



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:00 AM UTC

PDB ID : 8K2A / pdb_00008k2a
EMDB ID : EMD-36836
Title : Cryo-EM structure of the human 55S mitoribosome with Tigecycline
Authors : Li, X.; Wang, M.; Cheng, J.
Deposited on : 2023-07-12
Resolution : 2.90 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

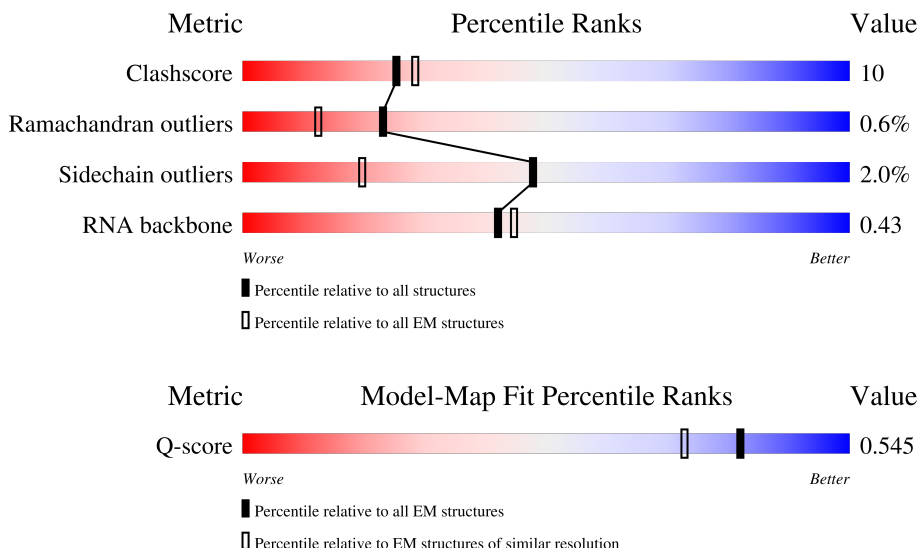
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



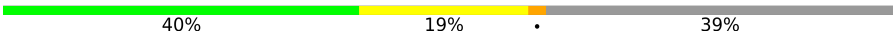
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	L1	1559	59% 32% 5% .
2	L2	69	48% 32% . 19%
3	LB	305	68% 10% 22%

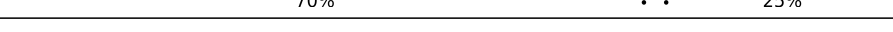
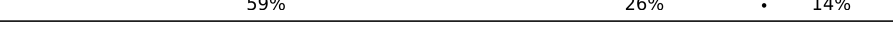
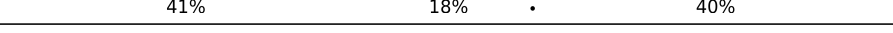
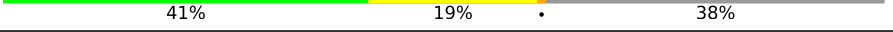
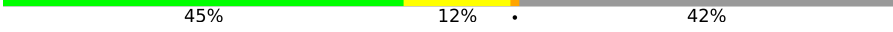
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Mol	Chain	Length	Quality of chain
4	LC	348	
5	LD	311	
6	LI	267	
7	LJ	261	
8	LK	192	
9	LM	178	
10	LN	145	
11	LO	296	
12	LP	251	
13	LQ	175	
14	LR	179	
15	LS	292	
16	LT	149	
17	LU	205	
18	LV	212	
19	LW	153	
20	LX	216	
21	La	148	
22	Lb	256	
23	Lu	250	
24	Ld	161	
25	Lf	188	
26	Lg	65	
27	Lh	92	
28	Li	188	

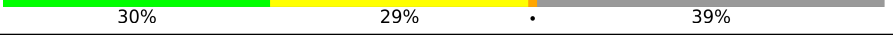
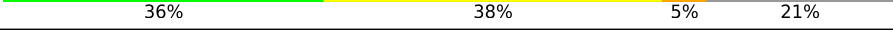
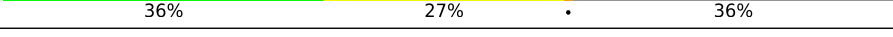
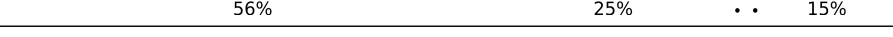
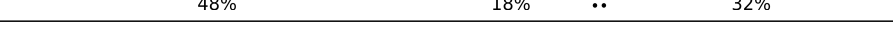
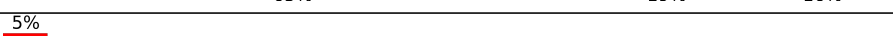
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Mol	Chain	Length	Quality of chain
29	Lj	103	
30	Lk	423	
31	Ll	380	
32	Lm	338	
33	Ln	206	
34	Lo	137	
35	Lp	142	
36	Lq	215	
37	Lr	332	
38	Ls	306	
39	Lt	279	
40	Lv	212	
41	Lw	166	
42	Lx	158	
43	Ly	128	
44	Lz	123	
45	L3	112	
46	L4	138	
47	L5	128	
48	L6	102	
49	L7	206	
50	L8	222	
51	SR	196	
52	Sf	439	
53	SB	296	

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Mol	Chain	Length	Quality of chain
54	SZ	167	
55	SE	430	
56	SF	125	
57	SG	242	
58	SI	396	
59	SJ	201	
60	SK	194	
61	SL	138	
62	SN	128	
63	SO	257	
64	SP	137	
65	SQ	130	
66	SS	258	
67	ST	142	
68	SW	87	
69	SX	360	
70	SY	190	
71	Sa	173	
72	Sb	205	
73	Sc	414	
74	Sd	187	
75	Se	398	
76	Sg	395	
77	Si	106	
78	Sj	218	

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Mol	Chain	Length	Quality of chain
79	Sk	323	
80	Sm	118	
81	Sn	199	
82	So	689	
83	S1	954	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 165285 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1500	Total	C	N	O	P	0	0
			31847	14290	5750	10307	1500		

- Molecule 2 is a RNA chain called Val tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	237	Total	C	N	O	S	0	0
			1851	1151	375	316	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LC	304	Total	C	N	O	S	0	0
			2393	1538	415	429	11		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LD	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LI	95	Total	C	N	O		0	0
			784	498	152	134			

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LJ	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LK	175	Total	C	N	O	S	0	0
			1323	841	237	243	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LM	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LN	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LO	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LP	221	Total	C	N	O	S	0	0
			1779	1138	325	306	10		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LQ	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LR	146	Total	C	N	O	S	0	0
			1189	743	226	215	5		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LS	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LT	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LU	160	Total	C	N	O	S	0	0
			1284	829	226	225	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LV	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LW	143	Total	C	N	O	S	0	0
			1188	752	224	208	4		

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LX	202	Total	C	N	O	S	0	0
			1652	1053	294	297	8		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	La	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Lb	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Lu	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ld	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Lf	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Lg	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Lh	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Li	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lj	38	Total	C	N	O	S	0	0
			341	217	72	48	4		

- Molecule 30 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lk	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 31 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ll	354	Total	C	N	O	S	0	0
			2947	1881	525	532	9		

- Molecule 32 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lm	293	Total	C	N	O	S	0	0
			2382	1525	404	435	18		

- Molecule 33 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ln	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 34 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lo	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 35 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lp	97	Total	C	N	O	S	0	0
			815	514	147	149	5		

- Molecule 36 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lq	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lr	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ls	214	Total	C	N	O	S	0	0
			1754	1117	304	320	13		

- Molecule 39 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lt	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lv	131	Total	C	N	O	S	0	0
			1035	661	169	201	4		

- Molecule 41 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lw	132	Total	C	N	O	S	0	0
			1097	710	191	194	2		

- Molecule 42 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lx	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 43 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ly	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lz	92	Total	C	N	O	S	0	0
			732	454	142	134	2		

- Molecule 45 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L3	96	Total	C	N	O	S	0	0
			743	462	143	133	5		

- Molecule 46 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L4	83	Total	C	N	O	S	0	0
			703	446	124	130	3		

- Molecule 47 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L5	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L6	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L7	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 50 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L8	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 51 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SR	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Sf	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 53 is a protein called Small ribosomal subunit protein uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SB	217	Total	C	N	O	S	0	0
			1768	1131	321	306	10		

- Molecule 54 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SZ	132	Total	C	N	O	S	0	0
			1082	699	195	184	4		

- Molecule 55 is a protein called Small ribosomal subunit protein uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SE	320	Total	C	N	O	S	0	0
			2540	1600	473	455	12		

- Molecule 56 is a protein called Small ribosomal subunit protein bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SF	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 57 is a protein called Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SG	201	Total	C	N	O	S	0	0
			1668	1069	305	283	11		

- Molecule 58 is a protein called Small ribosomal subunit protein uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SI	304	Total	C	N	O	S	0	0
			2501	1591	444	452	14		

- Molecule 59 is a protein called Small ribosomal subunit protein uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SJ	122	Total	C	N	O	S	0	0
			999	643	168	185	3		

- Molecule 60 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SK	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 61 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SL	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 62 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SN	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 63 is a protein called Small ribosomal subunit protein uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO	164	Total	C	N	O	S	0	0
			1382	883	257	235	7		

- Molecule 64 is a protein called Small ribosomal subunit protein bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 65 is a protein called Small ribosomal subunit protein uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 66 is a protein called Small ribosomal subunit protein mS40.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	185	Total	C	N	O	S	0	0
			1528	970	285	267	6		

- Molecule 67 is a protein called Small ribosomal subunit protein bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

- Molecule 68 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SW	86	Total	C	N	O	S	0	0
			740	458	150	124	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SW	50	ARG	CYS	variant	UNP P82921

- Molecule 69 is a protein called Small ribosomal subunit protein mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SX	295	Total	C	N	O	S	0	0
			2405	1530	413	454	8		

- Molecule 70 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SY	126	Total	C	N	O	S	0	0
			1042	673	183	185	1		

- Molecule 71 is a protein called Small ribosomal subunit protein mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Sa	162	Total	C	N	O	S	0	0
			1330	850	231	238	11		

- Molecule 72 is a protein called Small ribosomal subunit protein mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sb	173	Total	C	N	O	S	0	0
			1454	894	294	262	4		

- Molecule 73 is a protein called Small ribosomal subunit protein mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sc	385	Total	C	N	O	S	0	0
			3116	1980	522	603	11		

- Molecule 74 is a protein called Small ribosomal subunit protein bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sd	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 75 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Se	350	Total	C	N	O	S	0	0
			2836	1813	497	515	11		

- Molecule 76 is a protein called Small ribosomal subunit protein mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sg	108	Total	C	N	O	S	0	0
			903	587	145	169	2		

- Molecule 77 is a protein called Small ribosomal subunit protein mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Si	86	Total	C	N	O	S	0	0
			731	467	131	129	4		

- Molecule 78 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sj	201	Total	C	N	O	S	0	0
			1680	1062	321	292	5		

- Molecule 79 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sk	256	Total	C	N	O	S	0	0
			2068	1317	349	392	10		

- Molecule 80 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sm	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 81 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sn	69	Total	C	N	O	S	0	0
			610	393	130	86	1		

- Molecule 82 is a protein called Small ribosomal subunit protein mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	So	616	Total	C	N	O	S	0	0
			4981	3177	849	928	27		

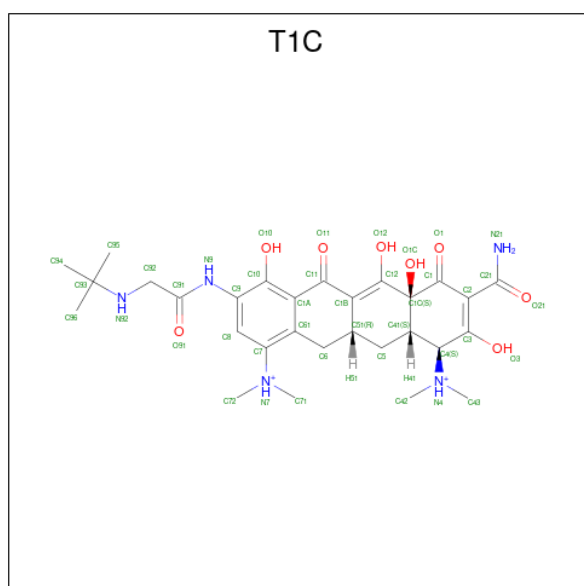
- Molecule 83 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	S1	928	Total	C	N	O	P	0	0
			19716	8840	3560	6388	928		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	L1	105	Total	Mg	0
			105	105	
84	LB	3	Total	Mg	0
			3	3	
84	LC	1	Total	Mg	0
			1	1	
84	La	1	Total	Mg	0
			1	1	
84	Lw	1	Total	Mg	0
			1	1	
84	L6	1	Total	Mg	0
			1	1	
84	S1	33	Total	Mg	0
			33	33	

- Molecule 85 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈).



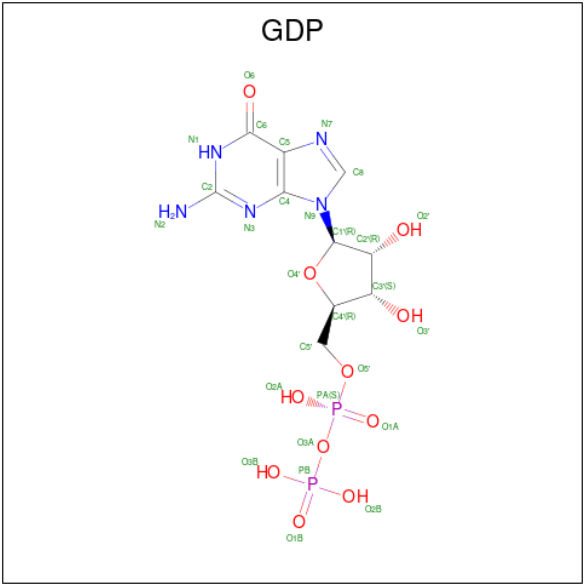
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
85	S1	1	Total	C	N	O	0
			42	29	5	8	
85	S1	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	Lf	1	Total	Zn	0
			1	1	
86	Lj	1	Total	Zn	0
			1	1	
86	SR	1	Total	Zn	0
			1	1	
86	SB	1	Total	Zn	0
			1	1	
86	SS	1	Total	Zn	0
			1	1	
86	ST	1	Total	Zn	0
			1	1	
86	Sa	1	Total	Zn	0
			1	1	

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

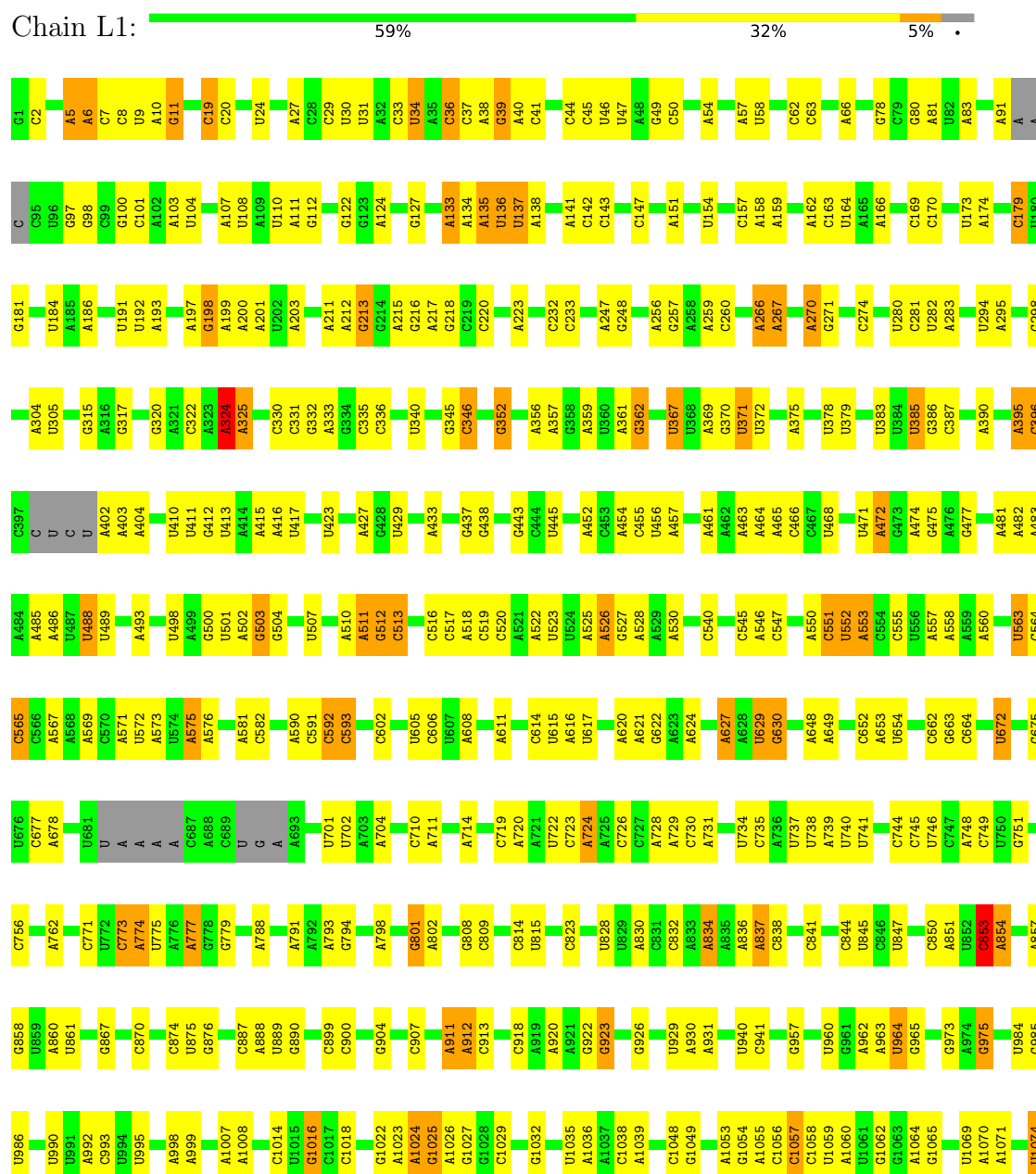


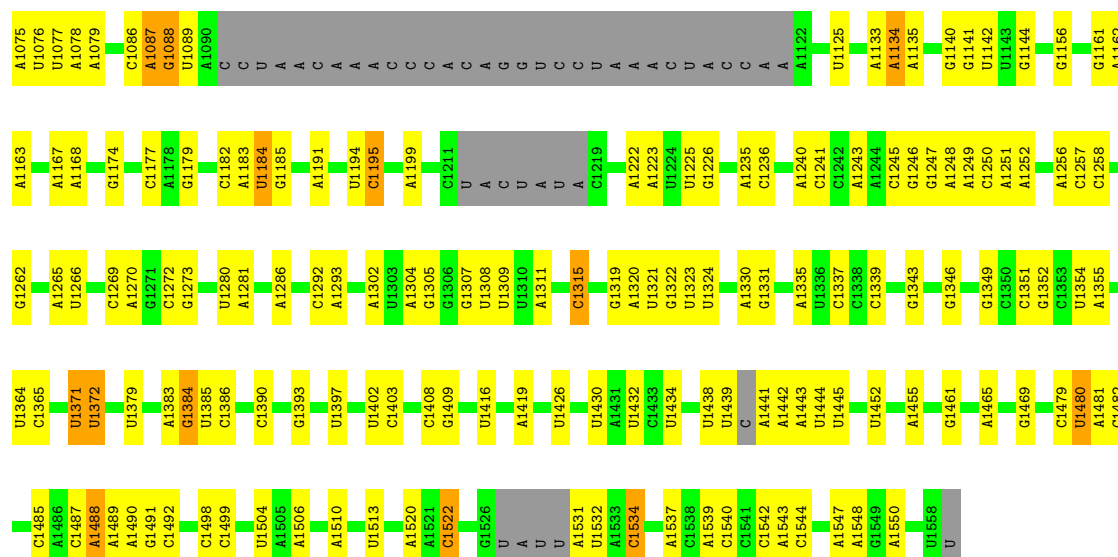
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	Se	1	28	10	5	11	2	0

3 Residue-property plots

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

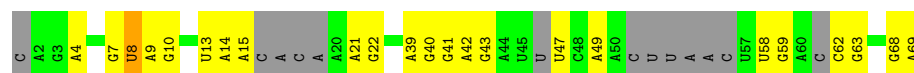
• Molecule 1: 16S rRNA





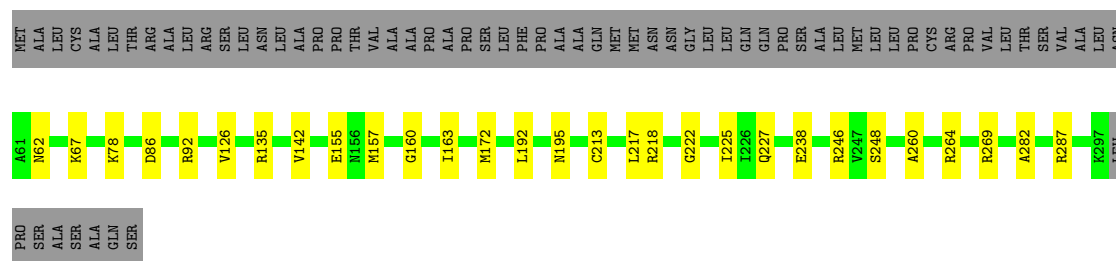
• Molecule 2: Val tRNA

Chain L2: 48% 32% 19%



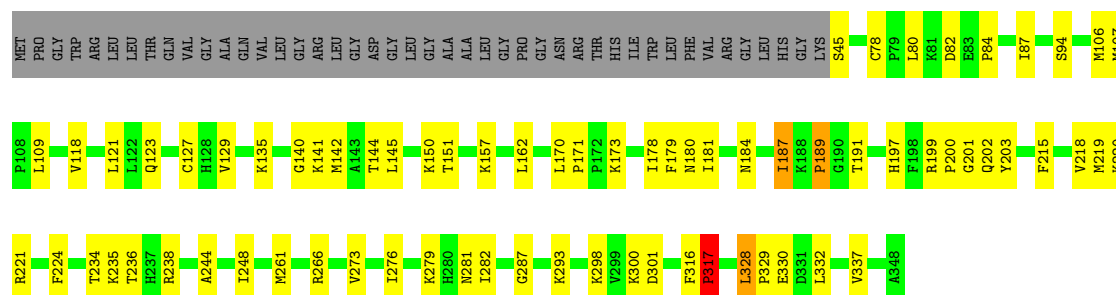
• Molecule 3: Large ribosomal subunit protein uL2m

Chain LB: 68% 10% 22%



• Molecule 4: Large ribosomal subunit protein uL3m

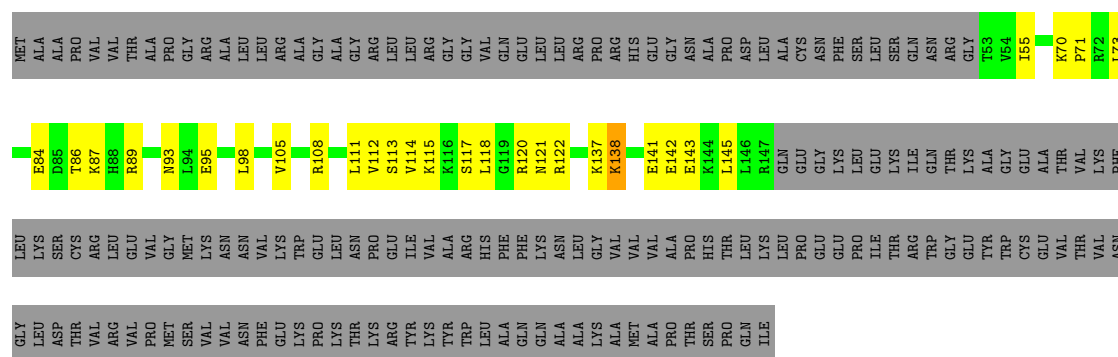
Chain LC: 66% 20% 13%



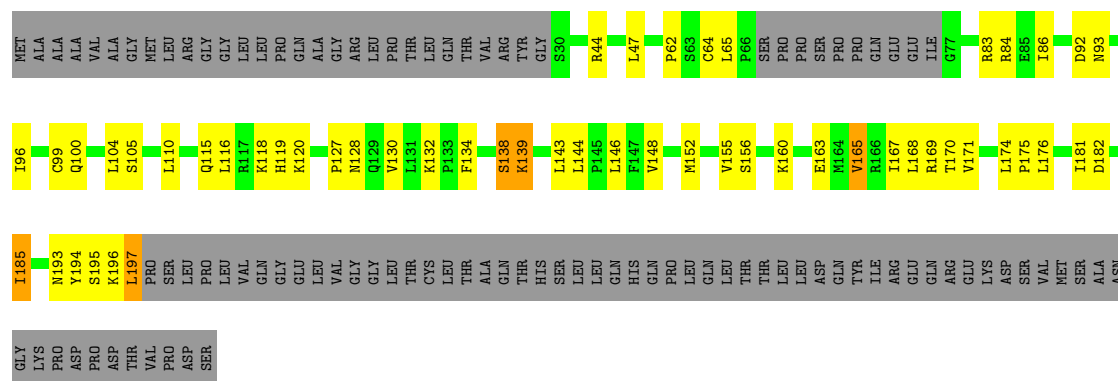
• Molecule 5: Large ribosomal subunit protein uL4m

L248	F72	LEU	MET
M253	V77	GLN	
H266	D81	PRO	
Q257	L82	VAL	
V260	F87	ARG	
T262	L93	ALA	
V266	H97	ARG	
L273	Q98	ALA	
M275	V99	TRP	
Q276	K113	LEU	
D277	R121	THR	
S278	R125	GLY	
R279	H138	GLN	
R281	W146	LEU	
P282	G157	SER	
Y284	P158	SER	
Y290	G173	LEU	
S291	L174	ALA	
D292	K175	ARG	
P293	M190	ALA	
P294	D191	THR	
ARG	S192	GLU	
PRO	L193	ASN	
HIS	E194	PRO	
THR	L195	GLU	
THR	P196	VAL	
GLN	Q201	ALA	
PRO	Y202	SER	
ALA	E205	GLY	
ALA	Y209	LEU	
THR	R210	PRO	
PRO	R211	THR	
HIS	D214	PRO	
CYS	H223	E45	
	M226	R49	
	V231	K50	
	L237	P56	
		R59	
		V62	
		W65	
		L69	
		R70	
		G74	

Chain LI: 25% 10% 64%

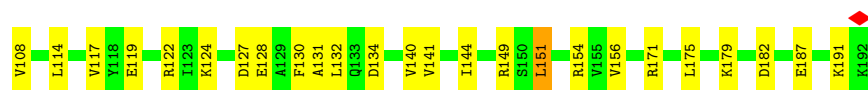


Chain LJ: 40% 19% 1% 39%



Chain LK: 65% 24% .. 9%





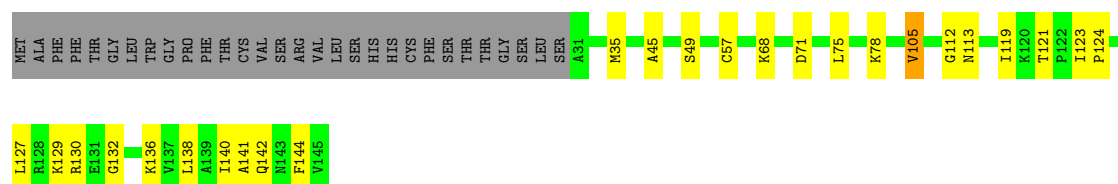
- Molecule 9: Large ribosomal subunit protein uL13m

Chain LM: 81% 17% ..



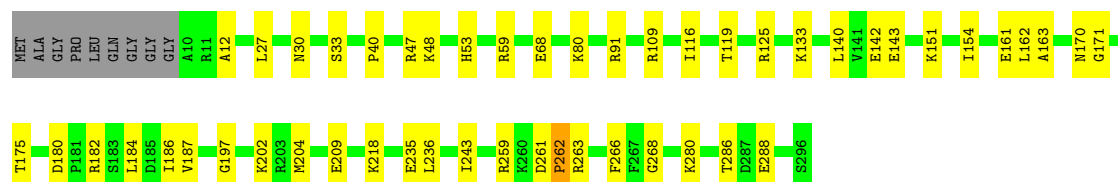
- Molecule 10: Large ribosomal subunit protein uL14m

Chain LN: 62% 17% 21%



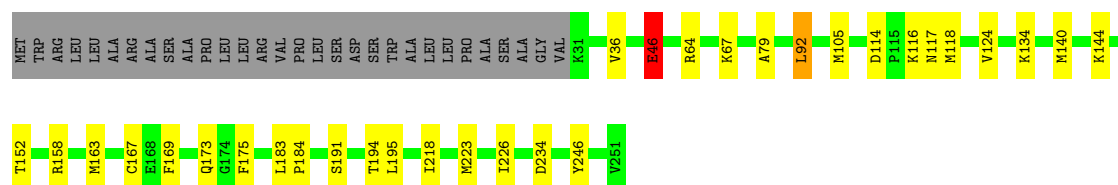
- Molecule 11: Large ribosomal subunit protein uL15m

Chain LO: 80% 17%



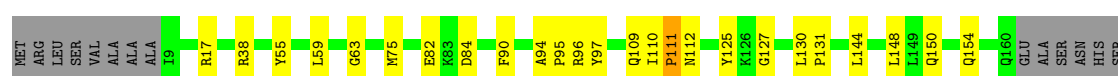
- Molecule 12: Large ribosomal subunit protein uL16m

Chain LP: 75% 12% 12%



- Molecule 13: Large ribosomal subunit protein bL17m

Chain LQ: 73% 14% 13%



SER
HIS
THR
ALA
GLN
THR
PRO
GLY
ILE

- Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain LR:  59% 22% 18%

MET ALA LEU ARG SER GLN PHE TRP GLY PHE SER PHE VAL CYS ARG ASN PRO GLY CYS ARG PHE ALA LEU ARG LEU THR SER CYS GLU PRO ALA LYS PRO E34 V43 N49 R50 N51 P52 R53 E56 R62 R65 E75 F76 W77 H78 R79 L80 I83 E90 A91

L32 V33 V101 V102 S105 T106 R107 A110 I111 H114 L115 A123 I127 L131 A132 Q133 R134 C135 L136 E137 M143 Q146 D155 S156 R159 L160 V169 V170 E179

- Molecule 15: Large ribosomal subunit protein bL19m

Chain LS:  64% 10% 25%

MET ALA ALA CYS ASP ILE LYS HIS ARG PRO VAL HIS TRP PHE MET ARG GLY LEU GLY ARG SER PHE GLN ALA ARG LEU THR LEU PRO PRO PRO ALA SER LEU ILE CYS ARG VAL HIS ALA GLY VAL ARG VAL GLN SER THR GLY PRO SER GLU PRO C248 L249 T250 E251 Q252 Q253 M254 K255 E256 K259

VAL ILE ASP LYS HIS ARG PRO VAL HIS TRP PHE MET ARG GLY LEU GLY ARG SER PHE GLN ALA ARG LEU THR LEU PRO PRO PRO ALA SER LEU ILE CYS ARG VAL HIS ALA GLY VAL ARG VAL GLN SER THR GLY PRO SER GLU PRO C248 L249 T250 E251 Q252 Q253 M254 K255 E256 K259

M289 I282 E285 I286 S292

- Molecule 16: Large ribosomal subunit protein bL20m

Chain LT:  82% 12% 6%

MET VAL PHE LEU THR ALA GLN LEU TRP L10 R11 R17 I21 Q22 E23 K26 K35 R40 R57 Y58 L59 K60 K61 N89 D104 Y108 R122 R123 E126 I141 H149

- Molecule 17: Large ribosomal subunit protein bL21m

Chain LU:  66% 11% 22%

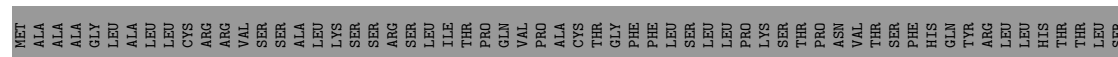
MET ALA ALA SER VAL LEU THR VAL THR LEU GLY ARG LEU ALA SER ASN CYS SER HIS SER ILE LEU ARG PRO SER GLY PRO GLY ALA ALA SER LEU TRP SER ALA SER ARG ARG PHE ASN SER GLN THR S45 V51 P52 K53 E71 E72 T73 R74 K82 R94 L95 F96

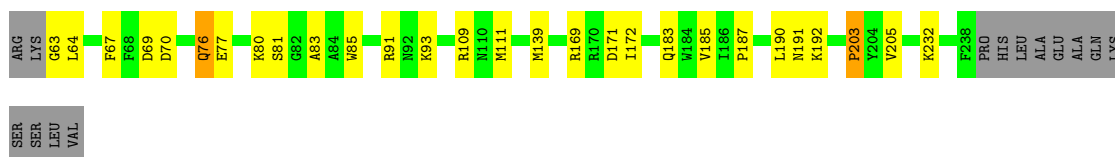
K107 E111 E119 C124 G125 L130 A138 L143 L144 L153 Y156 V160 M179 P189 C203 L204 LEU

- Molecule 18: 39S ribosomal protein L22, mitochondrial

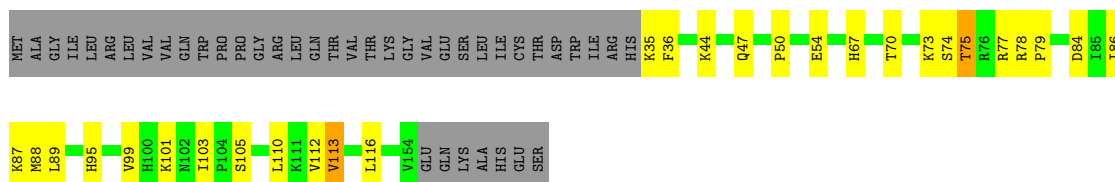
Chain LV:  64% 14% 22%

MET ALA ALA VAL LEU GLY GLN LEU GLY LEU TRP ILE HIS ASN LEU ARG SER ARG GLY LYS LEU ALA LEU GLY LEU LEU SER PHE HIS SER VAL LEU PRO GLN SER TYR THR ILE HIS THR SER ALA SER LEU ASP I47 K50 N55 R69 Y74 K81 Y82 M87

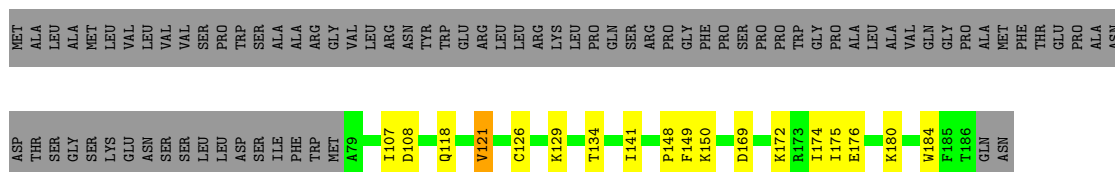




- Molecule 24: Large ribosomal subunit protein uL30m



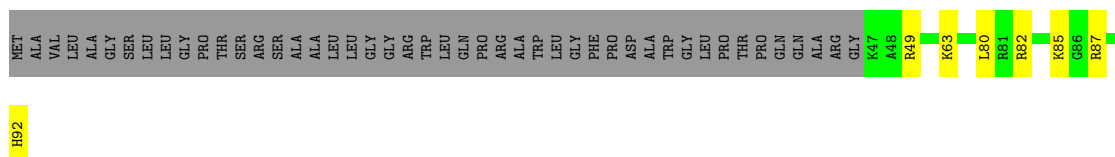
- Molecule 25: Large ribosomal subunit protein bL32m



- Molecule 26: Large ribosomal subunit protein bL33m

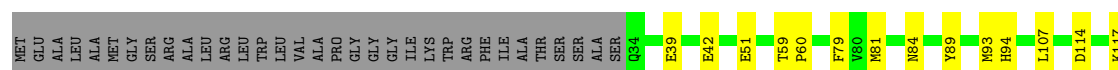
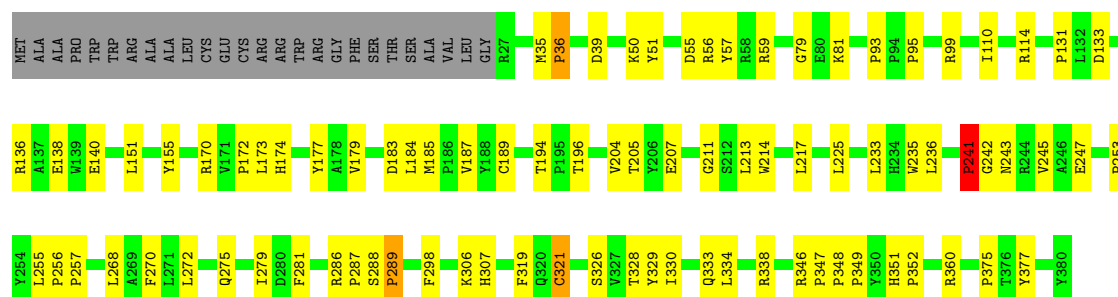
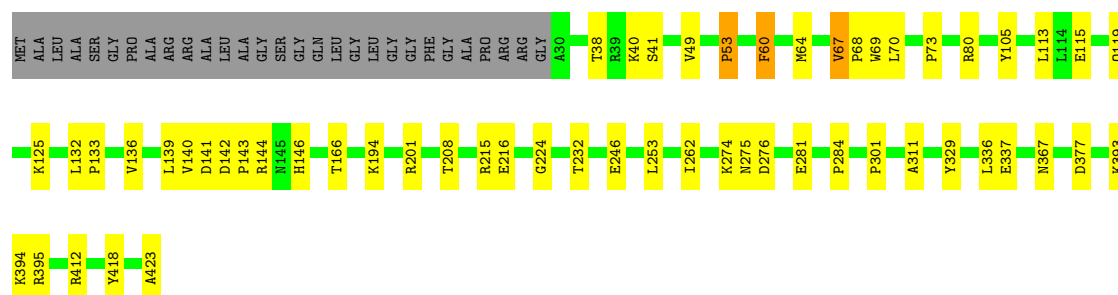
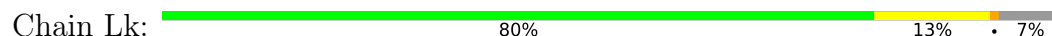
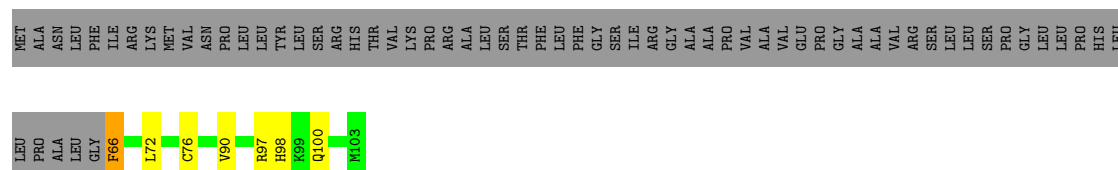


- Molecule 27: Large ribosomal subunit protein bL34m



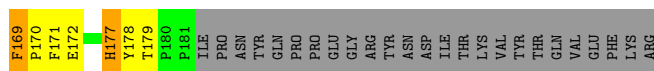
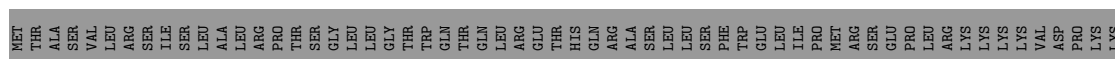
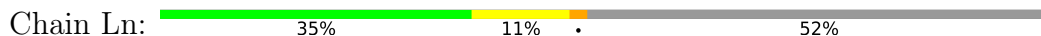
- Molecule 28: Large ribosomal subunit protein bL35m



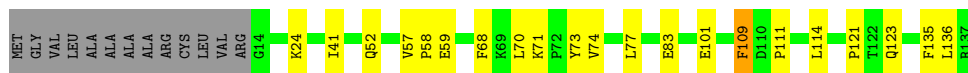




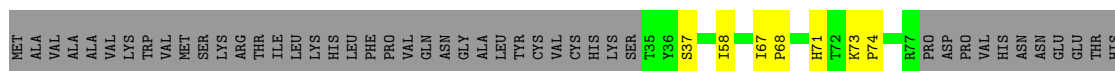
- Molecule 33: Large ribosomal subunit protein mL40



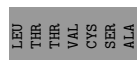
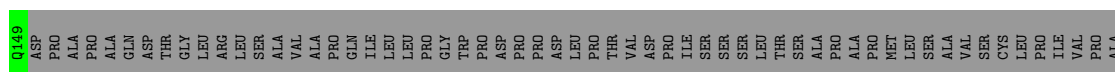
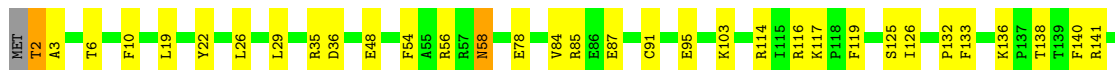
- Molecule 34: Large ribosomal subunit protein mL41



- Molecule 35: Large ribosomal subunit protein mL42



- Molecule 36: Large ribosomal subunit protein mL43



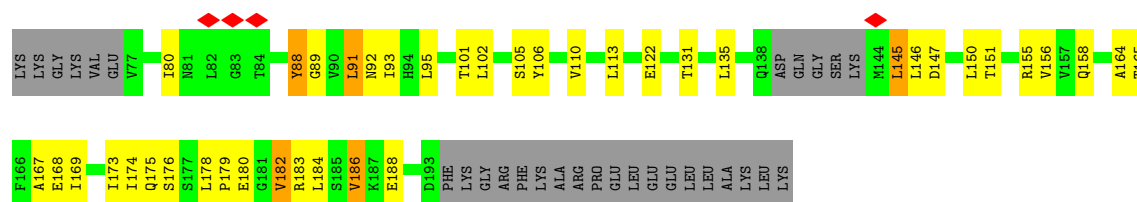
- Molecule 37: Large ribosomal subunit protein mL44

Y270	Y271	K279	P285	G286	E287	T288	V291	R302	Y305	G306	F307	Y316	SER	LYS	PRO	PRO	GLU	THR	LEU	ARG	ALA	GLU	LYS	SER	ILE	THR	ALA	SER													
ILE	GLU	LYS	GLU	ALA	VAL	LEU	ASN	L119	M122	G129	T130	S131	F132	S133	Q134	M148	P149	G152	L156	L173	A174	V175	E182	E183	F196	L203	G207	P208	F209	R210	T211	F218	E227	E230	L245	R248	P253	R259	T264	LEU	GLY
MET	ALA	SER	GLY	LEU	VAL	ARG	LEU	LEU	GLN	GLN	HIS	ARG	CYS	LEU	LEU	ALA	PRO	VAL	PRO	PRO	VAL	ARG	GLY	Y31	F39	K43	R47	L51	P56	F57	V58	E62	K63	I72	E81	L88	S95	K99	Q107	LEU	GLY

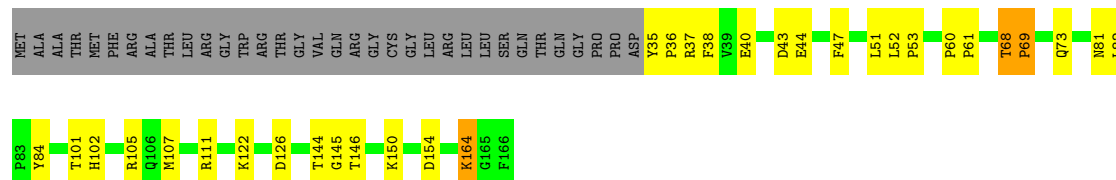
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K265	Q179	L74	MET
P266	E182	I77	ALA
L269	R185	E78	PRO
A270	G186	E80	VAL
R273	T187	R81	ARG
V276	A188	S82	ARG
	E189	L83	THR
	R190		LEU
L279	T191	E94	LEU
			GLY
	L195	R97	VAL
		L98	ALA
	M198	A99	GLY
	M199	K100	TRP
	M200		ARG
	E201		ARG
	A202	D104	PHE
	K203	LEU	GLU
		HIS	ASP
		GLU	ASP
	G206	GLU	LEU
	N207	GLU	TRP
		ASP	ALA
	G211	GLU	GLY
	H212	GLN	SER
	V213	ASP	LEU
	T214	ILE	SER
		LEU	SER
	F217	L116	ARG
	PRO		SER
	GLN	D119	LEU
	ALA		ALA
	MET	W124	LEU
	ARG		ALA
	THR	T138	ALA
	GLU		ALA
	SER	R146	PRO
	ASN	T147	SER
	L227	S148	SER
	G228	T149	ASN
	A229	M150	GLY
	K230	R151	
	V231	R152	S43
	F232	L153	
	F233		R46
	L237	L157	A50
	L238	V158	L51
	L239	L159	C52
	T240	L160	L53
	G241	Q168	Q54
	D242	D169	R55
	F243	V170	P56
		W171	P57
			V58
	W254		V59
	V255		
	T256	P174	P65
		E177	L66
	F259		

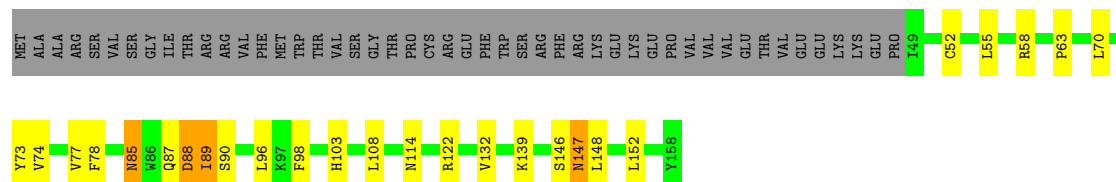
MET
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VAL
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VPS



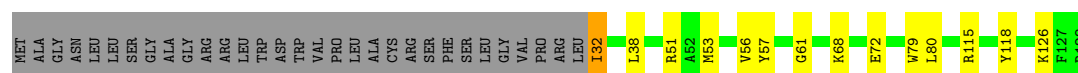
- Molecule 41: Large ribosomal subunit protein mL49



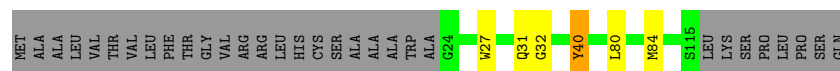
- Molecule 42: Large ribosomal subunit protein mL50



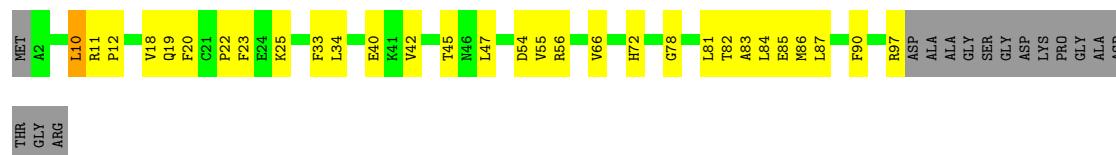
- Molecule 43: Large ribosomal subunit protein mL51



- Molecule 44: 39S ribosomal protein L52, mitochondrial



- Molecule 45: Large ribosomal subunit protein mL53



- | | | | | | | | | | | | | |
|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| Met | ALA | SER | VAL | ARG | GLN | ALA | ARG | SER | LEU | LEU | GLY | VAL | ALA | ALA | THR | LEU | ALA | PRO | GLY | SER | ARG | GLY | Y25 | Z26 | A27 | R28 | P29 | P30 | P31 | R32 | R33 | P37 | P40 | P48 | R49 | Q50 | Q51 | A62 | S68 | V71 | P72 | G73 | S74 | Q81 | E84 | L85 | L108 | G110 |
| | E123 | M128 | P129 | T132 | V133 | E141 | K145 | K150 | E151 | R152 | ARG | ALA | ALA | ARG | LEU | GLN | ALA | GLY | GLY | ALA | ALA | ALA | GLN | LEU | LEU | GLY | T79 | VAL | ASP | PRO | ARG | SER | ALA | PHE | GLN | GLY | LEU | LYS | LYS | GLU | ARG | LYS | LEU | LYS | GLU | GLY | GLN | |

ARG
LYS
LYS
GLU
ALA
ARG
ALA
ALA
ALA
ALA
ALA
VAL
ALA
GLN
ASP
PRO
PRO
ALA
ALA
SER
SER
SER

- Molecule 51: Large ribosomal subunit protein mL66

Chain SR: 58% 16% 26%

MET ALA ALA LEU LYS LEU VAL SER GLY CYS GLY ARG LEU LEU VAL SER TRP TRP ARG LEU PRO ALA ARG GLY F35 V38 V39 E40 T41 GLN GLN LYS THR T47 I48 I49 E50 E51 R52 T56 P57 K58 P71 I72 C73

N76 H79 Y83 Y86 L89 S90 P101 I104 T105 G106 L107 LEU LEU LEU LEU V119 K120 M121 L127 R132 P133 R134 LEU PRO GLY VAL VAL PRO LYS SER LYS PRO Q146 R149 P167 M174 P175 R182 D183 N184 R189 H196

- Molecule 52: Large ribosomal subunit protein mL65

Chain Sf: 69% 15% 16%

MET ALA ALA ALA ARG CYS TRP ARG PRO PRO LEU LEU ARG GLY PRO ARG ARG LEU LEU LEU HIS THR ALA ALA ASN ALA ALA THR LEU THR THR THR CYS GLN ASP VAL ALA ALA THR PRO V41 M51 R59 R62 I63 E64 R65 W66 T69 A73 K79 K85 M86

Q107 Y108 F109 V113 L118 P119 PRO PRO PRO PRO GLU PRO PRO PRO PRO PRO PRO PRO PRO PRO A140 R143 D148 C149 L150 R158 R165 F176 L177 D178 R212 R219 D235 N238 N239 Q240 Q240 I243 S244 K245 F250

V251 P252 L253 S256 V257 I264 L271 L272 L273 F283 K287 H296 F299 H300 D304 R307 R308 D318 Q319 LEU I320 I329 A330 S331 P354 I361 T362 D363 G364 Q373 L379 I392 N414 D415 D416 L419 Q420 Q420 L425 K430 F430 GLU

LYS SER GLN LEU LEU LEU ASN

- Molecule 53: Small ribosomal subunit protein uS2m

Chain SB: 50% 22% 27%

MET ALA THR SER SER ALA LEU PRO ARG ILE ARG LEU GLY ALA GLY ALA ALA ALA ALA PRO SER ARG TRP LEU PHE LEU LEU GLY LYS LEU ALA THR PRO ARG PRO PRO ALA ALA ARG ARG ARG ARG ARG LEU LEU SER ALA THR ALA THR ALA LEU MET ARG ILE GLU ASP GLU ASP THR ASP F58 N59 D60

K61 I62 E65 P66 L67 K68 F73 N74 N75 N76 F77 F78 V81 R82 H90 L91 K94 R98 M102 S109 S109 L118 Q126 F131 F131 M135 A136 Y137 I141 I142 N148 R149 Q150 F151 S152 I155 E156 H157 M158 C162 G163 E164 Y165 A166 H167

M175 L182 F183 V187 R188 L189 P190 L196 H197 V207 R210 D211 K214 T219 V220 G221 I222 V223 D224 T225 N226 C227 N228 P229 C230 L231 T232 T233 Y234 P235 V236 N239 S242 T255 R259 I62 A63 R65 T73 G74 N75 L76 H81 E84 R85

ASP GLN GLY PRO VAL HIS PRO PRO GLY ASP ALA MET SER HIS LEU

- Molecule 54: Small ribosomal subunit protein uS3m

Chain SZ: 52% 25% 21%

MET ALA ALA SER VAL CYS SER SER GLY LEU LEU GLY GLY PRO PRO ARG VAL LEU LEU TRP SER ARG GLU LEU PRO PRO CYS TRP ARG ALA LEU HIS THR SER PRO VAL CYS ALA K36 A40 V51 E54 P59 H60 Y61 I62 A63 R65 T73 G74 N75 L76 H81 E84 R85



- Molecule 55: Small ribosomal subunit protein uS5m

Chain SE: 61% 12% 26%



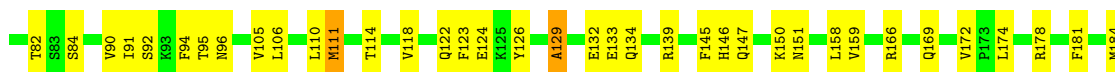
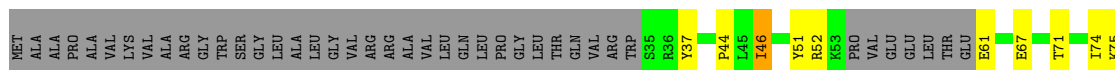
- Molecule 56: Small ribosomal subunit protein bS6m

Chain SF: 76% 22%



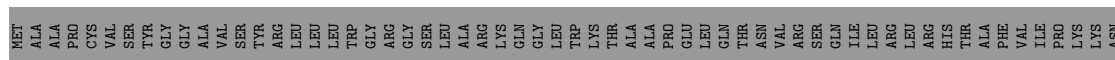
- Molecule 57: Small ribosomal subunit protein uS7m

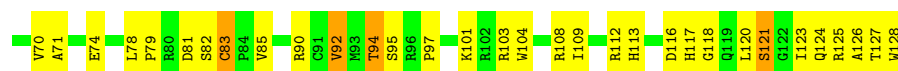
Chain SG: 57% 25% 17%



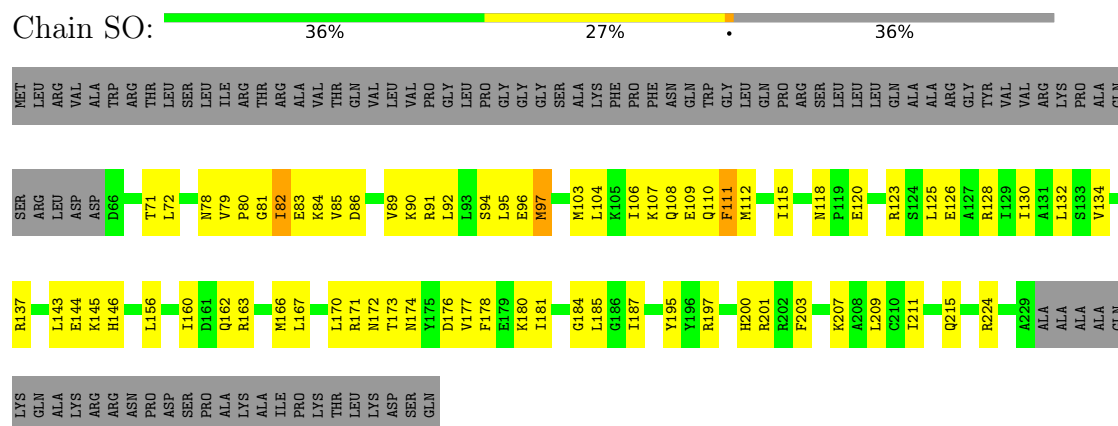
- Molecule 58: Small ribosomal subunit protein uS9m

Chain SI: 54% 21% 23%

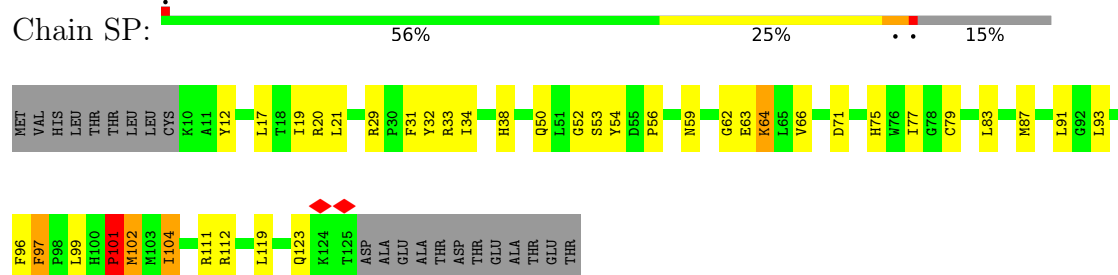




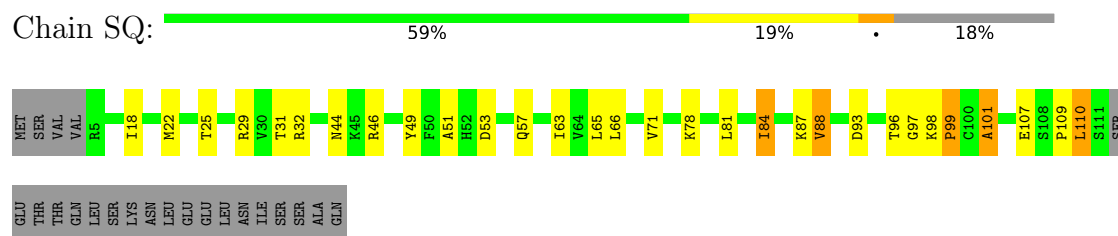
- Molecule 63: Small ribosomal subunit protein uS15m



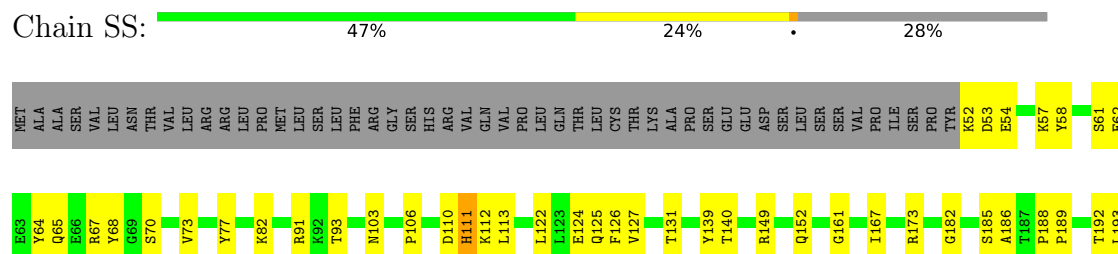
- Molecule 64: Small ribosomal subunit protein bS16m



- Molecule 65: Small ribosomal subunit protein uS17m



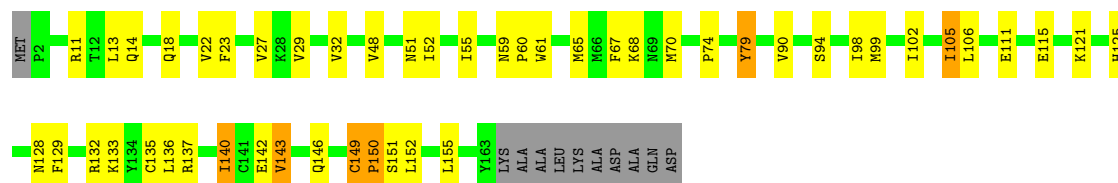
- Molecule 66: Small ribosomal subunit protein mS40





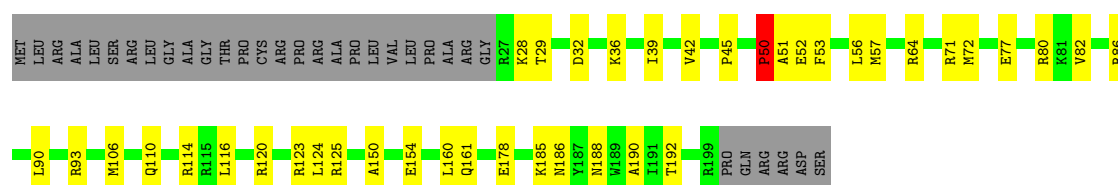
- Molecule 71: Small ribosomal subunit protein mS25

Chain Sa: 



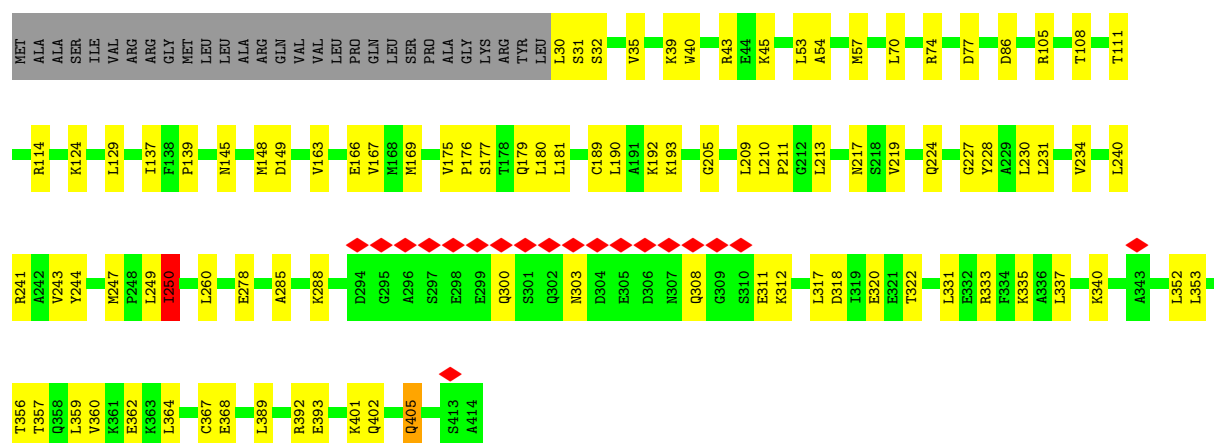
- Molecule 72: Small ribosomal subunit protein mS26

Chain Sb: 

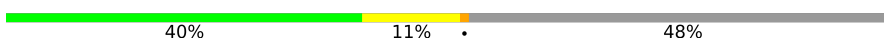


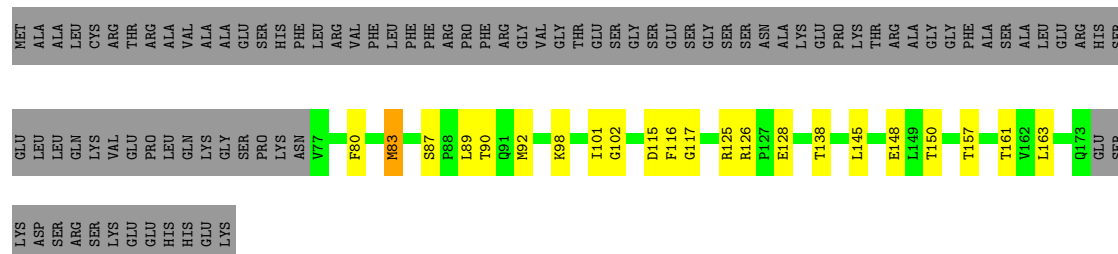
- Molecule 73: Small ribosomal subunit protein mS27

Chain Sc: 



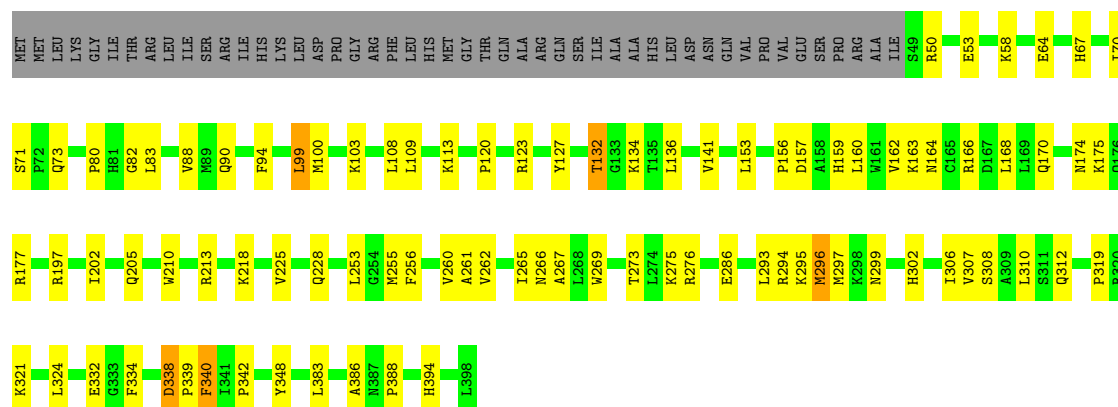
- Molecule 74: Small ribosomal subunit protein bS1m

Chain Sd: 



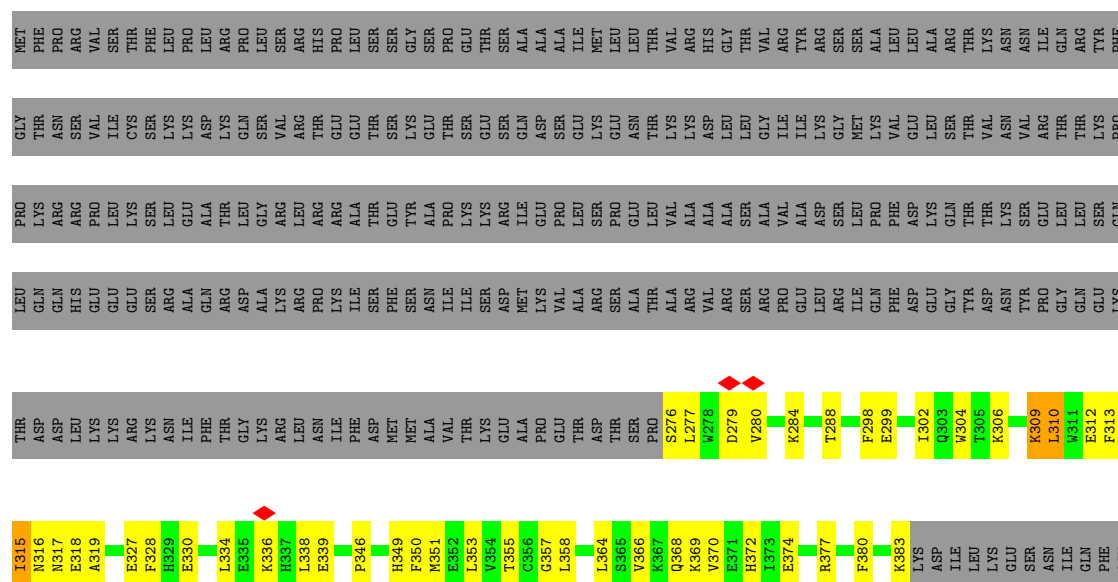
• Molecule 75: Small ribosomal subunit protein mS29

Chain Se:  66% 21% 12%



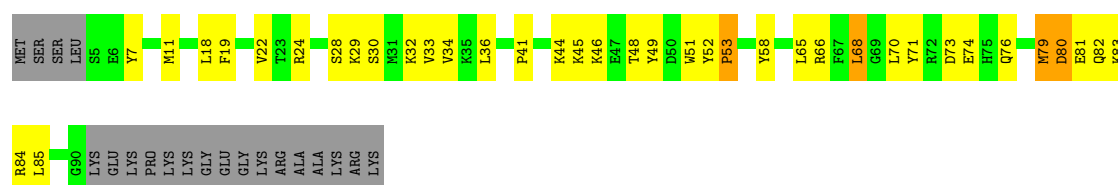
• Molecule 76: Small ribosomal subunit protein mS31

Chain Sg:  16% 11% 73%



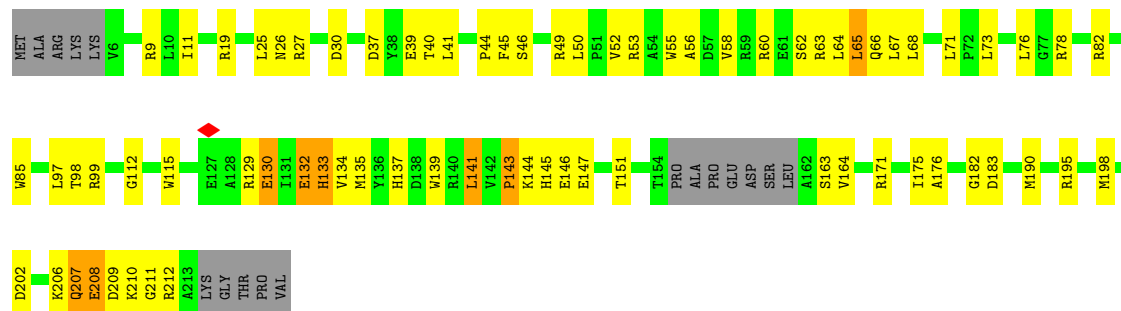
• Molecule 77: Small ribosomal subunit protein mS33

Chain Si:  45% 32% 19%



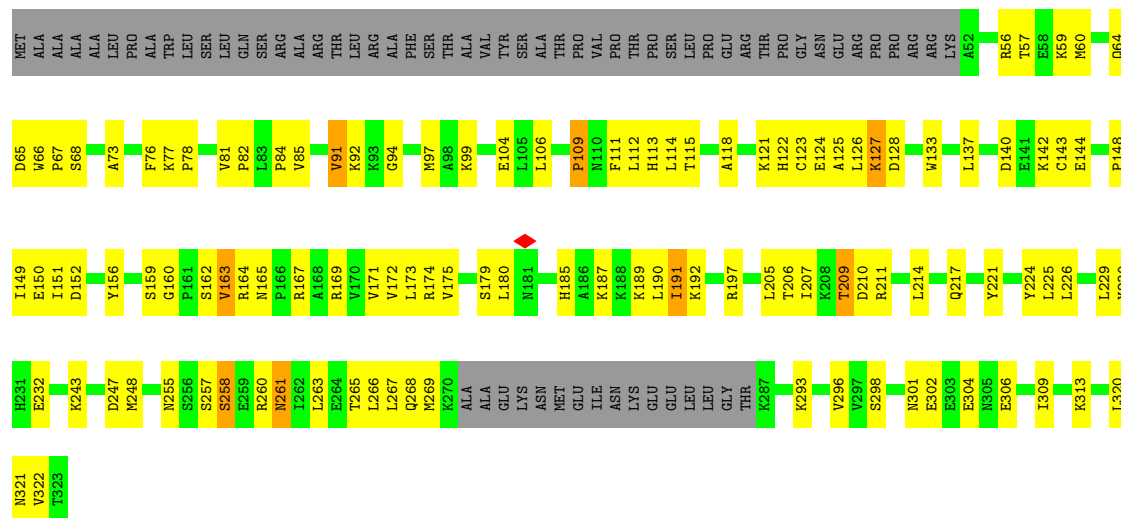
• Molecule 78: Small ribosomal subunit protein mS34

Chain Sj:  59% 30% 8%



- Molecule 79: Small ribosomal subunit protein mS35

Chain Sk:  44% 33% 21%



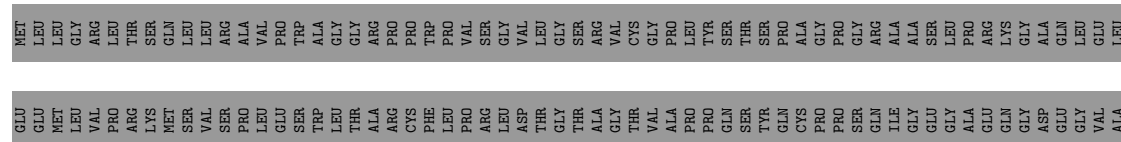
- Molecule 80: Small ribosomal subunit protein mS37

Chain Sm:  69% 29% 2%



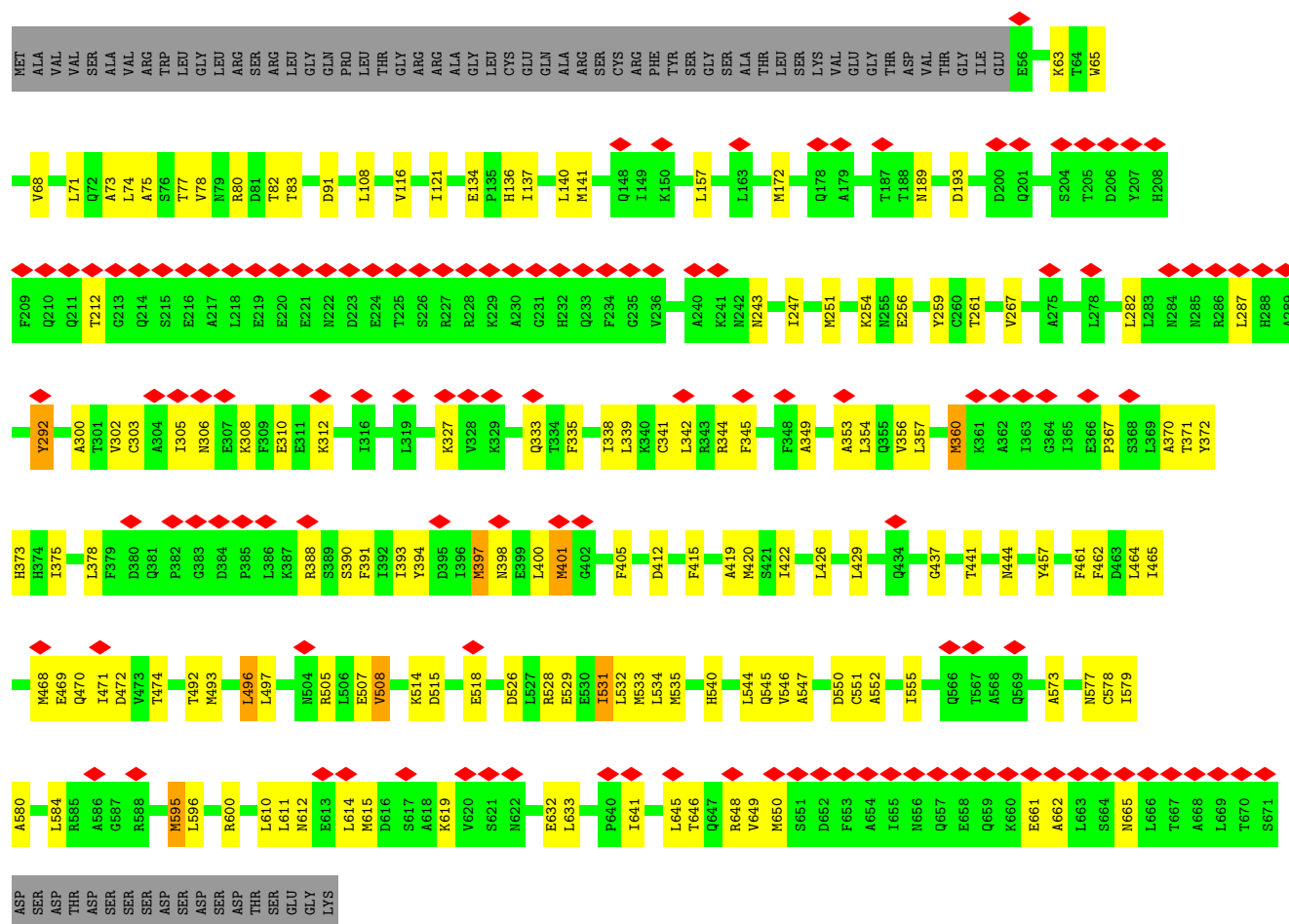
- Molecule 81: Small ribosomal subunit protein mS38

Chain Sn:  26% 9% 65%

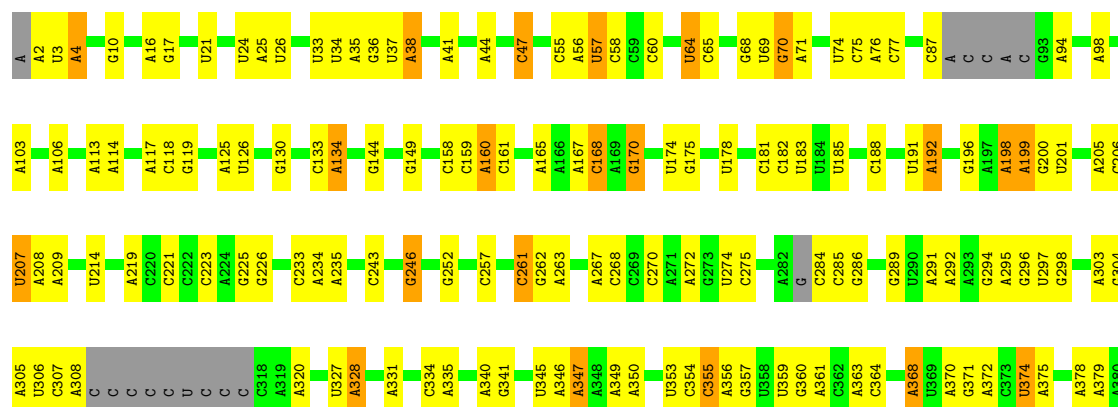




• Molecule 82: Small ribosomal subunit protein mS39



• Molecule 83: 12S rRNA



A883	C782	A706	U610	A507	G381
C884	A783	A706	A611	G508	U382
C885	A786	A709	U612	A514	G383
C887	A787	A709	A613	A515	G384
U888	U712	U712	C614	U395	C385
A889	A791	G713	C618	A519	U386
C890	A792	G714	U620	A520	U387
G891	G793	A720	C621	C525	U388
C892	A794	U721	U622	G532	U395
A893	G795	G723	U623	U533	C396
U894	U796	A797	C624	A537	U397
A897	G798	U723	A625	U402	A402
A910	A799	U726	C631	C405	A405
A911	G800	A727	C632	U540	G410
G912	U805	C728	C633	A541	C418
G915	A806	C729	A636	U542	C419
U916	G807	C731	U637	C544	A422
A917	U808	A732	G638	U546	U434
A918	U809	G733	C638	C547	A435
U921	G817	A734	C643	U548	U442
G922	C818	A735	U644	A549	A443
G923	C819	A736	A645	A554	C451
U930	A823	A	C646	G555	A456
A931	A824	C	A647	U567	A457
C932	G825	U	A648	U568	C458
G935	A831	G742	C654	A573	C459
A936	C832	U744	C655	C576	U460
A937	C834	A745	C656	C577	C461
A938	C835	U751	A662	C578	A462
G939	C841	A752	C663	C579	A463
U940	G842	U753	C667	G580	U468
G941	U843	G754	C670	U598	A
C942	U843	A755	A671	U599	A
A943	C847	A756	C671	G600	U
G947	C848	A757	C676	C601	C473
C948	U849	C	A679	U602	A474
G948	U849	U	C680	A593	A479
A952	C864	U760	C683	U598	A480
A953	A865	A761	A684	G600	C481
C954	A866	G762	C685	C601	C489
	A867	G763	A685	U602	U497
	A870	G764	C686	A604	A498
	A870	G765	C689	C607	C504
	U874	U766	C694	G607	
	U874	C767	C695		
	A877	G768	C696		
	C878	A769	C697		
	U880	A770	U697		
	A881	U773	C700		
	A882	A780	G701		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.669	Depositor
Minimum map value	-0.297	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	499.80002, 499.80002, 499.80002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T1C, ZN, GDP

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	0.34	0/35628	0.51	5/55448 (0.0%)
2	L2	0.18	0/1328	0.36	0/2056
3	LB	0.53	0/1888	0.83	0/2538
4	LC	0.61	0/2462	1.00	6/3340 (0.2%)
5	LD	0.55	0/2071	0.92	4/2817 (0.1%)
6	LI	0.46	0/798	0.84	1/1073 (0.1%)
7	LJ	0.66	2/1308 (0.2%)	1.18	6/1761 (0.3%)
8	LK	0.43	0/1340	0.81	3/1802 (0.2%)
9	LM	0.53	0/1495	0.88	1/2029 (0.0%)
10	LN	0.61	0/904	0.93	1/1218 (0.1%)
11	LO	0.51	0/2359	0.85	3/3185 (0.1%)
12	LP	0.51	0/1826	0.82	2/2458 (0.1%)
13	LQ	0.53	0/1269	0.90	2/1708 (0.1%)
14	LR	0.56	0/1215	0.92	1/1645 (0.1%)
15	LS	0.40	0/1863	0.71	3/2509 (0.1%)
16	LT	0.45	0/1174	0.81	0/1572
17	LU	0.55	1/1311 (0.1%)	0.87	2/1778 (0.1%)
18	LV	0.53	0/1402	0.88	3/1886 (0.2%)
19	LW	0.31	0/1217	0.61	0/1644
20	LX	0.52	0/1697	0.91	0/2302
21	La	0.61	0/893	0.94	3/1204 (0.2%)
22	Lb	0.45	0/2090	0.91	3/2825 (0.1%)
23	Lu	0.47	0/1552	0.83	4/2079 (0.2%)
24	Ld	0.63	0/1003	1.03	4/1354 (0.3%)
25	Lf	0.61	0/895	0.94	0/1201
26	Lg	0.53	0/438	0.89	0/583
27	Lh	0.56	0/382	0.92	0/507
28	Li	0.35	0/852	0.68	0/1136
29	Lj	0.57	0/349	0.97	2/461 (0.4%)
30	Lk	0.43	0/3305	0.75	6/4502 (0.1%)
31	Ll	0.58	0/3042	0.95	10/4140 (0.2%)
32	Lm	0.42	0/2439	0.78	2/3299 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ln	0.60	0/855	1.08	3/1152 (0.3%)
34	Lo	0.56	0/1025	0.90	3/1379 (0.2%)
35	Lp	0.40	0/839	0.82	2/1136 (0.2%)
36	Lq	0.62	0/1202	0.87	0/1626
37	Lr	0.61	0/2264	1.05	6/3059 (0.2%)
38	Ls	0.49	0/1800	0.85	2/2436 (0.1%)
39	Lt	0.36	0/1797	0.78	1/2422 (0.0%)
40	Lv	0.60	0/1051	1.01	2/1422 (0.1%)
41	Lw	0.57	0/1134	1.00	3/1547 (0.2%)
42	Lx	0.65	0/918	1.00	0/1249
43	Ly	0.51	0/849	0.89	1/1135 (0.1%)
44	Lz	0.48	0/747	0.85	1/1005 (0.1%)
45	L3	0.59	0/754	1.21	3/1017 (0.3%)
46	L4	0.58	0/722	1.09	0/978
47	L5	0.58	0/379	0.97	0/510
48	L6	0.52	0/818	0.85	0/1097
49	L7	0.55	0/1071	0.98	4/1433 (0.3%)
50	L8	0.39	0/1107	0.74	4/1498 (0.3%)
51	SR	0.47	0/1238	0.81	0/1676
52	Sf	0.53	0/3114	0.87	4/4225 (0.1%)
53	SB	0.61	0/1811	1.05	6/2451 (0.2%)
54	SZ	0.50	0/1112	0.99	2/1505 (0.1%)
55	SE	0.41	0/2590	0.80	6/3477 (0.2%)
56	SF	0.34	0/989	0.68	0/1335
57	SG	0.47	0/1708	0.87	5/2291 (0.2%)
58	SI	0.46	0/2555	0.85	0/3424
59	SJ	0.49	0/1019	1.10	4/1379 (0.3%)
60	SK	0.47	0/1031	0.79	0/1390
61	SL	0.68	0/854	1.11	6/1148 (0.5%)
62	SN	0.65	1/879 (0.1%)	1.17	2/1182 (0.2%)
63	SO	0.63	0/1406	1.13	3/1878 (0.2%)
64	SP	0.60	0/941	1.05	2/1265 (0.2%)
65	SQ	0.67	0/864	1.03	1/1169 (0.1%)
66	SS	0.55	0/1580	0.95	6/2150 (0.3%)
67	ST	0.66	0/791	1.08	4/1062 (0.4%)
68	SW	0.61	0/752	1.08	5/1001 (0.5%)
69	SX	0.46	0/2452	0.96	4/3310 (0.1%)
70	SY	0.52	0/1069	0.89	0/1441
71	Sa	0.58	0/1361	0.97	1/1829 (0.1%)
72	Sb	0.46	0/1474	0.82	1/1976 (0.1%)
73	Sc	0.33	0/3177	0.72	1/4292 (0.0%)
74	Sd	0.72	0/778	1.24	5/1048 (0.5%)
75	Se	0.36	0/2908	0.75	5/3936 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Sg	0.53	0/931	1.03	1/1259 (0.1%)
77	Si	0.54	0/748	1.05	3/1000 (0.3%)
78	Sj	0.51	0/1723	1.00	8/2334 (0.3%)
79	Sk	0.55	0/2113	1.06	8/2863 (0.3%)
80	Sm	0.43	0/939	0.84	2/1256 (0.2%)
81	Sn	0.46	0/621	0.89	0/820
82	So	0.33	0/5093	0.70	9/6891 (0.1%)
83	S1	0.26	0/22053	0.44	2/34324 (0.0%)
All	All	0.45	4/173801 (0.0%)	0.77	218/246748 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	LJ	0	1
8	LK	0	1
76	Sg	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	LJ	115	GLN	C-O	6.71	1.32	1.24
62	SN	59	LYS	CA-CB	5.59	1.60	1.52
7	LJ	144	LEU	C-N	5.46	1.38	1.33
17	LU	160	VAL	C-O	-5.06	1.19	1.24

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Lb	18	GLU	CA-C-N	-11.58	108.06	122.19
22	Lb	18	GLU	C-N-CA	-11.58	108.06	122.19
45	L3	45	THR	N-CA-C	-11.02	102.06	114.62
78	Sj	209	ASP	N-CA-C	-10.17	100.90	113.20
53	SB	148	ASN	CB-CA-C	-9.62	94.99	110.86

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	LJ	138	SER	Peptide
8	LK	58	LYS	Peptide
76	Sg	327	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	31847	0	16179	216	0
2	L2	1191	0	607	9	0
3	LB	1851	0	1909	25	0
4	LC	2393	0	2398	59	0
5	LD	2013	0	2044	49	0
6	LI	784	0	832	22	0
7	LJ	1283	0	1370	41	0
8	LK	1323	0	1400	38	0
9	LM	1451	0	1448	31	0
10	LN	889	0	941	22	0
11	LO	2305	0	2378	45	0
12	LP	1779	0	1808	33	0
13	LQ	1245	0	1283	15	0
14	LR	1189	0	1180	42	0
15	LS	1822	0	1859	29	0
16	LT	1153	0	1214	14	0
17	LU	1284	0	1354	18	0
18	LV	1368	0	1410	24	0
19	LW	1188	0	1180	27	0
20	LX	1652	0	1658	54	0
21	La	871	0	898	15	0
22	Lb	2035	0	2054	44	0
23	Lu	1517	0	1561	23	0
24	Ld	978	0	1030	25	0
25	Lf	880	0	902	17	0
26	Lg	433	0	475	29	0
27	Lh	376	0	406	6	0
28	Li	831	0	883	13	0
29	Lj	341	0	361	4	0
30	Lk	3210	0	3206	42	0
31	Ll	2947	0	2841	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Lm	2382	0	2393	56	0
33	Ln	836	0	844	37	0
34	Lo	997	0	987	20	0
35	Lp	815	0	792	12	0
36	Lq	1178	0	1180	31	0
37	Lr	2217	0	2220	39	0
38	Ls	1754	0	1732	69	0
39	Lt	1762	0	1767	67	0
40	Lv	1035	0	1040	56	0
41	Lw	1097	0	1085	26	0
42	Lx	895	0	881	24	0
43	Ly	827	0	857	15	0
44	Lz	732	0	730	6	0
45	L3	743	0	758	25	0
46	L4	703	0	693	29	0
47	L5	372	0	387	23	0
48	L6	797	0	804	23	0
49	L7	1058	0	1083	43	0
50	L8	1076	0	1049	25	0
51	SR	1203	0	1219	28	0
52	Sf	3036	0	3022	42	0
53	SB	1768	0	1765	61	0
54	SZ	1082	0	1088	44	0
55	SE	2540	0	2574	35	0
56	SF	972	0	1001	29	0
57	SG	1668	0	1716	53	0
58	SI	2501	0	2486	79	0
59	SJ	999	0	1024	79	0
60	SK	1011	0	1052	48	0
61	SL	838	0	887	23	0
62	SN	861	0	885	78	0
63	SO	1382	0	1472	85	0
64	SP	920	0	951	43	0
65	SQ	846	0	908	35	0
66	SS	1528	0	1488	57	0
67	ST	774	0	801	22	0
68	SW	740	0	754	25	0
69	SX	2405	0	2425	72	0
70	SY	1042	0	1037	45	0
71	Sa	1330	0	1342	51	0
72	Sb	1454	0	1464	53	0
73	Sc	3116	0	3069	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	Sd	766	0	785	16	0
75	Se	2836	0	2828	62	0
76	Sg	903	0	843	44	0
77	Si	731	0	734	84	0
78	Sj	1680	0	1674	66	0
79	Sk	2068	0	2087	148	0
80	Sm	925	0	962	25	0
81	Sn	610	0	682	20	0
82	So	4981	0	4959	181	0
83	S1	19716	0	10015	188	0
84	L1	105	0	0	1	0
84	L6	1	0	0	0	0
84	LB	3	0	0	0	0
84	LC	1	0	0	0	0
84	La	1	0	0	0	0
84	Lw	1	0	0	0	0
84	S1	33	0	0	0	0
85	L1	84	0	76	1	0
85	S1	84	0	76	1	0
86	Lf	1	0	0	0	0
86	Lj	1	0	0	0	0
86	SB	1	0	0	0	0
86	SR	1	0	0	0	0
86	SS	1	0	0	0	0
86	ST	1	0	0	0	0
86	Sa	1	0	0	0	0
87	Se	28	0	12	0	0
All	All	165285	0	140514	3173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 3173 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Sk:113:HIS:CD2	79:Sk:114:LEU:HG	1.43	1.50
73:Sc:180:LEU:HD12	73:Sc:181:LEU:N	1.27	1.49
40:Lv:146:LEU:HD23	40:Lv:147:ASP:N	1.19	1.47
40:Lv:146:LEU:CD2	40:Lv:147:ASP:H	1.25	1.45
79:Sk:320:LEU:HD13	79:Sk:321:ASN:N	1.33	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LB	235/305 (77%)	224 (95%)	9 (4%)	2 (1%)	14	41
4	LC	302/348 (87%)	275 (91%)	25 (8%)	2 (1%)	18	48
5	LD	248/311 (80%)	233 (94%)	15 (6%)	0	100	100
6	LI	93/267 (35%)	83 (89%)	10 (11%)	0	100	100
7	LJ	154/261 (59%)	132 (86%)	19 (12%)	3 (2%)	6	23
8	LK	173/192 (90%)	156 (90%)	15 (9%)	2 (1%)	10	34
9	LM	175/178 (98%)	164 (94%)	10 (6%)	1 (1%)	21	51
10	LN	113/145 (78%)	103 (91%)	10 (9%)	0	100	100
11	LO	285/296 (96%)	274 (96%)	10 (4%)	1 (0%)	30	59
12	LP	219/251 (87%)	214 (98%)	4 (2%)	1 (0%)	24	54
13	LQ	150/175 (86%)	141 (94%)	8 (5%)	1 (1%)	18	48
14	LR	144/179 (80%)	138 (96%)	6 (4%)	0	100	100
15	LS	217/292 (74%)	206 (95%)	11 (5%)	0	100	100
16	LT	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	LU	158/205 (77%)	150 (95%)	7 (4%)	1 (1%)	21	51
18	LV	164/212 (77%)	151 (92%)	12 (7%)	1 (1%)	21	51
19	LW	139/153 (91%)	138 (99%)	1 (1%)	0	100	100
20	LX	200/216 (93%)	184 (92%)	16 (8%)	0	100	100
21	La	109/148 (74%)	104 (95%)	5 (5%)	0	100	100
22	Lb	241/256 (94%)	225 (93%)	15 (6%)	1 (0%)	30	59
23	Lu	174/250 (70%)	167 (96%)	6 (3%)	1 (1%)	21	51
24	Ld	118/161 (73%)	111 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Lf	106/188 (56%)	101 (95%)	5 (5%)	0	100	100
26	Lg	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
27	Lh	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
28	Li	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
29	Lj	36/103 (35%)	36 (100%)	0	0	100	100
30	Lk	392/423 (93%)	375 (96%)	17 (4%)	0	100	100
31	Ll	352/380 (93%)	323 (92%)	26 (7%)	3 (1%)	14	41
32	Lm	291/338 (86%)	278 (96%)	12 (4%)	1 (0%)	36	65
33	Ln	97/206 (47%)	81 (84%)	14 (14%)	2 (2%)	5	21
34	Lo	122/137 (89%)	115 (94%)	6 (5%)	1 (1%)	16	44
35	Lp	93/142 (66%)	89 (96%)	4 (4%)	0	100	100
36	Lq	146/215 (68%)	133 (91%)	13 (9%)	0	100	100
37	Lr	271/332 (82%)	261 (96%)	10 (4%)	0	100	100
38	Ls	210/306 (69%)	200 (95%)	10 (5%)	0	100	100
39	Lt	211/279 (76%)	186 (88%)	23 (11%)	2 (1%)	14	41
40	Lv	125/212 (59%)	114 (91%)	10 (8%)	1 (1%)	16	44
41	Lw	130/166 (78%)	121 (93%)	8 (6%)	1 (1%)	16	44
42	Lx	108/158 (68%)	103 (95%)	4 (4%)	1 (1%)	14	41
43	Ly	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
44	Lz	90/123 (73%)	84 (93%)	6 (7%)	0	100	100
45	L3	94/112 (84%)	79 (84%)	14 (15%)	1 (1%)	11	36
46	L4	81/138 (59%)	73 (90%)	6 (7%)	2 (2%)	4	17
47	L5	43/128 (34%)	38 (88%)	4 (9%)	1 (2%)	5	19
48	L6	92/102 (90%)	90 (98%)	2 (2%)	0	100	100
49	L7	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
50	L8	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
51	SR	140/196 (71%)	134 (96%)	6 (4%)	0	100	100
52	Sf	366/439 (83%)	345 (94%)	19 (5%)	2 (0%)	24	54
53	SB	215/296 (73%)	200 (93%)	15 (7%)	0	100	100
54	SZ	130/167 (78%)	111 (85%)	18 (14%)	1 (1%)	16	44
55	SE	314/430 (73%)	289 (92%)	24 (8%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	SF	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
57	SG	197/242 (81%)	192 (98%)	4 (2%)	1 (0%)	24	54
58	SI	300/396 (76%)	267 (89%)	28 (9%)	5 (2%)	7	26
59	SJ	120/201 (60%)	101 (84%)	18 (15%)	1 (1%)	16	44
60	SK	134/194 (69%)	126 (94%)	8 (6%)	0	100	100
61	SL	106/138 (77%)	90 (85%)	12 (11%)	4 (4%)	2	10
62	SN	99/128 (77%)	86 (87%)	12 (12%)	1 (1%)	12	39
63	SO	162/257 (63%)	148 (91%)	12 (7%)	2 (1%)	10	34
64	SP	114/137 (83%)	105 (92%)	7 (6%)	2 (2%)	6	25
65	SQ	105/130 (81%)	91 (87%)	10 (10%)	4 (4%)	2	10
66	SS	183/258 (71%)	156 (85%)	24 (13%)	3 (2%)	7	27
67	ST	94/142 (66%)	89 (95%)	4 (4%)	1 (1%)	11	36
68	SW	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
69	SX	293/360 (81%)	274 (94%)	19 (6%)	0	100	100
70	SY	124/190 (65%)	115 (93%)	7 (6%)	2 (2%)	7	27
71	Sa	160/173 (92%)	143 (89%)	14 (9%)	3 (2%)	6	23
72	Sb	171/205 (83%)	168 (98%)	2 (1%)	1 (1%)	21	51
73	Sc	383/414 (92%)	364 (95%)	18 (5%)	1 (0%)	36	65
74	Sd	95/187 (51%)	85 (90%)	9 (10%)	1 (1%)	11	36
75	Se	348/398 (87%)	333 (96%)	13 (4%)	2 (1%)	21	51
76	Sg	106/395 (27%)	98 (92%)	7 (7%)	1 (1%)	14	41
77	Si	84/106 (79%)	78 (93%)	6 (7%)	0	100	100
78	Sj	197/218 (90%)	161 (82%)	31 (16%)	5 (2%)	4	17
79	Sk	252/323 (78%)	217 (86%)	33 (13%)	2 (1%)	16	44
80	Sm	114/118 (97%)	107 (94%)	6 (5%)	1 (1%)	14	41
81	Sn	67/199 (34%)	65 (97%)	2 (3%)	0	100	100
82	So	614/689 (89%)	595 (97%)	19 (3%)	0	100	100
All	All	13557/17977 (75%)	12631 (93%)	846 (6%)	80 (1%)	23	51

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	LC	82	ASP

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Mol	Chain	Res	Type
13	LQ	111	PRO
22	Lb	92	ALA
39	Lt	266	PRO
39	Lt	270	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	LB	191/245 (78%)	191 (100%)	0	100	100
4	LC	258/290 (89%)	254 (98%)	4 (2%)	55	83
5	LD	217/262 (83%)	216 (100%)	1 (0%)	81	93
6	LI	86/228 (38%)	85 (99%)	1 (1%)	63	86
7	LJ	145/232 (62%)	139 (96%)	6 (4%)	27	61
8	LK	137/150 (91%)	131 (96%)	6 (4%)	25	59
9	LM	155/156 (99%)	154 (99%)	1 (1%)	78	93
10	LN	98/124 (79%)	96 (98%)	2 (2%)	48	78
11	LO	245/249 (98%)	244 (100%)	1 (0%)	84	94
12	LP	188/211 (89%)	187 (100%)	1 (0%)	81	93
13	LQ	133/150 (89%)	129 (97%)	4 (3%)	36	70
14	LR	128/154 (83%)	128 (100%)	0	100	100
15	LS	201/256 (78%)	200 (100%)	1 (0%)	81	93
16	LT	118/126 (94%)	116 (98%)	2 (2%)	53	82
17	LU	145/180 (81%)	145 (100%)	0	100	100
18	LV	146/182 (80%)	146 (100%)	0	100	100
19	LW	128/135 (95%)	128 (100%)	0	100	100
20	LX	180/191 (94%)	174 (97%)	6 (3%)	33	67
21	La	91/119 (76%)	91 (100%)	0	100	100
22	Lb	219/229 (96%)	217 (99%)	2 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Lu	159/223 (71%)	158 (99%)	1 (1%)	78	93
24	Ld	111/147 (76%)	109 (98%)	2 (2%)	51	80
25	Lf	97/164 (59%)	95 (98%)	2 (2%)	47	77
26	Lg	49/60 (82%)	49 (100%)	0	100	100
27	Lh	40/72 (56%)	39 (98%)	1 (2%)	42	74
28	Li	88/166 (53%)	88 (100%)	0	100	100
29	Lj	37/89 (42%)	37 (100%)	0	100	100
30	Lk	353/368 (96%)	350 (99%)	3 (1%)	73	90
31	Ll	313/332 (94%)	309 (99%)	4 (1%)	61	86
32	Lm	269/303 (89%)	268 (100%)	1 (0%)	84	94
33	Ln	91/190 (48%)	88 (97%)	3 (3%)	33	67
34	Lo	104/112 (93%)	103 (99%)	1 (1%)	68	89
35	Lp	93/133 (70%)	92 (99%)	1 (1%)	65	88
36	Lq	130/186 (70%)	125 (96%)	5 (4%)	29	64
37	Lr	241/288 (84%)	241 (100%)	0	100	100
38	Ls	196/274 (72%)	195 (100%)	1 (0%)	81	93
39	Lt	188/236 (80%)	179 (95%)	9 (5%)	23	55
40	Lv	116/188 (62%)	108 (93%)	8 (7%)	14	41
41	Lw	122/148 (82%)	120 (98%)	2 (2%)	55	83
42	Lx	104/148 (70%)	98 (94%)	6 (6%)	18	49
43	Ly	86/110 (78%)	85 (99%)	1 (1%)	63	86
44	Lz	73/97 (75%)	73 (100%)	0	100	100
45	L3	81/90 (90%)	80 (99%)	1 (1%)	63	86
46	L4	78/116 (67%)	77 (99%)	1 (1%)	61	86
47	L5	40/113 (35%)	38 (95%)	2 (5%)	22	53
48	L6	80/87 (92%)	79 (99%)	1 (1%)	61	86
49	L7	117/181 (65%)	116 (99%)	1 (1%)	70	90
50	L8	110/178 (62%)	110 (100%)	0	100	100
51	SR	133/169 (79%)	132 (99%)	1 (1%)	73	90
52	Sf	326/381 (86%)	322 (99%)	4 (1%)	63	86
53	SB	191/249 (77%)	188 (98%)	3 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	SZ	115/143 (80%)	107 (93%)	8 (7%)	14	40
55	SE	267/357 (75%)	260 (97%)	7 (3%)	40	73
56	SF	104/107 (97%)	102 (98%)	2 (2%)	50	79
57	SG	178/209 (85%)	174 (98%)	4 (2%)	45	77
58	SI	263/342 (77%)	251 (95%)	12 (5%)	24	57
59	SJ	112/180 (62%)	109 (97%)	3 (3%)	39	73
60	SK	104/147 (71%)	103 (99%)	1 (1%)	68	89
61	SL	93/118 (79%)	90 (97%)	3 (3%)	34	68
62	SN	91/113 (80%)	80 (88%)	11 (12%)	5	16
63	SO	152/226 (67%)	149 (98%)	3 (2%)	48	78
64	SP	95/113 (84%)	89 (94%)	6 (6%)	16	45
65	SQ	93/115 (81%)	90 (97%)	3 (3%)	34	68
66	SS	166/230 (72%)	163 (98%)	3 (2%)	51	80
67	ST	87/123 (71%)	84 (97%)	3 (3%)	32	66
68	SW	78/79 (99%)	77 (99%)	1 (1%)	61	86
69	SX	263/318 (83%)	258 (98%)	5 (2%)	50	79
70	SY	109/164 (66%)	104 (95%)	5 (5%)	24	57
71	Sa	150/157 (96%)	146 (97%)	4 (3%)	39	73
72	Sb	148/174 (85%)	145 (98%)	3 (2%)	48	78
73	Sc	338/364 (93%)	335 (99%)	3 (1%)	70	90
74	Sd	84/158 (53%)	81 (96%)	3 (4%)	31	65
75	Se	310/351 (88%)	306 (99%)	4 (1%)	61	86
76	Sg	97/357 (27%)	92 (95%)	5 (5%)	21	52
77	Si	79/95 (83%)	75 (95%)	4 (5%)	21	53
78	Sj	175/190 (92%)	169 (97%)	6 (3%)	32	66
79	Sk	235/291 (81%)	218 (93%)	17 (7%)	13	39
80	Sm	99/101 (98%)	91 (92%)	8 (8%)	11	33
81	Sn	63/166 (38%)	62 (98%)	1 (2%)	55	83
82	So	548/609 (90%)	543 (99%)	5 (1%)	70	90
All	All	12121/15564 (78%)	11875 (98%)	246 (2%)	48	78

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	SE	240	SER
79	Sk	162	SER
62	SN	29	TYR
79	Sk	109	PRO
80	Sm	58	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
72	Sb	133	GLN
82	So	189	ASN
73	Sc	246	ASN
76	Sg	329	HIS
37	Lr	65	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1491/1559 (95%)	384 (25%)	27 (1%)
2	L2	52/69 (75%)	13 (25%)	0
83	S1	921/954 (96%)	208 (22%)	16 (1%)
All	All	2464/2582 (95%)	605 (24%)	43 (1%)

5 of 605 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	5	A
1	L1	6	A
1	L1	7	C
1	L1	8	C
1	L1	9	U

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
83	S1	117	A
83	S1	600	G
83	S1	374	U
83	S1	519	A
83	S1	684	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 157 ligands modelled in this entry, 152 are monoatomic - leaving 5 for Mogul analysis.

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$
85	T1C	L1	1706	84	45,45,45	1.13	4 (8%)	56,72,72	0.86	2 (3%)
85	T1C	L1	1707	84	45,45,45	1.15	4 (8%)	56,72,72	0.97	4 (7%)
85	T1C	S1	1034	84	45,45,45	1.18	4 (8%)	56,72,72	0.98	2 (3%)
87	GDP	Se	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.86	7 (15%)
85	T1C	S1	1035	-	45,45,45	1.13	4 (8%)	56,72,72	1.09	5 (8%)

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
85	T1C	L1	1706	84	-	10/22/80/80	0/4/4/4
85	T1C	L1	1707	84	-	9/22/80/80	0/4/4/4
85	T1C	S1	1034	84	-	10/22/80/80	0/4/4/4
87	GDP	Se	500	-	-	3/16/32/32	0/3/3/3
85	T1C	S1	1035	-	-	7/22/80/80	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	S1	1034	T1C	C21-N21	5.02	1.47	1.33
85	L1	1707	T1C	C21-N21	5.00	1.47	1.33
85	S1	1035	T1C	C21-N21	4.99	1.47	1.33
85	L1	1706	T1C	C21-N21	4.90	1.47	1.33
87	Se	500	GDP	C5-C4	3.19	1.47	1.38

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	Se	500	GDP	C5-C4-N3	-6.57	117.93	128.39
87	Se	500	GDP	C2-N3-C4	5.33	121.48	112.30
87	Se	500	GDP	N9-C4-N3	5.01	135.96	125.95
85	S1	1035	T1C	C11-C1B-C12	4.06	122.01	118.80
85	S1	1034	T1C	C1-C1C-C12	3.83	114.37	109.88

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	L1	1706	T1C	C41-C4-N4-C43
85	L1	1706	T1C	C3-C4-N4-C43
85	L1	1706	T1C	C3-C4-N4-C42
85	L1	1707	T1C	C41-C4-N4-C43
85	L1	1707	T1C	C3-C4-N4-C43

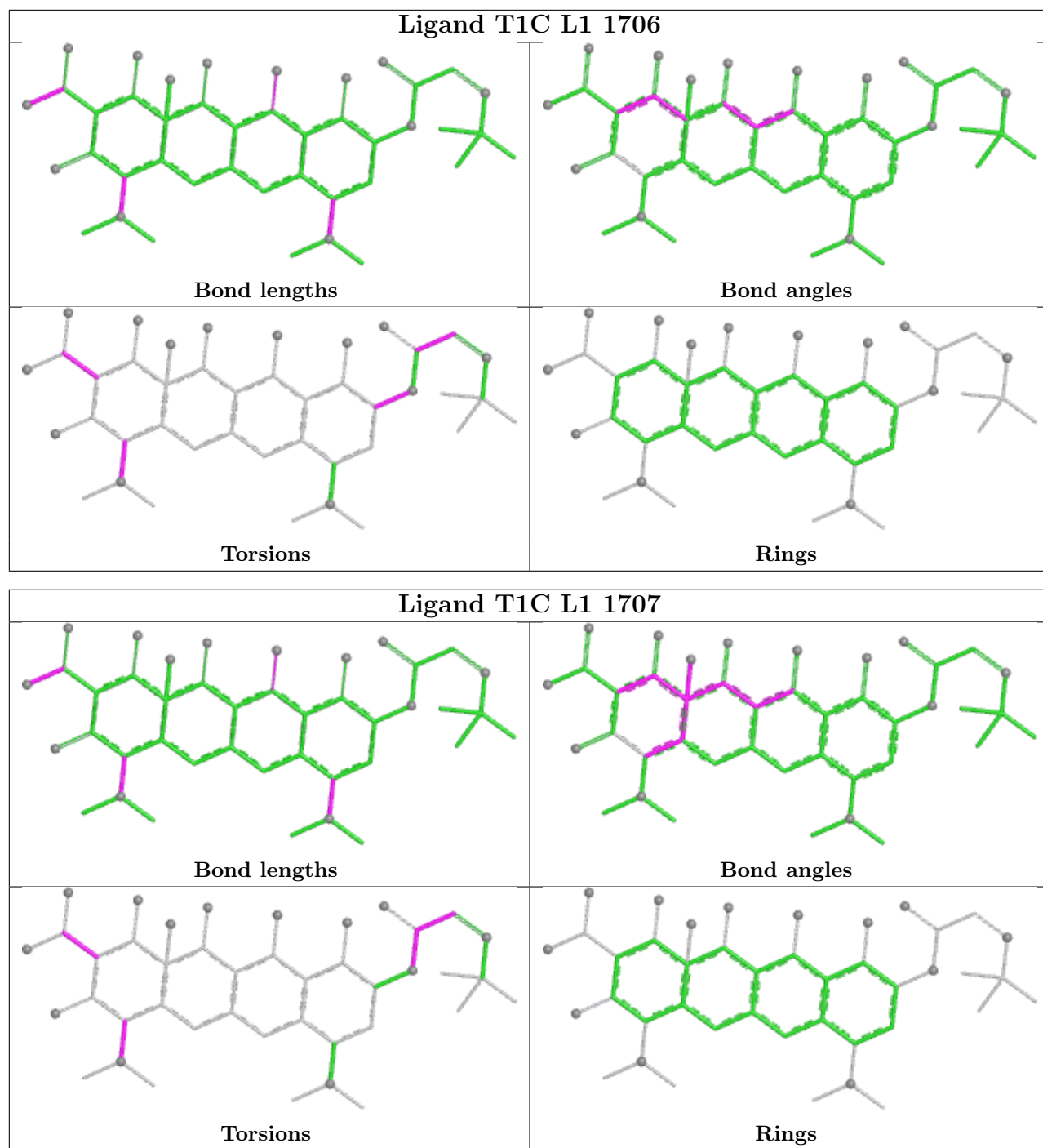
There are no ring outliers.

2 monomers are involved in 2 short contacts:

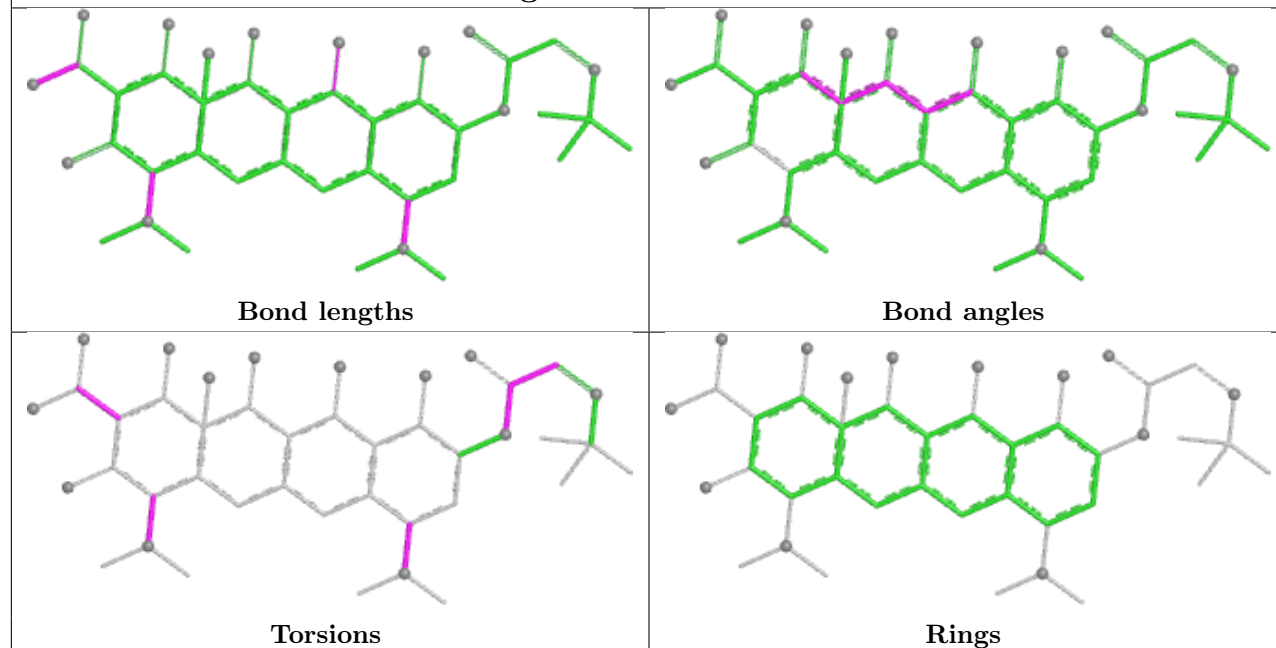
Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	L1	1707	T1C	1	0
85	S1	1034	T1C	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

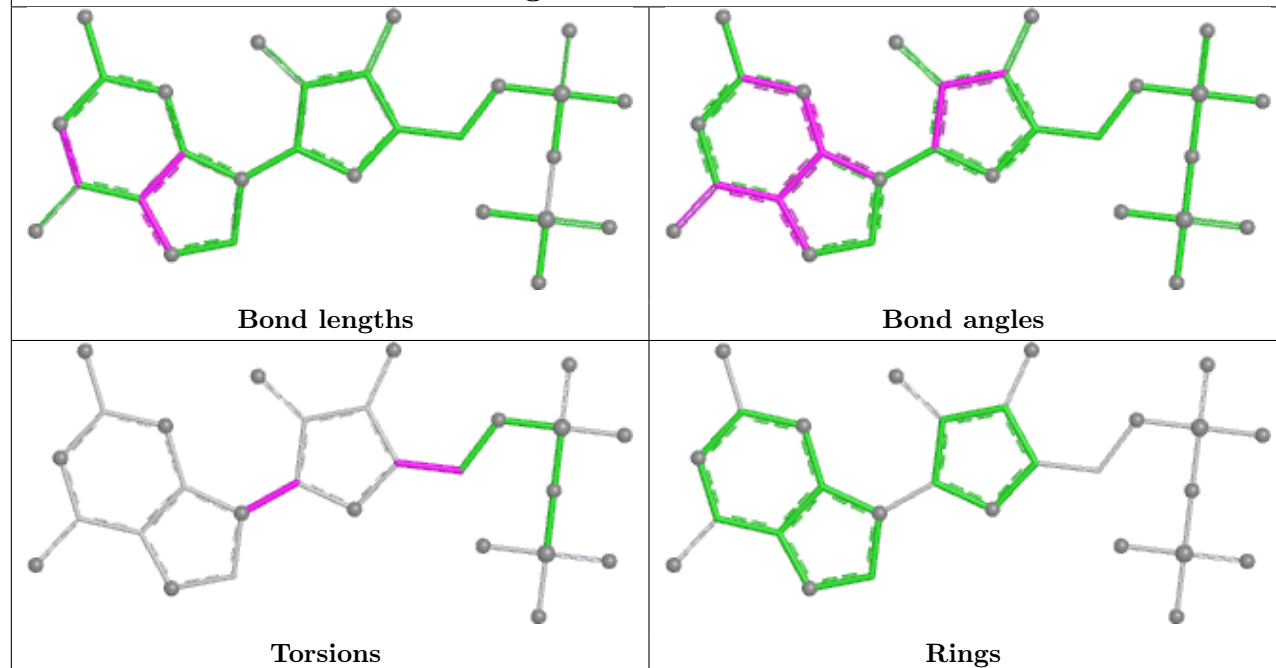
equivalents in the CSD to analyse the geometry.

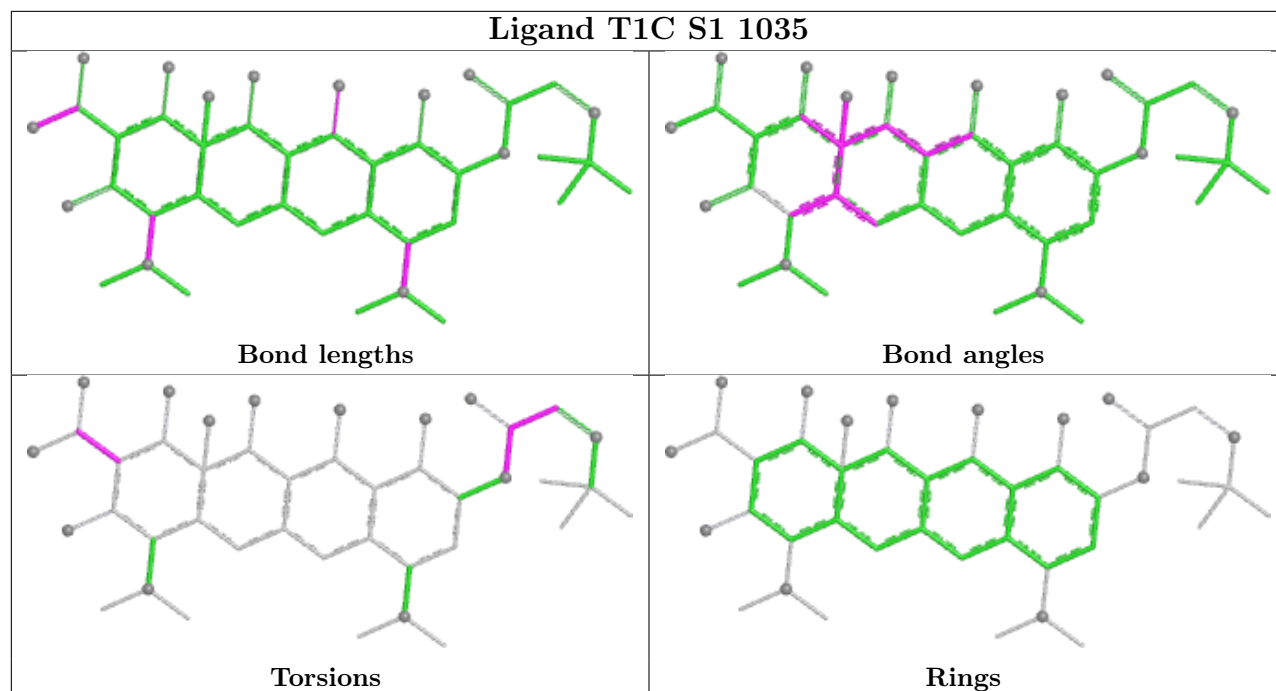


Ligand T1C S1 1034



Ligand GDP Se 500





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

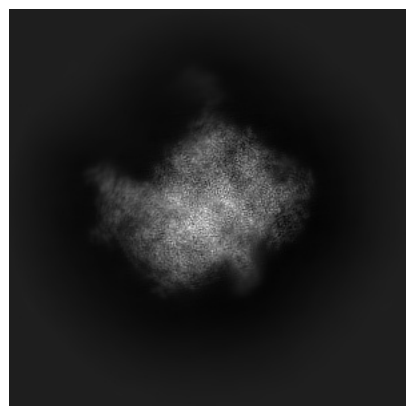
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36836. These allow visual inspection of the internal detail of the map and identification of artifacts.

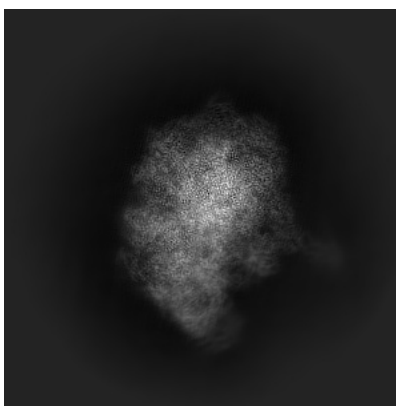
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

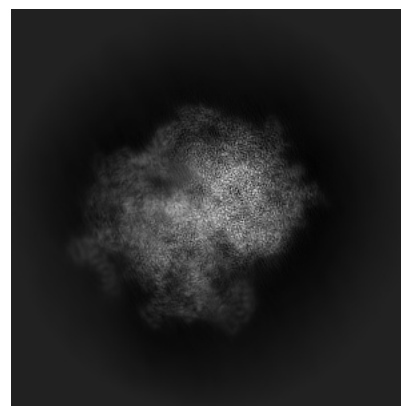
6.1.1 Primary map



X

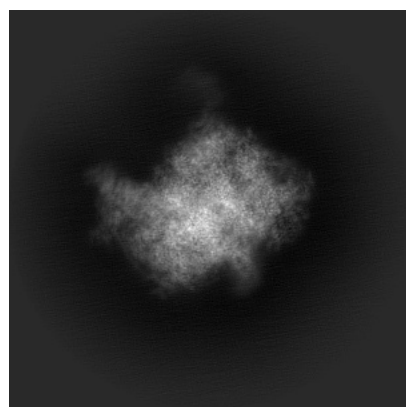


Y

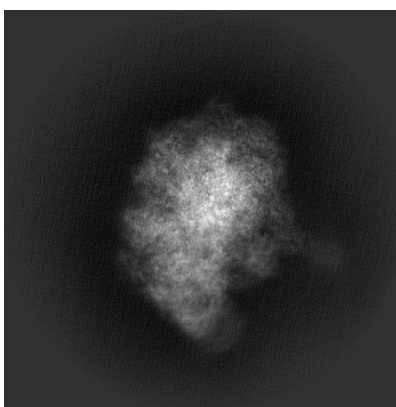


Z

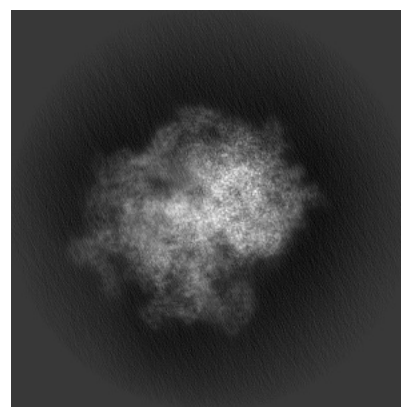
6.1.2 Raw map



X



Y

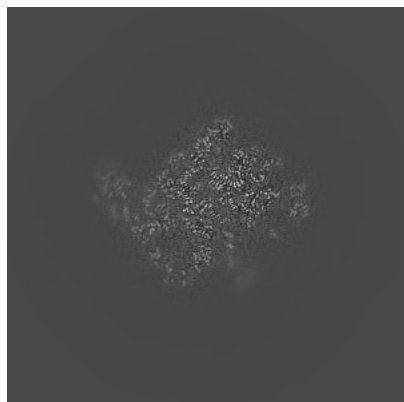


Z

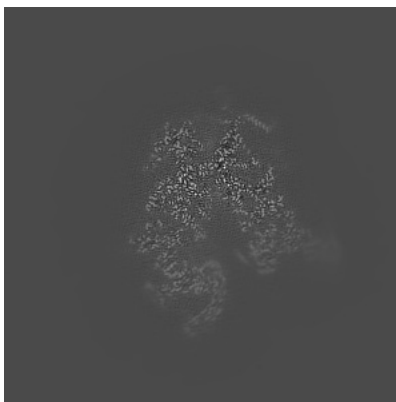
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

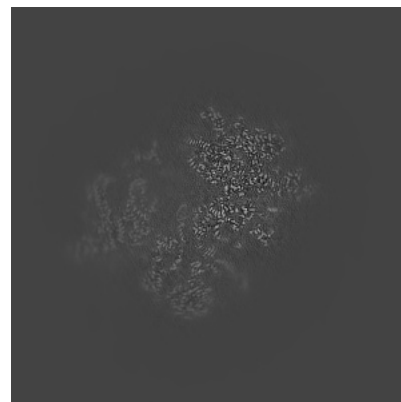
6.2.1 Primary map



X Index: 210

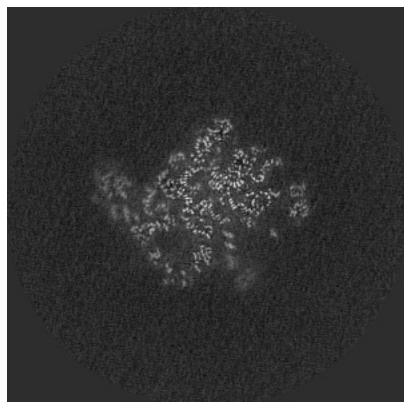


Y Index: 210

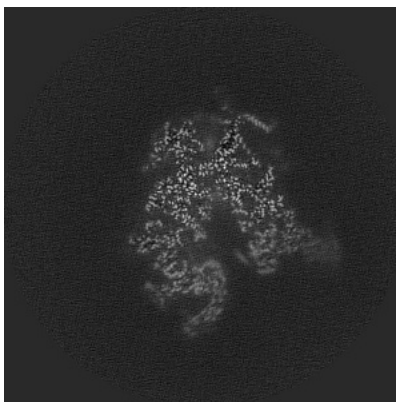


Z Index: 210

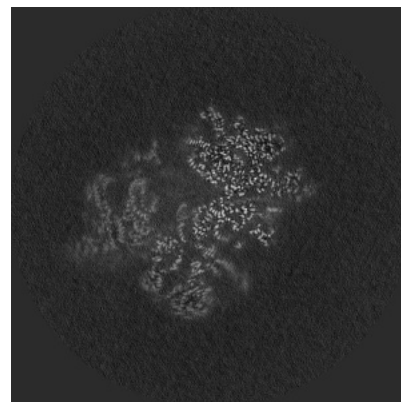
6.2.2 Raw map



X Index: 210



Y Index: 210

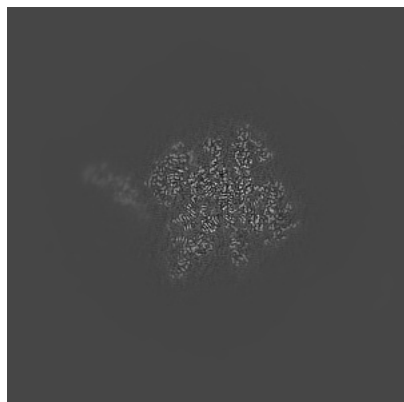


Z Index: 210

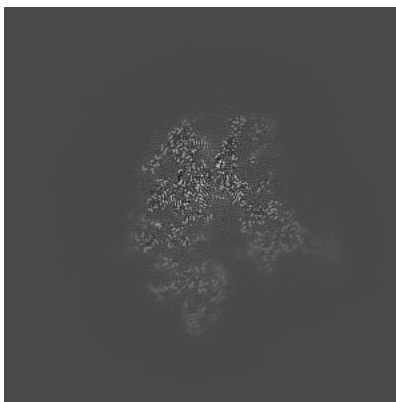
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

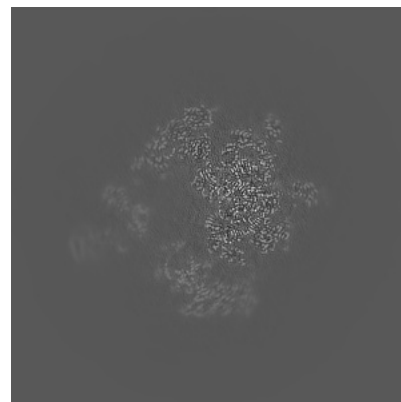
6.3.1 Primary map



X Index: 236

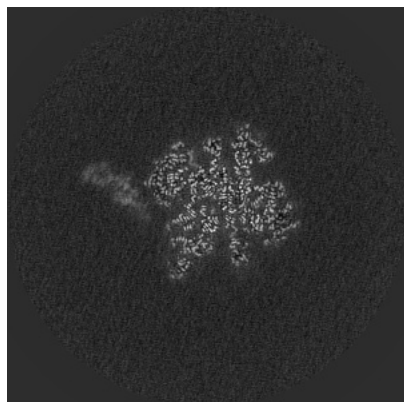


Y Index: 206

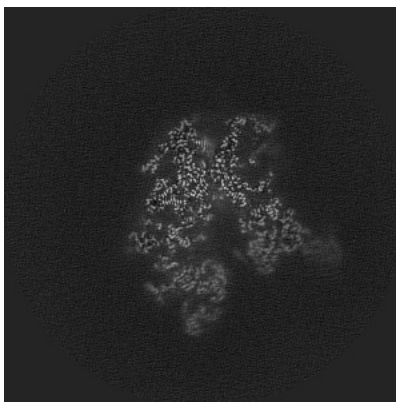


Z Index: 230

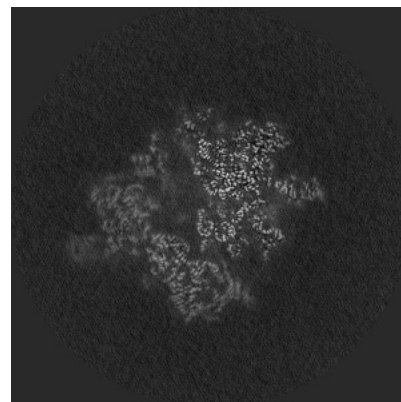
6.3.2 Raw map



X Index: 236



Y Index: 207

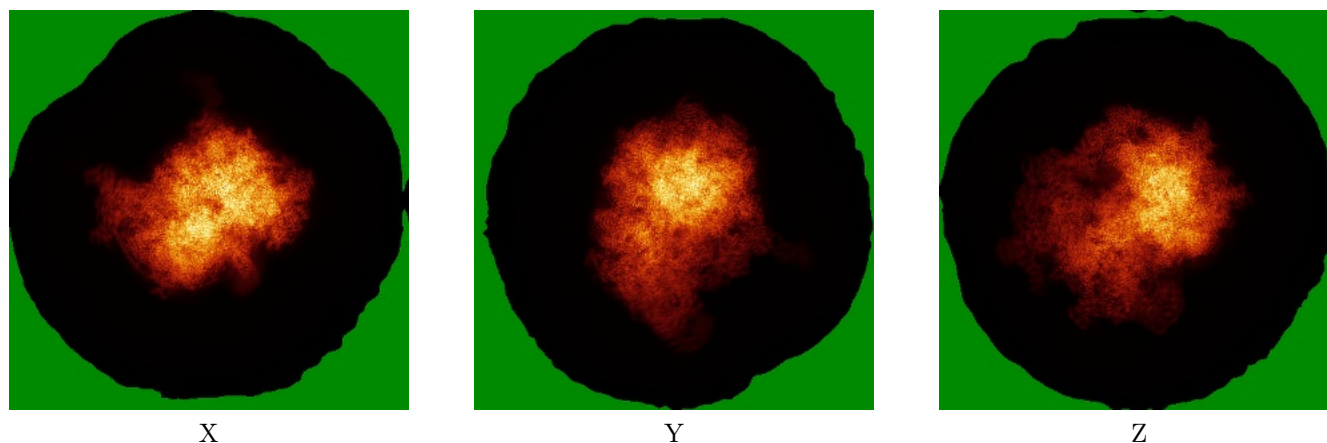


Z Index: 218

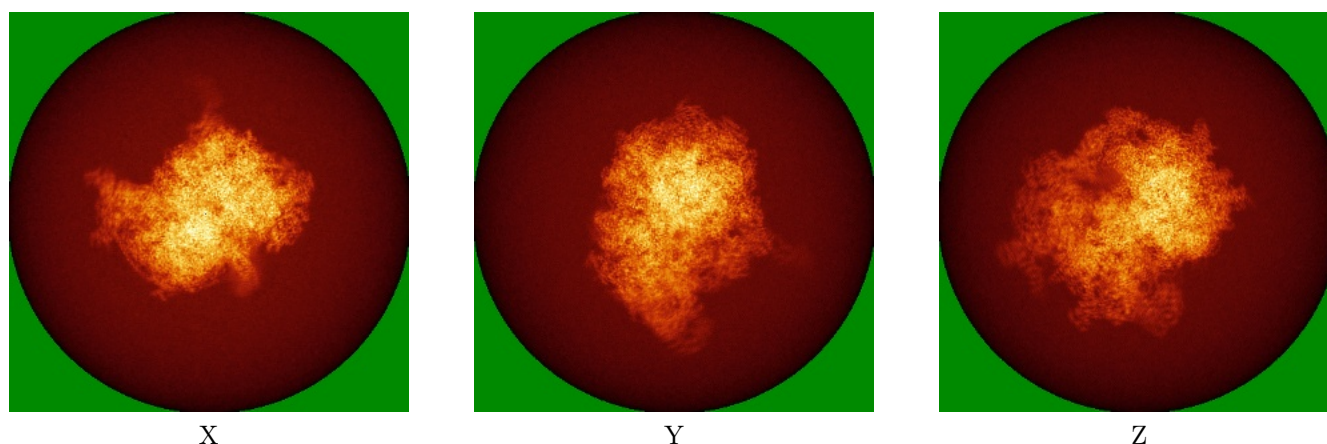
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

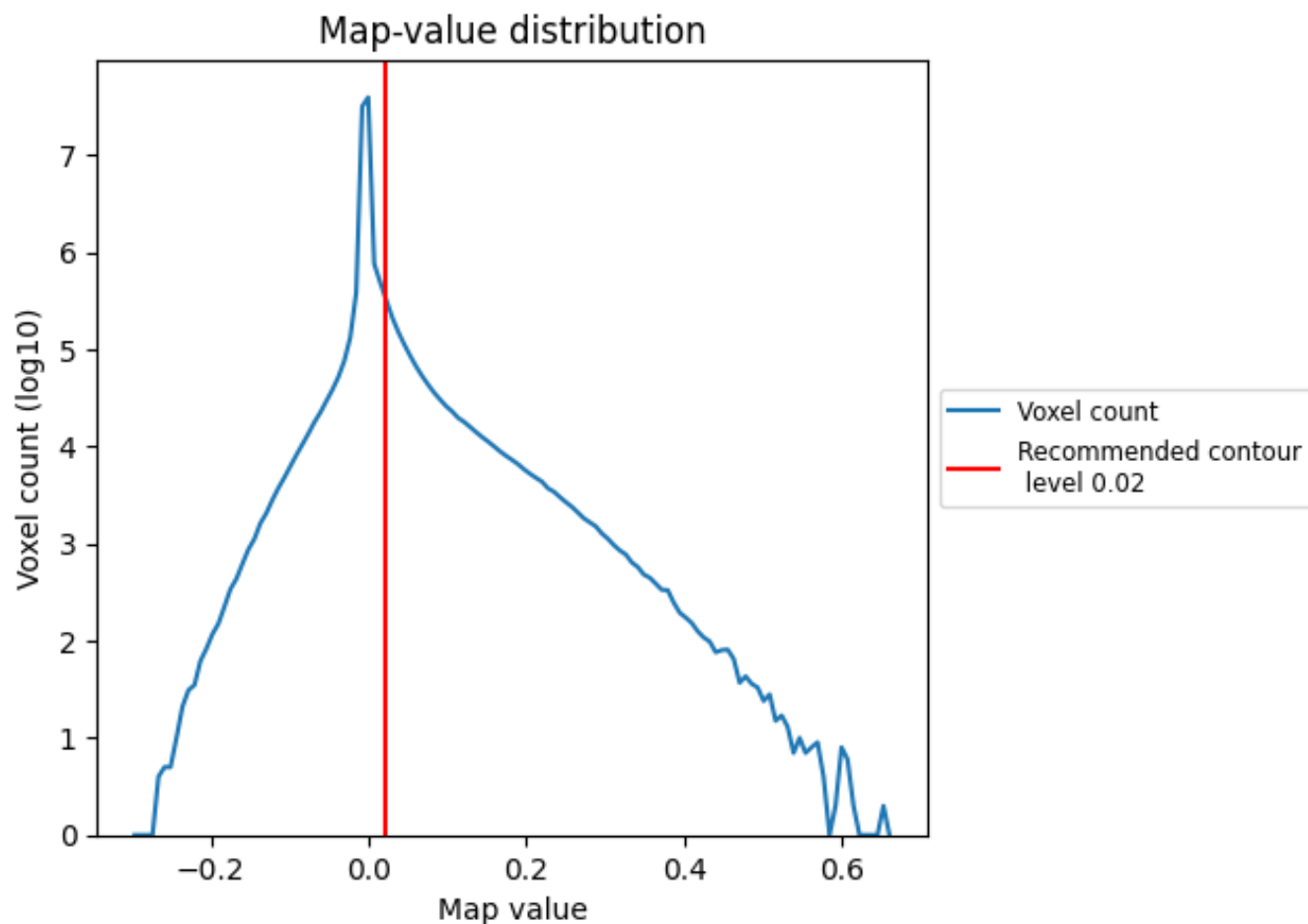
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

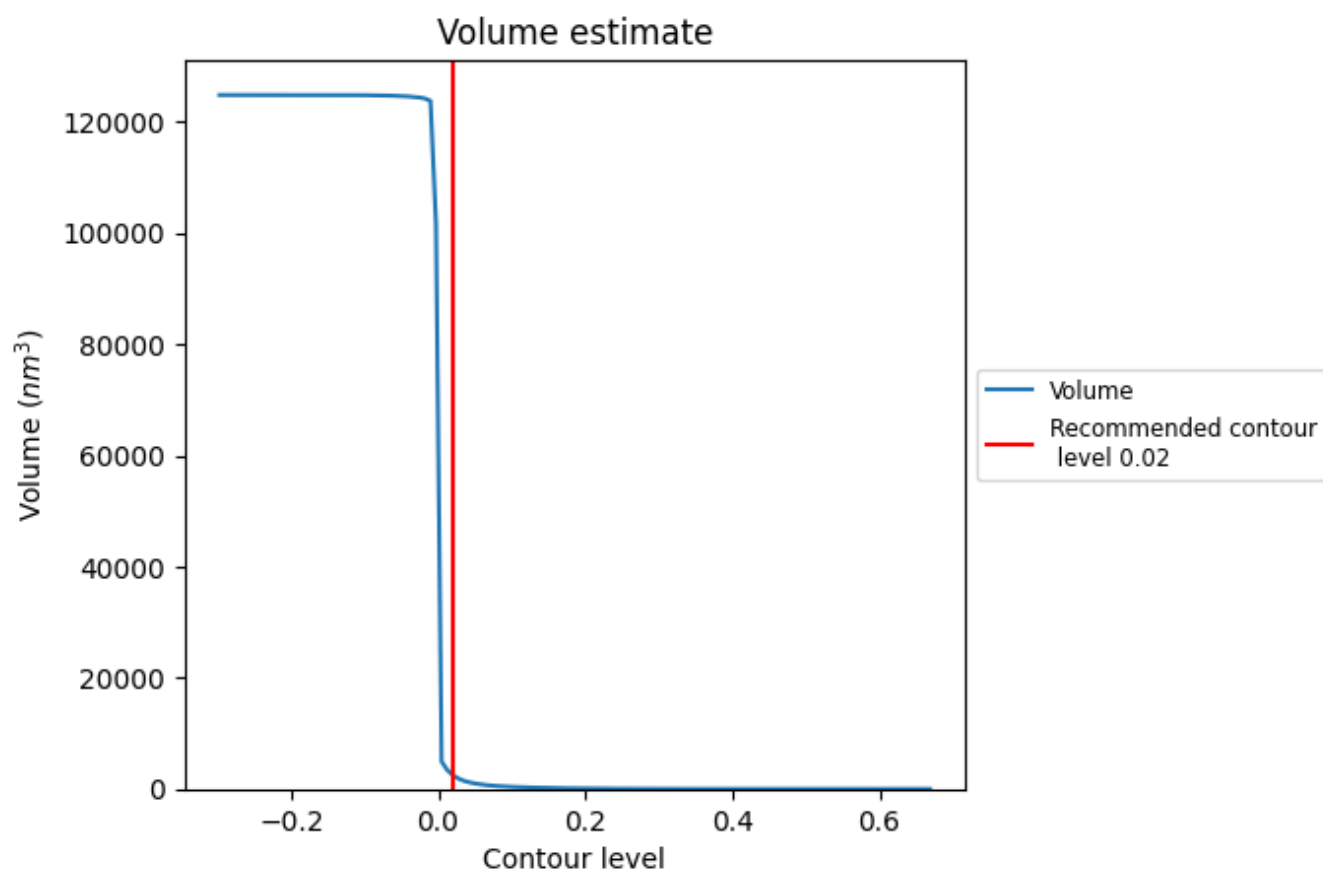
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

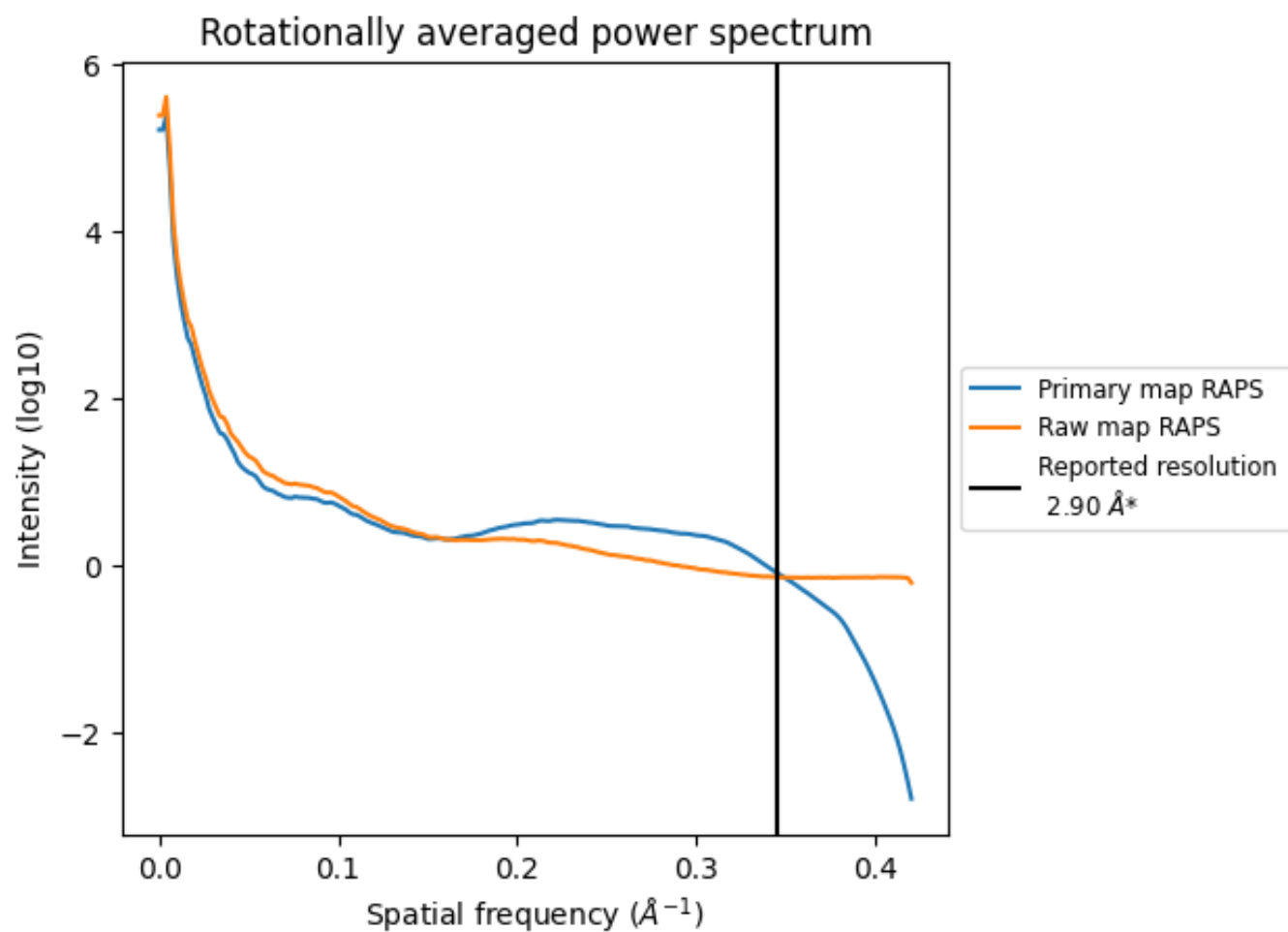
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2486 nm³; this corresponds to an approximate mass of 2246 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

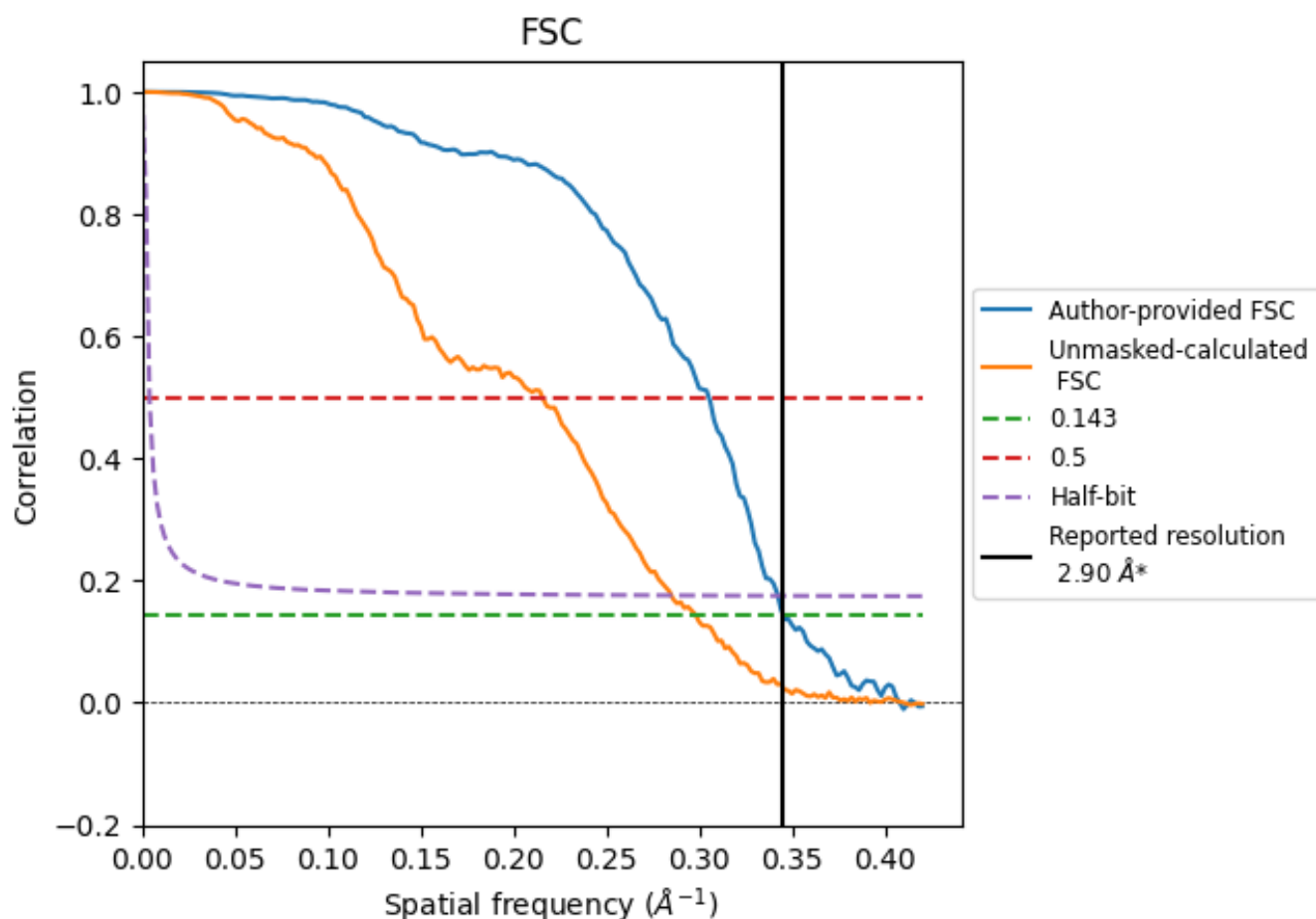


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.28	2.92
Unmasked-calculated*	3.35	4.64	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.9 by more than 10 %

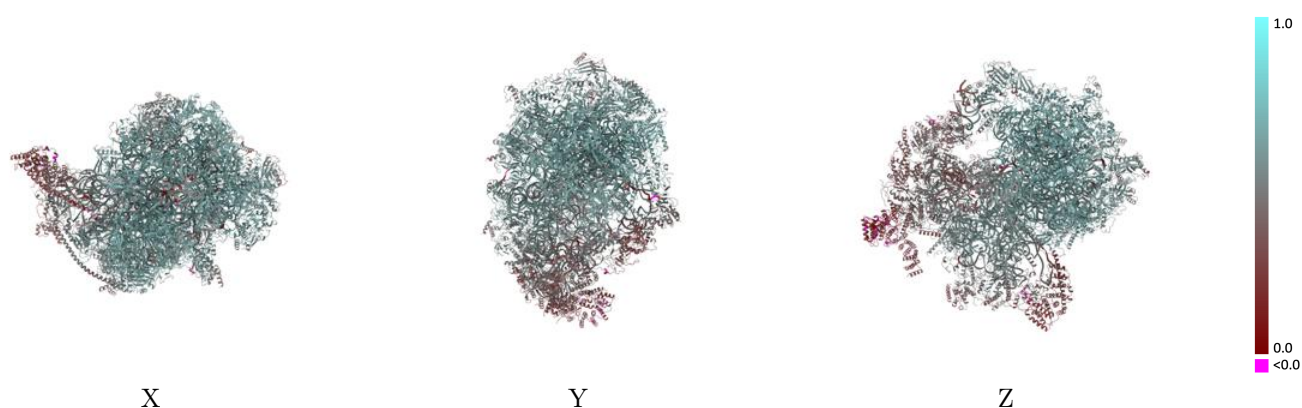
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-36836 and PDB model 8K2A. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)

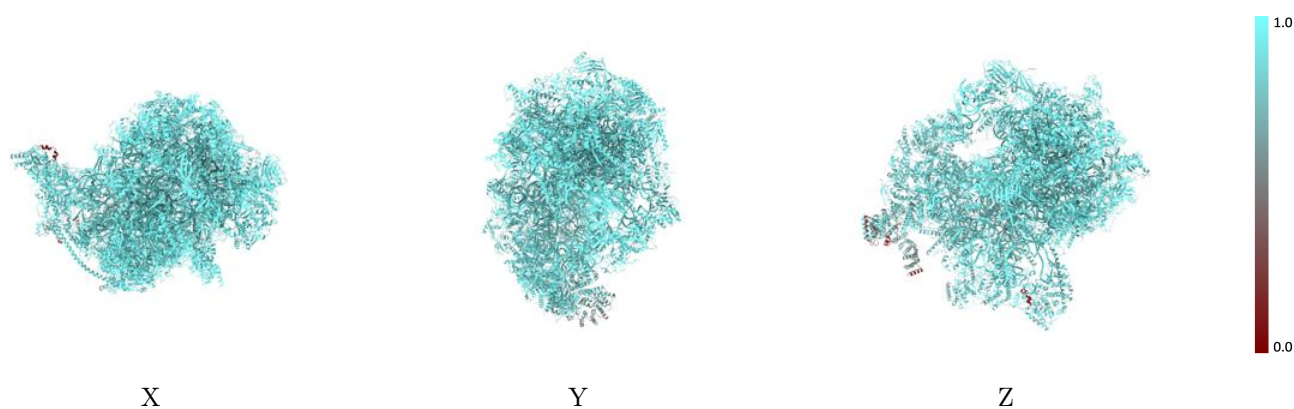
This section was not generated.

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



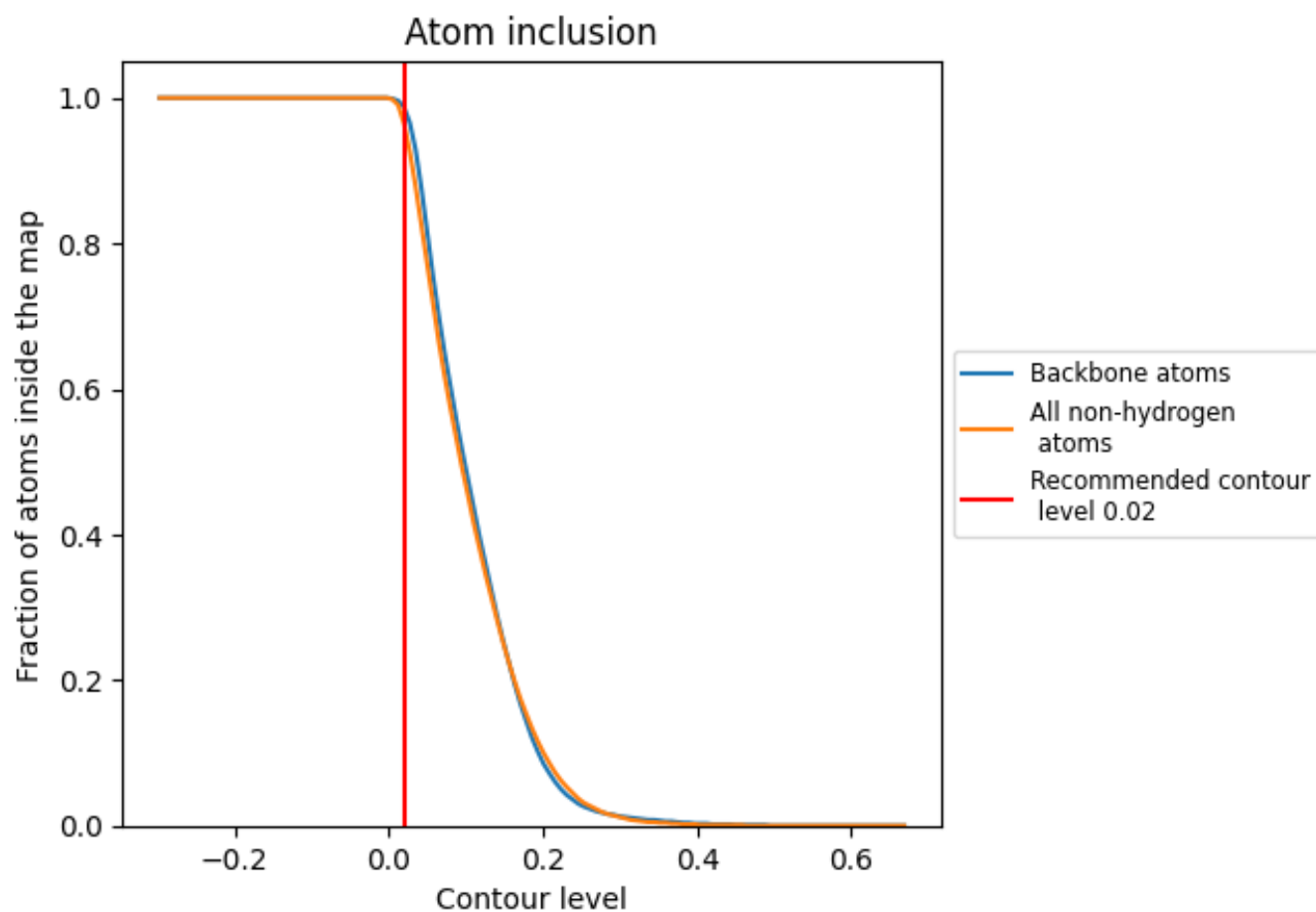
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.5450
L1	 0.9940	 0.6210
L2	 0.9920	 0.4300
L3	 0.9790	 0.4960
L4	 0.9110	 0.4000
L5	 0.9770	 0.4960
L6	 0.9960	 0.6560
L7	 0.9800	 0.5540
L8	 0.9730	 0.5510
LB	 0.9970	 0.6540
LC	 0.9850	 0.6220
LD	 0.9940	 0.6350
LI	 0.9880	 0.5600
LJ	 0.9590	 0.4850
LK	 0.8890	 0.3380
LM	 0.9900	 0.6470
LN	 0.9900	 0.6190
LO	 0.9930	 0.6340
LP	 0.9910	 0.6270
LQ	 0.9930	 0.6220
LR	 0.9750	 0.5880
LS	 0.9830	 0.5990
LT	 0.9860	 0.6500
LU	 0.9920	 0.6370
LV	 0.9960	 0.6440
LW	 0.9670	 0.6010
LX	 0.9760	 0.5600
La	 0.9910	 0.6450
Lb	 0.9820	 0.5910
Ld	 0.9920	 0.6440
Lf	 0.9840	 0.6230
Lg	 0.9930	 0.6170
Lh	 1.0000	 0.6760
Li	 0.9950	 0.6690
Lj	 0.9970	 0.6350



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Chain	Atom inclusion	Q-score
Lk	 0.9890	 0.6040
Ll	 0.9720	 0.5620
Lm	 0.9780	 0.5630
Ln	 0.9200	 0.4040
Lo	 0.9750	 0.5920
Lp	 0.9710	 0.5990
Lq	 0.9970	 0.6450
Lr	 0.9860	 0.5970
Ls	 0.9450	 0.5230
Lt	 0.8990	 0.3610
Lu	 0.9930	 0.6220
Lv	 0.9400	 0.4860
Lw	 0.9840	 0.6130
Lx	 0.9650	 0.5410
Ly	 0.9930	 0.6520
Lz	 0.9520	 0.5870
S1	 0.9960	 0.5510
SB	 0.9770	 0.5590
SE	 0.9630	 0.5260
SF	 0.9880	 0.5940
SG	 0.9580	 0.4690
SI	 0.9380	 0.4620
SJ	 0.9430	 0.4340
SK	 0.9900	 0.5760
SL	 0.9830	 0.5490
SN	 0.9490	 0.4350
SO	 0.9760	 0.5270
SP	 0.9580	 0.4970
SQ	 0.9960	 0.5790
SR	 0.9900	 0.6140
SS	 0.9560	 0.4790
ST	 0.9840	 0.5890
SW	 0.9890	 0.5990
SX	 0.9060	 0.4160
SY	 0.9540	 0.5130
SZ	 0.9670	 0.4840
Sa	 0.9730	 0.5360
Sb	 0.9540	 0.4660
Sc	 0.8410	 0.2790
Sd	 0.9770	 0.5540
Se	 0.9250	 0.4040
Sf	 0.9930	 0.6210

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Continued from previous page...

Chain	Atom inclusion	Q-score
Sg	 0.8670	 0.3230
Si	 0.9610	 0.3830
Sj	 0.9370	 0.3810
Sk	 0.8790	 0.3470
Sm	 0.9680	 0.5280
Sn	 0.9970	 0.6020
So	 0.6390	 0.1880