



Full wwPDB EM Validation Report ⓘ

Mar 19, 2025 – 05:37 PM EDT

PDB ID : 9B1Y
EMDB ID : EMD-44092
Title : WT strain WT mycobacterial ribosome
Authors : Chen, Y.; Young, I.D.; Fraser, J.S.; Javid, B.
Deposited on : 2024-03-14
Resolution : 2.47 Å(reported)
Based on initial models : 5o5j, 5o60

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.41.4

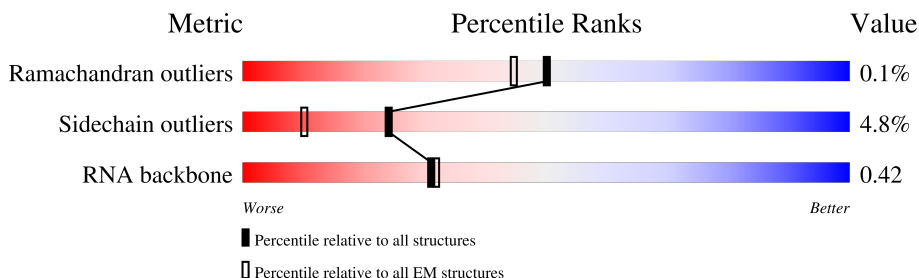
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1511	<div> <div>10%</div> <div>75%</div> <div>25%</div> </div>
2	C	208	<div> <div>44%</div> <div>93%</div> <div>7%</div> </div>
3	D	200	<div> <div>46%</div> <div>92%</div> <div>8%</div> </div>
4	E	180	<div> <div>32%</div> <div>97%</div> <div>.</div> </div>
5	F	96	<div> <div>29%</div> <div>98%</div> <div>.</div> </div>
6	G	155	<div> <div>53%</div> <div>97%</div> <div>.</div> </div>
7	H	131	<div> <div>34%</div> <div>94%</div> <div>6%</div> </div>
8	I	126	<div> <div>29%</div> <div>94%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
9	J	99	
10	K	115	
11	L	122	
12	M	116	
13	N	60	
14	O	88	
15	P	96	
16	Q	94	
17	R	65	
18	T	85	
19	V	228	
20	Y	3038	
21	U	118	
22	Z	275	
23	a	214	
24	b	209	
25	c	182	
26	d	176	
27	e	133	
28	f	146	
29	g	122	
30	h	145	
31	i	136	
32	j	118	
33	k	126	

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Mol	Chain	Length	Quality of chain
34	l	113	
35	m	124	
36	n	100	
37	o	114	
38	p	97	
39	q	97	
40	r	192	
41	s	79	
42	t	63	
43	u	64	
44	v	126	
45	w	59	
46	x	54	
47	y	49	
48	z	46	
49	1	63	
50	2	37	
51	4	81	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 146984 atoms, of which 3 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1511	Total	C	H	N	O	P	0	0
			32443	14449	3	5930	10550	1511		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	180	Total	C	N	O	S	0	0
			1296	812	245	235	4		

- Molecule 5 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

- Molecule 6 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	155	Total	C	N	O	S	0	0
			1232	768	241	221	2		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	131	Total	C	N	O	S	0	0
			1010	633	189	187	1		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	126	Total	C	N	O	S	0	0
			994	630	194	170			

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	99	Total	C	N	O	S	0	0
			788	495	146	144	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	115	Total	C	N	O	S	0	0
			855	528	170	156	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	88	Total	C	N	O	0	0
			720	449	147	124		

- Molecule 15 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	96	Total	C	N	O	0	0
			764	488	142	134		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	T	85	Total	C	N	O	0	0
			660	402	139	119		

- Molecule 19 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 20 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	3038	Total	C	N	O	P	0	0
			65241	29079	12000	21124	3038		

- Molecule 21 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 22 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 24 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 26 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 27 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 28 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 29 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 30 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 31 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 32 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 33 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	126	Total	C	N	O	S	0	0
			956	586	199	171			

- Molecule 34 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 35 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	m	124	Total	C	N	O	0	0
			988	613	203	172		

- Molecule 36 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	n	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 37 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	o	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 38 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	p	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 39 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	SER	deletion	UNP A0QSG0
q	?	-	ALA	deletion	UNP A0QSG0
q	?	-	ASN	deletion	UNP A0QSG0
q	?	-	GLU	deletion	UNP A0QSG0
q	?	-	ARG	deletion	UNP A0QSG0
q	?	-	GLY	deletion	UNP A0QSG0
q	?	-	ALA	deletion	UNP A0QSG0
q	?	-	SER	deletion	UNP A0QSG0

- Molecule 40 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	r	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 41 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	s	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 42 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 43 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 44 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	w	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 46 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 49 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	1	63	Total	C	N	O	0	0
			502	302	115	85		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 51 is a RNA chain called 23S rRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	81	Total	C	N	O	P	0	0
			1740	775	313	571	81		

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	A	208	Total	Mg	0
			208	208	
52	E	2	Total	Mg	0
			2	2	
52	H	1	Total	Mg	0
			1	1	
52	K	1	Total	Mg	0
			1	1	
52	N	1	Total	Mg	0
			1	1	
52	Q	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
52	R	1	Total 1	Mg 1	0
52	T	2	Total 2	Mg 2	0
52	Y	376	Total 376	Mg 376	0
52	U	10	Total 10	Mg 10	0
52	Z	10	Total 10	Mg 10	0
52	b	1	Total 1	Mg 1	0
52	c	1	Total 1	Mg 1	0
52	h	1	Total 1	Mg 1	0
52	i	2	Total 2	Mg 2	0
52	o	1	Total 1	Mg 1	0
52	p	1	Total 1	Mg 1	0
52	t	1	Total 1	Mg 1	0
52	y	2	Total 2	Mg 2	0
52	1	1	Total 1	Mg 1	0

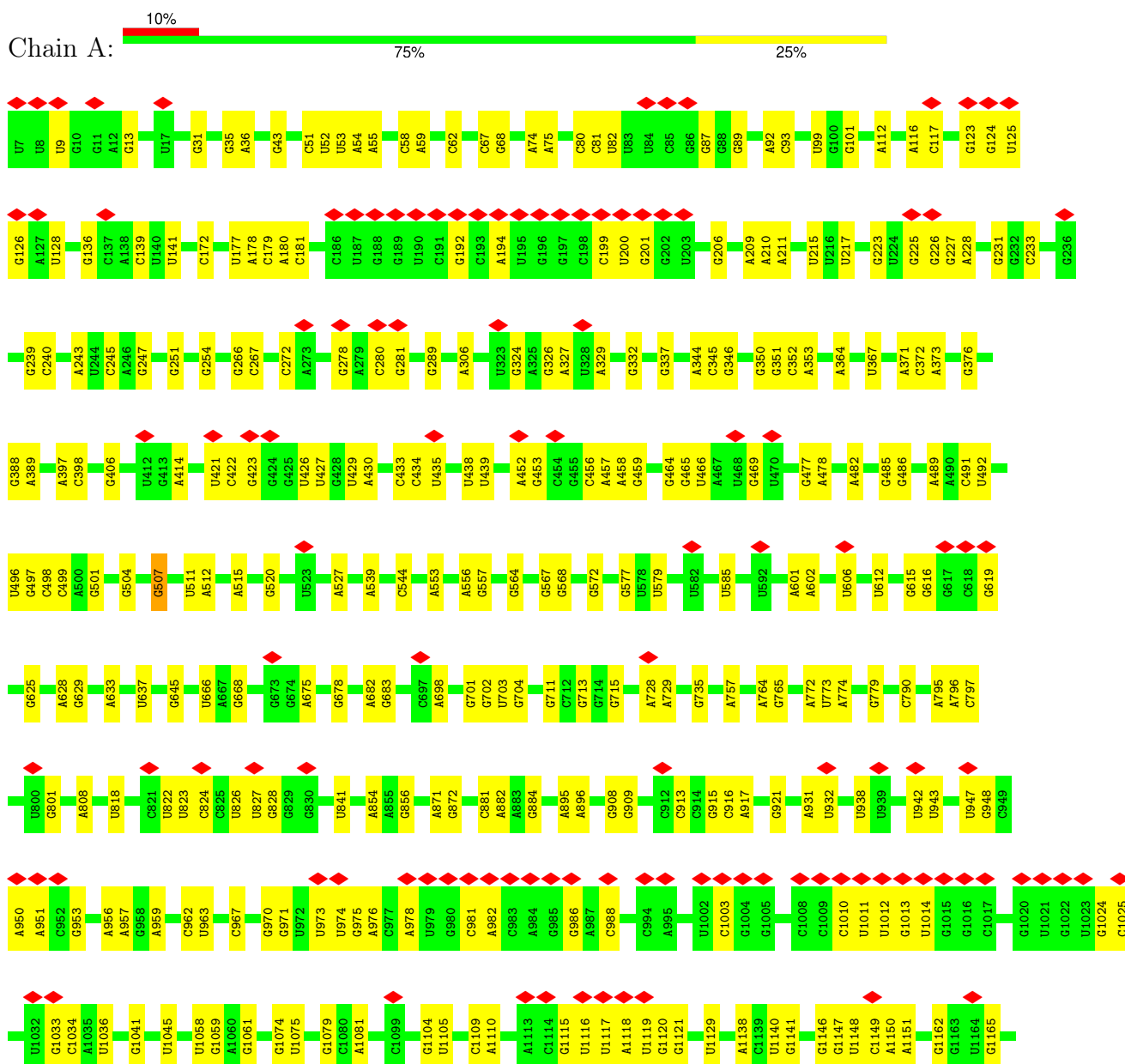
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

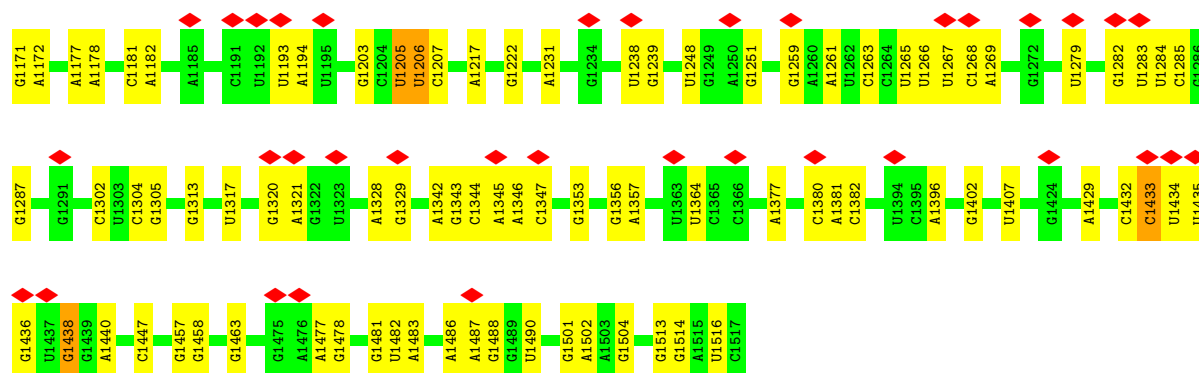
Mol	Chain	Residues	Atoms		AltConf
53	N	1	Total 1	Zn 1	0
53	R	1	Total 1	Zn 1	0
53	t	1	Total 1	Zn 1	0
53	y	1	Total 1	Zn 1	0
53	2	1	Total 1	Zn 1	0

3 Residue-property plots

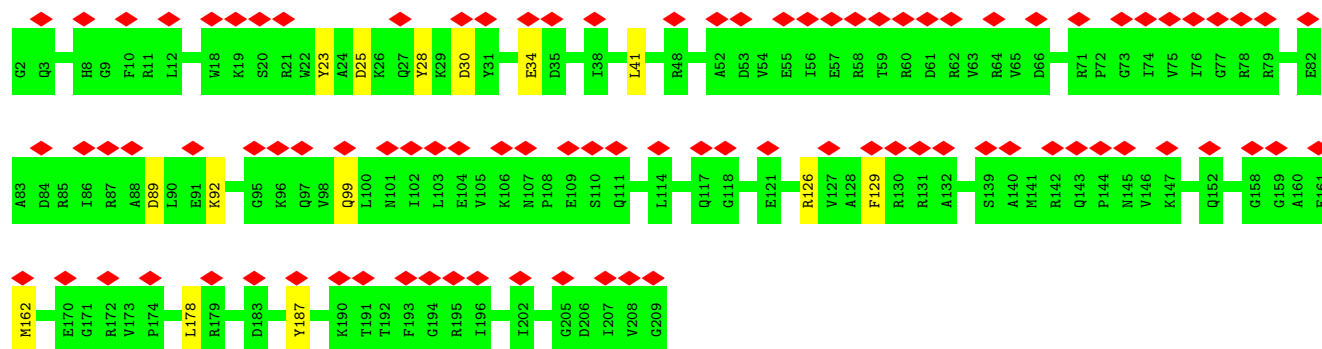
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

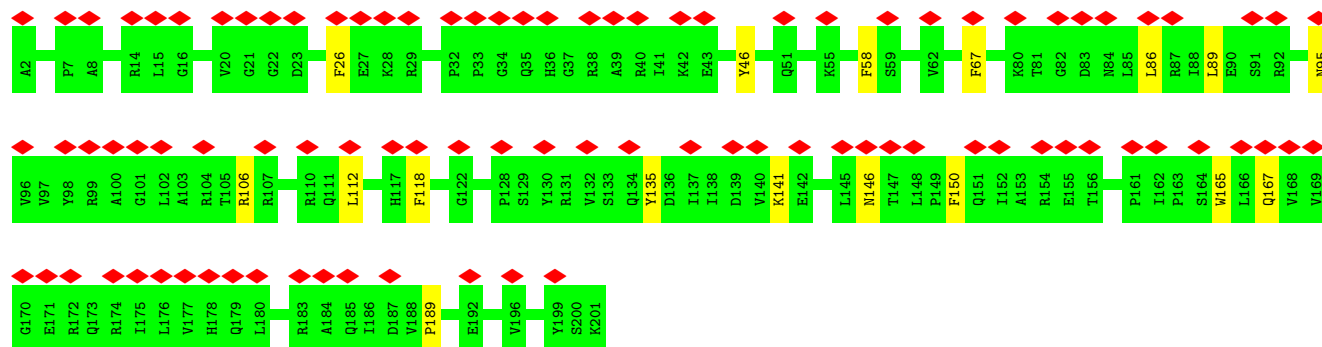
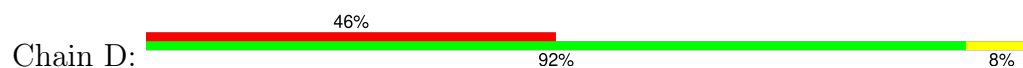




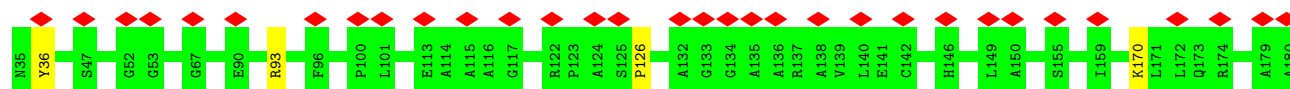
• Molecule 2: Small ribosomal subunit protein uS3

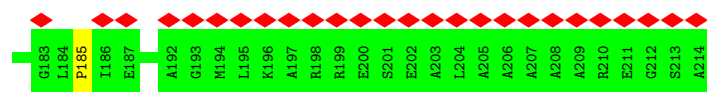


• Molecule 3: Small ribosomal subunit protein uS4

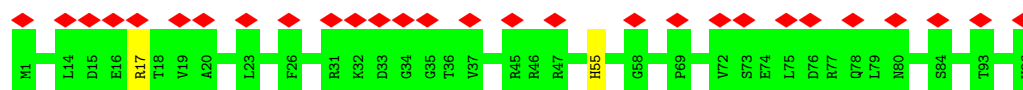


• Molecule 4: Small ribosomal subunit protein uS5

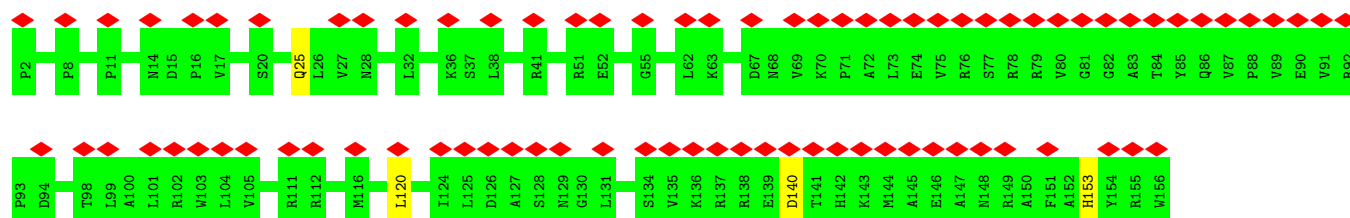




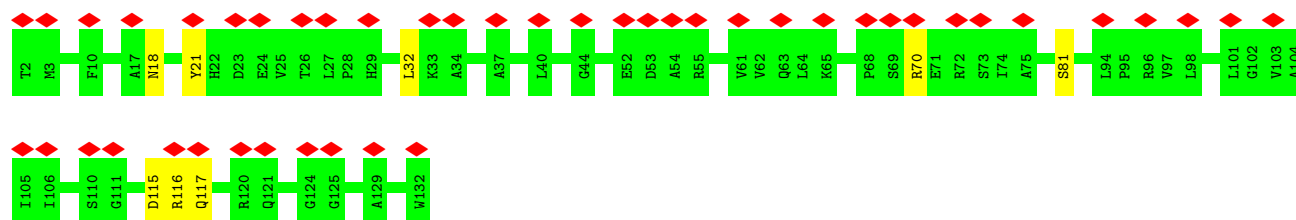
- Molecule 5: Small ribosomal subunit protein bS6



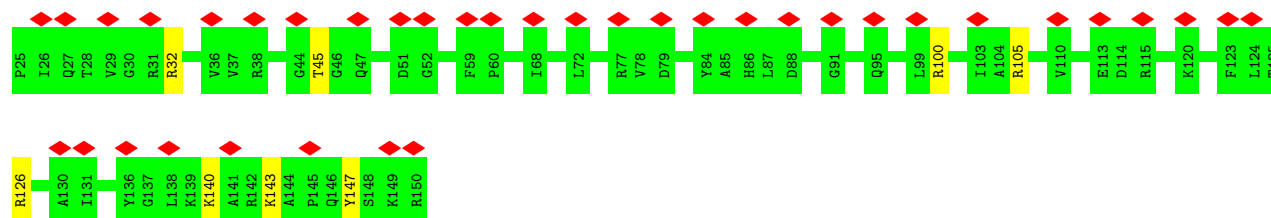
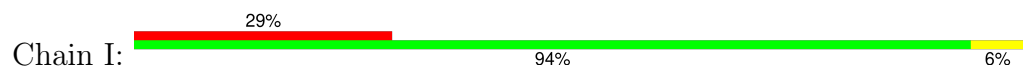
- Molecule 6: Small ribosomal subunit protein uS7



- Molecule 7: Small ribosomal subunit protein uS8

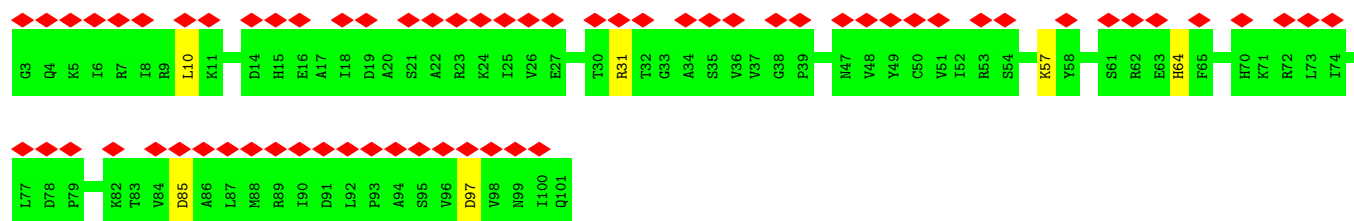


- Molecule 8: Small ribosomal subunit protein uS9



- Molecule 9: Small ribosomal subunit protein uS10





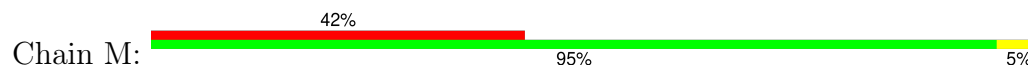
- Molecule 10: Small ribosomal subunit protein uS11



- Molecule 11: Small ribosomal subunit protein uS12



- Molecule 12: Small ribosomal subunit protein uS13



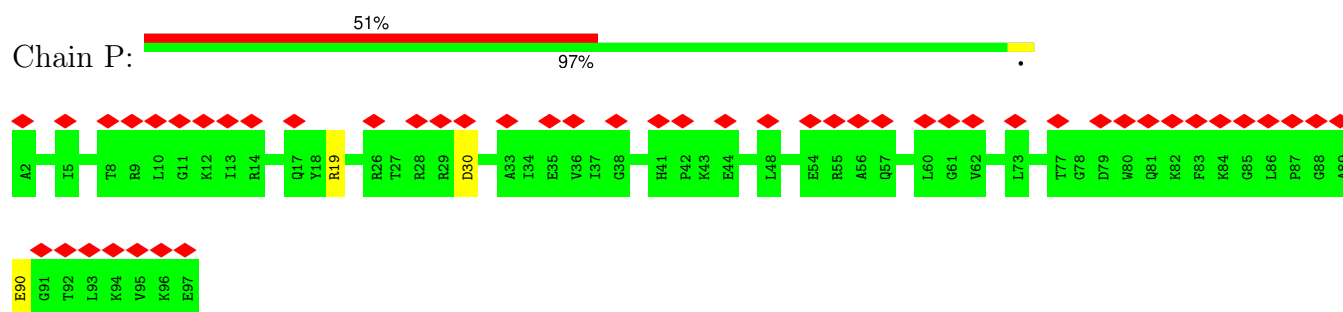
- Molecule 13: Small ribosomal subunit protein uS14B



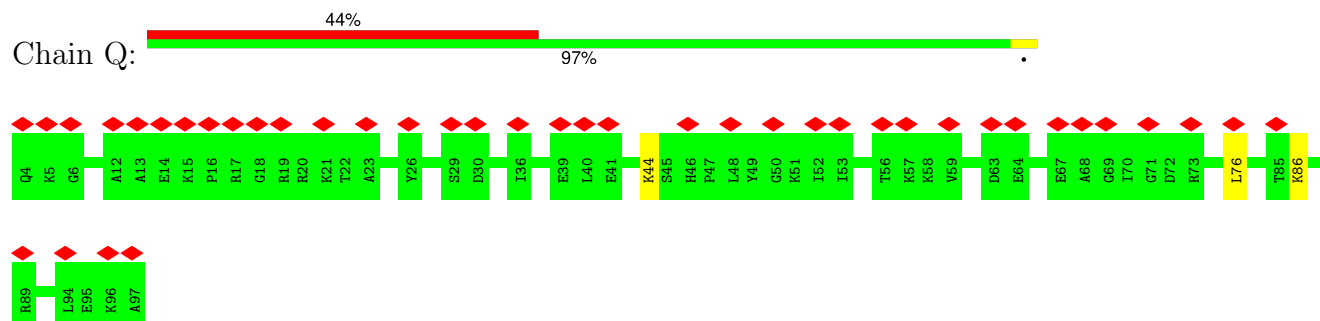
- Molecule 14: Small ribosomal subunit protein uS15



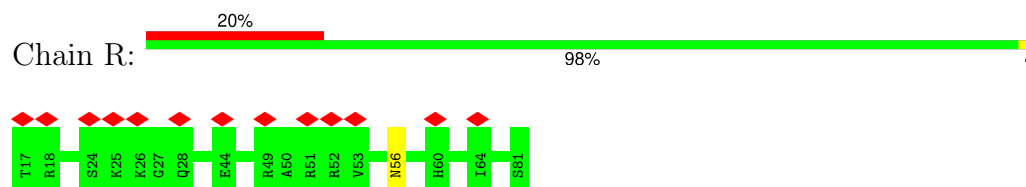
- Molecule 15: Small ribosomal subunit protein bS16



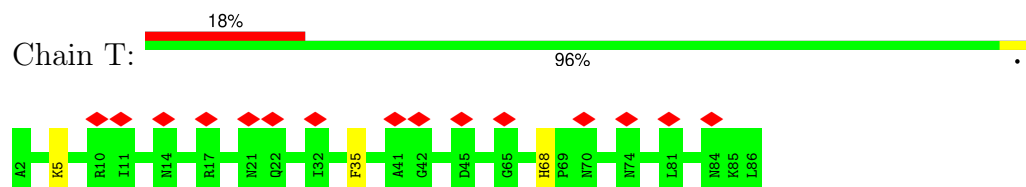
- Molecule 16: Small ribosomal subunit protein uS17



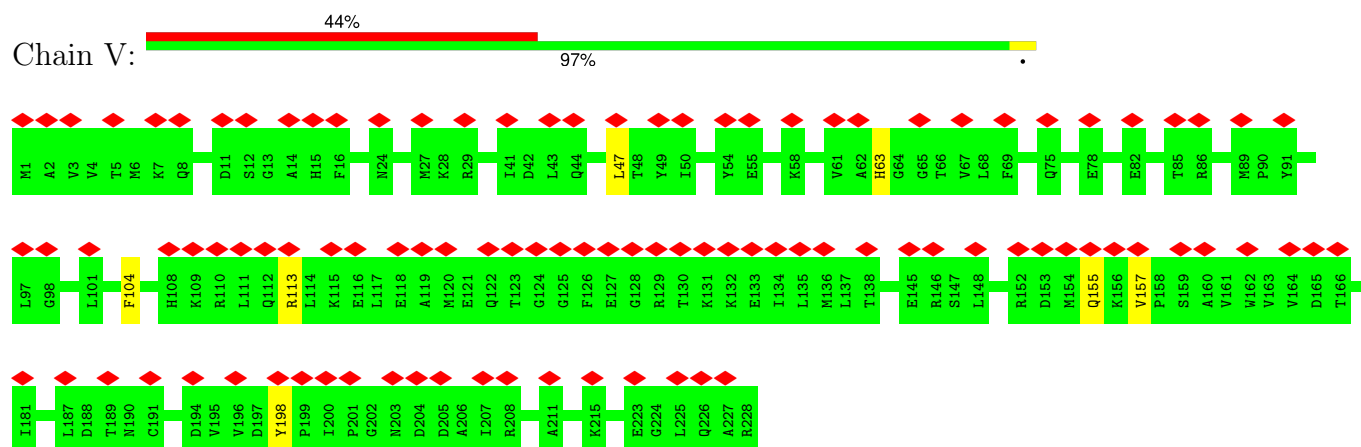
- Molecule 17: Small ribosomal subunit protein bS18B



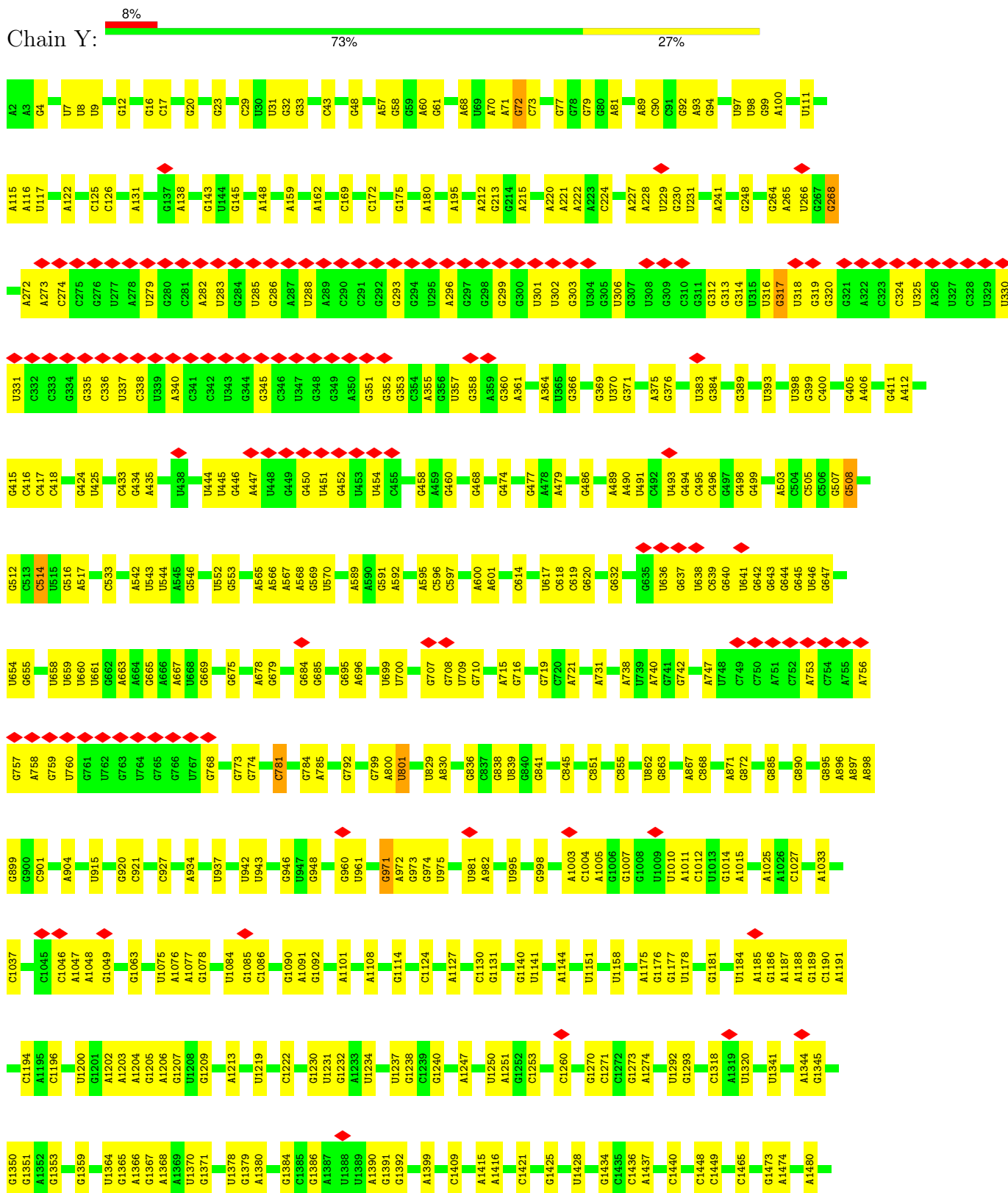
- Molecule 18: Small ribosomal subunit protein bS20

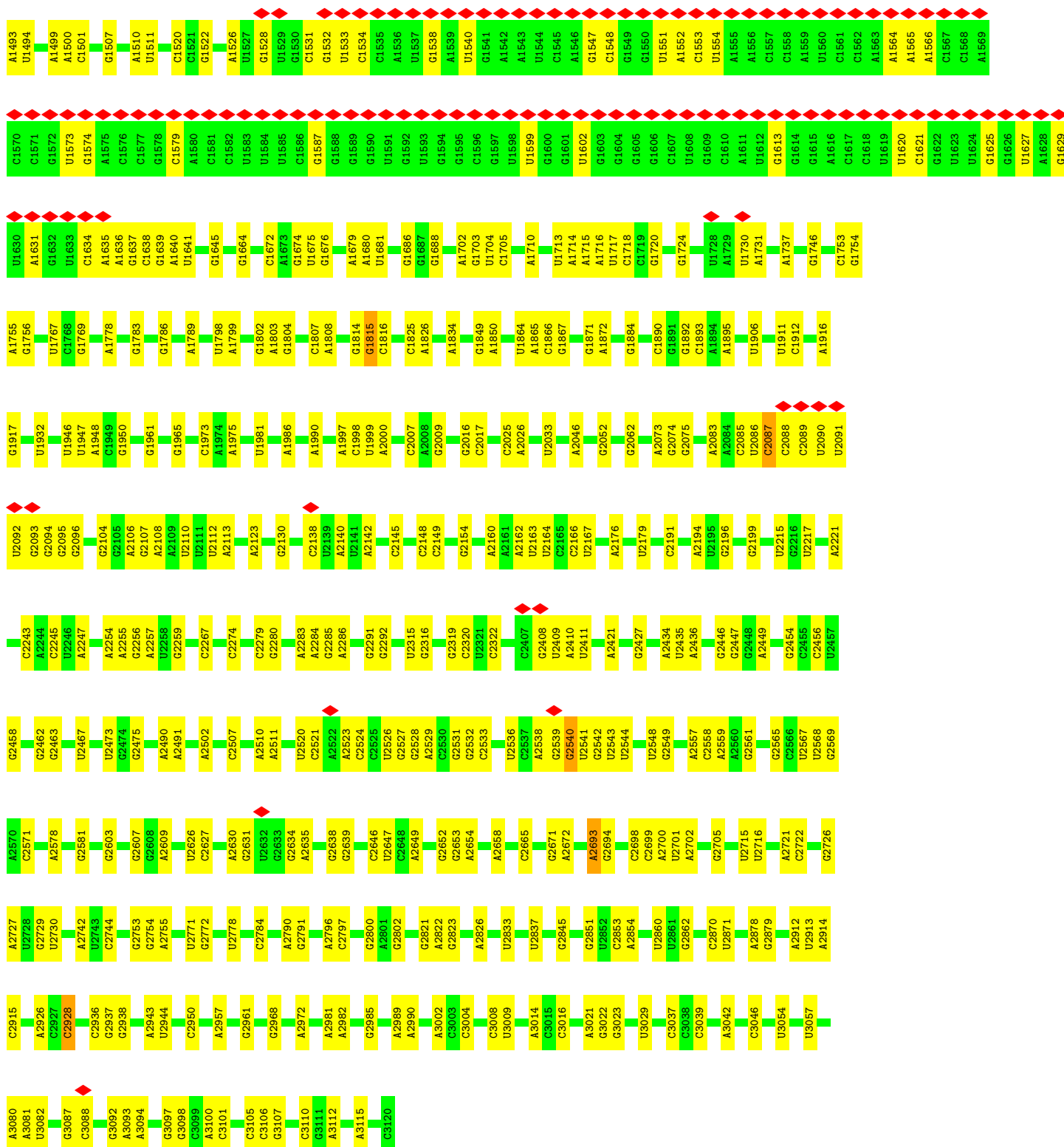


- Molecule 19: Small ribosomal subunit protein uS2



• Molecule 20: 23S rRNA



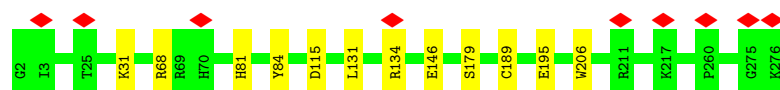


• Molecule 21: 5S rRNA

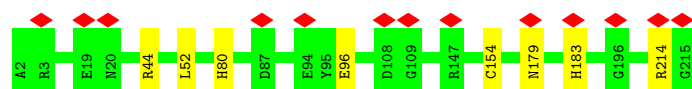
Chain U:



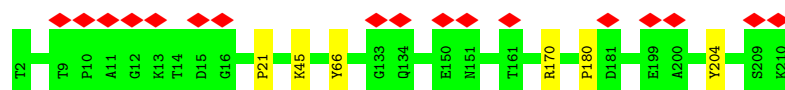
- Molecule 22: Large ribosomal subunit protein uL2



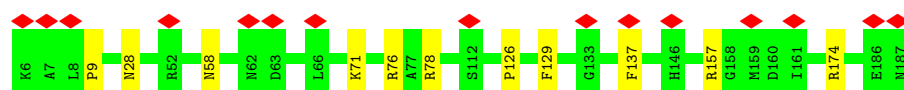
- Molecule 23: Large ribosomal subunit protein uL3



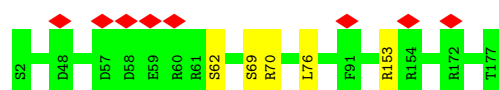
- Molecule 24: Large ribosomal subunit protein uL4



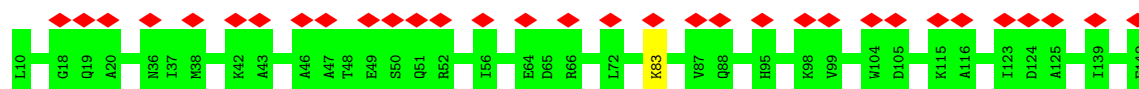
- Molecule 25: Large ribosomal subunit protein uL5



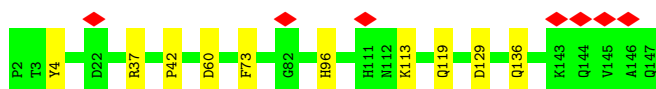
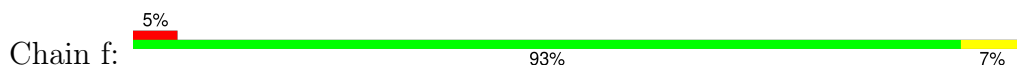
- Molecule 26: Large ribosomal subunit protein uL6



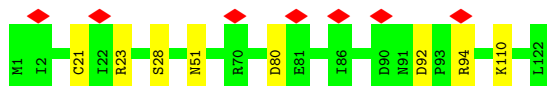
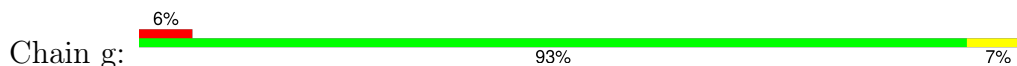
- Molecule 27: Large ribosomal subunit protein uL11



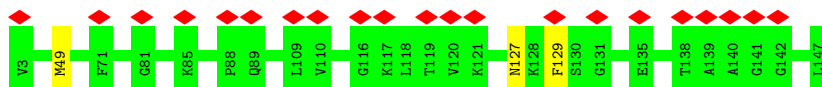
- Molecule 28: 50S ribosomal protein L13



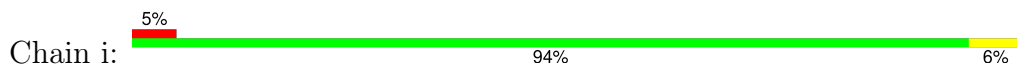
- Molecule 29: Large ribosomal subunit protein uL14



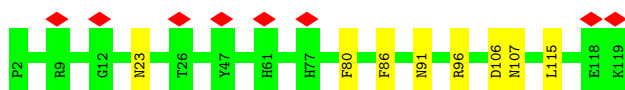
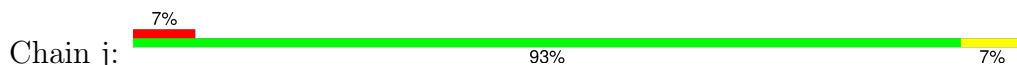
- Molecule 30: 50S ribosomal protein L15



- Molecule 31: Large ribosomal subunit protein uL16



- Molecule 32: Large ribosomal subunit protein bL17

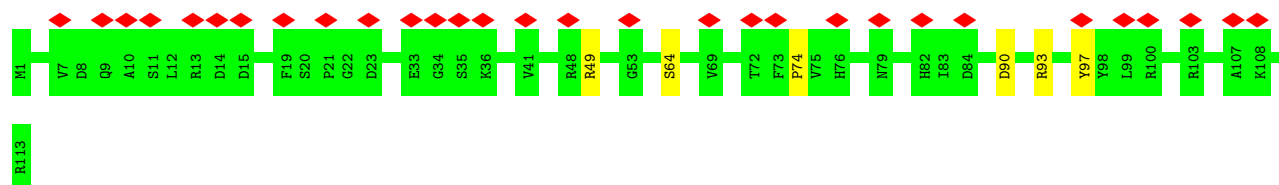


- Molecule 33: Large ribosomal subunit protein uL18



- Molecule 34: Large ribosomal subunit protein bL19

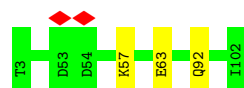




- Molecule 35: Large ribosomal subunit protein bL20



- Molecule 36: Large ribosomal subunit protein bL21



- Molecule 37: 50S ribosomal protein L22



- Molecule 38: Large ribosomal subunit protein uL23



- Molecule 39: Large ribosomal subunit protein uL24

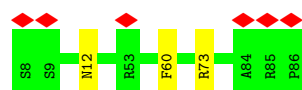


- Molecule 40: Large ribosomal subunit protein bL25

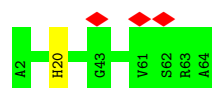




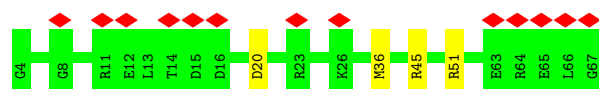
- Molecule 41: Large ribosomal subunit protein bL27



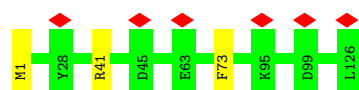
- Molecule 42: Large ribosomal subunit protein bL28



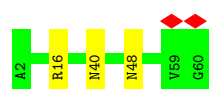
- Molecule 43: Large ribosomal subunit protein uL29



- Molecule 44: Large ribosomal subunit protein uL10

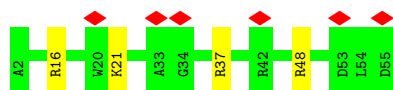


- Molecule 45: Large ribosomal subunit protein uL30

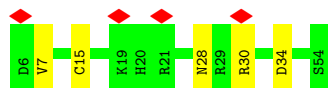
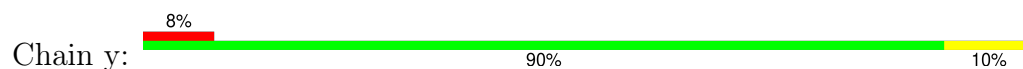


- Molecule 46: Large ribosomal subunit protein bL32

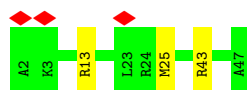
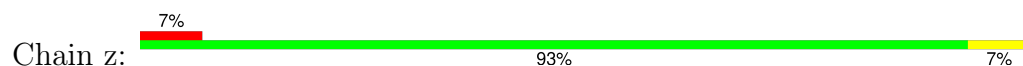




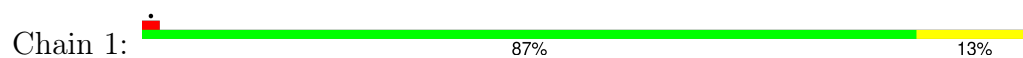
- Molecule 47: Large ribosomal subunit protein bL33A



- Molecule 48: 50S ribosomal protein L34



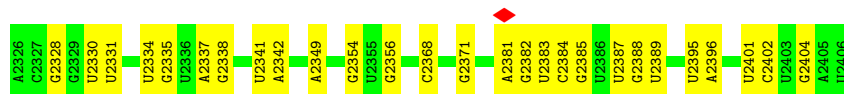
- Molecule 49: Large ribosomal subunit protein bL35



- Molecule 50: 50S ribosomal protein L36



- Molecule 51: 23S rRNA fragment



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1466881	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 ($e^-/\text{\AA}^2$)	901.165	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	96000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	17.420	Depositor
Minimum map value	-9.464	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.487	Depositor
Recommended contour level	0.968	Depositor
Map size (\AA)	539.784, 539.784, 539.784	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.833, 0.833, 0.833	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, G7M, MG

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	A	0.26	0/36278	0.77	14/56596 (0.0%)
2	C	0.26	0/1684	0.58	0/2261
3	D	0.29	0/1672	0.65	1/2251 (0.0%)
4	E	0.32	0/1312	0.68	2/1772 (0.1%)
5	F	0.25	0/782	0.58	0/1059
6	G	0.25	0/1252	0.58	0/1690
7	H	0.27	0/1025	0.59	0/1385
8	I	0.25	0/1012	0.53	0/1362
9	J	0.26	0/802	0.58	0/1086
10	K	0.33	0/873	0.65	2/1180 (0.2%)
11	L	0.27	0/969	0.60	0/1294
12	M	0.42	2/942 (0.2%)	0.80	4/1260 (0.3%)
13	N	0.66	2/488 (0.4%)	1.30	4/650 (0.6%)
14	O	0.25	0/729	0.59	0/977
15	P	0.28	0/778	0.55	0/1049
16	Q	0.25	0/759	0.57	0/1016
17	R	0.36	0/518	0.70	0/693
18	T	0.27	0/663	0.62	0/882
19	V	0.26	0/1822	0.54	1/2457 (0.0%)
20	Y	0.67	14/73003 (0.0%)	0.92	97/113787 (0.1%)
21	U	0.39	0/2821	0.81	0/4396
22	Z	0.33	0/2153	0.63	0/2895
23	a	0.31	0/1609	0.60	0/2165
24	b	0.35	1/1592 (0.1%)	0.67	2/2153 (0.1%)
25	c	0.44	3/1467 (0.2%)	0.87	5/1973 (0.3%)
26	d	0.30	0/1369	0.56	0/1848
27	e	0.23	0/986	0.42	0/1303
28	f	0.34	0/1157	0.59	1/1567 (0.1%)
29	g	0.37	0/946	0.63	0/1268
30	h	0.31	0/1091	0.59	0/1457
31	i	0.32	0/1118	0.60	0/1506
32	j	0.30	0/945	0.57	0/1267

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	k	0.28	0/966	0.59	0/1298
34	l	1.24	3/921 (0.3%)	1.32	5/1236 (0.4%)
35	m	0.35	0/1000	0.63	0/1341
36	n	0.32	0/764	0.52	0/1030
37	o	0.30	0/887	0.59	0/1204
38	p	0.32	0/766	0.56	0/1030
39	q	0.28	0/738	0.51	0/987
40	r	0.27	0/1443	0.55	0/1970
41	s	0.31	0/595	0.62	0/798
42	t	0.30	0/478	0.58	0/641
43	u	0.31	0/534	0.70	0/713
44	v	0.26	0/925	0.49	0/1246
45	w	0.29	0/477	0.58	0/640
46	x	0.33	0/427	0.70	0/572
47	y	0.35	0/413	0.63	0/553
48	z	0.35	0/380	0.77	0/500
49	1	0.36	0/507	0.75	2/672 (0.3%)
50	2	0.31	0/303	0.61	0/401
51	4	0.16	0/1943	0.71	0/3020
All	All	0.51	25/159084 (0.0%)	0.82	140/238357 (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
9	J	0	1
29	g	0	1
30	h	0	1
All	All	0	3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	360	G	C6-N1	58.77	1.80	1.39
20	Y	360	G	N1-C2	54.31	1.81	1.37
20	Y	360	G	N3-C4	49.24	1.70	1.35
20	Y	360	G	C2-N3	43.69	1.67	1.32
20	Y	360	G	C5-C4	39.41	1.66	1.38
34	l	74	PRO	CG-CD	-34.30	0.37	1.50
20	Y	268	G	C1'-N9	33.00	1.98	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	360	G	C5-C6	30.71	1.73	1.42
20	Y	268	G	N9-C8	25.21	1.55	1.37
20	Y	268	G	N9-C4	25.18	1.58	1.38
20	Y	268	G	N7-C5	-11.94	1.32	1.39
13	N	30	PRO	CG-CD	-11.13	1.14	1.50
34	l	74	PRO	CB-CG	9.08	1.95	1.50
12	M	113	PRO	CG-CD	-7.48	1.25	1.50
25	c	9	PRO	CG-CD	-7.38	1.26	1.50
34	l	74	PRO	N-CD	6.68	1.57	1.47
13	N	30	PRO	CB-CG	-6.43	1.17	1.50
12	M	113	PRO	N-CD	6.40	1.56	1.47
20	Y	268	G	C8-N7	-6.23	1.27	1.30
25	c	9	PRO	N-CD	5.78	1.55	1.47
20	Y	317	G	C6-O6	-5.72	1.19	1.24
25	c	126	PRO	CG-CD	-5.71	1.31	1.50
20	Y	495	C	C4-N4	-5.61	1.28	1.33
24	b	21	PRO	N-CD	-5.56	1.40	1.47
20	Y	268	G	C2'-C1'	5.51	1.59	1.53

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	268	G	C8-N9-C4	-72.53	77.39	106.40
20	Y	268	G	N7-C8-N9	48.47	137.33	113.10
34	l	74	PRO	N-CD-CG	-36.18	48.92	103.20
20	Y	317	G	N1-C6-O6	-32.75	100.25	119.90
20	Y	268	G	N9-C4-C5	31.84	118.14	105.40
20	Y	268	G	N3-C4-C5	-28.26	114.47	128.60
20	Y	317	G	C5-C6-O6	26.20	144.32	128.60
20	Y	360	G	C2-N3-C4	23.45	123.62	111.90
20	Y	495	C	N3-C4-N4	-21.46	102.98	118.00
13	N	30	PRO	N-CD-CG	-19.38	74.13	103.20
20	Y	360	G	N1-C2-N3	-17.69	113.29	123.90
20	Y	268	G	C2-N3-C4	17.23	120.52	111.90
25	c	126	PRO	CA-N-CD	-16.58	88.28	111.50
20	Y	268	G	C5-N7-C8	-16.55	96.02	104.30
20	Y	268	G	C4-N9-C1'	16.23	147.60	126.50
13	N	30	PRO	CA-N-CD	-15.04	90.45	111.50
20	Y	495	C	C5-C4-N4	14.38	130.27	120.20
13	N	30	PRO	CA-CB-CG	-13.92	77.55	104.00
24	b	21	PRO	CA-N-CD	-13.67	92.36	111.50
34	l	74	PRO	CA-CB-CG	-13.44	78.46	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	360	G	C4-C5-N7	-13.38	105.45	110.80
25	c	9	PRO	CA-N-CD	-13.29	92.90	111.50
20	Y	268	G	C6-C5-N7	-12.95	122.63	130.40
12	M	113	PRO	CA-N-CD	-12.93	93.40	111.50
20	Y	268	G	C4-C5-C6	12.58	126.35	118.80
20	Y	360	G	N3-C4-N9	12.21	133.33	126.00
20	Y	360	G	N7-C8-N9	11.79	118.99	113.10
20	Y	495	C	N3-C4-C5	11.78	126.61	121.90
20	Y	268	G	N9-C1'-C2'	11.49	128.94	114.00
25	c	9	PRO	N-CD-CG	-10.89	86.87	103.20
20	Y	72	G	OP2-P-O3'	-10.86	81.31	105.20
3	D	189	PRO	CA-N-CD	-10.81	96.36	111.50
20	Y	799	G	OP1-P-O3'	-10.80	81.43	105.20
20	Y	800	A	OP1-P-O3'	-10.80	81.43	105.20
20	Y	800	A	OP2-P-O3'	-10.78	81.48	105.20
1	A	1205	U	N3-C2-O2	-10.64	114.75	122.20
20	Y	799	G	OP2-P-O3'	-10.62	81.83	105.20
20	Y	360	G	N3-C4-C5	-10.55	123.33	128.60
4	E	126	PRO	CA-N-CD	-10.51	96.79	111.50
20	Y	72	G	OP1-P-O3'	-10.27	82.61	105.20
12	M	113	PRO	N-CD-CG	-10.13	88.00	103.20
10	K	126	PRO	CA-N-CD	-9.67	97.97	111.50
28	f	42	PRO	CA-N-CD	-9.50	98.19	111.50
20	Y	1409	C	N3-C2-O2	-9.26	115.42	121.90
13	N	30	PRO	CB-CG-CD	9.12	142.07	106.50
34	l	74	PRO	CA-N-CD	-9.03	98.86	111.50
4	E	185	PRO	CA-N-CD	-8.79	99.19	111.50
20	Y	2148	C	N3-C2-O2	-8.54	115.92	121.90
20	Y	1449	C	N3-C2-O2	-8.46	115.98	121.90
34	l	74	PRO	CB-CG-CD	-8.34	73.99	106.50
20	Y	268	G	O4'-C1'-N9	8.33	114.87	108.20
20	Y	514	C	N3-C2-O2	-8.30	116.09	121.90
1	A	1433	C	N3-C2-O2	-8.13	116.21	121.90
20	Y	495	C	C4-C5-C6	-8.04	113.38	117.40
1	A	1345	A	N1-C6-N6	-8.02	113.79	118.60
20	Y	508	G	N1-C6-O6	-7.89	115.16	119.90
20	Y	2087	C	N1-C2-O2	7.62	123.47	118.90
20	Y	801	U	OP1-P-OP2	7.59	130.98	119.60
12	M	56	LEU	CA-CB-CG	7.56	132.69	115.30
1	A	1205	U	N1-C2-N3	7.55	119.43	114.90
24	b	180	PRO	CA-N-CD	-7.49	101.02	111.50
20	Y	73	C	OP1-P-OP2	7.27	130.50	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	800	A	OP1-P-OP2	7.26	130.49	119.60
20	Y	2693	A	N1-C6-N6	7.22	122.93	118.60
20	Y	317	G	C4-C5-C6	-7.21	114.48	118.80
20	Y	1816	C	N3-C2-O2	-7.20	116.86	121.90
20	Y	360	G	N3-C2-N2	7.08	124.86	119.90
20	Y	2772	G	N3-C2-N2	-6.84	115.11	119.90
20	Y	508	G	C5-C6-O6	6.77	132.66	128.60
25	c	126	PRO	N-CD-CG	-6.67	93.20	103.20
20	Y	2148	C	N1-C2-O2	6.57	122.84	118.90
20	Y	2087	C	C2-N1-C1'	6.57	126.02	118.80
20	Y	1816	C	N1-C2-O2	6.53	122.82	118.90
20	Y	2243	C	C2-N1-C1'	6.52	125.97	118.80
20	Y	2772	G	N9-C4-C5	6.50	108.00	105.40
20	Y	317	G	C5-C6-N1	6.44	114.72	111.50
20	Y	360	G	C5-C6-N1	6.42	114.71	111.50
20	Y	2928	C	N3-C2-O2	-6.37	117.44	121.90
20	Y	971	G	N3-C4-N9	-6.30	122.22	126.00
20	Y	360	G	N1-C2-N2	6.25	121.83	116.20
20	Y	514	C	N1-C2-O2	6.23	122.64	118.90
20	Y	1425	G	N1-C6-O6	-6.22	116.17	119.90
25	c	9	PRO	CA-CB-CG	-6.18	92.26	104.00
1	A	80	C	N3-C2-O2	-6.14	117.60	121.90
20	Y	781	C	N3-C2-O2	-6.11	117.62	121.90
20	Y	268	G	C8-N9-C1'	6.10	134.93	127.00
20	Y	1815	G	N3-C4-N9	-6.05	122.37	126.00
1	A	1345	A	C5-C6-N6	6.04	128.53	123.70
20	Y	495	C	N1-C2-O2	6.01	122.50	118.90
20	Y	317	G	N1-C2-N3	-6.00	120.30	123.90
20	Y	1409	C	N3-C4-N4	-5.97	113.82	118.00
34	l	74	PRO	N-CA-CB	-5.90	96.11	102.60
12	M	113	PRO	CA-CB-CG	-5.89	92.81	104.00
20	Y	1434	G	C5-C6-O6	5.88	132.13	128.60
1	A	1205	U	C2-N3-C4	-5.88	123.47	127.00
20	Y	2243	C	C6-N1-C1'	-5.84	113.79	120.80
20	Y	1814	G	N3-C4-N9	-5.83	122.50	126.00
20	Y	2928	C	C6-N1-C2	-5.77	117.99	120.30
20	Y	268	G	C6-N1-C2	-5.70	121.68	125.10
1	A	233	C	N1-C2-O2	5.64	122.28	118.90
1	A	1438	G	C5-C6-O6	5.60	131.96	128.60
20	Y	710	G	C6-C5-N7	-5.57	127.06	130.40
10	K	126	PRO	N-CD-CG	-5.55	94.88	103.20
20	Y	317	G	C6-C5-N7	5.54	133.72	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1438	G	N1-C6-O6	-5.54	116.58	119.90
49	1	37	PRO	CA-N-CD	-5.53	103.75	111.50
20	Y	2087	C	C6-N1-C1'	-5.50	114.20	120.80
20	Y	2540	G	N3-C4-N9	-5.49	122.70	126.00
20	Y	1434	G	N3-C4-N9	-5.49	122.71	126.00
20	Y	360	G	C6-C5-N7	5.49	133.69	130.40
1	A	1206	U	C2-N1-C1'	5.48	124.28	117.70
20	Y	360	G	N9-C4-C5	-5.46	103.22	105.40
20	Y	1409	C	C5-C4-N4	5.41	123.98	120.20
20	Y	2961	G	N1-C6-O6	-5.39	116.66	119.90
20	Y	1037	C	N3-C2-O2	-5.35	118.16	121.90
20	Y	2693	A	C5-C6-N6	-5.32	119.44	123.70
49	1	2	PRO	CA-N-CD	-5.31	104.07	111.50
20	Y	2456	C	N3-C2-O2	-5.30	118.19	121.90
20	Y	2259	G	N3-C4-N9	5.28	129.17	126.00
20	Y	1449	C	N1-C2-O2	5.27	122.06	118.90
1	A	1438	G	N3-C4-N9	-5.27	122.84	126.00
20	Y	79	G	N3-C4-N9	-5.27	122.84	126.00
20	Y	2540	G	C8-N9-C1'	5.22	133.79	127.00
20	Y	710	G	C4-N9-C1'	5.21	133.27	126.50
20	Y	2784	C	C2-N3-C4	5.19	122.50	119.90
20	Y	1392	G	C5-C6-O6	5.18	131.71	128.60
20	Y	2149	C	N3-C2-O2	-5.17	118.28	121.90
20	Y	1434	G	C2-N3-C4	-5.17	109.32	111.90
1	A	1432	C	N1-C2-O2	5.17	122.00	118.90
20	Y	2540	G	C4-N9-C1'	-5.16	119.79	126.50
20	Y	1884	G	N1-C6-O6	-5.15	116.81	119.90
20	Y	2243	C	N1-C2-O2	5.15	121.99	118.90
20	Y	2540	G	C6-C5-N7	5.15	133.49	130.40
20	Y	2784	C	N3-C4-C5	-5.14	119.84	121.90
20	Y	496	C	N3-C2-O2	-5.14	118.30	121.90
20	Y	710	G	C8-N9-C1'	-5.13	120.33	127.00
1	A	206	G	N3-C4-N9	-5.09	122.94	126.00
19	V	47	LEU	CA-CB-CG	5.09	127.01	115.30
20	Y	971	G	N9-C4-C5	5.02	107.41	105.40
20	Y	533	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	J	10	LEU	Peptide

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Mol	Chain	Res	Type	Group
29	g	23	ARG	Sidechain
30	h	129	PHE	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	
2	C	206/208 (99%)	192 (93%)	14 (7%)	0	100	100
3	D	198/200 (99%)	186 (94%)	12 (6%)	0	100	100
4	E	178/180 (99%)	167 (94%)	11 (6%)	0	100	100
5	F	94/96 (98%)	87 (93%)	7 (7%)	0	100	100
6	G	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
7	H	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
8	I	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
9	J	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	13	23
10	K	113/115 (98%)	104 (92%)	9 (8%)	0	100	100
11	L	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
12	M	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
13	N	58/60 (97%)	50 (86%)	8 (14%)	0	100	100
14	O	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
15	P	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
16	Q	92/94 (98%)	84 (91%)	8 (9%)	0	100	100
17	R	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
18	T	83/85 (98%)	81 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	V	226/228 (99%)	211 (93%)	13 (6%)	2 (1%)	14	26
22	Z	273/275 (99%)	242 (89%)	31 (11%)	0	100	100
23	a	212/214 (99%)	185 (87%)	27 (13%)	0	100	100
24	b	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
25	c	180/182 (99%)	169 (94%)	11 (6%)	0	100	100
26	d	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
27	e	96/133 (72%)	96 (100%)	0	0	100	100
28	f	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
29	g	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
30	h	143/145 (99%)	121 (85%)	22 (15%)	0	100	100
31	i	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	19	32
32	j	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
33	k	124/126 (98%)	115 (93%)	9 (7%)	0	100	100
34	l	111/113 (98%)	92 (83%)	19 (17%)	0	100	100
35	m	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
36	n	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
37	o	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
38	p	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
39	q	93/97 (96%)	85 (91%)	8 (9%)	0	100	100
40	r	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
41	s	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
42	t	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
43	u	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
44	v	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
45	w	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
46	x	52/54 (96%)	45 (86%)	7 (14%)	0	100	100
47	y	47/49 (96%)	41 (87%)	5 (11%)	1 (2%)	5	8
48	z	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
49	1	61/63 (97%)	47 (77%)	14 (23%)	0	100	100
50	2	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	5592/5723 (98%)	5169 (92%)	418 (8%)	5 (0%)	50	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	V	155	GLN
31	i	29	PHE
19	V	157	VAL
9	J	57	LYS
47	y	7	VAL

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	
2	C	170/170 (100%)	156 (92%)	14 (8%)	9	18
3	D	175/175 (100%)	159 (91%)	16 (9%)	7	14
4	E	127/127 (100%)	124 (98%)	3 (2%)	44	68
5	F	85/85 (100%)	83 (98%)	2 (2%)	44	68
6	G	131/131 (100%)	127 (97%)	4 (3%)	35	59
7	H	107/107 (100%)	99 (92%)	8 (8%)	11	21
8	I	102/102 (100%)	94 (92%)	8 (8%)	10	19
9	J	89/89 (100%)	85 (96%)	4 (4%)	23	43
10	K	89/89 (100%)	84 (94%)	5 (6%)	17	33
11	L	103/103 (100%)	101 (98%)	2 (2%)	52	74
12	M	99/99 (100%)	95 (96%)	4 (4%)	27	48
13	N	49/49 (100%)	48 (98%)	1 (2%)	50	73
14	O	76/76 (100%)	75 (99%)	1 (1%)	65	83
15	P	79/79 (100%)	76 (96%)	3 (4%)	28	50
16	Q	80/80 (100%)	77 (96%)	3 (4%)	28	50
17	R	55/55 (100%)	54 (98%)	1 (2%)	54	76
18	T	69/69 (100%)	66 (96%)	3 (4%)	25	45
19	V	191/191 (100%)	187 (98%)	4 (2%)	48	72
22	Z	215/215 (100%)	203 (94%)	12 (6%)	17	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	a	160/160 (100%)	152 (95%)	8 (5%)	20	38
24	b	169/169 (100%)	165 (98%)	4 (2%)	44	68
25	c	151/151 (100%)	142 (94%)	9 (6%)	16	30
26	d	148/148 (100%)	143 (97%)	5 (3%)	32	55
27	e	102/102 (100%)	101 (99%)	1 (1%)	73	87
28	f	119/119 (100%)	110 (92%)	9 (8%)	11	20
29	g	100/100 (100%)	93 (93%)	7 (7%)	12	23
30	h	112/112 (100%)	110 (98%)	2 (2%)	54	76
31	i	114/114 (100%)	107 (94%)	7 (6%)	15	29
32	j	97/97 (100%)	89 (92%)	8 (8%)	9	18
33	k	93/93 (100%)	91 (98%)	2 (2%)	47	70
34	l	100/100 (100%)	95 (95%)	5 (5%)	20	38
35	m	97/97 (100%)	90 (93%)	7 (7%)	12	22
36	n	81/81 (100%)	78 (96%)	3 (4%)	29	52
37	o	90/90 (100%)	83 (92%)	7 (8%)	10	19
38	p	83/83 (100%)	78 (94%)	5 (6%)	16	30
39	q	81/81 (100%)	80 (99%)	1 (1%)	67	84
40	r	155/155 (100%)	152 (98%)	3 (2%)	52	74
41	s	58/58 (100%)	55 (95%)	3 (5%)	19	37
42	t	50/50 (100%)	49 (98%)	1 (2%)	50	73
43	u	58/58 (100%)	54 (93%)	4 (7%)	13	24
44	v	89/89 (100%)	86 (97%)	3 (3%)	32	55
45	w	52/52 (100%)	49 (94%)	3 (6%)	17	32
46	x	43/43 (100%)	39 (91%)	4 (9%)	7	13
47	y	47/47 (100%)	43 (92%)	4 (8%)	8	16
48	z	35/35 (100%)	32 (91%)	3 (9%)	8	16
49	1	53/53 (100%)	47 (89%)	6 (11%)	4	8
50	2	35/35 (100%)	32 (91%)	3 (9%)	8	16
All	All	4663/4663 (100%)	4438 (95%)	225 (5%)	24	40

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	23	TYR
2	C	25	ASP
2	C	28	TYR
2	C	30	ASP
2	C	34	GLU
2	C	41	LEU
2	C	89	ASP
2	C	92	LYS
2	C	99	GLN
2	C	126	ARG
2	C	129	PHE
2	C	162	MET
2	C	178	LEU
2	C	187	TYR
3	D	26	PHE
3	D	46	TYR
3	D	58	PHE
3	D	67	PHE
3	D	86	LEU
3	D	89	LEU
3	D	95	ASN
3	D	106	ARG
3	D	112	LEU
3	D	118	PHE
3	D	135	TYR
3	D	141	LYS
3	D	146	ASN
3	D	150	PHE
3	D	165	TRP
3	D	167	GLN
4	E	36	TYR
4	E	93	ARG
4	E	170	LYS
5	F	17	ARG
5	F	55	HIS
6	G	25	GLN
6	G	120	LEU
6	G	140	ASP
6	G	153	HIS
7	H	18	ASN
7	H	21	TYR
7	H	32	LEU
7	H	70	ARG

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Mol	Chain	Res	Type
7	H	81	SER
7	H	115	ASP
7	H	116	ARG
7	H	117	GLN
8	I	32	ARG
8	I	45	THR
8	I	100	ARG
8	I	105	ARG
8	I	126	ARG
8	I	140	LYS
8	I	143	LYS
8	I	147	TYR
9	J	31	ARG
9	J	64	HIS
9	J	85	ASP
9	J	97	ASP
10	K	27	HIS
10	K	36	PHE
10	K	81	ARG
10	K	96	LYS
10	K	128	ASN
11	L	12	ARG
11	L	103	ASP
12	M	15	MET
12	M	46	LYS
12	M	59	TYR
12	M	92	HIS
13	N	13	LYS
14	O	42	HIS
15	P	19	ARG
15	P	30	ASP
15	P	90	GLU
16	Q	44	LYS
16	Q	76	LEU
16	Q	86	LYS
17	R	56	ASN
18	T	5	LYS
18	T	35	PHE
18	T	68	HIS
19	V	63	HIS
19	V	104	PHE
19	V	113	ARG

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Mol	Chain	Res	Type
19	V	198	TYR
22	Z	31	LYS
22	Z	68	ARG
22	Z	81	HIS
22	Z	84	TYR
22	Z	115	ASP
22	Z	131	LEU
22	Z	134	ARG
22	Z	146	GLU
22	Z	179	SER
22	Z	189	CYS
22	Z	195	GLU
22	Z	206	TRP
23	a	44	ARG
23	a	52	LEU
23	a	80	HIS
23	a	96	GLU
23	a	154	CYS
23	a	179	ASN
23	a	183	HIS
23	a	214	ARG
24	b	45	LYS
24	b	66	TYR
24	b	170	ARG
24	b	204	TYR
25	c	28	ASN
25	c	58	ASN
25	c	71	LYS
25	c	76	ARG
25	c	78	ARG
25	c	129	PHE
25	c	137	PHE
25	c	157	ARG
25	c	174	ARG
26	d	62	SER
26	d	69	SER
26	d	70	ARG
26	d	76	LEU
26	d	153	ARG
27	e	83	LYS
28	f	4	TYR
28	f	37	ARG

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Mol	Chain	Res	Type
28	f	60	ASP
28	f	73	PHE
28	f	96	HIS
28	f	113	LYS
28	f	119	GLN
28	f	129	ASP
28	f	136	GLN
29	g	21	CYS
29	g	28	SER
29	g	51	ASN
29	g	80	ASP
29	g	92	ASP
29	g	94	ARG
29	g	110	LYS
30	h	49	MET
30	h	127	ASN
31	i	14	HIS
31	i	28	SER
31	i	51	ARG
31	i	57	HIS
31	i	60	ARG
31	i	98	LYS
31	i	112	LYS
32	j	23	ASN
32	j	80	PHE
32	j	86	PHE
32	j	91	ASN
32	j	96	ARG
32	j	106	ASP
32	j	107	ASN
32	j	115	LEU
33	k	90	GLU
33	k	118	ASP
34	l	49	ARG
34	l	64	SER
34	l	90	ASP
34	l	93	ARG
34	l	97	TYR
35	m	13	LYS
35	m	25	ARG
35	m	29	SER
35	m	41	HIS

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Mol	Chain	Res	Type
35	m	76	TYR
35	m	78	ARG
35	m	91	ASP
36	n	57	LYS
36	n	63	GLU
36	n	92	GLN
37	o	18	ARG
37	o	20	SER
37	o	26	ARG
37	o	45	TRP
37	o	51	SER
37	o	56	LYS
37	o	82	TYR
38	p	8	ARG
38	p	9	ASP
38	p	34	HIS
38	p	53	LYS
38	p	62	ARG
39	q	86	ARG
40	r	37	LEU
40	r	40	HIS
40	r	75	GLU
41	s	12	ASN
41	s	60	PHE
41	s	73	ARG
42	t	20	HIS
43	u	20	ASP
43	u	36	MET
43	u	45	ARG
43	u	51	ARG
44	v	1	MET
44	v	41	ARG
44	v	73	PHE
45	w	16	ARG
45	w	40	ASN
45	w	48	ASN
46	x	16	ARG
46	x	21	LYS
46	x	37	ARG
46	x	48	ARG
47	y	15	CYS
47	y	28	ASN

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Mol	Chain	Res	Type
47	y	30	ARG
47	y	34	ASP
48	z	13	ARG
48	z	25	MET
48	z	43	ARG
49	1	13	ARG
49	1	24	ARG
49	1	35	HIS
49	1	43	ARG
49	1	51	SER
49	1	54	ASP
50	2	20	HIS
50	2	24	MET
50	2	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	8	HIS
3	D	75	ASN
3	D	185	GLN
4	E	111	GLN
6	G	106	ASN
8	I	27	GLN
8	I	95	GLN
10	K	27	HIS
10	K	73	GLN
10	K	128	ASN
11	L	5	GLN
11	L	29	GLN
11	L	73	ASN
11	L	105	GLN
12	M	106	ASN
14	O	28	GLN
15	P	50	GLN
16	Q	62	HIS
22	Z	87	ASN
22	Z	91	ASN
22	Z	227	ASN
23	a	34	ASN
23	a	130	HIS
23	a	135	GLN

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Mol	Chain	Res	Type
23	a	178	GLN
24	b	76	GLN
24	b	182	GLN
24	b	208	ASN
25	c	58	ASN
25	c	134	ASN
26	d	7	GLN
26	d	75	ASN
26	d	102	GLN
29	g	3	GLN
31	i	17	GLN
31	i	55	ASN
32	j	31	HIS
33	k	9	ASN
34	l	79	ASN
35	m	27	GLN
35	m	72	ASN
36	n	90	HIS
39	q	70	ASN
40	r	76	GLN
40	r	126	GLN
40	r	129	ASN
48	z	9	GLN
48	z	19	HIS
50	2	32	HIS
50	2	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1511 (99%)	366 (24%)	18 (1%)
20	Y	2989/3038 (98%)	779 (26%)	57 (1%)
21	U	117/118 (99%)	27 (23%)	2 (1%)
51	4	76/81 (93%)	26 (34%)	1 (1%)
All	All	4687/4748 (98%)	1198 (25%)	78 (1%)

All (1198) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	13	G

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Mol	Chain	Res	Type
1	A	31	G
1	A	35	G
1	A	36	A
1	A	43	G
1	A	51	C
1	A	52	U
1	A	53	U
1	A	54	A
1	A	55	A
1	A	58	C
1	A	59	A
1	A	62	C
1	A	67	C
1	A	68	G
1	A	74	A
1	A	75	A
1	A	81	C
1	A	82	U
1	A	87	G
1	A	89	G
1	A	92	A
1	A	93	C
1	A	99	U
1	A	101	G
1	A	112	A
1	A	116	A
1	A	117	C
1	A	123	G
1	A	125	U
1	A	126	G
1	A	128	U
1	A	136	G
1	A	139	C
1	A	141	U
1	A	172	C
1	A	177	U
1	A	178	A
1	A	179	C
1	A	180	A
1	A	181	C
1	A	192	G
1	A	194	A

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Mol	Chain	Res	Type
1	A	199	C
1	A	200	U
1	A	201	G
1	A	209	A
1	A	210	A
1	A	211	A
1	A	215	U
1	A	217	U
1	A	223	G
1	A	225	G
1	A	226	G
1	A	227	G
1	A	228	A
1	A	231	G
1	A	239	G
1	A	240	C
1	A	243	A
1	A	245	C
1	A	247	G
1	A	251	G
1	A	254	G
1	A	266	G
1	A	267	C
1	A	272	C
1	A	278	G
1	A	280	C
1	A	281	G
1	A	289	G
1	A	306	A
1	A	324	G
1	A	326	G
1	A	327	A
1	A	329	A
1	A	332	G
1	A	337	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A

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Mol	Chain	Res	Type
1	A	364	A
1	A	367	U
1	A	371	A
1	A	372	C
1	A	373	A
1	A	376	G
1	A	388	G
1	A	389	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	426	U
1	A	427	U
1	A	429	U
1	A	430	A
1	A	433	C
1	A	434	C
1	A	435	U
1	A	438	U
1	A	439	U
1	A	452	A
1	A	453	G
1	A	456	C
1	A	457	A
1	A	458	A
1	A	459	G
1	A	464	G
1	A	465	G
1	A	466	U
1	A	469	G
1	A	477	G
1	A	478	A
1	A	482	A
1	A	486	G
1	A	489	A
1	A	491	C
1	A	492	U
1	A	496	U

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Mol	Chain	Res	Type
1	A	497	G
1	A	498	C
1	A	499	C
1	A	501	G
1	A	504	G
1	A	507	G7M
1	A	511	U
1	A	512	A
1	A	515	A
1	A	520	G
1	A	527	A
1	A	539	A
1	A	544	C
1	A	553	A
1	A	556	A
1	A	557	G
1	A	564	G
1	A	567	G
1	A	568	G
1	A	572	G
1	A	577	G
1	A	579	U
1	A	585	U
1	A	601	A
1	A	602	A
1	A	606	U
1	A	612	U
1	A	615	G
1	A	616	G
1	A	619	G
1	A	625	G
1	A	628	A
1	A	629	G
1	A	633	A
1	A	637	U
1	A	645	G
1	A	666	U
1	A	668	G
1	A	675	A
1	A	678	G
1	A	682	A
1	A	683	G

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Mol	Chain	Res	Type
1	A	698	A
1	A	701	G
1	A	702	G
1	A	703	U
1	A	704	G
1	A	711	G
1	A	713	G
1	A	715	G
1	A	728	A
1	A	729	A
1	A	735	G
1	A	757	A
1	A	764	A
1	A	765	G
1	A	772	A
1	A	773	U
1	A	774	A
1	A	779	G
1	A	790	C
1	A	795	A
1	A	796	A
1	A	797	C
1	A	801	G
1	A	808	A
1	A	818	U
1	A	822	U
1	A	823	U
1	A	824	C
1	A	826	U
1	A	827	U
1	A	828	G
1	A	841	U
1	A	854	A
1	A	856	G
1	A	871	A
1	A	872	G
1	A	881	C
1	A	882	A
1	A	884	G
1	A	896	A
1	A	908	G
1	A	909	G

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Mol	Chain	Res	Type
1	A	913	C
1	A	915	G
1	A	916	C
1	A	917	A
1	A	921	G
1	A	931	A
1	A	932	U
1	A	938	U
1	A	942	U
1	A	943	U
1	A	947	U
1	A	948	G
1	A	950	A
1	A	951	A
1	A	953	G
1	A	956	A
1	A	957	A
1	A	959	A
1	A	963	U
1	A	967	C
1	A	970	G
1	A	971	G
1	A	973	U
1	A	974	U
1	A	975	G
1	A	976	A
1	A	978	A
1	A	981	C
1	A	982	A
1	A	986	G
1	A	988	C
1	A	1003	C
1	A	1010	C
1	A	1012	U
1	A	1013	G
1	A	1014	U
1	A	1024	G
1	A	1025	C
1	A	1033	G
1	A	1034	C
1	A	1036	U
1	A	1041	G

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Mol	Chain	Res	Type
1	A	1045	U
1	A	1058	U
1	A	1059	G
1	A	1061	G
1	A	1074	G
1	A	1075	U
1	A	1079	G
1	A	1081	A
1	A	1104	G
1	A	1105	U
1	A	1110	A
1	A	1115	G
1	A	1116	U
1	A	1117	U
1	A	1118	A
1	A	1119	U
1	A	1120	G
1	A	1121	G
1	A	1129	U
1	A	1138	A
1	A	1140	U
1	A	1141	G
1	A	1146	G
1	A	1147	G
1	A	1148	U
1	A	1149	C
1	A	1150	A
1	A	1151	A
1	A	1162	G
1	A	1165	G
1	A	1171	G
1	A	1172	A
1	A	1177	A
1	A	1178	A
1	A	1181	C
1	A	1182	A
1	A	1193	U
1	A	1194	A
1	A	1203	G
1	A	1205	U
1	A	1206	U
1	A	1207	C

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Mol	Chain	Res	Type
1	A	1217	A
1	A	1222	G
1	A	1231	A
1	A	1238	U
1	A	1239	G
1	A	1248	U
1	A	1251	G
1	A	1259	G
1	A	1261	A
1	A	1263	C
1	A	1265	U
1	A	1266	U
1	A	1267	U
1	A	1268	C
1	A	1269	A
1	A	1279	U
1	A	1282	G
1	A	1283	U
1	A	1284	U
1	A	1285	C
1	A	1287	G
1	A	1302	C
1	A	1304	C
1	A	1305	G
1	A	1313	G
1	A	1317	U
1	A	1320	G
1	A	1321	A
1	A	1328	A
1	A	1329	G
1	A	1342	A
1	A	1343	G
1	A	1344	C
1	A	1346	A
1	A	1347	C
1	A	1353	G
1	A	1356	G
1	A	1357	A
1	A	1364	U
1	A	1377	A
1	A	1380	C
1	A	1381	A

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Mol	Chain	Res	Type
1	A	1382	C
1	A	1396	A
1	A	1402	G
1	A	1407	U
1	A	1429	A
1	A	1433	C
1	A	1434	U
1	A	1435	U
1	A	1436	G
1	A	1438	G
1	A	1440	A
1	A	1447	C
1	A	1457	G
1	A	1458	G
1	A	1463	G
1	A	1478	G
1	A	1481	G
1	A	1483	A
1	A	1486	A
1	A	1487	A
1	A	1488	G
1	A	1490	U
1	A	1501	G
1	A	1502	A
1	A	1504	G
1	A	1513	G
1	A	1514	G
1	A	1516	U
20	Y	4	G
20	Y	7	U
20	Y	8	U
20	Y	9	U
20	Y	12	G
20	Y	16	G
20	Y	17	C
20	Y	20	G
20	Y	23	G
20	Y	29	C
20	Y	31	U
20	Y	32	G
20	Y	33	G
20	Y	43	C

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Mol	Chain	Res	Type
20	Y	48	G
20	Y	57	A
20	Y	58	G
20	Y	60	A
20	Y	61	G
20	Y	68	A
20	Y	70	A
20	Y	71	A
20	Y	72	G
20	Y	77	G
20	Y	81	A
20	Y	89	A
20	Y	90	C
20	Y	92	G
20	Y	93	A
20	Y	94	G
20	Y	97	U
20	Y	98	U
20	Y	99	G
20	Y	100	A
20	Y	111	U
20	Y	115	A
20	Y	116	A
20	Y	117	U
20	Y	122	A
20	Y	125	C
20	Y	126	C
20	Y	131	A
20	Y	138	A
20	Y	143	G
20	Y	145	G
20	Y	148	A
20	Y	159	A
20	Y	162	A
20	Y	169	C
20	Y	172	C
20	Y	175	G
20	Y	180	A
20	Y	195	A
20	Y	212	A
20	Y	213	G
20	Y	215	A

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Mol	Chain	Res	Type
20	Y	220	A
20	Y	221	A
20	Y	222	A
20	Y	224	C
20	Y	227	A
20	Y	228	A
20	Y	229	U
20	Y	230	G
20	Y	231	U
20	Y	241	A
20	Y	248	G
20	Y	264	G
20	Y	265	A
20	Y	266	U
20	Y	268	G
20	Y	272	A
20	Y	273	A
20	Y	274	C
20	Y	279	U
20	Y	282	A
20	Y	283	U
20	Y	285	U
20	Y	286	G
20	Y	288	U
20	Y	293	G
20	Y	296	A
20	Y	299	G
20	Y	301	U
20	Y	302	U
20	Y	303	G
20	Y	306	U
20	Y	312	G
20	Y	313	G
20	Y	314	G
20	Y	316	U
20	Y	317	G
20	Y	318	U
20	Y	319	G
20	Y	320	G
20	Y	324	C
20	Y	325	U
20	Y	330	U

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Mol	Chain	Res	Type
20	Y	331	U
20	Y	336	C
20	Y	337	U
20	Y	338	C
20	Y	340	A
20	Y	345	G
20	Y	351	G
20	Y	352	G
20	Y	353	G
20	Y	355	A
20	Y	357	U
20	Y	358	G
20	Y	361	A
20	Y	364	A
20	Y	366	G
20	Y	369	G
20	Y	370	U
20	Y	371	G
20	Y	375	A
20	Y	376	G
20	Y	383	U
20	Y	384	G
20	Y	389	G
20	Y	393	U
20	Y	398	U
20	Y	399	G
20	Y	400	C
20	Y	405	G
20	Y	406	A
20	Y	411	G
20	Y	412	A
20	Y	415	G
20	Y	416	C
20	Y	417	C
20	Y	418	C
20	Y	424	G
20	Y	425	U
20	Y	433	C
20	Y	434	G
20	Y	435	A
20	Y	444	U
20	Y	445	U

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Mol	Chain	Res	Type
20	Y	446	G
20	Y	447	A
20	Y	450	G
20	Y	451	U
20	Y	452	G
20	Y	454	U
20	Y	458	G
20	Y	460	G
20	Y	468	G
20	Y	474	G
20	Y	477	G
20	Y	479	A
20	Y	486	G
20	Y	489	A
20	Y	490	A
20	Y	491	U
20	Y	494	G
20	Y	498	G
20	Y	499	G
20	Y	503	A
20	Y	505	C
20	Y	507	G
20	Y	508	G
20	Y	512	G
20	Y	514	C
20	Y	516	G
20	Y	517	A
20	Y	542	A
20	Y	543	U
20	Y	544	U
20	Y	546	G
20	Y	552	U
20	Y	553	G
20	Y	565	A
20	Y	566	A
20	Y	568	A
20	Y	569	G
20	Y	570	U
20	Y	589	A
20	Y	591	G
20	Y	592	A
20	Y	595	A

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Mol	Chain	Res	Type
20	Y	596	C
20	Y	597	C
20	Y	600	A
20	Y	601	A
20	Y	614	C
20	Y	617	U
20	Y	618	C
20	Y	619	C
20	Y	620	G
20	Y	632	G
20	Y	636	U
20	Y	637	G
20	Y	638	U
20	Y	639	C
20	Y	640	G
20	Y	641	U
20	Y	642	G
20	Y	644	G
20	Y	645	G
20	Y	646	U
20	Y	647	G
20	Y	654	U
20	Y	655	G
20	Y	658	U
20	Y	659	U
20	Y	660	U
20	Y	661	U
20	Y	663	A
20	Y	665	G
20	Y	667	A
20	Y	669	G
20	Y	675	G
20	Y	678	A
20	Y	679	G
20	Y	684	G
20	Y	685	G
20	Y	696	A
20	Y	699	U
20	Y	700	U
20	Y	707	G
20	Y	708	G
20	Y	709	U

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Mol	Chain	Res	Type
20	Y	715	A
20	Y	716	G
20	Y	719	G
20	Y	721	A
20	Y	731	A
20	Y	738	A
20	Y	740	A
20	Y	742	G
20	Y	747	A
20	Y	753	A
20	Y	756	A
20	Y	757	G
20	Y	758	A
20	Y	759	G
20	Y	760	U
20	Y	768	G
20	Y	773	G
20	Y	774	G
20	Y	781	C
20	Y	784	G
20	Y	785	A
20	Y	792	G
20	Y	801	U
20	Y	829	U
20	Y	830	A
20	Y	836	G
20	Y	838	G
20	Y	839	U
20	Y	841	G
20	Y	845	C
20	Y	851	C
20	Y	855	C
20	Y	862	U
20	Y	863	G
20	Y	867	A
20	Y	868	C
20	Y	871	A
20	Y	872	G
20	Y	885	G
20	Y	890	G
20	Y	896	A
20	Y	897	A

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Mol	Chain	Res	Type
20	Y	898	A
20	Y	899	G
20	Y	901	C
20	Y	904	A
20	Y	915	U
20	Y	920	G
20	Y	921	C
20	Y	927	C
20	Y	934	A
20	Y	937	U
20	Y	942	U
20	Y	943	U
20	Y	946	G
20	Y	948	G
20	Y	960	G
20	Y	961	U
20	Y	971	G
20	Y	972	A
20	Y	973	G
20	Y	974	G
20	Y	975	U
20	Y	981	U
20	Y	982	A
20	Y	995	U
20	Y	998	G
20	Y	1003	A
20	Y	1004	C
20	Y	1005	A
20	Y	1007	G
20	Y	1010	U
20	Y	1011	A
20	Y	1012	C
20	Y	1014	G
20	Y	1015	A
20	Y	1025	A
20	Y	1027	C
20	Y	1033	A
20	Y	1046	C
20	Y	1047	A
20	Y	1048	A
20	Y	1049	G
20	Y	1063	G

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Mol	Chain	Res	Type
20	Y	1075	U
20	Y	1076	A
20	Y	1078	G
20	Y	1084	U
20	Y	1085	G
20	Y	1086	C
20	Y	1090	G
20	Y	1091	A
20	Y	1092	G
20	Y	1101	A
20	Y	1108	A
20	Y	1114	G
20	Y	1124	C
20	Y	1127	A
20	Y	1130	C
20	Y	1131	G
20	Y	1140	G
20	Y	1141	U
20	Y	1144	A
20	Y	1151	U
20	Y	1158	U
20	Y	1175	A
20	Y	1176	G
20	Y	1177	G
20	Y	1178	U
20	Y	1181	G
20	Y	1184	U
20	Y	1185	A
20	Y	1186	G
20	Y	1187	A
20	Y	1188	A
20	Y	1189	G
20	Y	1190	C
20	Y	1191	A
20	Y	1194	C
20	Y	1196	C
20	Y	1200	U
20	Y	1202	A
20	Y	1203	A
20	Y	1204	A
20	Y	1205	G
20	Y	1206	A

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Mol	Chain	Res	Type
20	Y	1207	G
20	Y	1209	G
20	Y	1213	A
20	Y	1219	U
20	Y	1222	C
20	Y	1230	G
20	Y	1232	G
20	Y	1234	U
20	Y	1237	U
20	Y	1238	G
20	Y	1240	G
20	Y	1247	A
20	Y	1250	U
20	Y	1251	A
20	Y	1253	C
20	Y	1260	C
20	Y	1270	G
20	Y	1271	C
20	Y	1273	G
20	Y	1274	A
20	Y	1292	U
20	Y	1293	G
20	Y	1318	C
20	Y	1320	U
20	Y	1341	U
20	Y	1344	A
20	Y	1345	G
20	Y	1350	G
20	Y	1351	G
20	Y	1353	G
20	Y	1359	G
20	Y	1364	U
20	Y	1365	G
20	Y	1367	G
20	Y	1368	A
20	Y	1370	U
20	Y	1371	G
20	Y	1378	U
20	Y	1379	G
20	Y	1380	A
20	Y	1384	G
20	Y	1386	G

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Mol	Chain	Res	Type
20	Y	1390	A
20	Y	1391	G
20	Y	1399	A
20	Y	1415	A
20	Y	1416	A
20	Y	1421	C
20	Y	1428	U
20	Y	1436	C
20	Y	1437	A
20	Y	1440	C
20	Y	1448	C
20	Y	1465	C
20	Y	1474	A
20	Y	1480	A
20	Y	1493	A
20	Y	1494	U
20	Y	1499	A
20	Y	1501	C
20	Y	1507	G
20	Y	1510	A
20	Y	1511	U
20	Y	1520	C
20	Y	1522	G
20	Y	1526	A
20	Y	1528	G
20	Y	1531	C
20	Y	1532	G
20	Y	1533	U
20	Y	1534	C
20	Y	1538	G
20	Y	1540	U
20	Y	1548	C
20	Y	1551	U
20	Y	1552	A
20	Y	1553	C
20	Y	1554	U
20	Y	1564	A
20	Y	1565	A
20	Y	1566	A
20	Y	1574	G
20	Y	1579	C
20	Y	1587	G

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Mol	Chain	Res	Type
20	Y	1599	U
20	Y	1602	U
20	Y	1613	G
20	Y	1620	U
20	Y	1621	C
20	Y	1625	G
20	Y	1627	U
20	Y	1629	G
20	Y	1631	A
20	Y	1634	C
20	Y	1635	A
20	Y	1636	A
20	Y	1637	G
20	Y	1638	C
20	Y	1639	G
20	Y	1640	A
20	Y	1641	U
20	Y	1645	G
20	Y	1664	G
20	Y	1672	C
20	Y	1674	G
20	Y	1675	U
20	Y	1676	G
20	Y	1679	A
20	Y	1680	A
20	Y	1681	U
20	Y	1686	G
20	Y	1688	G
20	Y	1702	A
20	Y	1703	G
20	Y	1704	U
20	Y	1705	C
20	Y	1710	A
20	Y	1713	U
20	Y	1714	A
20	Y	1715	A
20	Y	1716	A
20	Y	1717	U
20	Y	1718	C
20	Y	1720	G
20	Y	1724	G
20	Y	1731	A

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Mol	Chain	Res	Type
20	Y	1737	A
20	Y	1746	G
20	Y	1753	C
20	Y	1754	G
20	Y	1755	A
20	Y	1756	G
20	Y	1767	U
20	Y	1769	G
20	Y	1778	A
20	Y	1783	G
20	Y	1786	G
20	Y	1789	A
20	Y	1798	U
20	Y	1799	A
20	Y	1802	G
20	Y	1804	G
20	Y	1807	C
20	Y	1808	A
20	Y	1815	G
20	Y	1825	C
20	Y	1826	A
20	Y	1834	A
20	Y	1849	G
20	Y	1850	A
20	Y	1864	U
20	Y	1865	A
20	Y	1866	C
20	Y	1867	G
20	Y	1871	G
20	Y	1872	A
20	Y	1890	C
20	Y	1892	G
20	Y	1893	C
20	Y	1895	A
20	Y	1906	U
20	Y	1911	U
20	Y	1912	C
20	Y	1916	A
20	Y	1917	G
20	Y	1932	U
20	Y	1946	U
20	Y	1947	U

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Mol	Chain	Res	Type
20	Y	1948	A
20	Y	1950	G
20	Y	1961	G
20	Y	1965	G
20	Y	1973	C
20	Y	1975	A
20	Y	1981	U
20	Y	1986	A
20	Y	1990	A
20	Y	1997	A
20	Y	1998	C
20	Y	1999	U
20	Y	2000	A
20	Y	2007	C
20	Y	2009	G
20	Y	2016	G
20	Y	2017	C
20	Y	2025	C
20	Y	2026	A
20	Y	2033	U
20	Y	2046	A
20	Y	2052	G
20	Y	2062	G
20	Y	2073	A
20	Y	2074	G
20	Y	2075	G
20	Y	2083	A
20	Y	2085	C
20	Y	2086	U
20	Y	2087	C
20	Y	2089	C
20	Y	2090	U
20	Y	2091	U
20	Y	2092	U
20	Y	2093	G
20	Y	2094	G
20	Y	2095	G
20	Y	2096	G
20	Y	2104	G
20	Y	2106	A
20	Y	2107	G
20	Y	2108	A

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Mol	Chain	Res	Type
20	Y	2110	U
20	Y	2112	U
20	Y	2113	A
20	Y	2123	A
20	Y	2130	G
20	Y	2138	C
20	Y	2140	A
20	Y	2142	A
20	Y	2145	C
20	Y	2154	G
20	Y	2160	A
20	Y	2162	A
20	Y	2163	U
20	Y	2164	U
20	Y	2166	C
20	Y	2167	U
20	Y	2176	A
20	Y	2179	U
20	Y	2191	C
20	Y	2194	A
20	Y	2196	G
20	Y	2199	G
20	Y	2215	U
20	Y	2217	U
20	Y	2221	A
20	Y	2245	C
20	Y	2247	A
20	Y	2254	A
20	Y	2255	A
20	Y	2256	G
20	Y	2257	A
20	Y	2267	C
20	Y	2274	C
20	Y	2279	C
20	Y	2280	G
20	Y	2283	A
20	Y	2284	A
20	Y	2285	G
20	Y	2286	A
20	Y	2291	G
20	Y	2292	G
20	Y	2315	U

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Mol	Chain	Res	Type
20	Y	2316	G
20	Y	2319	G
20	Y	2320	C
20	Y	2322	C
20	Y	2408	G
20	Y	2409	U
20	Y	2410	A
20	Y	2411	U
20	Y	2421	A
20	Y	2427	G
20	Y	2434	A
20	Y	2435	U
20	Y	2436	A
20	Y	2446	G
20	Y	2447	G
20	Y	2449	A
20	Y	2454	G
20	Y	2458	G
20	Y	2462	G
20	Y	2463	G
20	Y	2467	U
20	Y	2473	U
20	Y	2475	G
20	Y	2490	A
20	Y	2491	A
20	Y	2502	A
20	Y	2507	C
20	Y	2510	A
20	Y	2511	A
20	Y	2520	U
20	Y	2521	C
20	Y	2523	A
20	Y	2524	C
20	Y	2526	U
20	Y	2527	G
20	Y	2528	G
20	Y	2529	A
20	Y	2531	G
20	Y	2532	G
20	Y	2533	C
20	Y	2536	U
20	Y	2538	A

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Mol	Chain	Res	Type
20	Y	2539	G
20	Y	2540	G
20	Y	2541	U
20	Y	2542	G
20	Y	2543	U
20	Y	2544	U
20	Y	2548	U
20	Y	2549	G
20	Y	2557	A
20	Y	2558	C
20	Y	2559	A
20	Y	2561	G
20	Y	2565	G
20	Y	2568	U
20	Y	2569	G
20	Y	2571	C
20	Y	2578	A
20	Y	2581	G
20	Y	2603	G
20	Y	2607	G
20	Y	2609	A
20	Y	2626	U
20	Y	2627	C
20	Y	2630	A
20	Y	2631	G
20	Y	2634	G
20	Y	2635	A
20	Y	2638	G
20	Y	2639	G
20	Y	2646	C
20	Y	2647	U
20	Y	2649	A
20	Y	2652	G
20	Y	2653	G
20	Y	2654	A
20	Y	2658	A
20	Y	2665	C
20	Y	2671	G
20	Y	2672	A
20	Y	2693	A
20	Y	2694	G
20	Y	2698	C

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Mol	Chain	Res	Type
20	Y	2699	C
20	Y	2700	A
20	Y	2701	U
20	Y	2702	A
20	Y	2705	G
20	Y	2715	U
20	Y	2716	U
20	Y	2721	A
20	Y	2722	C
20	Y	2726	G
20	Y	2727	A
20	Y	2729	G
20	Y	2730	U
20	Y	2742	A
20	Y	2744	C
20	Y	2753	G
20	Y	2754	G
20	Y	2755	A
20	Y	2771	U
20	Y	2778	U
20	Y	2790	A
20	Y	2791	G
20	Y	2796	A
20	Y	2797	C
20	Y	2800	G
20	Y	2802	G
20	Y	2822	A
20	Y	2823	G
20	Y	2826	A
20	Y	2833	U
20	Y	2837	U
20	Y	2845	G
20	Y	2851	G
20	Y	2853	C
20	Y	2854	A
20	Y	2860	U
20	Y	2862	G
20	Y	2870	C
20	Y	2871	U
20	Y	2878	A
20	Y	2879	G
20	Y	2912	A

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Mol	Chain	Res	Type
20	Y	2913	U
20	Y	2914	A
20	Y	2915	C
20	Y	2926	A
20	Y	2928	C
20	Y	2936	C
20	Y	2937	G
20	Y	2938	G
20	Y	2943	A
20	Y	2944	U
20	Y	2950	C
20	Y	2957	A
20	Y	2968	G
20	Y	2972	A
20	Y	2981	A
20	Y	2982	A
20	Y	2985	G
20	Y	2989	A
20	Y	2990	A
20	Y	3002	A
20	Y	3004	C
20	Y	3009	U
20	Y	3014	A
20	Y	3016	C
20	Y	3021	A
20	Y	3022	G
20	Y	3023	G
20	Y	3029	U
20	Y	3037	C
20	Y	3039	C
20	Y	3042	A
20	Y	3046	C
20	Y	3054	U
20	Y	3057	U
20	Y	3080	A
20	Y	3081	A
20	Y	3082	U
20	Y	3087	G
20	Y	3088	C
20	Y	3092	G
20	Y	3093	A
20	Y	3094	A

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Mol	Chain	Res	Type
20	Y	3098	G
20	Y	3100	A
20	Y	3101	C
20	Y	3105	C
20	Y	3106	C
20	Y	3107	G
20	Y	3110	C
20	Y	3112	A
20	Y	3115	A
21	U	4	A
21	U	5	C
21	U	7	G
21	U	9	G
21	U	11	U
21	U	13	C
21	U	14	A
21	U	25	G
21	U	36	U
21	U	43	C
21	U	46	A
21	U	47	A
21	U	52	G
21	U	54	A
21	U	57	U
21	U	58	A
21	U	59	A
21	U	67	A
21	U	68	G
21	U	86	A
21	U	87	U
21	U	89	C
21	U	90	G
21	U	91	G
21	U	103	G
21	U	107	A
21	U	114	A
51	4	2328	G
51	4	2330	U
51	4	2331	U
51	4	2334	U
51	4	2335	G
51	4	2337	A

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Mol	Chain	Res	Type
51	4	2338	G
51	4	2341	U
51	4	2342	A
51	4	2349	A
51	4	2354	G
51	4	2356	G
51	4	2368	C
51	4	2371	G
51	4	2382	G
51	4	2383	U
51	4	2384	C
51	4	2385	G
51	4	2387	U
51	4	2388	G
51	4	2389	U
51	4	2395	U
51	4	2396	A
51	4	2401	U
51	4	2402	C
51	4	2404	G

All (78) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	92	A
1	A	124	G
1	A	209	A
1	A	350	G
1	A	422	C
1	A	429	U
1	A	485	G
1	A	498	C
1	A	895	A
1	A	962	C
1	A	1011	U
1	A	1058	U
1	A	1109	C
1	A	1117	U
1	A	1149	C
1	A	1342	A
1	A	1477	A
1	A	1482	U

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Mol	Chain	Res	Type
20	Y	97	U
20	Y	324	C
20	Y	335	G
20	Y	336	C
20	Y	357	U
20	Y	416	C
20	Y	445	U
20	Y	493	U
20	Y	552	U
20	Y	567	A
20	Y	591	G
20	Y	600	A
20	Y	617	U
20	Y	643	G
20	Y	695	G
20	Y	895	G
20	Y	972	A
20	Y	974	G
20	Y	981	U
20	Y	1004	C
20	Y	1010	U
20	Y	1046	C
20	Y	1077	A
20	Y	1084	U
20	Y	1177	G
20	Y	1186	G
20	Y	1205	G
20	Y	1231	U
20	Y	1364	U
20	Y	1366	A
20	Y	1390	A
20	Y	1436	C
20	Y	1473	G
20	Y	1500	A
20	Y	1532	G
20	Y	1547	G
20	Y	1573	U
20	Y	1730	U
20	Y	1803	A
20	Y	1947	U
20	Y	1999	U
20	Y	2088	C

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Mol	Chain	Res	Type
20	Y	2089	C
20	Y	2094	G
20	Y	2095	G
20	Y	2166	C
20	Y	2408	G
20	Y	2528	G
20	Y	2542	G
20	Y	2567	U
20	Y	2630	A
20	Y	2652	G
20	Y	2693	A
20	Y	2729	G
20	Y	2821	G
20	Y	3008	C
20	Y	3097	G
21	U	10	G
21	U	42	C
51	4	2381	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
1	G7M	A	507	1	20,26,27	0.94	1 (5%)	16,39,42	0.53	0

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
1	G7M	A	507	1	-	3/3/25/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	507	G7M	C8-N9	2.90	1.38	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	507	G7M	O4'-C4'-C5'-O5'
1	A	507	G7M	C3'-C4'-C5'-O5'
1	A	507	G7M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 629 ligands modelled in this entry, 629 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	Y	50
27	e	20
1	A	5
51	4	4
39	q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	2325:U	O3'	2407:C	P	19.51
1	4	2385:G	O3'	2386:U	P	13.58
1	Y	1549:G	O3'	1550:G	P	13.38
1	Y	1600:G	O3'	1601:G	P	12.25
1	Y	1008:G	O3'	1009:U	P	11.11
1	Y	1622:G	O3'	1623:U	P	10.68
1	Y	454:U	O3'	455:C	P	10.20
1	e	22:PRO	C	23:ALA	N	9.59
1	Y	299:G	O3'	300:G	P	9.56
1	e	15:ILE	C	16:GLN	N	9.39
1	Y	996:G	O3'	997:G	P	8.61
1	4	2344:G	O3'	2345:U	P	8.25
1	e	54:ASN	C	55:VAL	N	8.02
1	Y	2096:G	O3'	2097:G	P	7.93
1	e	118:LEU	C	119:ASN	N	7.77
1	Y	1001:C	O3'	1002:C	P	7.54
1	q	47:VAL	C	56:SER	N	7.27
1	A	1200:A	O3'	1201:G	P	7.21
1	4	2349:A	O3'	2350:G	P	7.06
1	e	25:PRO	C	26:VAL	N	6.89
1	e	125:ALA	C	126:ALA	N	6.57
1	Y	2411:U	O3'	2412:U	P	6.50
1	Y	995:U	O3'	996:G	P	6.32
1	e	124:ASP	C	125:ALA	N	6.10
1	e	42:LYS	C	43:ALA	N	6.07
1	4	2393:A	O3'	2394:A	P	5.94
1	Y	367:U	O3'	368:U	P	5.38
1	A	1199:C	O3'	1200:A	P	5.35
1	e	24:PRO	C	25:PRO	N	5.26
1	e	88:GLN	C	89:LYS	N	4.95
1	Y	1631:A	O3'	1632:G	P	4.91
1	Y	1545:C	O3'	1546:A	P	4.90
1	Y	1534:C	O3'	1535:C	P	4.76
1	Y	1196:C	O3'	1197:C	P	4.60
1	Y	999:C	O3'	1000:C	P	4.56

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	61:THR	C	62:VAL	N	4.54
1	Y	2087:C	O3'	2088:C	P	4.49
1	e	39:GLU	C	40:PHE	N	4.46
1	e	41:CYS	C	42:LYS	N	4.32
1	e	68:PHE	C	69:THR	N	4.26
1	Y	1000:C	O3'	1001:C	P	4.22
1	Y	1599:U	O3'	1600:G	P	4.09
1	Y	1005:A	O3'	1006:G	P	4.08
1	Y	2323:G	O3'	2324:A	P	3.94
1	e	55:VAL	C	56:ILE	N	3.71
1	e	67:SER	C	68:PHE	N	3.69
1	Y	1529:U	O3'	1530:G	P	3.66
1	Y	1542:A	O3'	1543:A	P	3.62
1	Y	1210:C	O3'	1211:G	P	3.57
1	Y	1543:A	O3'	1544:U	P	3.40
1	Y	1170:C	O3'	1171:C	P	3.39
1	Y	2142:A	O3'	2143:A	P	3.32
1	A	1000:U	O3'	1001:G	P	3.31
1	e	86:GLY	C	87:VAL	N	3.31
1	Y	437:G	O3'	438:U	P	3.26
1	A	1130:C	O3'	1131:G	P	3.20
1	e	63:TYR	C	64:GLU	N	3.18
1	Y	1800:G	O3'	1801:C	P	3.16
1	e	13:LEU	C	14:GLN	N	3.09
1	Y	2140:A	O3'	2141:U	P	3.08
1	Y	1019:C	O3'	1020:A	P	3.06
1	e	121:ASN	C	122:ASP	N	3.05
1	A	999:A	O3'	1000:U	P	3.03
1	Y	400:C	O3'	401:C	P	3.03
1	Y	1200:U	O3'	1201:G	P	3.03
1	Y	279:U	O3'	280:G	P	2.98
1	Y	2100:A	O3'	2101:A	P	2.96
1	Y	2415:G	O3'	2416:C	P	2.95
1	Y	988:U	O3'	989:G	P	2.94
1	Y	1016:C	O3'	1017:G	P	2.92
1	Y	500:A	O3'	501:C	P	2.91
1	Y	1499:A	O3'	1500:A	P	2.89
1	Y	2135:U	O3'	2136:A	P	2.88
1	Y	2143:A	O3'	2144:C	P	2.88
1	Y	2146:A	O3'	2147:U	P	2.88
1	Y	160:A	O3'	161:U	P	2.85
1	Y	1399:A	O3'	1400:G	P	2.81

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	499:G	O3'	500:A	P	2.80
1	Y	1708:A	O3'	1709:U	P	2.79
1	Y	1700:G	O3'	1701:G	P	2.77

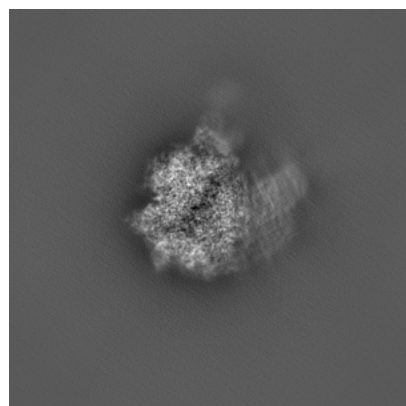
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44092. These allow visual inspection of the internal detail of the map and identification of artifacts.

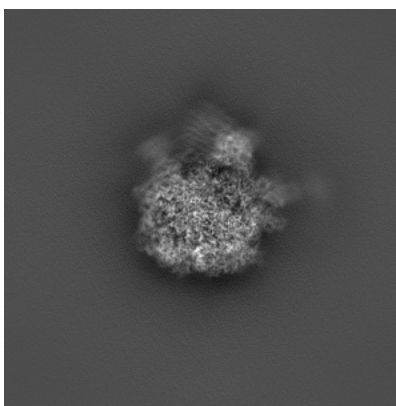
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

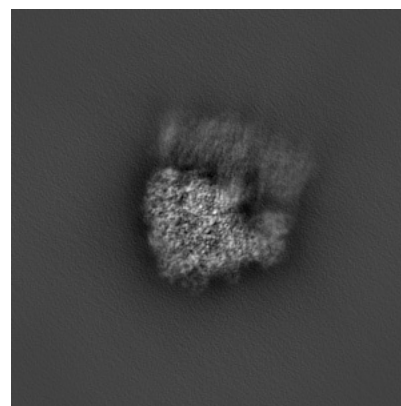
6.1.1 Primary map



X

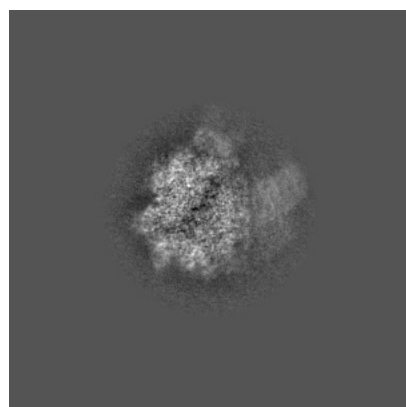


Y

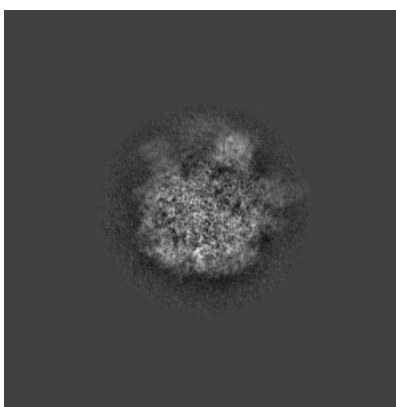


Z

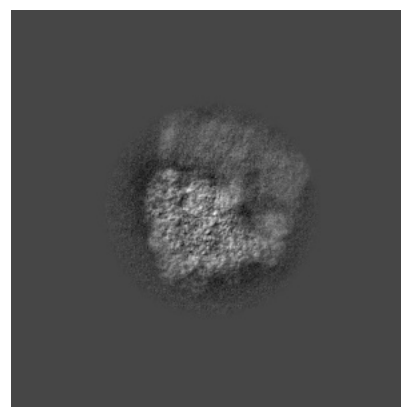
6.1.2 Raw map



X



Y

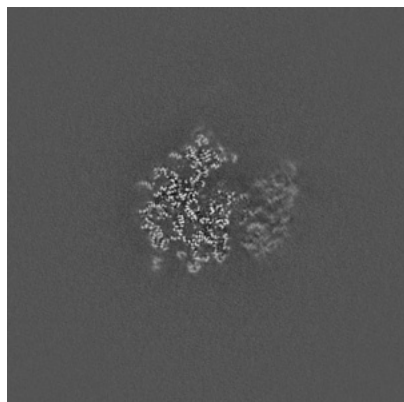


Z

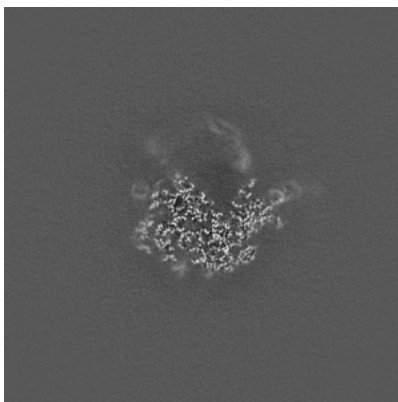
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

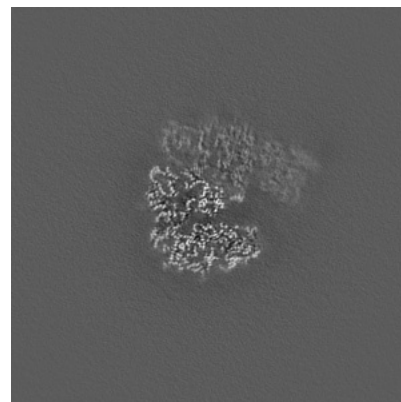
6.2.1 Primary map



X Index: 324

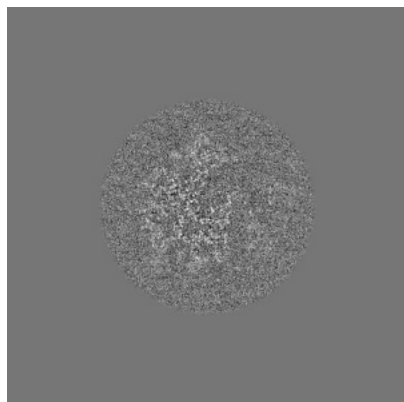


Y Index: 324

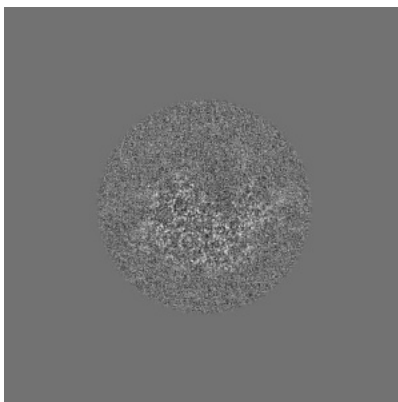


Z Index: 324

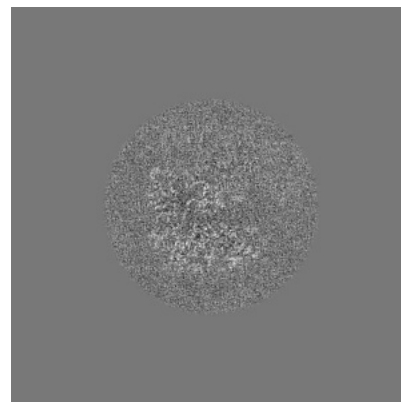
6.2.2 Raw map



X Index: 324



Y Index: 324

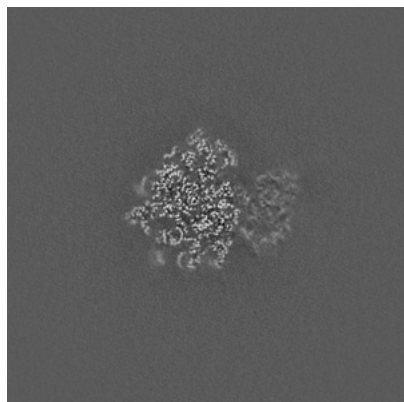


Z Index: 324

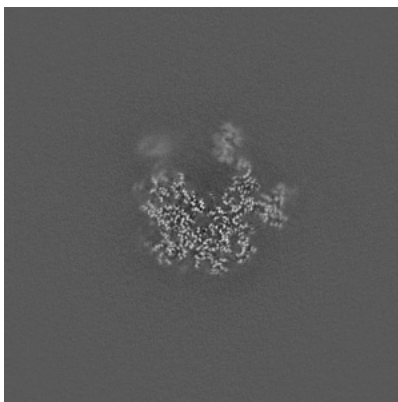
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

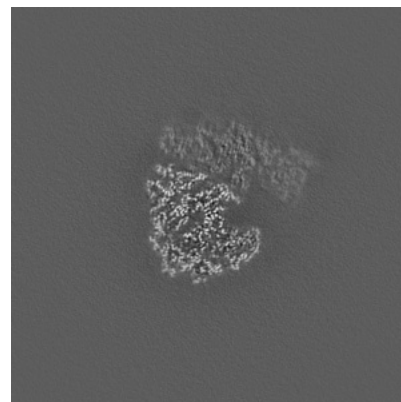
6.3.1 Primary map



X Index: 312

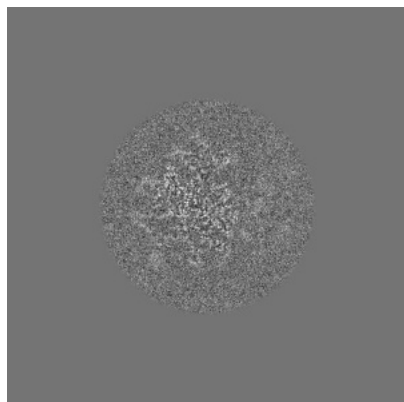


Y Index: 310

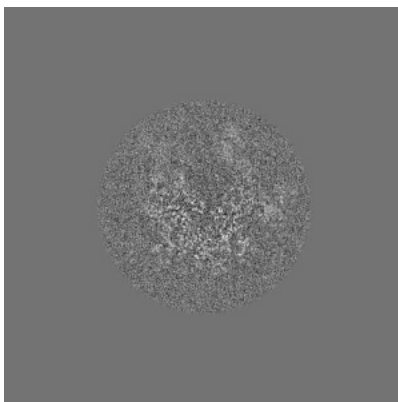


Z Index: 318

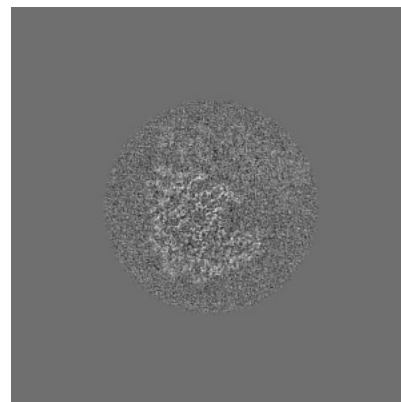
6.3.2 Raw map



X Index: 317



Y Index: 311

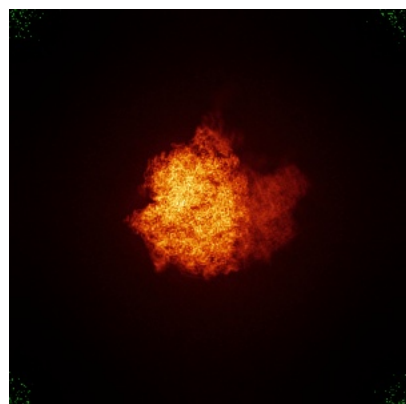


Z Index: 317

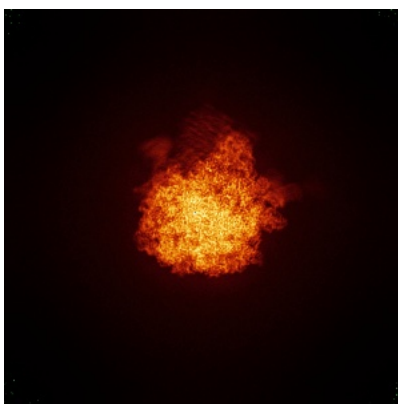
The images above show the largest variance slices of the map in three orthogonal directions.

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

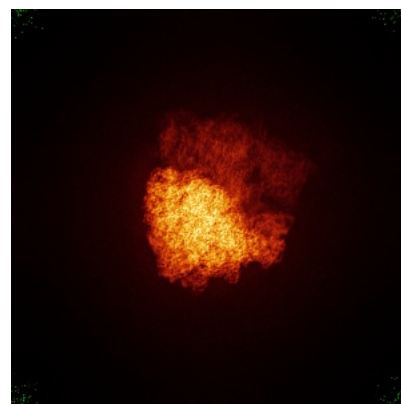
6.4.1 Primary map



X

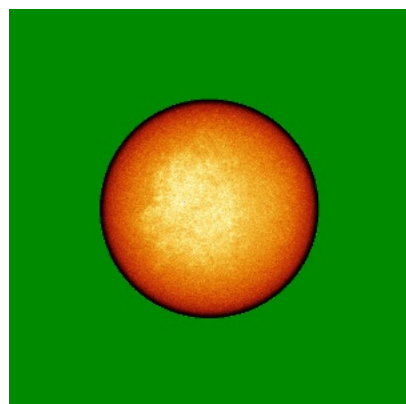


Y

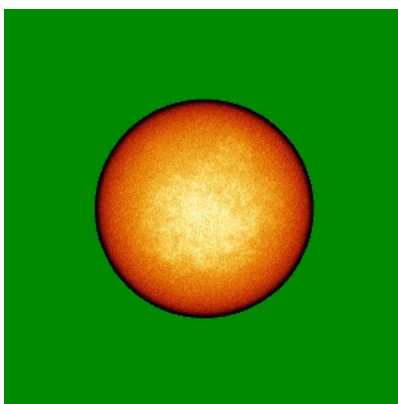


Z

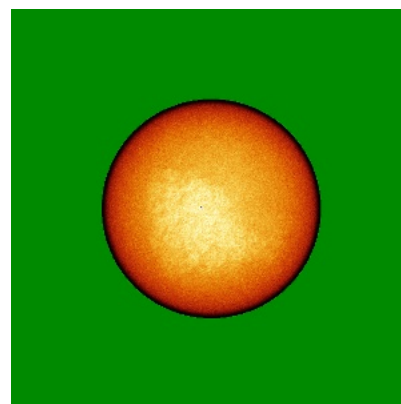
6.4.2 Raw map



X



Y

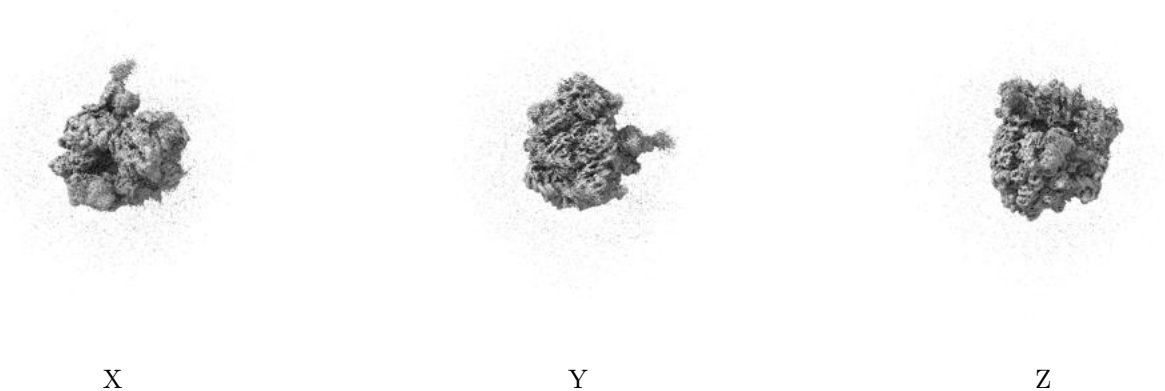


Z

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.

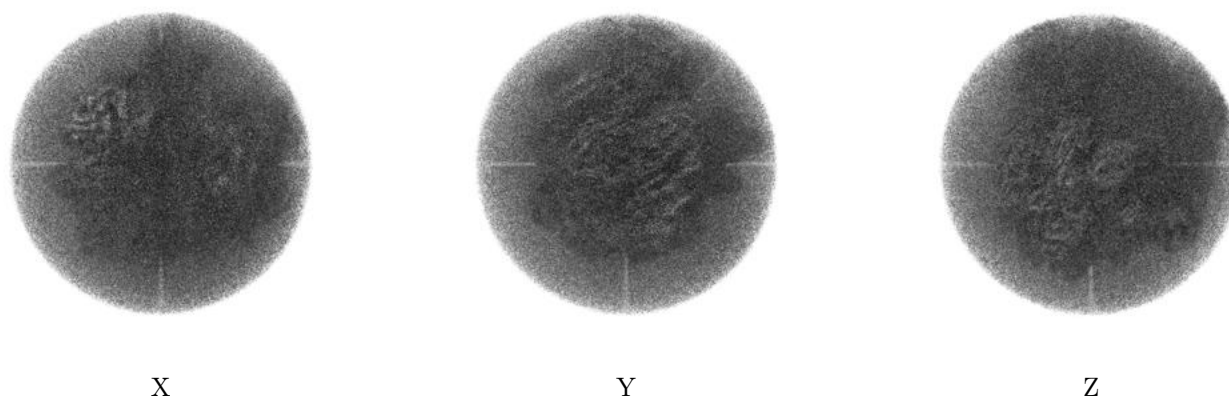
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.968. 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



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

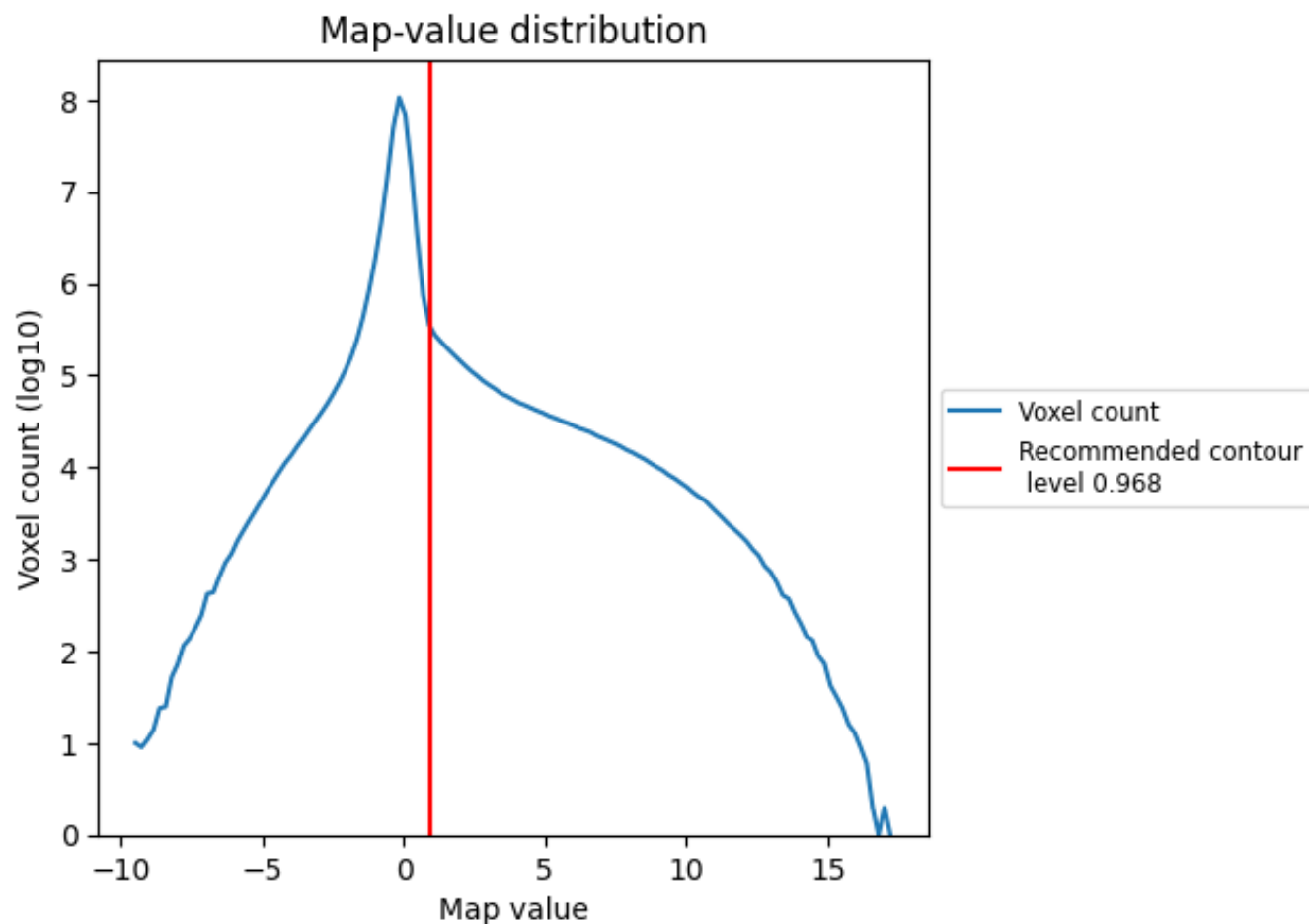
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

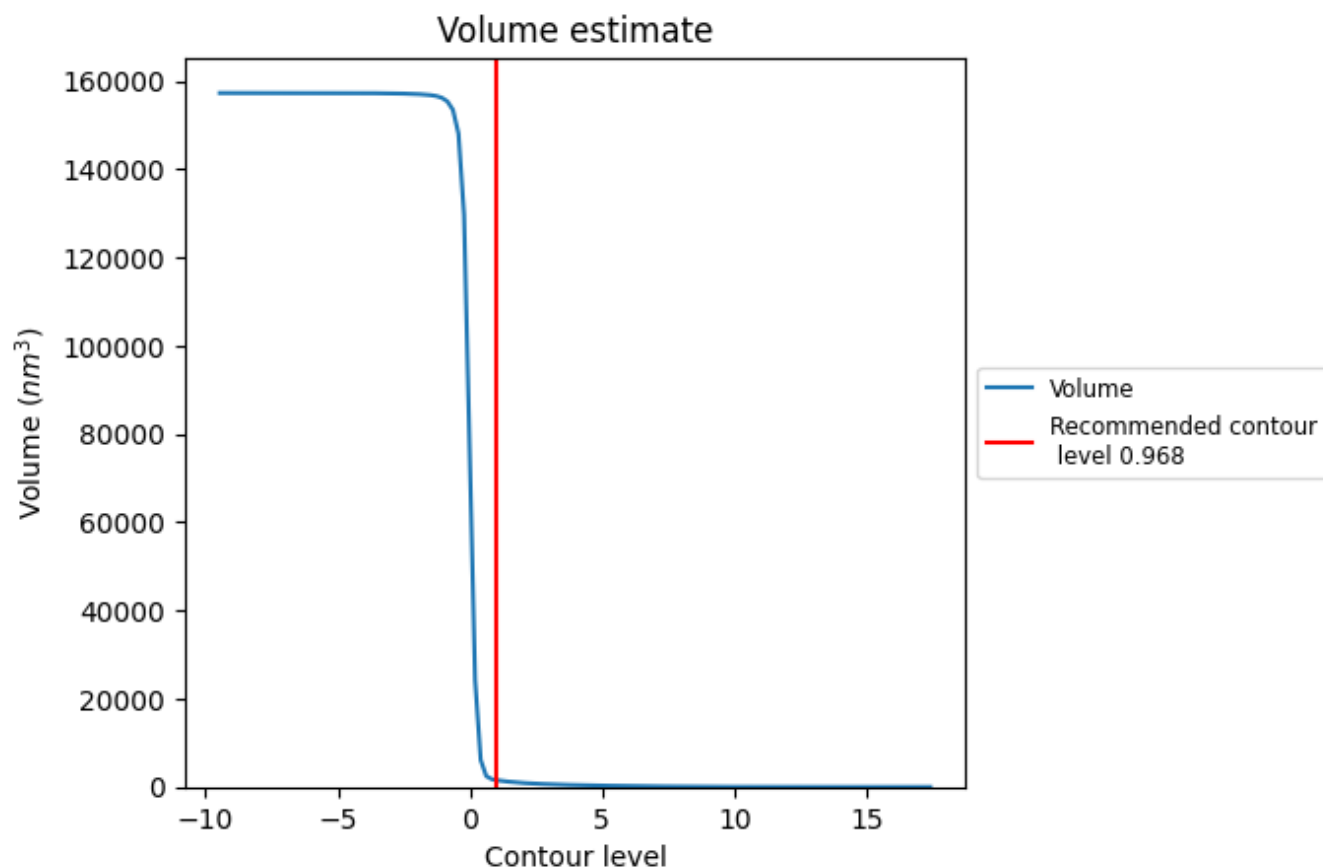
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

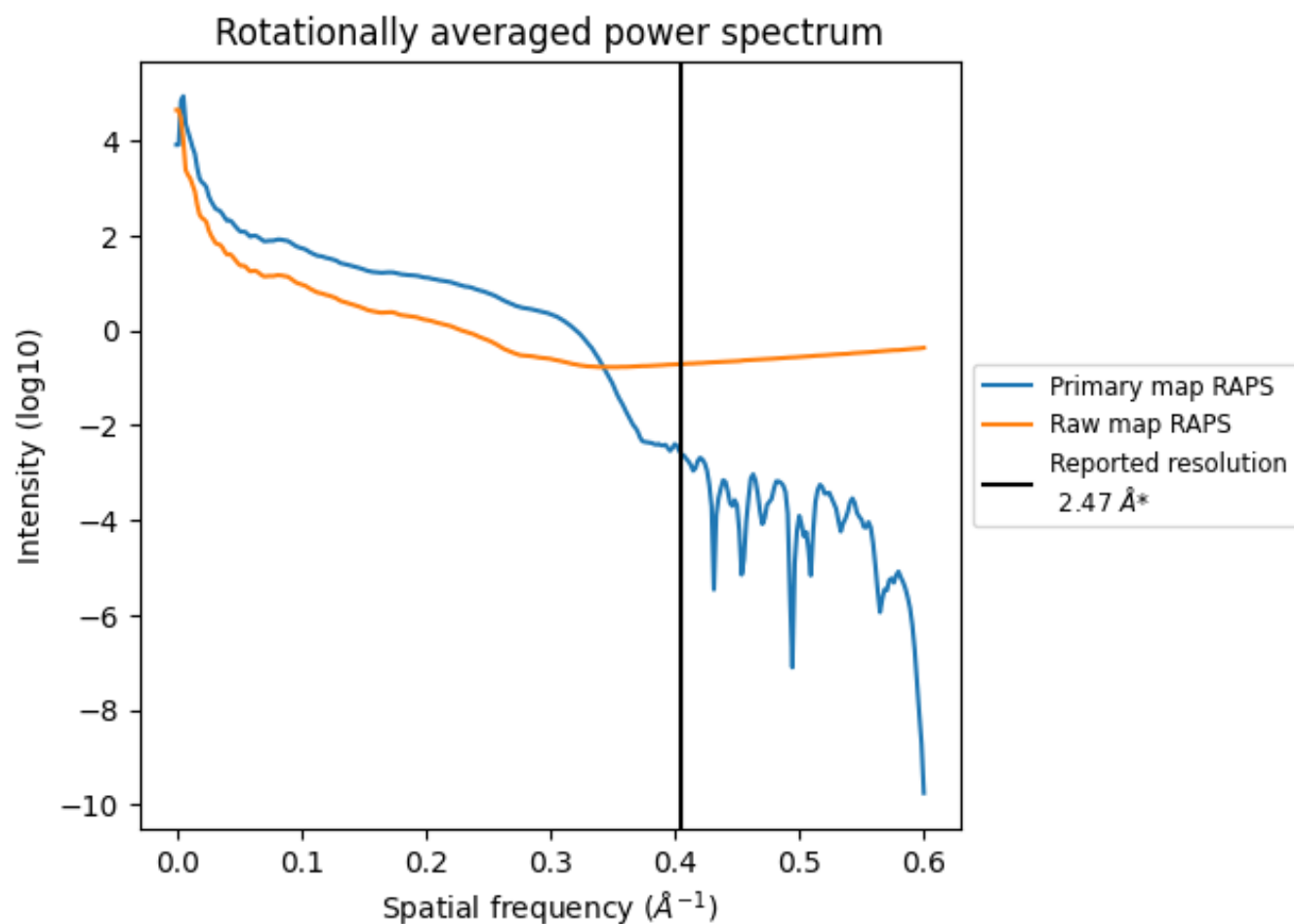
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1591 nm^3 ; this corresponds to an approximate mass of 1437 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 ⓘ

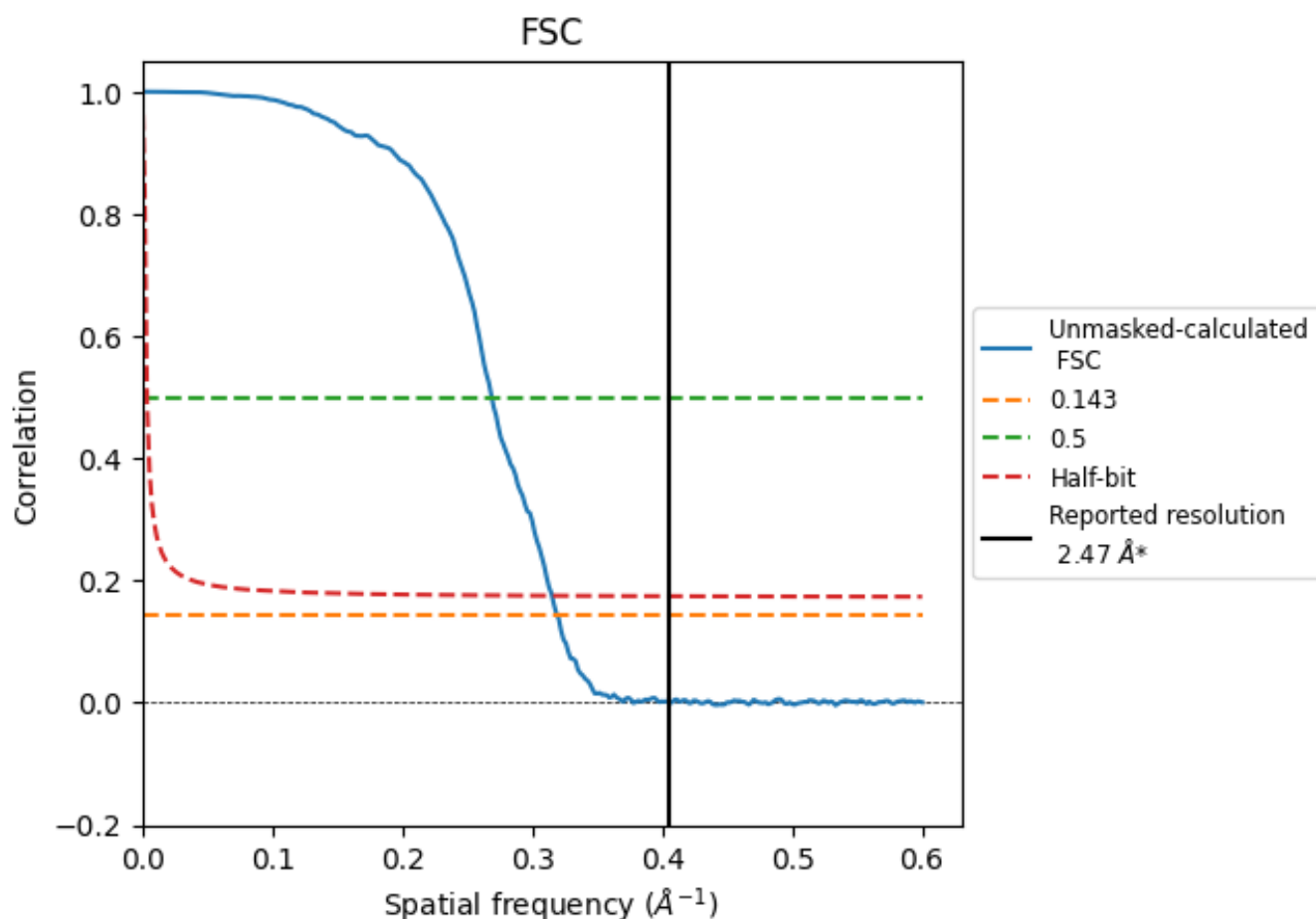


*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

8.2 Resolution estimates [i](#)

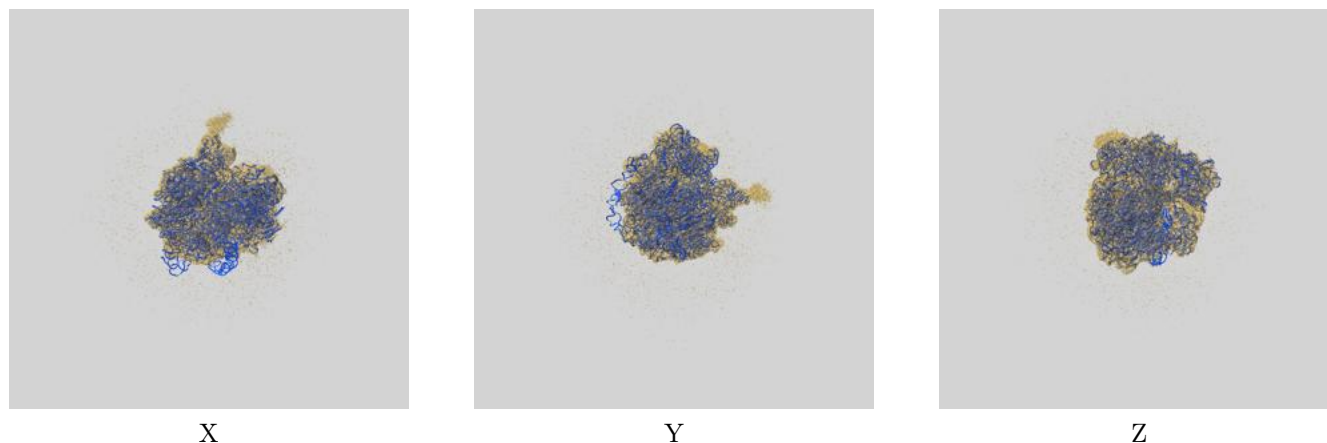
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	3.72	3.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.47 by more than 10 %

9 Map-model fit [i](#)

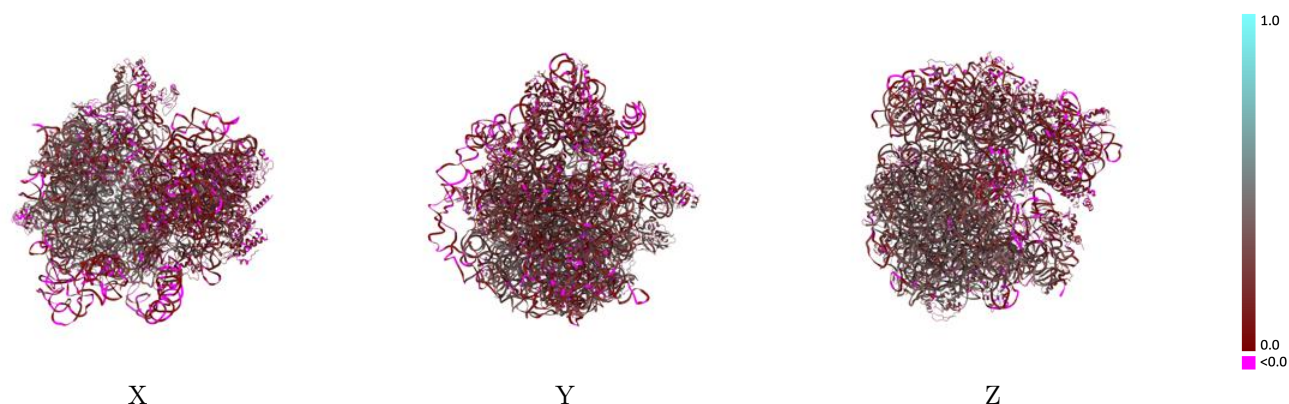
This section contains information regarding the fit between EMDB map EMD-44092 and PDB model 9B1Y. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



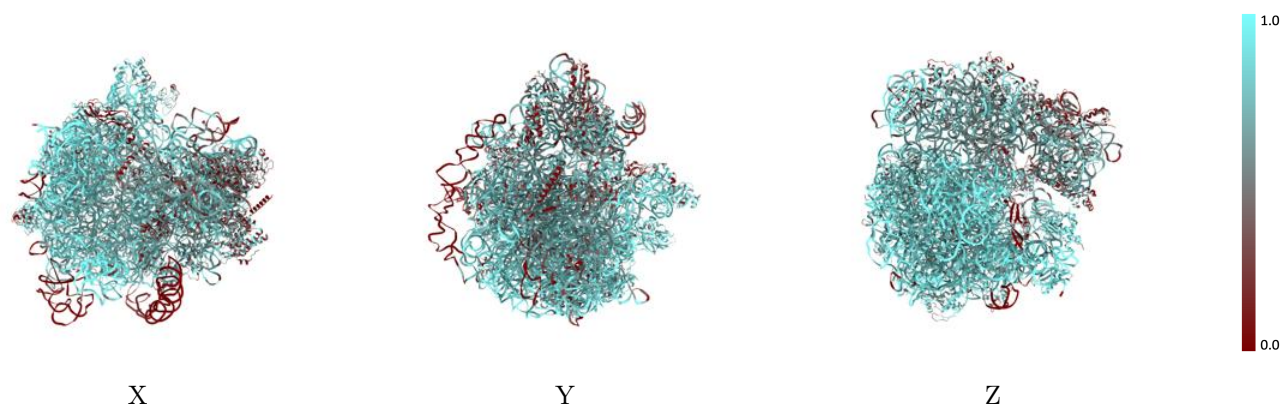
The images above show the 3D surface view of the map at the recommended contour level 0.968 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



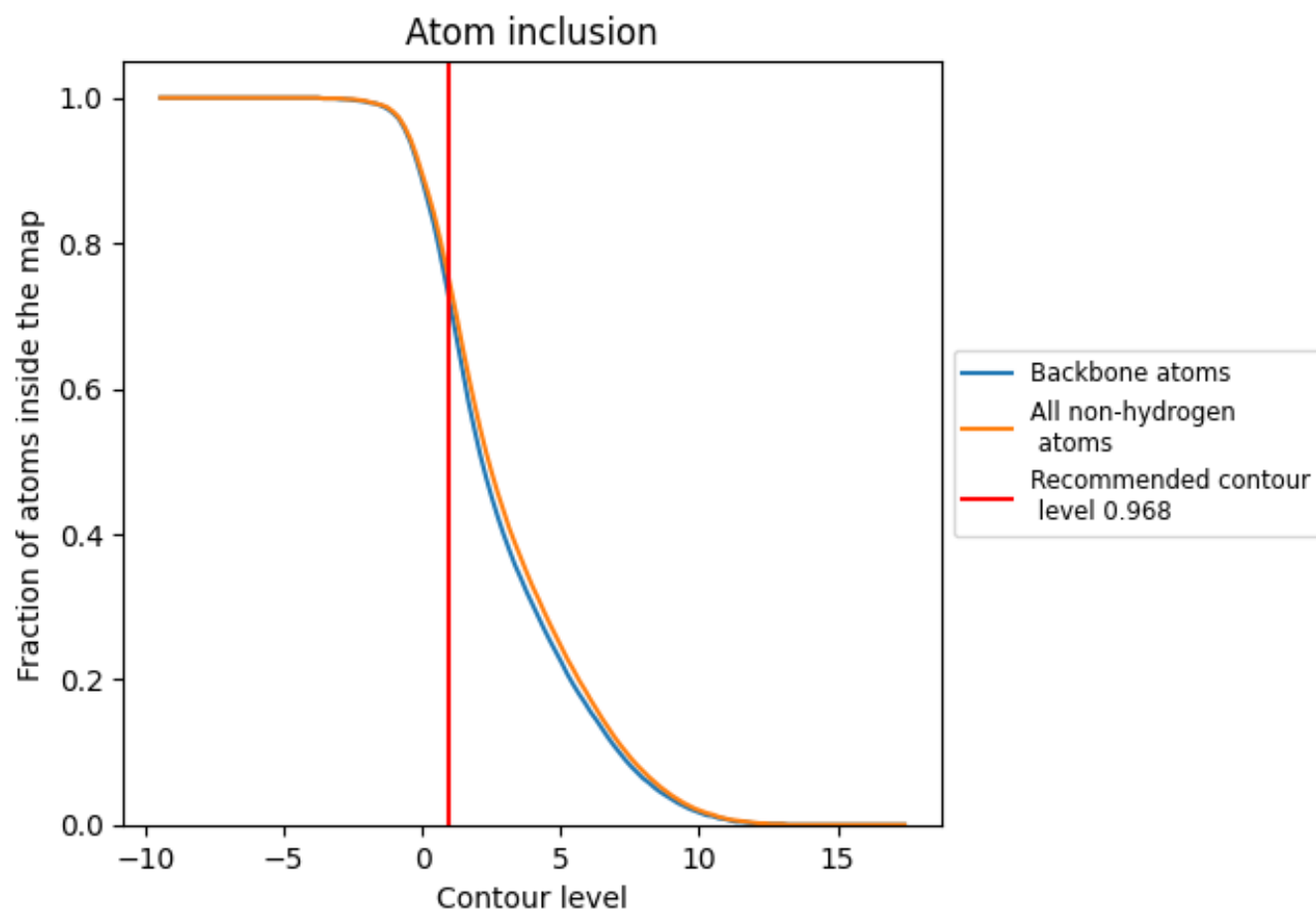
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.968).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 75% 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 (0.968) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.2350
1	 0.8070	 0.3320
2	 0.8580	 0.3260
4	 0.8940	 0.0730
A	 0.6890	 0.1760
C	 0.4590	 0.1440
D	 0.4610	 0.1290
E	 0.5590	 0.1700
F	 0.6250	 0.1990
G	 0.3960	 0.1300
H	 0.5540	 0.1860
I	 0.5690	 0.1350
J	 0.3330	 0.1210
K	 0.6440	 0.1920
L	 0.5560	 0.1880
M	 0.4870	 0.1230
N	 0.5090	 0.1060
O	 0.6310	 0.2320
P	 0.4260	 0.1280
Q	 0.4760	 0.1330
R	 0.6840	 0.1650
T	 0.6460	 0.1870
U	 0.9250	 0.2900
V	 0.4720	 0.1510
Y	 0.8340	 0.2800
Z	 0.7890	 0.2840
a	 0.7930	 0.2890
b	 0.7630	 0.2680
c	 0.8250	 0.1780
d	 0.8580	 0.2980
e	 0.6400	 0.0800
f	 0.8110	 0.3270
g	 0.7910	 0.2700
h	 0.6860	 0.2130
i	 0.7750	 0.2900



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Chain	Atom inclusion	Q-score
j	 0.7750	 0.2820
k	 0.7850	 0.2490
l	 0.6170	 0.1510
m	 0.7950	 0.3210
n	 0.8540	 0.3370
o	 0.7630	 0.3270
p	 0.7890	 0.2720
q	 0.8600	 0.3110
r	 0.4240	 0.1450
s	 0.7840	 0.3170
t	 0.8070	 0.2940
u	 0.7060	 0.1860
v	 0.8340	 0.1870
w	 0.8020	 0.3090
x	 0.6970	 0.2420
y	 0.7860	 0.2570
z	 0.7540	 0.3040