wwPDB EM Validation Summary Report

May 12, 2024 – 06:29 am BST

PDB ID	:	8RXX
EMDB ID	:	EMD-19582
Title	:	CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME WITH A/P/E-site tRNA AND mRNA : LM32Cs3H1 sKO STRAIN
Authors	:	Rajan, K.S.; Yonath, A.
Deposited on	:	2024-02-08
Resolution	:	2.97 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:

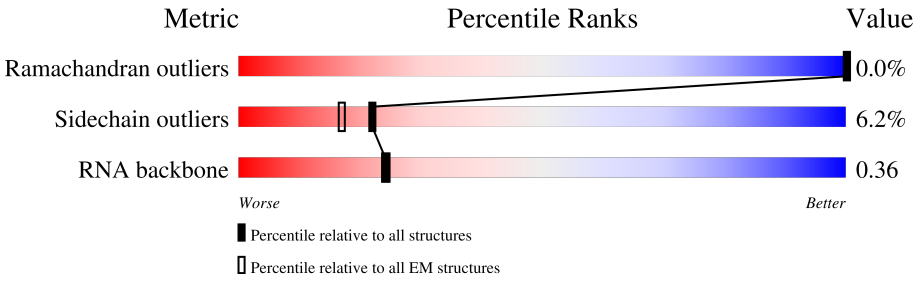
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	L1	1782	58% 33% · 7%
2	L2	1526	48% 26% · 25%
3	L3	216	53% 31% · 15%
4	L4	184	64% 35% ·
5	L5	135	59% 30% · 10%
6	L6	73	42% 51% · ·
7	L7	171	59% 36% · ·
8	L8	123	72% 24% · ·

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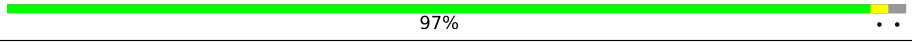
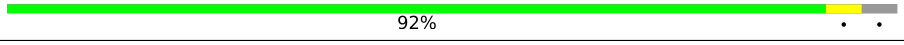
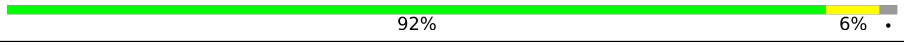
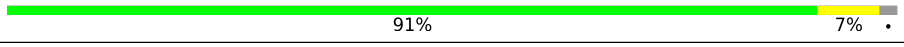
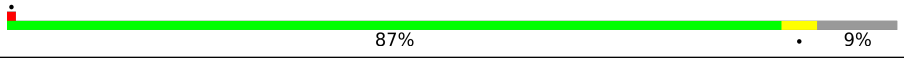
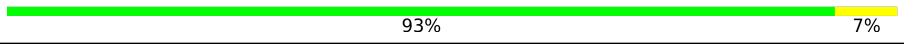
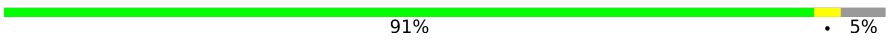
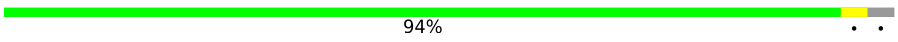
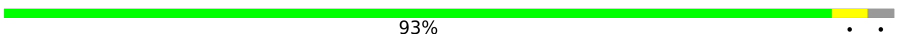
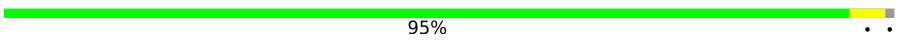
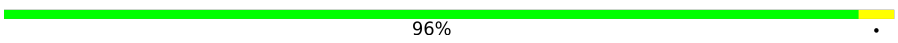
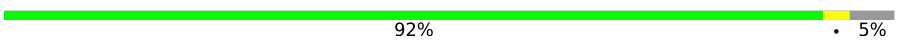
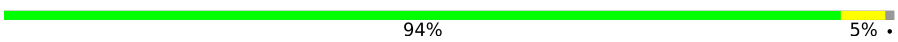
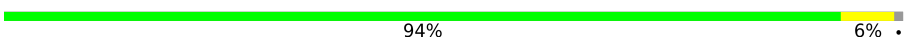
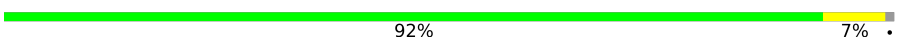
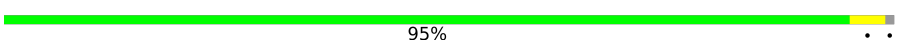
Mol	Chain	Length	Quality of chain
9	LA	260	
10	LB	419	
11	LC	373	
12	LD	188	
13	LE	190	
14	LF	195	
15	LG	264	
16	LH	222	
17	LI	220	
18	LJ	139	
19	LK	175	
20	LL	145	
21	LM	204	
22	LN	213	
23	LO	305	
24	LP	198	
25	LQ	254	
26	LR	179	
27	LS	159	
28	LT	166	
29	LU	129	
30	LV	145	
31	LW	143	
32	LX	124	
33	LY	134	

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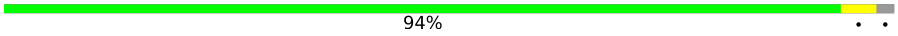
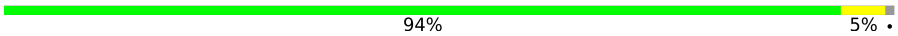
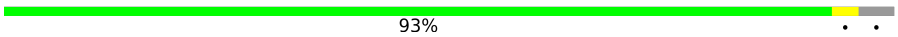
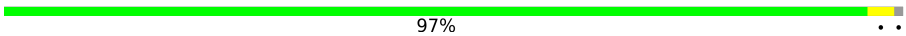
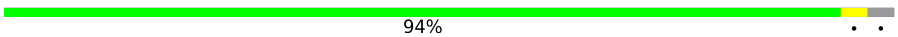
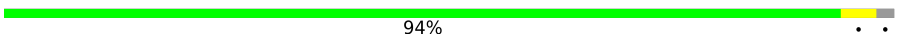
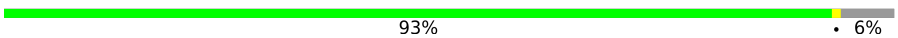
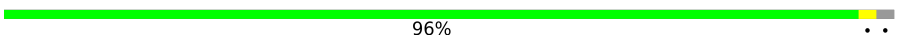
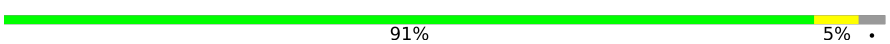
Mol	Chain	Length	Quality of chain
34	LZ	147	
35	La	127	
36	Lb	70	
37	Lc	252	
38	Ld	104	
39	Le	188	
40	Lf	133	
41	Lg	144	
42	Lh	168	
43	Li	105	
44	Lj	83	
45	Lk	83	
46	Ll	51	
47	Lm	128	
48	Ln	34	
49	Lo	92	
50	Lp	106	
51	S1	2204	
52	S2	76	
53	S3	77	
54	S4	76	
55	S5	13	
56	SA	264	
57	SB	246	
58	SC	219	

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Mol	Chain	Length	Quality of chain
59	SD	190	92%
60	SE	273	93% 5%
61	SF	265	80% 18%
62	SG	249	92% 6%
63	SH	190	95%
64	SI	200	96%
65	SJ	130	94% 5%
66	SK	220	85% 5% 10%
67	SL	149	91% 5%
68	SM	116	84% 12%
69	SN	168	55% 41%
70	SO	144	88% 6% 6%
71	SP	143	90% 9%
72	SQ	141	25% 65% 5% 30%
73	SR	153	77% 5% 17%
74	SS	57	93% 5%
75	ST	151	88% 6% 6%
76	SU	173	82% 7% 12%
77	SV	143	83% 15%
78	SW	152	72% 24%
79	SX	161	91% 6%
80	SY	164	51% 46%
81	SZ	137	91% 5%
82	Sa	120	51% 9% 40%
83	Sb	112	87% 6% 7%

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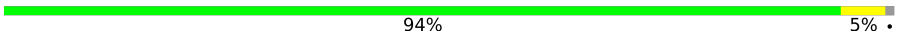
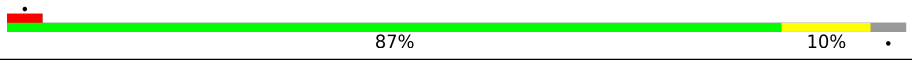
Mol	Chain	Length	Quality of chain
84	Sc	86	
85	Sd	87	
86	Se	66	
87	Sf	152	
88	Sg	312	
89	Sh	235	

2 Entry composition (i)

There are 94 unique types of molecules in this entry. The entry contains 213449 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 RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L1	1657	35568	15899	6506	11505	1658	1	0

- Molecule 2 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L2	1149	24609	11017	4437	8005	1150	1	0

- Molecule 3 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L3	183	3877	1735	669	1290	183	0	0

- Molecule 4 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L4	184	3937	1756	712	1285	184	0	0

- Molecule 5 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L5	122	2600	1160	466	852	122	0	0

- Molecule 6 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	L6	71	1506	675	271	489	71	0	0

- Molecule 7 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	166	Total	C	N	O	P	0	0
			3532	1583	626	1158	165		

- Molecule 8 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	255	Total	C	N	O	S	0	0
			1931	1201	394	326	10		

- Molecule 10 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LB	401	Total	C	N	O	S	0	0
			3169	1997	629	530	13		

- Molecule 11 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	366	Total	C	N	O	S	0	0
			2815	1759	561	480	15		

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	175	Total	C	N	O	S	0	0
			1340	849	258	225	8		

- Molecule 13 is a protein called Putative 60S ribosomal protein L9.

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

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LF	149	Total	C	N	O	S	0	0
			1151	731	216	202	2		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	241	Total	C	N	O	S	1	0
			1905	1200	380	318	7		

- Molecule 16 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	221	Total	C	N	O	S	0	0
			1764	1122	353	282	7		

- Molecule 17 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	208	Total	C	N	O	S	0	0
			1635	1022	331	274	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	135	Total	C	N	O	S	0	0
			1008	636	190	176	6		

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	169	Total	C	N	O	S	0	0
			1327	829	261	229	8		

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 21 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	203	Total	C	N	O	S	0	0
			1711	1079	362	262	8		

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

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

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	290	Total	C	N	O	S	0	0
			2212	1405	416	385	6		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	197	Total	C	N	O	S	0	0
			1535	965	306	258	6		

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	201	Total	C	N	O	S	0	0
			1679	1034	367	272	6		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	178	Total	C	N	O	S	0	0
			1455	925	279	246	5		

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LS	158	Total	C	N	O	S	0	0
			1247	793	243	207	4		

- Molecule 28 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	152	Total	C	N	O	S	0	0
			1218	761	241	205	11		

- Molecule 29 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	122	Total	C	N	O	S	0	0
			957	623	176	155	3		

- Molecule 30 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LV	119	Total	C	N	O	S	0	0
			945	599	180	164	2		

- Molecule 31 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LW	121	Total	C	N	O	S	0	0
			956	598	200	154	4		

- Molecule 32 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LX	85	Total	C	N	O	S	0	0
			714	461	140	109	4		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LY	133	Total	C	N	O	S	0	0
			1067	684	215	165	3		

- Molecule 34 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LZ	145	Total	C	N	O	S	0	0
			1113	682	237	189	5		

- Molecule 35 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	La	125	Total	C	N	O	S	0	0
			1043	650	217	172	4		

- Molecule 36 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Lb	68	Total	C	N	O	0	0
			546	335	125	86		

- Molecule 37 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lc	229	Total	C	N	O	S	0	0
			1862	1185	358	308	11		

- Molecule 38 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ld	97	Total	C	N	O	S	0	0
			744	464	136	139	5		

- Molecule 39 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Le	186	Total	C	N	O	S	0	0
			1469	922	296	247	4		

- Molecule 40 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lf	128	Total	C	N	O	S	0	0
			1046	658	210	174	4		

- Molecule 41 is a protein called Putative ribosomal protein l35a.

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

- Molecule 42 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lh	127	Total	C	N	O	S	0	0
			1029	633	224	166	6		

- Molecule 43 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Li	102	Total	C	N	O	S	0	0
			807	508	163	133	3		

- Molecule 44 is a protein called Ribosomal protein L37.

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

- Molecule 45 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lk	78	Total	C	N	O	S	0	0
			581	365	115	98	3		

- Molecule 46 is a protein called Putative 60S ribosomal protein L39.

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

- Molecule 47 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lm	51	Total	C	N	O	S	0	0
			402	254	80	63	5		

- Molecule 48 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ln	33	Total	C	N	O	S	0	0
			290	178	73	37	2		

- Molecule 49 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lo	89	Total	C	N	O	S	0	0
			693	431	143	113	6		

- Molecule 50 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lp	97	Total	C	N	O	S	0	0
			780	494	158	123	5		

- Molecule 51 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S1	1836	Total	C	N	O	P	1	0
			39285	17572	7085	12791	1837		

- Molecule 52 is a RNA chain called A-site_tRNA_chain_S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	S2	12	Total	C	N	O	P	S	0	0
			263	121	47	82	12	1		

- Molecule 53 is a RNA chain called P-site_tRNA_chain_S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	71	Total	C	N	O	P	0	0
			1513	676	277	490	70		

- Molecule 54 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S4	66	Total	C	N	O	P	0	0
			1406	628	253	460	65		

- Molecule 55 is a RNA chain called mRNA_chain_S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S5	11	Total	C	N	O	P	0	0
			229	103	38	77	11		

- Molecule 56 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SA	238	Total	C	N	O	S	0	0
			1909	1194	366	338	11		

- Molecule 57 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SB	211	Total	C	N	O	S	0	0
			1649	1047	301	290	11		

- Molecule 58 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SC	212	Total	C	N	O	S	0	0
			1627	1030	297	287	13		

- Molecule 59 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SD	183	Total	C	N	O	S	0	0
			1504	947	305	244	8		

- Molecule 60 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SE	260	Total	C	N	O	S	0	0
			2054	1301	393	351	9		

- Molecule 61 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SF	218	Total	C	N	O	S	0	0
			1662	1063	297	293	9		

- Molecule 62 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SG	245	Total	C	N	O	S	0	0
			1948	1213	401	331	3		

- Molecule 63 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SH	182	Total	C	N	O	S	0	0
			1430	889	275	259	7		

- Molecule 64 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SI	200	Total	C	N	O	S	0	0
			1639	1044	316	271	8		

- Molecule 65 is a protein called Putative 40S ribosomal protein S15A.

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

- Molecule 66 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SK	198	Total	C	N	O	S	0	0
			1600	998	330	270	2		

- Molecule 67 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SL	144	Total	C	N	O	S	0	0
			1140	731	210	196	3		

- Molecule 68 is a protein called Putative ribosomal protein S20.

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

- Molecule 69 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SN	99	Total	C	N	O	S	0	0
			808	518	141	142	7		

- Molecule 70 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SO	136	Total	C	N	O	S	0	0
			1010	624	197	182	7		

- Molecule 71 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SP	141	Total	C	N	O	S	0	0
			1096	691	216	186	3		

- Molecule 72 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SQ	98	Total	C	N	O	S	0	0
			655	400	119	131	5		

- Molecule 73 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SR	127	Total	C	N	O	S	0	0
			1011	641	195	171	4		

- Molecule 74 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SS	56	Total	C	N	O	S	0	0
			451	279	94	73	5		

- Molecule 75 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	ST	142	Total	C	N	O	S	0	0
			1159	731	230	190	8		

- Molecule 76 is a protein called Ribosomal protein S17 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SU	153	Total	C	N	O	S	0	0
			1251	792	248	206	5		

- Molecule 77 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SV	122	Total	C	N	O	S	0	0
			936	588	180	164	4		

- Molecule 78 is a protein called Putative 40S ribosomal protein S15.

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

- Molecule 79 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SX	152	Total	C	N	O	S	0	0
			1206	766	237	199	4		

- Molecule 80 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SY	88	Total	C	N	O	S	0	0
			659	407	121	127	4		

- Molecule 81 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SZ	130	Total	C	N	O	S	0	0
			1051	675	204	169	3		

- Molecule 82 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sa	72	Total	C	N	O	S	0	0
			567	361	100	103	3		

- Molecule 83 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sb	104	Total	C	N	O	S	0	0
			827	513	177	130	7		

- Molecule 84 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sc	85	Total	C	N	O	S	0	0
			674	416	131	119	8		

- Molecule 85 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sd	66	Total	C	N	O	S	0	0
			479	293	96	86	4		

- Molecule 86 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Se	58	Total	C	N	O	S	0	0
			465	293	97	74	1		

- Molecule 87 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms				AltConf	Trace
87	Sf	46	Total	C	N	O	0	0
			300	187	63	50		

- Molecule 88 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Sg	301	Total	C	N	O	S	0	0
			2341	1468	418	442	13		

- Molecule 89 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Sh	103	Total	C	N	O	S	0	0
			826	520	158	145	3		

- Molecule 90 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
90	L1	34	Total K 34 34	0
90	L2	22	Total K 22 22	0
90	L3	3	Total K 3 3	0
90	L4	6	Total K 6 6	0
90	L5	1	Total K 1 1	0
90	L7	2	Total K 2 2	0
90	LA	1	Total K 1 1	0
90	LM	1	Total K 1 1	0
90	S1	19	Total K 19 19	0

- Molecule 91 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
91	L1	16	Total Na 16 16	0
91	L2	14	Total Na 14 14	0
91	L8	1	Total Na 1 1	0
91	LA	1	Total Na 1 1	0
91	Lh	1	Total Na 1 1	0
91	S1	7	Total Na 7 7	0
91	SK	1	Total Na 1 1	0

- Molecule 92 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
92	L1	73	Total Mg 73 73	0
92	L2	42	Total Mg 42 42	0

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Mol	Chain	Residues	Atoms	AltConf
92	L3	3	Total Mg 3 3	0
92	L4	2	Total Mg 2 2	0
92	L5	2	Total Mg 2 2	0
92	L6	1	Total Mg 1 1	0
92	L7	3	Total Mg 3 3	0
92	L8	2	Total Mg 2 2	0
92	LB	1	Total Mg 1 1	0
92	LJ	1	Total Mg 1 1	0
92	LT	1	Total Mg 1 1	0
92	Lf	1	Total Mg 1 1	0
92	Lj	1	Total Mg 1 1	0
92	S1	31	Total Mg 31 31	0
92	S5	1	Total Mg 1 1	0
92	SK	1	Total Mg 1 1	0

- Molecule 93 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
93	Lm	1	Total Zn 1 1	0
93	SS	1	Total Zn 1 1	0
93	Sb	1	Total Zn 1 1	0

- Molecule 94 is water.

Mol	Chain	Residues	Atoms	AltConf
94	L1	337	Total O 337 337	0
94	L2	235	Total O 235 235	0
94	L3	21	Total O 21 21	0
94	L4	39	Total O 39 39	0
94	L5	30	Total O 30 30	0
94	L6	6	Total O 6 6	0
94	L7	38	Total O 38 38	0
94	L8	2	Total O 2 2	0
94	LA	14	Total O 14 14	0
94	LB	20	Total O 20 20	0
94	LC	18	Total O 18 18	0
94	LF	3	Total O 3 3	0
94	LG	2	Total O 2 2	0
94	LH	6	Total O 6 6	0
94	LI	5	Total O 5 5	0
94	LJ	6	Total O 6 6	0
94	LK	1	Total O 1 1	0
94	LL	8	Total O 8 8	0
94	LM	12	Total O 12 12	0
94	LP	6	Total O 6 6	0
94	LQ	8	Total O 8 8	0
94	LR	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
94	LT	11	Total O 11 11	0
94	LV	4	Total O 4 4	0
94	LW	2	Total O 2 2	0
94	LX	3	Total O 3 3	0
94	LZ	1	Total O 1 1	0
94	La	3	Total O 3 3	0
94	Lb	1	Total O 1 1	0
94	Lc	5	Total O 5 5	0
94	Ld	1	Total O 1 1	0
94	Le	3	Total O 3 3	0
94	Lf	8	Total O 8 8	0
94	Lg	7	Total O 7 7	0
94	Lh	7	Total O 7 7	0
94	Lj	11	Total O 11 11	0
94	Lk	1	Total O 1 1	0
94	Ll	4	Total O 4 4	0
94	Lm	1	Total O 1 1	0
94	Ln	1	Total O 1 1	0
94	Lo	6	Total O 6 6	0
94	Lp	1	Total O 1 1	0
94	S1	78	Total O 78 78	0

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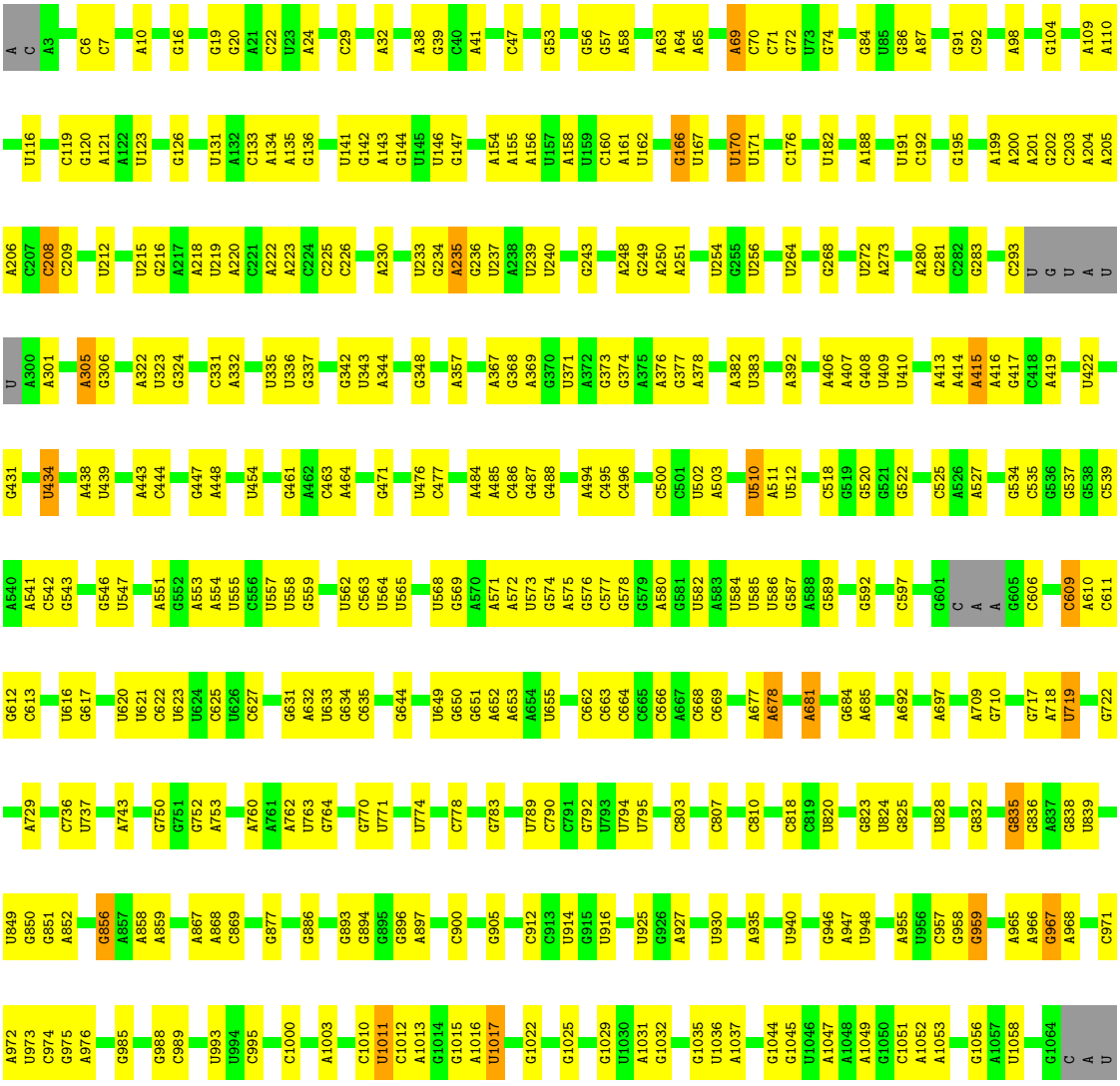
Mol	Chain	Residues	Atoms	AltConf
94	S3	1	Total O 1 1	0
94	S4	1	Total O 1 1	0
94	S5	3	Total O 3 3	0
94	SK	2	Total O 2 2	0
94	SO	1	Total O 1 1	0
94	SP	1	Total O 1 1	0
94	ST	3	Total O 3 3	0
94	Sb	1	Total O 1 1	0

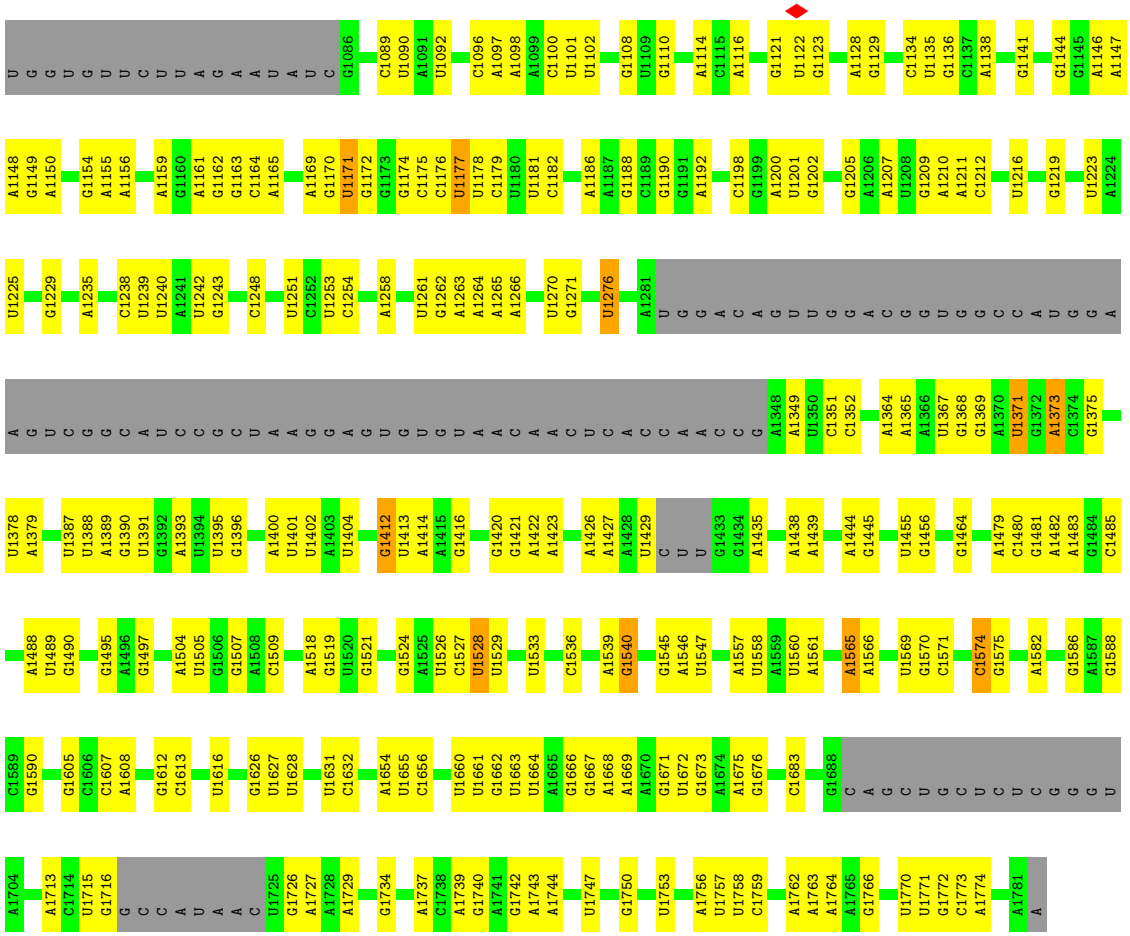
3 Residue-property plots (i)

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

- Molecule 1: LSUa_rRNA_chain_1

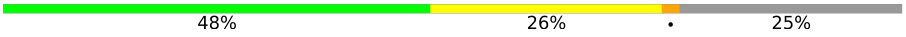
Chain L1:

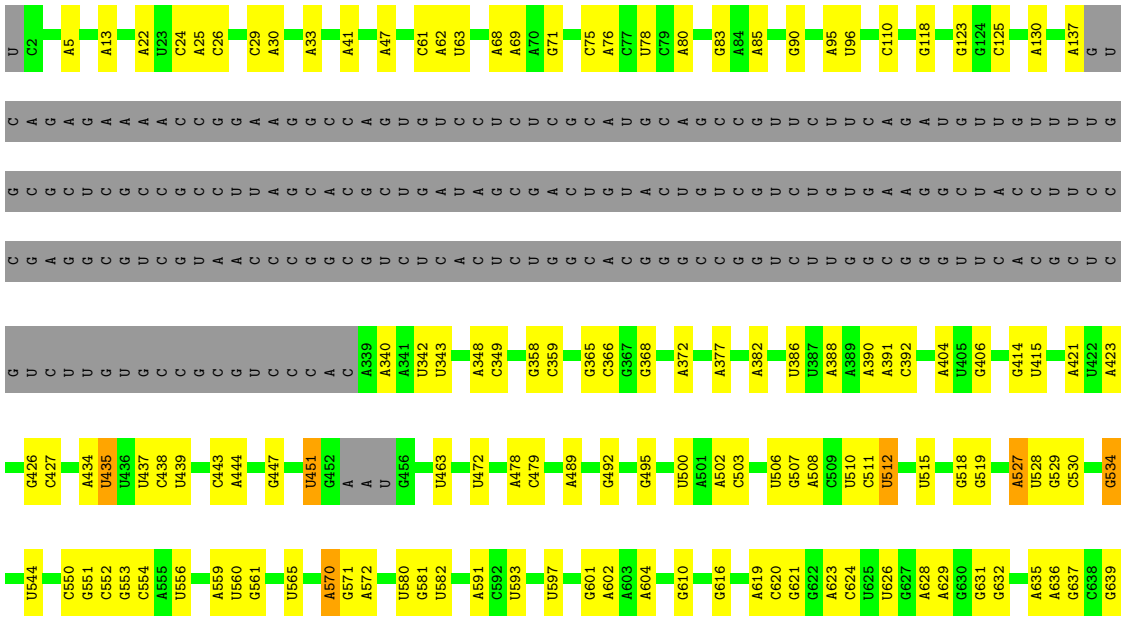


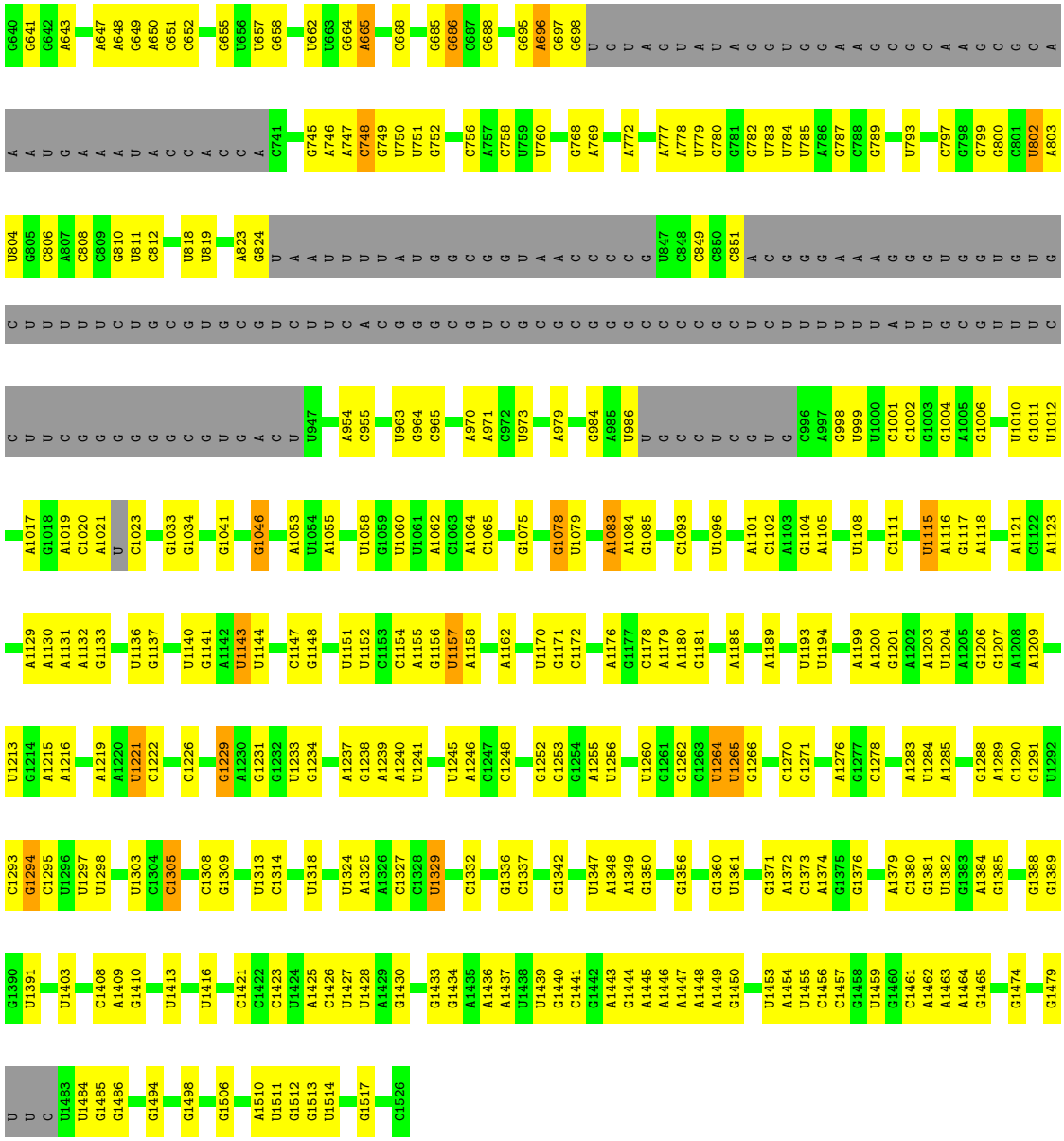


• Molecule 2: LSUb_rRNA_chain_2

Chain L2:

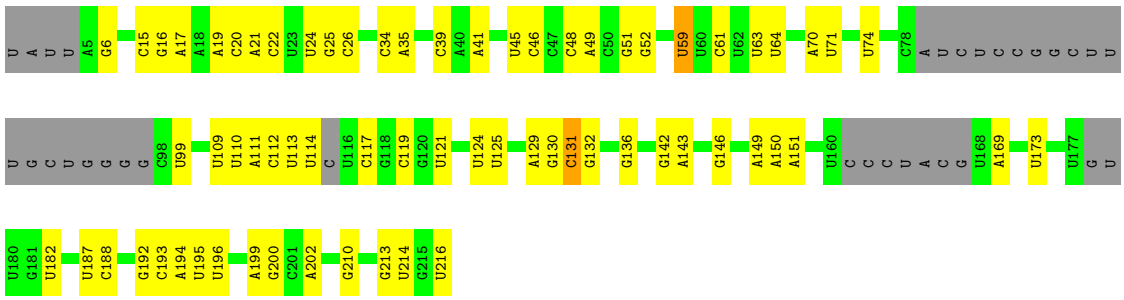






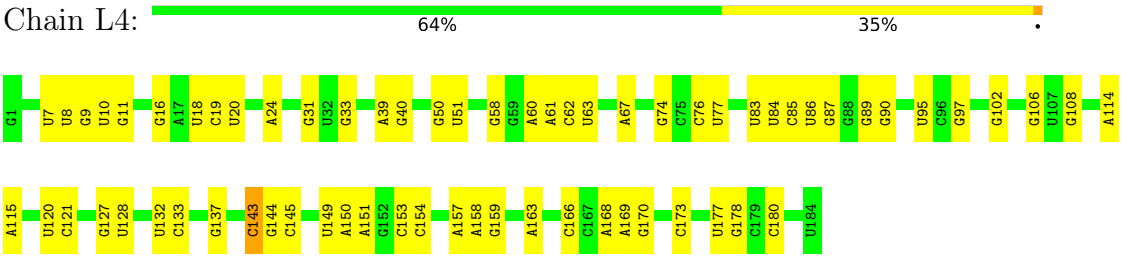
• Molecule 3: SR1_chain_3

Chain L3:



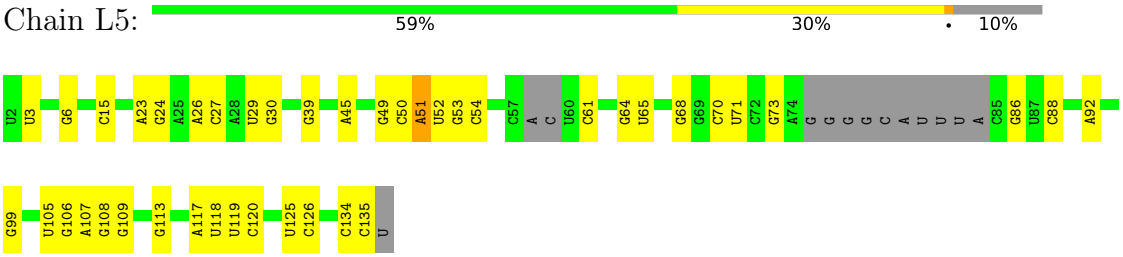
• Molecule 4: SR2_chain_4

Chain L4:



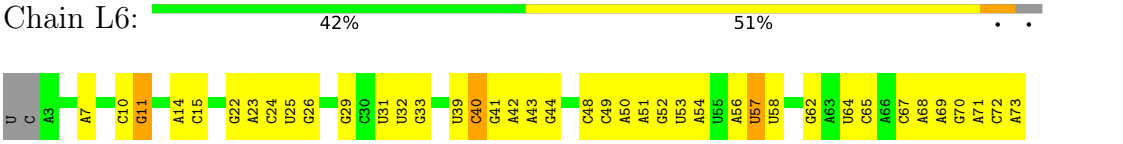
• Molecule 5: SR4_chain_5

Chain L5:



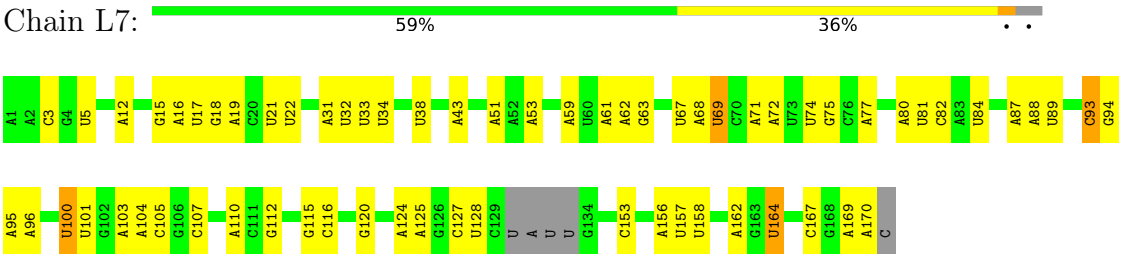
• Molecule 6: SR6_chain_6

Chain L6:



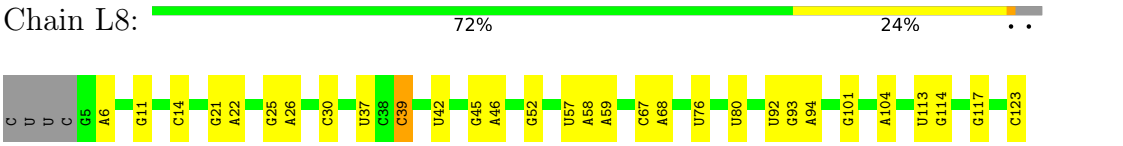
• Molecule 7: 5.8S_rRNA_chain_7

Chain L7:



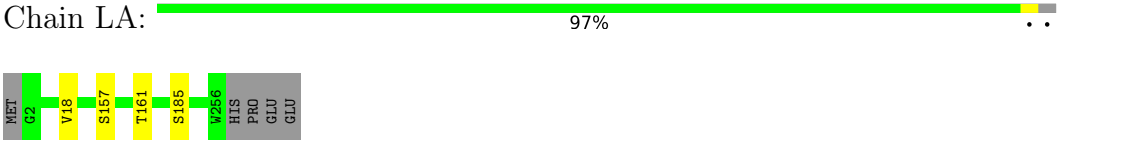
• Molecule 8: 5S_rRNA_chain_8

Chain L8:



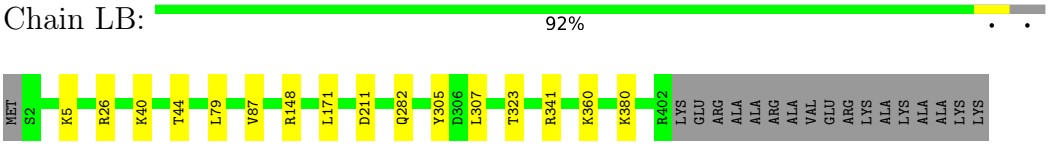
• Molecule 9: Putative 60S ribosomal protein L2

Chain LA:



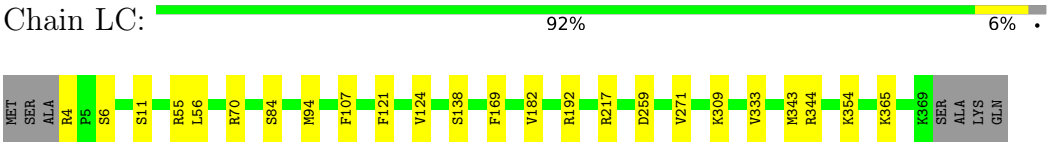
• Molecule 10: Putative ribosomal protein L3

Chain LB:



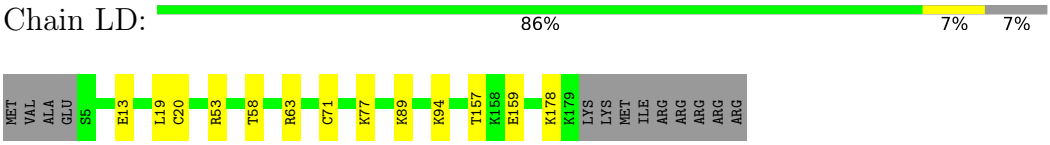
• Molecule 11: Putative ribosomal protein L1a

Chain LC:



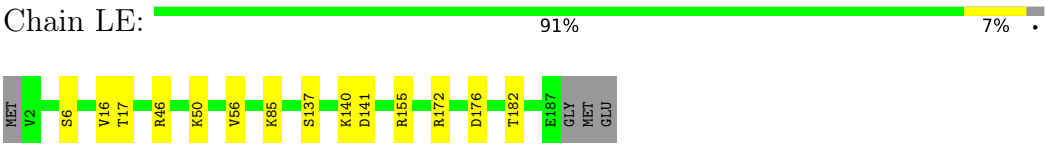
• Molecule 12: 60S ribosomal protein L11

Chain LD:



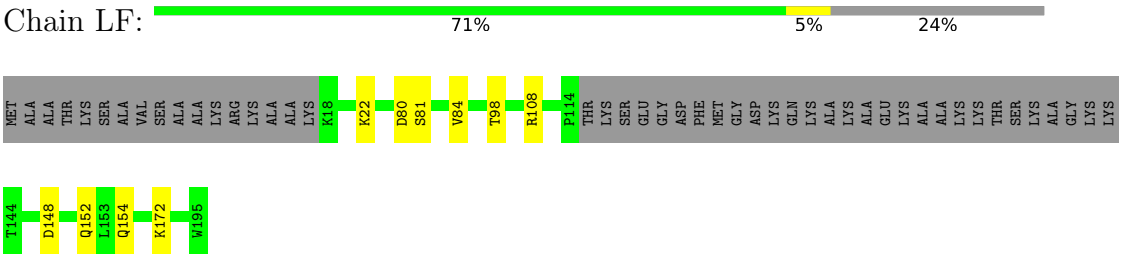
• Molecule 13: Putative 60S ribosomal protein L9

Chain LE:



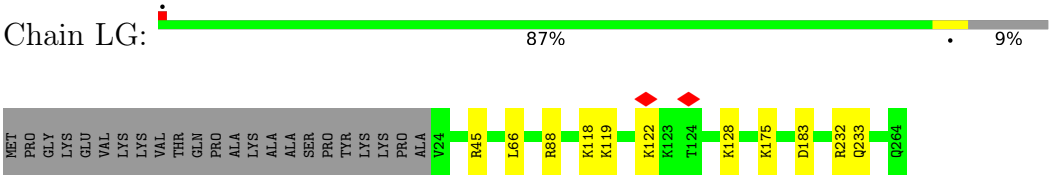
• Molecule 14: Putative 60S ribosomal protein L6

Chain LF:



• Molecule 15: 60S ribosomal protein L7a

Chain LG:



• Molecule 16: Putative 60S ribosomal protein L13a

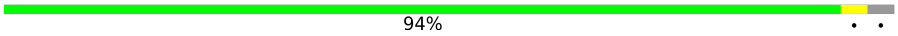
Chain LH:

• Molecule 17: Putative 60S ribosomal protein L13

Chain LI:

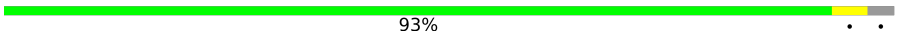
• Molecule 18: Putative 60S ribosomal protein L23

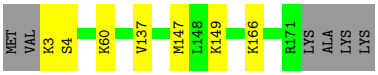
Chain LJ:



• Molecule 19: Putative 40S ribosomal protein L14

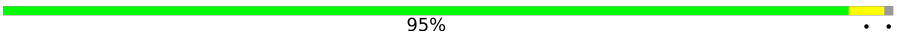
Chain LK:

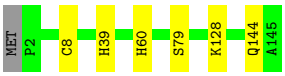




• Molecule 20: Putative 60S ribosomal protein L27A/L29

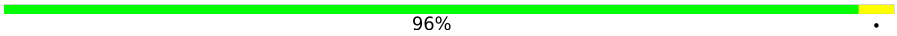
Chain LL:

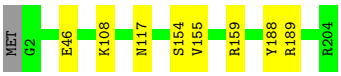




• Molecule 21: Ribosomal protein L15

Chain LM:





• Molecule 22: Putative 60S ribosomal protein L10

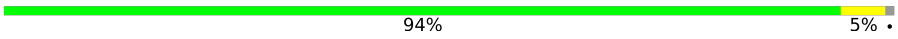
Chain LN:

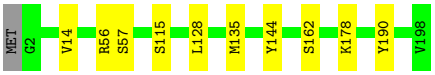
• Molecule 23: Putative 60S ribosomal protein L5

Chain LO:

• Molecule 24: 60S ribosomal protein L18

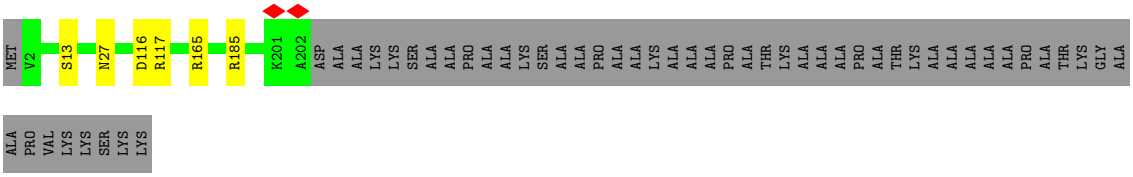
Chain LP:





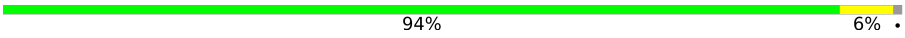
• Molecule 25: Putative 60S ribosomal protein L19

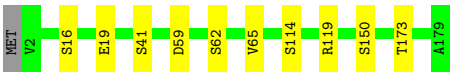
Chain LQ:



• Molecule 26: 60S ribosomal protein L18a

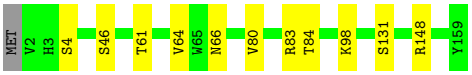
Chain LR:





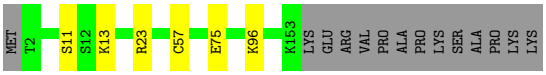
• Molecule 27: Putative 60S ribosomal protein L21

Chain LS:



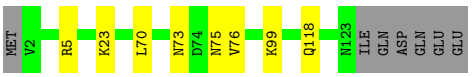
• Molecule 28: Putative 60S ribosomal protein L17

Chain LT:



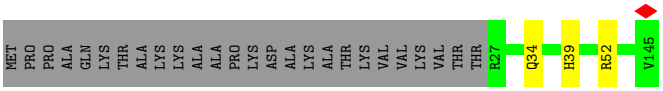
• Molecule 29: Putative 60S ribosomal protein L22

Chain LU:



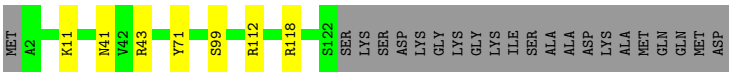
• Molecule 30: Putative 60S ribosomal protein L23a

Chain LV:



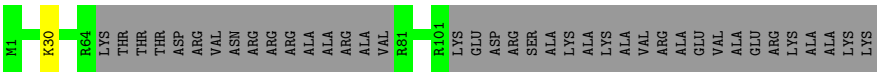
• Molecule 31: Putative 60S ribosomal protein L26

Chain LW:



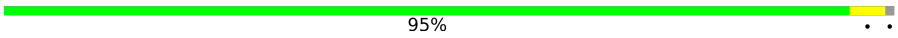
• Molecule 32: Putative ribosomal protein L24

Chain LX:



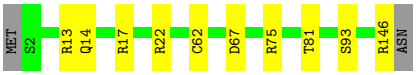
• Molecule 33: 60S ribosomal protein L27

Chain LY:



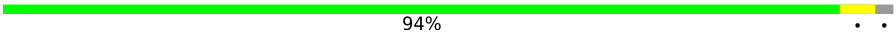
• Molecule 34: Putative 60S ribosomal protein L28

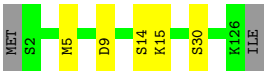
Chain LZ:



• Molecule 35: Putative 60S ribosomal protein L35

Chain La:



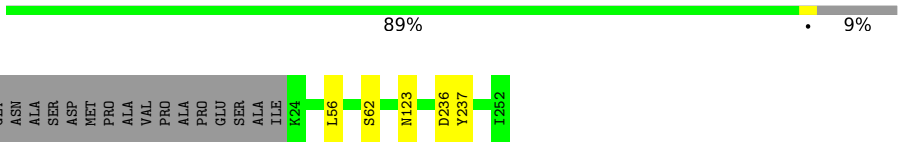


• Molecule 36: 60S ribosomal protein L29

Chain Lb:

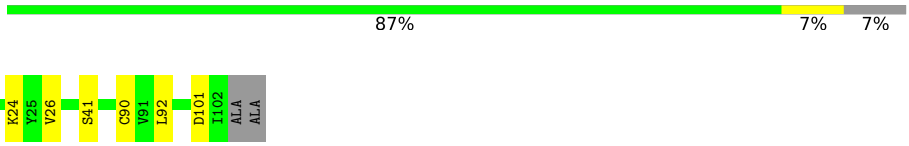
• Molecule 37: Putative 60S ribosomal protein L7

Chain Lc:



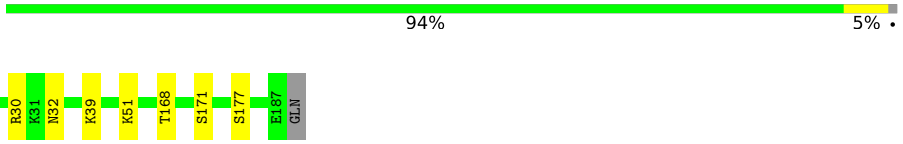
• Molecule 38: 60S ribosomal protein L30

Chain Ld:



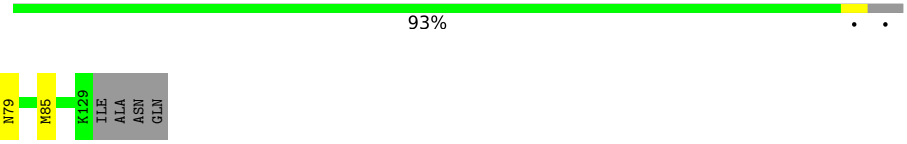
• Molecule 39: Putative 60S ribosomal subunit protein L31

Chain Le:



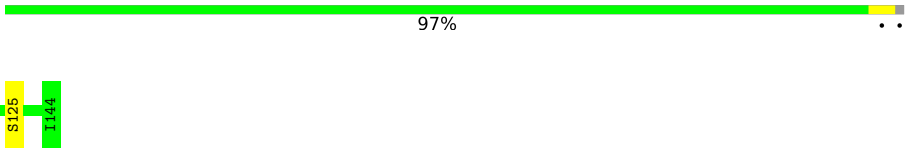
• Molecule 40: 60S ribosomal protein L32

Chain Lf:



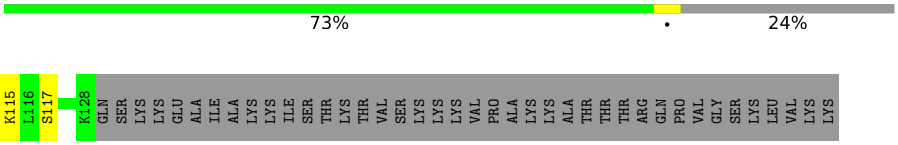
• Molecule 41: Putative ribosomal protein l35a

Chain Lg:



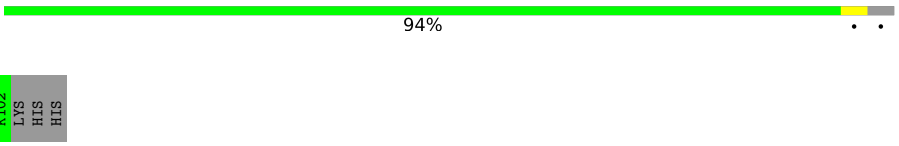
• Molecule 42: Putative 60S ribosomal protein L34

Chain Lh:



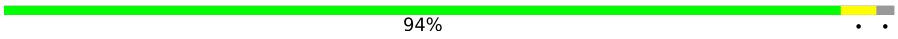
• Molecule 43: Putative 60S Ribosomal protein L36

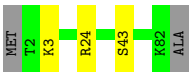
Chain Li:



• Molecule 44: Ribosomal protein L37

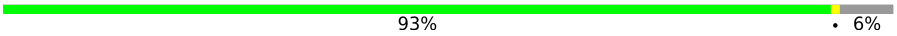
Chain Lj:

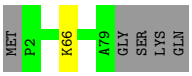




• Molecule 45: Putative ribosomal protein L38

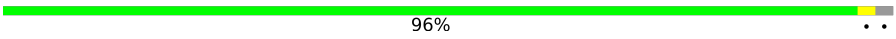
Chain Lk:





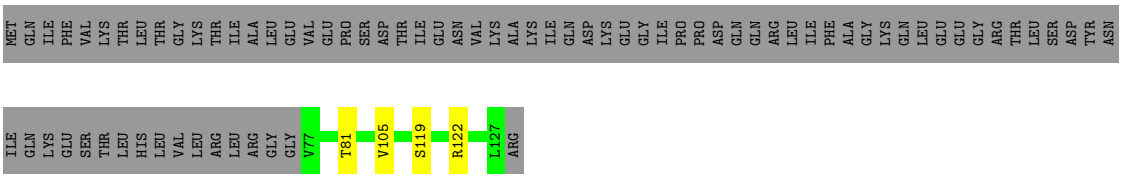
• Molecule 46: Putative 60S ribosomal protein L39

Chain Ll:



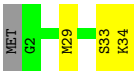
• Molecule 47: Ubiquitin-60S ribosomal protein L40

Chain Lm:



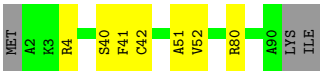
• Molecule 48: 60S ribosomal protein L41

Chain Ln:



• Molecule 49: 60S ribosomal protein L37a

Chain Lo:

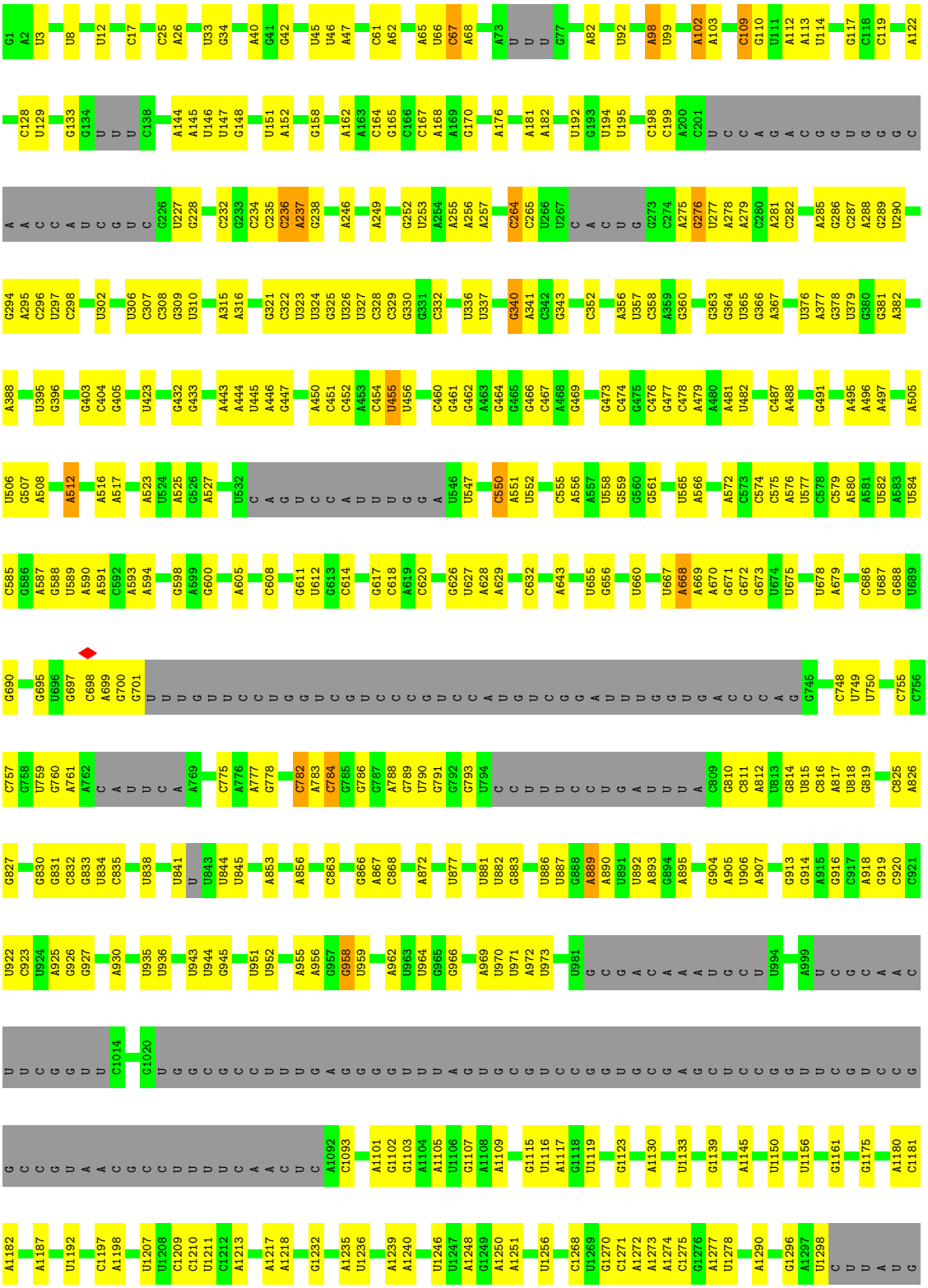


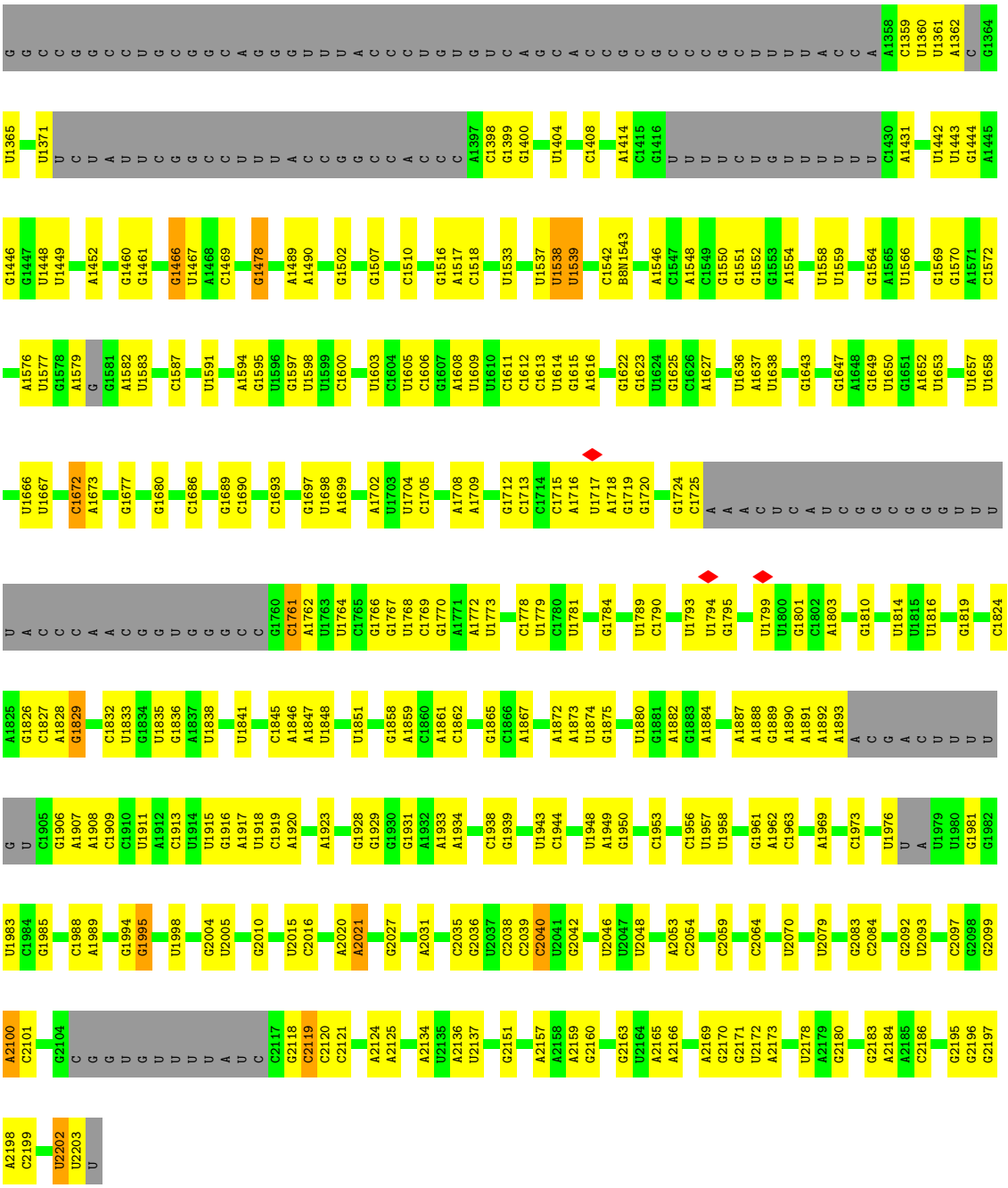
• Molecule 50: Putative 60S ribosomal protein L44

Chain Lp:

• Molecule 51: SSU_rRNA_chain_S1

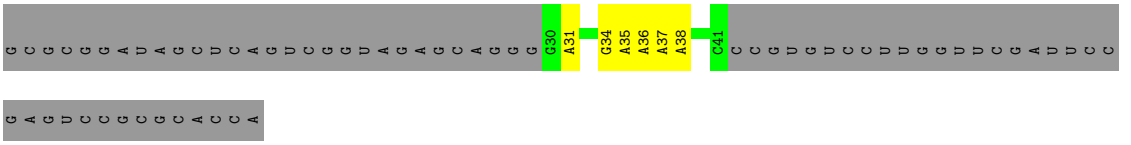
Chain S1:





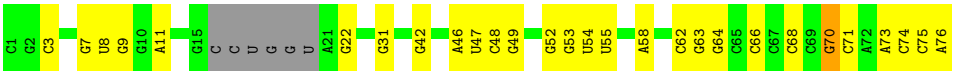
• Molecule 52: A-site_tRNA_chain_S2

Chain S2:



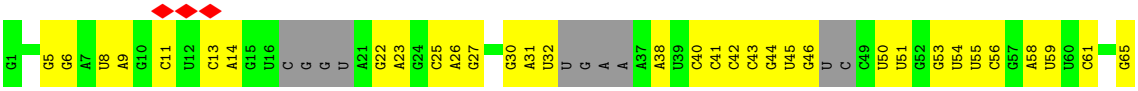
• Molecule 53: P-site_tRNA_chain_S3

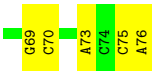
Chain S3:



• Molecule 54: E-site_tRNA_chain_S4

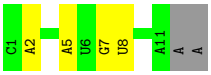
Chain S4:





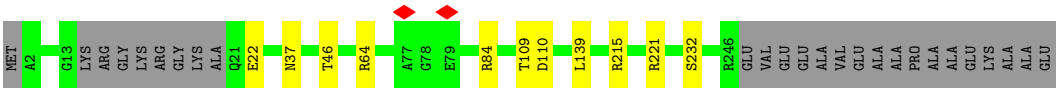
• Molecule 55: mRNA_chain_S5

Chain S5:



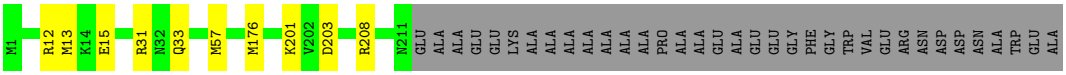
• Molecule 56: 40S ribosomal protein S3a

Chain SA:



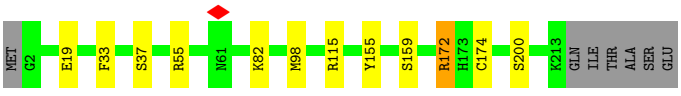
• Molecule 57: 40S ribosomal protein SA

Chain SB:



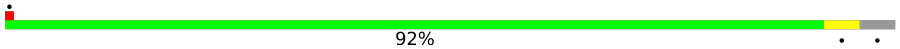
• Molecule 58: Putative 40S ribosomal protein S3

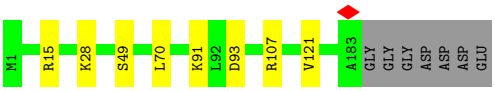
Chain SC:



• Molecule 59: Putative 40S ribosomal protein S9

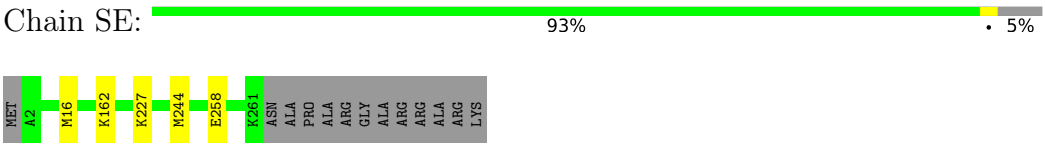
Chain SD:





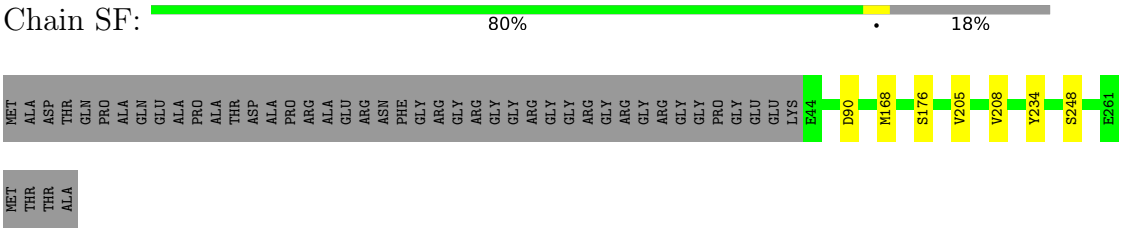
• Molecule 60: 40S ribosomal protein S4

Chain SE:



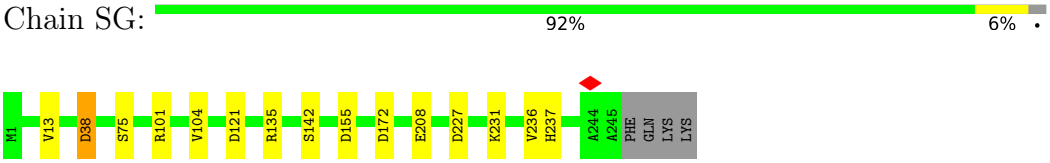
• Molecule 61: 40S ribosomal protein S2

Chain SF:



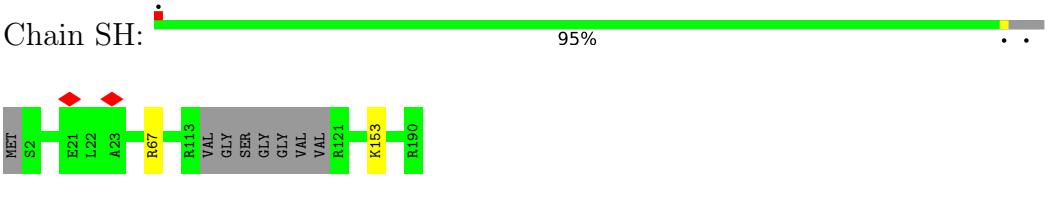
• Molecule 62: 40S ribosomal protein S6

Chain SG:



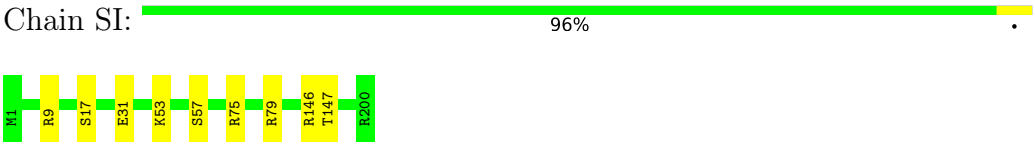
• Molecule 63: 40S ribosomal protein S5

Chain SH:



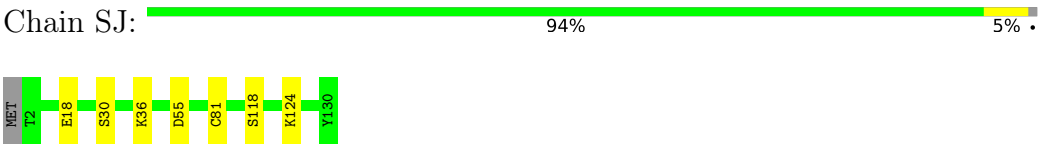
• Molecule 64: 40S ribosomal protein S7

Chain SI:



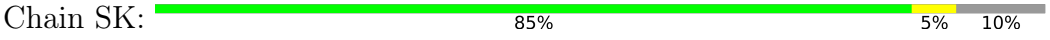
• Molecule 65: Putative 40S ribosomal protein S15A

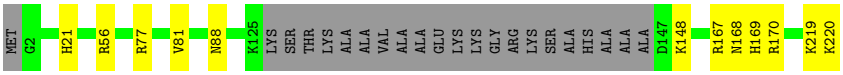
Chain SJ:



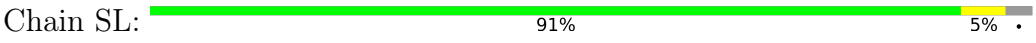
• Molecule 66: 40S ribosomal protein S8

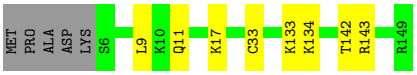
Chain SK:



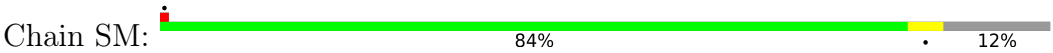


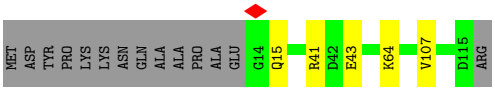
• Molecule 67: Putative 40S ribosomal protein S16



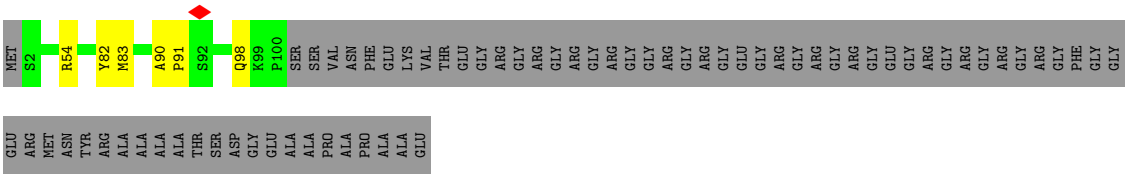


• Molecule 68: Putative ribosomal protein S20

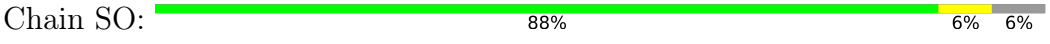


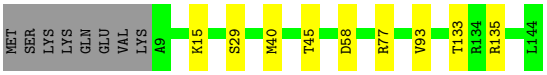


• Molecule 69: Putative 40S ribosomal protein S10

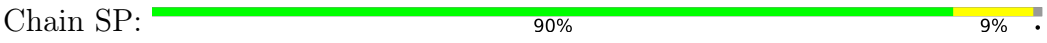


• Molecule 70: 40S ribosomal protein S14

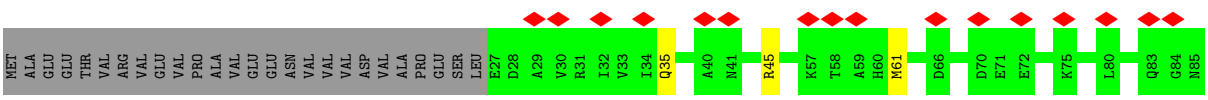


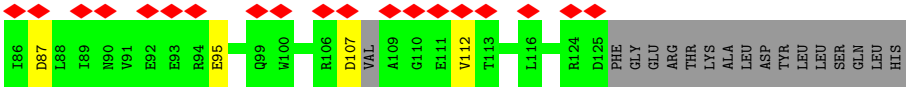


• Molecule 71: Putative 40S ribosomal protein S23



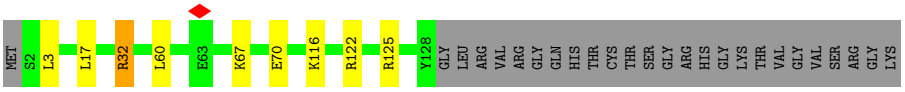
• Molecule 72: 40S ribosomal protein S12





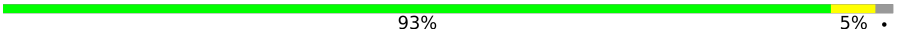
• Molecule 73: Putative 40S ribosomal protein S18

Chain SR:



• Molecule 74: Putative ribosomal protein S29

Chain SS:

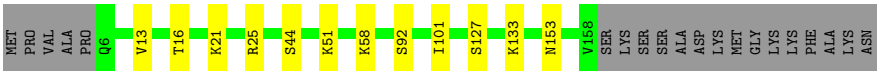


• Molecule 75: Putative 40S ribosomal protein S13

Chain ST:

• Molecule 76: Ribosomal protein S17 family protein

Chain SU:

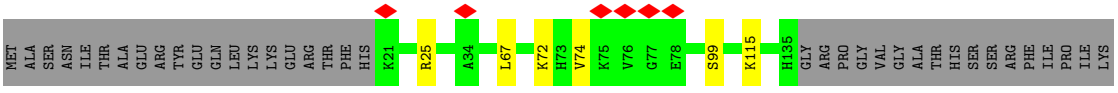


• Molecule 77: Putative 40S ribosomal protein S17

Chain SV:

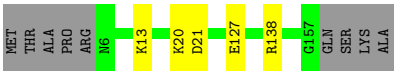
• Molecule 78: Putative 40S ribosomal protein S15

Chain SW:

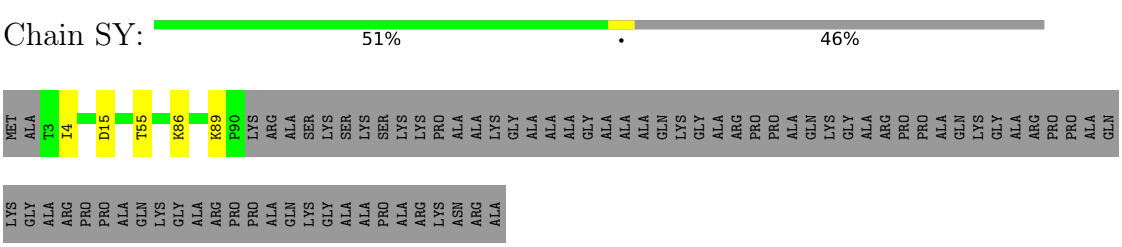


• Molecule 79: 40S ribosomal protein S19-like protein

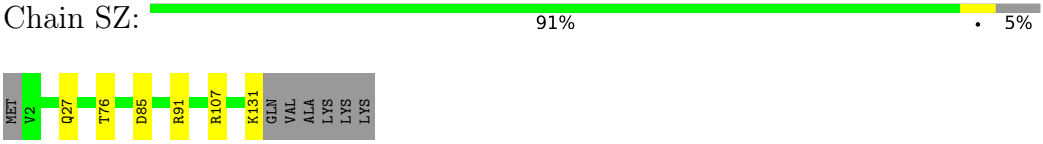
Chain SX:



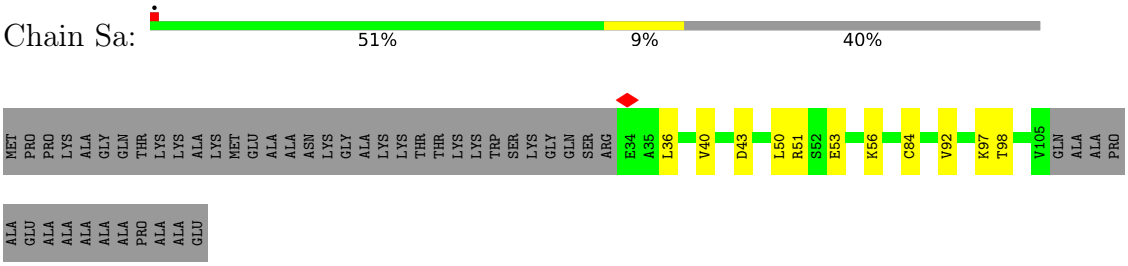
• Molecule 80: Putative 40S ribosomal protein S21



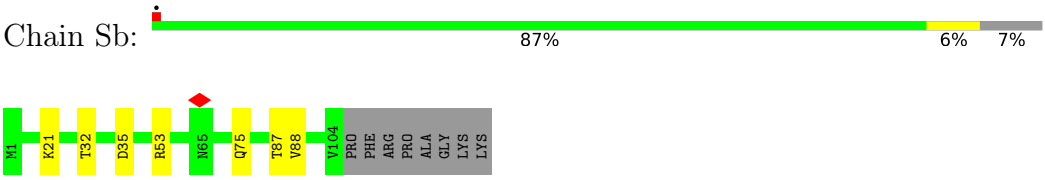
• Molecule 81: 40S ribosomal protein S24



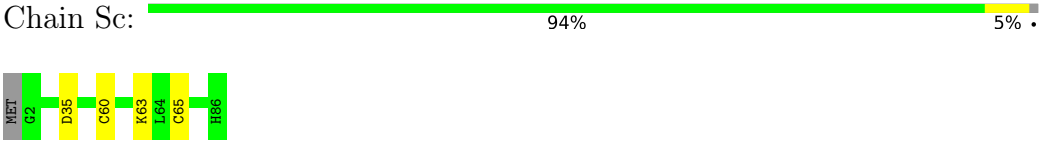
• Molecule 82: 40S ribosomal protein S25



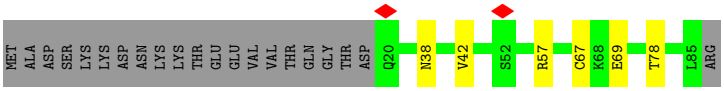
• Molecule 83: 40S ribosomal protein S26



• Molecule 84: Putative 40S ribosomal protein S27-1

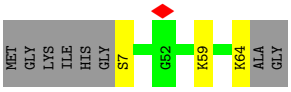


• Molecule 85: Putative 40S ribosomal protein S33



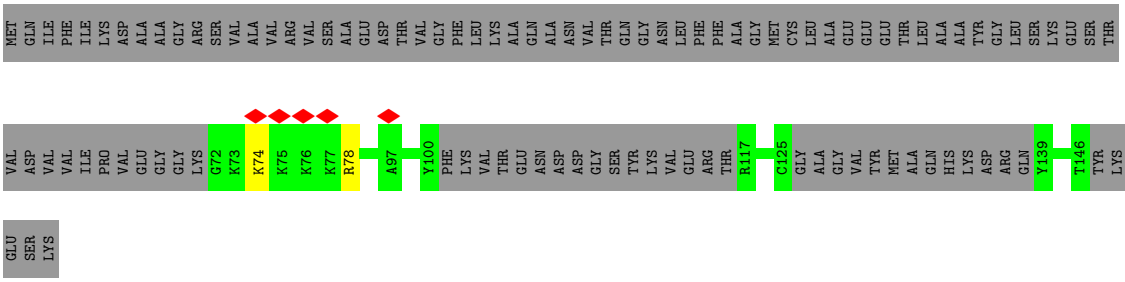
• Molecule 86: 40S ribosomal protein S30

Chain Se:



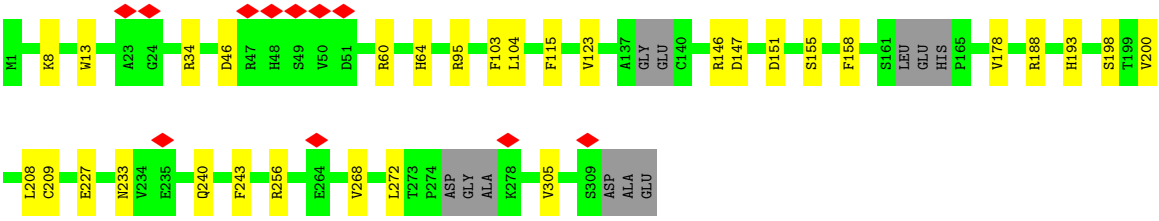
• Molecule 87: Ubiquitin-60S ribosomal protein L40

Chain Sf:



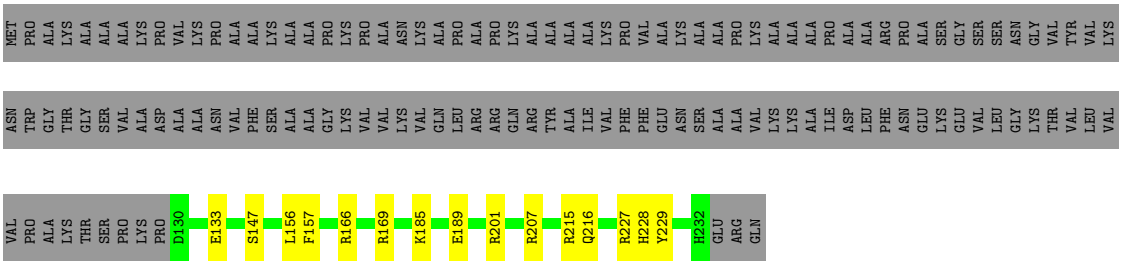
• Molecule 88: Guanine nucleotide-binding protein subunit beta-like protein

Chain Sg:



• Molecule 89: Putative RNA binding protein

Chain Sh:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	490938	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 ($e^-/Å^2$)	1.273	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, OMG, NA, K, MA6, ZN, B8N, PSU, MG, OMC, OMU, A2M, MIA, 7MG, 5MC

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	L1	0.66	0/38810	1.11	28/60514 (0.0%)
2	L2	0.67	0/25898	1.11	25/40361 (0.1%)
3	L3	0.67	0/4302	1.13	5/6687 (0.1%)
4	L4	0.66	0/4376	1.10	4/6822 (0.1%)
5	L5	0.68	0/2903	1.14	3/4518 (0.1%)
6	L6	0.70	0/1683	1.14	3/2618 (0.1%)
7	L7	0.65	0/3802	1.11	3/5917 (0.1%)
8	L8	0.68	0/2829	1.08	4/4405 (0.1%)
9	LA	0.28	0/1972	0.58	0/2646
10	LB	0.27	0/3236	0.55	0/4354
11	LC	0.27	0/2865	0.54	0/3854
12	LD	0.30	0/1363	0.53	0/1825
13	LE	0.27	0/1492	0.53	0/2011
14	LF	0.27	0/1173	0.52	0/1586
15	LG	0.26	0/1932	0.54	0/2599
16	LH	0.26	0/1800	0.53	0/2418
17	LI	0.31	0/1668	0.54	0/2236
18	LJ	0.27	0/1025	0.52	0/1383
19	LK	0.27	0/1346	0.49	0/1805
20	LL	0.29	0/1151	0.53	0/1538
21	LM	0.27	0/1751	0.57	0/2338
22	LN	0.25	0/1647	0.54	0/2203
23	LO	0.29	0/2252	0.50	0/3024
24	LP	0.27	0/1560	0.55	0/2088
25	LQ	0.26	0/1698	0.55	0/2246
26	LR	0.28	0/1489	0.53	0/2008
27	LS	0.27	0/1276	0.53	0/1720
28	LT	0.28	0/1242	0.53	0/1666
29	LU	0.26	0/973	0.51	0/1299
30	LV	0.26	0/960	0.52	0/1293
31	LW	0.27	0/970	0.56	0/1296
32	LX	0.27	0/735	0.55	0/989

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	LY	0.26	0/1088	0.53	0/1455
34	LZ	0.29	0/1129	0.55	0/1512
35	La	0.26	0/1054	0.55	0/1399
36	Lb	0.25	0/557	0.53	0/743
37	Lc	0.28	0/1896	0.53	0/2540
38	Ld	0.28	0/754	0.52	0/1019
39	Le	0.26	0/1488	0.54	0/1979
40	Lf	0.27	0/1066	0.55	0/1424
41	Lg	0.32	0/1172	0.59	0/1573
42	Lh	0.33	0/1045	0.59	0/1390
43	Li	0.28	0/822	0.53	0/1099
44	Lj	0.27	0/686	0.62	0/915
45	Lk	0.26	0/590	0.52	0/798
46	Ll	0.26	0/463	0.52	0/617
47	Lm	0.24	0/408	0.52	0/545
48	Ln	0.25	0/294	0.67	0/383
49	Lo	0.32	0/705	0.61	0/940
50	Lp	0.27	0/793	0.50	0/1048
51	S1	0.69	0/42900	1.10	49/66828 (0.1%)
52	S2	0.73	0/260	1.07	0/400
53	S3	0.73	0/1690	1.06	1/2631 (0.0%)
54	S4	0.73	0/1568	1.11	0/2436
55	S5	0.69	0/254	1.12	0/392
56	SA	0.24	0/1933	0.56	0/2596
57	SB	0.25	0/1683	0.50	0/2279
58	SC	0.31	0/1650	0.54	0/2209
59	SD	0.26	0/1532	0.55	0/2054
60	SE	0.25	0/2092	0.52	0/2819
61	SF	0.26	0/1698	0.50	0/2301
62	SG	0.27	0/1972	0.58	1/2635 (0.0%)
63	SH	0.24	0/1452	0.50	0/1948
64	SI	0.25	0/1669	0.52	0/2244
65	SJ	0.26	0/1038	0.52	0/1391
66	SK	0.25	0/1623	0.57	0/2169
67	SL	0.33	0/1161	0.53	0/1559
68	SM	0.24	0/806	0.54	0/1093
69	SN	3.35	1/831 (0.1%)	1.21	3/1127 (0.3%)
70	SO	0.26	0/1025	0.59	0/1379
71	SP	0.25	0/1116	0.51	0/1496
72	SQ	0.26	0/655	0.57	0/890
73	SR	0.28	0/1029	0.56	0/1384
74	SS	0.23	0/457	0.52	0/606
75	ST	0.26	0/1182	0.54	0/1584

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SU	0.27	0/1280	0.53	0/1720
77	SV	0.24	0/945	0.50	0/1265
78	SW	0.25	0/945	0.53	0/1271
79	SX	0.24	0/1237	0.51	0/1661
80	SY	0.24	0/669	0.50	0/908
81	SZ	0.25	0/1071	0.51	0/1425
82	Sa	0.24	0/572	0.55	0/769
83	Sb	0.25	0/844	0.58	0/1129
84	Sc	0.26	0/688	0.57	0/921
85	Sd	0.24	0/481	0.55	0/647
86	Se	0.25	0/473	0.51	0/627
87	Sf	0.73	0/303	0.63	0/408
88	Sg	0.24	0/2398	0.51	0/3256
89	Sh	0.26	0/843	0.54	0/1134
All	All	0.58	1/224214 (0.0%)	0.94	129/329237 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	LE	0	1
17	LI	0	1
25	LQ	0	1
34	LZ	0	2
49	Lo	0	1
58	SC	0	1
73	SR	0	1
87	Sf	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	SN	91	PRO	N-CD	95.85	2.82	1.47

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	SN	91	PRO	N-CD-CG	-33.16	53.46	103.20
69	SN	91	PRO	CA-N-CD	-14.57	91.11	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	S1	99	U	O4'-C1'-N1	6.82	113.65	108.20
51	S1	92	U	O4'-C1'-N1	6.81	113.65	108.20
51	S1	337	U	O4'-C1'-N1	6.77	113.61	108.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	LE	155	ARG	Sidechain
17	LI	157	ARG	Sidechain
25	LQ	117	ARG	Sidechain
34	LZ	13	ARG	Sidechain
34	LZ	22	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LA	253/260 (97%)	246 (97%)	7 (3%)	0	100	100
10	LB	399/419 (95%)	391 (98%)	8 (2%)	0	100	100
11	LC	364/373 (98%)	352 (97%)	12 (3%)	0	100	100
12	LD	173/188 (92%)	169 (98%)	4 (2%)	0	100	100
13	LE	184/190 (97%)	177 (96%)	7 (4%)	0	100	100
14	LF	145/195 (74%)	138 (95%)	7 (5%)	0	100	100
15	LG	240/264 (91%)	238 (99%)	2 (1%)	0	100	100
16	LH	219/222 (99%)	215 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	LI	206/220 (94%)	202 (98%)	3 (2%)	1 (0%)	29	66
18	LJ	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
19	LK	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
20	LL	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
21	LM	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
22	LN	195/213 (92%)	191 (98%)	4 (2%)	0	100	100
23	LO	284/305 (93%)	279 (98%)	5 (2%)	0	100	100
24	LP	195/198 (98%)	191 (98%)	4 (2%)	0	100	100
25	LQ	199/254 (78%)	199 (100%)	0	0	100	100
26	LR	176/179 (98%)	176 (100%)	0	0	100	100
27	LS	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
28	LT	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
29	LU	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
30	LV	117/145 (81%)	116 (99%)	1 (1%)	0	100	100
31	LW	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
32	LX	81/124 (65%)	78 (96%)	3 (4%)	0	100	100
33	LY	131/134 (98%)	129 (98%)	2 (2%)	0	100	100
34	LZ	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
35	La	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
36	Lb	66/70 (94%)	62 (94%)	4 (6%)	0	100	100
37	Lc	227/252 (90%)	222 (98%)	5 (2%)	0	100	100
38	Ld	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
39	Le	184/188 (98%)	182 (99%)	2 (1%)	0	100	100
40	Lf	126/133 (95%)	123 (98%)	3 (2%)	0	100	100
41	Lg	141/144 (98%)	140 (99%)	1 (1%)	0	100	100
42	Lh	125/168 (74%)	123 (98%)	2 (2%)	0	100	100
43	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
44	Lj	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
45	Lk	76/83 (92%)	76 (100%)	0	0	100	100
46	Ll	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
47	Lm	49/128 (38%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	Ln	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
49	Lo	87/92 (95%)	80 (92%)	5 (6%)	2 (2%)	6	28
50	Lp	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
56	SA	234/264 (89%)	225 (96%)	9 (4%)	0	100	100
57	SB	209/246 (85%)	203 (97%)	6 (3%)	0	100	100
58	SC	210/219 (96%)	208 (99%)	2 (1%)	0	100	100
59	SD	181/190 (95%)	180 (99%)	1 (1%)	0	100	100
60	SE	258/273 (94%)	251 (97%)	7 (3%)	0	100	100
61	SF	216/265 (82%)	214 (99%)	2 (1%)	0	100	100
62	SG	243/249 (98%)	239 (98%)	4 (2%)	0	100	100
63	SH	178/190 (94%)	176 (99%)	2 (1%)	0	100	100
64	SI	198/200 (99%)	196 (99%)	2 (1%)	0	100	100
65	SJ	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
66	SK	194/220 (88%)	194 (100%)	0	0	100	100
67	SL	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
68	SM	100/116 (86%)	95 (95%)	5 (5%)	0	100	100
69	SN	97/168 (58%)	94 (97%)	3 (3%)	0	100	100
70	SO	134/144 (93%)	129 (96%)	5 (4%)	0	100	100
71	SP	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
72	SQ	94/141 (67%)	89 (95%)	5 (5%)	0	100	100
73	SR	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
74	SS	54/57 (95%)	54 (100%)	0	0	100	100
75	ST	140/151 (93%)	138 (99%)	2 (1%)	0	100	100
76	SU	151/173 (87%)	147 (97%)	4 (3%)	0	100	100
77	SV	120/143 (84%)	118 (98%)	2 (2%)	0	100	100
78	SW	113/152 (74%)	111 (98%)	2 (2%)	0	100	100
79	SX	150/161 (93%)	147 (98%)	3 (2%)	0	100	100
80	SY	86/164 (52%)	85 (99%)	1 (1%)	0	100	100
81	SZ	128/137 (93%)	126 (98%)	2 (2%)	0	100	100
82	Sa	70/120 (58%)	68 (97%)	2 (3%)	0	100	100
83	Sb	102/112 (91%)	102 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	Sc	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
85	Sd	64/87 (74%)	63 (98%)	1 (2%)	0	100	100
86	Se	56/66 (85%)	55 (98%)	1 (2%)	0	100	100
87	Sf	40/152 (26%)	38 (95%)	2 (5%)	0	100	100
88	Sg	293/312 (94%)	289 (99%)	4 (1%)	0	100	100
89	Sh	101/235 (43%)	100 (99%)	1 (1%)	0	100	100
All	All	11374/12926 (88%)	11132 (98%)	239 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	Lo	51	ALA
17	LI	66	PRO
49	Lo	52	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	LA	197/204 (97%)	193 (98%)	4 (2%)	55	81
10	LB	329/351 (94%)	313 (95%)	16 (5%)	25	59
11	LC	289/301 (96%)	265 (92%)	24 (8%)	11	37
12	LD	131/162 (81%)	118 (90%)	13 (10%)	8	28
13	LE	164/172 (95%)	151 (92%)	13 (8%)	12	39
14	LF	122/153 (80%)	112 (92%)	10 (8%)	11	37
15	LG	196/221 (89%)	185 (94%)	11 (6%)	21	54
16	LH	181/188 (96%)	166 (92%)	15 (8%)	11	37
17	LI	170/183 (93%)	165 (97%)	5 (3%)	42	74
18	LJ	105/111 (95%)	101 (96%)	4 (4%)	33	67
19	LK	136/145 (94%)	129 (95%)	7 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	LL	113/114 (99%)	107 (95%)	6 (5%)	22 56
21	LM	178/180 (99%)	170 (96%)	8 (4%)	27 62
22	LN	168/179 (94%)	153 (91%)	15 (9%)	9 33
23	LO	210/242 (87%)	201 (96%)	9 (4%)	29 64
24	LP	162/164 (99%)	152 (94%)	10 (6%)	18 50
25	LQ	169/198 (85%)	164 (97%)	5 (3%)	41 73
26	LR	157/159 (99%)	147 (94%)	10 (6%)	17 49
27	LS	128/134 (96%)	117 (91%)	11 (9%)	10 35
28	LT	128/143 (90%)	122 (95%)	6 (5%)	26 61
29	LU	92/114 (81%)	84 (91%)	8 (9%)	10 35
30	LV	100/124 (81%)	97 (97%)	3 (3%)	41 73
31	LW	101/122 (83%)	94 (93%)	7 (7%)	15 46
32	LX	74/104 (71%)	73 (99%)	1 (1%)	67 86
33	LY	111/116 (96%)	105 (95%)	6 (5%)	22 55
34	LZ	113/118 (96%)	105 (93%)	8 (7%)	14 44
35	La	114/118 (97%)	109 (96%)	5 (4%)	28 63
36	Lb	56/58 (97%)	51 (91%)	5 (9%)	9 33
37	Lc	191/209 (91%)	186 (97%)	5 (3%)	46 76
38	Ld	85/89 (96%)	78 (92%)	7 (8%)	11 37
39	Le	154/158 (98%)	144 (94%)	10 (6%)	17 48
40	Lf	111/115 (96%)	107 (96%)	4 (4%)	35 68
41	Lg	120/121 (99%)	116 (97%)	4 (3%)	38 71
42	Lh	107/146 (73%)	102 (95%)	5 (5%)	26 61
43	Li	84/88 (96%)	81 (96%)	3 (4%)	35 68
44	Lj	68/70 (97%)	65 (96%)	3 (4%)	28 63
45	Lk	57/74 (77%)	56 (98%)	1 (2%)	59 83
46	Ll	46/47 (98%)	45 (98%)	1 (2%)	52 80
47	Lm	41/113 (36%)	37 (90%)	4 (10%)	8 29
48	Ln	30/32 (94%)	27 (90%)	3 (10%)	7 27
49	Lo	69/74 (93%)	65 (94%)	4 (6%)	20 53
50	Lp	82/92 (89%)	73 (89%)	9 (11%)	6 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	SA	205/222 (92%)	194 (95%)	11 (5%)	22 55
57	SB	175/202 (87%)	165 (94%)	10 (6%)	20 54
58	SC	170/184 (92%)	158 (93%)	12 (7%)	14 44
59	SD	158/164 (96%)	150 (95%)	8 (5%)	24 57
60	SE	216/225 (96%)	211 (98%)	5 (2%)	50 79
61	SF	174/208 (84%)	167 (96%)	7 (4%)	31 66
62	SG	201/208 (97%)	186 (92%)	15 (8%)	13 41
63	SH	150/159 (94%)	148 (99%)	2 (1%)	69 88
64	SI	179/186 (96%)	170 (95%)	9 (5%)	24 58
65	SJ	110/111 (99%)	103 (94%)	7 (6%)	17 49
66	SK	162/176 (92%)	150 (93%)	12 (7%)	13 42
67	SL	116/120 (97%)	108 (93%)	8 (7%)	15 46
68	SM	92/104 (88%)	87 (95%)	5 (5%)	22 55
69	SN	86/128 (67%)	82 (95%)	4 (5%)	26 61
70	SO	101/113 (89%)	92 (91%)	9 (9%)	9 33
71	SP	113/117 (97%)	100 (88%)	13 (12%)	5 22
72	SQ	56/120 (47%)	49 (88%)	7 (12%)	4 18
73	SR	105/130 (81%)	96 (91%)	9 (9%)	10 35
74	SS	46/49 (94%)	43 (94%)	3 (6%)	17 48
75	ST	125/132 (95%)	116 (93%)	9 (7%)	14 43
76	SU	134/152 (88%)	122 (91%)	12 (9%)	9 33
77	SV	96/126 (76%)	92 (96%)	4 (4%)	30 64
78	SW	97/130 (75%)	91 (94%)	6 (6%)	18 50
79	SX	122/131 (93%)	117 (96%)	5 (4%)	30 65
80	SY	71/116 (61%)	66 (93%)	5 (7%)	15 45
81	SZ	111/118 (94%)	105 (95%)	6 (5%)	22 55
82	Sa	64/95 (67%)	53 (83%)	11 (17%)	2 9
83	Sb	85/93 (91%)	78 (92%)	7 (8%)	11 37
84	Sc	75/76 (99%)	71 (95%)	4 (5%)	22 56
85	Sd	48/75 (64%)	42 (88%)	6 (12%)	4 18
86	Se	50/54 (93%)	47 (94%)	3 (6%)	19 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
87	Sf	19/126 (15%)	18 (95%)	1 (5%)	22 56
88	Sg	258/265 (97%)	227 (88%)	31 (12%)	5 20
89	Sh	85/177 (48%)	70 (82%)	15 (18%)	2 9
All	All	9494/10798 (88%)	8905 (94%)	589 (6%)	22 50

5 of 589 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
74	SS	57	ARG
88	Sg	305	VAL
76	SU	25	ARG
74	SS	15	MET
82	Sa	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
58	SC	74	GLN
83	Sb	7	ASN
66	SK	169	HIS
86	Se	60	GLN
69	SN	98	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1648/1782 (92%)	571 (34%)	54 (3%)
2	L2	1139/1526 (74%)	369 (32%)	38 (3%)
3	L3	178/216 (82%)	66 (37%)	7 (3%)
4	L4	183/184 (99%)	60 (32%)	5 (2%)
5	L5	119/135 (88%)	37 (31%)	6 (5%)
51	S1	1809/2204 (82%)	632 (34%)	50 (2%)
52	S2	10/76 (13%)	5 (50%)	1 (10%)
53	S3	69/77 (89%)	27 (39%)	2 (2%)
54	S4	62/76 (81%)	37 (59%)	2 (3%)
55	S5	10/13 (76%)	4 (40%)	1 (10%)
6	L6	70/73 (95%)	40 (57%)	5 (7%)
7	L7	162/171 (94%)	58 (35%)	5 (3%)
8	L8	118/123 (95%)	27 (22%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5577/6656 (83%)	1933 (34%)	178 (3%)

5 of 1933 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	C
1	L1	7	C
1	L1	10	A
1	L1	16	G
1	L1	19	G

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	L7	21	U
51	S1	687	U
7	L7	104	A
51	S1	294	G
51	S1	958	G

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

162 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	$\#\|Z\| > 2$
2	OMC	L2	583	2	19,22,23	0.28	0	26,31,34	0.42	0
4	OMG	L4	74	4	18,26,27	1.00	2 (11%)	19,38,41	0.64	0
2	OMG	L2	1231	2	18,26,27	1.02	3 (16%)	19,38,41	0.71	0
2	PSU	L2	500	2	18,21,22	0.86	1 (5%)	22,30,33	0.60	0
51	PSU	S1	2048	51	18,21,22	0.89	1 (5%)	22,30,33	0.66	0
1	A2M	L1	305	1	18,25,26	0.61	0	18,36,39	1.05	3 (16%)
51	PSU	S1	12	51	18,21,22	0.87	1 (5%)	22,30,33	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	L1	695	1	19,22,23	0.29	0	26,31,34	0.44	0
51	OMU	S1	1833	51	19,22,23	0.21	0	26,31,34	0.37	0
2	OMG	L2	686	2	18,26,27	1.01	2 (11%)	19,38,41	0.77	0
1	OMU	L1	1039	1	19,22,23	0.20	0	26,31,34	0.53	0
2	PSU	L2	472	2	18,21,22	0.85	1 (5%)	22,30,33	0.65	0
2	PSU	L2	1194	2	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
51	OMG	S1	1478	51	18,26,27	1.01	2 (11%)	19,38,41	0.69	1 (5%)
1	PSU	L1	940	1	18,21,22	0.87	1 (5%)	22,30,33	0.74	1 (4%)
1	OMC	L1	1010	92,1	19,22,23	0.30	0	26,31,34	0.39	0
51	OMC	S1	18	51	19,22,23	0.29	0	26,31,34	0.42	0
2	PSU	L2	510	2	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
51	OMG	S1	1829	51,92	18,26,27	1.01	2 (11%)	19,38,41	0.66	0
1	A2M	L1	678	2,1	18,25,26	0.61	0	18,36,39	0.75	1 (5%)
2	A2M	L2	572	2	18,25,26	0.60	0	18,36,39	0.89	1 (5%)
2	OMG	L2	1229	2	18,26,27	1.02	3 (16%)	19,38,41	0.70	1 (5%)
51	OMU	S1	8	51	19,22,23	0.24	0	26,31,34	0.56	0
1	OMG	L1	856	1	18,26,27	1.02	3 (16%)	19,38,41	0.73	0
2	OMU	L2	560	2,91	19,22,23	0.21	0	26,31,34	1.00	1 (3%)
1	PSU	L1	1171	1	18,21,22	0.89	1 (5%)	22,30,33	0.66	0
51	7MG	S1	1995	51,53	22,26,27	1.05	1 (4%)	29,39,42	0.70	0
1	PSU	L1	1529	1	18,21,22	0.88	1 (5%)	22,30,33	0.70	0
51	PSU	S1	455	51	18,21,22	0.88	1 (5%)	22,30,33	0.66	0
2	PSU	L2	1264	2	18,21,22	0.86	1 (5%)	22,30,33	0.76	1 (4%)
1	OMU	L1	845	1	19,22,23	0.30	0	26,31,34	0.86	0
2	OMG	L2	641	2	18,26,27	1.00	3 (16%)	19,38,41	0.84	0
2	A2M	L2	1372	2	18,25,26	0.61	0	18,36,39	0.83	1 (5%)
1	PSU	L1	1177	1	18,21,22	0.87	1 (5%)	22,30,33	0.52	0
1	PSU	L1	1664	1	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
2	OMG	L2	71	2	18,26,27	0.99	2 (11%)	19,38,41	0.80	0
1	A2M	L1	235	1	18,25,26	0.61	0	18,36,39	0.81	1 (5%)
2	5MC	L2	1308	2	18,22,23	0.32	0	26,32,35	0.63	1 (3%)
1	PSU	L1	239	1	18,21,22	0.89	1 (5%)	22,30,33	0.60	0
1	PSU	L1	510	1	18,21,22	0.89	1 (5%)	22,30,33	0.59	0
2	A2M	L2	527	2	18,25,26	0.63	0	18,36,39	0.77	1 (5%)
3	OMU	L3	13	3	19,22,23	0.23	0	26,31,34	0.51	0
2	PSU	L2	1284	2	18,21,22	0.85	1 (5%)	22,30,33	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PSU	L7	69	7,92	18,21,22	0.86	1 (5%)	22,30,33	0.75	0
1	A2M	L1	69	1	18,25,26	0.61	0	18,36,39	0.82	1 (5%)
1	OMG	L1	959	1	18,26,27	1.02	2 (11%)	19,38,41	0.97	1 (5%)
2	A2M	L2	570	2,1	18,25,26	0.61	0	18,36,39	0.83	1 (5%)
1	A2M	L1	681	1	18,25,26	0.59	0	18,36,39	0.73	1 (5%)
2	PSU	L2	1303	2	18,21,22	0.84	1 (5%)	22,30,33	0.73	0
2	OMC	L2	1159	2	19,22,23	0.28	0	26,31,34	0.45	0
51	PSU	S1	1841	51	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
1	1MA	L1	677	1	16,25,26	0.78	1 (6%)	18,37,40	0.71	0
51	OMC	S1	2140	51	19,22,23	0.29	0	26,31,34	0.52	0
2	PSU	L2	802	2,92	18,21,22	0.87	1 (5%)	22,30,33	0.59	0
2	A2M	L2	1185	2	18,25,26	0.61	0	18,36,39	0.76	1 (5%)
51	PSU	S1	1657	51	18,21,22	0.85	1 (5%)	22,30,33	0.58	0
51	OMC	S1	1866	51	19,22,23	0.28	0	26,31,34	0.46	0
2	A2M	L2	502[B]	2	18,25,26	0.64	0	18,36,39	1.03	2 (11%)
51	PSU	S1	1246	51	18,21,22	0.87	1 (5%)	22,30,33	0.58	0
1	OMC	L1	1527	1	19,22,23	0.29	0	26,31,34	0.35	0
51	5MC	S1	1544	51	18,22,23	0.31	0	26,32,35	0.50	0
51	PSU	S1	1156	51	18,21,22	0.87	1 (5%)	22,30,33	0.62	0
2	OMC	L2	1397	2	19,22,23	0.27	0	26,31,34	0.56	0
51	OMG	S1	1550	51	18,26,27	1.00	2 (11%)	19,38,41	0.70	0
2	PSU	L2	1152	2	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
51	PSU	S1	2046	51	18,21,22	0.88	1 (5%)	22,30,33	0.74	0
1	A2M	L1	927	1	18,25,26	0.60	0	18,36,39	0.72	1 (5%)
2	PSU	L2	593	2	18,21,22	0.87	1 (5%)	22,30,33	0.56	0
51	A2M	S1	98	51,92	18,25,26	0.62	0	18,36,39	0.79	1 (5%)
1	A2M	L1	1373	1	18,25,26	0.61	0	18,36,39	0.79	1 (5%)
51	PSU	S1	33	51	18,21,22	0.88	1 (5%)	22,30,33	0.66	0
2	OMC	L2	443	2,91,90	19,22,23	0.34	0	26,31,34	0.50	0
51	OMC	S1	38	51	19,22,23	0.28	0	26,31,34	0.52	0
2	PSU	L2	1382	2,92	18,21,22	0.87	1 (5%)	22,30,33	0.69	0
51	A2M	S1	2021	51	18,25,26	0.62	0	18,36,39	0.80	1 (5%)
51	OMG	S1	1623	51	18,26,27	1.00	3 (16%)	19,38,41	0.66	0
2	A2M	L2	382	2	18,25,26	0.60	0	18,36,39	0.73	1 (5%)
2	PSU	L2	1403	2	18,21,22	0.87	1 (5%)	22,30,33	0.71	0
1	OMG	L1	1190	1	18,26,27	1.01	2 (11%)	19,38,41	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	OMG	S1	2151	51	18,26,27	1.01	2 (11%)	19,38,41	0.76	0
2	A2M	L2	604	2,1	18,25,26	0.62	1 (5%)	18,36,39	0.78	1 (5%)
2	OMG	L2	1046	2,53	18,26,27	1.01	2 (11%)	19,38,41	0.65	0
1	PSU	L1	1528	1	18,21,22	0.87	1 (5%)	22,30,33	0.52	0
2	OMC	L2	1248	2	19,22,23	0.28	0	26,31,34	0.49	0
2	PSU	L2	1058	2	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
1	PSU	L1	1533	2,1	18,21,22	0.86	1 (5%)	22,30,33	0.63	0
2	OMG	L2	1517	2	18,26,27	1.01	2 (11%)	19,38,41	0.71	0
51	5MC	S1	2061	51	18,22,23	0.30	0	26,32,35	0.56	0
1	PSU	L1	1181	1	18,21,22	0.86	1 (5%)	22,30,33	0.74	1 (4%)
7	A2M	L7	162	7,1	18,25,26	0.59	0	18,36,39	0.73	1 (5%)
2	PSU	L2	1318	2	18,21,22	0.85	1 (5%)	22,30,33	0.64	0
51	B8N	S1	1543	-	24,29,30	0.80	1 (4%)	29,42,45	0.76	0
2	A2M	L2	1384	2,92	18,25,26	0.61	0	18,36,39	0.85	1 (5%)
1	A2M	L1	407	1	18,25,26	0.60	0	18,36,39	0.85	1 (5%)
51	PSU	S1	1533	51	18,21,22	0.88	1 (5%)	22,30,33	0.71	0
2	PSU	L2	626	2	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
2	OMU	L2	1419	2	19,22,23	0.20	0	26,31,34	0.32	0
2	OMU	L2	1359	2	19,22,23	0.20	0	26,31,34	0.51	0
51	PSU	S1	1566	51	18,21,22	0.86	1 (5%)	22,30,33	0.58	0
7	PSU	L7	74	7,90	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
2	PSU	L2	565	2	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
51	PSU	S1	1539	51	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
51	OMU	S1	29	51	19,22,23	0.19	0	26,31,34	0.58	0
51	OMG	S1	1647	51	18,26,27	1.00	2 (11%)	19,38,41	0.84	1 (5%)
2	PSU	L2	597	2	18,21,22	0.87	1 (5%)	22,30,33	0.65	0
1	PSU	L1	1017	1	18,21,22	0.87	1 (5%)	22,30,33	0.74	0
2	A2M	L2	95	2	18,25,26	0.61	0	18,36,39	0.75	1 (5%)
51	OMU	S1	1979	51	19,22,23	0.21	0	26,31,34	0.39	0
2	OMG	L2	655	2	18,26,27	1.01	2 (11%)	19,38,41	0.75	0
2	OMG	L2	534	2	18,26,27	1.01	2 (11%)	19,38,41	0.67	1 (5%)
2	OMG	L2	1078	2	18,26,27	1.01	3 (16%)	19,38,41	0.86	2 (10%)
2	A2M	L2	591	2	18,25,26	0.61	0	18,36,39	0.77	1 (5%)
1	A2M	L1	1539	2,92,1	18,25,26	0.61	0	18,36,39	0.74	1 (5%)
2	OMU	L2	667	2	19,22,23	0.20	0	26,31,34	0.60	0
51	OMU	S1	1621	51	19,22,23	0.21	0	26,31,34	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMU	L1	1659	92,1	19,22,23	0.21	0	26,31,34	0.40	0
1	PSU	L1	774	1	18,21,22	0.87	1 (5%)	22,30,33	0.75	1 (4%)
2	OMC	L2	14	2,1	19,22,23	0.27	0	26,31,34	0.33	0
2	A2M	L2	628	2	18,25,26	0.60	0	18,36,39	0.74	1 (5%)
2	5MC	L2	524	2,92	18,22,23	0.33	0	26,32,35	0.50	0
2	A2M	L2	665	2	18,25,26	0.60	0	18,36,39	0.72	1 (5%)
1	A2M	L1	955	1	18,25,26	0.59	0	18,36,39	0.78	1 (5%)
2	PSU	L2	1060	2	18,21,22	0.89	1 (5%)	22,30,33	0.83	1 (4%)
2	PSU	L2	78	2	18,21,22	0.88	1 (5%)	22,30,33	0.75	1 (4%)
1	A2M	L1	858	1	18,25,26	0.62	1 (5%)	18,36,39	0.83	1 (5%)
2	OMG	L2	1253	2	18,26,27	1.00	2 (11%)	19,38,41	0.66	1 (5%)
51	OMG	S1	1865	51	18,26,27	0.99	2 (11%)	19,38,41	0.80	0
2	OMC	L2	1317	2	19,22,23	0.27	0	26,31,34	0.33	0
7	A2M	L7	43	7	18,25,26	0.60	0	18,36,39	0.87	1 (5%)
2	OMU	L2	73	2	19,22,23	0.22	0	26,31,34	0.42	0
51	PSU	S1	1192	51	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
52	MIA	S2	37	52	24,31,32	0.82	1 (4%)	26,44,47	4.50	2 (7%)
51	MA6	S1	2185	51,90	18,26,27	0.72	0	19,38,41	0.41	0
1	PSU	L1	422	1	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
51	PSU	S1	2202	51	18,21,22	0.85	1 (5%)	22,30,33	0.57	0
1	OMG	L1	1524	1	18,26,27	1.02	2 (11%)	19,38,41	0.94	1 (5%)
2	PSU	L2	512	2	18,21,22	0.87	1 (5%)	22,30,33	0.73	0
51	MA6	S1	2184	51,90	18,26,27	0.75	1 (5%)	19,38,41	0.50	0
2	OMG	L2	1360	2	18,26,27	1.01	2 (11%)	19,38,41	0.66	0
51	A2M	S1	479	51	18,25,26	0.59	0	18,36,39	0.74	1 (5%)
1	OMG	L1	1540	2,1,90	18,26,27	1.02	2 (11%)	19,38,41	0.64	0
7	PSU	L7	101	7	18,21,22	0.86	1 (5%)	22,30,33	0.76	1 (4%)
2	PSU	L2	437	2	18,21,22	0.85	1 (5%)	22,30,33	0.65	0
51	A2M	S1	668	51,92	18,25,26	0.60	0	18,36,39	0.81	1 (5%)
2	PSU	L2	1265	2	18,21,22	0.87	1 (5%)	22,30,33	0.71	0
1	OMG	L1	1626	1	18,26,27	1.01	3 (16%)	19,38,41	0.69	0
2	A2M	L2	502[A]	2,51	18,25,26	0.63	0	18,36,39	1.12	3 (16%)
2	OMC	L2	359	2	19,22,23	0.27	0	26,31,34	0.41	0
2	PSU	L2	1144	2	18,21,22	0.83	1 (5%)	22,30,33	0.64	0
1	OMU	L1	1107	1	19,22,23	0.20	0	26,31,34	0.60	0
2	PSU	L2	1413	2,90	18,21,22	0.88	1 (5%)	22,30,33	0.71	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	L1	1011	2,1	18,21,22	0.83	1 (5%)	22,30,33	0.74	1 (4%)
1	OMU	L1	847	1	19,22,23	0.20	0	26,31,34	0.51	0
7	OMG	L7	75	7	18,26,27	1.00	2 (11%)	19,38,41	0.75	1 (5%)
51	A2M	S1	512	51	18,25,26	0.60	0	18,36,39	0.85	1 (5%)
51	OMU	S1	661	51	19,22,23	0.20	0	26,31,34	0.39	0
2	OMU	L2	1077	2	19,22,23	0.20	0	26,31,34	0.40	0
2	PSU	L2	662	2,92	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
51	OMG	S1	600	51	18,26,27	1.00	2 (11%)	19,38,41	0.68	0
1	A2M	L1	697	1	18,25,26	0.60	0	18,36,39	0.81	1 (5%)
1	OMU	L1	1371	1	19,22,23	0.28	0	26,31,34	0.99	1 (3%)
2	PSU	L2	1213	2	18,21,22	0.85	1 (5%)	22,30,33	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L2	583	2	-	0/9/27/28	0/2/2/2
4	OMG	L4	74	4	-	2/5/27/28	0/3/3/3
2	OMG	L2	1231	2	-	0/5/27/28	0/3/3/3
2	PSU	L2	500	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	2048	51	-	0/7/25/26	0/2/2/2
1	A2M	L1	305	1	-	2/5/27/28	0/3/3/3
51	PSU	S1	12	51	-	0/7/25/26	0/2/2/2
1	OMC	L1	695	1	-	0/9/27/28	0/2/2/2
51	OMU	S1	1833	51	-	2/9/27/28	0/2/2/2
2	OMG	L2	686	2	-	2/5/27/28	0/3/3/3
1	OMU	L1	1039	1	-	0/9/27/28	0/2/2/2
2	PSU	L2	472	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1194	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1478	51	-	1/5/27/28	0/3/3/3
1	PSU	L1	940	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	1010	92,1	-	2/9/27/28	0/2/2/2
51	OMC	S1	18	51	-	1/9/27/28	0/2/2/2
2	PSU	L2	510	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1829	51,92	-	2/5/27/28	0/3/3/3
1	A2M	L1	678	2,1	-	4/5/27/28	0/3/3/3
2	A2M	L2	572	2	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L2	1229	2	-	2/5/27/28	0/3/3/3
51	OMU	S1	8	51	-	6/9/27/28	0/2/2/2
1	OMG	L1	856	1	-	0/5/27/28	0/3/3/3
2	OMU	L2	560	2,91	-	3/9/27/28	0/2/2/2
1	PSU	L1	1171	1	-	2/7/25/26	0/2/2/2
51	7MG	S1	1995	51,53	-	0/7/37/38	0/3/3/3
1	PSU	L1	1529	1	-	0/7/25/26	0/2/2/2
51	PSU	S1	455	51	-	1/7/25/26	0/2/2/2
2	PSU	L2	1264	2	-	2/7/25/26	0/2/2/2
1	OMU	L1	845	1	-	3/9/27/28	0/2/2/2
2	OMG	L2	641	2	-	0/5/27/28	0/3/3/3
2	A2M	L2	1372	2	-	0/5/27/28	0/3/3/3
1	PSU	L1	1177	1	-	2/7/25/26	0/2/2/2
1	PSU	L1	1664	1	-	0/7/25/26	0/2/2/2
2	OMG	L2	71	2	-	0/5/27/28	0/3/3/3
1	A2M	L1	235	1	-	2/5/27/28	0/3/3/3
2	5MC	L2	1308	2	-	4/7/25/26	0/2/2/2
1	PSU	L1	239	1	-	0/7/25/26	0/2/2/2
1	PSU	L1	510	1	-	3/7/25/26	0/2/2/2
2	A2M	L2	527	2	-	2/5/27/28	0/3/3/3
3	OMU	L3	13	3	-	1/9/27/28	0/2/2/2
2	PSU	L2	1284	2	-	0/7/25/26	0/2/2/2
7	PSU	L7	69	7,92	-	0/7/25/26	0/2/2/2
1	A2M	L1	69	1	-	0/5/27/28	0/3/3/3
1	OMG	L1	959	1	-	3/5/27/28	0/3/3/3
2	A2M	L2	570	2,1	-	2/5/27/28	0/3/3/3
1	A2M	L1	681	1	-	3/5/27/28	0/3/3/3
2	PSU	L2	1303	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	1159	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1841	51	-	0/7/25/26	0/2/2/2
1	1MA	L1	677	1	-	0/3/25/26	0/3/3/3
51	OMC	S1	2140	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	802	2,92	-	2/7/25/26	0/2/2/2
2	A2M	L2	1185	2	-	2/5/27/28	0/3/3/3
51	PSU	S1	1657	51	-	2/7/25/26	0/2/2/2
51	OMC	S1	1866	51	-	0/9/27/28	0/2/2/2
2	A2M	L2	502[B]	2	-	2/5/27/28	0/3/3/3
51	PSU	S1	1246	51	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	L1	1527	1	-	2/9/27/28	0/2/2/2
51	5MC	S1	1544	51	-	1/7/25/26	0/2/2/2
51	PSU	S1	1156	51	-	0/7/25/26	0/2/2/2
2	OMC	L2	1397	2	-	0/9/27/28	0/2/2/2
51	OMG	S1	1550	51	-	0/5/27/28	0/3/3/3
2	PSU	L2	1152	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	2046	51	-	0/7/25/26	0/2/2/2
1	A2M	L1	927	1	-	0/5/27/28	0/3/3/3
2	PSU	L2	593	2	-	2/7/25/26	0/2/2/2
51	A2M	S1	98	51,92	-	2/5/27/28	0/3/3/3
1	A2M	L1	1373	1	-	2/5/27/28	0/3/3/3
51	PSU	S1	33	51	-	0/7/25/26	0/2/2/2
2	OMC	L2	443	2,91,90	-	4/9/27/28	0/2/2/2
51	OMC	S1	38	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	1382	2,92	-	0/7/25/26	0/2/2/2
51	A2M	S1	2021	51	-	2/5/27/28	0/3/3/3
51	OMG	S1	1623	51	-	0/5/27/28	0/3/3/3
2	A2M	L2	382	2	-	0/5/27/28	0/3/3/3
2	PSU	L2	1403	2	-	0/7/25/26	0/2/2/2
1	OMG	L1	1190	1	-	0/5/27/28	0/3/3/3
51	OMG	S1	2151	51	-	2/5/27/28	0/3/3/3
2	A2M	L2	604	2,1	-	0/5/27/28	0/3/3/3
2	OMG	L2	1046	2,53	-	3/5/27/28	0/3/3/3
1	PSU	L1	1528	1	-	2/7/25/26	0/2/2/2
2	OMC	L2	1248	2	-	1/9/27/28	0/2/2/2
2	PSU	L2	1058	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	1533	2,1	-	0/7/25/26	0/2/2/2
2	OMG	L2	1517	2	-	0/5/27/28	0/3/3/3
51	5MC	S1	2061	51	-	2/7/25/26	0/2/2/2
1	PSU	L1	1181	1	-	0/7/25/26	0/2/2/2
7	A2M	L7	162	7,1	-	1/5/27/28	0/3/3/3
2	PSU	L2	1318	2	-	0/7/25/26	0/2/2/2
51	B8N	S1	1543	-	-	6/16/34/35	0/2/2/2
2	A2M	L2	1384	2,92	-	1/5/27/28	0/3/3/3
1	A2M	L1	407	1	-	0/5/27/28	0/3/3/3
51	PSU	S1	1533	51	-	0/7/25/26	0/2/2/2
2	PSU	L2	626	2	-	0/7/25/26	0/2/2/2
2	OMU	L2	1419	2	-	0/9/27/28	0/2/2/2
2	OMU	L2	1359	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1566	51	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PSU	L7	74	7,90	-	0/7/25/26	0/2/2/2
2	PSU	L2	565	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	1539	51	-	2/7/25/26	0/2/2/2
51	OMU	S1	29	51	-	1/9/27/28	0/2/2/2
51	OMG	S1	1647	51	-	0/5/27/28	0/3/3/3
2	PSU	L2	597	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	1017	1	-	2/7/25/26	0/2/2/2
2	A2M	L2	95	2	-	1/5/27/28	0/3/3/3
51	OMU	S1	1979	51	-	1/9/27/28	0/2/2/2
2	OMG	L2	655	2	-	1/5/27/28	0/3/3/3
2	OMG	L2	534	2	-	2/5/27/28	0/3/3/3
2	OMG	L2	1078	2	-	2/5/27/28	0/3/3/3
2	A2M	L2	591	2	-	0/5/27/28	0/3/3/3
1	A2M	L1	1539	2,92,1	-	0/5/27/28	0/3/3/3
2	OMU	L2	667	2	-	1/9/27/28	0/2/2/2
51	OMU	S1	1621	51	-	0/9/27/28	0/2/2/2
1	OMU	L1	1659	92,1	-	0/9/27/28	0/2/2/2
1	PSU	L1	774	1	-	0/7/25/26	0/2/2/2
2	OMC	L2	14	2,1	-	0/9/27/28	0/2/2/2
2	A2M	L2	628	2	-	0/5/27/28	0/3/3/3
2	5MC	L2	524	2,92	-	0/7/25/26	0/2/2/2
2	A2M	L2	665	2	-	3/5/27/28	0/3/3/3
1	A2M	L1	955	1	-	1/5/27/28	0/3/3/3
2	PSU	L2	1060	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	78	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	858	1	-	1/5/27/28	0/3/3/3
2	OMG	L2	1253	2	-	0/5/27/28	0/3/3/3
51	OMG	S1	1865	51	-	0/5/27/28	0/3/3/3
2	OMC	L2	1317	2	-	0/9/27/28	0/2/2/2
7	A2M	L7	43	7	-	0/5/27/28	0/3/3/3
2	OMU	L2	73	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1192	51	-	0/7/25/26	0/2/2/2
52	MIA	S2	37	52	-	4/11/33/34	0/3/3/3
51	MA6	S1	2185	51,90	-	4/7/29/30	0/3/3/3
1	PSU	L1	422	1	-	0/7/25/26	0/2/2/2
51	PSU	S1	2202	51	-	1/7/25/26	0/2/2/2
1	OMG	L1	1524	1	-	3/5/27/28	0/3/3/3
2	PSU	L2	512	2	-	2/7/25/26	0/2/2/2
51	MA6	S1	2184	51,90	-	3/7/29/30	0/3/3/3
2	OMG	L2	1360	2	-	1/5/27/28	0/3/3/3

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A2M	S1	479	51	-	0/5/27/28	0/3/3/3
1	OMG	L1	1540	2,1,90	-	2/5/27/28	0/3/3/3
7	PSU	L7	101	7	-	0/7/25/26	0/2/2/2
2	PSU	L2	437	2	-	0/7/25/26	0/2/2/2
51	A2M	S1	668	51,92	-	2/5/27/28	0/3/3/3
2	PSU	L2	1265	2	-	1/7/25/26	0/2/2/2
1	OMG	L1	1626	1	-	0/5/27/28	0/3/3/3
2	A2M	L2	502[A]	2,51	-	3/5/27/28	0/3/3/3
2	OMC	L2	359	2	-	2/9/27/28	0/2/2/2
2	PSU	L2	1144	2	-	2/7/25/26	0/2/2/2
1	OMU	L1	1107	1	-	1/9/27/28	0/2/2/2
2	PSU	L2	1413	2,90	-	0/7/25/26	0/2/2/2
1	PSU	L1	1011	2,1	-	0/7/25/26	0/2/2/2
1	OMU	L1	847	1	-	0/9/27/28	0/2/2/2
7	OMG	L7	75	7	-	1/5/27/28	0/3/3/3
51	A2M	S1	512	51	-	2/5/27/28	0/3/3/3
51	OMU	S1	661	51	-	0/9/27/28	0/2/2/2
2	OMU	L2	1077	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	662	2,92	-	0/7/25/26	0/2/2/2
51	OMG	S1	600	51	-	1/5/27/28	0/3/3/3
1	A2M	L1	697	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	1371	1	-	5/9/27/28	0/2/2/2
2	PSU	L2	1213	2	-	0/7/25/26	0/2/2/2

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1995	7MG	C5-N7	4.26	1.40	1.35
1	L1	510	PSU	C6-C5	3.48	1.39	1.35
1	L1	1171	PSU	C6-C5	3.44	1.39	1.35
51	S1	455	PSU	C6-C5	3.41	1.39	1.35
51	S1	2048	PSU	C6-C5	3.40	1.39	1.35

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	S2	37	MIA	C11-S10-C2	22.64	119.17	102.27
2	L2	560	OMU	O3'-C3'-C4'	3.39	120.86	111.05
52	S2	37	MIA	C5-C6-N1	-2.98	118.33	120.81
2	L2	1060	PSU	C2'-C3'-C4'	-2.59	97.60	102.64
1	L1	959	OMG	O2'-C2'-C1'	2.56	114.17	109.09

There are no chirality outliers.

5 of 158 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L7	75	OMG	C1'-C2'-O2'-CM2
7	L7	162	A2M	C1'-C2'-O2'-CM'
1	L1	235	A2M	O4'-C4'-C5'-O5'
1	L1	235	A2M	C3'-C4'-C5'-O5'
1	L1	510	PSU	C2'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 299 ligands modelled in this entry, 299 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
51	S1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S1	1543:B8N	O3'	1544:5MC	P	3.91
1	S1	1542:C	O3'	1543:B8N	P	3.22

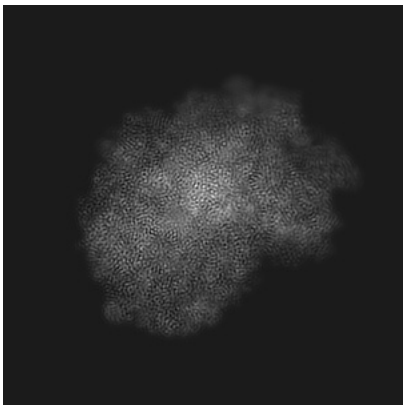
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19582. These allow visual inspection of the internal detail of the map and identification of artifacts.

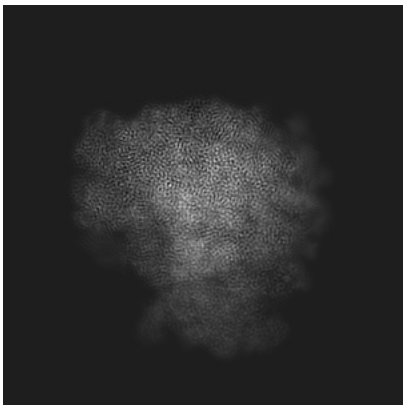
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

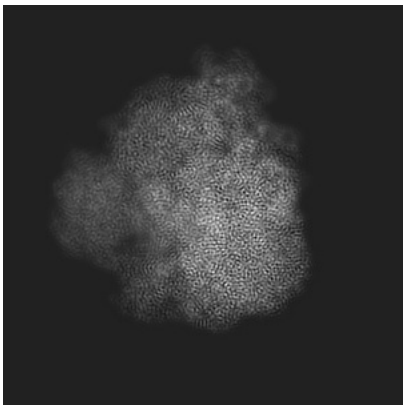
6.1.1 Primary map



X

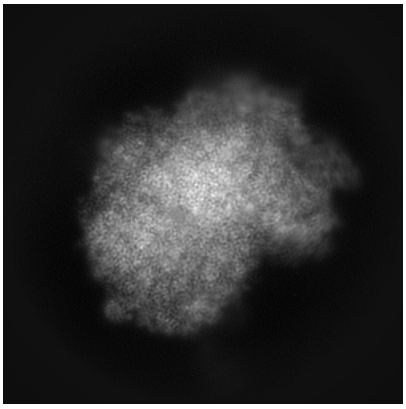


Y

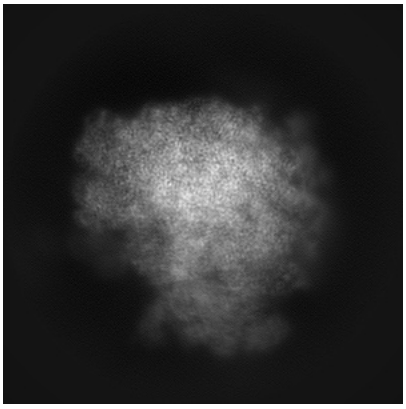


Z

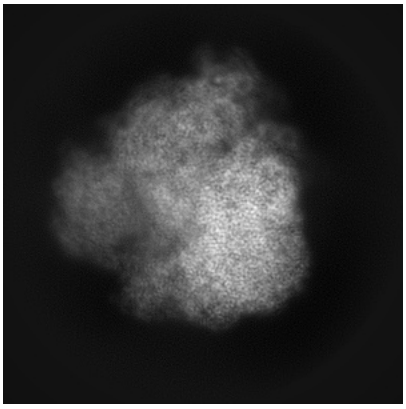
6.1.2 Raw map



X



Y

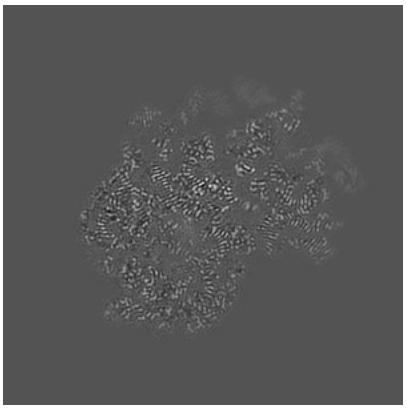


Z

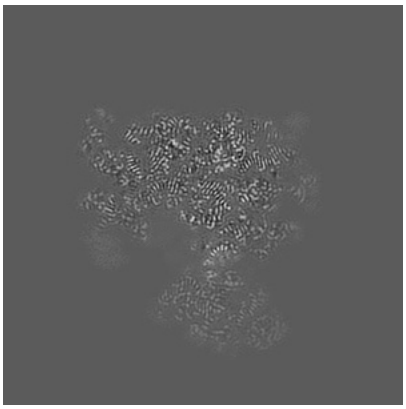
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

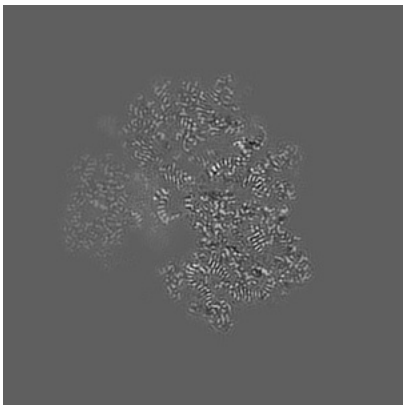
6.2.1 Primary map



X Index: 240

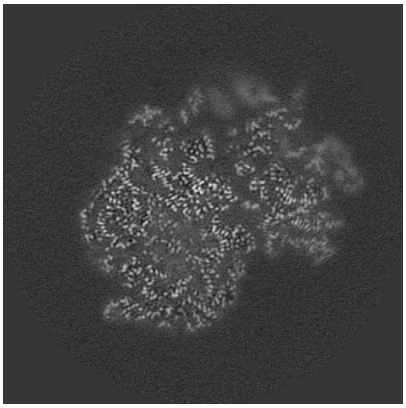


Y Index: 240

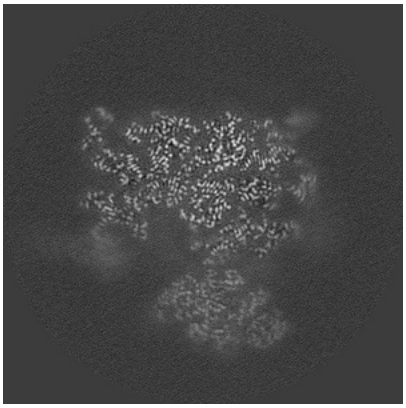


Z Index: 240

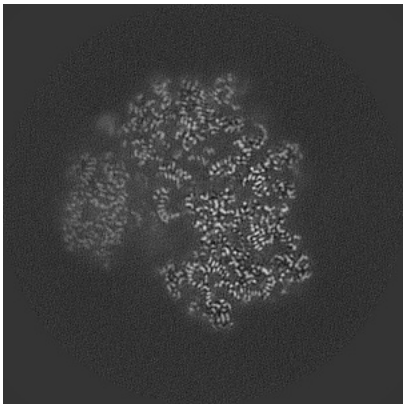
6.2.2 Raw map



X Index: 240



Y Index: 240

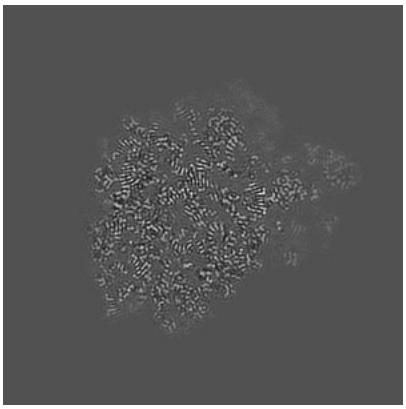


Z Index: 240

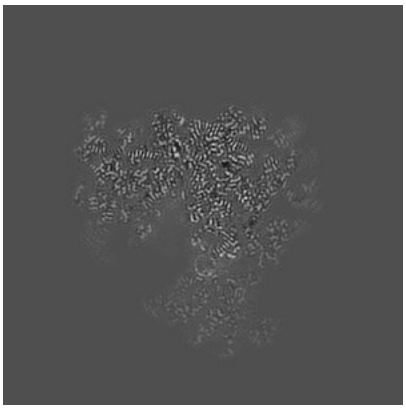
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

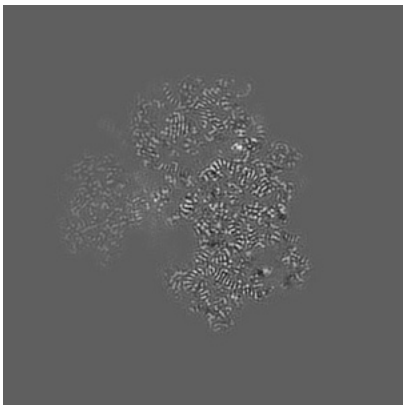
6.3.1 Primary map



X Index: 286

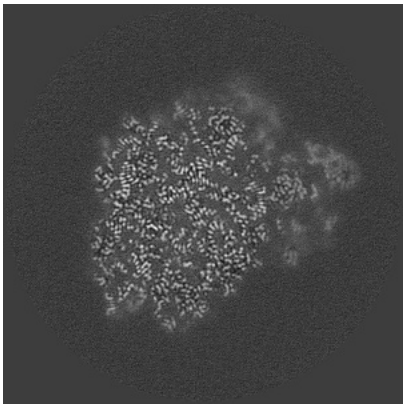


Y Index: 230

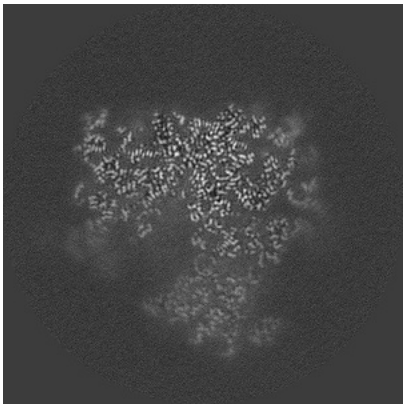


Z Index: 245

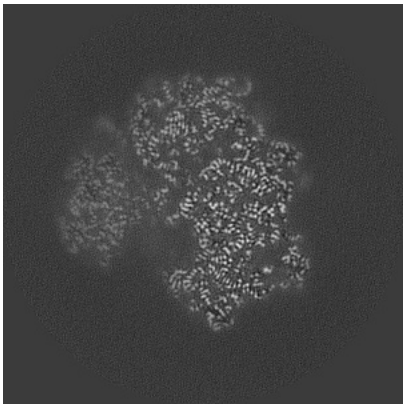
6.3.2 Raw map



X Index: 286



Y Index: 230

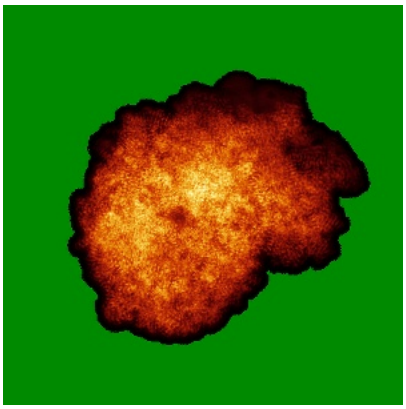


Z Index: 245

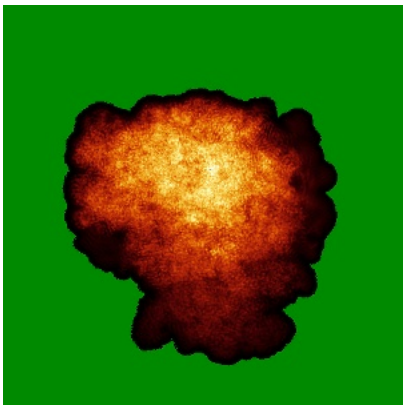
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

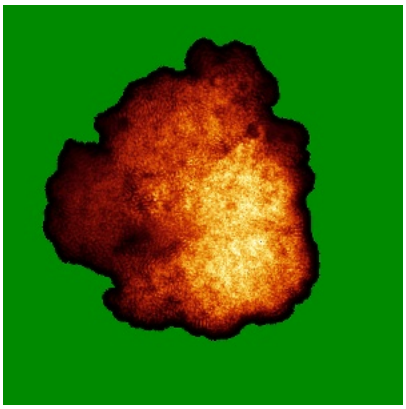
6.4.1 Primary map



X

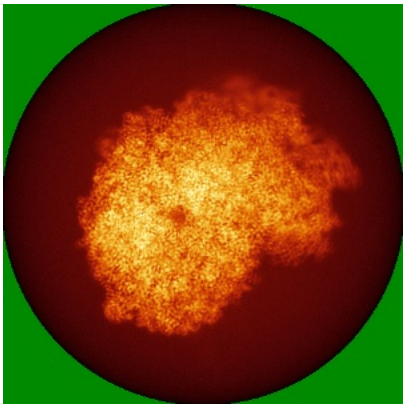


Y

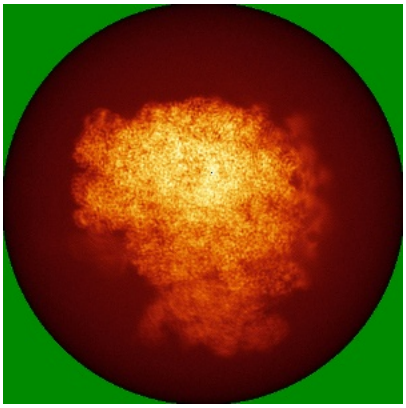


Z

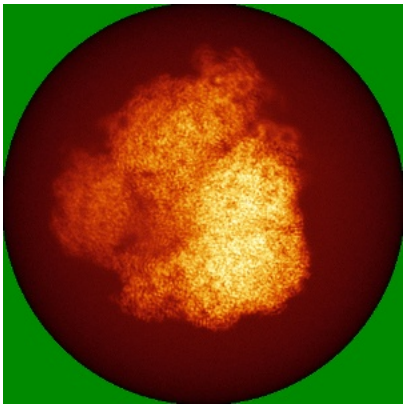
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

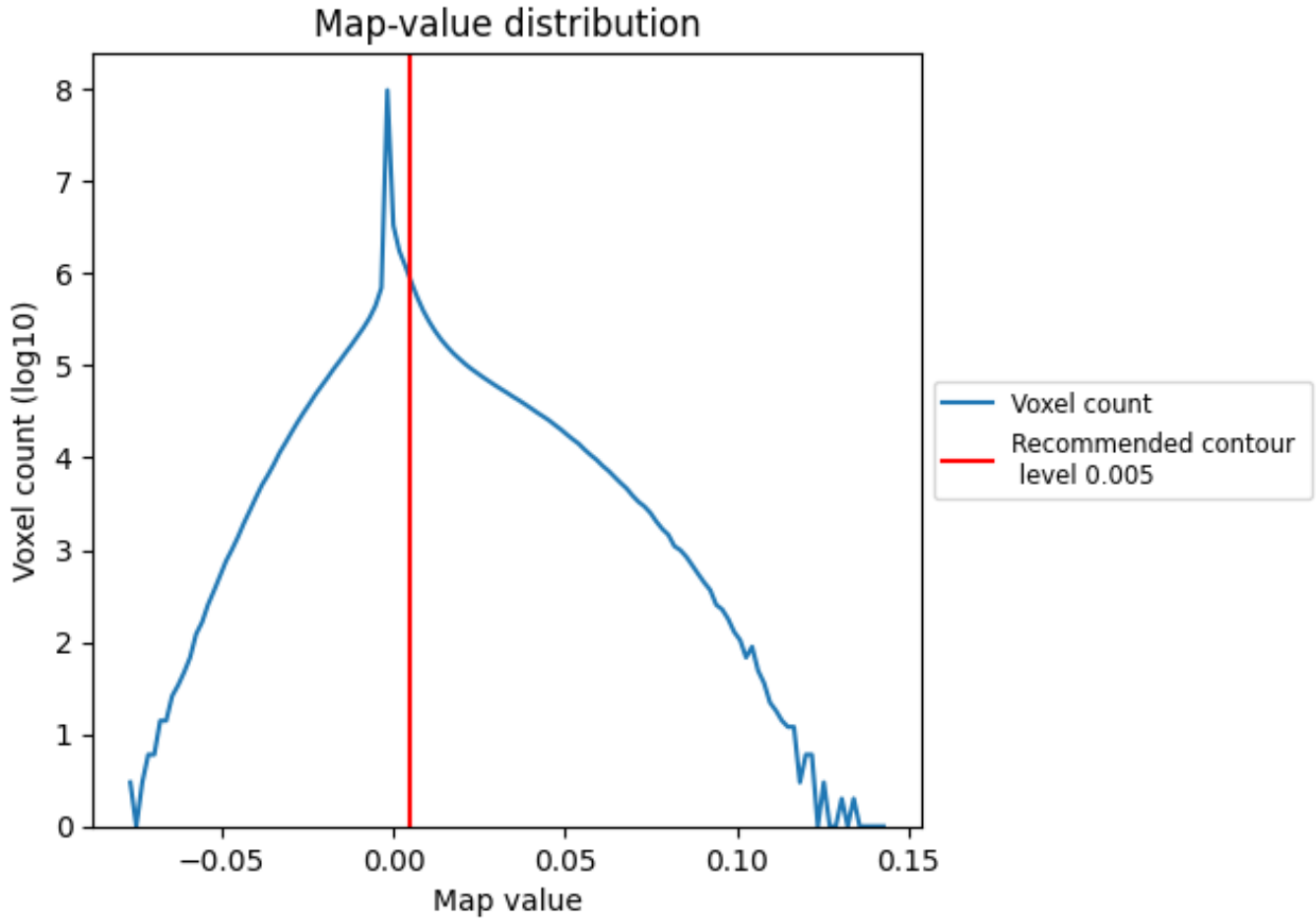
6.6 Mask visualisation (i)

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

7 Map analysis

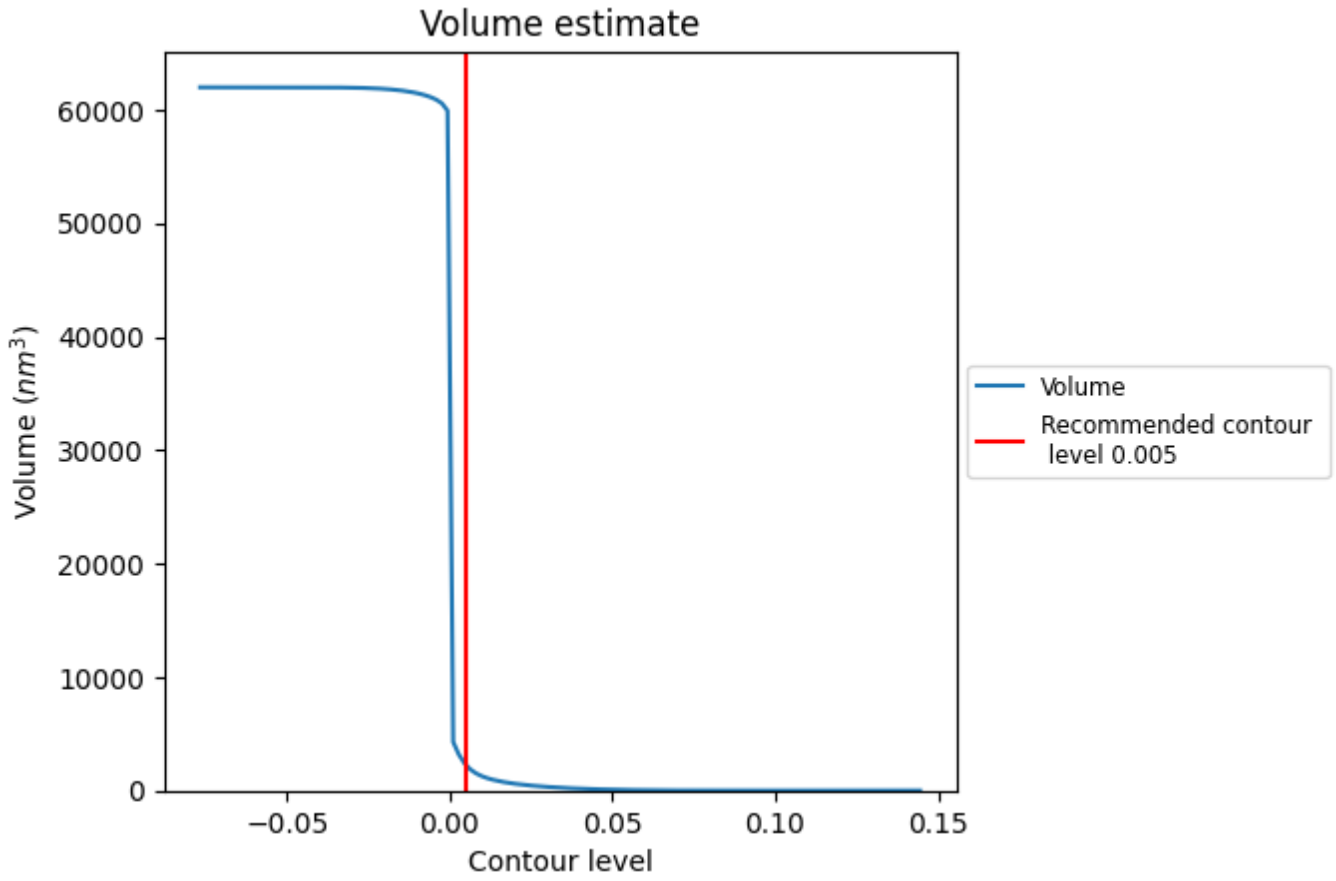
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

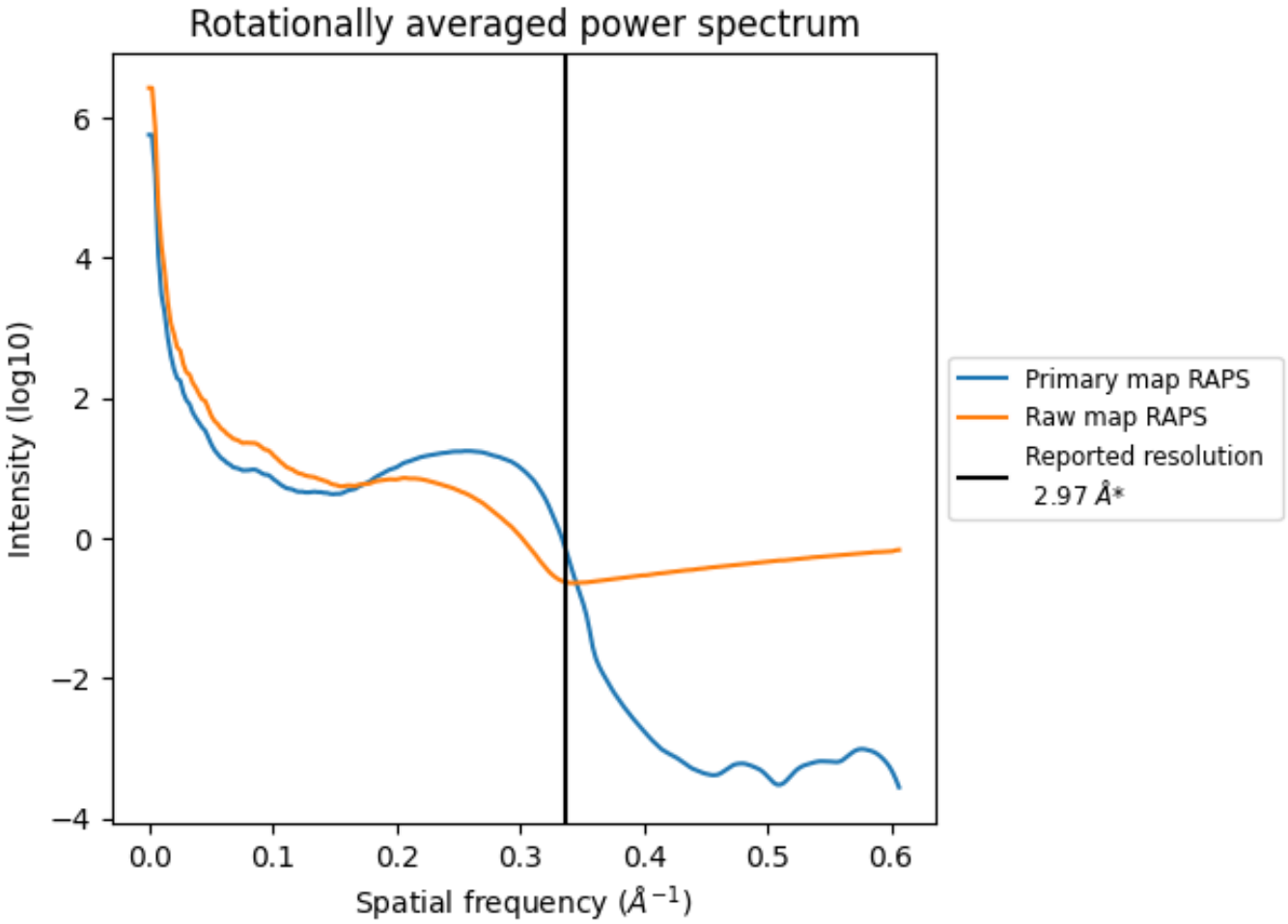
7.2 Volume estimate (i)



The volume at the recommended contour level is 2282 nm^3; this corresponds to an approximate mass of 2062 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

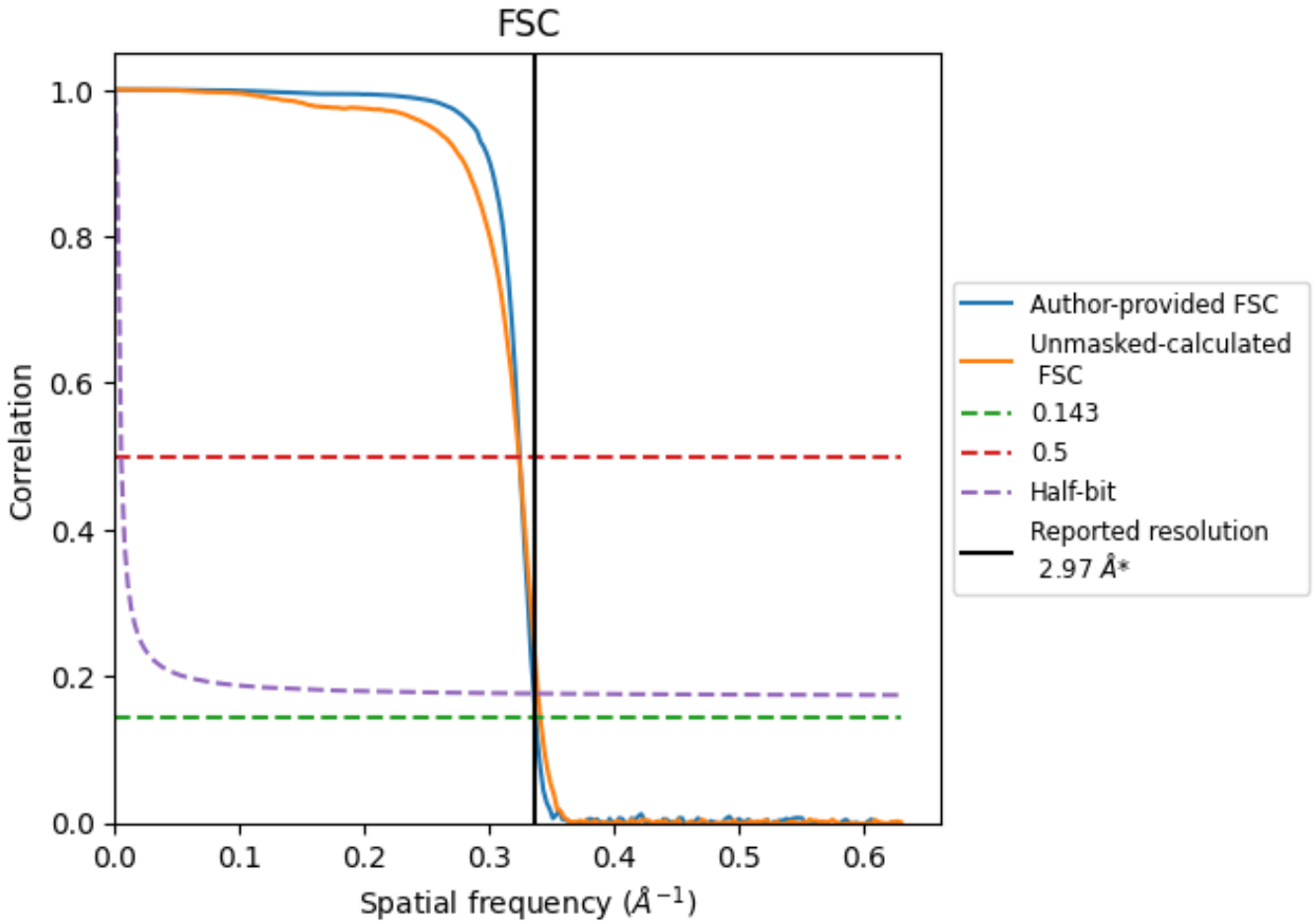


*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8.2 Resolution estimates (i)

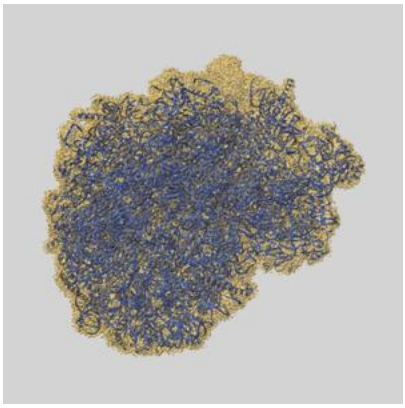
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.96	3.08	2.98
Unmasked-calculated*	2.93	3.09	2.95

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

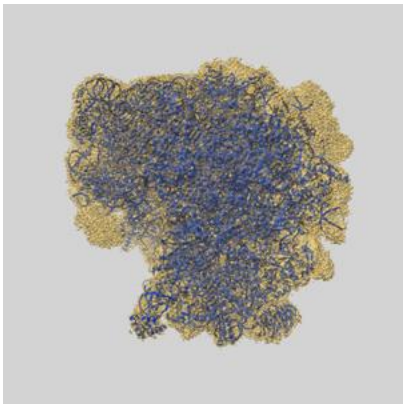
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19582 and PDB model 8RXX. Per-residue inclusion information can be found in section 3 on page 25.

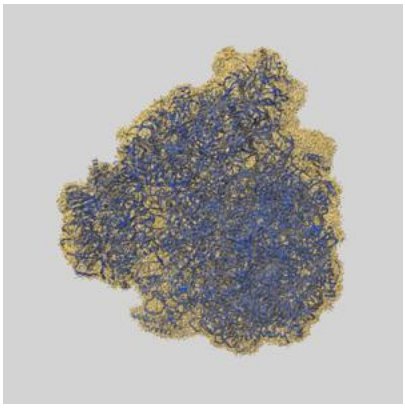
9.1 Map-model overlay



X



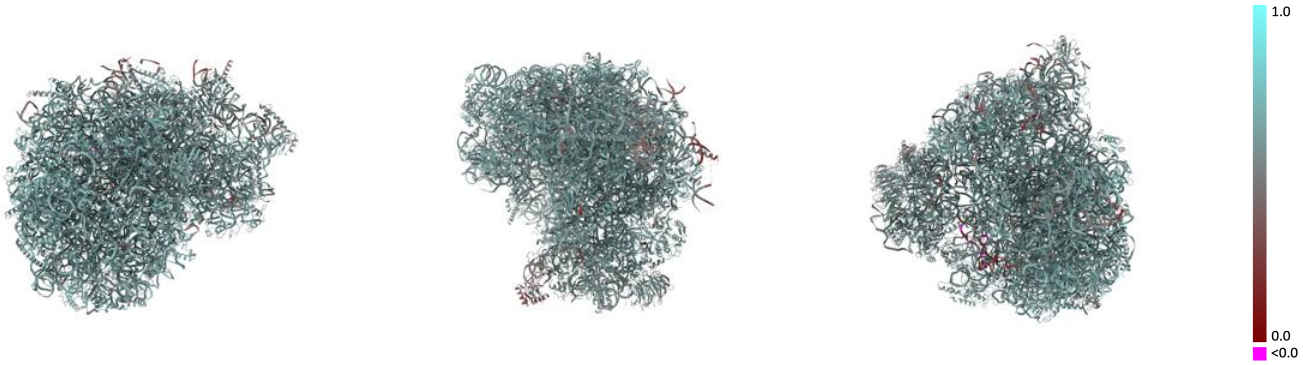
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

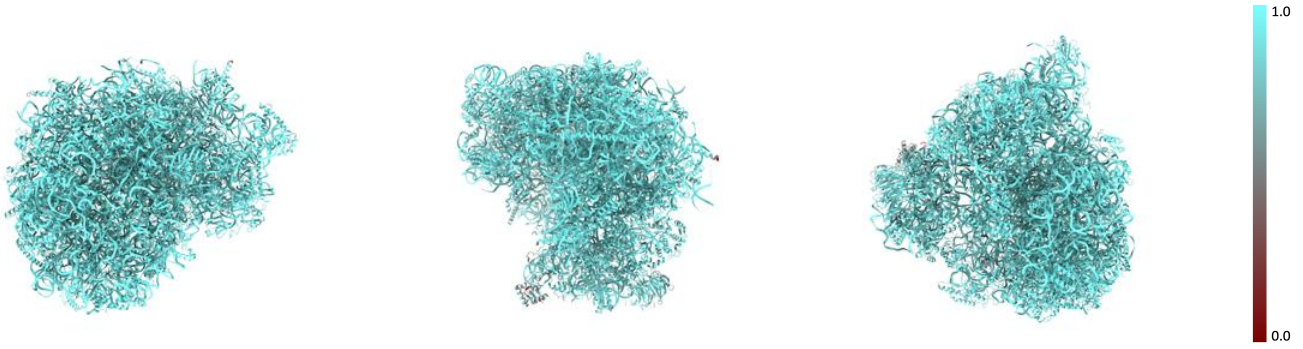
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

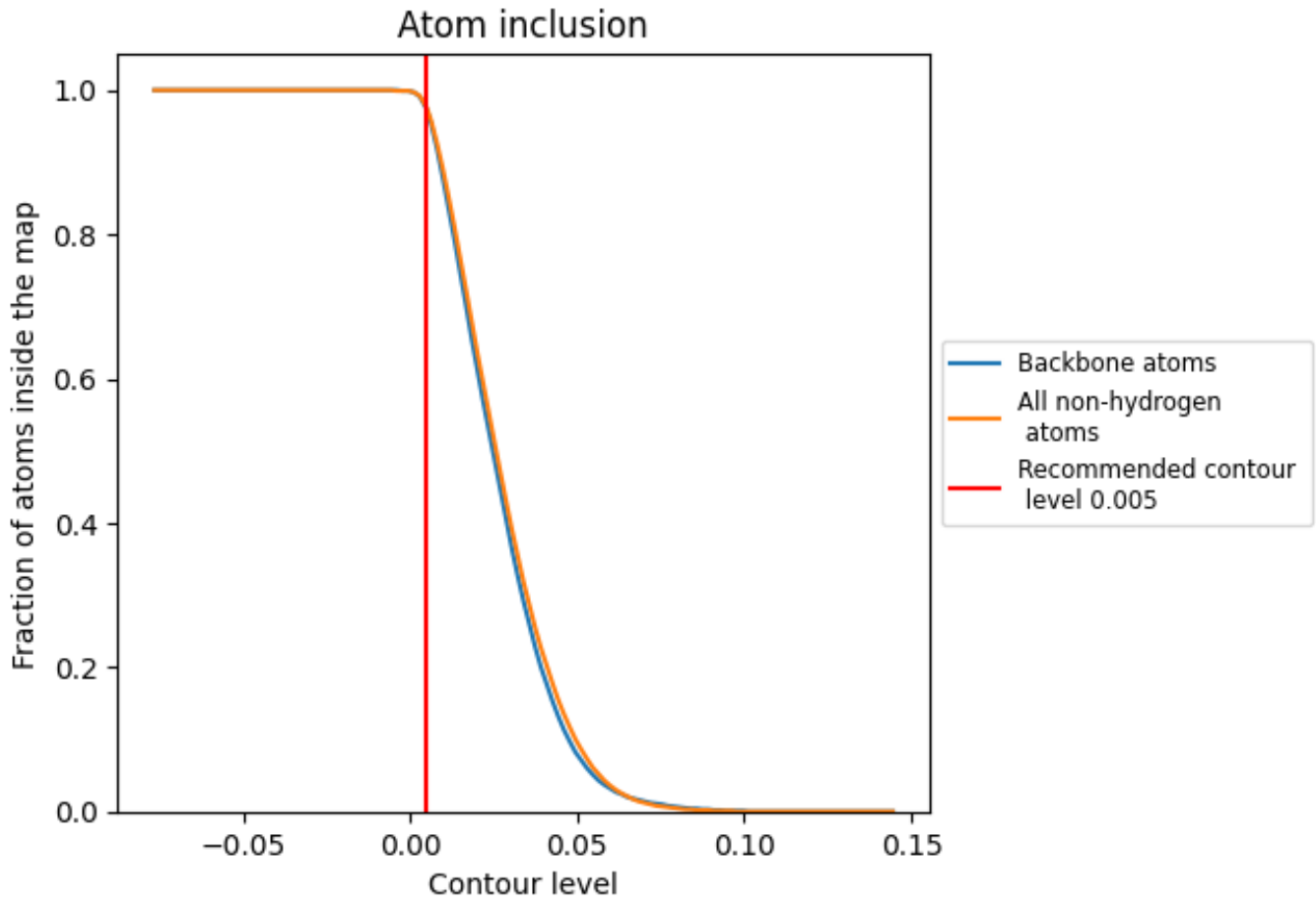
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.6010
L1	0.9900	0.6160
L2	0.9860	0.6050
L3	0.9830	0.6020
L4	0.9940	0.6220
L5	0.9820	0.6000
L6	0.9780	0.5990
L7	0.9900	0.6210
L8	0.9950	0.6100
LA	0.9940	0.6460
LB	0.9910	0.6410
LC	0.9910	0.6370
LD	0.9760	0.5850
LE	0.9810	0.6230
LF	0.9760	0.6200
LG	0.9710	0.6130
LH	0.9880	0.6360
LI	0.9870	0.6360
LJ	0.9930	0.6370
LK	0.9860	0.6210
LL	0.9890	0.6450
LM	0.9950	0.6450
LN	0.9650	0.6080
LO	0.9740	0.6110
LP	0.9950	0.6380
LQ	0.9780	0.6010
LR	0.9890	0.6360
LS	0.9910	0.6280
LT	0.9960	0.6440
LU	0.9790	0.6120
LV	0.9860	0.6370
LW	0.9910	0.6410
LX	0.9740	0.6200
LY	0.9780	0.6200
LZ	0.9900	0.6370

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Chain	Atom inclusion	Q-score
La	0.9870	0.6300
Lb	0.9810	0.6270
Lc	0.9880	0.6380
Ld	0.9810	0.6110
Le	0.9780	0.6260
Lf	0.9910	0.6360
Lg	0.9940	0.6480
Lh	0.9710	0.6140
Li	0.9600	0.6060
Lj	0.9920	0.6440
Lk	0.9810	0.6310
Ll	0.9930	0.6460
Lm	0.9820	0.6220
Ln	0.9930	0.6020
Lo	0.9930	0.6290
Lp	0.9920	0.6370
S1	0.9780	0.5780
S2	0.9390	0.3690
S3	0.9900	0.4260
S4	0.8410	0.2800
S5	1.0000	0.5370
SA	0.9570	0.6080
SB	0.9720	0.6000
SC	0.8880	0.5730
SD	0.9630	0.6020
SE	0.9810	0.6170
SF	0.9770	0.6140
SG	0.9670	0.5930
SH	0.9320	0.5810
SI	0.9820	0.6100
SJ	0.9870	0.6230
SK	0.9920	0.6190
SL	0.9600	0.5890
SM	0.8980	0.5670
SN	0.8740	0.5500
SO	0.9680	0.6110
SP	0.9770	0.6090
SQ	0.5140	0.3640
SR	0.8760	0.5510
SS	0.9450	0.5940
ST	0.9810	0.6140
SU	0.9930	0.6310

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Chain	Atom inclusion	Q-score
SV	0.9300	0.5740
SW	0.8330	0.5420
SX	0.9560	0.5760
SY	0.9660	0.5940
SZ	0.9710	0.6020
Sa	0.8930	0.5580
Sb	0.9750	0.6120
Sc	0.9800	0.6050
Sd	0.9070	0.5710
Se	0.9070	0.5600
Sf	0.7700	0.4760
Sg	0.8350	0.5300
Sh	0.9290	0.5350