



## wwPDB EM Validation Summary Report ⓘ

Feb 3, 2025 – 08:04 pm GMT

PDB ID : 8QHU  
EMDB ID : EMD-18419  
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :  
LM32Cs1C1 snoRNA overexpression  
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.  
Deposited on : 2023-09-10  
Resolution : 2.72 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

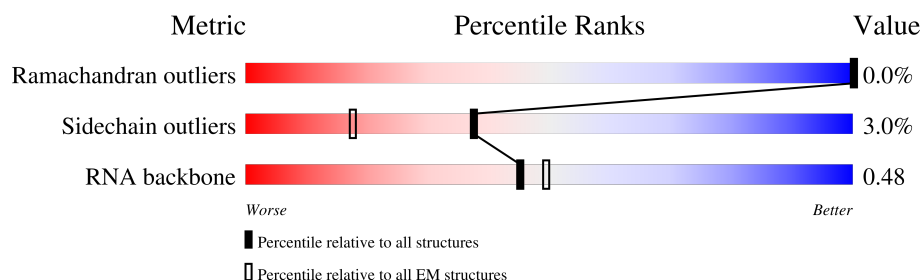
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 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 2.72 Å.

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



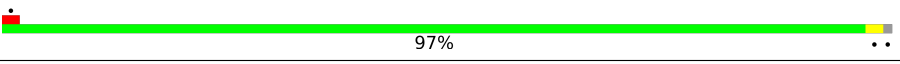

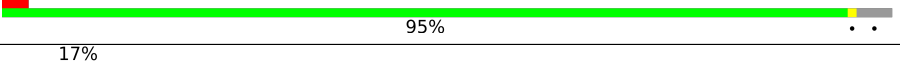


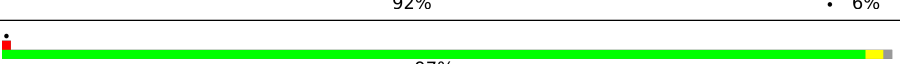
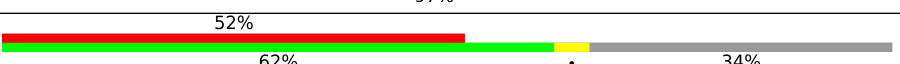
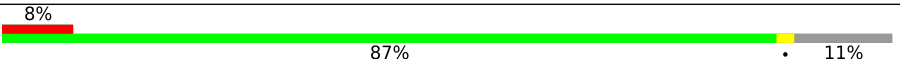
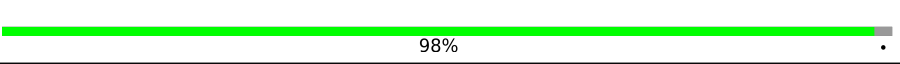
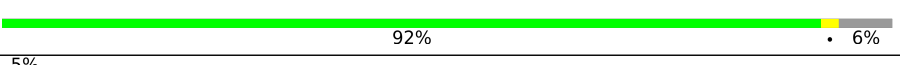
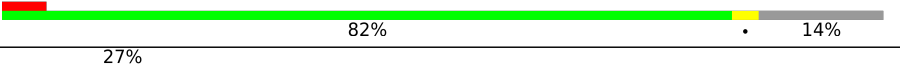
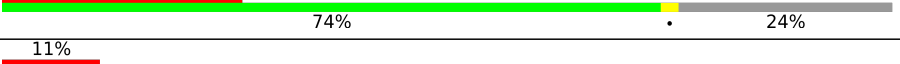

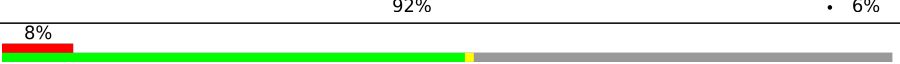
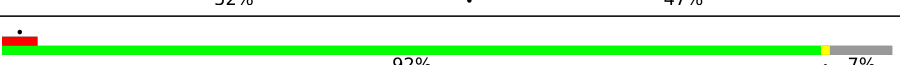


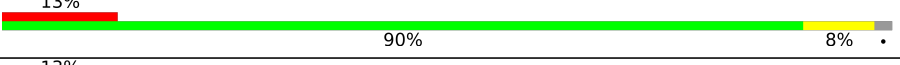


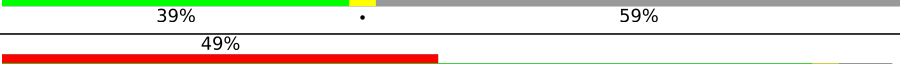
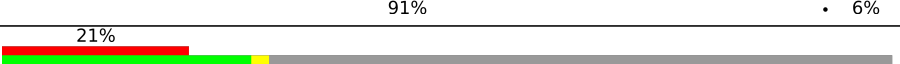



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	SB	246	<div> <div>8%</div> <div>81%</div> <div>15%</div> </div>
2	SC	219	<div> <div>11%</div> <div>94%</div> <div>•</div> </div>
3	SD	190	<div> <div>6%</div> <div>94%</div> <div>•</div> </div>
4	SE	273	<div> <div>6%</div> <div>94%</div> <div>• 5%</div> </div>
5	SF	265	<div> <div>6%</div> <div>81%</div> <div>• 17%</div> </div>
6	SG	249	<div> <div>12%</div> <div>89%</div> <div>• 7%</div> </div>
7	SH	190	<div> <div>•</div> <div>93%</div> <div>•</div> </div>
8	SI	200	<div> <div>13%</div> <div>98%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	SJ	130	
10	SK	220	
11	SL	149	
12	SM	116	
13	SN	168	
14	SO	144	
15	SP	143	
16	SQ	141	
17	SR	153	
18	SS	57	
19	ST	151	
20	SU	173	
21	SV	143	
22	SW	152	
23	SX	161	
24	SY	164	
25	SZ	137	
26	Sa	120	
27	Sb	112	
28	Sc	86	
29	Sd	87	
30	Se	66	
31	Sf	152	
32	Sg	312	
33	Sh	235	


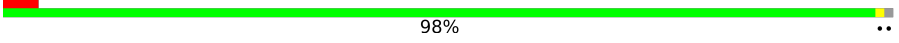
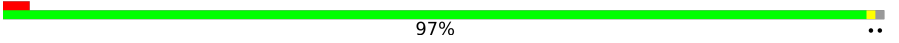
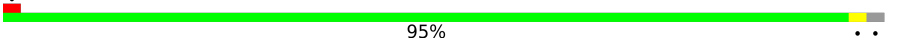
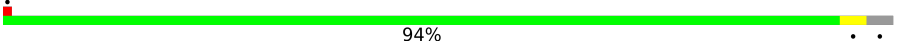



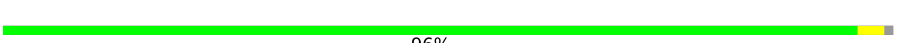

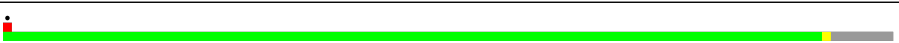



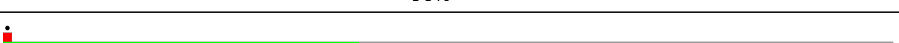
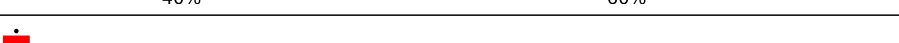
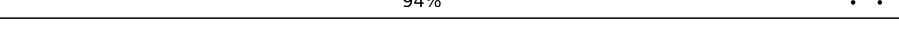
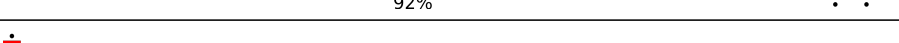





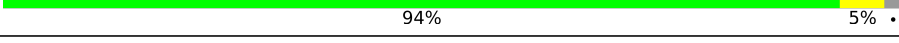
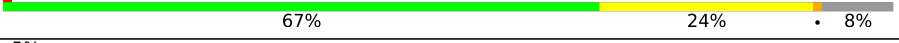
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Mol	Chain	Length	Quality of chain
34	S4	76	
35	S1	2204	
36	SA	264	
37	4	184	
38	6	73	
39	8	123	
40	A	260	
41	B	419	
42	C	373	
43	D	188	
44	E	190	
45	H	222	
46	I	220	
47	J	139	
48	K	175	
49	L	145	
50	M	204	
51	P	198	
52	Q	254	
53	R	179	
54	S	159	
55	T	166	
56	U	129	
57	V	145	
58	W	143	




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Mol	Chain	Length	Quality of chain
59	X	124	
60	Y	134	
61	Z	147	
62	a	127	
63	b	70	
64	c	252	
65	d	104	
66	f	133	
67	g	144	
68	h	168	
69	i	105	
70	j	83	
71	k	83	
72	l	51	
73	m	128	
74	n	34	
75	o	92	
76	p	106	
77	F	195	
78	G	264	
79	N	213	
80	O	305	
81	e	188	
82	1	1782	
83	3	216	

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Mol	Chain	Length	Quality of chain
84	5	135	
85	7	171	
86	2	1526	

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 209021 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SB	208	Total	C	N	O	S	0	0
			1627	1034	297	284	12		

- Molecule 2 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SC	212	Total	C	N	O	S	1	0
			1630	1032	299	286	13		

- Molecule 3 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SD	182	Total	C	N	O	S	0	0
			1482	933	300	241	8		

- Molecule 4 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SE	260	Total	C	N	O	S	0	0
			2050	1299	393	349	9		

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SF	219	Total	C	N	O	S	0	0
			1670	1068	298	294	10		

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SG	231	Total	C	N	O	S	0	0
			1831	1144	374	310	3		

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SH	182	Total	C	N	O	S	0	0
			1436	892	278	259	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SI	199	Total	C	N	O	S	0	0
			1619	1032	313	267	7		

- Molecule 9 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	182	Total	C	N	O	S	0	0
			1443	906	305	230	2		

- Molecule 11 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SL	143	Total	C	N	O	S	0	0
			1124	724	206	191	3		

- Molecule 12 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SM	102	Total	C	N	O	S	0	0
			796	498	145	151	2		

- Molecule 13 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SN	100	Total	C	N	O	S	0	0
			813	521	142	143	7		

- Molecule 14 is a protein called 40S ribosomal protein S14.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	SO	136	Total	C	N	O	S	0	0
			1015	627	198	182	8		

- Molecule 15 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SP	141	Total	C	N	O	S	0	0
			1100	694	217	186	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SQ	93	Total	C	N	O	S	0	0
			656	406	121	124	5		

- Molecule 17 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SR	136	Total	C	N	O	S	0	0
			1080	682	213	181	4		

- Molecule 18 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SS	56	Total	C	N	O	S	0	0
			452	279	94	73	6		

- Molecule 19 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	ST	142	Total	C	N	O	S	0	0
			1155	728	229	190	8		

- Molecule 20 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SU	148	Total	C	N	O	S	0	0
			1184	749	236	194	5		

- Molecule 21 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SV	109	Total	C	N	O	S	0	0
			850	538	164	144	4		

- Molecule 22 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SW	115	Total	C	N	O	S	0	0
			925	590	176	155	4		

- Molecule 23 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SX	152	Total	C	N	O	S	0	0
			1202	764	237	197	4		

- Molecule 24 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SY	87	Total	C	N	O	S	0	0
			640	397	120	119	4		

- Molecule 25 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SZ	127	Total	C	N	O	S	0	0
			1031	662	200	166	3		

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sa	71	Total	C	N	O	S	0	0
			558	356	99	100	3		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Sb	103	Total	C	N	O	S	0	0
			820	508	176	129	7		

- Molecule 28 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sc	84	Total	C	N	O	S	0	0
			647	400	125	114	8		

- Molecule 29 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Sd	65	Total	C	N	O	S	0	0
			474	290	95	85	4		

- Molecule 30 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Se	51	Total	C	N	O	S	0	0
			405	255	87	62	1		

- Molecule 31 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Sf	63	Total	C	N	O	S	0	0
			530	337	103	84	6		

- Molecule 32 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sg	294	Total	C	N	O	S	0	0
			2219	1396	393	419	11		

- Molecule 33 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sh	71	Total	C	N	O	S	0	0
			522	334	96	90	2		

- Molecule 34 is a RNA chain called E-site\_tRNA\_chain\_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S4	68	Total	C	N	O	P	0	0
			1447	646	258	476	67		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S4	3	G	C	conflict	GB 1851743410
S4	70	C	G	conflict	GB 1851743410

- Molecule 35 is a RNA chain called SSU\_rRNA\_chain\_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S1	1847	Total	C	N	O	P	1	0
			39517	17680	7108	12881	1848		

- Molecule 36 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SA	225	Total	C	N	O	S	1	0
			1820	1141	346	321	12		

- Molecule 37 is a RNA chain called SR2\_chain\_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	184	Total	C	N	O	P	1	0
			3956	1765	714	1292	185		

- Molecule 38 is a RNA chain called SR6\_chain\_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 39 is a RNA chain called 5S\_rRNA\_chain\_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 40 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A	255	Total	C	N	O	S	1	0
			1927	1200	395	321	11		

- Molecule 41 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B	401	Total	C	N	O	S	0	0
			3145	1985	625	522	13		

- Molecule 42 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C	366	Total	C	N	O	S	0	0
			2799	1752	558	474	15		

- Molecule 43 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	D	173	Total	C	N	O	S	0	0
			1290	819	245	218	8		

- Molecule 44 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	E	186	Total	C	N	O	S	0	0
			1472	934	273	259	6		

- Molecule 45 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H	221	Total	C	N	O	S	0	0
			1765	1123	353	282	7		

- Molecule 46 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	I	209	Total	C	N	O	S	0	0
			1645	1026	334	277	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 47 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	J	134	Total	C	N	O	S	0	0
			996	630	189	171	6		

- Molecule 48 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	K	170	Total	C	N	O	S	0	0
			1313	823	263	219	8		

- Molecule 49 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L	144	Total	C	N	O	S	0	0
			1110	700	225	179	6		

- Molecule 50 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	M	203	Total	C	N	O	S	0	0
			1704	1076	362	258	8		

- Molecule 51 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	P	197	Total	C	N	O	S	0	0
			1532	964	306	256	6		

- Molecule 52 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Q	185	Total	C	N	O	S	0	0
			1527	947	336	238	6		

- Molecule 53 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	R	178	Total	C	N	O	S	0	0
			1452	925	279	243	5		

- Molecule 54 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S	158	Total	C	N	O	S	0	0
			1253	797	243	209	4		

- Molecule 55 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	T	151	Total	C	N	O	S	0	0
			1215	760	241	203	11		

- Molecule 56 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	U	12	Total	C	N	O	0	0
			81	48	19	14		

- Molecule 57 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	V	118	Total	C	N	O	S	0	0
			934	593	180	159	2		

- Molecule 58 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	W	120	Total	C	N	O	S	0	0
			955	597	199	155	4		

- Molecule 59 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	X	64	Total	C	N	O	S	0	0
			548	359	105	80	4		

- Molecule 60 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Y	133	Total	C	N	O	S	0	0
			1048	674	212	159	3		

- Molecule 61 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Z	145	Total	C	N	O	S	0	0
			1121	687	238	191	5		

- Molecule 62 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	a	124	Total	C	N	O	S	0	0
			1028	644	216	164	4		

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	b	68	Total	C	N	O	S	0	0
			546	335	125	86			

- Molecule 64 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	c	229	Total	C	N	O	S	0	0
			1866	1188	359	308	11		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	d	92	Total	C	N	O	S	0	0
			705	438	129	133	5		

- Molecule 66 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f	126	Total	C	N	O	S	0	0
			1023	645	203	171	4		

- Molecule 67 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g	143	Total	C	N	O	S	0	0
			1149	714	240	190	5		

- Molecule 68 is a protein called Putative 60S ribosomal protein L34.



Mol	Chain	Residues	Atoms					AltConf	Trace
68	h	125	Total	C	N	O	S	0	0
			1011	621	220	164	6		

- Molecule 69 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i	98	Total	C	N	O	S	0	0
			777	492	159	124	2		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j	81	Total	C	N	O	S	0	0
			672	409	154	103	6		

- Molecule 71 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k	77	Total	C	N	O	S	0	0
			614	388	120	103	3		

- Molecule 72 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 73 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m	51	Total	C	N	O	S	0	0
			410	258	84	61	7		

- Molecule 74 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n	33	Total	C	N	O	S	0	0
			292	178	75	37	2		

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	88	Total	C	N	O	S	0	0
			689	428	142	113	6		

- Molecule 76 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p	98	Total	C	N	O	S	0	0
			787	498	159	125	5		

- Molecule 77 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	F	148	Total	C	N	O	S	0	0
			1118	714	212	190	2		

- Molecule 78 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	G	228	Total	C	N	O	S	0	0
			1792	1130	354	301	7		

- Molecule 79 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	N	199	Total	C	N	O	S	0	0
			1615	1018	321	262	14		

- Molecule 80 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	O	282	Total	C	N	O	S	0	0
			2125	1359	409	351	6		

- Molecule 81 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	e	185	Total	C	N	O	S	0	0
			1456	915	295	242	4		

- Molecule 82 is a RNA chain called RNA (1646-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
82	1	1646	Total	C	N	O	P	0	0
			35315	15785	6473	11411	1646		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	164	G	U	conflict	GB 321438308
1	165	U	C	conflict	GB 321438308
1	198	A	C	conflict	GB 321438308
1	523	A	G	conflict	GB 321438308
1	593	C	U	conflict	GB 321438308
1	1428	A	C	conflict	GB 321438308

- Molecule 83 is a RNA chain called SR1\_chain\_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	3	178	Total	C	N	O	P	0	0
			3776	1689	656	1253	178		

- Molecule 84 is a RNA chain called SR4\_chain\_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	5	117	Total	C	N	O	P	0	0
			2496	1113	447	819	117		

- Molecule 85 is a RNA chain called 5.8S\_rRNA\_chain\_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	7	163	Total	C	N	O	P	0	0
			3472	1556	616	1138	162		

- Molecule 86 is a RNA chain called LSUB\_rRNA\_chain\_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	2	1190	Total	C	N	O	P	0	0
			25463	11395	4598	8280	1190		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	SG	1	Total	Mg	0
			1	1	

*Continued on next page...*

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Mol	Chain	Residues	Atoms		AltConf
87	SK	1	Total 1	Mg 1	0
87	SS	1	Total 1	Mg 1	0
87	SX	2	Total 2	Mg 2	0
87	Sb	1	Total 1	Mg 1	0
87	S1	79	Total 79	Mg 79	0
87	4	7	Total 7	Mg 7	0
87	6	1	Total 1	Mg 1	0
87	8	6	Total 6	Mg 6	0
87	B	2	Total 2	Mg 2	0
87	I	1	Total 1	Mg 1	0
87	J	1	Total 1	Mg 1	0
87	S	1	Total 1	Mg 1	0
87	T	1	Total 1	Mg 1	0
87	f	1	Total 1	Mg 1	0
87	N	1	Total 1	Mg 1	0
87	1	119	Total 119	Mg 119	0
87	3	4	Total 4	Mg 4	0
87	5	1	Total 1	Mg 1	0
87	7	7	Total 7	Mg 7	0
87	2	97	Total 97	Mg 97	0

- Molecule 88 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
88	S1	11	Total 11	K 11	0
88	4	4	Total 4	K 4	0
88	A	1	Total 1	K 1	0
88	B	1	Total 1	K 1	0
88	M	1	Total 1	K 1	0
88	N	1	Total 1	K 1	0
88	1	11	Total 11	K 11	0
88	3	1	Total 1	K 1	0
88	5	2	Total 2	K 2	0
88	2	13	Total 13	K 13	0

- Molecule 89 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
89	S1	2	Total 2	Na 2	0
89	1	2	Total 2	Na 2	0
89	3	1	Total 1	Na 1	0
89	5	1	Total 1	Na 1	0
89	7	1	Total 1	Na 1	0
89	2	3	Total 3	Na 3	0

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	S1	44	Total 44	O 44	0
90	4	9	Total 9	O 9	0

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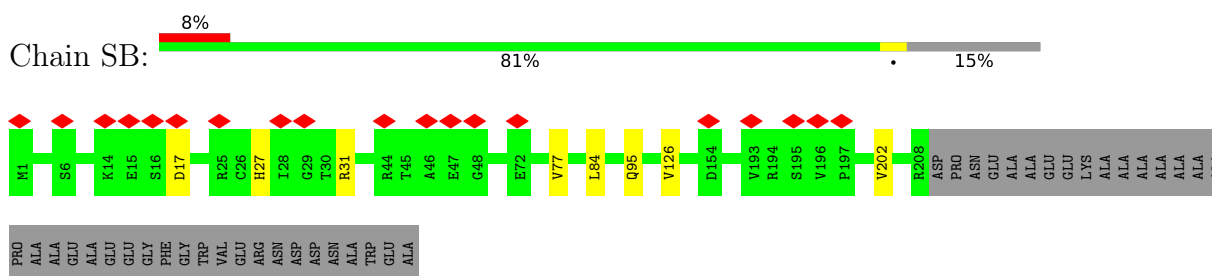
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Mol	Chain	Residues	Atoms		AltConf
90	8	4	Total 4	O 4	0
90	A	4	Total 4	O 4	0
90	B	4	Total 4	O 4	0
90	E	1	Total 1	O 1	0
90	H	1	Total 1	O 1	0
90	J	1	Total 1	O 1	0
90	T	2	Total 2	O 2	0
90	W	1	Total 1	O 1	0
90	b	1	Total 1	O 1	0
90	h	2	Total 2	O 2	0
90	j	3	Total 3	O 3	0
90	1	135	Total 135	O 135	0
90	3	4	Total 4	O 4	0
90	5	4	Total 4	O 4	0
90	7	6	Total 6	O 6	0
90	2	141	Total 141	O 141	0

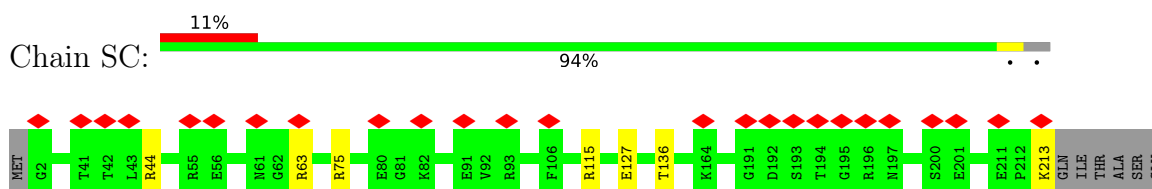
### 3 Residue-property plots [i](#)

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.

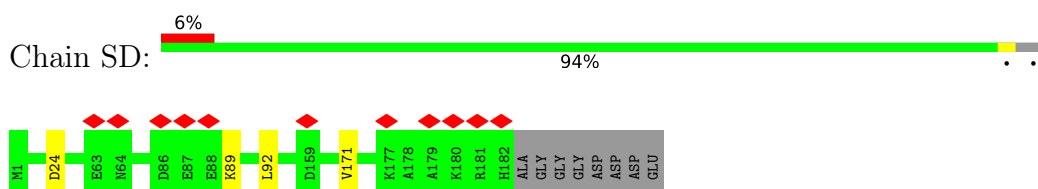
- Molecule 1: 40S ribosomal protein SA



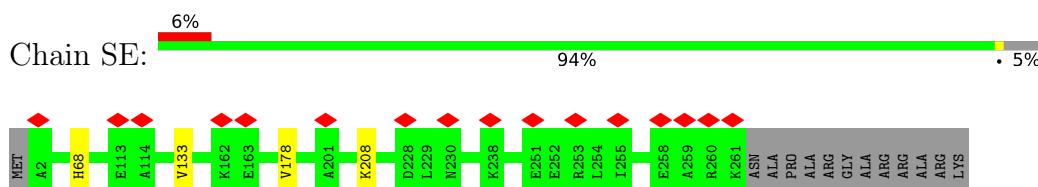
- Molecule 2: Putative 40S ribosomal protein S3



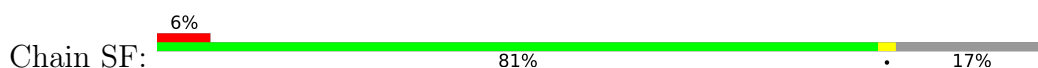
- Molecule 3: Putative 40S ribosomal protein S9

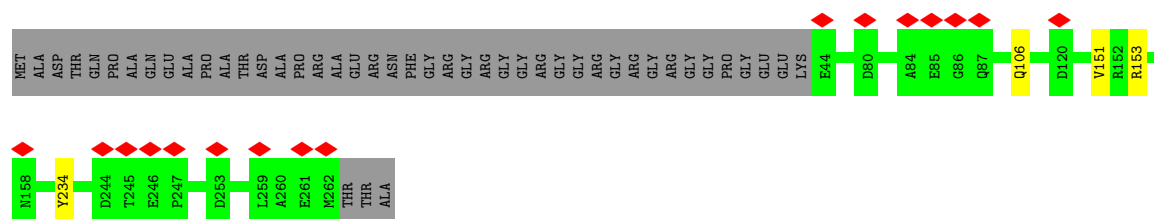


- Molecule 4: 40S ribosomal protein S4



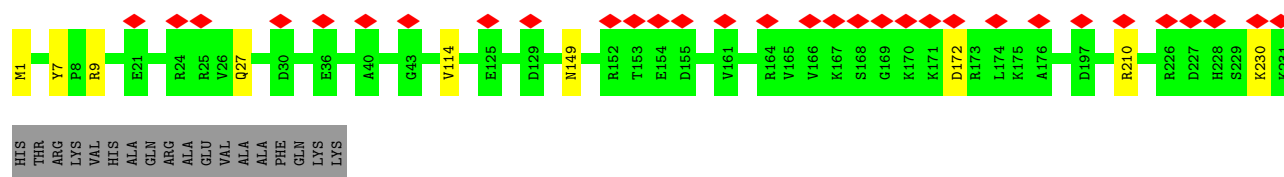
- Molecule 5: 40S ribosomal protein S2





- Molecule 6: 40S ribosomal protein S6

Chain SG: 12% 89% 7%



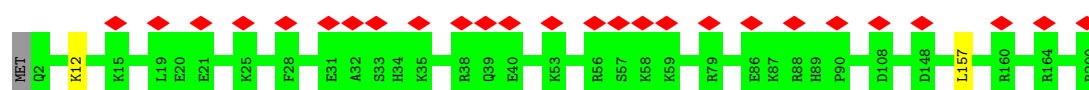
- Molecule 7: 40S ribosomal protein S5

Chain SH: 93% 7%



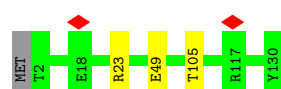
- Molecule 8: 40S ribosomal protein S7

Chain SI: 13% 98% 9%



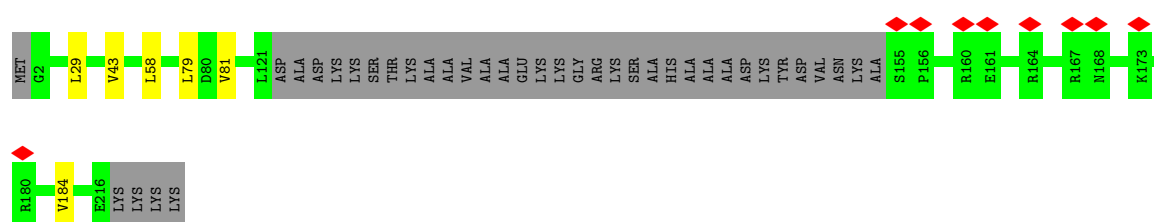
- Molecule 9: Putative 40S ribosomal protein S15A

Chain SJ: 97% 3%



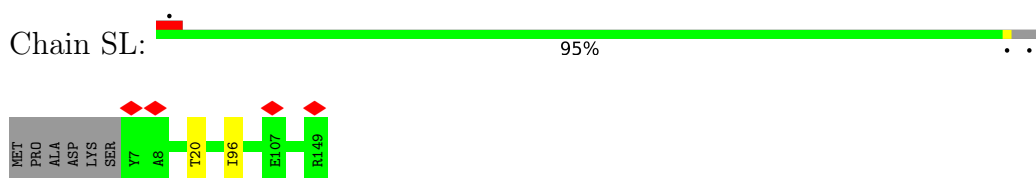
- Molecule 10: 40S ribosomal protein S8

Chain SK: 80% 17% 3%

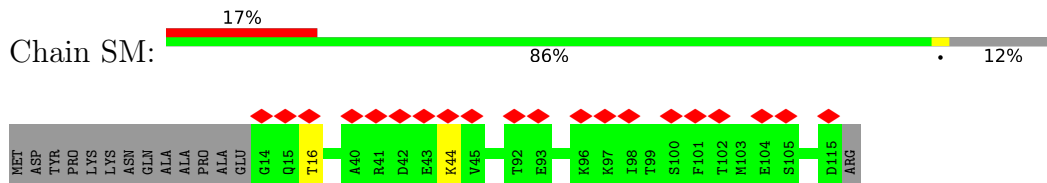




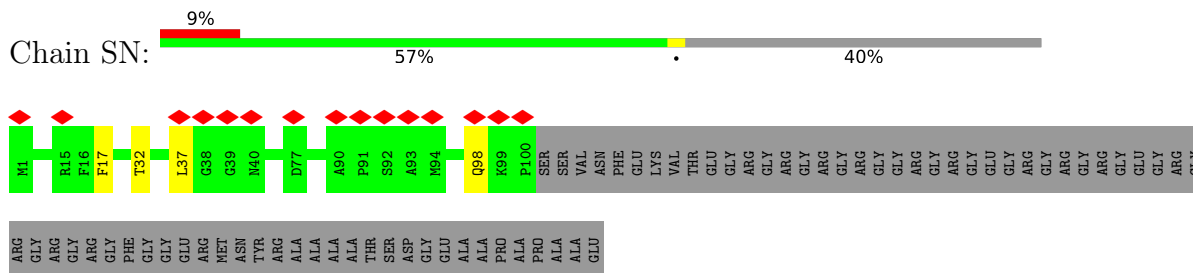
- Molecule 11: Putative 40S ribosomal protein S16



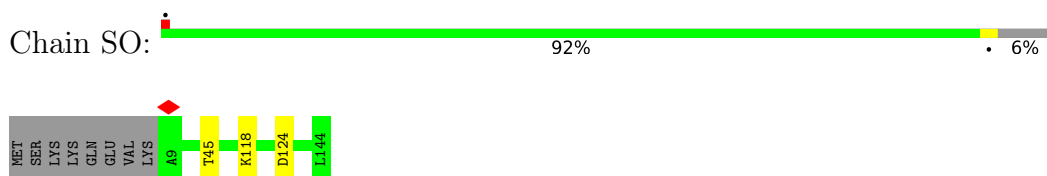
- Molecule 12: Putative ribosomal protein S20



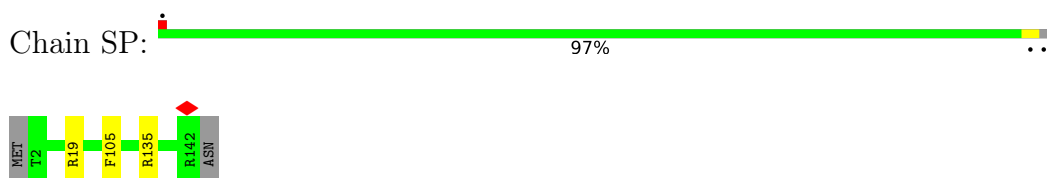
- Molecule 13: Putative 40S ribosomal protein S10



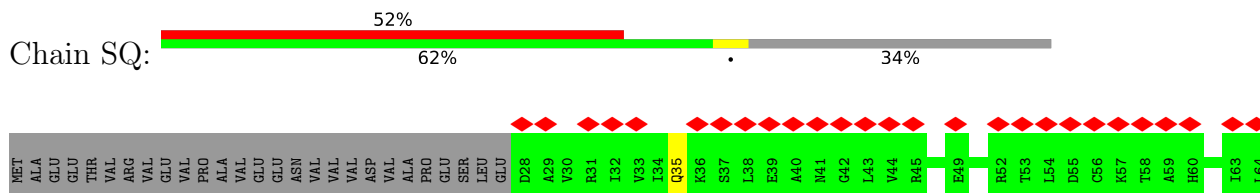
- Molecule 14: 40S ribosomal protein S14

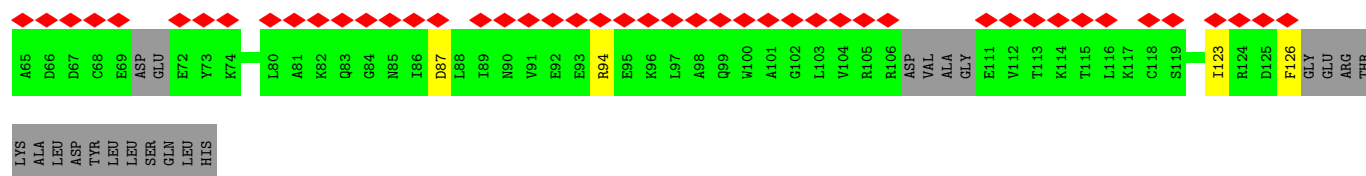


- Molecule 15: Putative 40S ribosomal protein S23



- Molecule 16: 40S ribosomal protein S12





- Molecule 17: Putative 40S ribosomal protein S18



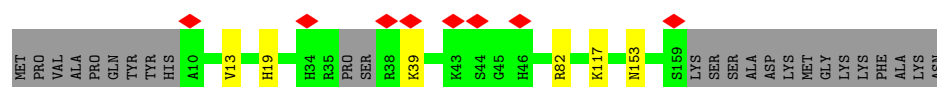
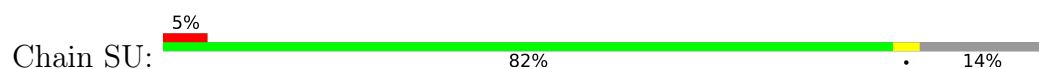
- Molecule 18: Putative ribosomal protein S29



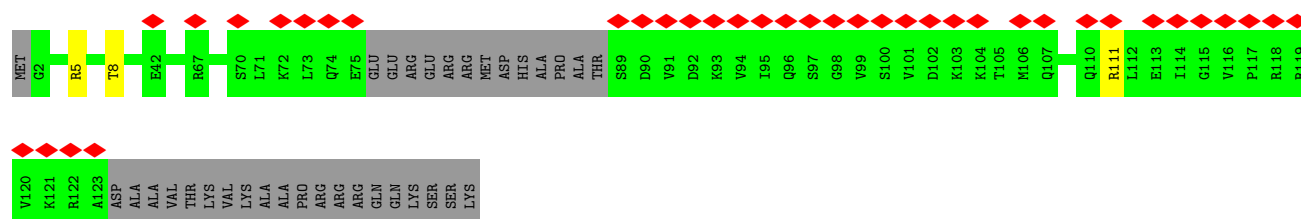
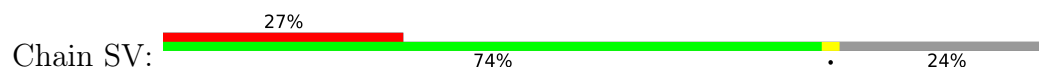
- Molecule 19: Putative 40S ribosomal protein S13



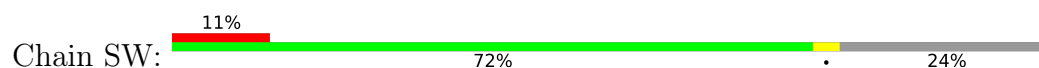
- Molecule 20: Putative 40S ribosomal protein S11

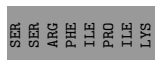


- Molecule 21: Putative 40S ribosomal protein S17



- Molecule 22: Putative 40S ribosomal protein S15





- 
- Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows amino acids: MET, THR, ALA, PRO, ARG, N6, H9, L19, L113, H114, Q131, R138, G157, GLN, SER, LYS, ALA. Red diamonds are placed above the N6, Q131, and G157 positions.

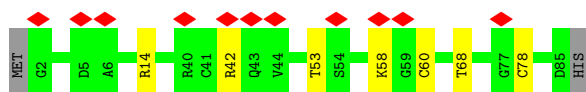
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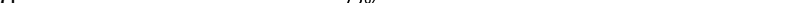
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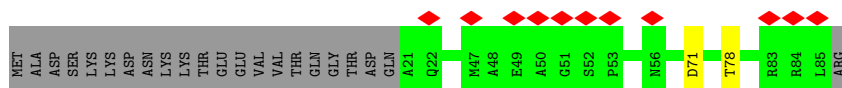
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ALA | GLU | MET | PRO | PRO | LYS | ALA | GLY | GLN | THR | LYS | LYS | ALA | LYS | MET | GLU | ALA | ALA | ASN | LYS | GLY | LYS | LYS | THR | THR | LYS | LYS | TRP | SER | LYS | GLY | GLN | SER | ARG | GLU | A35 | E45 | D48 | R56 | D67 | Q82 | V106 | GLN | ALA | ALA | PRO | PRO | GLU | ALA | ALA | ALA | ALA | ALA | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- 
- Sequence logo for the 1000bp upstream region of the H19 gene. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows amino acid positions from MET to LYS. Red diamonds indicate positions with a p-value < 0.05. The sequence is: MET, T2, R17, D48, R53, A64, N65, I98, K103, V104, PRO, PHE, ARG, PRO, ALA, GLY, LYS, LYS.

- 



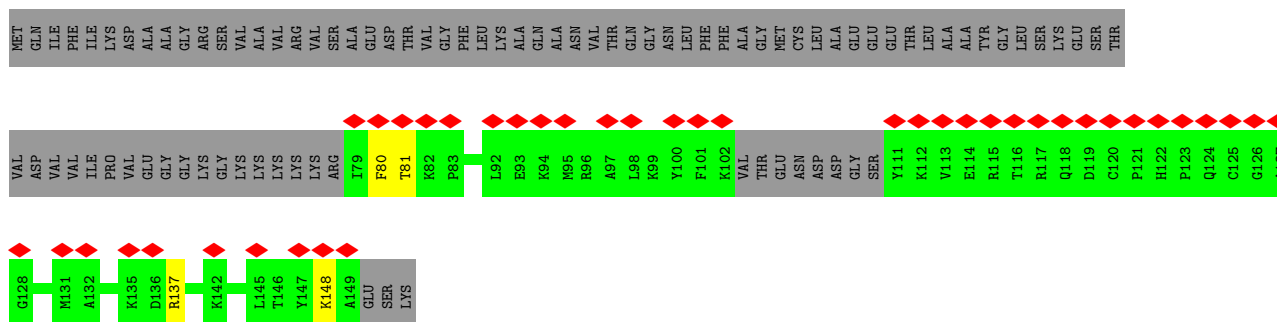
- Chain Sd: 

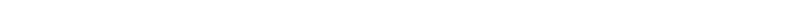


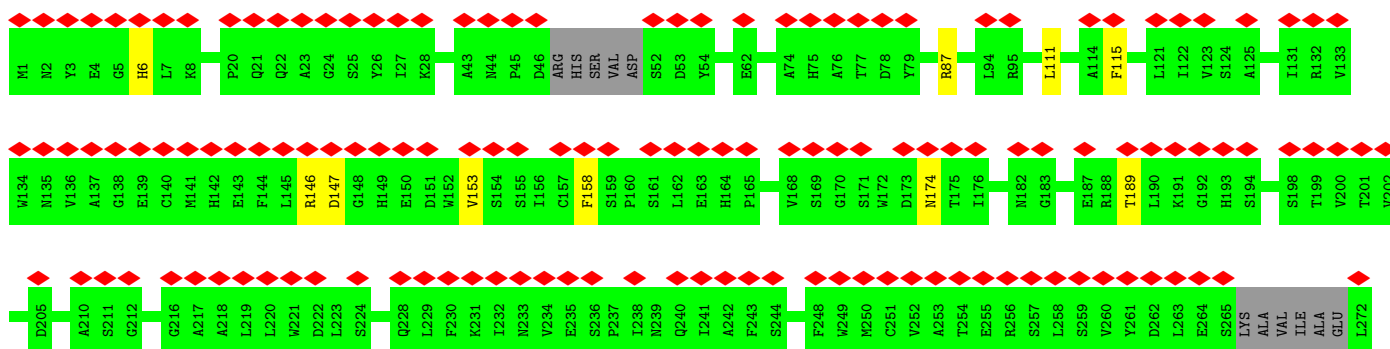
- Chain Se:  77% 23%



- Chain Sf: 

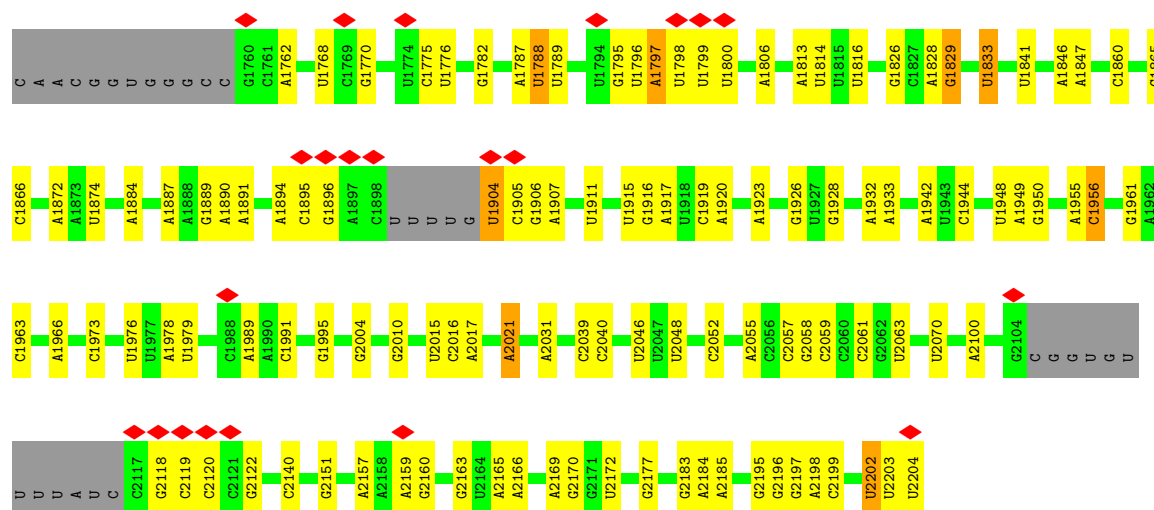


- Chain Sg: 

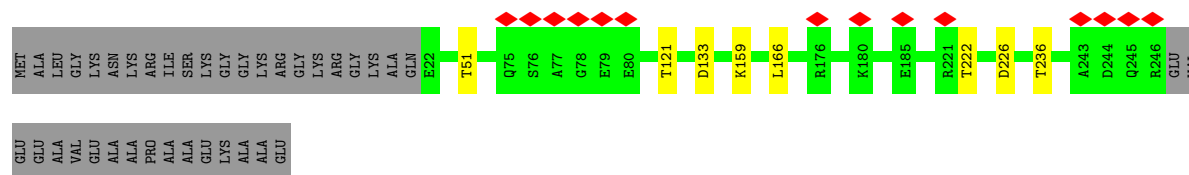
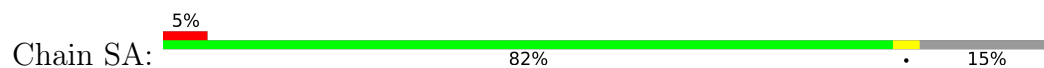




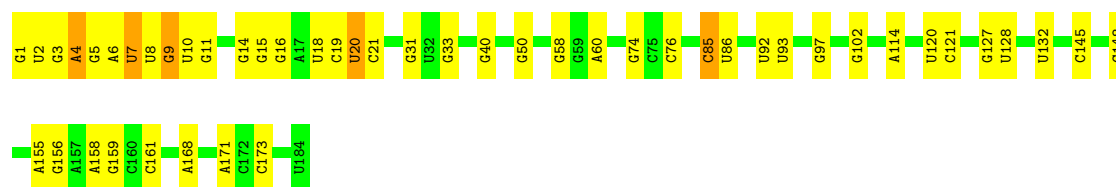




• Molecule 36: 40S ribosomal protein S3a



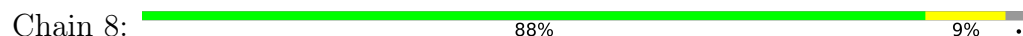
• Molecule 37: SR2\_chain\_4



• Molecule 38: SR6\_chain\_6

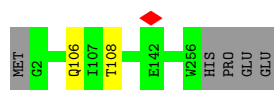


• Molecule 39: 5S\_rRNA\_chain\_8



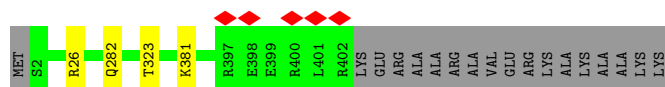
- Molecule 40: Putative 60S ribosomal protein L2

Chain A:  97%



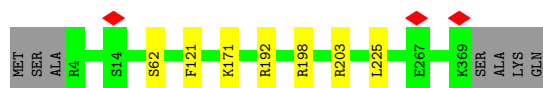
- Molecule 41: Putative ribosomal protein L3

Chain B:  95%

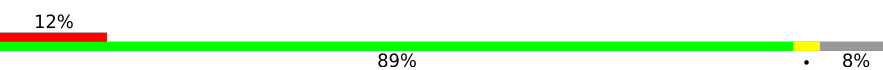


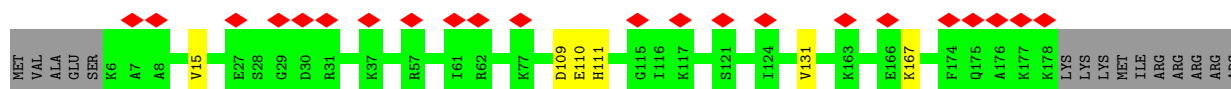
- Molecule 42: Putative ribosomal protein L1a

Chain C:  96%



- Molecule 43: 60S ribosomal protein L11

Chain D:  12% 89% 8%



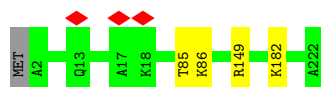
- Molecule 44: Putative 60S ribosomal protein L9

Chain E:  95%



- Molecule 45: Putative 60S ribosomal protein L13a

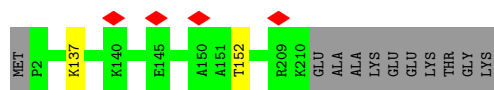
Chain H:  98%



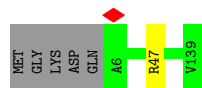
- Molecule 46: Putative 60S ribosomal protein L13

Chain I:  94% 5%





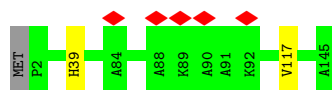
- Molecule 47: Putative 60S ribosomal protein L23



- Molecule 48: Putative 40S ribosomal protein L14



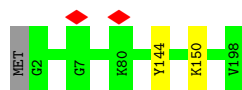
- Molecule 49: Putative 60S ribosomal protein L27A/L29



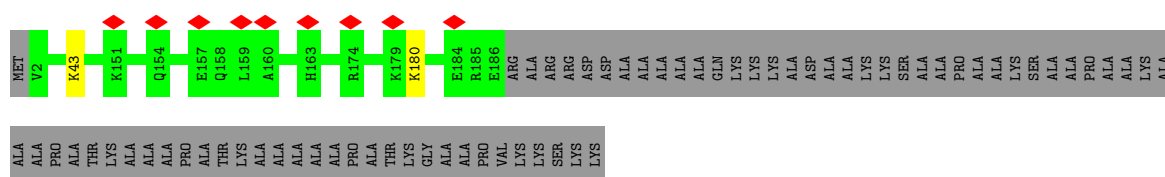
- Molecule 50: Ribosomal protein L15



- Molecule 51: 60S ribosomal protein L18

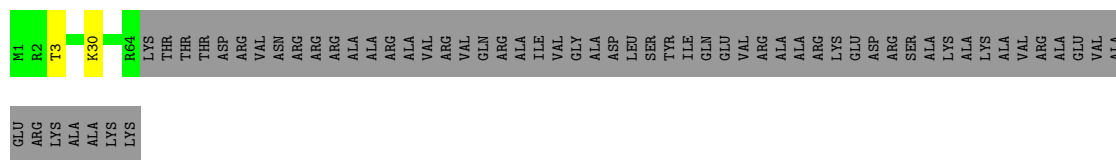


- Molecule 52: Putative 60S ribosomal protein L19





Chain X:  50% 48%



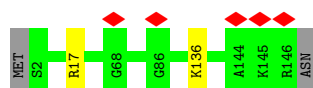
- Molecule 60: 60S ribosomal protein L27

Chain Y:  98%



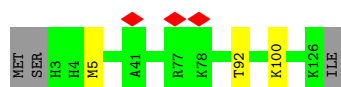
- Molecule 61: Putative 60S ribosomal protein L28

Chain Z:  97%



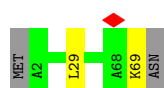
- Molecule 62: Putative 60S ribosomal protein L35

Chain a:  95%




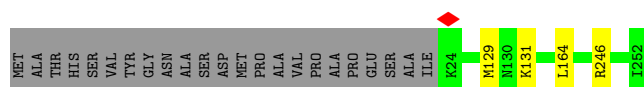
- Molecule 63: 60S ribosomal protein L29

Chain b:  94%




- Molecule 64: Putative 60S ribosomal protein L7

Chain c:  89% 9%



- Molecule 65: 60S ribosomal protein L30

Chain d:  5% 85% 12%



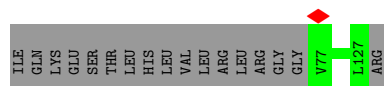
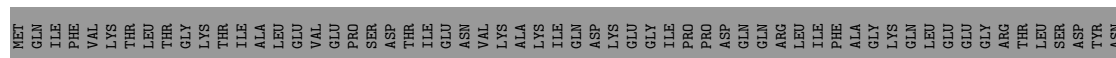
- Molecule 72: Putative 60S ribosomal protein L39

Chain l:  96%



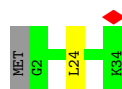
- Molecule 73: Ubiquitin-60S ribosomal protein L40

Chain m:  40% 60%



- Molecule 74: 60S ribosomal protein L41

Chain n:  94%




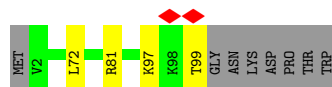
- Molecule 75: 60S ribosomal protein L37a

Chain o:  92%




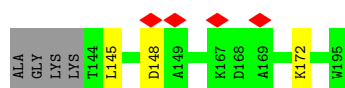
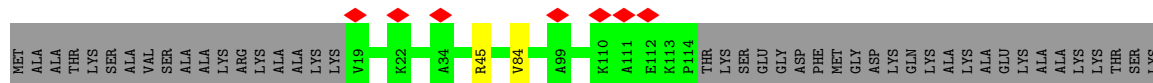
- Molecule 76: Putative 60S ribosomal protein L44

Chain p:  89% 8%




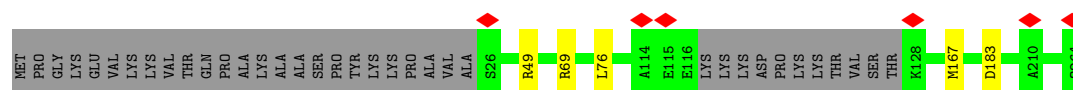
- Molecule 77: Putative 60S ribosomal protein L6

Chain F:  6% 73% 24%




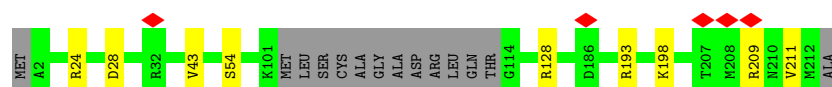
- Molecule 78: 60S ribosomal protein L7a

Chain G: 

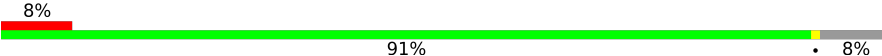


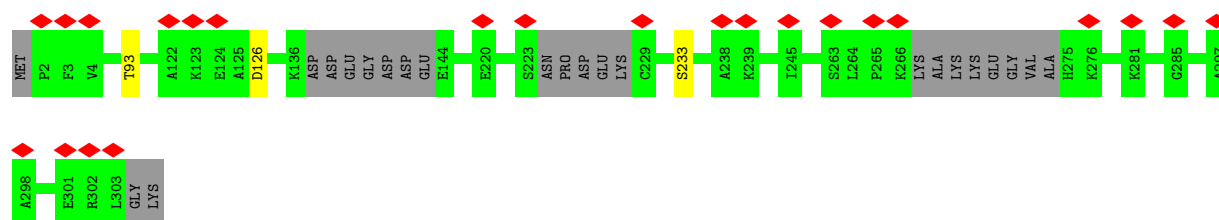
- Molecule 79: Putative 60S ribosomal protein L10

Chain N: 



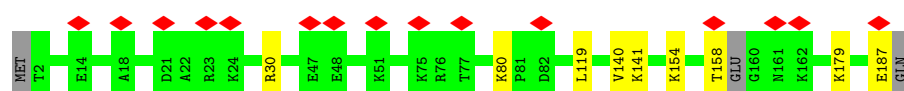
- Molecule 80: Putative 60S ribosomal protein L5

Chain O: 



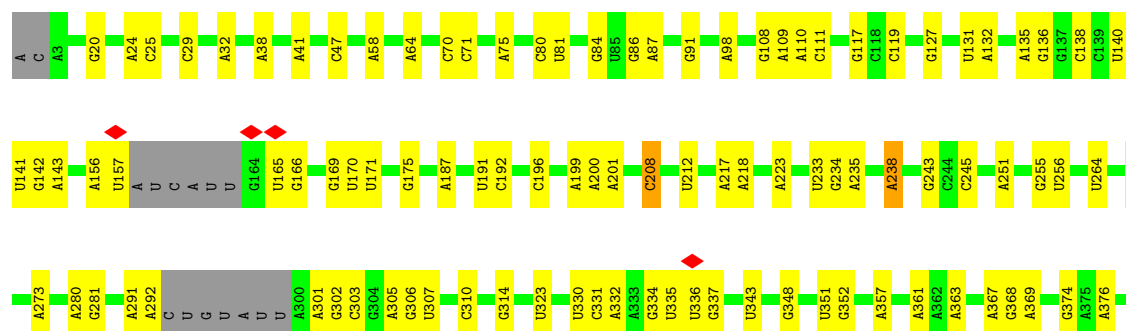
- Molecule 81: Putative 60S ribosomal subunit protein L31

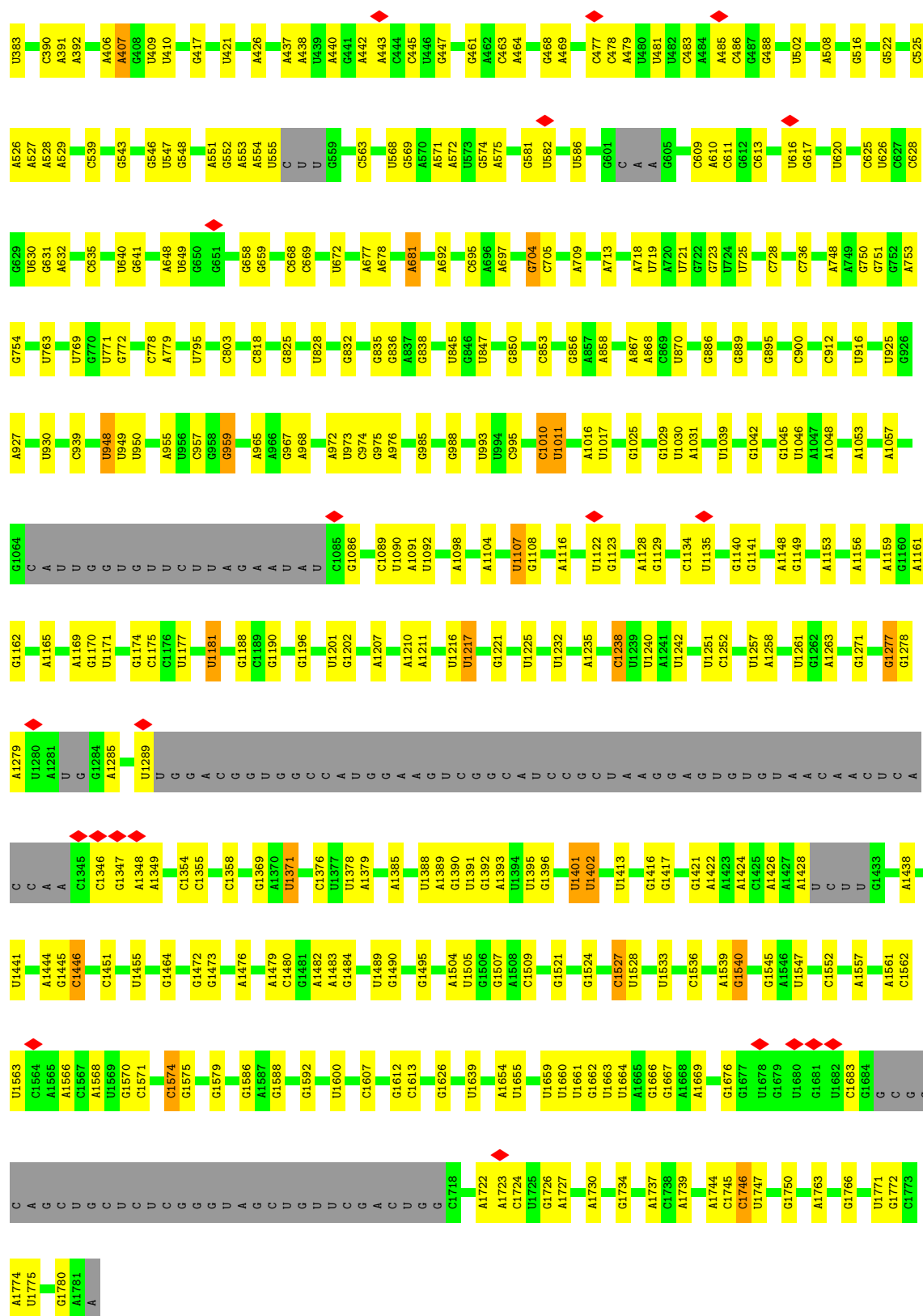
Chain e: 



- Molecule 82: RNA (1646-MER)

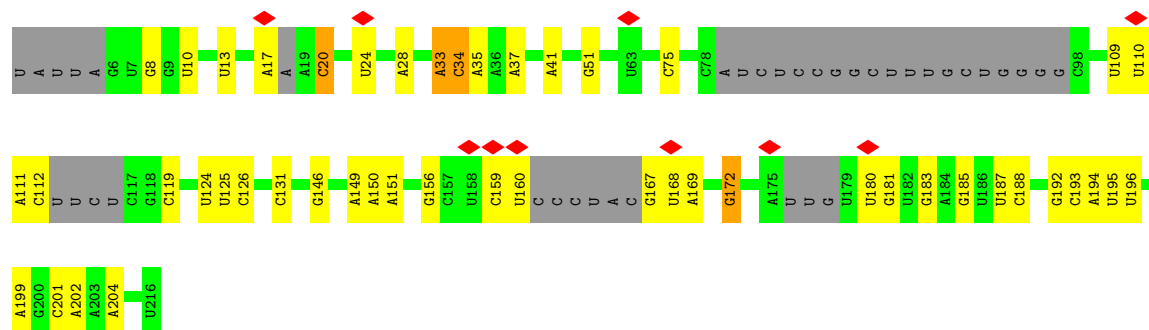
Chain 1: 



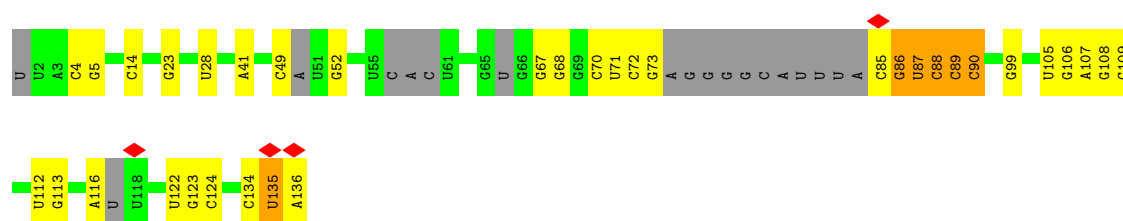


• Molecule 83: SR1\_chain\_3

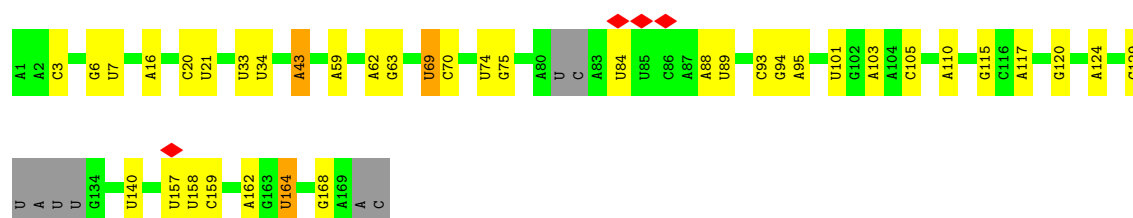
Chain 3: 5% 60% 21% 18%



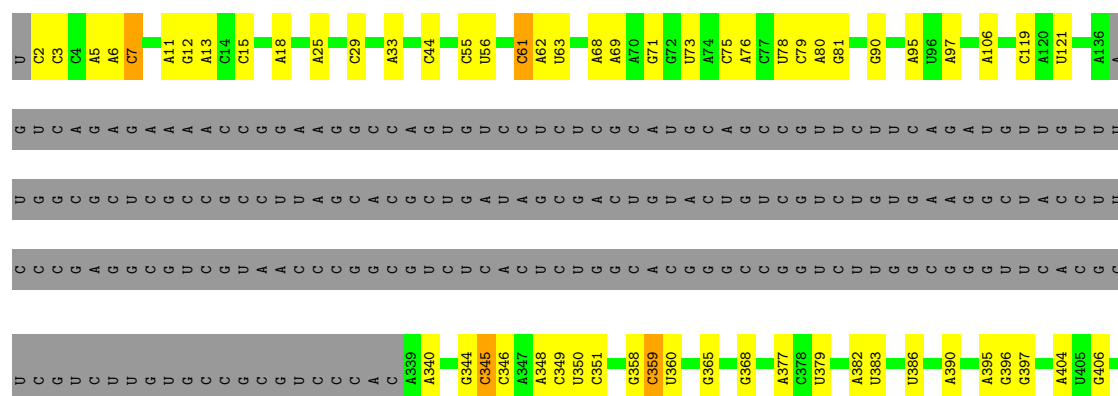
• Molecule 84: SR4\_chain\_5



• Molecule 85: 5.8S\_rRNA\_chain\_7



• Molecule 86: LSUb\_rRNA\_chain\_2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134493	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 ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	358.56, 358.56, 358.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.747, 0.747, 0.747	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: PSU, 7MG, MA6, OMG, NA, A2M, MG, K, 5MC, 1MA, OMC, C4J, OMU

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	SB	0.26	0/1660	0.50	0/2246
2	SC	0.26	0/1658	0.50	0/2219
3	SD	0.25	0/1509	0.54	0/2026
4	SE	0.26	0/2088	0.53	0/2814
5	SF	0.26	0/1706	0.48	0/2311
6	SG	0.26	0/1853	0.56	0/2475
7	SH	0.24	0/1458	0.50	0/1955
8	SI	0.25	0/1649	0.52	0/2220
9	SJ	0.26	0/1038	0.51	0/1391
10	SK	0.27	0/1465	0.58	0/1964
11	SL	0.25	0/1145	0.48	0/1540
12	SM	0.24	0/806	0.52	0/1093
13	SN	0.26	0/836	0.47	0/1134
14	SO	0.26	0/1030	0.54	0/1384
15	SP	0.26	0/1120	0.51	0/1500
16	SQ	0.23	0/658	0.52	0/890
17	SR	0.25	0/1099	0.53	0/1477
18	SS	0.25	0/458	0.52	0/607
19	ST	0.28	0/1178	0.53	0/1580
20	SU	0.27	0/1208	0.51	0/1622
21	SV	0.24	0/856	0.50	0/1141
22	SW	0.26	0/945	0.49	0/1271
23	SX	0.26	0/1233	0.51	0/1656
24	SY	0.24	0/650	0.49	0/883
25	SZ	0.26	0/1051	0.49	0/1399
26	Sa	0.25	0/563	0.53	0/757
27	Sb	0.28	0/837	0.58	0/1120
28	Sc	0.31	0/660	0.57	0/888
29	Sd	0.26	0/476	0.57	0/640
30	Se	0.25	0/411	0.51	0/544
31	Sf	0.25	0/544	0.48	0/723
32	Sg	0.25	0/2274	0.48	0/3100

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Sh	0.27	0/532	0.51	0/718
34	S4	0.31	0/1613	1.25	8/2506 (0.3%)
35	S1	0.37	0/42994	0.85	41/66965 (0.1%)
36	SA	0.26	0/1848	0.53	0/2487
37	4	0.47	0/4397	0.95	27/6854 (0.4%)
38	6	0.35	0/1683	0.86	1/2618 (0.0%)
39	8	0.39	0/2829	0.86	5/4405 (0.1%)
40	A	0.29	0/1969	0.57	0/2643
41	B	0.27	0/3212	0.54	0/4324
42	C	0.27	0/2849	0.54	0/3835
43	D	0.26	0/1313	0.52	0/1766
44	E	0.27	0/1492	0.51	0/2011
45	H	0.27	0/1801	0.53	0/2419
46	I	0.26	0/1678	0.53	0/2250
47	J	0.28	0/1013	0.53	0/1367
48	K	0.26	0/1332	0.51	0/1788
49	L	0.29	0/1137	0.53	0/1521
50	M	0.28	0/1744	0.58	0/2329
51	P	0.28	0/1557	0.56	0/2084
52	Q	0.26	0/1546	0.56	0/2047
53	R	0.29	0/1486	0.52	0/2003
54	S	0.29	0/1282	0.53	0/1728
55	T	0.29	0/1239	0.54	0/1660
56	U	0.23	0/80	0.60	0/105
57	V	0.27	0/949	0.52	0/1277
58	W	0.26	0/969	0.55	0/1294
59	X	0.29	0/569	0.53	0/767
60	Y	0.28	0/1069	0.54	0/1434
61	Z	0.26	0/1137	0.55	0/1521
62	a	0.26	0/1039	0.55	0/1379
63	b	0.26	0/557	0.50	0/743
64	c	0.28	0/1900	0.53	0/2544
65	d	0.28	0/715	0.49	0/968
66	f	0.28	0/1043	0.57	0/1395
67	g	0.29	0/1172	0.58	0/1573
68	h	0.27	0/1027	0.57	0/1368
69	i	0.28	0/792	0.53	0/1059
70	j	0.29	0/686	0.62	0/915
71	k	0.27	0/623	0.51	0/833
72	l	0.27	0/463	0.55	0/617
73	m	0.29	0/416	0.55	0/553
74	n	0.28	0/296	0.73	0/386
75	o	0.28	0/701	0.58	0/934

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	p	0.32	0/800	0.53	0/1058
77	F	0.27	0/1140	0.52	0/1546
78	G	0.26	0/1817	0.53	0/2447
79	N	0.28	0/1647	0.57	0/2203
80	O	0.27	0/2164	0.50	0/2904
81	e	0.26	0/1474	0.54	0/1959
82	1	0.44	1/38669 (0.0%)	0.86	54/60289 (0.1%)
83	3	0.39	0/4189	0.89	19/6510 (0.3%)
84	5	0.46	0/2785	0.97	11/4330 (0.3%)
85	7	0.41	0/3712	0.82	1/5778 (0.0%)
86	2	0.44	0/27120	0.90	46/42264 (0.1%)
All	All	0.36	1/220388 (0.0%)	0.76	213/323851 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	157	U	C1'-N1	6.28	1.58	1.48

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	S4	12	U	O5'-P-OP1	-26.31	79.13	110.70
34	S4	12	U	O5'-P-OP2	-16.96	90.35	110.70
34	S4	11	C	OP1-P-O3'	-15.32	71.50	105.20
34	S4	12	U	OP1-P-OP2	15.27	142.50	119.60
86	2	55	C	OP1-P-O3'	-14.02	74.35	105.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SB	206/246 (84%)	196 (95%)	10 (5%)	0	100	100
2	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
3	SD	180/190 (95%)	179 (99%)	1 (1%)	0	100	100
4	SE	258/273 (94%)	254 (98%)	4 (2%)	0	100	100
5	SF	217/265 (82%)	214 (99%)	3 (1%)	0	100	100
6	SG	229/249 (92%)	222 (97%)	6 (3%)	1 (0%)	30	53
7	SH	178/190 (94%)	174 (98%)	4 (2%)	0	100	100
8	SI	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
9	SJ	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
10	SK	178/220 (81%)	178 (100%)	0	0	100	100
11	SL	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
12	SM	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
13	SN	98/168 (58%)	94 (96%)	4 (4%)	0	100	100
14	SO	134/144 (93%)	130 (97%)	4 (3%)	0	100	100
15	SP	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
16	SQ	87/141 (62%)	78 (90%)	9 (10%)	0	100	100
17	SR	134/153 (88%)	128 (96%)	6 (4%)	0	100	100
18	SS	54/57 (95%)	54 (100%)	0	0	100	100
19	ST	140/151 (93%)	139 (99%)	1 (1%)	0	100	100
20	SU	144/173 (83%)	141 (98%)	3 (2%)	0	100	100
21	SV	103/143 (72%)	98 (95%)	5 (5%)	0	100	100
22	SW	113/152 (74%)	111 (98%)	2 (2%)	0	100	100
23	SX	150/161 (93%)	145 (97%)	5 (3%)	0	100	100
24	SY	85/164 (52%)	81 (95%)	4 (5%)	0	100	100
25	SZ	125/137 (91%)	124 (99%)	1 (1%)	0	100	100
26	Sa	69/120 (58%)	67 (97%)	2 (3%)	0	100	100
27	Sb	101/112 (90%)	97 (96%)	4 (4%)	0	100	100
28	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
29	Sd	63/87 (72%)	63 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Se	47/66 (71%)	46 (98%)	1 (2%)	0	100	100
31	Sf	59/152 (39%)	56 (95%)	3 (5%)	0	100	100
32	Sg	286/312 (92%)	273 (96%)	13 (4%)	0	100	100
33	Sh	67/235 (28%)	62 (92%)	5 (8%)	0	100	100
36	SA	224/264 (85%)	216 (96%)	8 (4%)	0	100	100
40	A	254/260 (98%)	246 (97%)	8 (3%)	0	100	100
41	B	399/419 (95%)	392 (98%)	7 (2%)	0	100	100
42	C	364/373 (98%)	356 (98%)	8 (2%)	0	100	100
43	D	171/188 (91%)	165 (96%)	6 (4%)	0	100	100
44	E	184/190 (97%)	178 (97%)	6 (3%)	0	100	100
45	H	219/222 (99%)	217 (99%)	2 (1%)	0	100	100
46	I	207/220 (94%)	204 (99%)	3 (1%)	0	100	100
47	J	132/139 (95%)	130 (98%)	2 (2%)	0	100	100
48	K	168/175 (96%)	162 (96%)	6 (4%)	0	100	100
49	L	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
50	M	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
51	P	195/198 (98%)	187 (96%)	8 (4%)	0	100	100
52	Q	183/254 (72%)	182 (100%)	1 (0%)	0	100	100
53	R	176/179 (98%)	175 (99%)	1 (1%)	0	100	100
54	S	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
55	T	149/166 (90%)	147 (99%)	2 (1%)	0	100	100
56	U	10/129 (8%)	10 (100%)	0	0	100	100
57	V	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
58	W	118/143 (82%)	115 (98%)	3 (2%)	0	100	100
59	X	62/124 (50%)	61 (98%)	1 (2%)	0	100	100
60	Y	131/134 (98%)	129 (98%)	2 (2%)	0	100	100
61	Z	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
62	a	122/127 (96%)	119 (98%)	3 (2%)	0	100	100
63	b	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
64	c	227/252 (90%)	221 (97%)	6 (3%)	0	100	100
65	d	90/104 (86%)	89 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	f	124/133 (93%)	120 (97%)	4 (3%)	0	100	100
67	g	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
68	h	123/168 (73%)	120 (98%)	3 (2%)	0	100	100
69	i	96/105 (91%)	96 (100%)	0	0	100	100
70	j	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
71	k	75/83 (90%)	75 (100%)	0	0	100	100
72	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
73	m	49/128 (38%)	49 (100%)	0	0	100	100
74	n	31/34 (91%)	26 (84%)	5 (16%)	0	100	100
75	o	86/92 (94%)	81 (94%)	5 (6%)	0	100	100
76	p	96/106 (91%)	94 (98%)	2 (2%)	0	100	100
77	F	144/195 (74%)	140 (97%)	4 (3%)	0	100	100
78	G	224/264 (85%)	221 (99%)	3 (1%)	0	100	100
79	N	195/213 (92%)	188 (96%)	7 (4%)	0	100	100
80	O	274/305 (90%)	270 (98%)	4 (2%)	0	100	100
81	e	181/188 (96%)	175 (97%)	6 (3%)	0	100	100
All	All	11077/12926 (86%)	10807 (98%)	269 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	SG	172	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SB	173/202 (86%)	165 (95%)	8 (5%)	23	47
2	SC	171/184 (93%)	164 (96%)	7 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	SD	154/164 (94%)	150 (97%)	4 (3%)	41	69
4	SE	215/225 (96%)	211 (98%)	4 (2%)	52	77
5	SF	175/208 (84%)	171 (98%)	4 (2%)	45	73
6	SG	189/208 (91%)	181 (96%)	8 (4%)	25	51
7	SH	151/159 (95%)	146 (97%)	5 (3%)	33	61
8	SI	175/186 (94%)	173 (99%)	2 (1%)	70	87
9	SJ	110/111 (99%)	107 (97%)	3 (3%)	40	68
10	SK	141/176 (80%)	135 (96%)	6 (4%)	25	50
11	SL	113/120 (94%)	111 (98%)	2 (2%)	54	78
12	SM	92/104 (88%)	90 (98%)	2 (2%)	47	74
13	SN	86/128 (67%)	82 (95%)	4 (5%)	22	47
14	SO	103/113 (91%)	100 (97%)	3 (3%)	37	65
15	SP	114/117 (97%)	111 (97%)	3 (3%)	41	69
16	SQ	59/120 (49%)	54 (92%)	5 (8%)	8	20
17	SR	111/130 (85%)	108 (97%)	3 (3%)	40	68
18	SS	47/49 (96%)	47 (100%)	0	100	100
19	ST	124/132 (94%)	121 (98%)	3 (2%)	44	71
20	SU	125/152 (82%)	119 (95%)	6 (5%)	21	46
21	SV	89/126 (71%)	86 (97%)	3 (3%)	32	59
22	SW	97/130 (75%)	92 (95%)	5 (5%)	19	42
23	SX	121/131 (92%)	117 (97%)	4 (3%)	33	61
24	SY	67/116 (58%)	65 (97%)	2 (3%)	36	64
25	SZ	109/118 (92%)	108 (99%)	1 (1%)	75	89
26	Sa	63/95 (66%)	61 (97%)	2 (3%)	34	62
27	Sb	85/93 (91%)	82 (96%)	3 (4%)	31	58
28	Sc	70/76 (92%)	63 (90%)	7 (10%)	6	15
29	Sd	48/75 (64%)	46 (96%)	2 (4%)	25	51
30	Se	42/54 (78%)	42 (100%)	0	100	100
31	Sf	56/126 (44%)	52 (93%)	4 (7%)	12	29
32	Sg	235/265 (89%)	225 (96%)	10 (4%)	25	50
33	Sh	47/177 (27%)	42 (89%)	5 (11%)	5	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	SA	197/222 (89%)	189 (96%)	8 (4%)	26	52
40	A	195/204 (96%)	193 (99%)	2 (1%)	73	88
41	B	324/351 (92%)	320 (99%)	4 (1%)	67	85
42	C	286/301 (95%)	279 (98%)	7 (2%)	44	71
43	D	121/162 (75%)	115 (95%)	6 (5%)	20	44
44	E	164/172 (95%)	158 (96%)	6 (4%)	29	56
45	H	181/188 (96%)	177 (98%)	4 (2%)	47	74
46	I	171/183 (93%)	169 (99%)	2 (1%)	67	85
47	J	103/111 (93%)	102 (99%)	1 (1%)	73	88
48	K	129/145 (89%)	122 (95%)	7 (5%)	18	41
49	L	109/114 (96%)	107 (98%)	2 (2%)	54	78
50	M	176/180 (98%)	170 (97%)	6 (3%)	32	59
51	P	160/164 (98%)	158 (99%)	2 (1%)	65	84
52	Q	152/198 (77%)	150 (99%)	2 (1%)	65	84
53	R	156/159 (98%)	155 (99%)	1 (1%)	84	93
54	S	130/134 (97%)	128 (98%)	2 (2%)	60	82
55	T	128/143 (90%)	126 (98%)	2 (2%)	58	81
56	U	7/114 (6%)	6 (86%)	1 (14%)	2	6
57	V	98/124 (79%)	93 (95%)	5 (5%)	20	43
58	W	102/122 (84%)	98 (96%)	4 (4%)	27	54
59	X	58/104 (56%)	56 (97%)	2 (3%)	32	59
60	Y	104/116 (90%)	102 (98%)	2 (2%)	52	77
61	Z	115/118 (98%)	113 (98%)	2 (2%)	56	80
62	a	110/118 (93%)	107 (97%)	3 (3%)	40	68
63	b	56/58 (97%)	54 (96%)	2 (4%)	30	57
64	c	192/209 (92%)	188 (98%)	4 (2%)	48	75
65	d	80/89 (90%)	76 (95%)	4 (5%)	20	44
66	f	108/115 (94%)	106 (98%)	2 (2%)	52	77
67	g	120/121 (99%)	115 (96%)	5 (4%)	25	51
68	h	105/146 (72%)	103 (98%)	2 (2%)	52	77
69	i	79/88 (90%)	78 (99%)	1 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	j	68/70 (97%)	66 (97%)	2 (3%)	37	65
71	k	67/74 (90%)	67 (100%)	0	100	100
72	l	46/47 (98%)	45 (98%)	1 (2%)	47	74
73	m	44/113 (39%)	44 (100%)	0	100	100
74	n	30/32 (94%)	29 (97%)	1 (3%)	33	61
75	o	70/74 (95%)	67 (96%)	3 (4%)	25	50
76	p	83/92 (90%)	79 (95%)	4 (5%)	21	46
77	F	113/153 (74%)	108 (96%)	5 (4%)	24	49
78	G	183/221 (83%)	178 (97%)	5 (3%)	40	68
79	N	168/179 (94%)	159 (95%)	9 (5%)	18	41
80	O	195/242 (81%)	192 (98%)	3 (2%)	60	82
81	e	152/158 (96%)	143 (94%)	9 (6%)	16	37
All	All	9192/10798 (85%)	8917 (97%)	275 (3%)	37	64

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	h	110	GLU
75	o	42	CYS
79	N	198	LYS
26	Sa	67	ASP
24	SY	26	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
7	SH	189	ASN
21	SV	107	GLN
21	SV	110	GLN
22	SW	121	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	S4	64/76 (84%)	31 (48%)	2 (3%)
35	S1	1819/2204 (82%)	442 (24%)	12 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	4	182/184 (98%)	35 (19%)	2 (1%)
38	6	70/73 (95%)	24 (34%)	2 (2%)
39	8	118/123 (95%)	9 (7%)	0
82	1	1636/1782 (91%)	391 (23%)	13 (0%)
83	3	173/216 (80%)	41 (23%)	4 (2%)
84	5	112/135 (82%)	30 (26%)	3 (2%)
85	7	160/171 (93%)	32 (20%)	2 (1%)
86	2	1181/1526 (77%)	311 (26%)	6 (0%)
All	All	5515/6490 (84%)	1346 (24%)	46 (0%)

5 of 1346 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	S4	4	C
34	S4	5	G
34	S4	6	G
34	S4	7	A
34	S4	8	U

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
82	1	1479	A
84	5	71	U
82	1	1562	C
83	3	150	A
84	5	134	C

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

151 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
86	A2M	2	604	86,82	18,25,26	4.34	6 (33%)	18,36,39	2.68	3 (16%)
35	OMU	S1	661	35	19,22,23	3.01	8 (42%)	26,31,34	1.69	5 (19%)
35	5MC	S1	2061	35	18,22,23	3.55	7 (38%)	26,32,35	1.03	2 (7%)
86	PSU	2	597	86	18,21,22	4.48	7 (38%)	22,30,33	2.06	5 (22%)
82	PSU	1	1039	82	18,21,22	4.52	7 (38%)	22,30,33	1.73	4 (18%)
35	MA6	S1	2185	35	18,26,27	1.15	3 (16%)	19,38,41	3.14	2 (10%)
85	OMG	7	75	85	18,26,27	2.56	8 (44%)	19,38,41	1.54	4 (21%)
86	A2M	2	1372	86	18,25,26	4.34	6 (33%)	18,36,39	2.44	3 (16%)
35	OMG	S1	2151	35	18,26,27	2.50	8 (44%)	19,38,41	1.49	4 (21%)
86	OMC	2	1248	86	19,22,23	2.97	8 (42%)	26,31,34	0.87	1 (3%)
86	PSU	2	662	86,87	18,21,22	4.43	7 (38%)	22,30,33	1.79	5 (22%)
82	OMG	1	1524	82	18,26,27	2.54	8 (44%)	19,38,41	1.64	4 (21%)
85	A2M	7	162	85,82	18,25,26	4.36	8 (44%)	18,36,39	2.72	3 (16%)
35	OMU	S1	1979	35	19,22,23	3.01	8 (42%)	26,31,34	1.72	5 (19%)
35	PSU	S1	104	35	18,21,22	4.49	7 (38%)	22,30,33	1.71	5 (22%)
86	5MC	2	524	86,87	18,22,23	3.50	7 (38%)	26,32,35	1.04	2 (7%)
35	OMU	S1	1621	87,35	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
85	PSU	7	69	85	18,21,22	4.48	9 (50%)	22,30,33	1.69	4 (18%)
35	A2M	S1	479	35	18,25,26	4.23	7 (38%)	18,36,39	2.76	3 (16%)
86	PSU	2	626	86	18,21,22	4.43	7 (38%)	22,30,33	1.72	4 (18%)
86	OMG	2	655	86	18,26,27	2.46	8 (44%)	19,38,41	1.35	3 (15%)
86	A2M	2	527	86,87	18,25,26	4.03	8 (44%)	18,36,39	2.65	3 (16%)
35	PSU	S1	12	35	18,21,22	4.45	7 (38%)	22,30,33	1.76	5 (22%)
86	PSU	2	593	86	18,21,22	4.36	7 (38%)	22,30,33	1.71	5 (22%)
86	OMG	2	1229	86	18,26,27	2.50	8 (44%)	19,38,41	1.52	4 (21%)
86	OMC	2	1317	86	19,22,23	3.02	8 (42%)	26,31,34	0.98	1 (3%)
86	OMU	2	73	86	19,22,23	2.95	8 (42%)	26,31,34	1.55	4 (15%)
82	A2M	1	955	82	18,25,26	4.29	7 (38%)	18,36,39	2.81	3 (16%)
35	PSU	S1	1657	35	18,21,22	4.43	7 (38%)	22,30,33	1.70	3 (13%)
35	A2M	S1	98	87,35	18,25,26	4.32	7 (38%)	18,36,39	2.66	3 (16%)
35	A2M	S1	918	35	18,25,26	4.22	7 (38%)	18,36,39	2.55	3 (16%)
86	PSU	2	1194	86	18,21,22	4.45	7 (38%)	22,30,33	1.66	4 (18%)
35	A2M	S1	753	35	18,25,26	4.35	7 (38%)	18,36,39	2.69	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
82	PSU	1	1177	82	18,21,22	4.47	7 (38%)	22,30,33	1.80	5 (22%)
86	PSU	2	1144	86	18,21,22	4.60	8 (44%)	22,30,33	1.91	4 (18%)
86	OMG	2	1078	86	18,26,27	2.47	8 (44%)	19,38,41	1.69	5 (26%)
86	PSU	2	1058	86	18,21,22	4.46	7 (38%)	22,30,33	2.13	5 (22%)
35	OMG	S1	600	35	18,26,27	2.54	8 (44%)	19,38,41	1.51	4 (21%)
35	PSU	S1	1539	35	18,21,22	4.47	7 (38%)	22,30,33	1.72	4 (18%)
35	OMC	S1	1866	35	19,22,23	2.97	8 (42%)	26,31,34	0.81	0
35	A2M	S1	28	87,35	18,25,26	4.26	6 (33%)	18,36,39	2.77	3 (16%)
82	OMC	1	1527	82	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
35	PSU	S1	1246	35	18,21,22	4.45	7 (38%)	22,30,33	1.83	5 (22%)
86	OMC	2	1397	86	19,22,23	2.95	8 (42%)	26,31,34	0.79	0
35	7MG	S1	1995	35	22,26,27	4.28	10 (45%)	29,39,42	2.03	9 (31%)
82	1MA	1	677	87,82	16,25,26	3.66	5 (31%)	18,37,40	1.87	4 (22%)
86	5MC	2	1308	86,88	18,22,23	4.65	13 (72%)	26,32,35	1.32	2 (7%)
82	A2M	1	858	82	18,25,26	4.22	7 (38%)	18,36,39	3.12	4 (22%)
86	OMC	2	443	86,87,88	19,22,23	2.88	8 (42%)	26,31,34	0.82	0
82	PSU	1	1011	86,82	18,21,22	4.38	9 (50%)	22,30,33	1.73	6 (27%)
86	OMC	2	359	86	19,22,23	3.01	8 (42%)	26,31,34	0.77	0
85	A2M	7	43	85	18,25,26	4.33	7 (38%)	18,36,39	2.73	4 (22%)
35	OMG	S1	1478	35	18,26,27	2.45	8 (44%)	19,38,41	1.61	5 (26%)
35	OMC	S1	2140	35	19,22,23	2.98	8 (42%)	26,31,34	0.81	0
86	OMU	2	1419	86	19,22,23	2.96	8 (42%)	26,31,34	1.66	4 (15%)
86	PSU	2	1265	86,87	18,21,22	4.45	7 (38%)	22,30,33	1.84	5 (22%)
82	OMG	1	1626	82	18,26,27	2.53	8 (44%)	19,38,41	1.53	4 (21%)
82	OMU	1	1107	82	19,22,23	2.98	8 (42%)	26,31,34	1.74	5 (19%)
35	OMG	S1	1550	35	18,26,27	2.54	8 (44%)	19,38,41	1.48	4 (21%)
35	MA6	S1	2184	35	18,26,27	1.15	1 (5%)	19,38,41	3.00	2 (10%)
35	OMU	S1	29	35	19,22,23	3.01	8 (42%)	26,31,34	1.69	4 (15%)
86	PSU	2	437	86,88	18,21,22	4.47	8 (44%)	22,30,33	1.81	5 (22%)
86	OMG	2	1360	86	18,26,27	2.55	8 (44%)	19,38,41	1.51	4 (21%)
86	PSU	2	1382	86,87,88	18,21,22	4.42	8 (44%)	22,30,33	2.06	6 (27%)
35	PSU	S1	1566	35	18,21,22	4.47	8 (44%)	22,30,33	1.68	4 (18%)
82	PSU	1	672	87,82	18,21,22	4.47	7 (38%)	22,30,33	1.88	6 (27%)
37	OMG	4	74	37	18,26,27	2.46	8 (44%)	19,38,41	1.46	5 (26%)
86	OMG	2	641	86,87	18,26,27	2.49	8 (44%)	19,38,41	1.60	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
82	PSU	1	1664	82	18,21,22	4.51	7 (38%)	22,30,33	1.75	5 (22%)
86	A2M	2	572	86	18,25,26	4.32	7 (38%)	18,36,39	2.74	3 (16%)
82	PSU	1	870	87,82	18,21,22	4.45	7 (38%)	22,30,33	2.02	5 (22%)
83	OMU	3	13	83	19,22,23	3.01	8 (42%)	26,31,34	1.72	4 (15%)
86	PSU	2	1403	86	18,21,22	4.52	7 (38%)	22,30,33	1.79	6 (27%)
85	OMU	7	7	85,82	19,22,23	3.03	8 (42%)	26,31,34	1.71	4 (15%)
35	PSU	S1	2046	35	18,21,22	4.53	7 (38%)	22,30,33	1.94	4 (18%)
35	OMU	S1	1833	35	19,22,23	3.04	8 (42%)	26,31,34	1.82	5 (19%)
82	A2M	1	678	86,82	18,25,26	4.35	8 (44%)	18,36,39	2.75	3 (16%)
82	OMU	1	847	82	19,22,23	3.00	8 (42%)	26,31,34	1.77	5 (19%)
35	OMC	S1	2059	35	19,22,23	2.97	8 (42%)	26,31,34	1.16	2 (7%)
86	OMG	2	534	86	18,26,27	2.50	8 (44%)	19,38,41	1.48	3 (15%)
35	A2M	S1	969	35	18,25,26	4.30	7 (38%)	18,36,39	2.80	4 (22%)
86	A2M	2	1185	86	18,25,26	4.36	7 (38%)	18,36,39	2.67	3 (16%)
86	OMG	2	71	86	18,26,27	2.52	8 (44%)	19,38,41	1.55	3 (15%)
35	A2M	S1	897	35	18,25,26	4.29	8 (44%)	18,36,39	2.68	3 (16%)
35	5MC	S1	1544	35	18,22,23	3.58	7 (38%)	26,32,35	1.03	1 (3%)
35	OMU	S1	8	35	19,22,23	2.96	8 (42%)	26,31,34	1.81	5 (19%)
35	A2M	S1	2021	35	18,25,26	4.13	7 (38%)	18,36,39	2.74	3 (16%)
35	OMG	S1	1829	87,35	18,26,27	2.52	8 (44%)	19,38,41	1.51	3 (15%)
82	PSU	1	1528	82	18,21,22	4.51	7 (38%)	22,30,33	1.98	5 (22%)
35	PSU	S1	1533	35	18,21,22	4.46	7 (38%)	22,30,33	1.85	5 (22%)
82	OMU	1	845	82	19,22,23	2.98	8 (42%)	26,31,34	2.24	8 (30%)
82	OMG	1	1190	87,82	18,26,27	2.46	8 (44%)	19,38,41	1.64	4 (21%)
86	PSU	2	1318	86	18,21,22	4.51	7 (38%)	22,30,33	1.99	6 (27%)
82	A2M	1	235	82	18,25,26	4.43	7 (38%)	18,36,39	2.73	4 (22%)
82	A2M	1	697	82	18,25,26	4.36	6 (33%)	18,36,39	2.61	3 (16%)
35	OMG	S1	1865	35	18,26,27	2.58	8 (44%)	19,38,41	1.57	4 (21%)
86	A2M	2	382	86	18,25,26	4.44	6 (33%)	18,36,39	2.55	3 (16%)
82	OMC	1	695	82	19,22,23	2.91	8 (42%)	26,31,34	0.68	0
82	A2M	1	681	82	18,25,26	4.24	6 (33%)	18,36,39	2.75	3 (16%)
86	OMU	2	1077	86	19,22,23	3.04	8 (42%)	26,31,34	1.68	4 (15%)
35	PSU	S1	609	35	18,21,22	4.51	7 (38%)	22,30,33	1.80	5 (22%)
86	A2M	2	591	86	18,25,26	4.34	6 (33%)	18,36,39	2.74	3 (16%)
82	PSU	1	1181	82	18,21,22	4.50	8 (44%)	22,30,33	2.00	5 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	PSU	2	1303	86	18,21,22	4.51	7 (38%)	22,30,33	2.17	6 (27%)
35	OMC	S1	38	35	19,22,23	2.97	8 (42%)	26,31,34	0.76	0
82	OMG	1	1540	86,82	18,26,27	2.48	8 (44%)	19,38,41	1.50	4 (21%)
86	PSU	2	510	86	18,21,22	4.51	7 (38%)	22,30,33	1.76	5 (22%)
35	PSU	S1	2048	35	18,21,22	4.48	7 (38%)	22,30,33	2.06	5 (22%)
86	OMC	2	1159	86	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
82	OMU	1	1371	82	19,22,23	3.05	8 (42%)	26,31,34	1.96	7 (26%)
82	PSU	1	1017	82	18,21,22	4.44	7 (38%)	22,30,33	1.86	5 (22%)
86	OMC	2	583	86	19,22,23	3.04	8 (42%)	26,31,34	0.84	1 (3%)
86	PSU	2	512	86	18,21,22	4.51	7 (38%)	22,30,33	1.83	5 (22%)
82	PSU	1	1171	82	18,21,22	4.42	7 (38%)	22,30,33	1.76	6 (27%)
82	OMG	1	856	82	18,26,27	2.50	8 (44%)	19,38,41	1.51	6 (31%)
86	PSU	2	1060	86	18,21,22	4.48	7 (38%)	22,30,33	2.07	5 (22%)
86	PSU	2	78	86	18,21,22	4.49	7 (38%)	22,30,33	1.99	4 (18%)
35	OMG	S1	1623	35	18,26,27	2.53	8 (44%)	19,38,41	1.52	5 (26%)
82	A2M	1	407	87,82	18,25,26	4.30	8 (44%)	18,36,39	2.62	4 (22%)
86	OMG	2	1231	86	18,26,27	2.52	8 (44%)	19,38,41	1.50	4 (21%)
82	OMG	1	959	82	18,26,27	2.51	8 (44%)	19,38,41	1.47	4 (21%)
35	PSU	S1	1841	35	18,21,22	4.50	7 (38%)	22,30,33	1.81	5 (22%)
86	PSU	2	1264	86	18,21,22	4.41	7 (38%)	22,30,33	1.79	6 (27%)
35	A2M	S1	912	35	18,25,26	4.39	7 (38%)	18,36,39	2.80	4 (22%)
82	PSU	1	1533	86,82	18,21,22	4.49	7 (38%)	22,30,33	1.82	6 (27%)
35	A2M	S1	668	87,35	18,25,26	3.92	8 (44%)	18,36,39	2.72	4 (22%)
82	A2M	1	927	82	18,25,26	4.33	6 (33%)	18,36,39	2.76	3 (16%)
82	A2M	1	305	82	18,25,26	4.15	7 (38%)	18,36,39	2.95	3 (16%)
82	A2M	1	1539	86,87,82	18,25,26	4.29	8 (44%)	18,36,39	2.60	3 (16%)
82	OMU	1	1659	87,82	19,22,23	3.01	8 (42%)	26,31,34	1.68	4 (15%)
86	OMG	2	1046	86	18,26,27	2.42	8 (44%)	19,38,41	1.39	5 (26%)
35	OMC	S1	115	35	19,22,23	2.96	8 (42%)	26,31,34	0.71	0
86	PSU	2	1413	86,87	18,21,22	4.41	7 (38%)	22,30,33	1.75	4 (18%)
35	OMC	S1	18	35	19,22,23	2.95	8 (42%)	26,31,34	0.74	0
86	PSU	2	1361	86	18,21,22	4.49	7 (38%)	22,30,33	1.82	4 (18%)
85	PSU	7	101	85	18,21,22	4.44	7 (38%)	22,30,33	1.82	6 (27%)
35	OMG	S1	1647	35	18,26,27	2.52	8 (44%)	19,38,41	1.59	3 (15%)
35	C4J	S1	1543	35	24,29,30	2.96	8 (33%)	29,42,45	1.28	2 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	A2M	2	570	86,82	18,25,26	4.15	7 (38%)	18,36,39	2.73	5 (27%)
86	A2M	2	95	86	18,25,26	4.35	7 (38%)	18,36,39	2.70	4 (22%)
86	OMU	2	667	86	19,22,23	3.04	8 (42%)	26,31,34	1.74	4 (15%)
86	A2M	2	1384	86,87	18,25,26	4.27	6 (33%)	18,36,39	2.57	3 (16%)
86	A2M	2	628	86	18,25,26	4.28	7 (38%)	18,36,39	2.72	3 (16%)
86	OMU	2	560	86,87	19,22,23	2.97	8 (42%)	26,31,34	1.79	5 (19%)
86	PSU	2	472	86	18,21,22	4.52	8 (44%)	22,30,33	1.78	4 (18%)
86	OMG	2	1253	86	18,26,27	2.46	8 (44%)	19,38,41	1.51	4 (21%)
85	PSU	7	74	85	18,21,22	4.49	7 (38%)	22,30,33	1.76	5 (22%)
86	OMU	2	1359	86	19,22,23	3.03	8 (42%)	26,31,34	1.73	4 (15%)
35	PSU	S1	33	35	18,21,22	4.61	8 (44%)	22,30,33	1.82	3 (13%)
35	A2M	S1	512	87,35	18,25,26	4.32	8 (44%)	18,36,39	2.74	3 (16%)
82	OMC	1	1010	87,82	19,22,23	2.95	8 (42%)	26,31,34	0.86	1 (3%)

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
86	A2M	2	604	86,82	-	0/5/27/28	0/3/3/3
35	OMU	S1	661	35	-	0/9/27/28	0/2/2/2
35	5MC	S1	2061	35	-	2/7/25/26	0/2/2/2
86	PSU	2	597	86	-	0/7/25/26	0/2/2/2
82	PSU	1	1039	82	-	1/7/25/26	0/2/2/2
35	MA6	S1	2185	35	-	3/7/29/30	0/3/3/3
85	OMG	7	75	85	-	0/5/27/28	0/3/3/3
86	A2M	2	1372	86	-	0/5/27/28	0/3/3/3
35	OMG	S1	2151	35	-	0/5/27/28	0/3/3/3
86	OMC	2	1248	86	-	1/9/27/28	0/2/2/2
86	PSU	2	662	86,87	-	0/7/25/26	0/2/2/2
82	OMG	1	1524	82	-	1/5/27/28	0/3/3/3
85	A2M	7	162	85,82	-	2/5/27/28	0/3/3/3
35	OMU	S1	1979	35	-	0/9/27/28	0/2/2/2
35	PSU	S1	104	35	-	0/7/25/26	0/2/2/2
86	5MC	2	524	86,87	-	0/7/25/26	0/2/2/2
35	OMU	S1	1621	87,35	-	1/9/27/28	0/2/2/2
85	PSU	7	69	85	-	2/7/25/26	0/2/2/2
35	A2M	S1	479	35	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PSU	2	626	86	-	0/7/25/26	0/2/2/2
86	OMG	2	655	86	-	0/5/27/28	0/3/3/3
86	A2M	2	527	86,87	-	2/5/27/28	0/3/3/3
35	PSU	S1	12	35	-	0/7/25/26	0/2/2/2
86	PSU	2	593	86	-	0/7/25/26	0/2/2/2
86	OMG	2	1229	86	-	0/5/27/28	0/3/3/3
86	OMC	2	1317	86	-	0/9/27/28	0/2/2/2
86	OMU	2	73	86	-	1/9/27/28	0/2/2/2
82	A2M	1	955	82	-	1/5/27/28	0/3/3/3
35	PSU	S1	1657	35	-	2/7/25/26	0/2/2/2
35	A2M	S1	98	87,35	-	3/5/27/28	0/3/3/3
35	A2M	S1	918	35	-	1/5/27/28	0/3/3/3
86	PSU	2	1194	86	-	0/7/25/26	0/2/2/2
35	A2M	S1	753	35	-	0/5/27/28	0/3/3/3
82	PSU	1	1177	82	-	0/7/25/26	0/2/2/2
86	PSU	2	1144	86	-	2/7/25/26	0/2/2/2
86	OMG	2	1078	86	-	1/5/27/28	0/3/3/3
86	PSU	2	1058	86	-	0/7/25/26	0/2/2/2
35	OMG	S1	600	35	-	2/5/27/28	0/3/3/3
35	PSU	S1	1539	35	-	1/7/25/26	0/2/2/2
35	OMC	S1	1866	35	-	3/9/27/28	0/2/2/2
35	A2M	S1	28	87,35	-	1/5/27/28	0/3/3/3
82	OMC	1	1527	82	-	2/9/27/28	0/2/2/2
35	PSU	S1	1246	35	-	0/7/25/26	0/2/2/2
86	OMC	2	1397	86	-	0/9/27/28	0/2/2/2
35	7MG	S1	1995	35	-	2/7/37/38	0/3/3/3
82	1MA	1	677	87,82	-	0/3/25/26	0/3/3/3
86	5MC	2	1308	86,88	-	4/7/25/26	0/2/2/2
82	A2M	1	858	82	-	1/5/27/28	0/3/3/3
86	OMC	2	443	86,87,88	-	4/9/27/28	0/2/2/2
82	PSU	1	1011	86,82	-	2/7/25/26	0/2/2/2
86	OMC	2	359	86	-	2/9/27/28	0/2/2/2
85	A2M	7	43	85	-	2/5/27/28	0/3/3/3
35	OMG	S1	1478	35	-	1/5/27/28	0/3/3/3
35	OMC	S1	2140	35	-	0/9/27/28	0/2/2/2
86	OMU	2	1419	86	-	1/9/27/28	0/2/2/2
86	PSU	2	1265	86,87	-	0/7/25/26	0/2/2/2
82	OMG	1	1626	82	-	0/5/27/28	0/3/3/3
82	OMU	1	1107	82	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	OMG	S1	1550	35	-	0/5/27/28	0/3/3/3
35	MA6	S1	2184	35	-	0/7/29/30	0/3/3/3
35	OMU	S1	29	35	-	1/9/27/28	0/2/2/2
86	PSU	2	437	86,88	-	2/7/25/26	0/2/2/2
86	OMG	2	1360	86	-	0/5/27/28	0/3/3/3
86	PSU	2	1382	86,87,88	-	0/7/25/26	0/2/2/2
35	PSU	S1	1566	35	-	2/7/25/26	0/2/2/2
82	PSU	1	672	87,82	-	0/7/25/26	0/2/2/2
37	OMG	4	74	37	-	2/5/27/28	0/3/3/3
86	OMG	2	641	86,87	-	0/5/27/28	0/3/3/3
82	PSU	1	1664	82	-	0/7/25/26	0/2/2/2
86	A2M	2	572	86	-	0/5/27/28	0/3/3/3
82	PSU	1	870	87,82	-	0/7/25/26	0/2/2/2
83	OMU	3	13	83	-	1/9/27/28	0/2/2/2
86	PSU	2	1403	86	-	0/7/25/26	0/2/2/2
85	OMU	7	7	85,82	-	1/9/27/28	0/2/2/2
35	PSU	S1	2046	35	-	0/7/25/26	0/2/2/2
35	OMU	S1	1833	35	-	2/9/27/28	0/2/2/2
82	A2M	1	678	86,82	-	0/5/27/28	0/3/3/3
82	OMU	1	847	82	-	0/9/27/28	0/2/2/2
35	OMC	S1	2059	35	-	2/9/27/28	0/2/2/2
86	OMG	2	534	86	-	2/5/27/28	0/3/3/3
35	A2M	S1	969	35	-	2/5/27/28	0/3/3/3
86	A2M	2	1185	86	-	3/5/27/28	0/3/3/3
86	OMG	2	71	86	-	0/5/27/28	0/3/3/3
35	A2M	S1	897	35	-	0/5/27/28	0/3/3/3
35	5MC	S1	1544	35	-	0/7/25/26	0/2/2/2
35	OMU	S1	8	35	-	4/9/27/28	0/2/2/2
35	A2M	S1	2021	35	-	3/5/27/28	0/3/3/3
35	OMG	S1	1829	87,35	-	3/5/27/28	0/3/3/3
82	PSU	1	1528	82	-	0/7/25/26	0/2/2/2
35	PSU	S1	1533	35	-	0/7/25/26	0/2/2/2
82	OMU	1	845	82	-	3/9/27/28	0/2/2/2
82	OMG	1	1190	87,82	-	0/5/27/28	0/3/3/3
86	PSU	2	1318	86	-	0/7/25/26	0/2/2/2
82	A2M	1	235	82	-	0/5/27/28	0/3/3/3
82	A2M	1	697	82	-	0/5/27/28	0/3/3/3
35	OMG	S1	1865	35	-	0/5/27/28	0/3/3/3
86	A2M	2	382	86	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	OMC	1	695	82	-	1/9/27/28	0/2/2/2
82	A2M	1	681	82	-	3/5/27/28	0/3/3/3
86	OMU	2	1077	86	-	0/9/27/28	0/2/2/2
35	PSU	S1	609	35	-	0/7/25/26	0/2/2/2
86	A2M	2	591	86	-	0/5/27/28	0/3/3/3
82	PSU	1	1181	82	-	2/7/25/26	0/2/2/2
86	PSU	2	1303	86	-	0/7/25/26	0/2/2/2
35	OMC	S1	38	35	-	0/9/27/28	0/2/2/2
82	OMG	1	1540	86,82	-	2/5/27/28	0/3/3/3
86	PSU	2	510	86	-	0/7/25/26	0/2/2/2
35	PSU	S1	2048	35	-	0/7/25/26	0/2/2/2
86	OMC	2	1159	86	-	0/9/27/28	0/2/2/2
82	OMU	1	1371	82	-	4/9/27/28	0/2/2/2
82	PSU	1	1017	82	-	0/7/25/26	0/2/2/2
86	OMC	2	583	86	-	0/9/27/28	0/2/2/2
86	PSU	2	512	86	-	0/7/25/26	0/2/2/2
82	PSU	1	1171	82	-	0/7/25/26	0/2/2/2
82	OMG	1	856	82	-	0/5/27/28	0/3/3/3
86	PSU	2	1060	86	-	0/7/25/26	0/2/2/2
86	PSU	2	78	86	-	0/7/25/26	0/2/2/2
35	OMG	S1	1623	35	-	0/5/27/28	0/3/3/3
82	A2M	1	407	87,82	-	3/5/27/28	0/3/3/3
86	OMG	2	1231	86	-	0/5/27/28	0/3/3/3
82	OMG	1	959	82	-	2/5/27/28	0/3/3/3
35	PSU	S1	1841	35	-	0/7/25/26	0/2/2/2
86	PSU	2	1264	86	-	0/7/25/26	0/2/2/2
35	A2M	S1	912	35	-	1/5/27/28	0/3/3/3
82	PSU	1	1533	86,82	-	0/7/25/26	0/2/2/2
35	A2M	S1	668	87,35	-	2/5/27/28	0/3/3/3
82	A2M	1	927	82	-	1/5/27/28	0/3/3/3
82	A2M	1	305	82	-	0/5/27/28	0/3/3/3
82	A2M	1	1539	86,87,82	-	0/5/27/28	0/3/3/3
82	OMU	1	1659	87,82	-	0/9/27/28	0/2/2/2
86	OMG	2	1046	86	-	1/5/27/28	0/3/3/3
35	OMC	S1	115	35	-	0/9/27/28	0/2/2/2
86	PSU	2	1413	86,87	-	0/7/25/26	0/2/2/2
35	OMC	S1	18	35	-	0/9/27/28	0/2/2/2
86	PSU	2	1361	86	-	1/7/25/26	0/2/2/2
85	PSU	7	101	85	-	0/7/25/26	0/2/2/2
35	OMG	S1	1647	35	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	C4J	S1	1543	35	-	7/16/34/35	0/2/2/2
86	A2M	2	570	86,82	-	1/5/27/28	0/3/3/3
86	A2M	2	95	86	-	0/5/27/28	0/3/3/3
86	OMU	2	667	86	-	1/9/27/28	0/2/2/2
86	A2M	2	1384	86,87	-	1/5/27/28	0/3/3/3
86	A2M	2	628	86	-	0/5/27/28	0/3/3/3
86	OMU	2	560	86,87	-	1/9/27/28	0/2/2/2
86	PSU	2	472	86	-	2/7/25/26	0/2/2/2
86	OMG	2	1253	86	-	0/5/27/28	0/3/3/3
85	PSU	7	74	85	-	0/7/25/26	0/2/2/2
86	OMU	2	1359	86	-	0/9/27/28	0/2/2/2
35	PSU	S1	33	35	-	2/7/25/26	0/2/2/2
35	A2M	S1	512	87,35	-	2/5/27/28	0/3/3/3
82	OMC	1	1010	87,82	-	1/9/27/28	0/2/2/2

The worst 5 of 1126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	382	A2M	O4'-C1'	16.06	1.63	1.41
82	1	235	A2M	O4'-C1'	16.01	1.63	1.41
35	S1	912	A2M	O4'-C1'	15.84	1.63	1.41
86	2	1185	A2M	O4'-C1'	15.73	1.63	1.41
82	1	697	A2M	O4'-C1'	15.69	1.63	1.41

The worst 5 of 570 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	2185	MA6	N1-C6-N6	-12.27	104.14	117.06
35	S1	2184	MA6	N1-C6-N6	-11.49	104.97	117.06
82	1	858	A2M	C5-C6-N6	9.27	134.43	120.35
82	1	305	A2M	C5-C6-N6	8.78	133.70	120.35
35	S1	28	A2M	C5-C6-N6	8.68	133.55	120.35

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	1	407	A2M	C3'-C4'-C5'-O5'
82	1	681	A2M	O4'-C4'-C5'-O5'
82	1	695	OMC	C1'-C2'-O2'-CM2
82	1	845	OMU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
82	1	845	OMU	O4'-C1'-N1-C6

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 391 ligands modelled in this entry, 391 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	S1	1
21	SV	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S1	1543:C4J	O3'	1544:5MC	P	4.41
1	SV	72:LYS	C	73:LEU	N	3.06

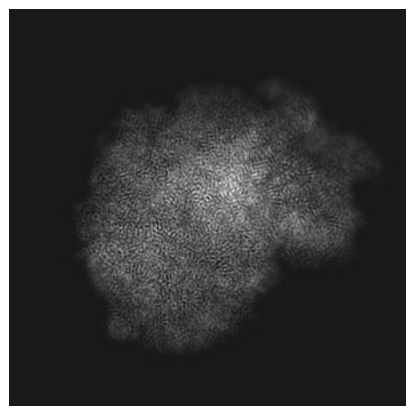
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18419. These allow visual inspection of the internal detail of the map and identification of artifacts.

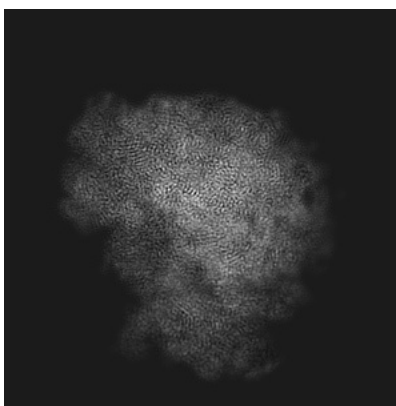
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

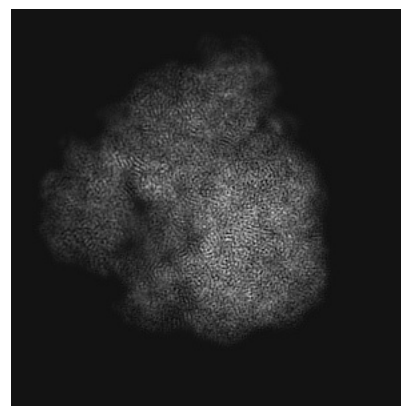
#### 6.1.1 Primary map



X

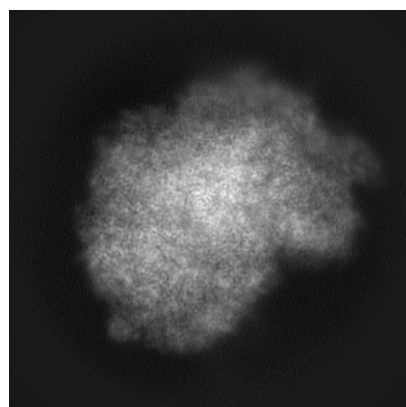


Y

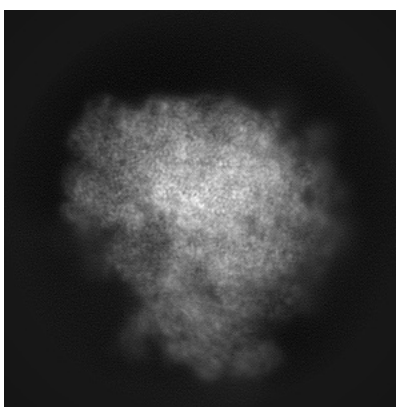


Z

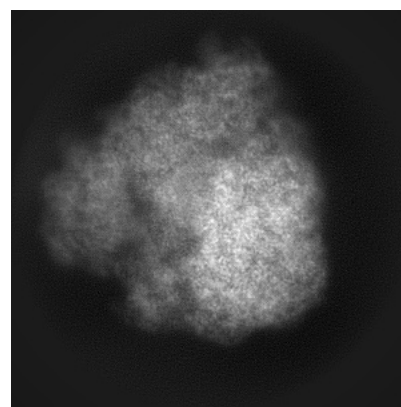
#### 6.1.2 Raw map



X



Y



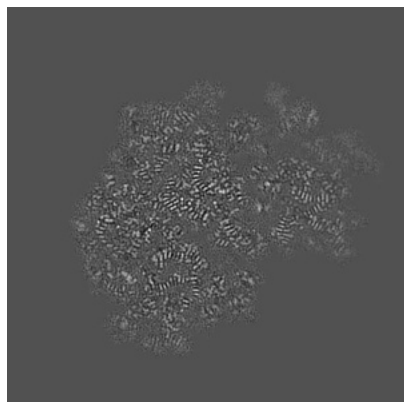
Z

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

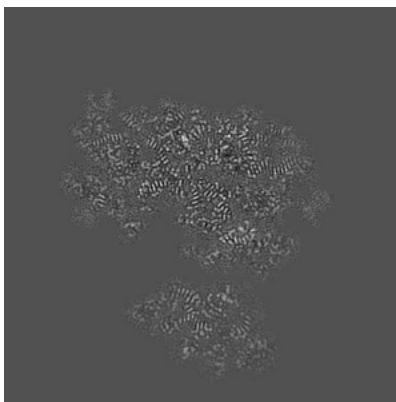


## 6.2 Central slices [i](#)

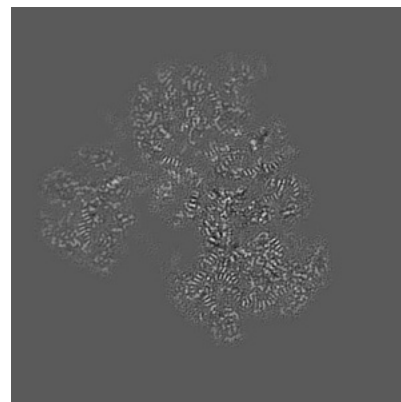
### 6.2.1 Primary map



X Index: 240

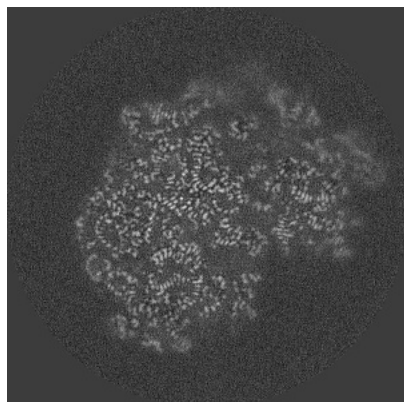


Y Index: 240

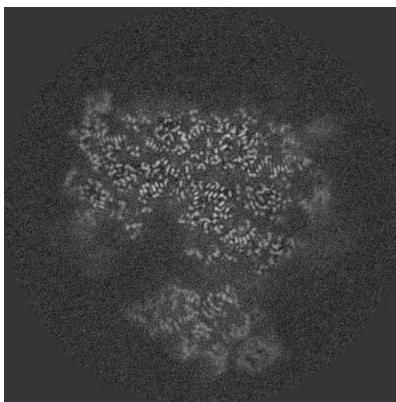


Z Index: 240

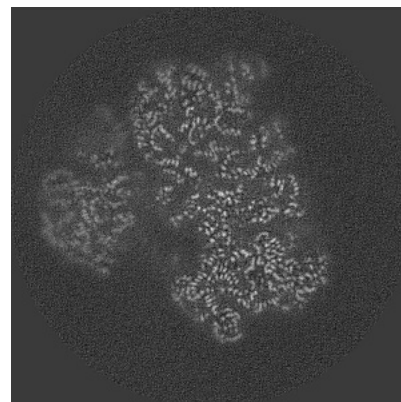
### 6.2.2 Raw map



X Index: 240



Y Index: 240



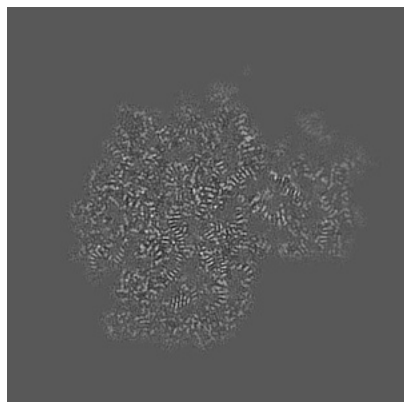
Z Index: 240

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



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

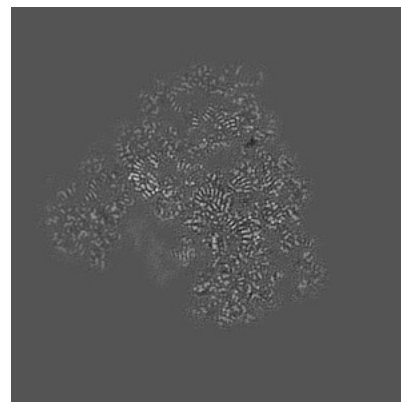
### 6.3.1 Primary map



X Index: 261

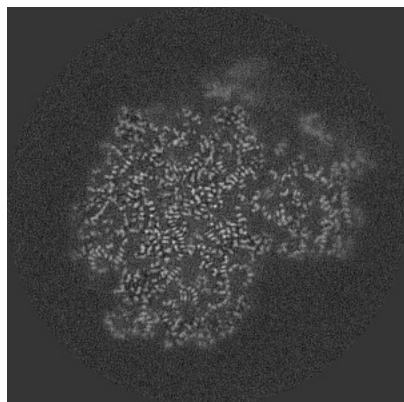


Y Index: 266

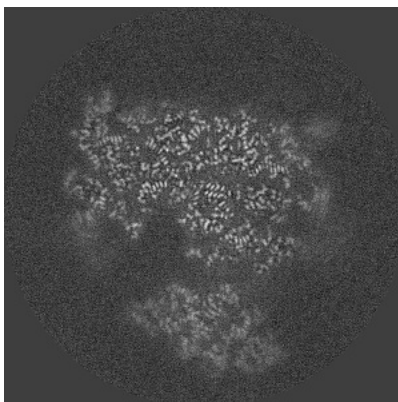


Z Index: 260

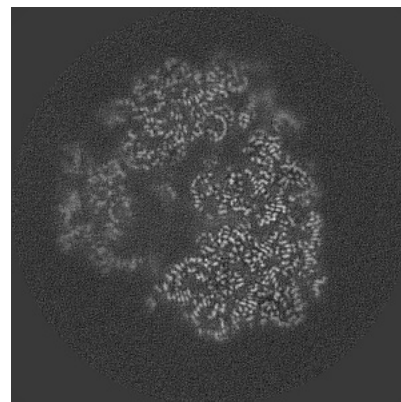
### 6.3.2 Raw map



X Index: 261



Y Index: 241

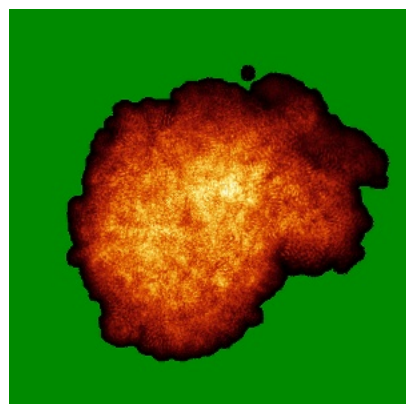


Z Index: 215

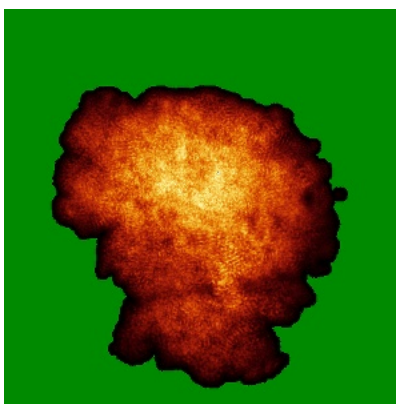
The images above show the largest variance slices of the map in three orthogonal directions.

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

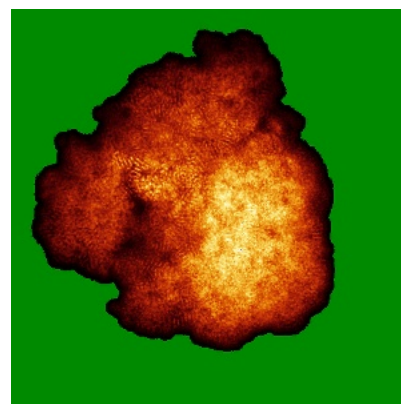
### 6.4.1 Primary map



X

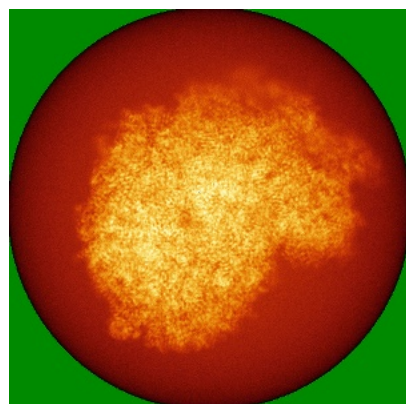


Y

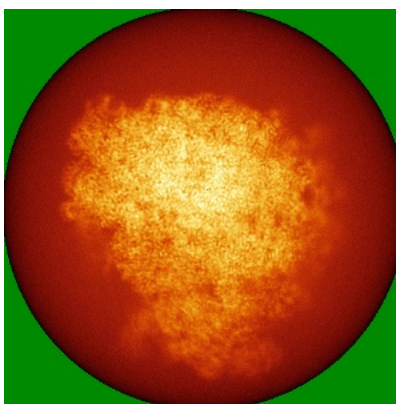


Z

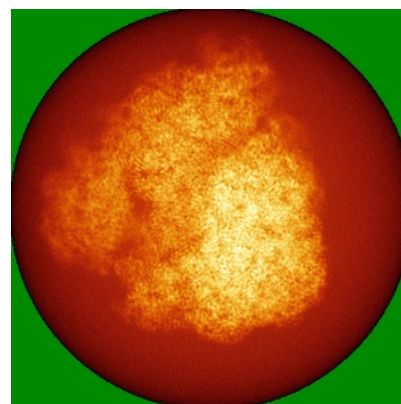
### 6.4.2 Raw map



X



Y

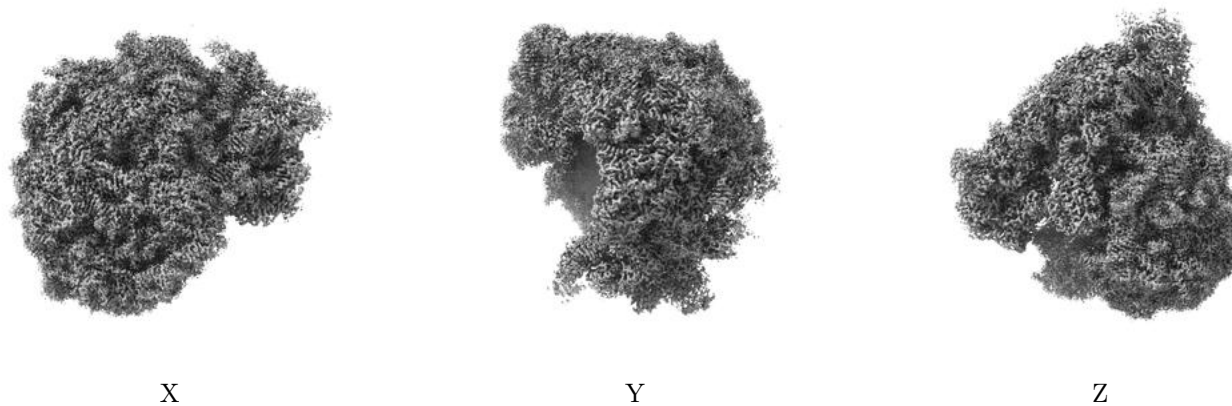


Z

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.

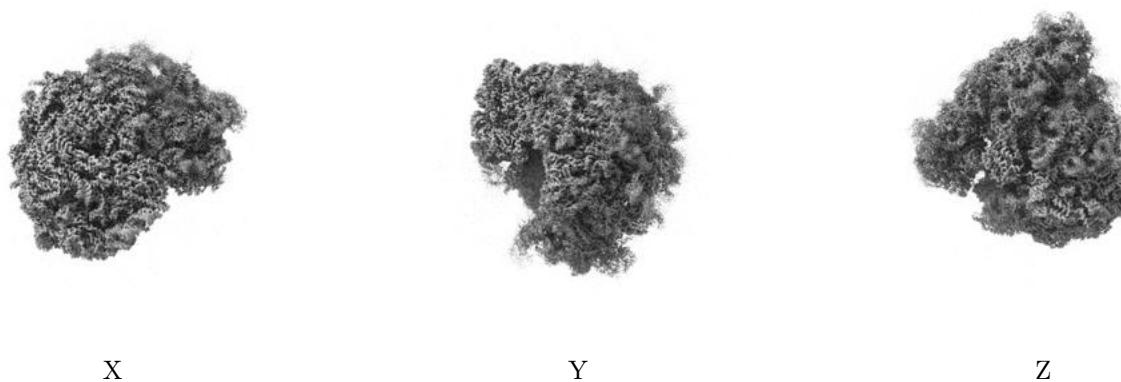
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

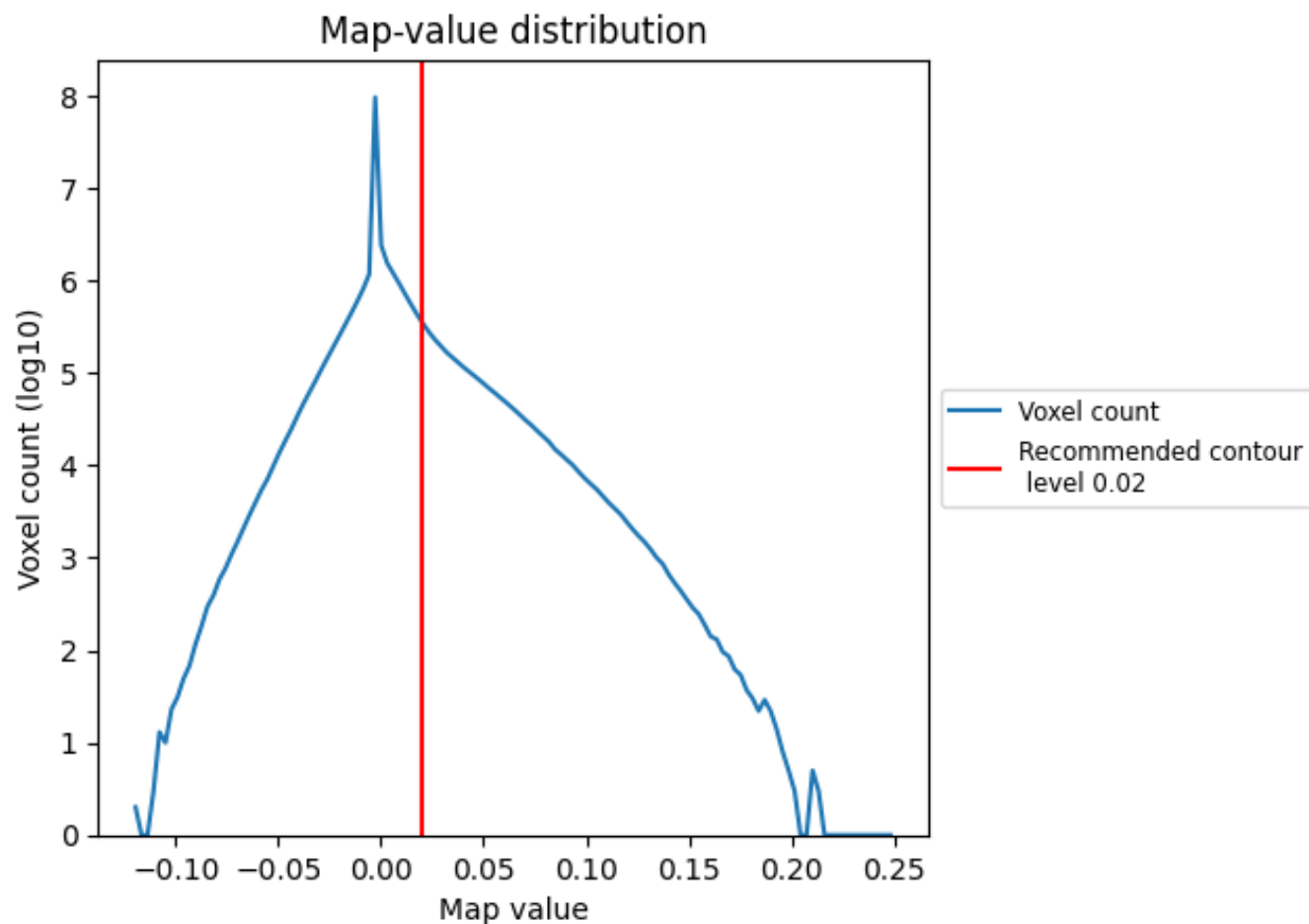
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

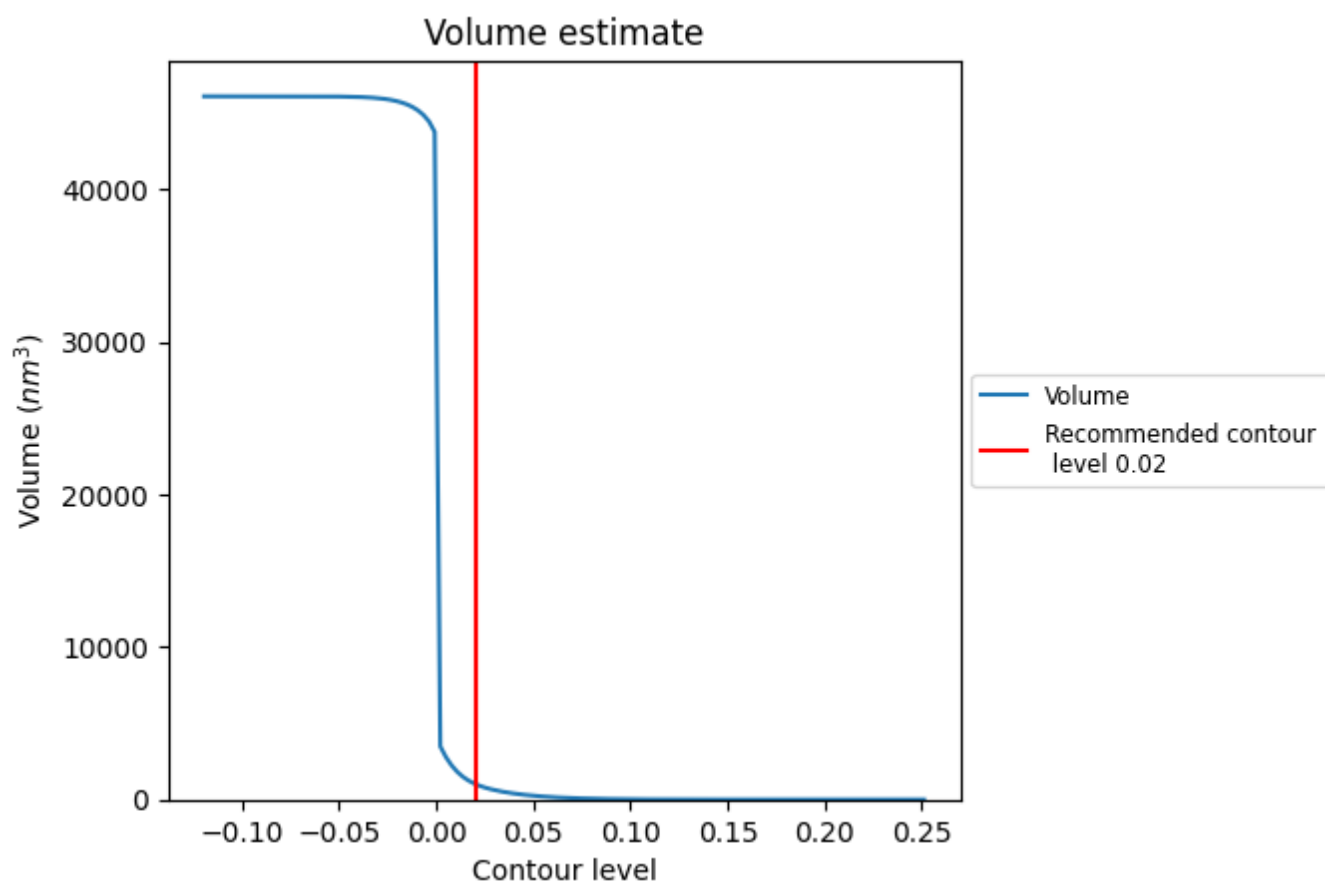
This section contains the results of statistical analysis of the map.

### 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.

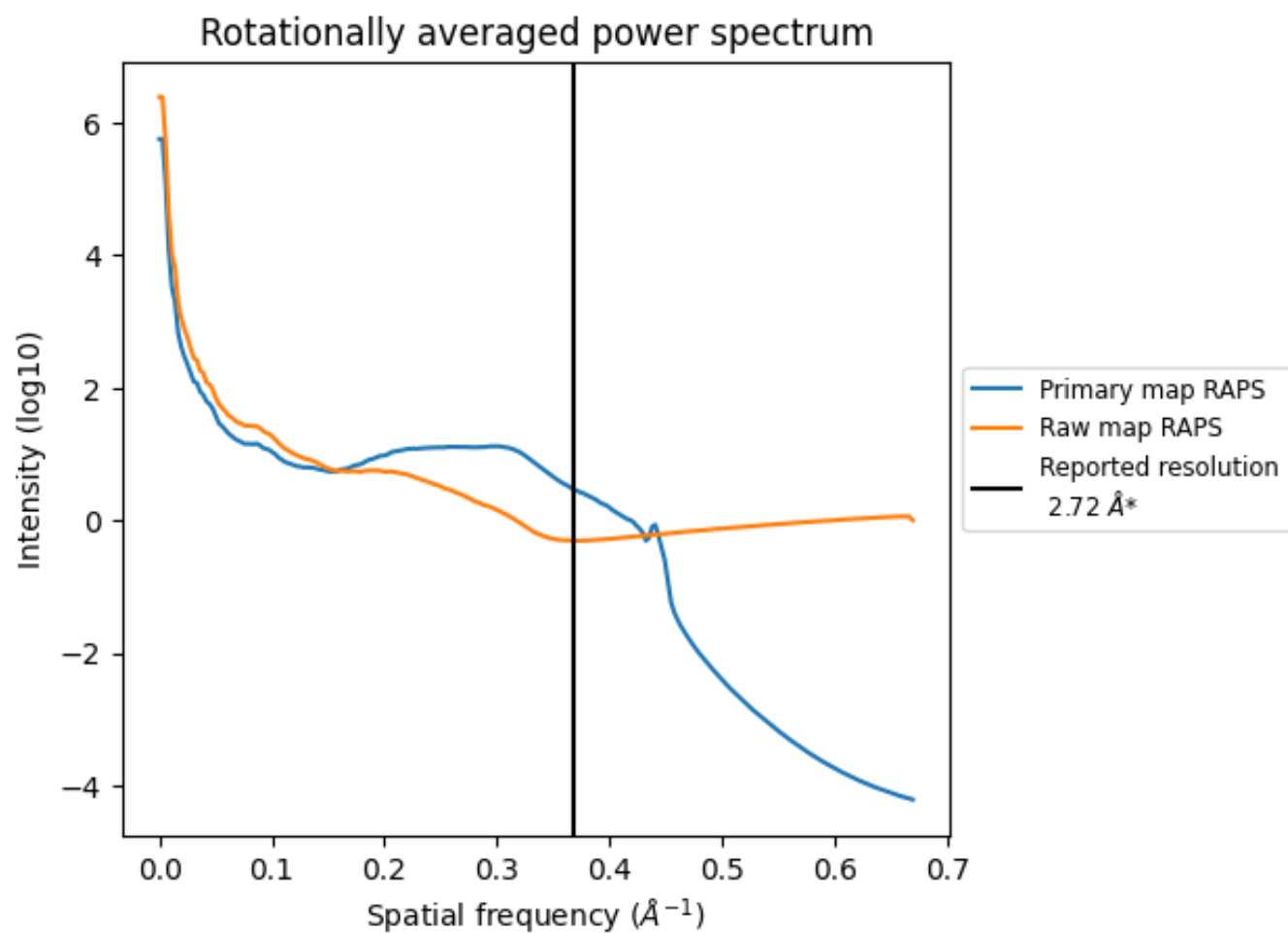
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1029  $\text{nm}^3$ ; this corresponds to an approximate mass of 929 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 ⓘ

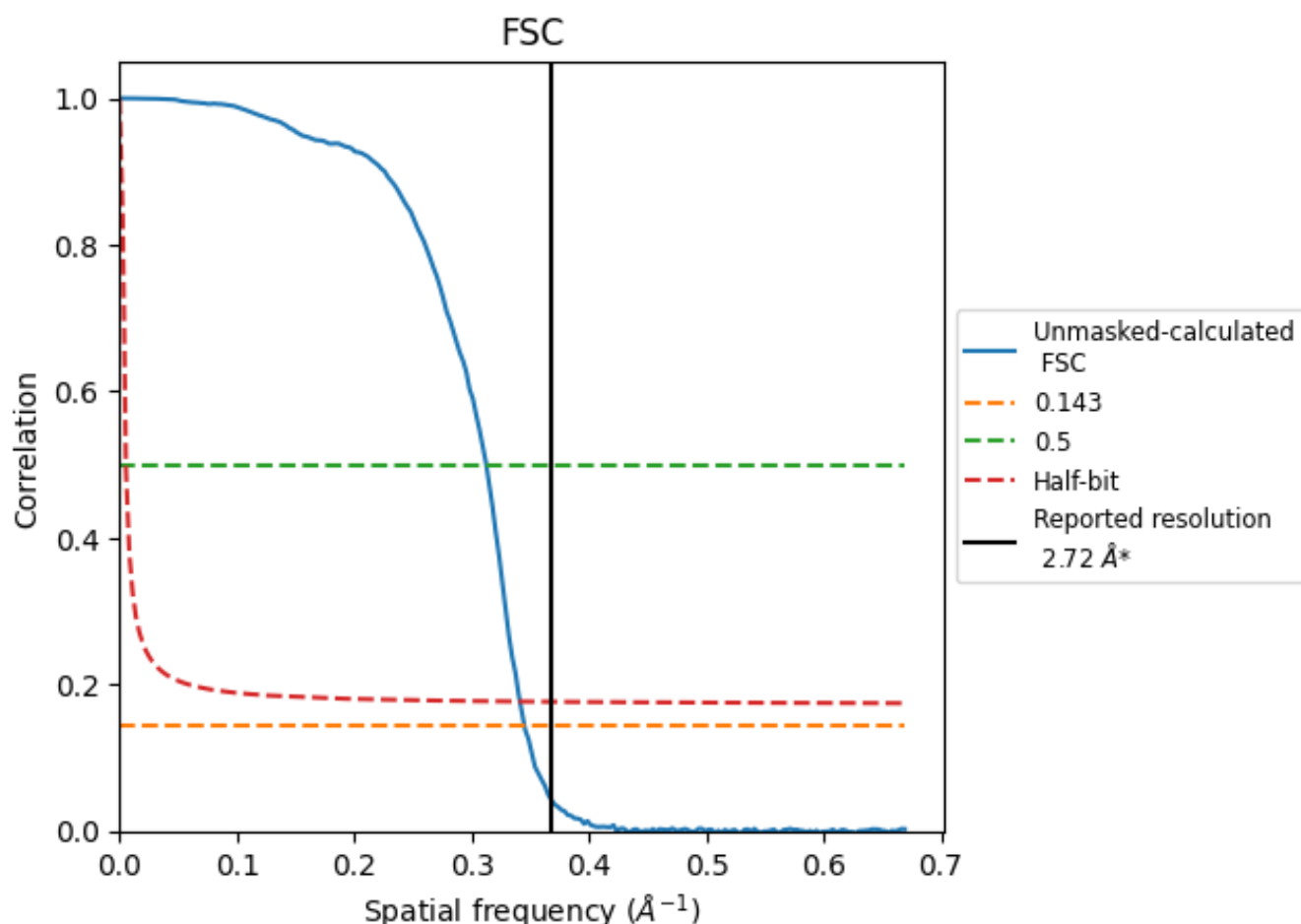


\*Reported resolution corresponds to spatial frequency of 0.368 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.368 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.90	3.20	2.93

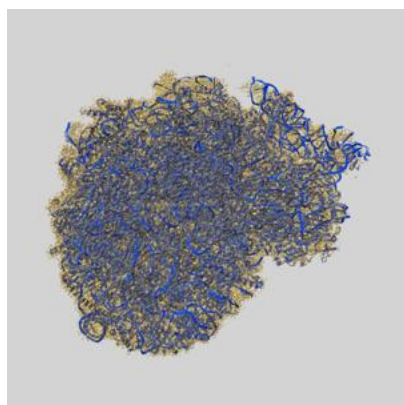
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



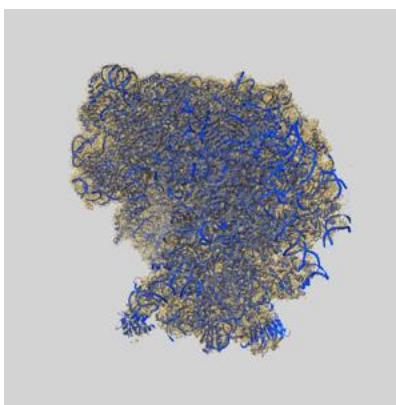
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18419 and PDB model 8QHU. Per-residue inclusion information can be found in section [3](#) on page [23](#).

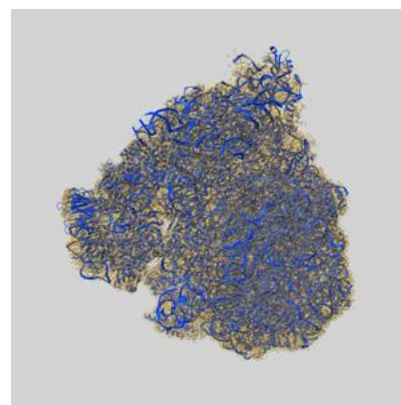
### 9.1 Map-model overlay [i](#)



X



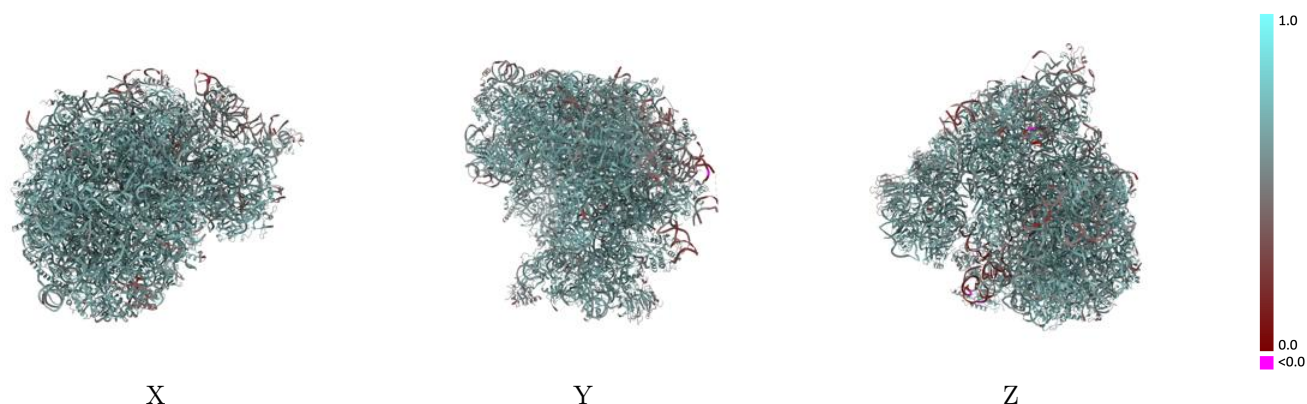
Y



Z

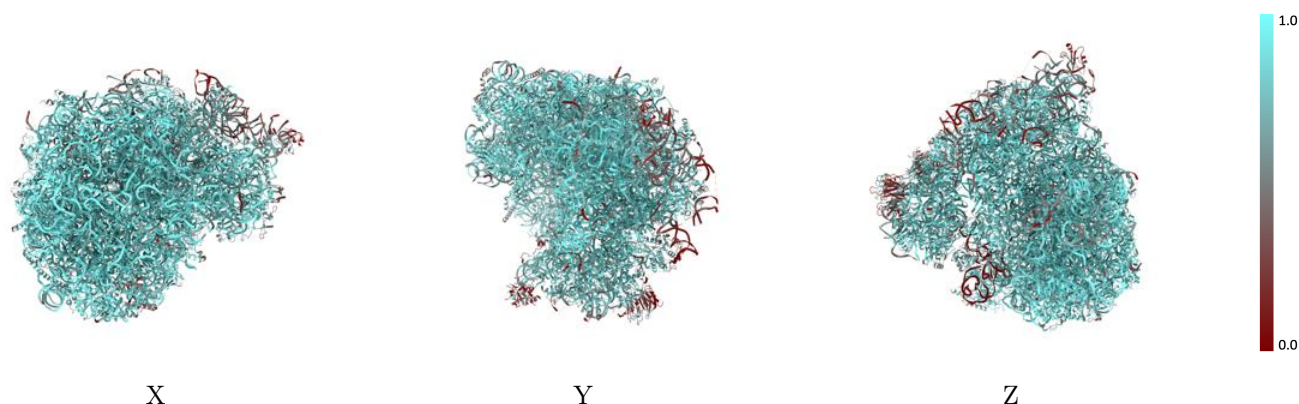
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



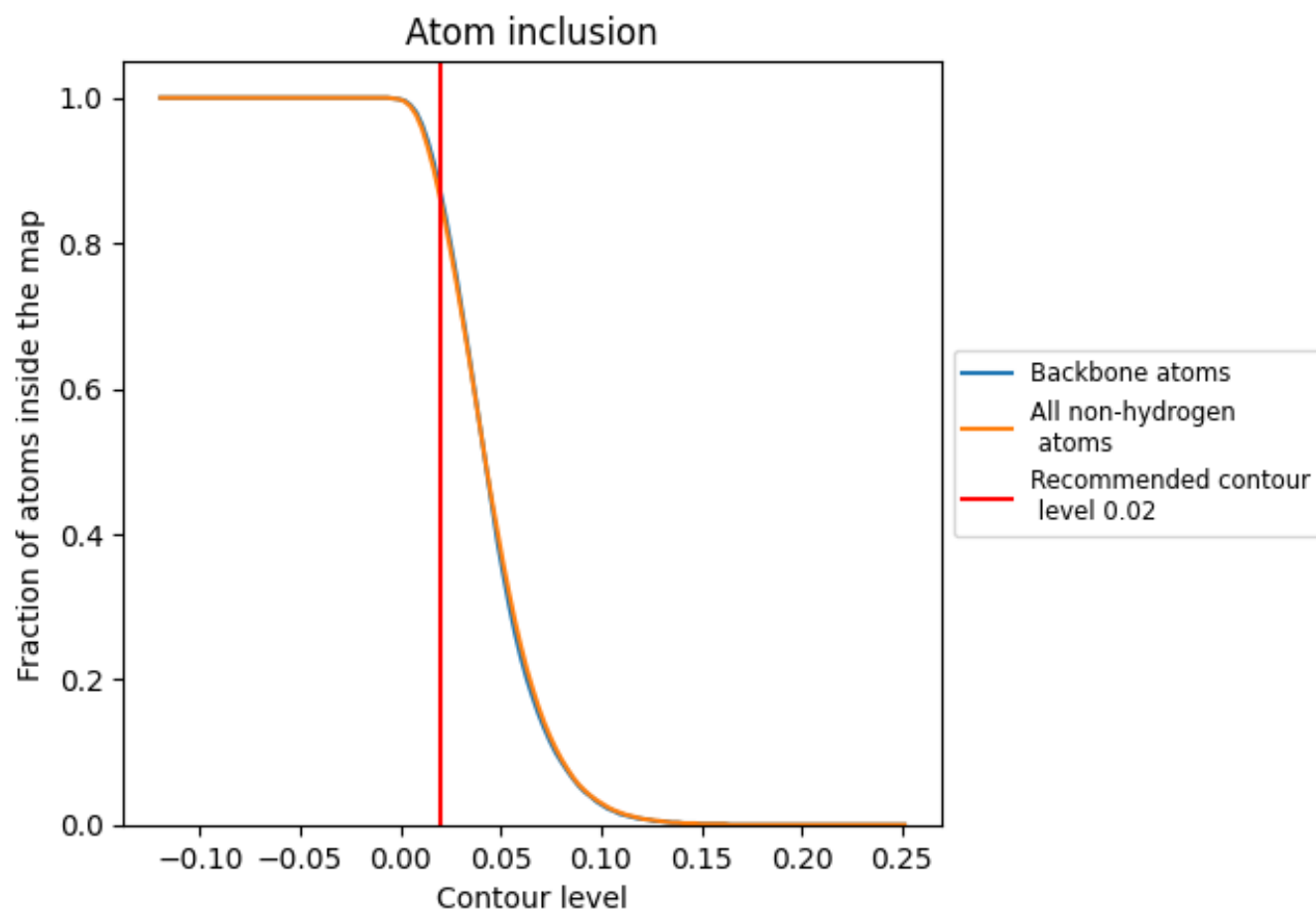
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.6220
1	 0.9280	 0.6380
2	 0.8730	 0.6080
3	 0.8700	 0.6040
4	 0.9500	 0.6550
5	 0.9040	 0.6120
6	 0.8570	 0.5870
7	 0.9230	 0.6360
8	 0.9430	 0.6380
A	 0.9680	 0.6840
B	 0.9470	 0.6820
C	 0.9290	 0.6540
D	 0.7250	 0.5510
E	 0.8810	 0.6450
F	 0.8220	 0.5990
G	 0.8810	 0.6240
H	 0.9390	 0.6700
I	 0.8840	 0.6420
J	 0.9350	 0.6700
K	 0.8220	 0.6040
L	 0.9380	 0.6700
M	 0.9810	 0.6850
N	 0.8900	 0.6490
O	 0.8470	 0.6100
P	 0.9390	 0.6640
Q	 0.8560	 0.6170
R	 0.9400	 0.6660
S	 0.8930	 0.6440
S1	 0.8400	 0.6000
S4	 0.2350	 0.2690
SA	 0.8060	 0.6210
SB	 0.7810	 0.6020
SC	 0.7150	 0.6090
SD	 0.8260	 0.6450
SE	 0.8240	 0.6480























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Chain	Atom inclusion	Q-score
SF	 0.8120	 0.6390
SG	 0.7250	 0.6150
SH	 0.8310	 0.6420
SI	 0.7500	 0.6100
SJ	 0.8880	 0.6620
SK	 0.8820	 0.6490
SL	 0.8660	 0.6540
SM	 0.6720	 0.6080
SN	 0.7240	 0.6130
SO	 0.8640	 0.6490
SP	 0.8780	 0.6580
SQ	 0.2120	 0.4660
SR	 0.7390	 0.6180
SS	 0.8740	 0.6570
ST	 0.8930	 0.6190
SU	 0.8660	 0.6540
SV	 0.5910	 0.5740
SW	 0.7230	 0.6150
SX	 0.8520	 0.6500
SY	 0.6860	 0.5960
SZ	 0.7720	 0.6310
Sa	 0.7420	 0.6180
Sb	 0.9130	 0.6470
Sc	 0.7510	 0.6090
Sd	 0.6950	 0.5920
Se	 0.7600	 0.6160
Sf	 0.3150	 0.5210
Sg	 0.4150	 0.5470
Sh	 0.3240	 0.4930
T	 0.9620	 0.6820
U	 0.3900	 0.4930
V	 0.9040	 0.6460
W	 0.9100	 0.6460
X	 0.9450	 0.6660
Y	 0.8520	 0.6130
Z	 0.8800	 0.6310
a	 0.8490	 0.6150
b	 0.9280	 0.6550
c	 0.9330	 0.6650
d	 0.8580	 0.6200
e	 0.8180	 0.6060
f	 0.9440	 0.6690

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Chain	Atom inclusion	Q-score
g	 0.9390	 0.6670
h	 0.8790	 0.6370
i	 0.8630	 0.6260
j	 0.9760	 0.6910
k	 0.7620	 0.5860
l	 0.9440	 0.6730
m	 0.9190	 0.6580
n	 0.8770	 0.5740
o	 0.9470	 0.6670
p	 0.9150	 0.6660