	1/1301 (0.1%)
15	W	0.54	0/902	0.74	0/1209
16	X	0.59	0/929	0.71	0/1242
17	Y	0.81	0/960	0.99	7/1278 (0.5%)
18	Z	0.64	0/829	0.86	4/1107 (0.4%)
19	a	0.58	0/864	0.70	0/1156
20	b	0.55	0/745	0.62	0/994
21	c	0.52	0/788	0.71	0/1051
22	d	0.55	0/766	0.61	0/1025
23	e	0.70	0/582	0.79	1/769 (0.1%)
24	f	0.68	0/635	0.88	3/848 (0.4%)
25	g	0.46	0/502	0.62	0/667
26	h	0.59	0/453	0.69	0/605
27	i	0.68	0/450	0.84	0/599
28	j	0.60	0/416	0.67	0/554
29	k	0.75	0/380	1.06	2/498 (0.4%)
30	l	0.70	0/513	0.76	0/676
31	m	0.60	0/303	0.76	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.03	5/98363 (0.0%)	1.00	88/147600 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
8	P	0	1
9	Q	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2605	PSU	O3'-P	-6.01	1.53	1.61
1	I	1254	A	N9-C4	-5.43	1.34	1.37
1	I	727	A	N9-C4	-5.35	1.34	1.37
4	L	81	GLU	CD-OE2	-5.05	1.20	1.25
1	I	1652	A	N9-C4	-5.00	1.34	1.37

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2607	G	N9-C1'-C2'	-10.93	99.80	114.00
1	I	12	U	C2-N1-C1'	10.18	129.91	117.70
1	I	846	U	C2-N1-C1'	9.83	129.49	117.70
1	I	2606	C	N1-C1'-C2'	-9.79	101.24	112.00
17	Y	6	ARG	NE-CZ-NH1	-8.52	116.04	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	203[B]	ARG	Mainchain
8	P	114	GLU	Peptide
9	Q	19	ASN	Peptide
9	Q	46	THR	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	270/271 (100%)	254 (94%)	16 (6%)	0	100	100
4	L	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	29	31
5	M	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
6	N	175/177 (99%)	152 (87%)	23 (13%)	0	100	100
7	O	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
8	P	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
9	Q	132/134 (98%)	110 (83%)	22 (17%)	0	100	100
10	R	140/142 (99%)	140 (100%)	0	0	100	100
11	S	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
12	T	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
13	U	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
14	V	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
15	W	114/117 (97%)	105 (92%)	9 (8%)	0	100	100
16	X	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
17	Y	115/117 (98%)	115 (100%)	0	0	100	100
18	Z	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	15	14
19	a	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
20	b	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
21	c	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
22	d	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	e	73/75 (97%)	73 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	f	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	g	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
26	h	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
27	i	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	j	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
29	k	44/46 (96%)	44 (100%)	0	0	100	100
30	l	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	3298/3357 (98%)	3112 (94%)	184 (6%)	2 (0%)	54	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	Z	52	PRO
4	L	151	THR

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	
3	K	217/216 (100%)	213 (98%)	4 (2%)	59	72
4	L	164/164 (100%)	159 (97%)	5 (3%)	41	53
5	M	165/165 (100%)	163 (99%)	2 (1%)	71	83
6	N	148/148 (100%)	146 (99%)	2 (1%)	67	80
7	O	137/137 (100%)	131 (96%)	6 (4%)	28	35
8	P	114/114 (100%)	112 (98%)	2 (2%)	59	72
9	Q	104/104 (100%)	104 (100%)	0	100	100
10	R	116/116 (100%)	113 (97%)	3 (3%)	46	58
11	S	103/103 (100%)	99 (96%)	4 (4%)	32	41
12	T	103/103 (100%)	101 (98%)	2 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	U	108/108 (100%)	104 (96%)	4 (4%)	34	43
14	V	100/100 (100%)	95 (95%)	5 (5%)	24	30
15	W	86/87 (99%)	85 (99%)	1 (1%)	71	83
16	X	99/99 (100%)	99 (100%)	0	100	100
17	Y	89/89 (100%)	87 (98%)	2 (2%)	52	65
18	Z	84/84 (100%)	83 (99%)	1 (1%)	71	83
19	a	93/93 (100%)	93 (100%)	0	100	100
20	b	80/80 (100%)	79 (99%)	1 (1%)	69	81
21	c	83/83 (100%)	81 (98%)	2 (2%)	49	62
22	d	78/78 (100%)	78 (100%)	0	100	100
23	e	57/57 (100%)	56 (98%)	1 (2%)	59	72
24	f	67/67 (100%)	66 (98%)	1 (2%)	65	78
25	g	54/54 (100%)	53 (98%)	1 (2%)	57	71
26	h	48/48 (100%)	47 (98%)	1 (2%)	53	67
27	i	47/47 (100%)	47 (100%)	0	100	100
28	j	45/45 (100%)	45 (100%)	0	100	100
29	k	38/38 (100%)	37 (97%)	1 (3%)	46	58
30	l	51/51 (100%)	49 (96%)	2 (4%)	32	41
31	m	34/34 (100%)	33 (97%)	1 (3%)	42	54
All	All	2712/2712 (100%)	2658 (98%)	54 (2%)	57	69

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	T	40	SER
14	V	14	SER
26	h	10	THR
12	T	70	LYS
13	U	65	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
17	Y	52	GLN

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Mol	Chain	Res	Type
25	g	15	ASN
30	l	31	HIS
7	O	115	HIS
9	Q	30	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2892/2904 (99%)	449 (15%)	23 (0%)
2	J	117/118 (99%)	14 (11%)	0
All	All	3009/3022 (99%)	463 (15%)	23 (0%)

5 of 463 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	G
1	I	10	A
1	I	12	U
1	I	14	A
1	I	15	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	2162	G
1	I	2430	A
1	I	2425	A
1	I	2447	G
1	I	784	G

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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
13	4D4	U	81	13	9,11,12	2.58	3 (33%)	8,13,15	1.14	0
1	1MG	I	745	1	18,26,27	2.66	5 (27%)	19,39,42	1.50	5 (26%)
1	OMC	I	2498	32,1	19,22,23	2.70	7 (36%)	26,31,34	0.68	0
1	PSU	I	955	1	18,21,22	1.65	5 (27%)	22,30,33	1.77	4 (18%)
1	OMU	I	2552	1	19,22,23	2.84	8 (42%)	26,31,34	1.67	5 (19%)
1	5MC	I	1962	1	18,22,23	3.11	7 (38%)	26,32,35	1.16	2 (7%)
1	PSU	I	2605	1	18,21,22	3.03	10 (55%)	22,30,33	2.54	6 (27%)
1	PSU	I	2604	1	18,21,22	2.65	9 (50%)	22,30,33	2.65	5 (22%)
1	PSU	I	2580	1	18,21,22	1.84	6 (33%)	22,30,33	1.69	5 (22%)
1	5MU	I	1939	1	19,22,23	4.71	7 (36%)	28,32,35	3.59	9 (32%)
1	2MA	I	2503	1	17,25,26	2.33	5 (29%)	17,37,40	1.51	4 (23%)
1	5MU	I	747	1	19,22,23	4.56	7 (36%)	28,32,35	3.59	8 (28%)
1	3TD	I	1915	1	18,22,23	4.18	6 (33%)	22,32,35	1.53	2 (9%)
1	PSU	I	746	1	18,21,22	1.64	6 (33%)	22,30,33	1.71	4 (18%)
1	6MZ	I	1618	1	18,25,26	1.85	3 (16%)	16,36,39	2.61	3 (18%)
1	2MG	I	1835	1	18,26,27	2.22	7 (38%)	16,38,41	1.25	3 (18%)
1	PSU	I	2457	1	18,21,22	1.65	4 (22%)	22,30,33	1.89	3 (13%)
1	H2U	I	2449	1	18,21,22	1.56	3 (16%)	21,30,33	0.60	0
1	PSU	I	1911	1	18,21,22	1.37	3 (16%)	22,30,33	2.17	3 (13%)
1	2MG	I	2445	1	18,26,27	2.23	7 (38%)	16,38,41	1.15	2 (12%)
1	PSU	I	1917	1	18,21,22	1.43	2 (11%)	22,30,33	1.87	4 (18%)
1	6MZ	I	2030	1	18,25,26	1.91	4 (22%)	16,36,39	2.98	4 (25%)
1	G7M	I	2069	1	20,26,27	2.10	7 (35%)	17,39,42	1.10	2 (11%)
1	OMG	I	2251	1	18,26,27	2.25	8 (44%)	19,38,41	1.32	3 (15%)
1	PSU	I	2504	32,1	18,21,22	1.69	5 (27%)	22,30,33	1.66	4 (18%)

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
13	4D4	U	81	13	-	2/11/12/14	-
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
1	OMC	I	2498	32,1	-	0/9/27/28	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2605	1	-	2/7/25/26	0/2/2/2
1	PSU	I	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	I	2503	1	-	1/3/25/26	0/3/3/3
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	3TD	I	1915	1	-	3/7/25/26	0/2/2/2
1	PSU	I	746	1	-	2/7/25/26	0/2/2/2
1	6MZ	I	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	I	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	H2U	I	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	I	1911	1	-	2/7/25/26	0/2/2/2
1	2MG	I	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	I	1917	1	-	2/7/25/26	0/2/2/2
1	6MZ	I	2030	1	-	2/5/27/28	0/3/3/3
1	G7M	I	2069	1	-	2/3/25/26	0/3/3/3
1	OMG	I	2251	1	-	0/5/27/28	0/3/3/3
1	PSU	I	2504	32,1	-	2/7/25/26	0/2/2/2

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1915	3TD	C6-C5	12.30	1.49	1.35
1	I	1939	5MU	C2-N1	10.56	1.55	1.38
1	I	747	5MU	C2-N1	10.13	1.54	1.38
1	I	1939	5MU	C6-N1	10.11	1.55	1.38
1	I	747	5MU	C6-N1	9.91	1.55	1.38

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1939	5MU	C5-C4-N3	12.20	125.73	115.31
1	I	747	5MU	C5-C4-N3	11.59	125.20	115.31
1	I	747	5MU	C5-C6-N1	-9.34	113.73	123.34
1	I	2030	6MZ	C1'-N9-C4	-9.14	110.59	126.64
1	I	1939	5MU	C5-C6-N1	-9.06	114.02	123.34

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1911	PSU	O4'-C4'-C5'-O5'
1	I	1915	3TD	C3'-C4'-C5'-O5'
1	I	1915	3TD	O4'-C4'-C5'-O5'
1	I	2445	2MG	C3'-C4'-C5'-O5'
1	I	2504	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 187 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

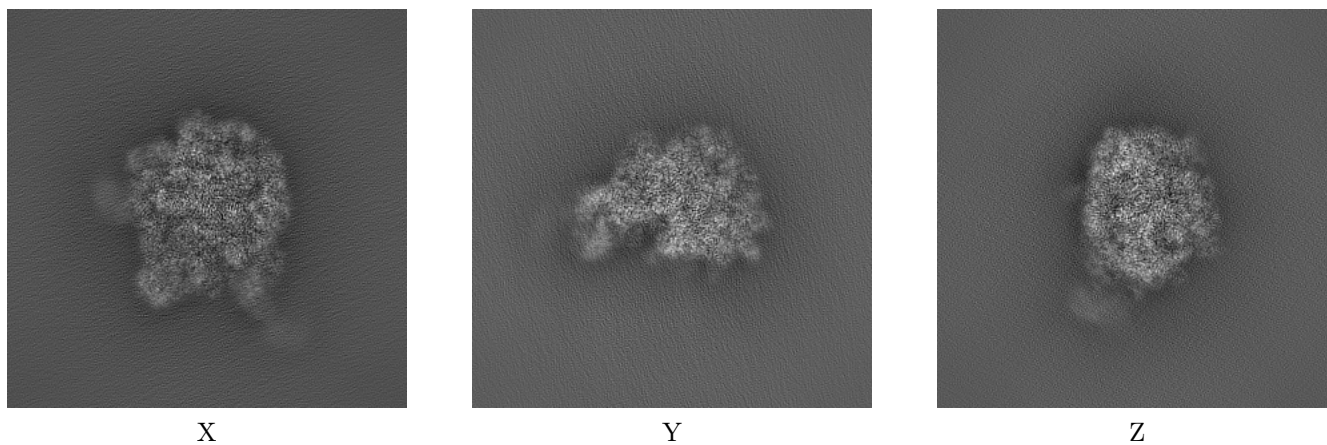
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20353. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

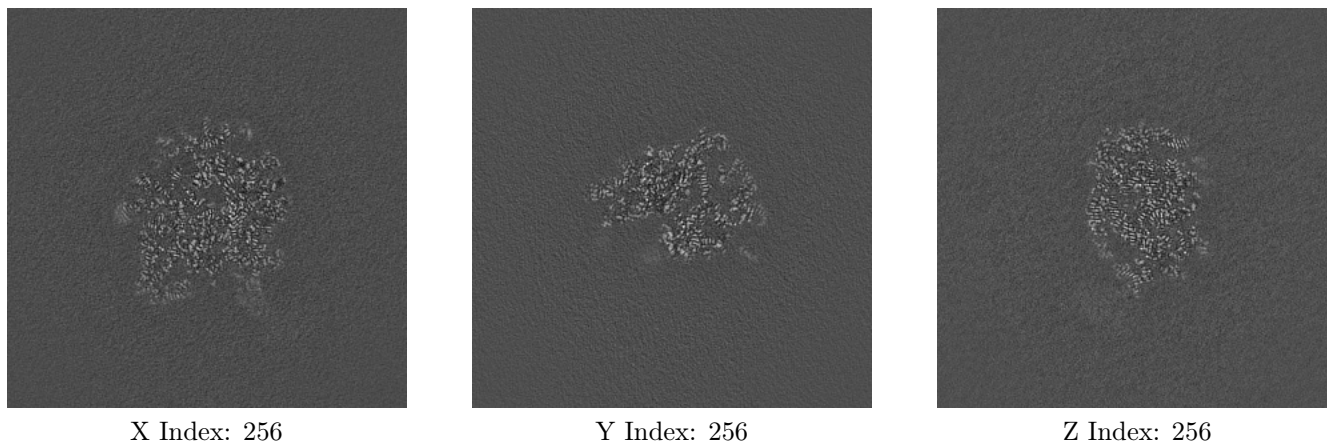
6.1.1 Primary map



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

6.2 Central slices [i](#)

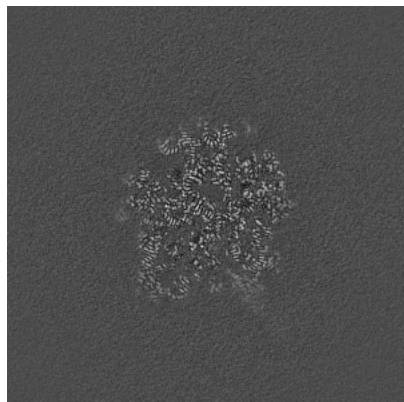
6.2.1 Primary map



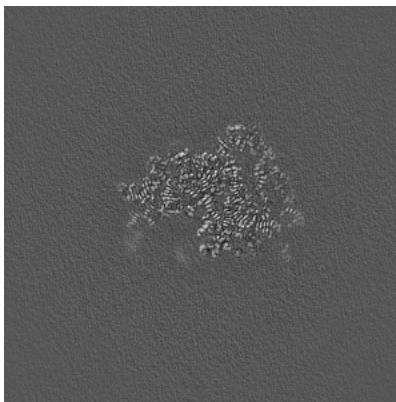
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

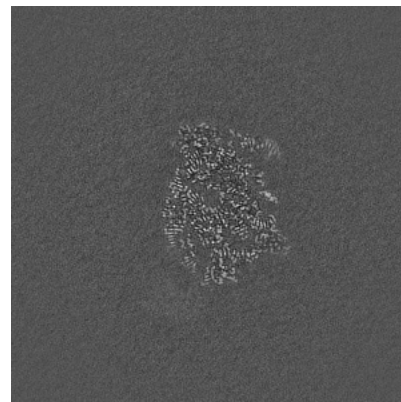
6.3.1 Primary map



X Index: 261



Y Index: 247

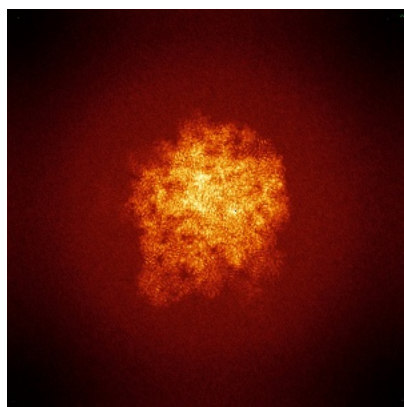


Z Index: 266

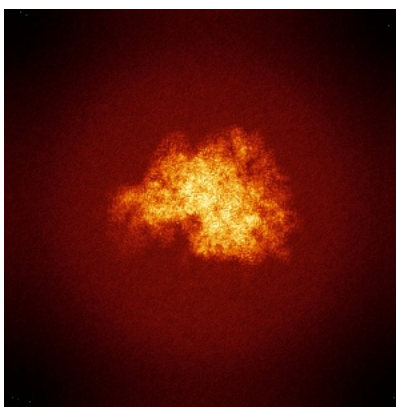
The images above show the largest variance slices of the map in three orthogonal directions.

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

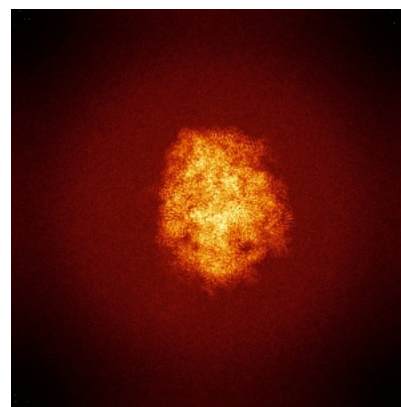
6.4.1 Primary map



X



Y

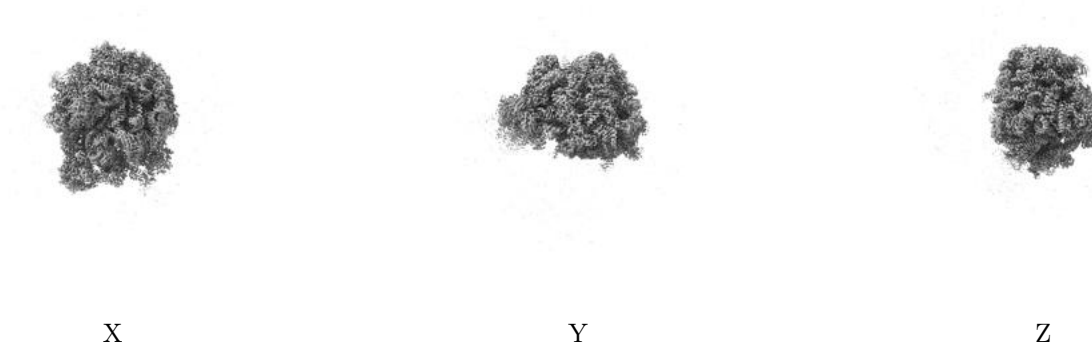


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

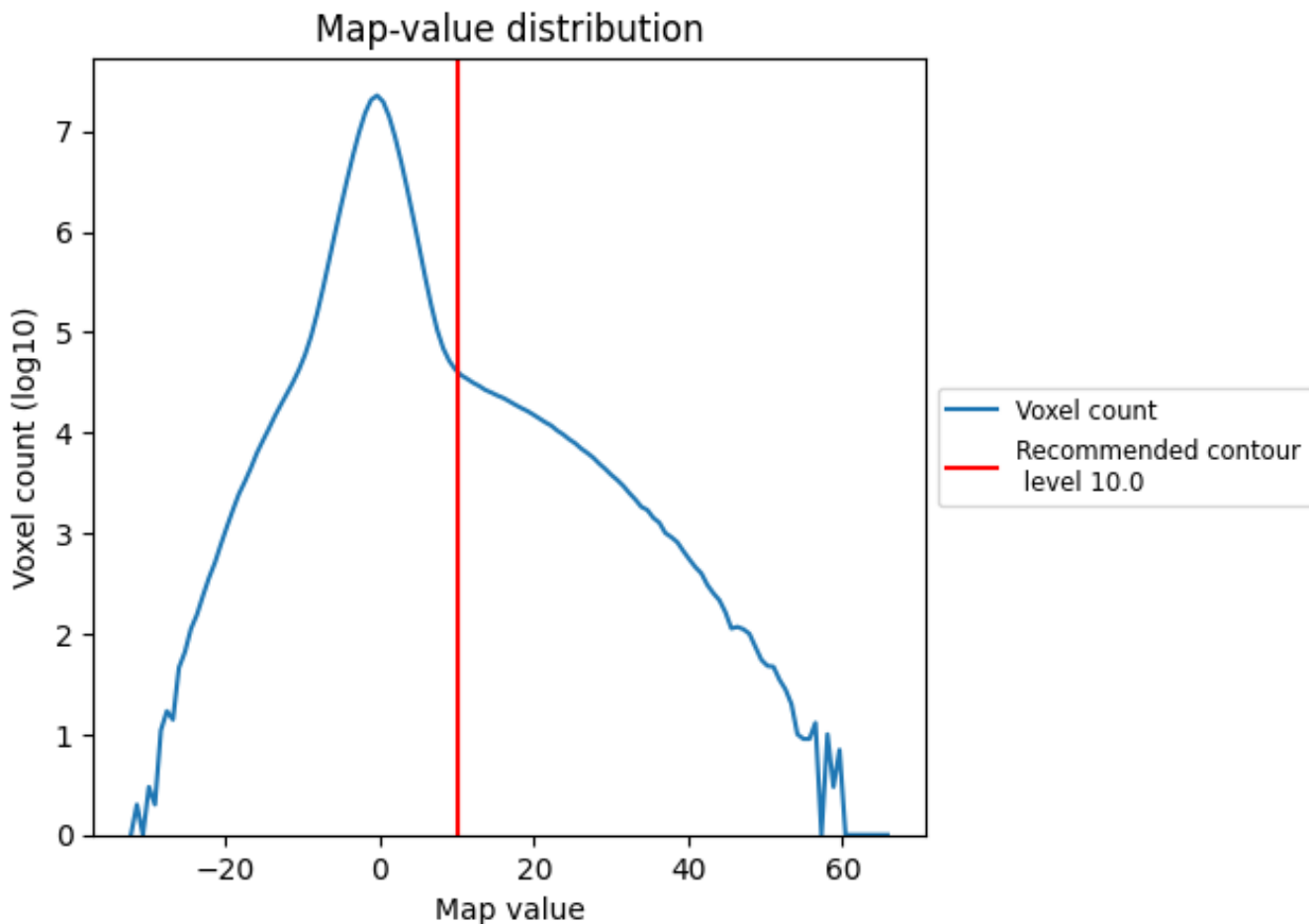
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

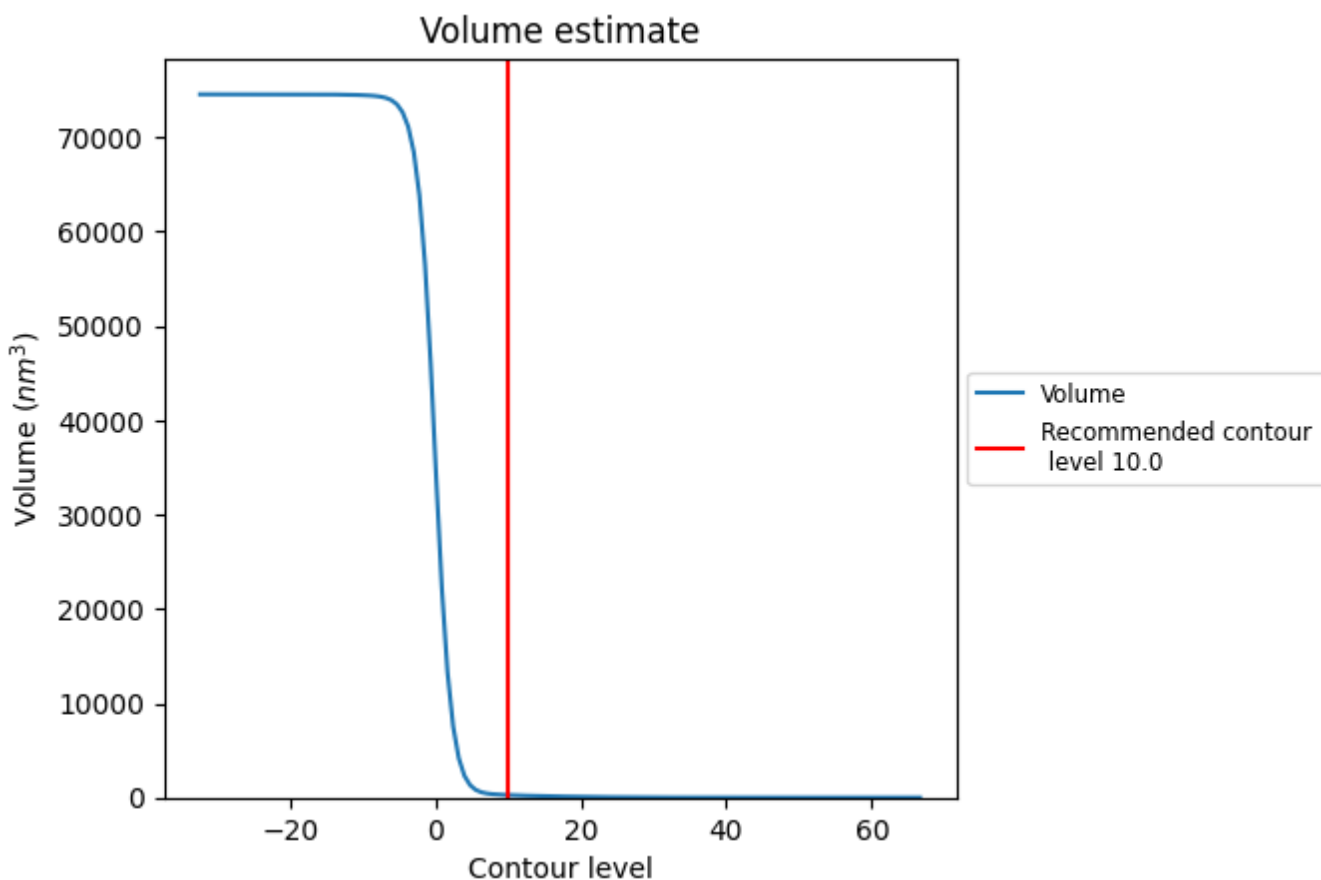
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

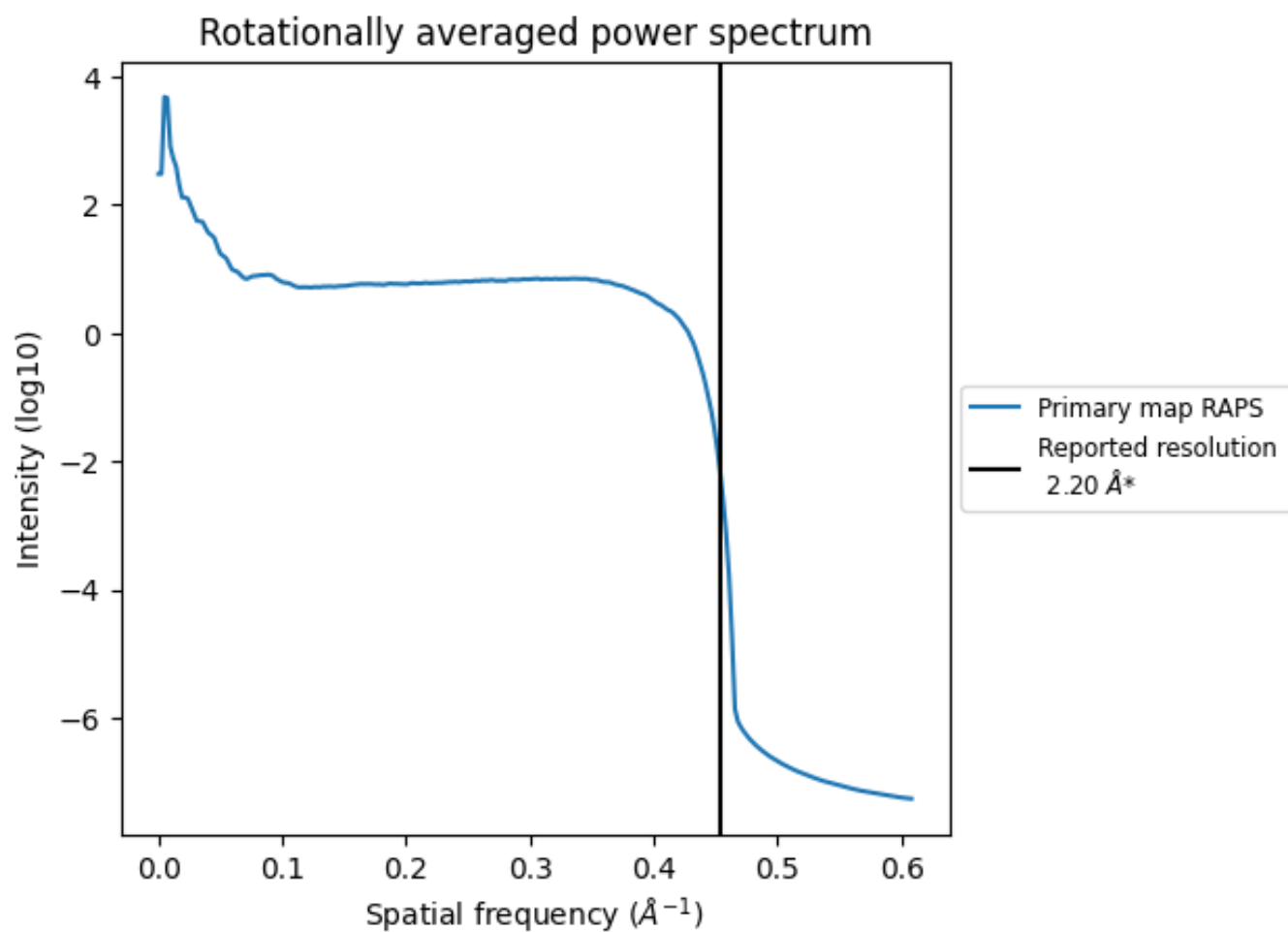
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 266 nm³; this corresponds to an approximate mass of 240 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 0.455\AA^{-1}

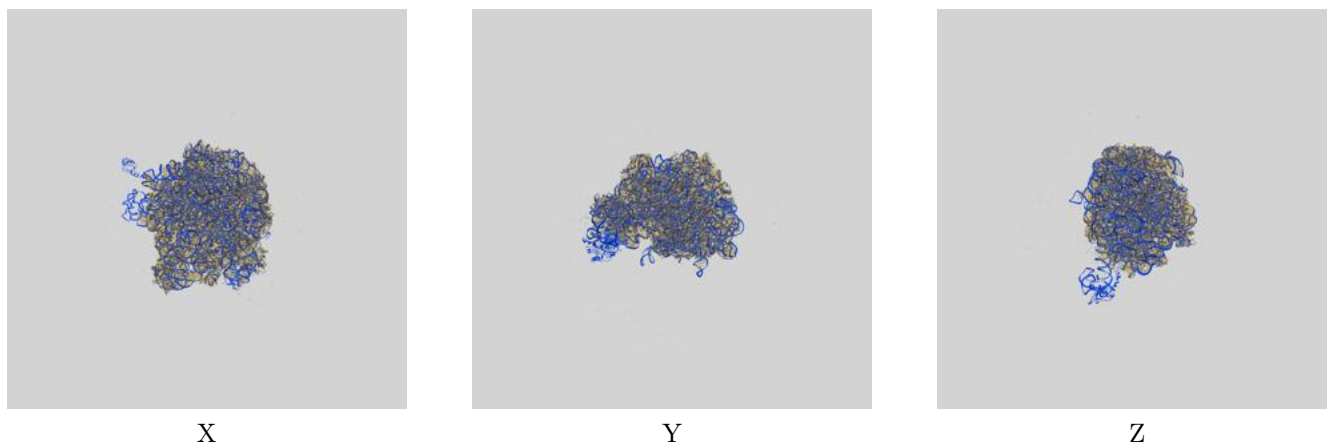
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

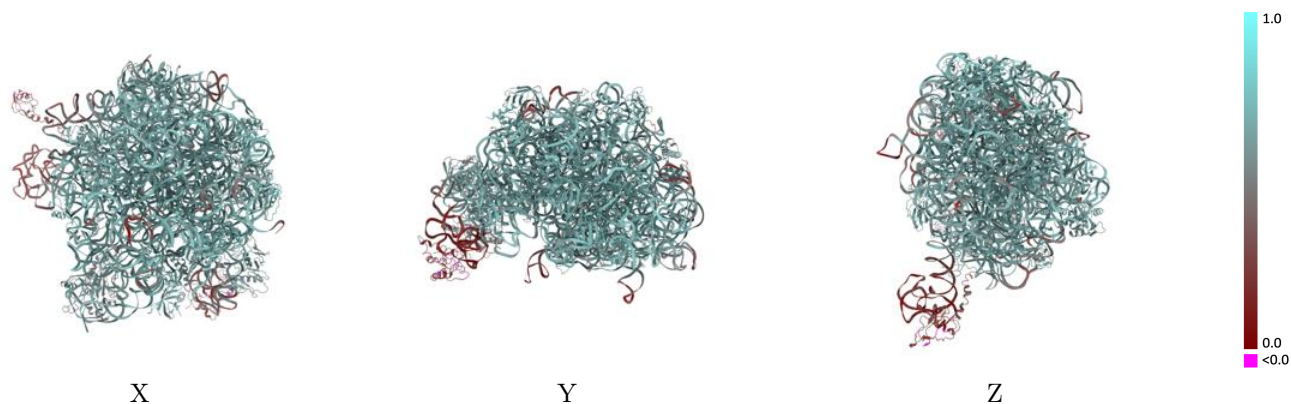
This section contains information regarding the fit between EMDB map EMD-20353 and PDB model 6PJ6. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



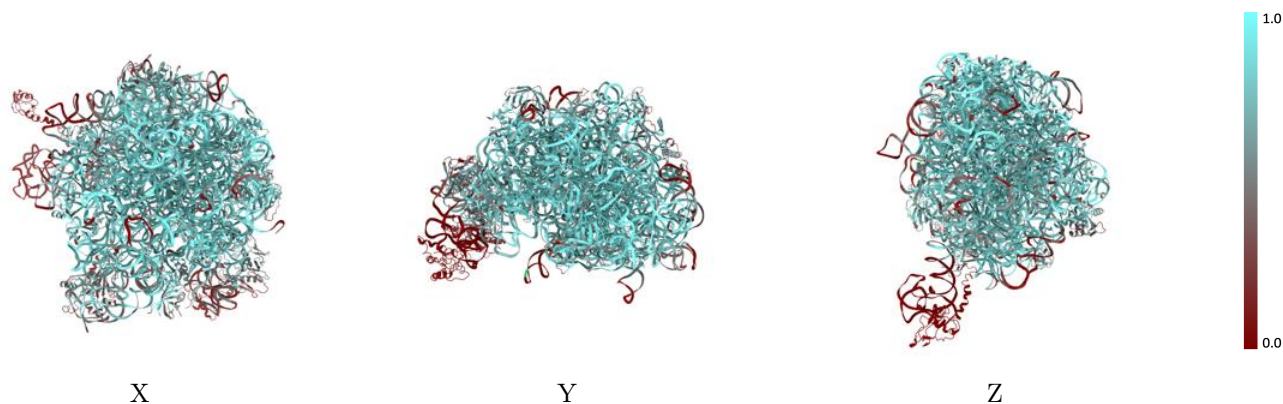
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



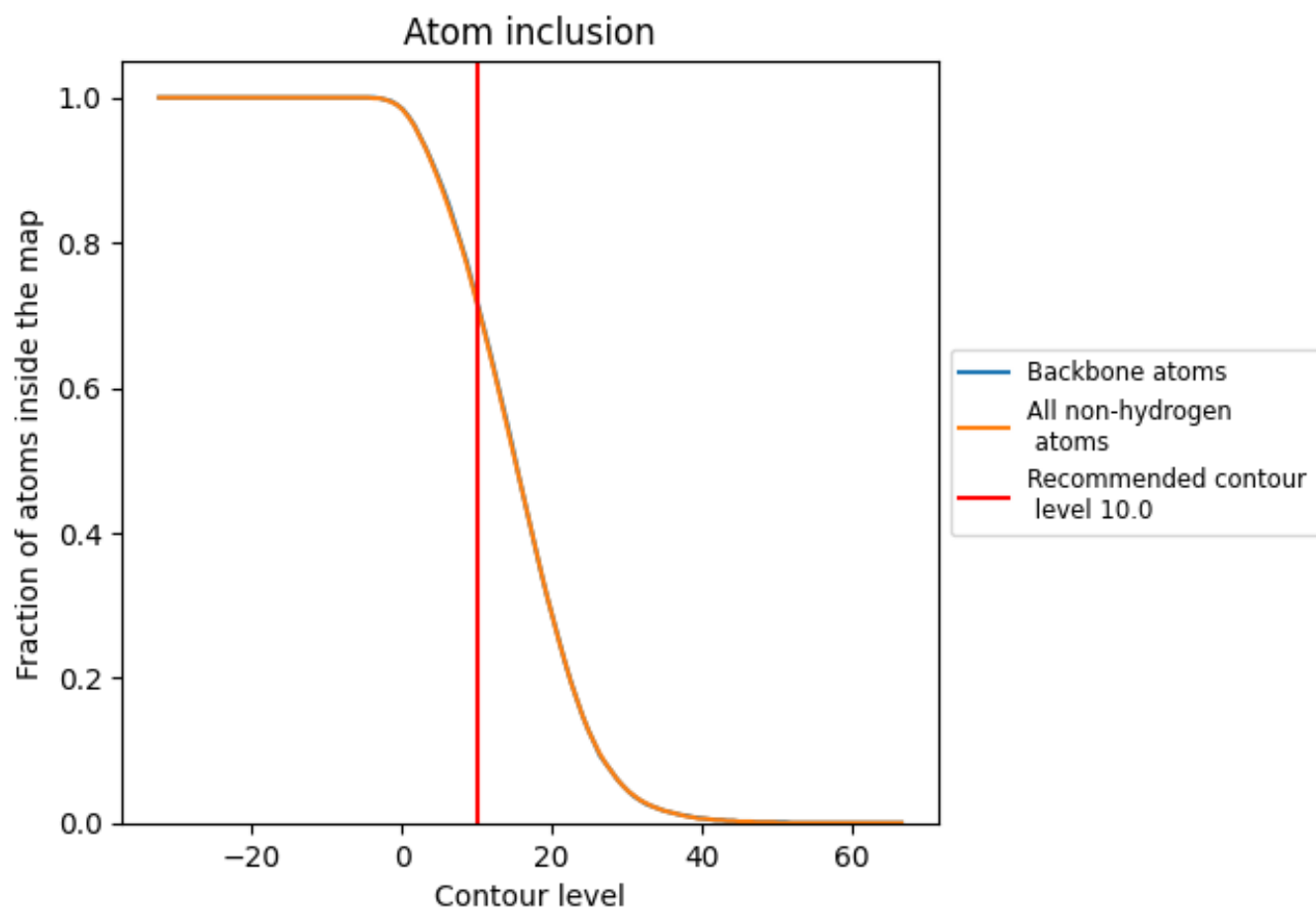
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10.0).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.6160
I	 0.7610	 0.6180
J	 0.6860	 0.6150
K	 0.7910	 0.6730
L	 0.7800	 0.6700
M	 0.6780	 0.6470
N	 0.1220	 0.4500
O	 0.4460	 0.5820
P	 0.1270	 0.3310
Q	 0.0000	 0.2260
R	 0.7690	 0.6740
S	 0.6980	 0.6520
T	 0.7520	 0.6650
U	 0.7400	 0.6650
V	 0.8400	 0.6810
W	 0.5700	 0.6060
X	 0.6670	 0.6330
Y	 0.8390	 0.6930
Z	 0.7290	 0.6440
a	 0.7490	 0.6570
b	 0.6390	 0.6360
c	 0.5990	 0.6150
d	 0.6350	 0.6360
e	 0.7910	 0.6630
f	 0.7140	 0.6620
g	 0.5400	 0.6070
h	 0.7480	 0.6580
i	 0.7520	 0.6600
j	 0.5960	 0.6200
k	 0.8370	 0.6900
l	 0.8370	 0.6870
m	 0.7070	 0.6500

