



wwPDB EM Validation Summary Report ⓘ

Jul 16, 2026 – 11:32 am BST

PDB ID : 8QHU / pdb_00008qhu
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

A user guide is available at

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

The types of validation reports are described at

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

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

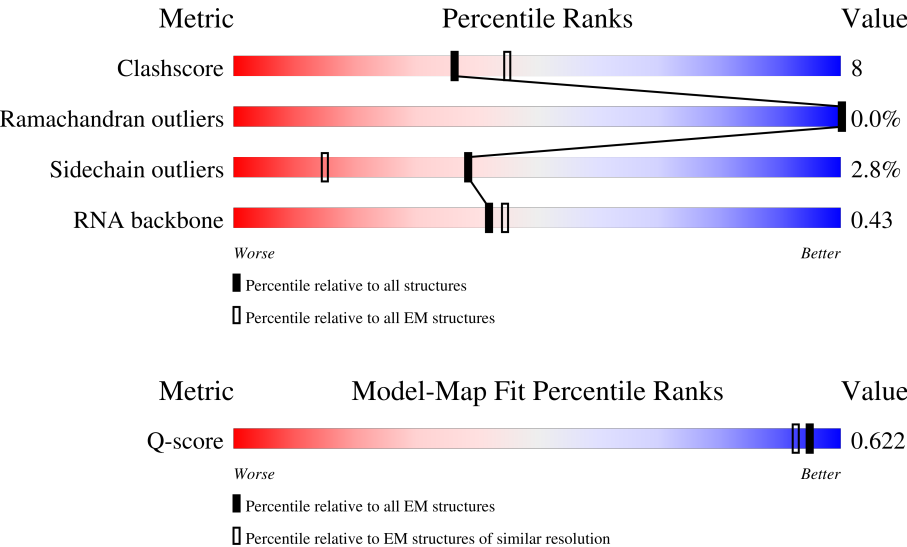
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10355 (2.22 - 3.22)

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

Mol	Chain	Length	Quality of chain
1	SB	246	
2	SC	219	
3	SD	190	

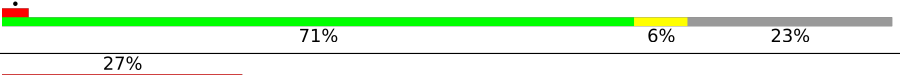
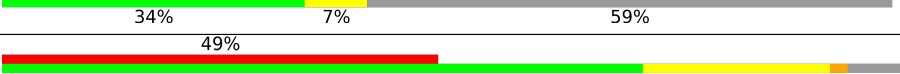
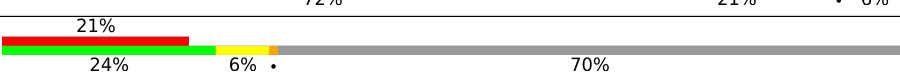
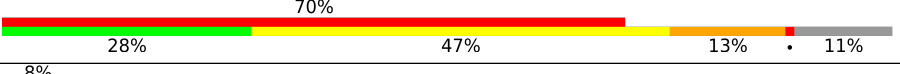
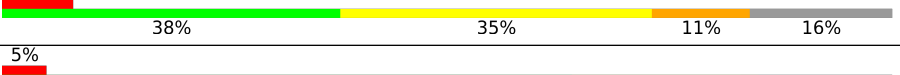
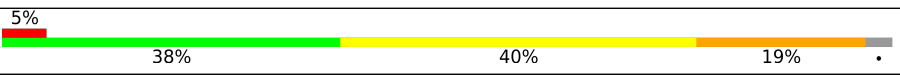
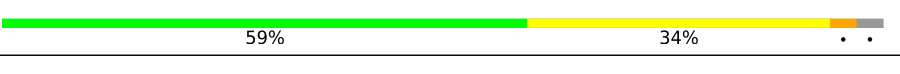
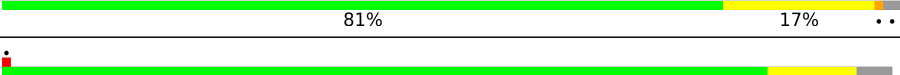
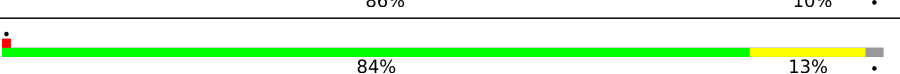
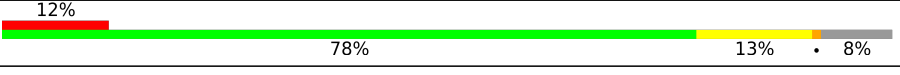
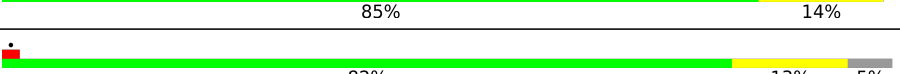
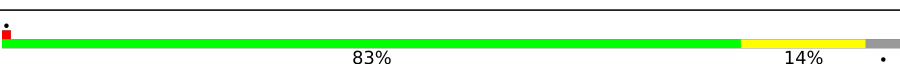
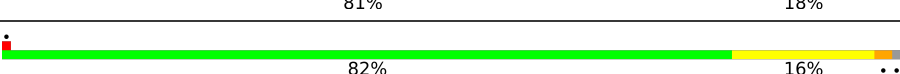
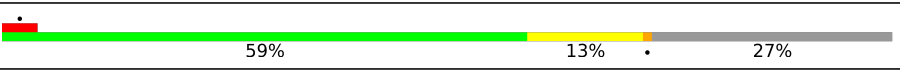
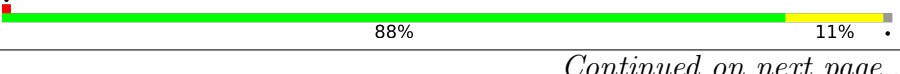
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	SE	273	
5	SF	265	
6	SG	249	
7	SH	190	
8	SI	200	
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	

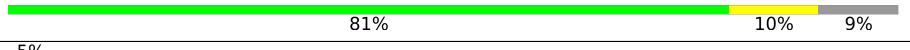
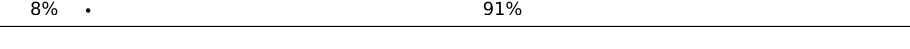
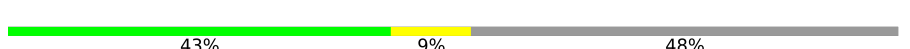
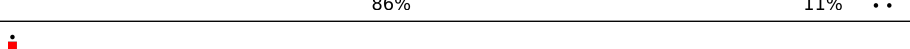
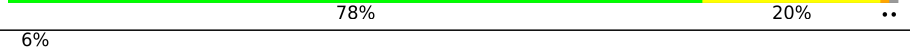
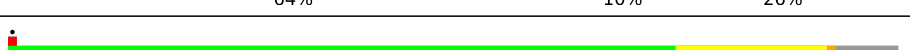
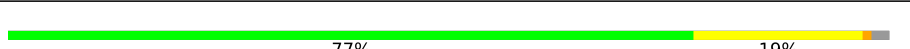
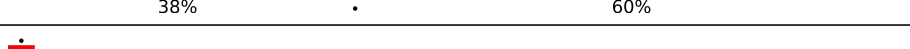
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Sd	87	
30	Se	66	
31	Sf	152	
32	Sg	312	
33	Sh	235	
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	

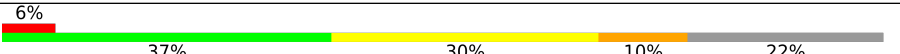
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	S	159	
55	T	166	
56	U	129	
57	V	145	
58	W	143	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	N	213	
80	O	305	
81	e	188	
82	1	1782	
83	3	216	
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		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 (CCD ID: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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 (CCD ID: 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.

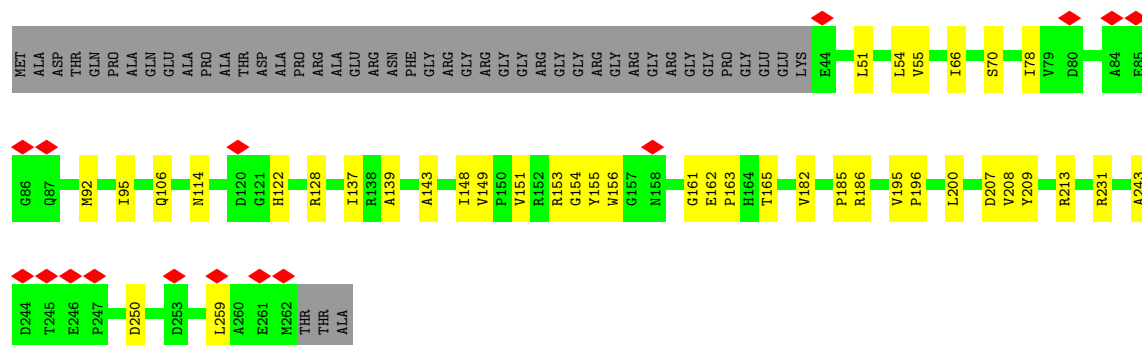
Mol	Chain	Residues	Atoms		AltConf
90	S1	44	Total 44	O 44	0
90	4	9	Total 9	O 9	0

Continued on next page...

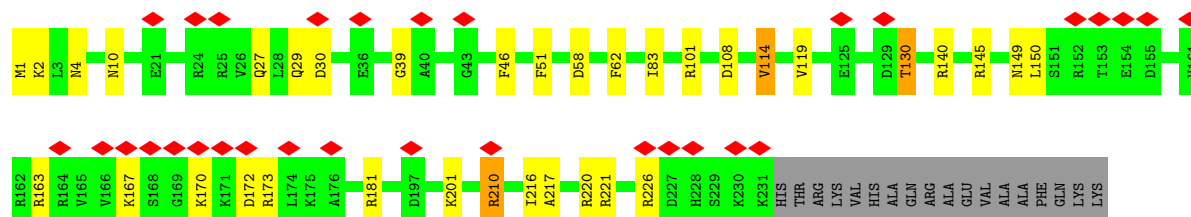
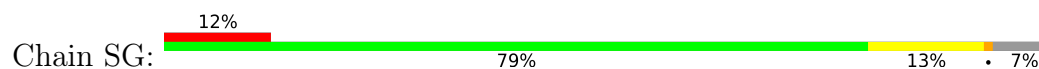
Continued from previous page...

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

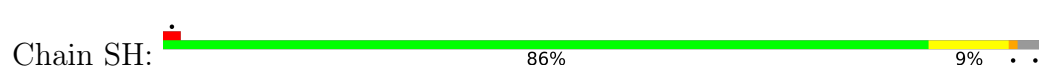
- Molecule 5: 40S ribosomal protein S2



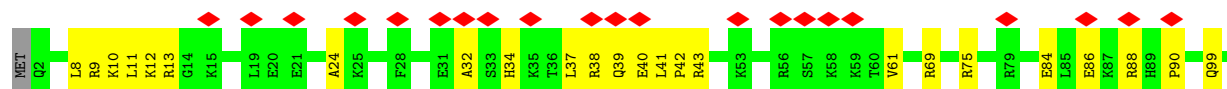
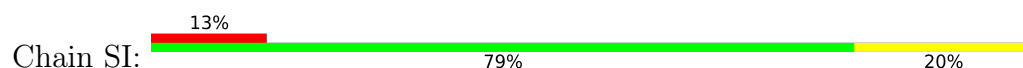
- Molecule 6: 40S ribosomal protein S6



- Molecule 7: 40S ribosomal protein S5



- Molecule 8: 40S ribosomal protein S7



ALA
ALA
GLU

- Molecule 14: 40S ribosomal protein S14

Chain SO:  76% 18% 6%

MET SER LYS LYS GLN VAL VAL LYS A9 L19 F27 T33 F34 T45 Y46 V47 T50 R59 A67 R77 C81 N84 V88 K89 A92 V96 L109 R114 V125 T126 P127 T128 P129 S132 R139 L144

- Molecule 15: Putative 40S ribosomal protein S23

Chain SP:  87% 12%

MET T2 K3 R11 T32 F33 S34 K48 K68 F84 V85 P86 L91 F106 G109 R119 F120 K121 K124 G129 R135 R142 ASN

- Molecule 16: 40S ribosomal protein S12

Chain SQ:  52% 51% 15% 34%

MET ALA GLU THR VAL ARG VAL ASP VAL ALA VAL GLU GLU ASN VAL VAL ASP VAL VAL SER LEU D28 A29 V30 R31 I32 V33 I34 Q35 K36 S37 L38 E39 A40 M41 G42 L43 V44 R45 G46 L47 S48 E49 R52 T53 L54 D55 C56 K57 T58 A59 H60 I63 L64 A65 D66 D67 C68 E69 ASP GLU E72 Y73 R74 L80 A81 K82 Q83 G84 N85 I86 D87 L88 I89 N90 V91 E92 E93 R94 E95 K96 L97 A98 Q99 W100 A101 G102 L103 V104 R105 R106 ASP VAL ALA GLY E111 V112 T113 K114 T115 L116 K117 C118 S119 I123 R124 D125 F126 GLU ARG THR LYS ALA LEU ASP TYR LEU LEU SER GLN LEU HIS

- Molecule 17: Putative 40S ribosomal protein S18

Chain SR:  8% 71% 16% 11%

M1 S2 L3 H12 R15 N18 V27 P28 R40 F41 L44 V53 E54 R55 R56 T59 L60 T61 A62 E63 E66 D74 R87 Q88 R89 T96 R109 D110 D111 K116 K117 M118 R119 R122 A127 Y128 G129 L130 R131 V132 R133 G134 Q135 H136 THR CYS THR SER GLY ARG HIS GLY LYS THR VAL GLY VAL SER ARG GLY LYS

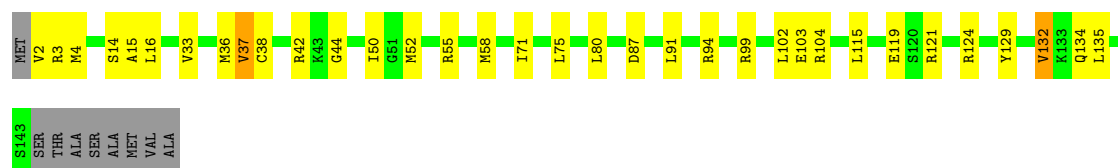
- Molecule 18: Putative ribosomal protein S29

Chain SS:  81% 18%

MET G2 H3 L4 M7 R10 Q11 K12 R20 A30 R33 R41 F53 R57

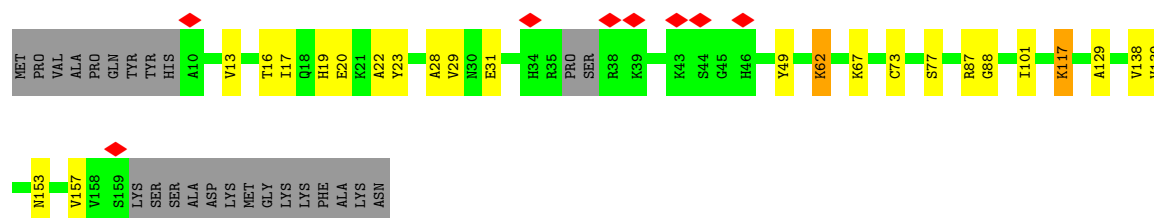
- Molecule 19: Putative 40S ribosomal protein S13

Chain ST:  72% 21% • 6%



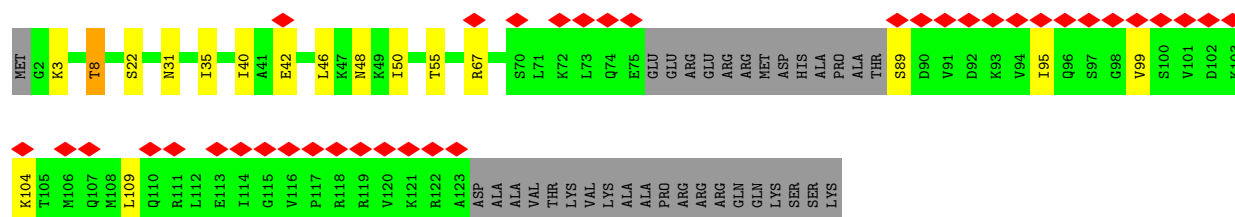
- Molecule 20: Putative 40S ribosomal protein S11

Chain SU:  72% 13% • 14%



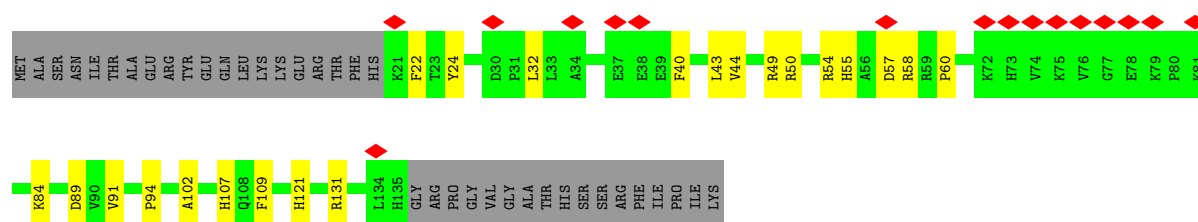
- Molecule 21: Putative 40S ribosomal protein S17

Chain SV:  27% 64% 11% • 24%



- Molecule 22: Putative 40S ribosomal protein S15

Chain SW:  11% 61% 14% 24%

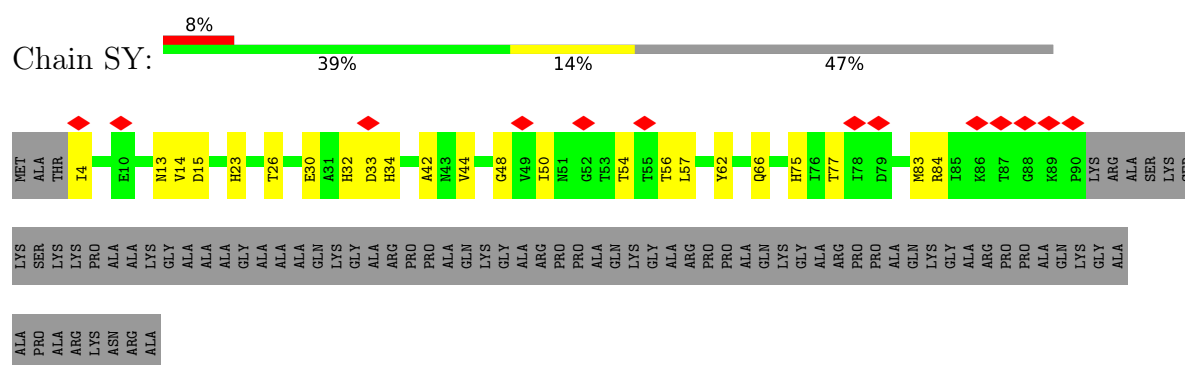


- Molecule 23: 40S ribosomal protein S19-like protein

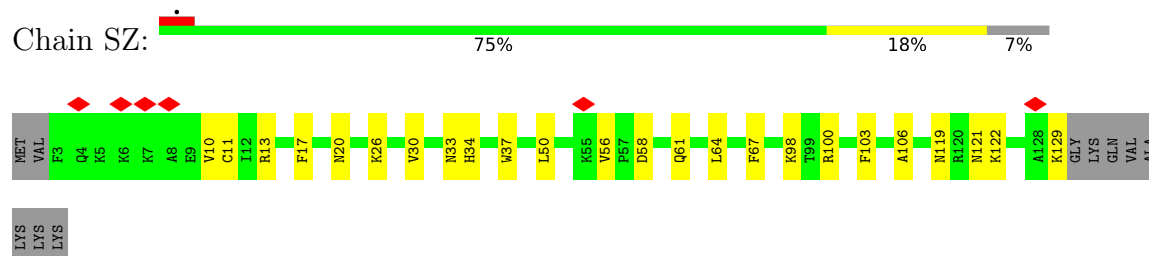
Chain SX:  83% 11% • 6%



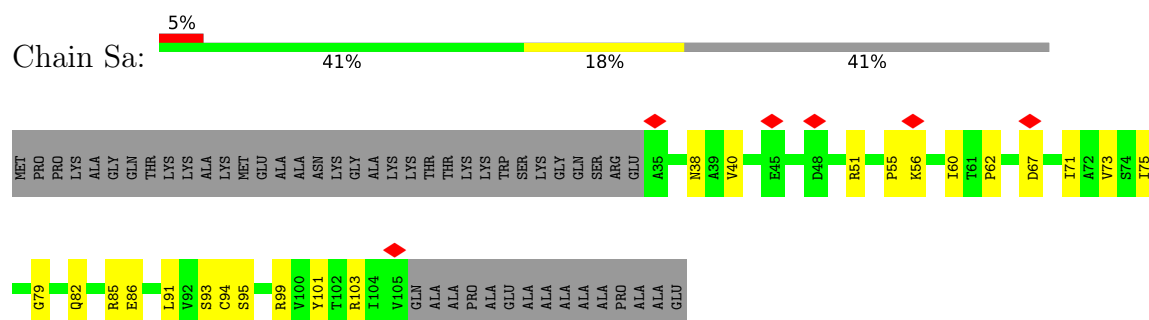
- Molecule 24: Putative 40S ribosomal protein S21



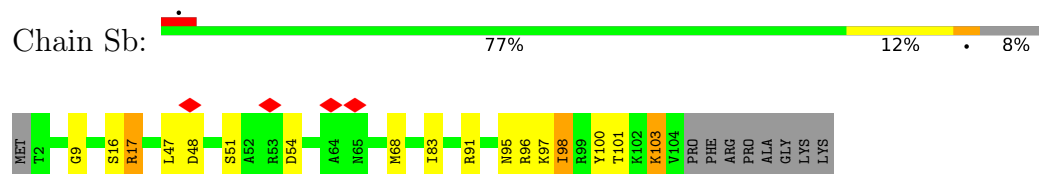
- Molecule 25: 40S ribosomal protein S24



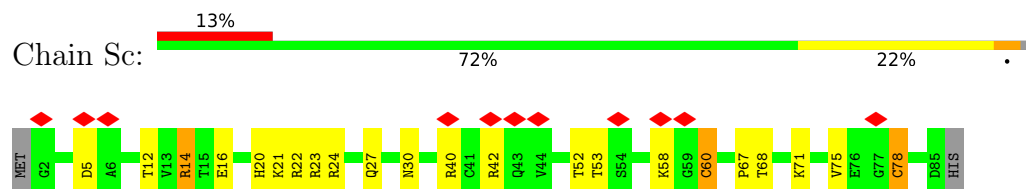
- Molecule 26: 40S ribosomal protein S25



- Molecule 27: 40S ribosomal protein S26



- Molecule 28: Putative 40S ribosomal protein S27-1



- Molecule 29: Putative 40S ribosomal protein S33

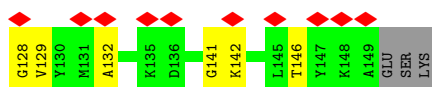
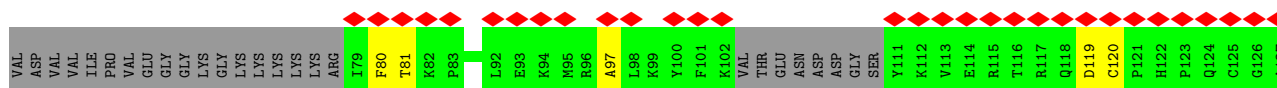
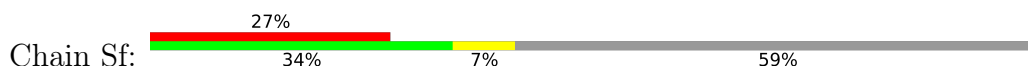




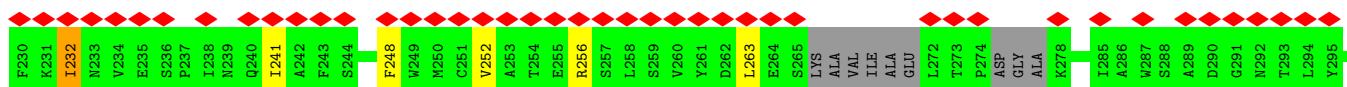
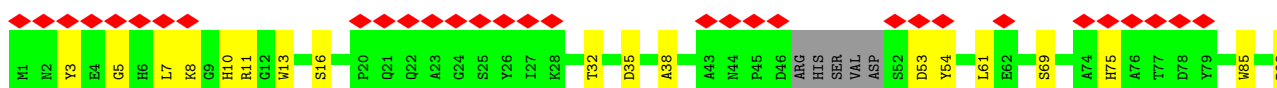
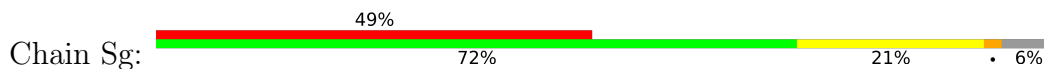
- Molecule 30: 40S ribosomal protein S30



- Molecule 31: Ubiquitin-60S ribosomal protein L40

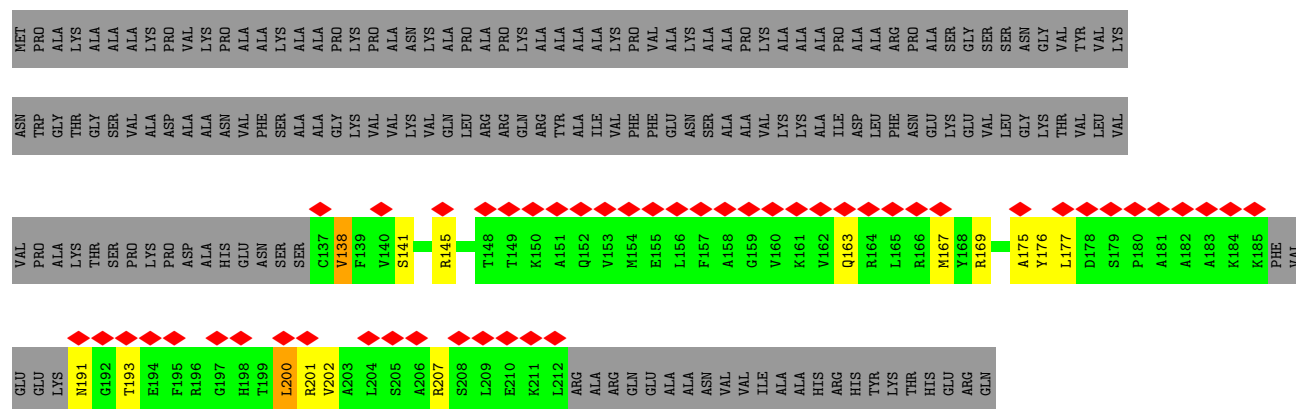


- Molecule 32: Small ribosomal subunit protein RACK1

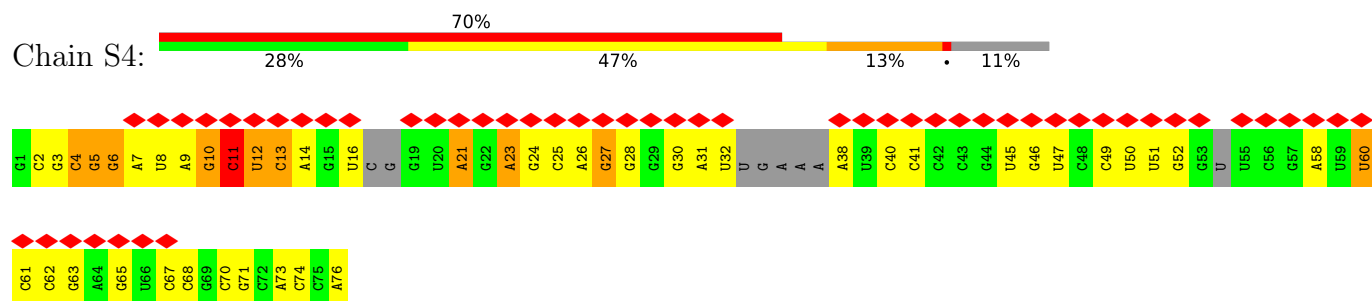


- Molecule 33: Putative RNA binding protein

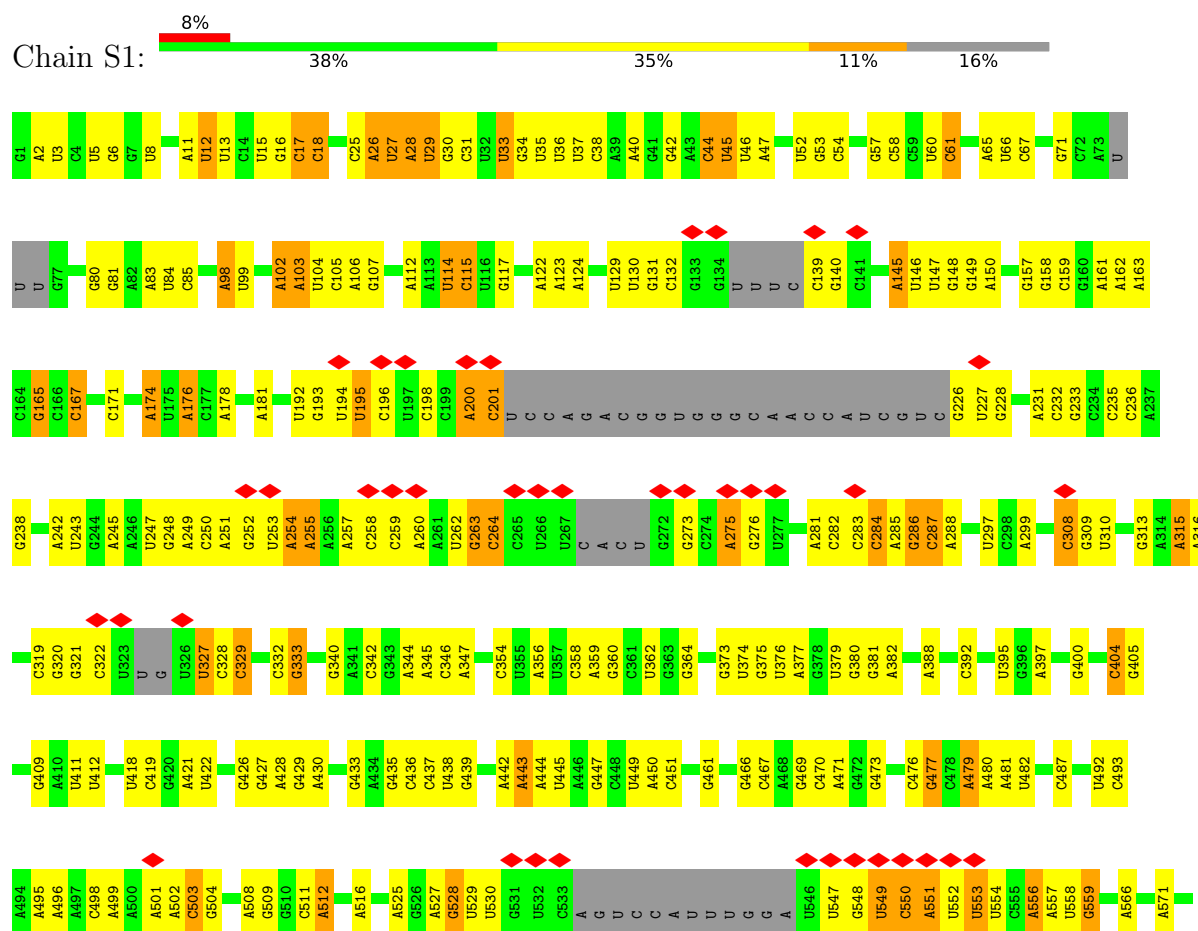




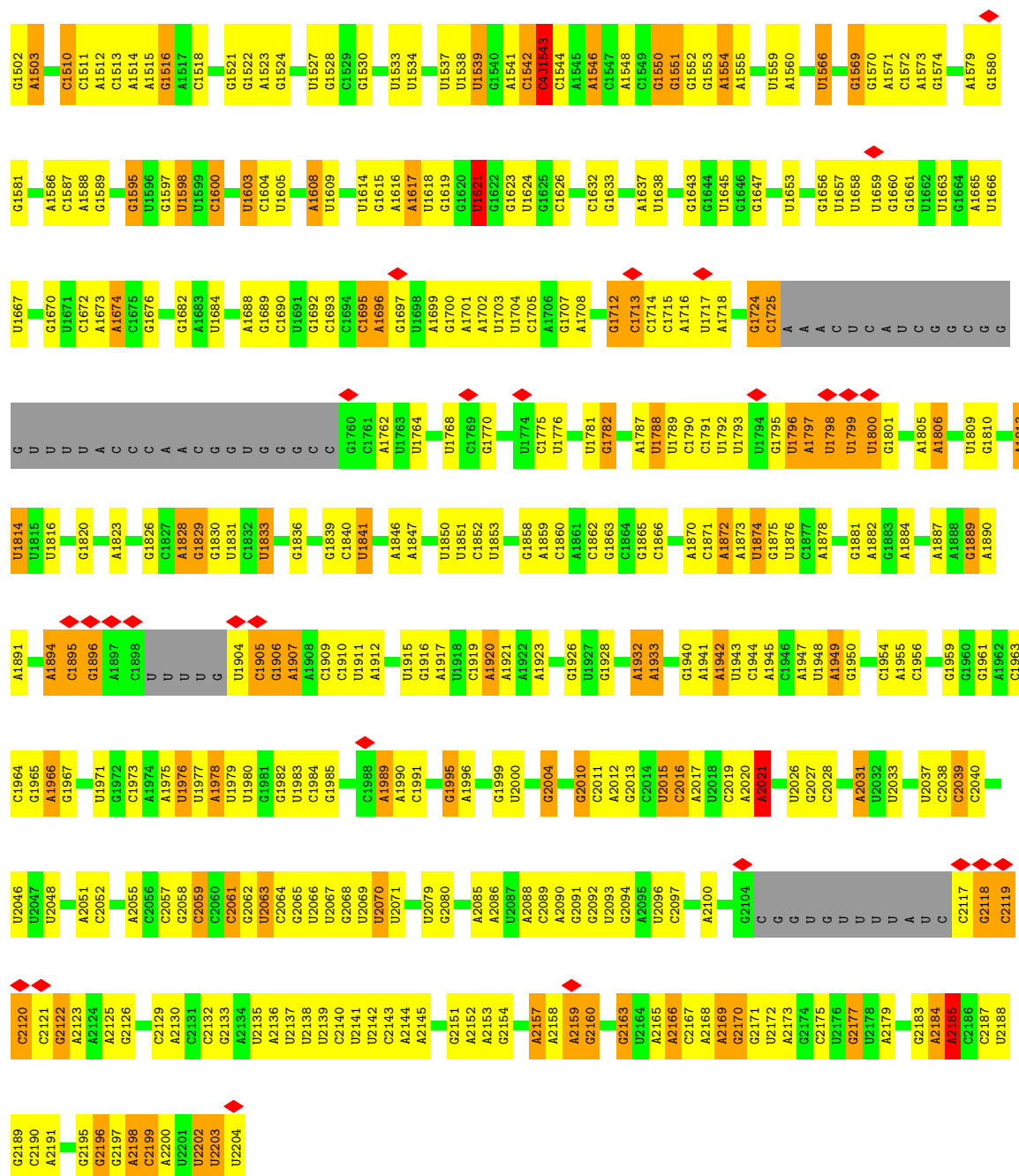
• Molecule 34: E-site_tRNA_chain_S4



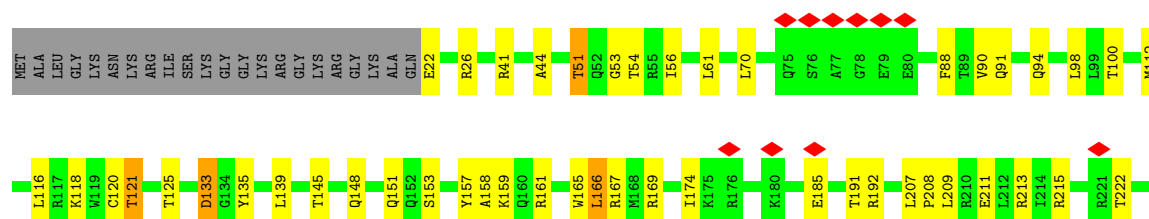
• Molecule 35: SSU_rRNA_chain_S1

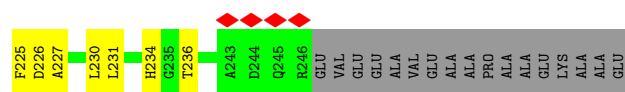






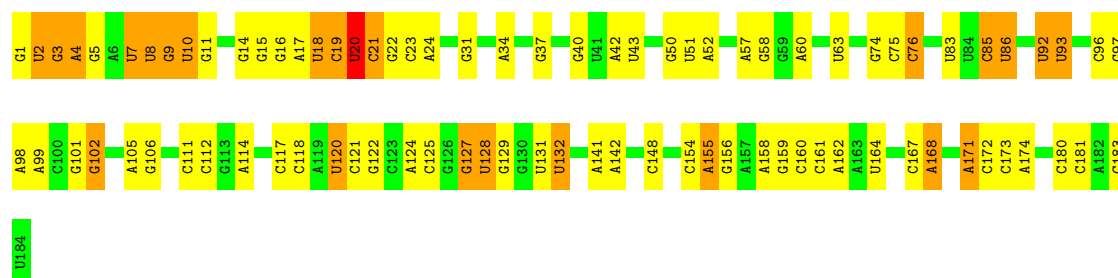
• Molecule 36: 40S ribosomal protein S3a





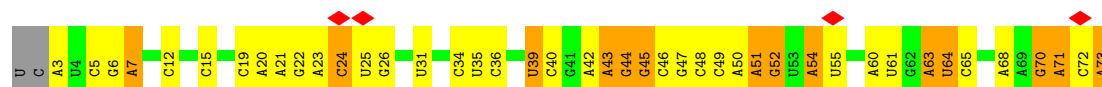
• Molecule 37: SR2_chain_4

Chain 4: 53% 34% 12% .



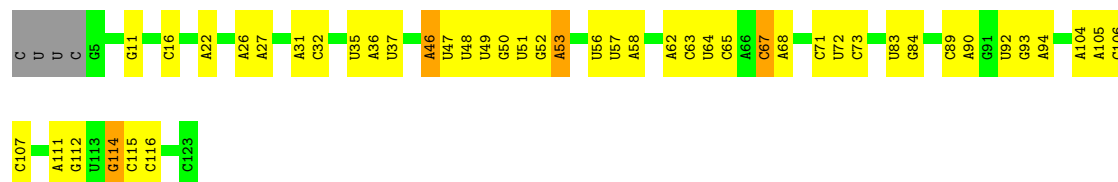
• Molecule 38: SR6_chain_6

Chain 6: 5% 38% 40% 19% .



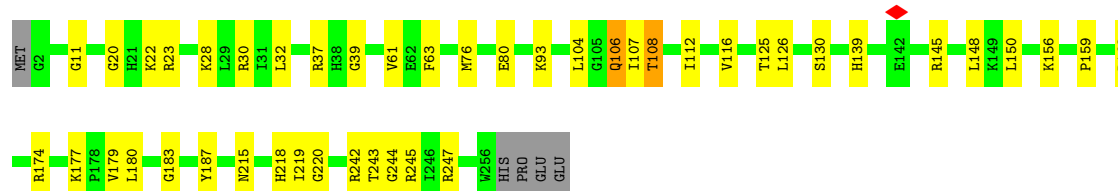
• Molecule 39: 5S_rRNA_chain_8

Chain 8: 59% 34% . .



• Molecule 40: Putative 60S ribosomal protein L2

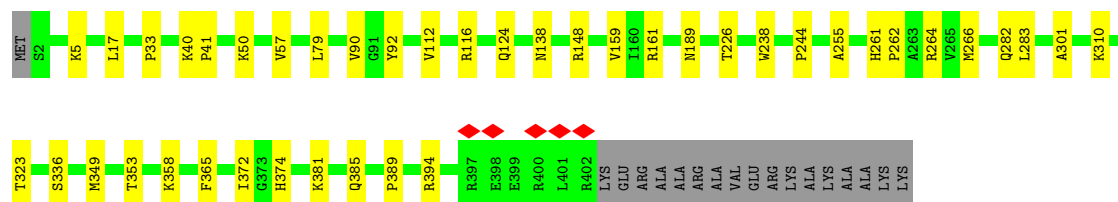
Chain A: 81% 17% . .



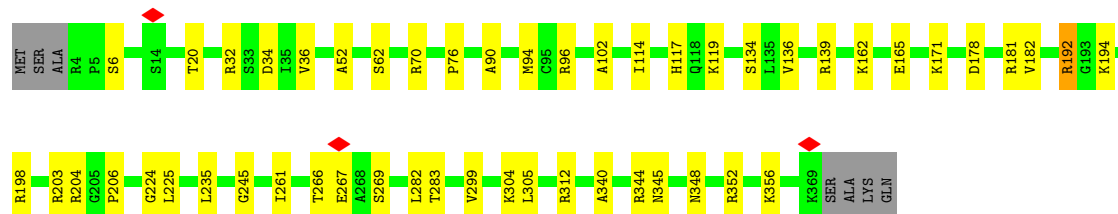
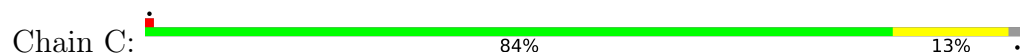
• Molecule 41: Putative ribosomal protein L3

Chain B: 86% 10% .

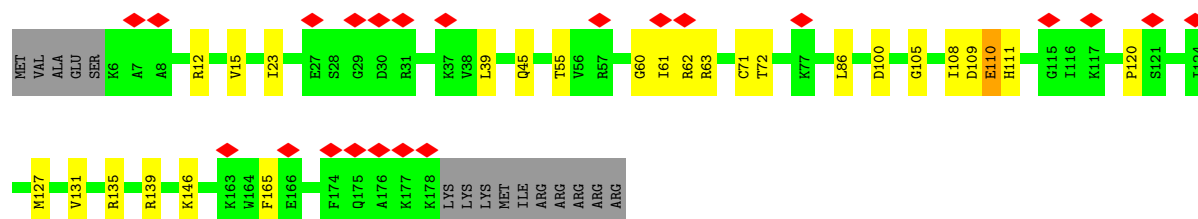
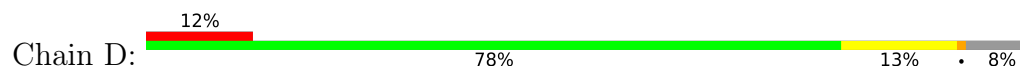




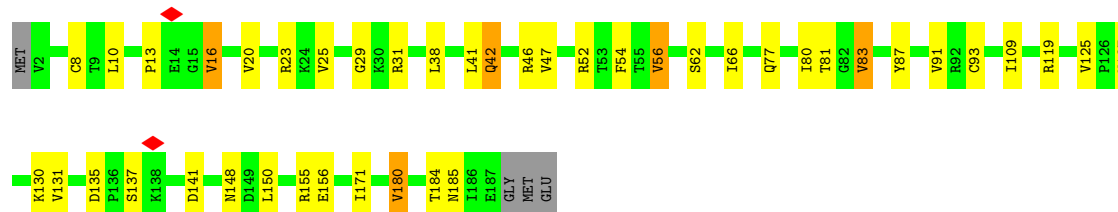
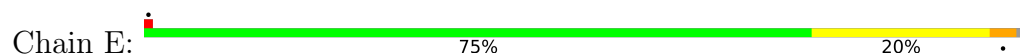
• Molecule 42: Putative ribosomal protein L1a



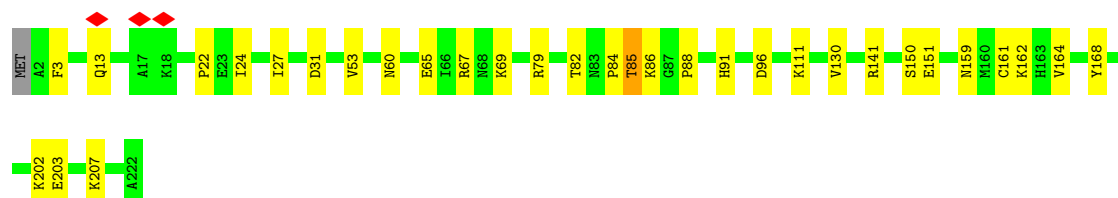
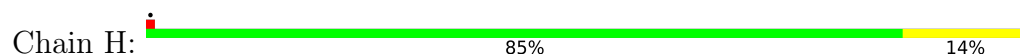
• Molecule 43: 60S ribosomal protein L11



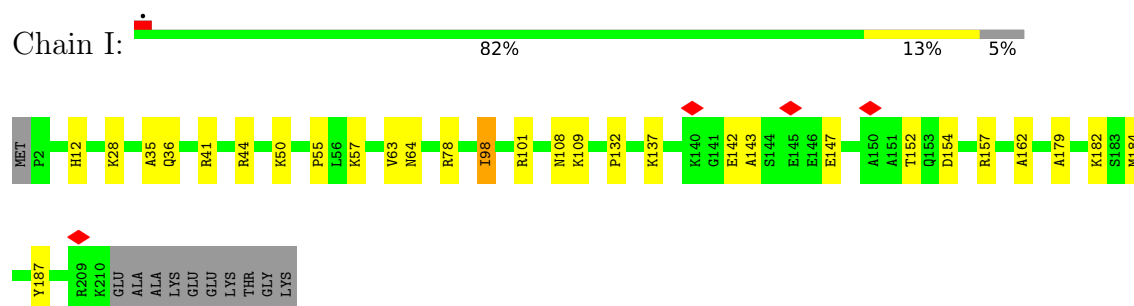
• Molecule 44: Putative 60S ribosomal protein L9



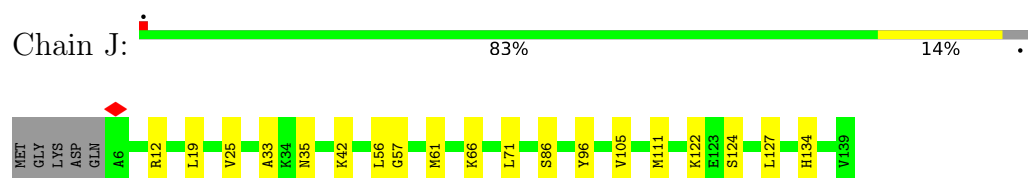
• Molecule 45: Putative 60S ribosomal protein L13a



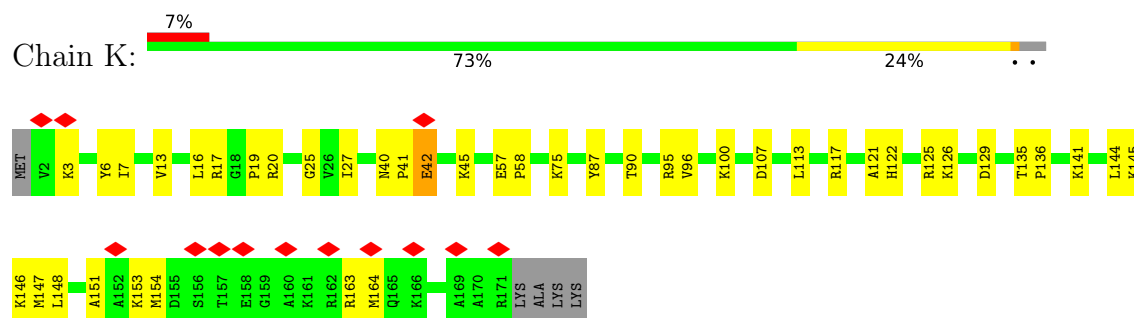
- Molecule 46: Putative 60S ribosomal protein L13



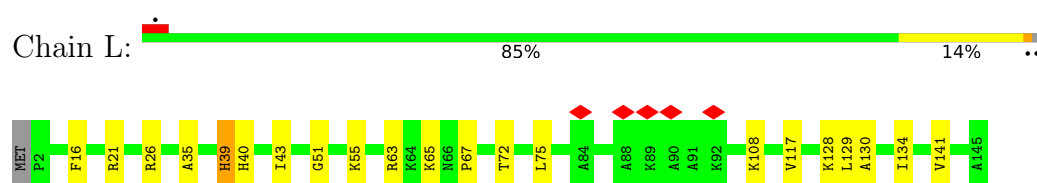
- Molecule 47: Putative 60S ribosomal protein L23



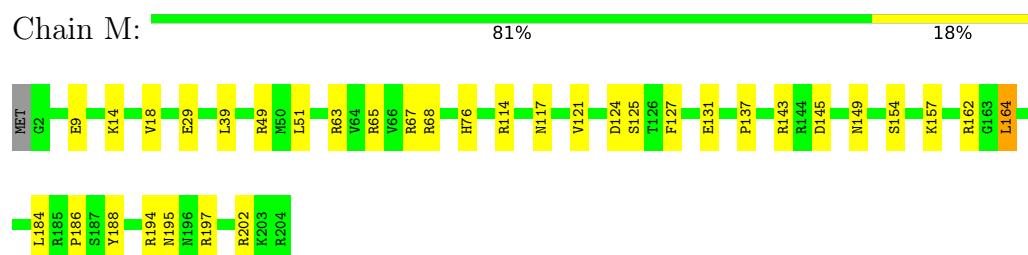
- Molecule 48: Putative 40S ribosomal protein L14



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

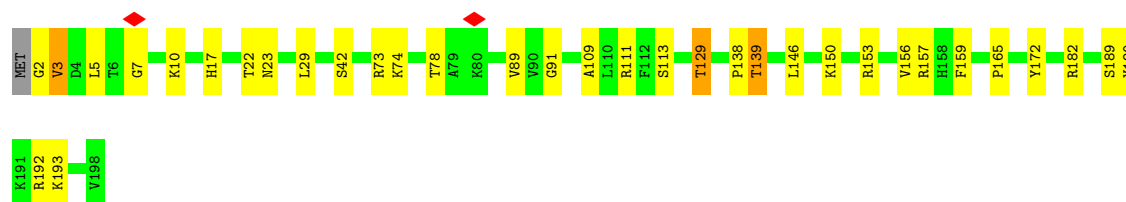


- Molecule 50: Ribosomal protein L15



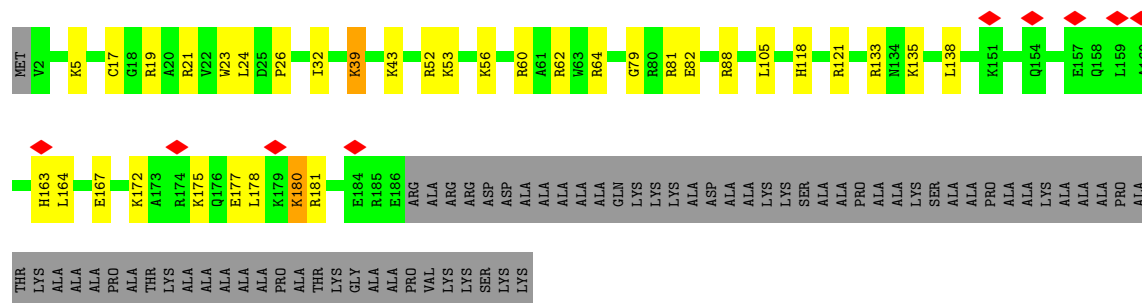
- Molecule 51: 60S ribosomal protein L18

Chain P:  82% 16% ..



- Molecule 52: Putative 60S ribosomal protein L19

Chain Q:  59% 13% 27%



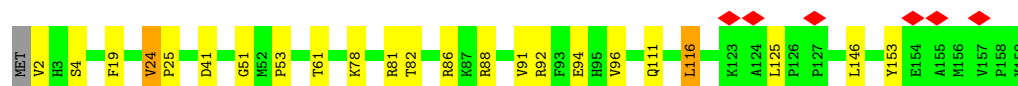
- Molecule 53: 60S ribosomal protein L18a

Chain R:  88% 11%



- Molecule 54: Putative 60S ribosomal protein L21

Chain S:  85% 13% ..



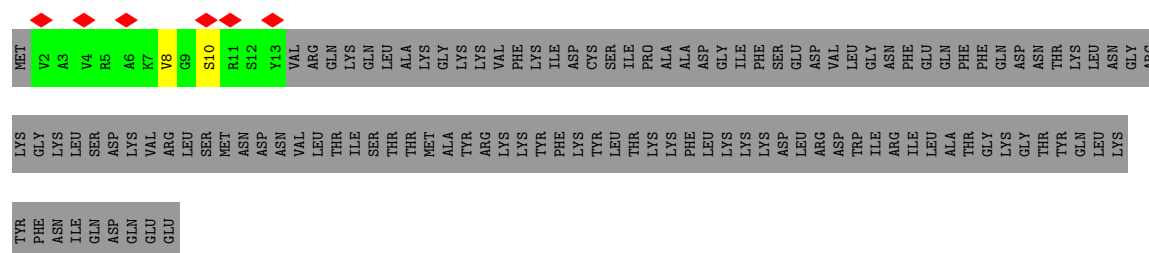
- Molecule 55: Putative 60S ribosomal protein L17

Chain T:  81% 10% 9%



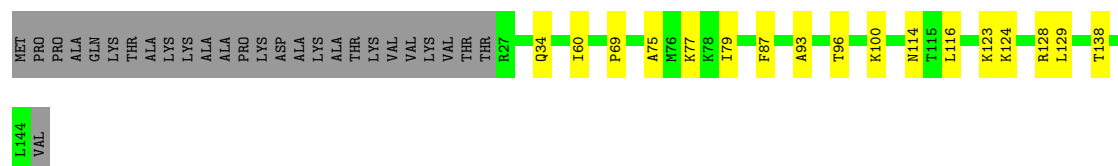
- Molecule 56: Putative 60S ribosomal protein L22

Chain U:  5% 8% 91%



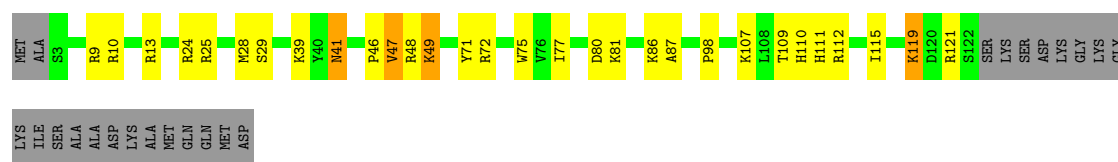
- Molecule 57: Putative 60S ribosomal protein L23a

Chain V: 70% 12% 19%



- Molecule 58: Putative 60S ribosomal protein L26

Chain W: 63% 18% 16%



- Molecule 59: Putative ribosomal protein L24

Chain X: 43% 9% 48%



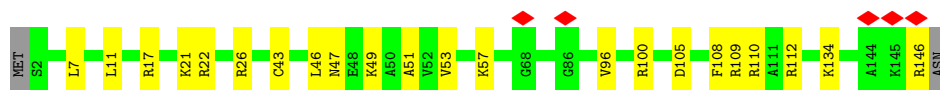
- Molecule 60: 60S ribosomal protein L27

Chain Y: 79% 20%



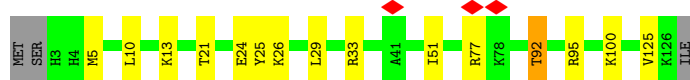
- Molecule 61: Putative 60S ribosomal protein L28

Chain Z: 84% 15%



- Molecule 62: Putative 60S ribosomal protein L35

Chain a: 86% 11% ..



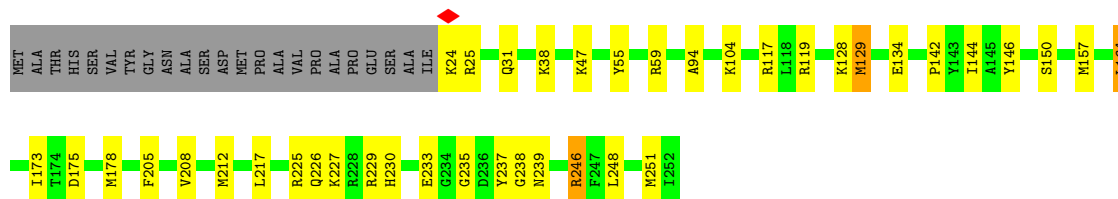
- Molecule 63: 60S ribosomal protein L29

Chain b: 79% 19% .



- Molecule 64: Putative 60S ribosomal protein L7

Chain c: 75% 15% . 9%



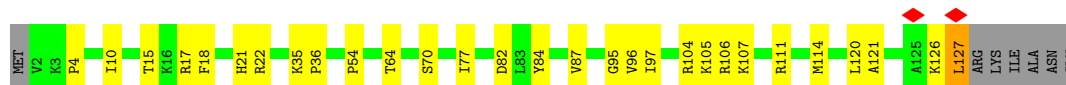
- Molecule 65: 60S ribosomal protein L30

Chain d: 5% 70% 17% . 12%



- Molecule 66: 60S ribosomal protein L32

Chain f: 73% 21% . 5%

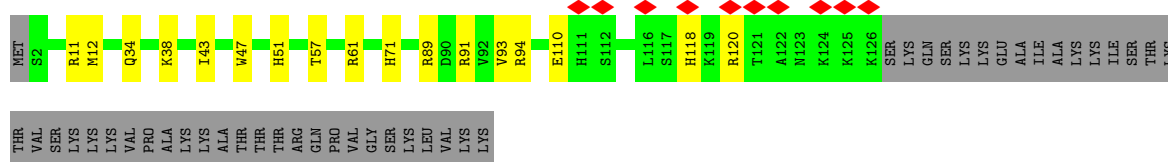


- Molecule 67: Putative ribosomal protein l35a

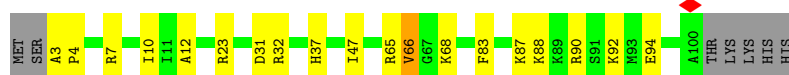
Chain g: 78% 20% ..



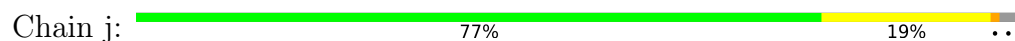
- Molecule 68: Putative 60S ribosomal protein L34



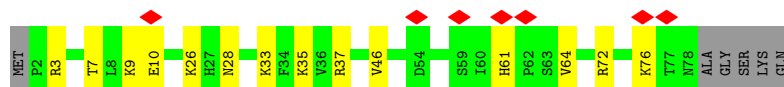
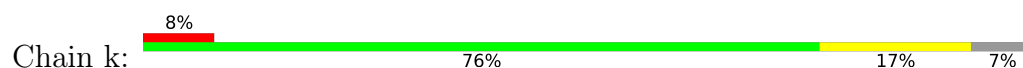
- Molecule 69: Putative 60S Ribosomal protein L36



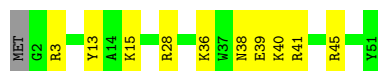
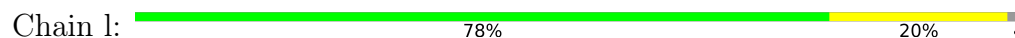
- Molecule 70: Ribosomal protein L37



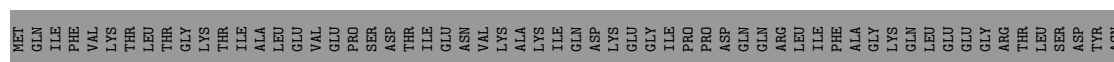
- Molecule 71: Putative ribosomal protein L38

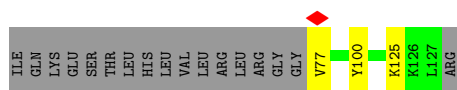


- Molecule 72: Putative 60S ribosomal protein L39



- Molecule 73: Ubiquitin-60S ribosomal protein L40

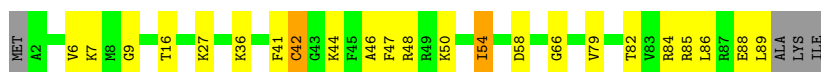




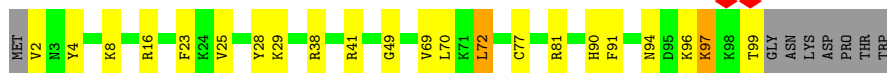
- Molecule 74: 60S ribosomal protein L41



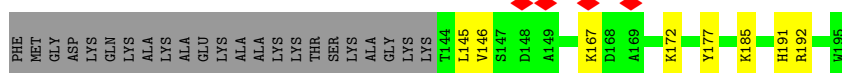
- Molecule 75: 60S ribosomal protein L37a



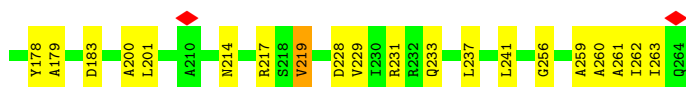
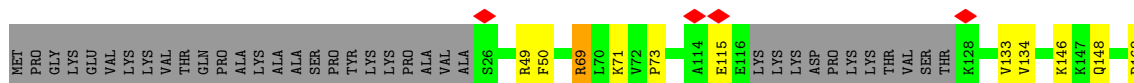
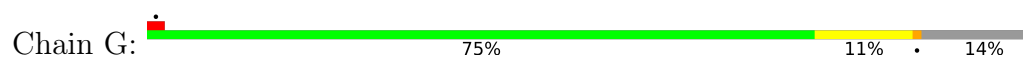
- Molecule 76: Putative 60S ribosomal protein L44



- Molecule 77: Putative 60S ribosomal protein L6

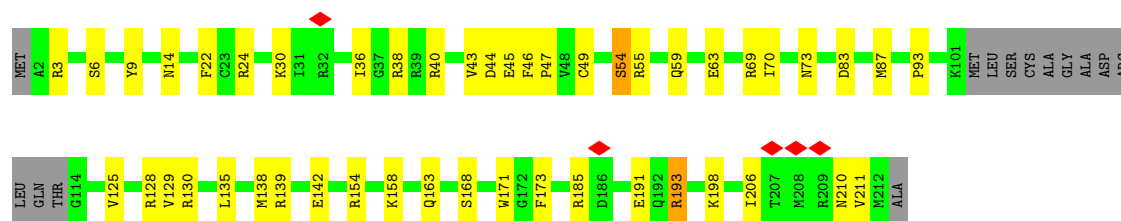


- Molecule 78: 60S ribosomal protein L7a



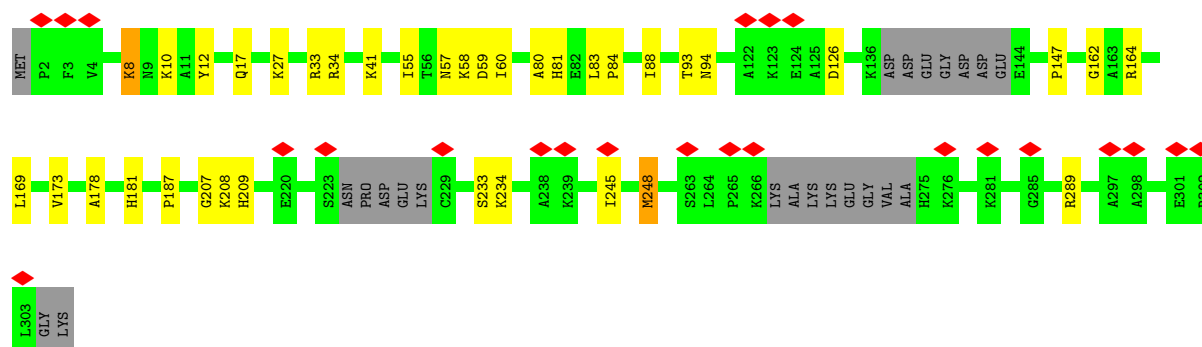
- Molecule 79: Putative 60S ribosomal protein L10

Chain N: 



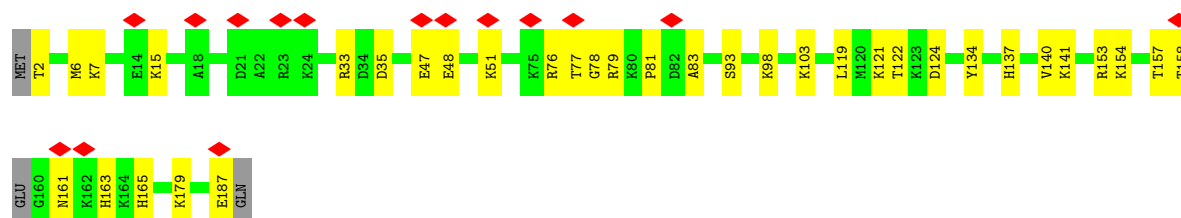
- Molecule 80: Putative 60S ribosomal protein L5

Chain O: 



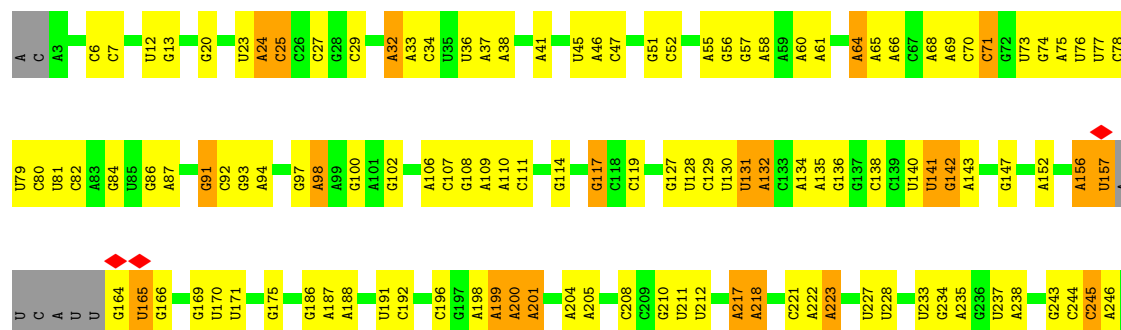
- Molecule 81: Putative 60S ribosomal subunit protein L31

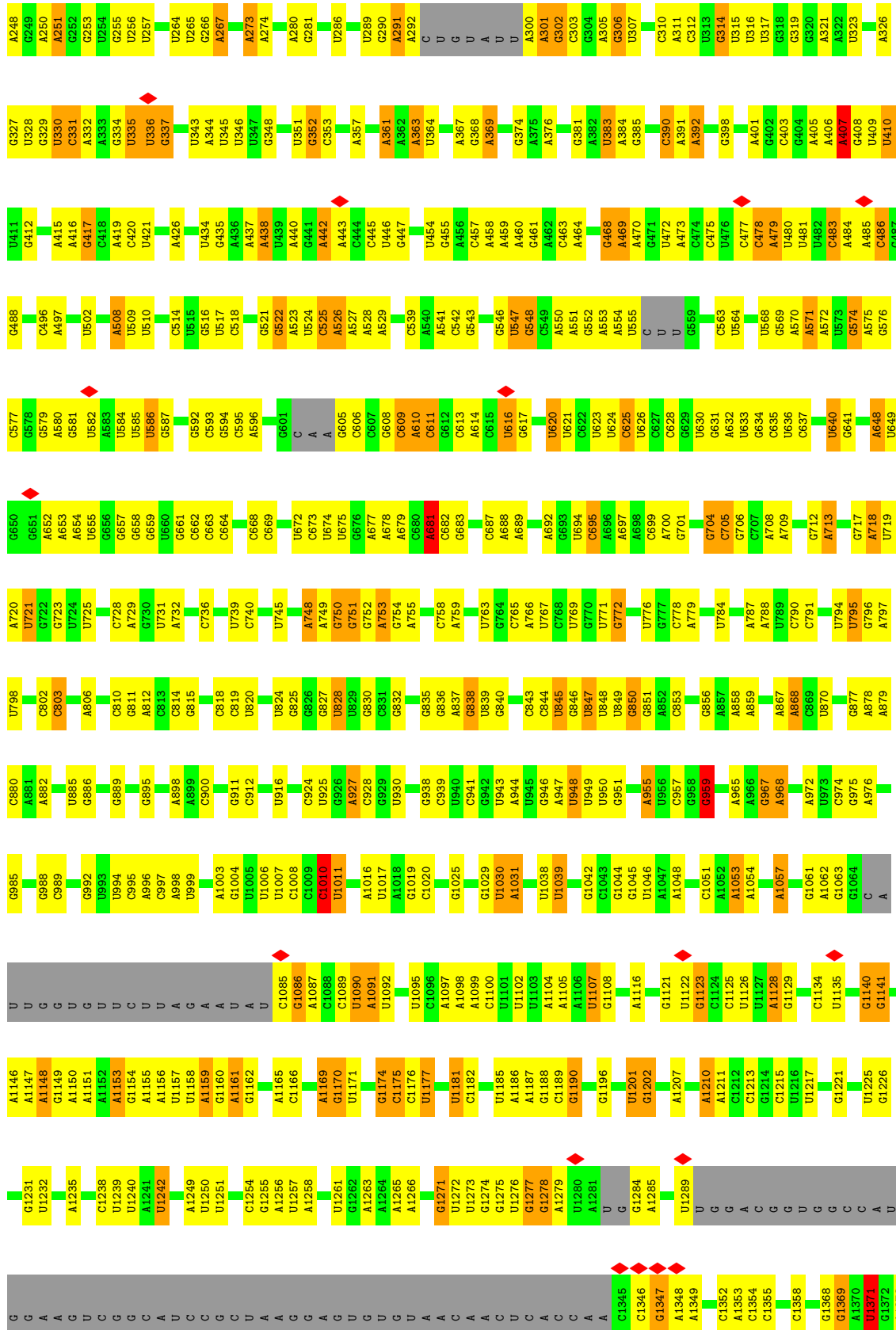
Chain e: 

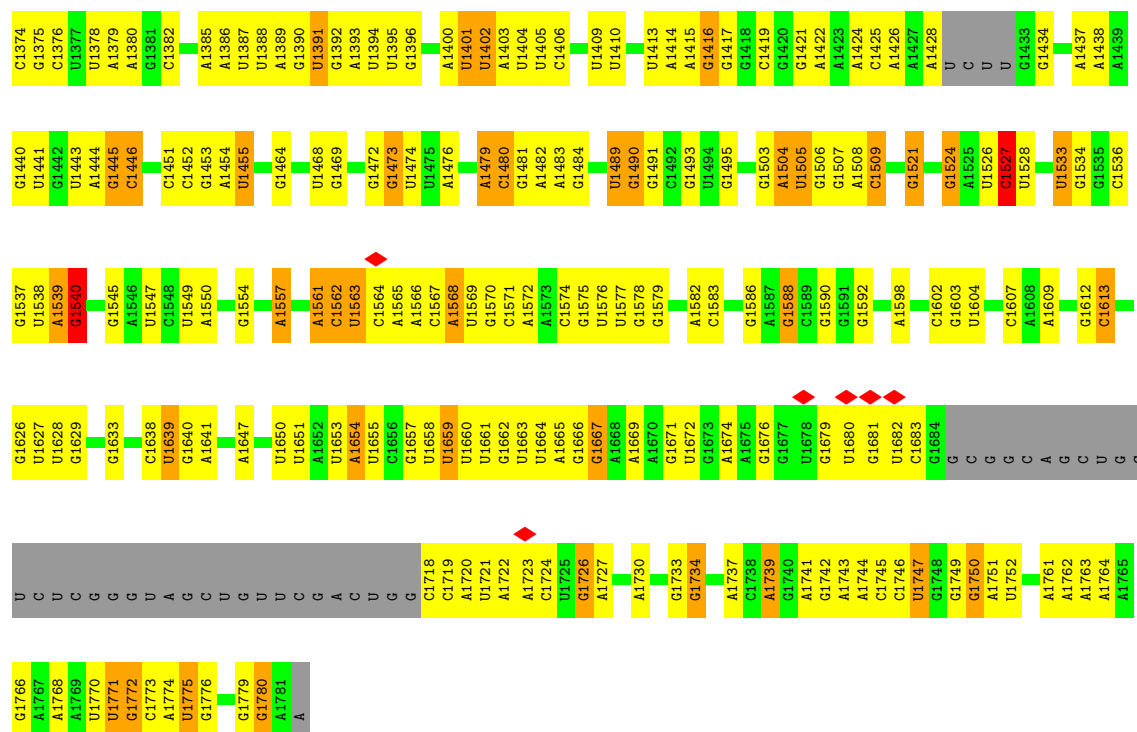


- Molecule 82: RNA (1646-MER)

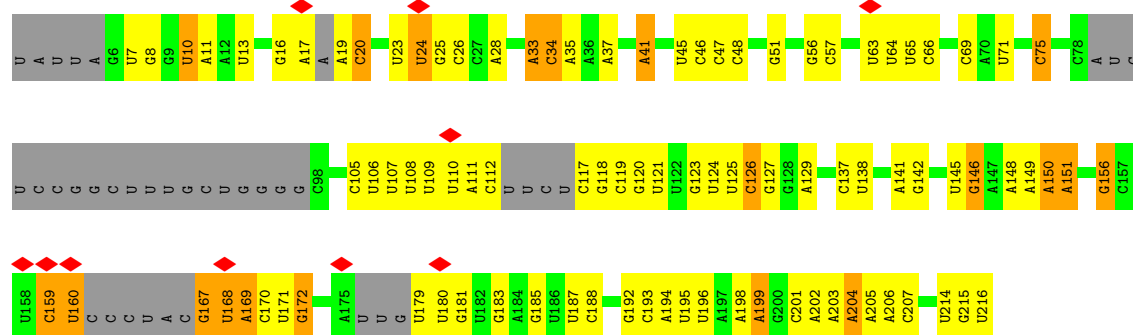
Chain 1: 



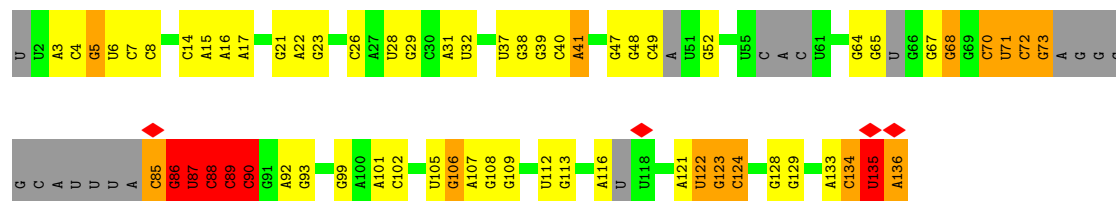




• Molecule 83: SR1_chain_3

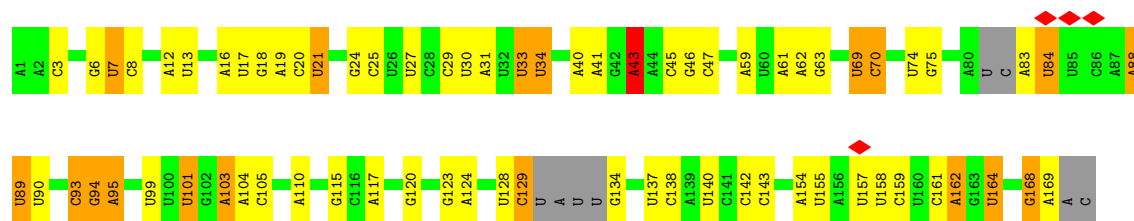


• Molecule 84: SR4_chain_5

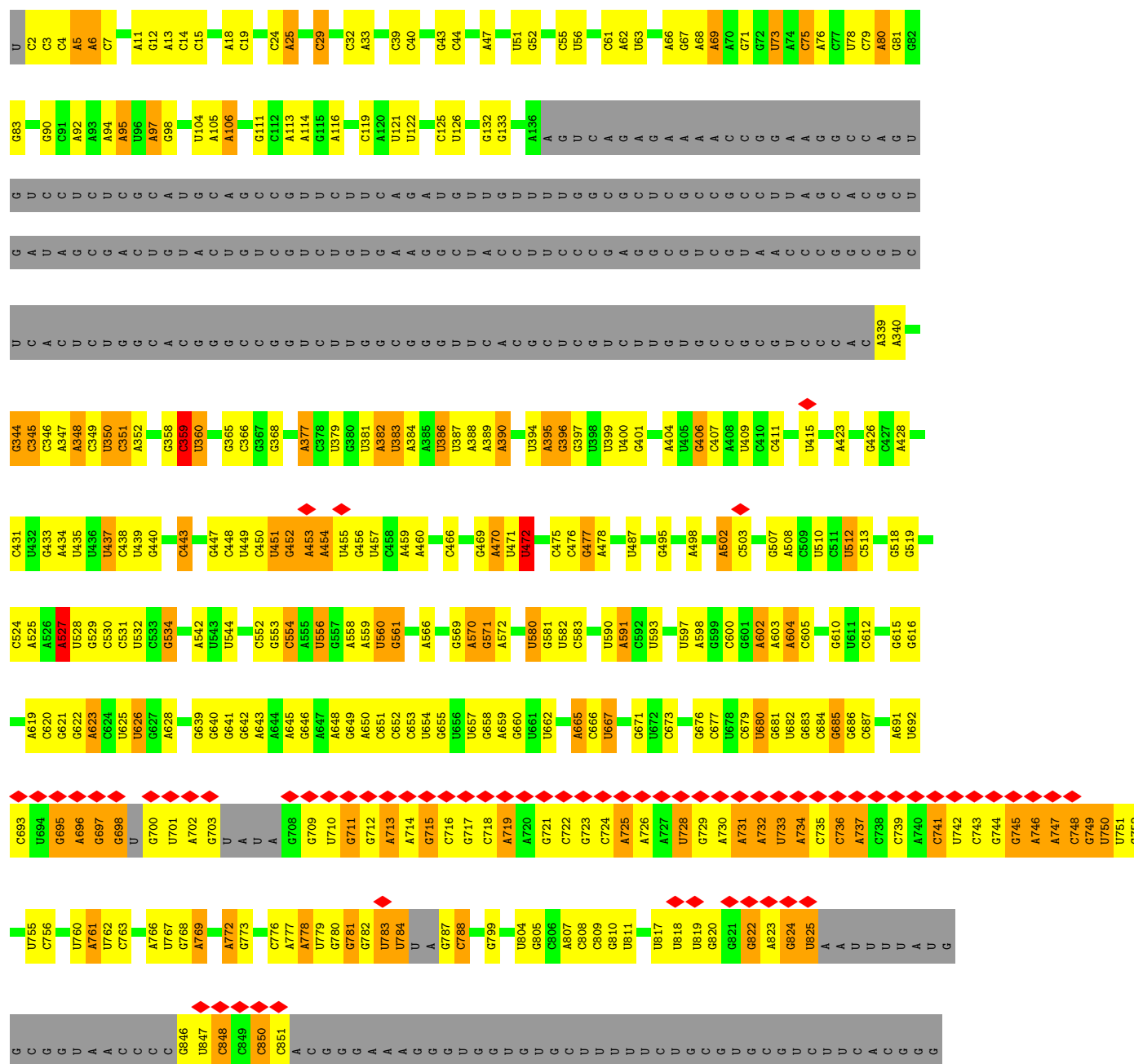


• Molecule 85: 5.8S_rRNA_chain_7





• 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, A2M, MG, PSU, 5MC, MA6, OMU, NA, OMG, 1MA, OMC, C4J, K

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	0.12	0/1660	0.27	0/2246
2	SC	0.11	0/1658	0.23	0/2219
3	SD	0.11	0/1509	0.23	0/2026
4	SE	0.13	0/2088	0.27	0/2814
5	SF	0.13	0/1706	0.25	0/2311
6	SG	0.11	0/1853	0.24	0/2475
7	SH	0.11	0/1458	0.24	0/1955
8	SI	0.12	0/1649	0.25	0/2220
9	SJ	0.13	0/1038	0.26	0/1391
10	SK	0.14	0/1465	0.27	0/1964
11	SL	0.11	0/1145	0.24	0/1540
12	SM	0.12	0/806	0.26	0/1093
13	SN	0.12	0/836	0.26	0/1134
14	SO	0.12	0/1030	0.26	0/1384
15	SP	0.12	0/1120	0.29	0/1500
16	SQ	0.10	0/658	0.33	0/890
17	SR	0.11	0/1099	0.27	0/1477
18	SS	0.13	0/458	0.24	0/607
19	ST	0.15	0/1178	0.27	0/1580
20	SU	0.14	0/1208	0.26	0/1622
21	SV	0.10	0/856	0.21	0/1141
22	SW	0.11	0/945	0.22	0/1271
23	SX	0.12	0/1233	0.24	0/1656
24	SY	0.11	0/650	0.27	0/883
25	SZ	0.11	0/1051	0.22	0/1399
26	Sa	0.12	0/563	0.29	0/757
27	Sb	0.17	0/837	0.27	0/1120
28	Sc	0.20	0/660	0.35	0/888
29	Sd	0.11	0/476	0.23	0/640
30	Se	0.11	0/411	0.24	0/544
31	Sf	0.08	0/544	0.27	0/723
32	Sg	0.11	0/2274	0.27	0/3100

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sh	0.10	0/532	0.27	0/718
34	S4	0.16	0/1613	0.55	6/2506 (0.2%)
35	S1	0.20	3/42994 (0.0%)	0.32	0/66965
36	SA	0.13	0/1848	0.27	0/2487
37	4	0.28	0/4397	0.53	17/6854 (0.2%)
38	6	0.18	0/1683	0.37	0/2618
39	8	0.19	0/2829	0.32	0/4405
40	A	0.17	0/1969	0.32	0/2643
41	B	0.16	0/3212	0.28	0/4324
42	C	0.15	0/2849	0.30	0/3835
43	D	0.13	0/1313	0.28	0/1766
44	E	0.14	0/1492	0.27	0/2011
45	H	0.16	0/1801	0.30	0/2419
46	I	0.15	0/1678	0.32	0/2250
47	J	0.16	0/1013	0.32	0/1367
48	K	0.15	0/1332	0.28	0/1788
49	L	0.16	0/1137	0.32	0/1521
50	M	0.18	0/1744	0.31	0/2329
51	P	0.16	0/1557	0.33	0/2084
52	Q	0.15	0/1546	0.26	0/2047
53	R	0.16	0/1486	0.28	0/2003
54	S	0.17	0/1282	0.29	0/1728
55	T	0.18	0/1239	0.32	0/1660
56	U	0.11	0/80	0.27	0/105
57	V	0.16	0/949	0.27	0/1277
58	W	0.14	0/969	0.29	0/1294
59	X	0.15	0/569	0.27	0/767
60	Y	0.14	0/1069	0.25	0/1434
61	Z	0.15	0/1137	0.26	0/1521
62	a	0.14	0/1039	0.27	0/1379
63	b	0.17	0/557	0.30	0/743
64	c	0.16	0/1900	0.30	0/2544
65	d	0.15	0/715	0.28	0/968
66	f	0.16	0/1043	0.33	0/1395
67	g	0.16	0/1172	0.29	0/1573
68	h	0.15	0/1027	0.29	0/1368
69	i	0.15	0/792	0.27	0/1059
70	j	0.19	0/686	0.34	0/915
71	k	0.13	0/623	0.24	0/833
72	l	0.17	0/463	0.28	0/617
73	m	0.15	0/416	0.28	0/553
74	n	0.21	0/296	0.42	0/386
75	o	0.18	0/701	0.36	0/934

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	p	0.23	0/800	0.38	0/1058
77	F	0.14	0/1140	0.28	0/1546
78	G	0.15	0/1817	0.29	0/2447
79	N	0.15	0/1647	0.30	0/2203
80	O	0.13	0/2164	0.27	0/2904
81	e	0.14	0/1474	0.29	0/1959
82	1	0.23	2/38669 (0.0%)	0.35	1/60289 (0.0%)
83	3	0.21	0/4189	0.34	0/6510
84	5	0.29	0/2785	0.52	7/4330 (0.2%)
85	7	0.24	0/3712	0.32	0/5778
86	2	0.24	1/27120 (0.0%)	0.37	2/42264 (0.0%)
All	All	0.20	6/220388 (0.0%)	0.33	33/323851 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	157	U	C1'-N1	6.48	1.58	1.48
86	2	527	A2M	O3'-P	5.39	1.61	1.56
35	S1	668	A2M	O3'-P	5.31	1.61	1.56
35	S1	29	OMU	O3'-P	5.17	1.61	1.56
82	1	1371	OMU	O3'-P	5.13	1.61	1.56

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	S4	11	C	OP1-P-O3'	-12.17	71.50	108.00
86	2	55	C	OP1-P-O3'	-11.22	74.35	108.00
37	4	8[A]	U	O3'-P-O5'	-11.00	87.50	104.00
37	4	8[B]	U	O3'-P-O5'	-11.00	87.50	104.00
86	2	55	C	OP2-P-O3'	-10.16	77.52	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SB	1627	0	1649	27	0
2	SC	1630	0	1688	19	0
3	SD	1482	0	1542	16	0
4	SE	2050	0	2144	20	0
5	SF	1670	0	1717	24	0
6	SG	1831	0	1955	24	0
7	SH	1436	0	1467	10	0
8	SI	1619	0	1697	29	0
9	SJ	1021	0	1050	17	0
10	SK	1443	0	1524	23	0
11	SL	1124	0	1179	12	0
12	SM	796	0	838	12	0
13	SN	813	0	791	17	0
14	SO	1015	0	1039	19	0
15	SP	1100	0	1146	12	0
16	SQ	656	0	611	11	0
17	SR	1080	0	1118	23	0
18	SS	452	0	462	11	0
19	ST	1155	0	1220	24	0
20	SU	1184	0	1219	14	0
21	SV	850	0	904	16	0
22	SW	925	0	953	14	0
23	SX	1202	0	1227	13	0
24	SY	640	0	635	17	0
25	SZ	1031	0	1105	16	0
26	Sa	558	0	606	15	0
27	Sb	820	0	858	15	0
28	Sc	647	0	639	12	0
29	Sd	474	0	486	7	0
30	Se	405	0	447	3	0
31	Sf	530	0	541	7	0
32	Sg	2219	0	2088	38	0
33	Sh	522	0	493	8	0
34	S4	1447	0	739	19	0
35	S1	39517	0	19970	686	0
36	SA	1820	0	1904	42	0
37	4	3956	0	1999	62	0
38	6	1506	0	768	34	0
39	8	2531	0	1283	38	0
40	A	1927	0	1980	36	0
41	B	3145	0	3244	30	0
42	C	2799	0	2906	38	0
43	D	1290	0	1253	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	E	1472	0	1551	26	0
45	H	1765	0	1872	21	0
46	I	1645	0	1700	22	0
47	J	996	0	1043	11	0
48	K	1313	0	1366	33	0
49	L	1110	0	1132	17	0
50	M	1704	0	1785	26	0
51	P	1532	0	1629	30	0
52	Q	1527	0	1632	27	0
53	R	1452	0	1495	16	0
54	S	1253	0	1289	19	0
55	T	1215	0	1258	11	0
56	U	81	0	83	2	0
57	V	934	0	995	11	0
58	W	955	0	1028	27	0
59	X	548	0	553	6	0
60	Y	1048	0	1099	19	0
61	Z	1121	0	1169	16	0
62	a	1028	0	1131	9	0
63	b	546	0	575	8	0
64	c	1866	0	1970	26	0
65	d	705	0	719	13	0
66	f	1023	0	1076	21	0
67	g	1149	0	1203	26	0
68	h	1011	0	1058	16	0
69	i	777	0	834	13	0
70	j	672	0	688	13	0
71	k	614	0	659	9	0
72	l	450	0	483	10	0
73	m	410	0	450	2	0
74	n	292	0	329	14	0
75	o	689	0	714	15	0
76	p	787	0	848	15	0
77	F	1118	0	1168	16	0
78	G	1792	0	1895	24	0
79	N	1615	0	1678	32	0
80	O	2125	0	2155	25	0
81	e	1456	0	1588	22	0
82	1	35315	0	17805	512	0
83	3	3776	0	1915	70	0
84	5	2496	0	1268	54	0
85	7	3472	0	1762	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	2	25463	0	12895	387	0
87	1	119	0	0	0	0
87	2	97	0	0	0	0
87	3	4	0	0	0	0
87	4	7	0	0	0	0
87	5	1	0	0	0	0
87	6	1	0	0	0	0
87	7	7	0	0	0	0
87	8	6	0	0	0	0
87	B	2	0	0	0	0
87	I	1	0	0	0	0
87	J	1	0	0	0	0
87	N	1	0	0	0	0
87	S	1	0	0	0	0
87	S1	79	0	0	0	0
87	SG	1	0	0	0	0
87	SK	1	0	0	0	0
87	SS	1	0	0	0	0
87	SX	2	0	0	0	0
87	Sb	1	0	0	0	0
87	T	1	0	0	0	0
87	f	1	0	0	0	0
88	1	11	0	0	0	0
88	2	13	0	0	0	0
88	3	1	0	0	0	0
88	4	4	0	0	0	0
88	5	2	0	0	0	0
88	A	1	0	0	0	0
88	B	1	0	0	0	0
88	M	1	0	0	0	0
88	N	1	0	0	0	0
88	S1	11	0	0	0	0
89	1	2	0	0	0	0
89	2	3	0	0	0	0
89	3	1	0	0	0	0
89	5	1	0	0	0	0
89	7	1	0	0	0	0
89	S1	2	0	0	0	0
90	1	135	0	0	2	0
90	2	141	0	0	5	0
90	3	4	0	0	0	0
90	4	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	5	4	0	0	0	0
90	7	6	0	0	1	0
90	8	4	0	0	0	0
90	A	4	0	0	0	0
90	B	4	0	0	0	0
90	E	1	0	0	0	0
90	H	1	0	0	0	0
90	J	1	0	0	0	0
90	S1	44	0	0	2	0
90	T	2	0	0	0	0
90	W	1	0	0	1	0
90	b	1	0	0	0	0
90	h	2	0	0	0	0
90	j	3	0	0	0	0
All	All	209021	0	152629	2716	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2716 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:1:1679:G:N2	82:1:1721:U:O2	1.79	1.13
86:2:382:A2M:C1'	86:2:382:A2M:O4'	1.63	1.11
82:1:164:G:H1	82:1:291:A:N6	1.51	1.07
35:S1:955:A:H61	35:S1:980:G:H1	1.04	0.99
35:S1:694:U:H3	35:S1:751:G:H1	0.99	0.98

There are no symmetry-related clashes.

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	52
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	50
2	SC	171/184 (93%)	165 (96%)	6 (4%)	32	59
3	SD	154/164 (94%)	149 (97%)	5 (3%)	34	62
4	SE	215/225 (96%)	212 (99%)	3 (1%)	59	80
5	SF	175/208 (84%)	173 (99%)	2 (1%)	65	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	SG	189/208 (91%)	183 (97%)	6 (3%)	34	62
7	SH	151/159 (95%)	149 (99%)	2 (1%)	61	81
8	SI	175/186 (94%)	174 (99%)	1 (1%)	78	90
9	SJ	110/111 (99%)	108 (98%)	2 (2%)	51	76
10	SK	141/176 (80%)	135 (96%)	6 (4%)	26	52
11	SL	113/120 (94%)	110 (97%)	3 (3%)	39	68
12	SM	92/104 (88%)	90 (98%)	2 (2%)	45	72
13	SN	86/128 (67%)	81 (94%)	5 (6%)	18	41
14	SO	103/113 (91%)	101 (98%)	2 (2%)	50	75
15	SP	114/117 (97%)	113 (99%)	1 (1%)	70	86
16	SQ	59/120 (49%)	54 (92%)	5 (8%)	10	24
17	SR	111/130 (85%)	108 (97%)	3 (3%)	39	68
18	SS	47/49 (96%)	46 (98%)	1 (2%)	47	73
19	ST	124/132 (94%)	119 (96%)	5 (4%)	28	55
20	SU	125/152 (82%)	120 (96%)	5 (4%)	28	55
21	SV	89/126 (71%)	87 (98%)	2 (2%)	45	72
22	SW	97/130 (75%)	94 (97%)	3 (3%)	35	63
23	SX	121/131 (92%)	116 (96%)	5 (4%)	27	54
24	SY	67/116 (58%)	65 (97%)	2 (3%)	36	64
25	SZ	109/118 (92%)	107 (98%)	2 (2%)	51	76
26	Sa	63/95 (66%)	61 (97%)	2 (3%)	34	62
27	Sb	85/93 (91%)	82 (96%)	3 (4%)	32	59
28	Sc	70/76 (92%)	63 (90%)	7 (10%)	7	18
29	Sd	48/75 (64%)	47 (98%)	1 (2%)	47	73
30	Se	42/54 (78%)	41 (98%)	1 (2%)	43	70
31	Sf	56/126 (44%)	54 (96%)	2 (4%)	31	58
32	Sg	235/265 (89%)	223 (95%)	12 (5%)	21	46
33	Sh	47/177 (27%)	42 (89%)	5 (11%)	6	16
36	SA	197/222 (89%)	189 (96%)	8 (4%)	27	54
40	A	195/204 (96%)	193 (99%)	2 (1%)	68	85
41	B	324/351 (92%)	322 (99%)	2 (1%)	78	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	C	286/301 (95%)	281 (98%)	5 (2%)	53	77
43	D	121/162 (75%)	116 (96%)	5 (4%)	27	54
44	E	164/172 (95%)	156 (95%)	8 (5%)	22	47
45	H	181/188 (96%)	178 (98%)	3 (2%)	53	77
46	I	171/183 (93%)	168 (98%)	3 (2%)	51	76
47	J	103/111 (93%)	102 (99%)	1 (1%)	68	85
48	K	129/145 (89%)	126 (98%)	3 (2%)	44	71
49	L	109/114 (96%)	107 (98%)	2 (2%)	51	76
50	M	176/180 (98%)	172 (98%)	4 (2%)	44	71
51	P	160/164 (98%)	156 (98%)	4 (2%)	42	69
52	Q	152/198 (77%)	148 (97%)	4 (3%)	40	69
53	R	156/159 (98%)	156 (100%)	0	100	100
54	S	130/134 (97%)	126 (97%)	4 (3%)	35	63
55	T	128/143 (90%)	126 (98%)	2 (2%)	55	78
56	U	7/114 (6%)	7 (100%)	0	100	100
57	V	98/124 (79%)	97 (99%)	1 (1%)	68	85
58	W	102/122 (84%)	97 (95%)	5 (5%)	22	47
59	X	58/104 (56%)	56 (97%)	2 (3%)	32	60
60	Y	104/116 (90%)	103 (99%)	1 (1%)	68	85
61	Z	115/118 (98%)	114 (99%)	1 (1%)	70	86
62	a	110/118 (93%)	107 (97%)	3 (3%)	39	68
63	b	56/58 (97%)	54 (96%)	2 (4%)	31	58
64	c	192/209 (92%)	186 (97%)	6 (3%)	35	63
65	d	80/89 (90%)	77 (96%)	3 (4%)	29	56
66	f	108/115 (94%)	106 (98%)	2 (2%)	50	75
67	g	120/121 (99%)	113 (94%)	7 (6%)	18	41
68	h	105/146 (72%)	103 (98%)	2 (2%)	50	75
69	i	79/88 (90%)	77 (98%)	2 (2%)	42	69
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%)	45	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	m	44/113 (39%)	43 (98%)	1 (2%)	44	71
74	n	30/32 (94%)	29 (97%)	1 (3%)	33	61
75	o	70/74 (95%)	66 (94%)	4 (6%)	18	41
76	p	83/92 (90%)	79 (95%)	4 (5%)	23	48
77	F	113/153 (74%)	110 (97%)	3 (3%)	39	68
78	G	183/221 (83%)	179 (98%)	4 (2%)	45	72
79	N	168/179 (94%)	162 (96%)	6 (4%)	31	58
80	O	195/242 (81%)	187 (96%)	8 (4%)	27	54
81	e	152/158 (96%)	146 (96%)	6 (4%)	28	56
All	All	9192/10798 (85%)	8935 (97%)	257 (3%)	38	67

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
77	F	84	VAL
79	N	54	SER
28	Sc	68	THR
28	Sc	53	THR
80	O	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
50	M	117	ASN
62	a	37	GLN
52	Q	143	HIS
57	V	64	ASN
63	b	17	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	S4	64/76 (84%)	31 (48%)	2 (3%)
35	S1	1822/2204 (82%)	444 (24%)	12 (0%)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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	5518/6490 (85%)	1348 (24%)	46 (0%)

5 of 1348 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
82	PSU	1	1171	82	18,21,22	4.42	7 (38%)	22,30,33	1.76	6 (27%)
82	OMU	1	1371	82	19,22,23	3.05	8 (42%)	26,31,34	1.96	7 (26%)
82	OMG	1	1524	82	23,26,27	2.39	9 (39%)	33,38,41	2.45	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	A2M	2	1185	86	22,25,26	3.49	9 (40%)	31,36,39	2.58	12 (38%)
35	A2M	S1	753	35	22,25,26	3.52	8 (36%)	31,36,39	2.40	11 (35%)
82	OMG	1	1540	82,86	23,26,27	2.36	9 (39%)	33,38,41	2.41	11 (33%)
86	OMG	2	1253	86	23,26,27	2.35	9 (39%)	33,38,41	2.43	12 (36%)
35	PSU	S1	1841	35	18,21,22	4.50	7 (38%)	22,30,33	1.81	5 (22%)
82	PSU	1	1181	82	18,21,22	4.50	8 (44%)	22,30,33	2.00	5 (22%)
86	OMC	2	443	87,86,88	19,22,23	2.88	8 (42%)	26,31,34	0.82	0
35	OMU	S1	661	35	19,22,23	3.01	8 (42%)	26,31,34	1.69	5 (19%)
86	OMG	2	1360	86	23,26,27	2.41	9 (39%)	33,38,41	2.53	10 (30%)
35	OMG	S1	1550	35	23,26,27	2.40	9 (39%)	33,38,41	2.46	10 (30%)
86	OMG	2	1229	86	23,26,27	2.37	9 (39%)	33,38,41	2.39	10 (30%)
82	A2M	1	678	82,86	22,25,26	3.52	10 (45%)	31,36,39	2.53	10 (32%)
86	A2M	2	604	82,86	22,25,26	3.53	9 (40%)	31,36,39	2.42	11 (35%)
35	5MC	S1	1544	35	18,22,23	3.58	7 (38%)	26,32,35	1.03	1 (3%)
82	A2M	1	1539	82,87,86	22,25,26	3.47	10 (45%)	31,36,39	2.41	11 (35%)
86	OMC	2	1397	86	19,22,23	2.95	8 (42%)	26,31,34	0.79	0
86	OMG	2	1078	86	23,26,27	2.34	9 (39%)	33,38,41	2.29	12 (36%)
35	PSU	S1	12	35	18,21,22	4.45	7 (38%)	22,30,33	1.76	5 (22%)
82	A2M	1	305	82	22,25,26	3.40	10 (45%)	31,36,39	2.58	11 (35%)
82	PSU	1	1528	82	18,21,22	4.51	7 (38%)	22,30,33	1.98	5 (22%)
86	PSU	2	1144	86	18,21,22	4.60	8 (44%)	22,30,33	1.91	4 (18%)
86	OMC	2	1317	86	19,22,23	3.02	8 (42%)	26,31,34	0.98	1 (3%)
86	PSU	2	1318	86	18,21,22	4.51	7 (38%)	22,30,33	1.99	6 (27%)
86	PSU	2	597	86	18,21,22	4.48	7 (38%)	22,30,33	2.06	5 (22%)
35	OMC	S1	2140	35	19,22,23	2.98	8 (42%)	26,31,34	0.81	0
86	OMU	2	1077	86	19,22,23	3.04	8 (42%)	26,31,34	1.68	4 (15%)
82	PSU	1	870	82,87	18,21,22	4.45	7 (38%)	22,30,33	2.02	5 (22%)
86	PSU	2	626	86	18,21,22	4.43	7 (38%)	22,30,33	1.72	4 (18%)
35	PSU	S1	104	35	18,21,22	4.49	7 (38%)	22,30,33	1.71	5 (22%)
86	OMG	2	71	86	23,26,27	2.39	9 (39%)	33,38,41	2.44	12 (36%)
86	PSU	2	1060	86	18,21,22	4.48	7 (38%)	22,30,33	2.07	5 (22%)
86	OMU	2	1419	86	19,22,23	2.96	8 (42%)	26,31,34	1.66	4 (15%)
86	OMC	2	583	86	19,22,23	3.04	8 (42%)	26,31,34	0.84	1 (3%)
82	OMU	1	1659	82,87	19,22,23	3.01	8 (42%)	26,31,34	1.68	4 (15%)
86	OMC	2	359	86	19,22,23	3.01	8 (42%)	26,31,34	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OMG	1	1190	82,87	23,26,27	2.32	9 (39%)	33,38,41	2.34	13 (39%)
82	PSU	1	1664	82	18,21,22	4.51	7 (38%)	22,30,33	1.75	5 (22%)
86	A2M	2	570	82,86	22,25,26	3.39	9 (40%)	31,36,39	2.53	12 (38%)
35	OMC	S1	38	35	19,22,23	2.97	8 (42%)	26,31,34	0.76	0
35	OMC	S1	1866	35	19,22,23	2.97	8 (42%)	26,31,34	0.81	0
35	A2M	S1	912	35	22,25,26	3.53	9 (40%)	31,36,39	2.55	13 (41%)
82	A2M	1	681	82	22,25,26	3.48	9 (40%)	31,36,39	2.42	11 (35%)
82	OMG	1	856	82	23,26,27	2.37	9 (39%)	33,38,41	2.38	13 (39%)
35	MA6	S1	2185	35	23,26,27	1.42	4 (17%)	34,38,41	3.11	12 (35%)
35	PSU	S1	2046	35	18,21,22	4.53	7 (38%)	22,30,33	1.94	4 (18%)
86	PSU	2	472	86	18,21,22	4.52	8 (44%)	22,30,33	1.78	4 (18%)
86	OMG	2	655	86	23,26,27	2.38	9 (39%)	33,38,41	2.37	9 (27%)
35	OMU	S1	1979	35	19,22,23	3.01	8 (42%)	26,31,34	1.72	5 (19%)
82	A2M	1	858	82	22,25,26	3.43	10 (45%)	31,36,39	2.57	13 (41%)
82	PSU	1	1177	82	18,21,22	4.47	7 (38%)	22,30,33	1.80	5 (22%)
86	OMC	2	1248	86	19,22,23	2.97	8 (42%)	26,31,34	0.87	1 (3%)
35	A2M	S1	897	35	22,25,26	3.48	10 (45%)	31,36,39	2.48	12 (38%)
86	PSU	2	437	86,88	18,21,22	4.47	8 (44%)	22,30,33	1.81	5 (22%)
82	A2M	1	235	82	22,25,26	3.52	9 (40%)	31,36,39	2.53	11 (35%)
35	A2M	S1	98	35,87	22,25,26	3.46	9 (40%)	31,36,39	2.28	10 (32%)
35	7MG	S1	1995	35	22,26,27	4.28	10 (45%)	29,39,42	2.03	9 (31%)
35	PSU	S1	1566	35	18,21,22	4.47	8 (44%)	22,30,33	1.68	4 (18%)
35	A2M	S1	479	35	22,25,26	3.37	9 (40%)	31,36,39	2.31	10 (32%)
82	PSU	1	1011	82,86	18,21,22	4.38	9 (50%)	22,30,33	1.73	6 (27%)
86	OMC	2	1159	86	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
82	A2M	1	927	82	22,25,26	3.52	9 (40%)	31,36,39	2.54	11 (35%)
86	OMG	2	1231	86	23,26,27	2.38	9 (39%)	33,38,41	2.43	10 (30%)
35	PSU	S1	2048	35	18,21,22	4.48	7 (38%)	22,30,33	2.06	5 (22%)
82	PSU	1	1017	82	18,21,22	4.44	7 (38%)	22,30,33	1.86	5 (22%)
35	OMU	S1	8	35	19,22,23	2.96	8 (42%)	26,31,34	1.81	5 (19%)
82	1MA	1	677	82,87	21,25,26	2.84	7 (33%)	31,37,40	2.86	9 (29%)
35	OMC	S1	115	35	19,22,23	2.96	8 (42%)	26,31,34	0.71	0
35	A2M	S1	668	35,87	22,25,26	3.32	9 (40%)	31,36,39	2.48	12 (38%)
86	OMG	2	1046	86	23,26,27	2.32	9 (39%)	33,38,41	2.32	10 (30%)
86	5MC	2	524	87,86	18,22,23	3.50	7 (38%)	26,32,35	1.04	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	A2M	7	43	85	22,25,26	3.52	9 (40%)	31,36,39	2.55	13 (41%)
35	OMC	S1	18	35	19,22,23	2.95	8 (42%)	26,31,34	0.74	0
86	A2M	2	382	86	22,25,26	3.57	8 (36%)	31,36,39	2.37	11 (35%)
35	OMG	S1	1829	35,87	23,26,27	2.38	9 (39%)	33,38,41	2.49	10 (30%)
82	OMC	1	695	82	19,22,23	2.91	8 (42%)	26,31,34	0.68	0
35	PSU	S1	1657	35	18,21,22	4.43	7 (38%)	22,30,33	1.70	3 (13%)
35	A2M	S1	512	35,87	22,25,26	3.50	10 (45%)	31,36,39	2.51	10 (32%)
35	OMU	S1	1833	35	19,22,23	3.04	8 (42%)	26,31,34	1.82	5 (19%)
35	MA6	S1	2184	35	23,26,27	1.43	4 (17%)	34,38,41	2.99	12 (35%)
86	5MC	2	1308	86,88	18,22,23	4.65	13 (72%)	26,32,35	1.32	2 (7%)
82	OMU	1	1107	82	19,22,23	2.98	8 (42%)	26,31,34	1.74	5 (19%)
82	OMU	1	845	82	19,22,23	2.98	8 (42%)	26,31,34	2.24	8 (30%)
86	A2M	2	527	87,86	22,25,26	3.33	9 (40%)	31,36,39	2.65	12 (38%)
86	OMG	2	534	86	23,26,27	2.38	9 (39%)	33,38,41	2.48	10 (30%)
35	OMG	S1	1478	35	23,26,27	2.34	9 (39%)	33,38,41	2.44	12 (36%)
85	A2M	7	162	82,85	22,25,26	3.52	10 (45%)	31,36,39	2.50	11 (35%)
35	A2M	S1	969	35	22,25,26	3.43	8 (36%)	31,36,39	2.54	12 (38%)
37	OMG	4	74	37	23,26,27	2.35	9 (39%)	33,38,41	2.36	11 (33%)
35	OMC	S1	2059	35	19,22,23	2.97	8 (42%)	26,31,34	1.16	2 (7%)
35	OMG	S1	2151	35	23,26,27	2.38	9 (39%)	33,38,41	2.51	10 (30%)
86	A2M	2	591	86	22,25,26	3.53	9 (40%)	31,36,39	2.46	11 (35%)
86	PSU	2	512	86	18,21,22	4.51	7 (38%)	22,30,33	1.83	5 (22%)
86	OMU	2	667	86	19,22,23	3.04	8 (42%)	26,31,34	1.74	4 (15%)
35	5MC	S1	2061	35	18,22,23	3.55	7 (38%)	26,32,35	1.03	2 (7%)
35	PSU	S1	33	35	18,21,22	4.61	8 (44%)	22,30,33	1.82	3 (13%)
35	OMG	S1	1865	35	23,26,27	2.42	9 (39%)	33,38,41	2.47	10 (30%)
82	PSU	1	1533	82,86	18,21,22	4.49	7 (38%)	22,30,33	1.82	6 (27%)
82	A2M	1	407	82,87	22,25,26	3.43	10 (45%)	31,36,39	2.36	13 (41%)
35	PSU	S1	1246	35	18,21,22	4.45	7 (38%)	22,30,33	1.83	5 (22%)
86	PSU	2	593	86	18,21,22	4.36	7 (38%)	22,30,33	1.71	5 (22%)
86	A2M	2	95	86	22,25,26	3.53	9 (40%)	31,36,39	2.47	12 (38%)
86	PSU	2	1361	86	18,21,22	4.49	7 (38%)	22,30,33	1.82	4 (18%)
86	PSU	2	78	86	18,21,22	4.49	7 (38%)	22,30,33	1.99	4 (18%)
85	OMG	7	75	85	23,26,27	2.40	9 (39%)	33,38,41	2.43	10 (30%)
86	A2M	2	1384	87,86	22,25,26	3.40	9 (40%)	31,36,39	2.35	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PSU	2	510	86	18,21,22	4.51	7 (38%)	22,30,33	1.76	5 (22%)
82	A2M	1	697	82	22,25,26	3.52	9 (40%)	31,36,39	2.42	11 (35%)
86	PSU	2	1264	86	18,21,22	4.41	7 (38%)	22,30,33	1.79	6 (27%)
86	PSU	2	1058	86	18,21,22	4.46	7 (38%)	22,30,33	2.13	5 (22%)
35	OMU	S1	29	35	19,22,23	3.01	8 (42%)	26,31,34	1.69	4 (15%)
86	PSU	2	1382	87,86,88	18,21,22	4.42	8 (44%)	22,30,33	2.06	6 (27%)
86	PSU	2	1265	87,86	18,21,22	4.45	7 (38%)	22,30,33	1.84	5 (22%)
35	OMU	S1	1621	35,87	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
35	A2M	S1	918	35	22,25,26	3.42	8 (36%)	31,36,39	2.45	12 (38%)
35	OMG	S1	600	35	23,26,27	2.40	9 (39%)	33,38,41	2.49	10 (30%)
82	OMU	1	847	82	19,22,23	3.00	8 (42%)	26,31,34	1.77	5 (19%)
86	OMU	2	1359	86	19,22,23	3.03	8 (42%)	26,31,34	1.73	4 (15%)
35	A2M	S1	28	35,87	22,25,26	3.44	9 (40%)	31,36,39	2.33	10 (32%)
85	PSU	7	101	85	18,21,22	4.44	7 (38%)	22,30,33	1.82	6 (27%)
86	PSU	2	1413	87,86	18,21,22	4.41	7 (38%)	22,30,33	1.75	4 (18%)
83	OMU	3	13	83	19,22,23	3.01	8 (42%)	26,31,34	1.72	4 (15%)
35	PSU	S1	1533	35	18,21,22	4.46	7 (38%)	22,30,33	1.85	5 (22%)
86	A2M	2	1372	86	22,25,26	3.52	9 (40%)	31,36,39	2.33	9 (29%)
35	OMG	S1	1623	35	23,26,27	2.38	9 (39%)	33,38,41	2.52	11 (33%)
35	A2M	S1	2021	35	22,25,26	3.39	9 (40%)	31,36,39	2.45	11 (35%)
85	PSU	7	69	85	18,21,22	4.48	9 (50%)	22,30,33	1.69	4 (18%)
85	PSU	7	74	85	18,21,22	4.49	7 (38%)	22,30,33	1.76	5 (22%)
82	PSU	1	1039	82	18,21,22	4.52	7 (38%)	22,30,33	1.73	4 (18%)
86	A2M	2	572	86	22,25,26	3.51	10 (45%)	31,36,39	2.47	10 (32%)
82	A2M	1	955	82	22,25,26	3.48	10 (45%)	31,36,39	2.46	11 (35%)
35	PSU	S1	1539	35	18,21,22	4.47	7 (38%)	22,30,33	1.72	4 (18%)
82	OMG	1	959	82	23,26,27	2.38	9 (39%)	33,38,41	2.57	10 (30%)
35	C4J	S1	1543	35	24,29,30	2.96	8 (33%)	29,42,45	1.28	2 (6%)
82	PSU	1	672	82,87	18,21,22	4.47	7 (38%)	22,30,33	1.88	6 (27%)
86	PSU	2	1194	86	18,21,22	4.45	7 (38%)	22,30,33	1.66	4 (18%)
35	PSU	S1	609	35	18,21,22	4.51	7 (38%)	22,30,33	1.80	5 (22%)
86	PSU	2	662	87,86	18,21,22	4.43	7 (38%)	22,30,33	1.79	5 (22%)
86	A2M	2	628	86	22,25,26	3.48	10 (45%)	31,36,39	2.40	11 (35%)
82	OMG	1	1626	82	23,26,27	2.39	9 (39%)	33,38,41	2.45	10 (30%)
86	PSU	2	1403	86	18,21,22	4.52	7 (38%)	22,30,33	1.79	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OMU	7	7	82,85	19,22,23	3.03	8 (42%)	26,31,34	1.71	4 (15%)
86	OMG	2	641	87,86	23,26,27	2.35	9 (39%)	33,38,41	2.37	14 (42%)
82	OMC	1	1527	82	19,22,23	2.97	8 (42%)	26,31,34	0.80	0
82	OMC	1	1010	82,87	19,22,23	2.95	8 (42%)	26,31,34	0.86	1 (3%)
86	OMU	2	560	87,86	19,22,23	2.97	8 (42%)	26,31,34	1.79	5 (19%)
86	PSU	2	1303	86	18,21,22	4.51	7 (38%)	22,30,33	2.17	6 (27%)
35	OMG	S1	1647	35	23,26,27	2.39	9 (39%)	33,38,41	2.43	12 (36%)
86	OMU	2	73	86	19,22,23	2.95	8 (42%)	26,31,34	1.55	4 (15%)

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
82	PSU	1	1171	82	-	0/7/25/26	0/2/2/2
82	OMU	1	1371	82	-	4/9/27/28	0/2/2/2
82	OMG	1	1524	82	-	1/9/27/28	0/3/3/3
86	A2M	2	1185	86	-	3/9/27/28	0/3/3/3
35	A2M	S1	753	35	-	0/9/27/28	0/3/3/3
82	OMG	1	1540	82,86	-	2/9/27/28	0/3/3/3
86	OMG	2	1253	86	-	0/9/27/28	0/3/3/3
35	PSU	S1	1841	35	-	0/7/25/26	0/2/2/2
82	PSU	1	1181	82	-	2/7/25/26	0/2/2/2
86	OMC	2	443	87,86,88	-	4/9/27/28	0/2/2/2
35	OMU	S1	661	35	-	0/9/27/28	0/2/2/2
86	OMG	2	1360	86	-	0/9/27/28	0/3/3/3
35	OMG	S1	1550	35	-	0/9/27/28	0/3/3/3
86	OMG	2	1229	86	-	0/9/27/28	0/3/3/3
82	A2M	1	678	82,86	-	0/9/27/28	0/3/3/3
86	A2M	2	604	82,86	-	0/9/27/28	0/3/3/3
35	5MC	S1	1544	35	-	0/7/25/26	0/2/2/2
82	A2M	1	1539	82,87,86	-	0/9/27/28	0/3/3/3
86	OMC	2	1397	86	-	0/9/27/28	0/2/2/2
86	OMG	2	1078	86	-	1/9/27/28	0/3/3/3
35	PSU	S1	12	35	-	0/7/25/26	0/2/2/2
82	A2M	1	305	82	-	0/9/27/28	0/3/3/3
82	PSU	1	1528	82	-	0/7/25/26	0/2/2/2
86	PSU	2	1144	86	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OMC	2	1317	86	-	0/9/27/28	0/2/2/2
86	PSU	2	1318	86	-	0/7/25/26	0/2/2/2
86	PSU	2	597	86	-	0/7/25/26	0/2/2/2
35	OMC	S1	2140	35	-	0/9/27/28	0/2/2/2
86	OMU	2	1077	86	-	0/9/27/28	0/2/2/2
82	PSU	1	870	82,87	-	0/7/25/26	0/2/2/2
86	PSU	2	626	86	-	0/7/25/26	0/2/2/2
35	PSU	S1	104	35	-	0/7/25/26	0/2/2/2
86	OMG	2	71	86	-	0/9/27/28	0/3/3/3
86	PSU	2	1060	86	-	0/7/25/26	0/2/2/2
86	OMU	2	1419	86	-	1/9/27/28	0/2/2/2
86	OMC	2	583	86	-	0/9/27/28	0/2/2/2
82	OMU	1	1659	82,87	-	0/9/27/28	0/2/2/2
86	OMC	2	359	86	-	2/9/27/28	0/2/2/2
82	OMG	1	1190	82,87	-	0/9/27/28	0/3/3/3
82	PSU	1	1664	82	-	0/7/25/26	0/2/2/2
86	A2M	2	570	82,86	-	4/9/27/28	0/3/3/3
35	OMC	S1	38	35	-	0/9/27/28	0/2/2/2
35	OMC	S1	1866	35	-	3/9/27/28	0/2/2/2
35	A2M	S1	912	35	-	1/9/27/28	0/3/3/3
82	A2M	1	681	82	-	3/9/27/28	0/3/3/3
82	OMG	1	856	82	-	0/9/27/28	0/3/3/3
35	MA6	S1	2185	35	-	3/11/29/30	0/3/3/3
35	PSU	S1	2046	35	-	0/7/25/26	0/2/2/2
86	PSU	2	472	86	-	2/7/25/26	0/2/2/2
86	OMG	2	655	86	-	0/9/27/28	0/3/3/3
35	OMU	S1	1979	35	-	0/9/27/28	0/2/2/2
82	A2M	1	858	82	-	2/9/27/28	0/3/3/3
82	PSU	1	1177	82	-	0/7/25/26	0/2/2/2
86	OMC	2	1248	86	-	1/9/27/28	0/2/2/2
35	A2M	S1	897	35	-	0/9/27/28	0/3/3/3
86	PSU	2	437	86,88	-	2/7/25/26	0/2/2/2
82	A2M	1	235	82	-	0/9/27/28	0/3/3/3
35	A2M	S1	98	35,87	-	3/9/27/28	0/3/3/3
35	7MG	S1	1995	35	-	2/7/37/38	0/3/3/3
35	PSU	S1	1566	35	-	2/7/25/26	0/2/2/2
35	A2M	S1	479	35	-	0/9/27/28	0/3/3/3
82	PSU	1	1011	82,86	-	2/7/25/26	0/2/2/2
86	OMC	2	1159	86	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	A2M	1	927	82	-	1/9/27/28	0/3/3/3
86	OMG	2	1231	86	-	0/9/27/28	0/3/3/3
35	PSU	S1	2048	35	-	0/7/25/26	0/2/2/2
82	PSU	1	1017	82	-	0/7/25/26	0/2/2/2
35	OMU	S1	8	35	-	4/9/27/28	0/2/2/2
82	1MA	1	677	82,87	-	1/7/25/26	0/3/3/3
35	OMC	S1	115	35	-	0/9/27/28	0/2/2/2
35	A2M	S1	668	35,87	-	5/9/27/28	0/3/3/3
86	OMG	2	1046	86	-	1/9/27/28	0/3/3/3
86	5MC	2	524	87,86	-	0/7/25/26	0/2/2/2
85	A2M	7	43	85	-	2/9/27/28	0/3/3/3
35	OMC	S1	18	35	-	0/9/27/28	0/2/2/2
86	A2M	2	382	86	-	0/9/27/28	0/3/3/3
35	OMG	S1	1829	35,87	-	3/9/27/28	0/3/3/3
82	OMC	1	695	82	-	1/9/27/28	0/2/2/2
35	PSU	S1	1657	35	-	2/7/25/26	0/2/2/2
35	A2M	S1	512	35,87	-	2/9/27/28	0/3/3/3
35	OMU	S1	1833	35	-	2/9/27/28	0/2/2/2
35	MA6	S1	2184	35	-	0/11/29/30	0/3/3/3
86	5MC	2	1308	86,88	-	4/7/25/26	0/2/2/2
82	OMU	1	1107	82	-	2/9/27/28	0/2/2/2
82	OMU	1	845	82	-	3/9/27/28	0/2/2/2
86	A2M	2	527	87,86	-	2/9/27/28	0/3/3/3
86	OMG	2	534	86	-	2/9/27/28	0/3/3/3
35	OMG	S1	1478	35	-	1/9/27/28	0/3/3/3
85	A2M	7	162	82,85	-	2/9/27/28	0/3/3/3
35	A2M	S1	969	35	-	2/9/27/28	0/3/3/3
37	OMG	4	74	37	-	2/9/27/28	0/3/3/3
35	OMC	S1	2059	35	-	2/9/27/28	0/2/2/2
35	OMG	S1	2151	35	-	0/9/27/28	0/3/3/3
86	A2M	2	591	86	-	0/9/27/28	0/3/3/3
86	PSU	2	512	86	-	0/7/25/26	0/2/2/2
86	OMU	2	667	86	-	1/9/27/28	0/2/2/2
35	5MC	S1	2061	35	-	2/7/25/26	0/2/2/2
35	PSU	S1	33	35	-	2/7/25/26	0/2/2/2
35	OMG	S1	1865	35	-	0/9/27/28	0/3/3/3
82	PSU	1	1533	82,86	-	0/7/25/26	0/2/2/2
82	A2M	1	407	82,87	-	3/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	S1	1246	35	-	0/7/25/26	0/2/2/2
86	PSU	2	593	86	-	0/7/25/26	0/2/2/2
86	A2M	2	95	86	-	0/9/27/28	0/3/3/3
86	PSU	2	1361	86	-	1/7/25/26	0/2/2/2
86	PSU	2	78	86	-	0/7/25/26	0/2/2/2
85	OMG	7	75	85	-	0/9/27/28	0/3/3/3
86	A2M	2	1384	87,86	-	1/9/27/28	0/3/3/3
86	PSU	2	510	86	-	0/7/25/26	0/2/2/2
82	A2M	1	697	82	-	0/9/27/28	0/3/3/3
86	PSU	2	1264	86	-	0/7/25/26	0/2/2/2
86	PSU	2	1058	86	-	0/7/25/26	0/2/2/2
35	OMU	S1	29	35	-	1/9/27/28	0/2/2/2
86	PSU	2	1382	87,86,88	-	0/7/25/26	0/2/2/2
86	PSU	2	1265	87,86	-	0/7/25/26	0/2/2/2
35	OMU	S1	1621	35,87	-	1/9/27/28	0/2/2/2
35	A2M	S1	918	35	-	4/9/27/28	0/3/3/3
35	OMG	S1	600	35	-	2/9/27/28	0/3/3/3
82	OMU	1	847	82	-	0/9/27/28	0/2/2/2
86	OMU	2	1359	86	-	0/9/27/28	0/2/2/2
35	A2M	S1	28	35,87	-	1/9/27/28	0/3/3/3
85	PSU	7	101	85	-	0/7/25/26	0/2/2/2
86	PSU	2	1413	87,86	-	0/7/25/26	0/2/2/2
83	OMU	3	13	83	-	1/9/27/28	0/2/2/2
35	PSU	S1	1533	35	-	0/7/25/26	0/2/2/2
86	A2M	2	1372	86	-	0/9/27/28	0/3/3/3
35	OMG	S1	1623	35	-	0/9/27/28	0/3/3/3
35	A2M	S1	2021	35	-	3/9/27/28	0/3/3/3
85	PSU	7	69	85	-	2/7/25/26	0/2/2/2
85	PSU	7	74	85	-	0/7/25/26	0/2/2/2
82	PSU	1	1039	82	-	1/7/25/26	0/2/2/2
86	A2M	2	572	86	-	0/9/27/28	0/3/3/3
82	A2M	1	955	82	-	1/9/27/28	0/3/3/3
35	PSU	S1	1539	35	-	1/7/25/26	0/2/2/2
82	OMG	1	959	82	-	2/9/27/28	0/3/3/3
35	C4J	S1	1543	35	-	7/16/34/35	0/2/2/2
82	PSU	1	672	82,87	-	0/7/25/26	0/2/2/2
86	PSU	2	1194	86	-	0/7/25/26	0/2/2/2
35	PSU	S1	609	35	-	0/7/25/26	0/2/2/2
86	PSU	2	662	87,86	-	0/7/25/26	0/2/2/2
86	A2M	2	628	86	-	0/9/27/28	0/3/3/3
82	OMG	1	1626	82	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PSU	2	1403	86	-	0/7/25/26	0/2/2/2
85	OMU	7	7	82,85	-	1/9/27/28	0/2/2/2
86	OMG	2	641	87,86	-	0/9/27/28	0/3/3/3
82	OMC	1	1527	82	-	2/9/27/28	0/2/2/2
82	OMC	1	1010	82,87	-	1/9/27/28	0/2/2/2
86	OMU	2	560	87,86	-	1/9/27/28	0/2/2/2
86	PSU	2	1303	86	-	0/7/25/26	0/2/2/2
35	OMG	S1	1647	35	-	0/9/27/28	0/3/3/3
86	OMU	2	73	86	-	1/9/27/28	0/2/2/2

The worst 5 of 1234 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	2	1144	PSU	C6-C5	12.05	1.49	1.35
35	S1	33	PSU	C6-C5	12.00	1.49	1.35
86	2	472	PSU	C6-C5	11.90	1.49	1.35
82	1	1039	PSU	C6-C5	11.83	1.49	1.35
86	2	437	PSU	C6-C5	11.78	1.49	1.35

The worst 5 of 1042 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S1	2185	MA6	N1-C6-N6	-11.84	104.14	117.08
35	S1	2184	MA6	N1-C6-N6	-11.08	104.97	117.08
82	1	677	1MA	C1'-N9-C8	-9.02	101.02	126.70
82	1	677	1MA	C1'-N9-C4	8.65	152.21	126.50
82	1	959	OMG	C1'-N9-C8	-8.14	103.52	126.70

There are no chirality outliers.

5 of 141 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
82	1	845	OMU	O4'-C1'-N1-C6

There are no ring outliers.

73 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	1371	OMU	1	0
82	1	1524	OMG	1	0
35	S1	753	A2M	3	0
82	1	1540	OMG	1	0
86	2	1253	OMG	2	0
35	S1	1841	PSU	1	0
86	2	443	OMC	1	0
35	S1	661	OMU	1	0
86	2	1360	OMG	1	0
35	S1	1550	OMG	2	0
86	2	604	A2M	2	0
82	1	1539	A2M	1	0
86	2	1397	OMC	1	0
86	2	1078	OMG	1	0
35	S1	12	PSU	1	0
86	2	1144	PSU	1	0
86	2	1317	OMC	1	0
86	2	626	PSU	1	0
86	2	1419	OMU	1	0
82	1	1659	OMU	2	0
86	2	359	OMC	1	0
82	1	1190	OMG	2	0
86	2	570	A2M	3	0
35	S1	912	A2M	2	0
82	1	681	A2M	1	0
35	S1	2185	MA6	1	0
86	2	472	PSU	2	0
82	1	1177	PSU	1	0
35	S1	897	A2M	1	0
35	S1	1995	7MG	2	0
35	S1	479	A2M	2	0
82	1	927	A2M	1	0
35	S1	115	OMC	1	0
35	S1	668	A2M	1	0
86	2	1046	OMG	1	0
85	7	43	A2M	2	0
35	S1	18	OMC	1	0
86	2	382	A2M	5	0
82	1	695	OMC	2	0
35	S1	512	A2M	1	0
35	S1	2184	MA6	2	0
86	2	1308	5MC	1	0
82	1	845	OMU	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	527	A2M	1	0
85	7	162	A2M	2	0
35	S1	969	A2M	1	0
35	S1	2059	OMC	1	0
86	2	591	A2M	2	0
86	2	512	PSU	2	0
86	2	667	OMU	1	0
35	S1	2061	5MC	1	0
82	1	1533	PSU	1	0
82	1	407	A2M	1	0
86	2	95	A2M	1	0
86	2	1384	A2M	2	0
35	S1	29	OMU	2	0
35	S1	1621	OMU	1	0
82	1	847	OMU	1	0
35	S1	28	A2M	2	0
85	7	101	PSU	1	0
86	2	1413	PSU	1	0
86	2	1372	A2M	1	0
35	S1	2021	A2M	1	0
82	1	1039	PSU	1	0
82	1	955	A2M	1	0
35	S1	1539	PSU	2	0
82	1	959	OMG	1	0
35	S1	1543	C4J	1	0
85	7	7	OMU	2	0
82	1	1527	OMC	4	0
82	1	1010	OMC	1	0
86	2	560	OMU	2	0
86	2	73	OMU	1	0

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

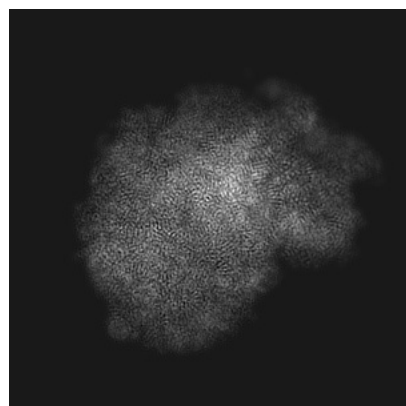
6 Map visualisation [i](#)

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.

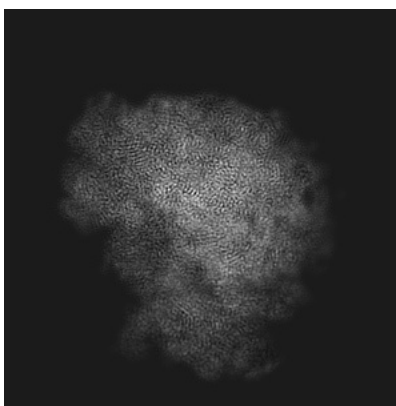
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

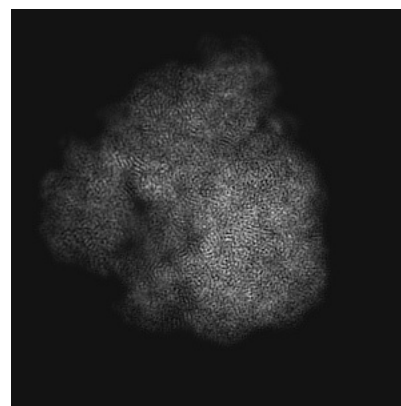
6.1.1 Primary map



X

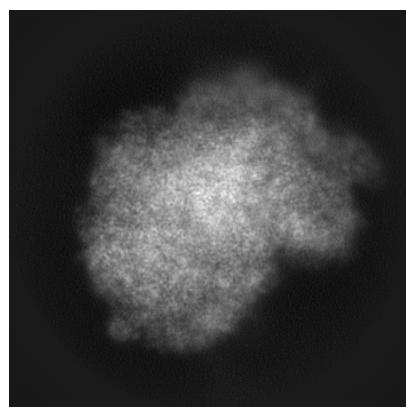


Y

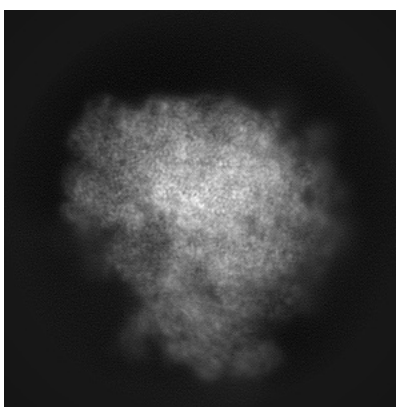


Z

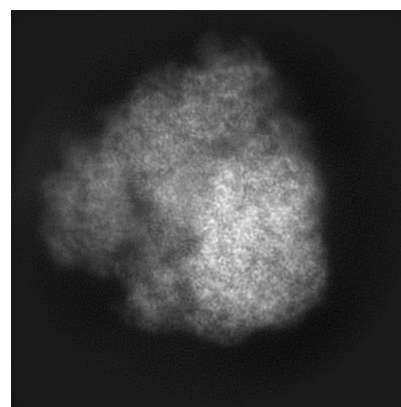
6.1.2 Raw map



X



Y

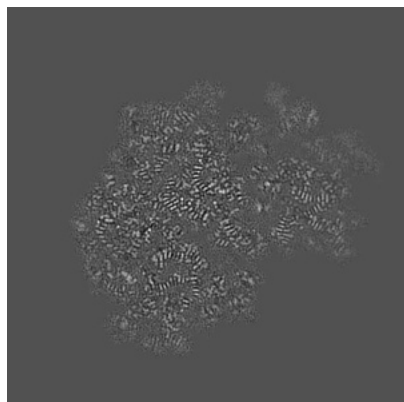


Z

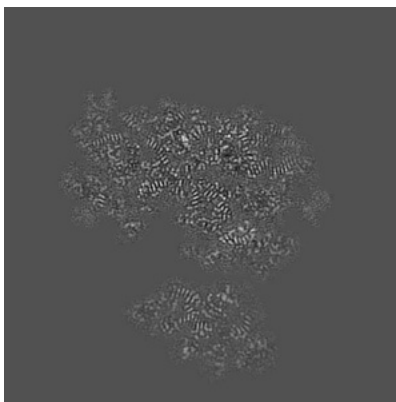
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

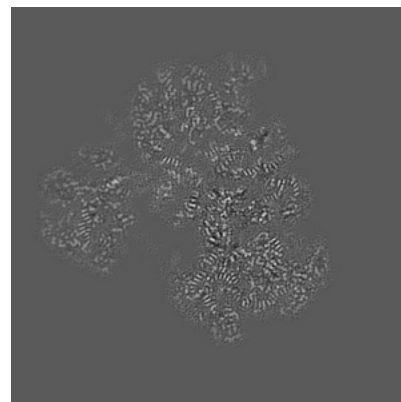
6.2.1 Primary map



X Index: 240

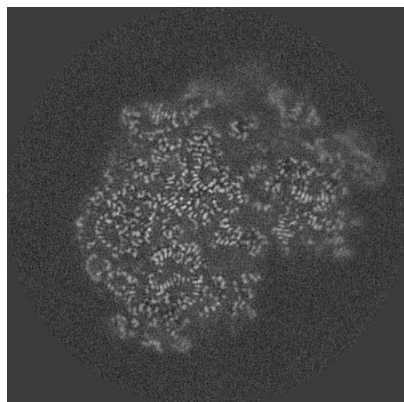


Y Index: 240

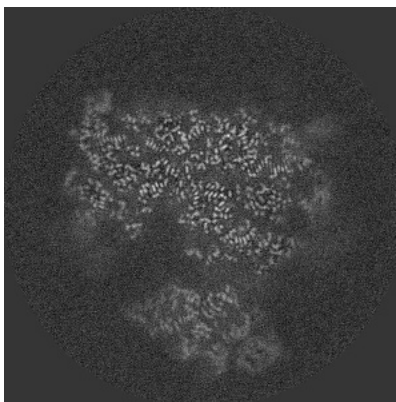


Z Index: 240

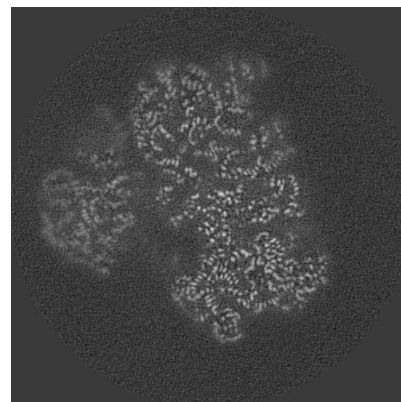
6.2.2 Raw map



X Index: 240



Y Index: 240

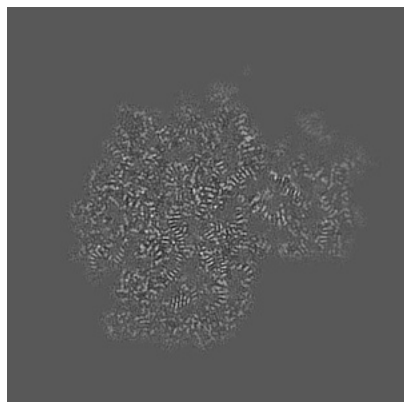


Z Index: 240

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

6.3 Largest variance slices [i](#)

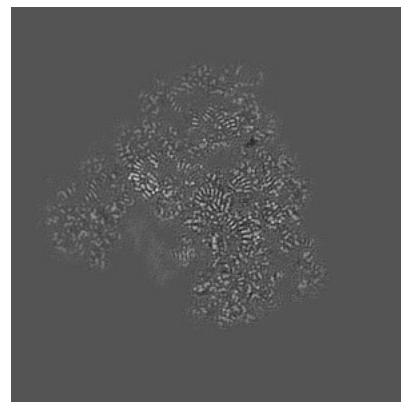
6.3.1 Primary map



X Index: 261

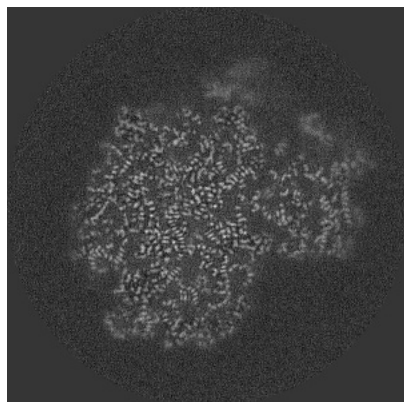


Y Index: 266

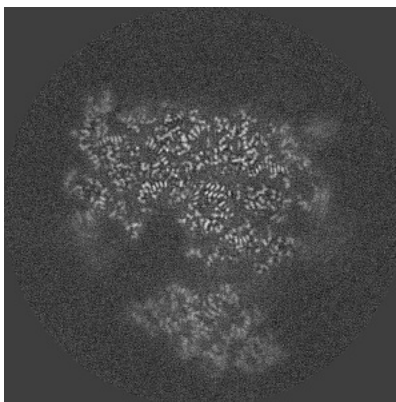


Z Index: 260

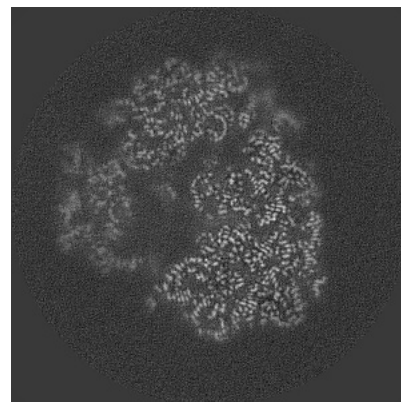
6.3.2 Raw map



X Index: 261



Y Index: 241

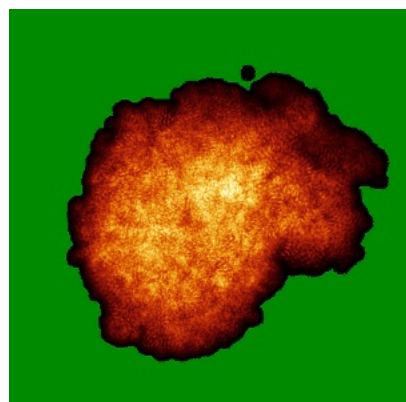


Z Index: 215

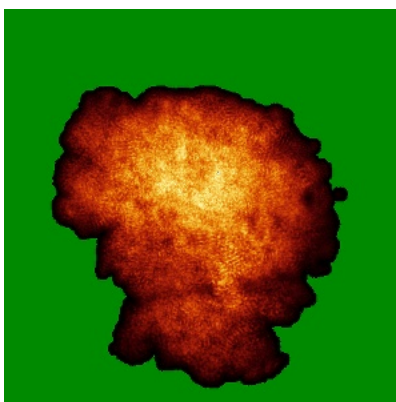
The images above show the largest variance slices of the map in three orthogonal directions.

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

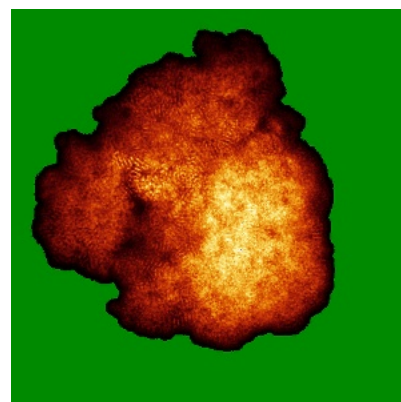
6.4.1 Primary map



X

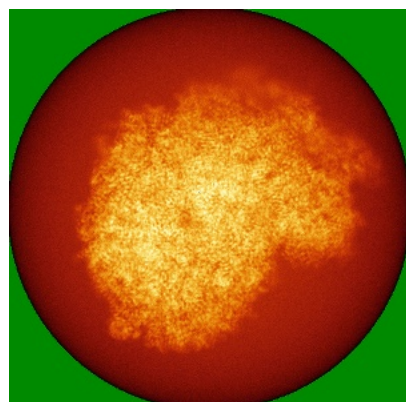


Y

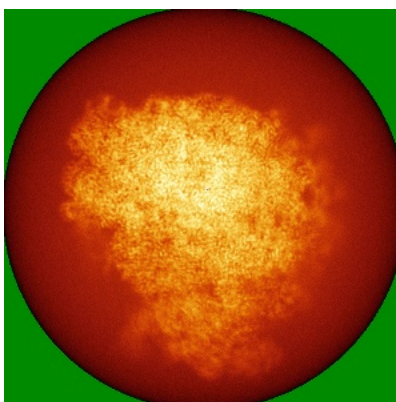


Z

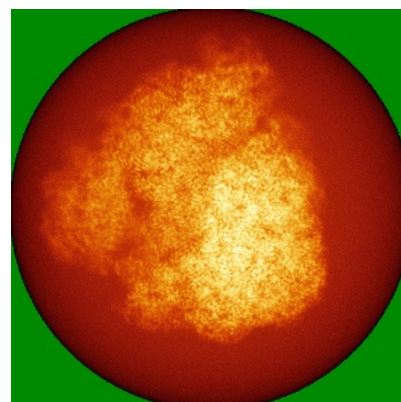
6.4.2 Raw map



X



Y

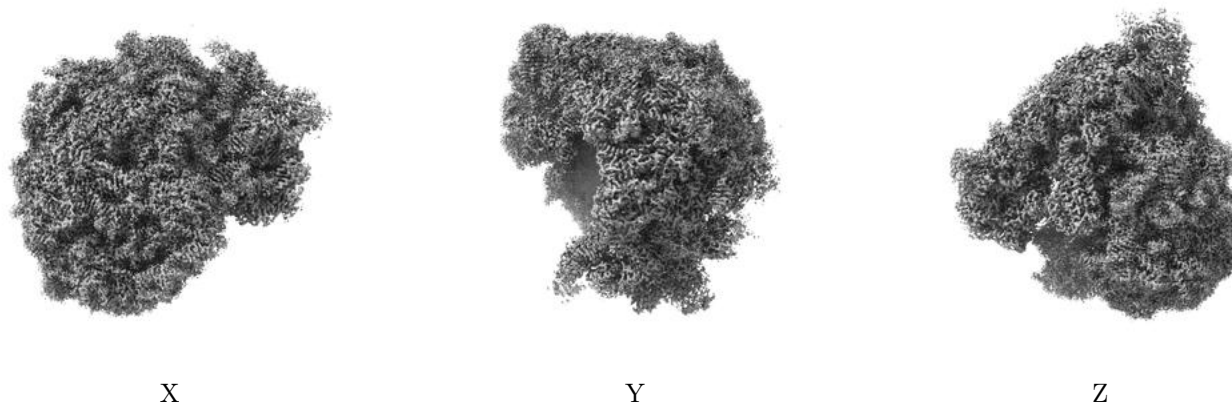


Z

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.

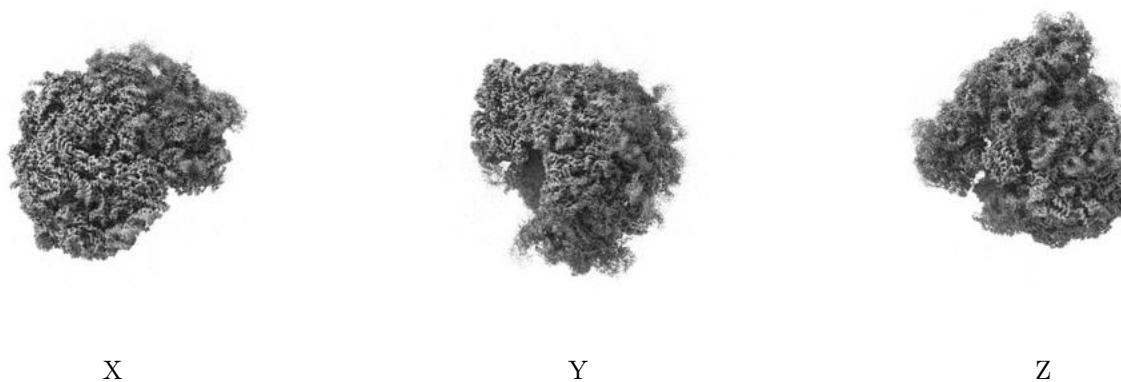
6.5 Orthogonal surface views [i](#)

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.

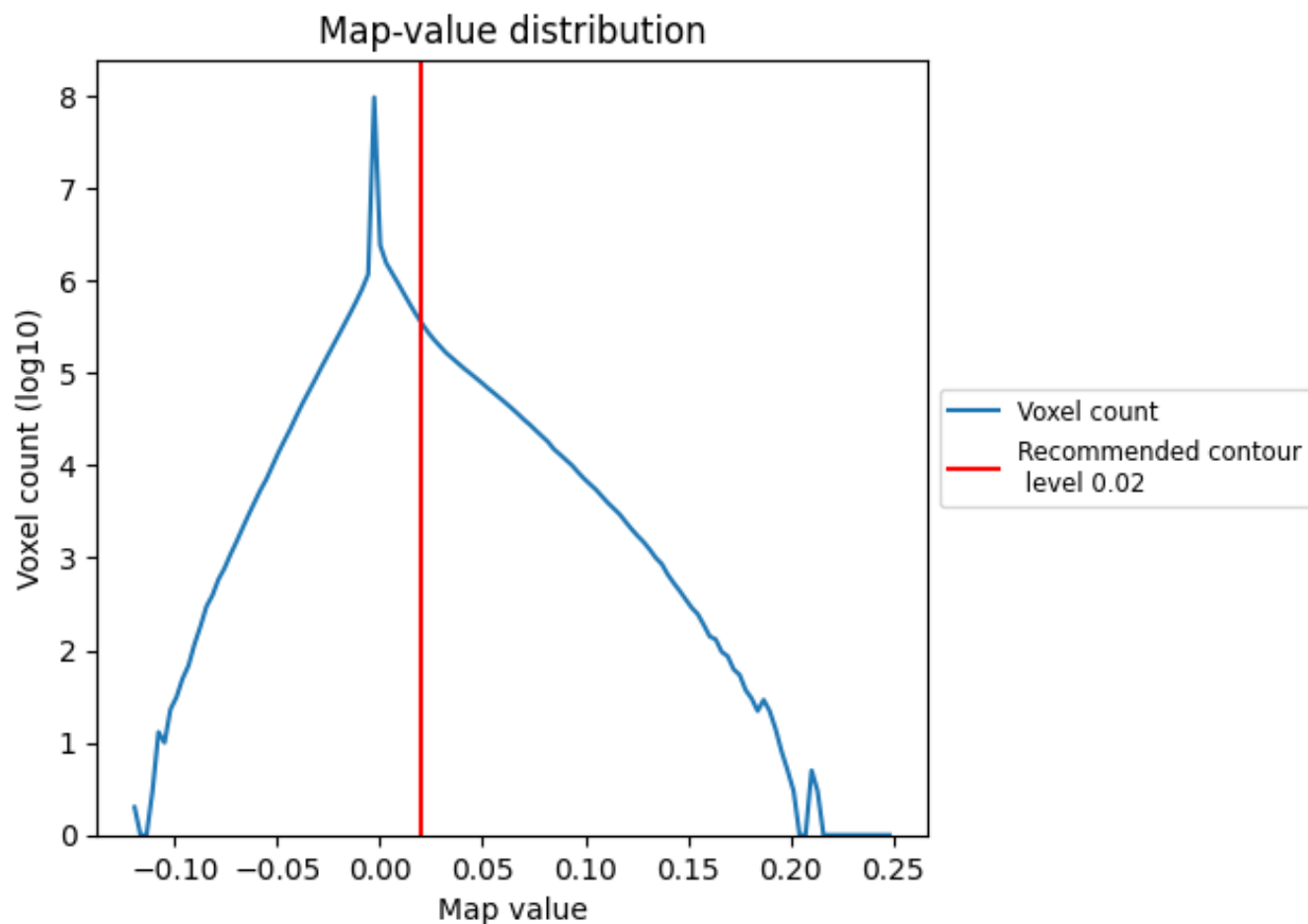
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

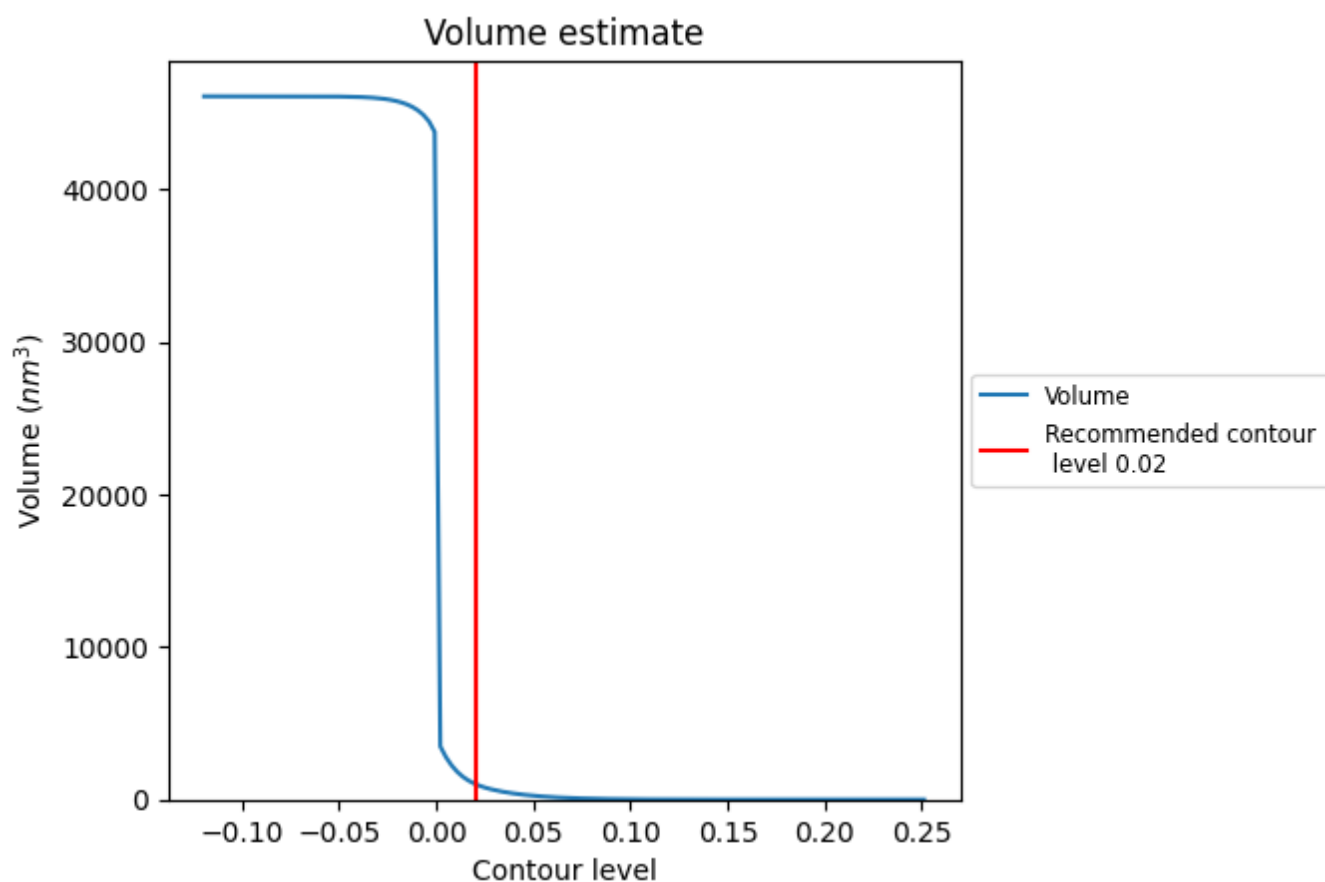
This section contains the results of statistical analysis of the map.

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.

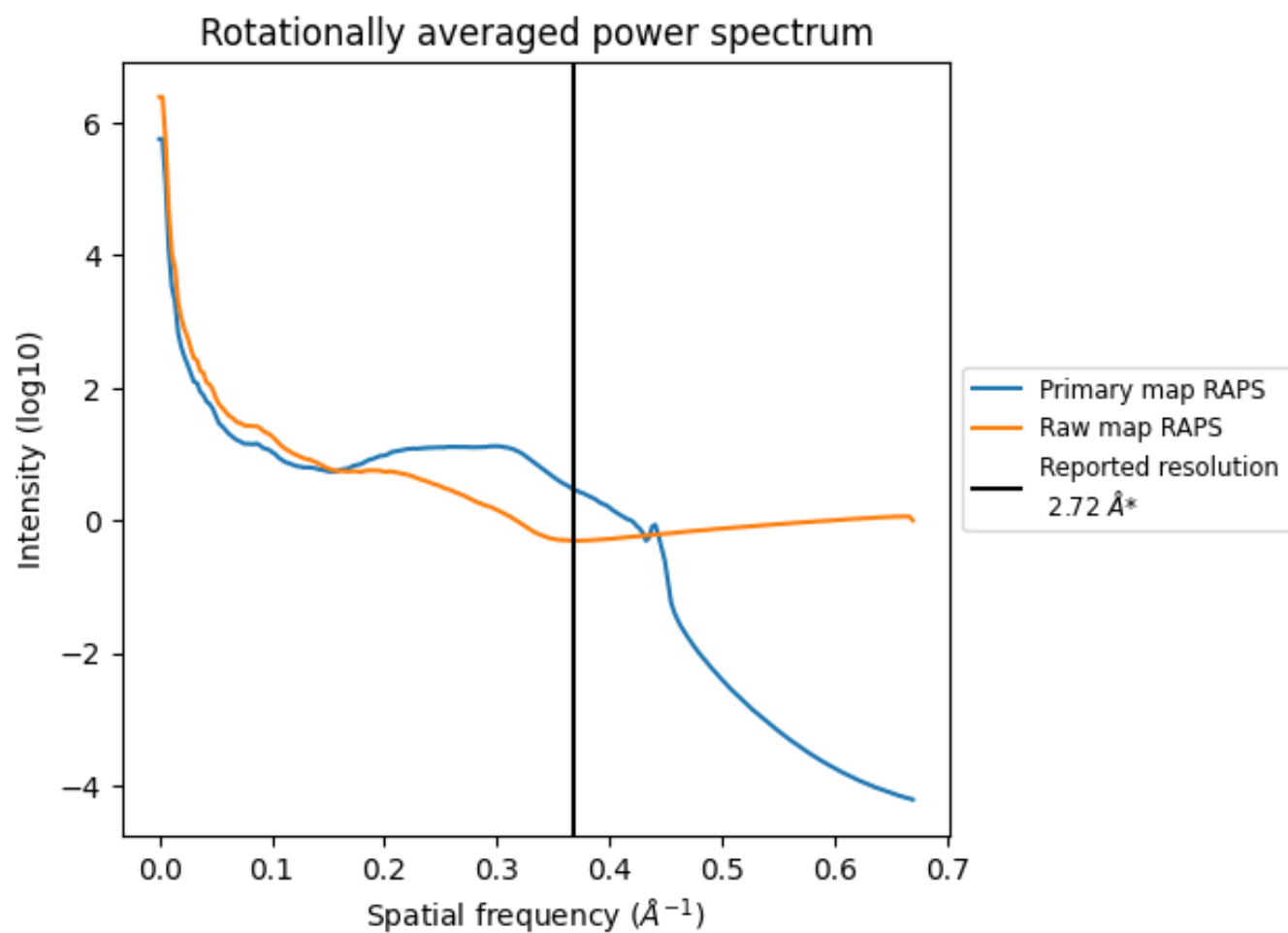
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1029 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 ⓘ

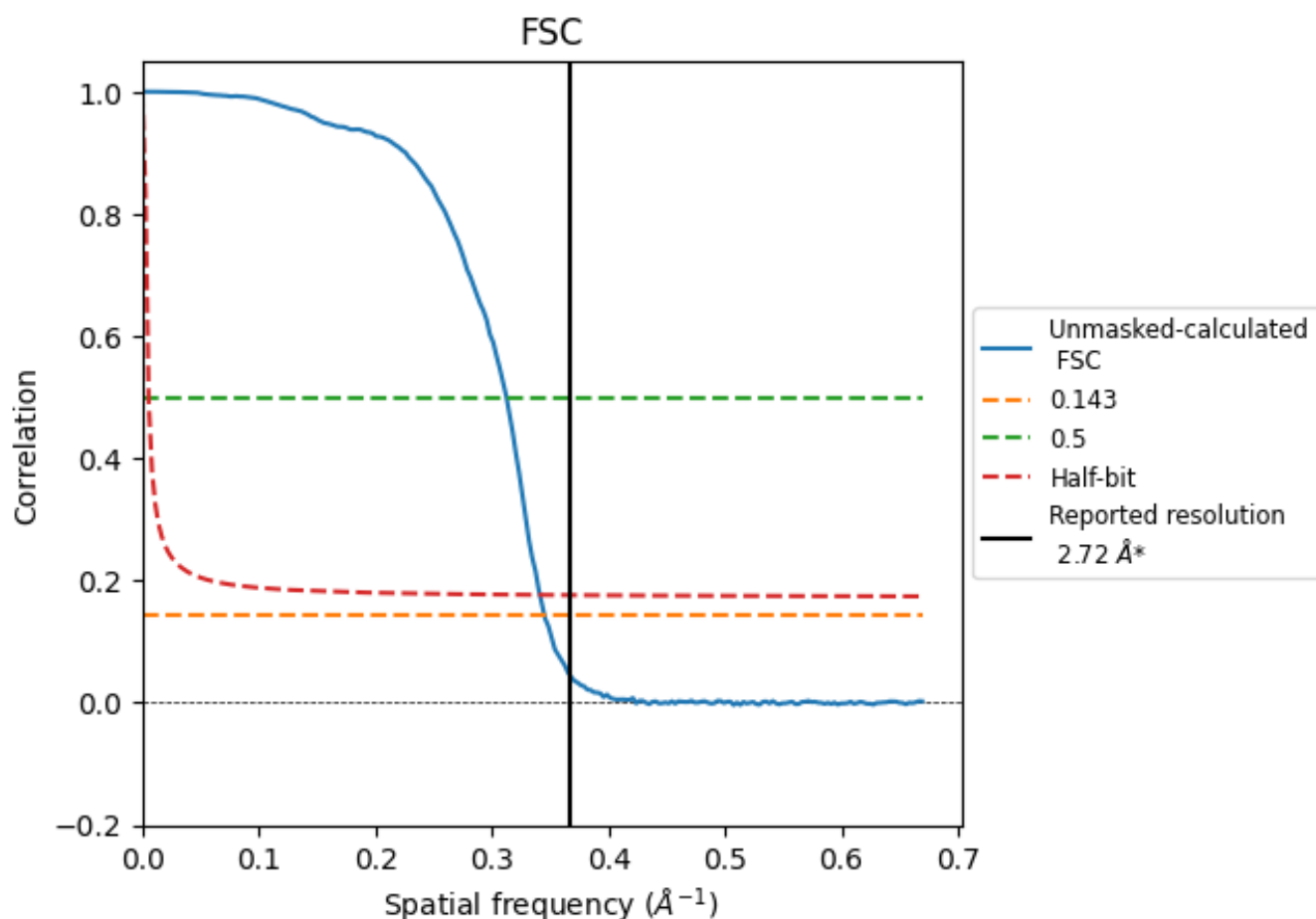


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

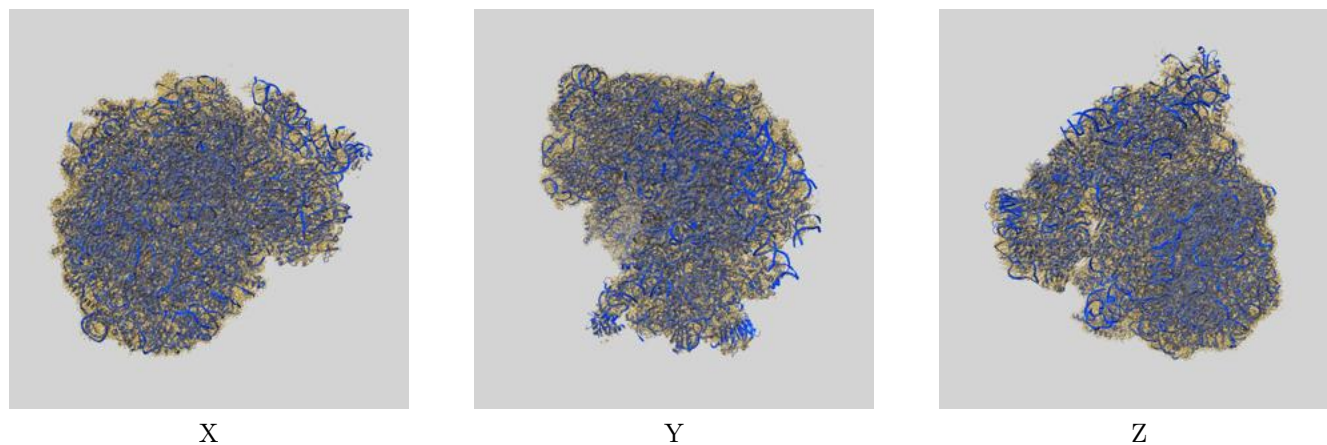
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.90	3.20	2.93

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

9 Map-model fit [i](#)

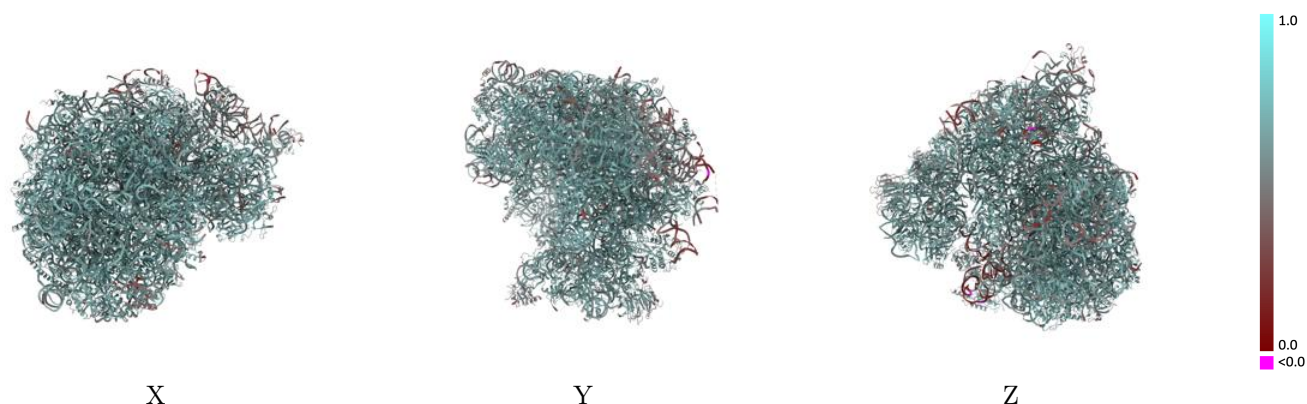
This section contains information regarding the fit between EMDB map EMD-18419 and PDB model 8QHU. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



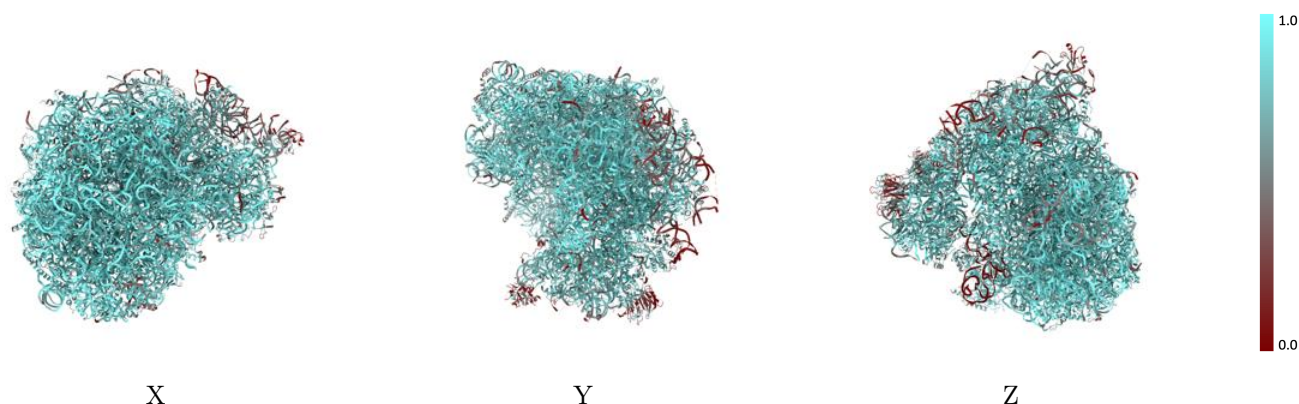
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



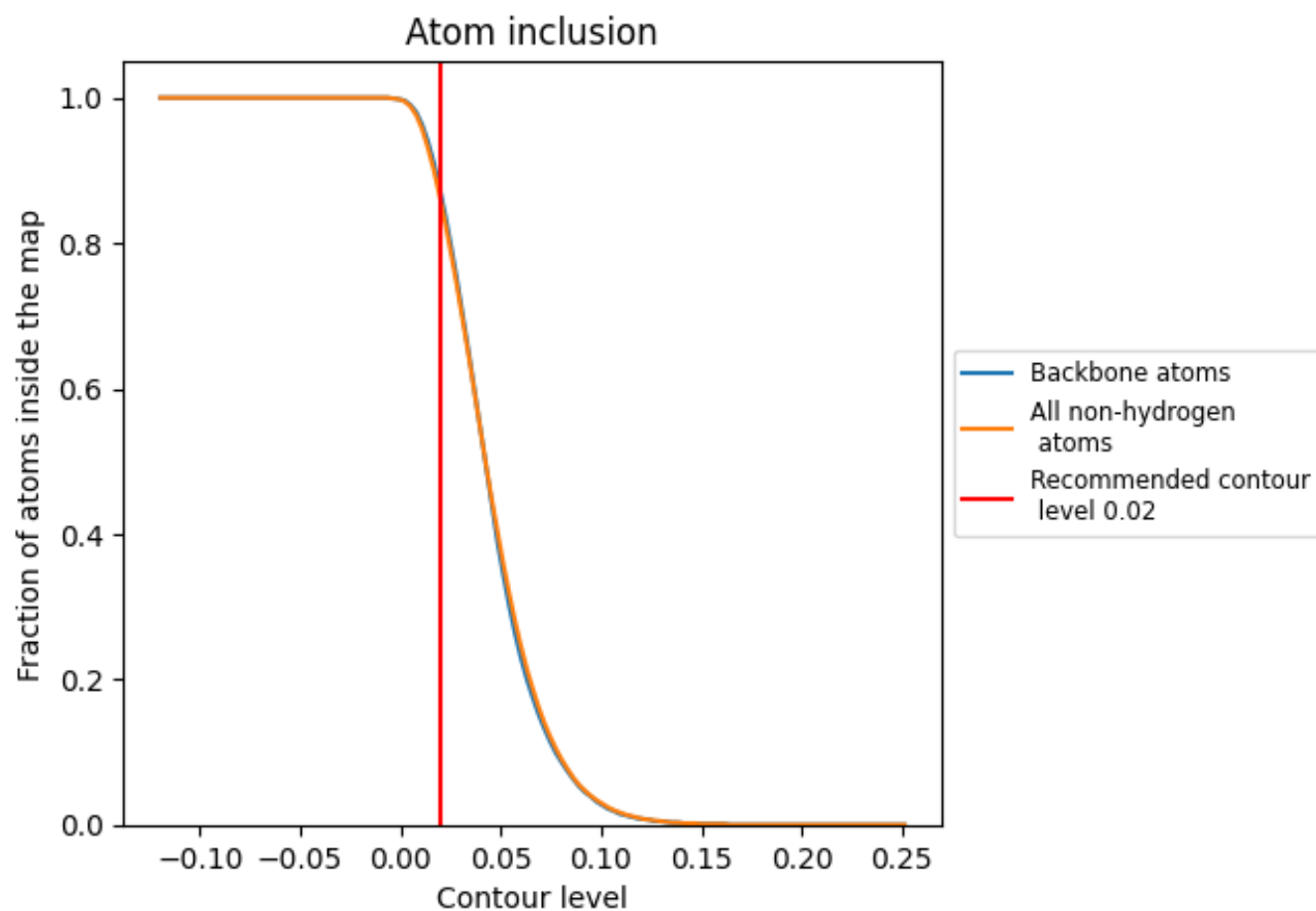
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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