



# wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 06:33 AM JST

PDB ID : 8XT0  
EMDB ID : EMD-38632  
Title : Cryo-EM structure of the human 55S mitoribosome with 5um Tigecycline  
Authors : Li, X.; Wang, M.; Cheng, J.  
Deposited on : 2024-01-10  
Resolution : 3.20 Å(reported)  
Based on initial model : 7A5I

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

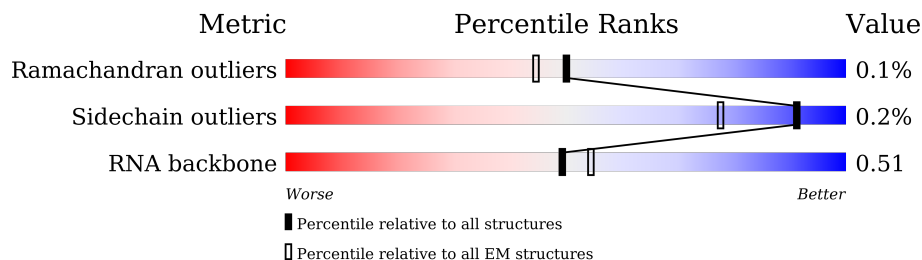
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



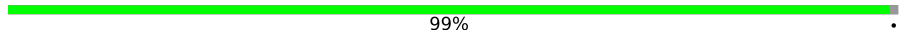

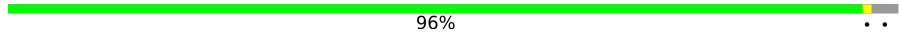




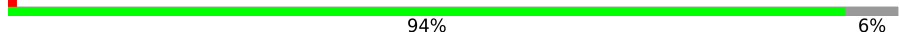


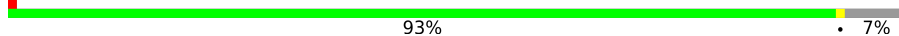


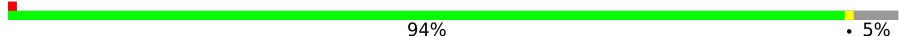











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	L1	1559	
2	L2	69	
3	LB	305	
4	LC	348	
5	LD	311	
6	LI	267	
7	LJ	261	
8	LK	192	

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Mol	Chain	Length	Quality of chain
9	LM	178	 99%
10	LN	145	 79%
11	LO	296	 96%
12	LP	251	 88%
13	LQ	175	 85%
14	LR	179	 81%
15	LS	292	 75%
16	LT	149	 94%
17	LU	205	 78%
18	LV	212	 78%
19	LW	153	 93%
20	LX	216	 92%
21	La	148	 75%
22	Lb	256	 94%
23	Lu	250	 70%
24	Ld	161	 75%
25	Lf	188	 57%
26	Lg	65	 80%
27	Lh	92	 50%
28	Li	188	 50%
29	Lj	103	 37%
30	Lk	423	 93%
31	Ll	380	 93%
32	Lm	338	 86%
33	Ln	206	 47%

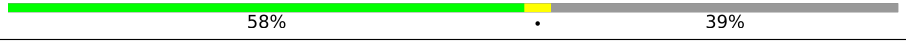








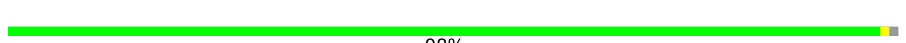

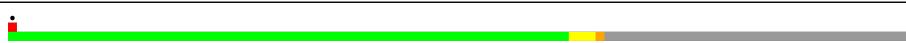



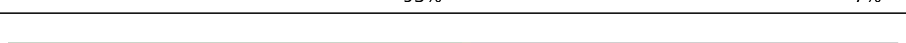
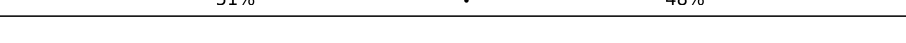
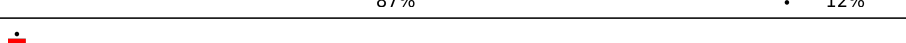


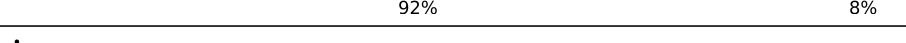
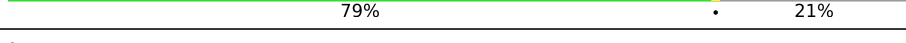
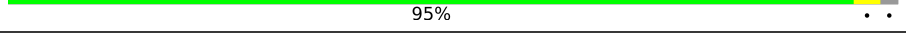


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Mol	Chain	Length	Quality of chain
34	Lo	137	90% 9%
35	Lp	142	66% 32%
36	Lq	215	69% 31%
37	Lr	332	83% 17%
38	Ls	306	69% 30%
39	Lt	279	76% 22%
40	Lv	212	61% 38%
41	Lw	166	80% 20%
42	Lx	158	68% 30%
43	Ly	128	76% 24%
44	Lz	123	75% 25%
45	L3	112	85% 14%
46	L4	138	59% 40%
47	L5	128	34% 65%
48	L6	102	92% 8%
49	L7	206	61% 38%
50	L8	222	57% 42%
51	SR	196	74% 26%
52	Sf	439	83% 16%
53	SB	296	72% 27%
54	SZ	167	77% 21%
55	SE	430	74% 26%
56	SF	125	98%
57	SG	242	81% 17%
58	SI	396	76% 23%

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Mol	Chain	Length	Quality of chain
59	SJ	201	 58% 39%
60	SK	194	 70% 30%
61	SL	138	 76% 22%
62	SN	128	 77% 21%
63	SO	257	 63% 36%
64	SP	137	 83% 15%
65	SQ	130	 82% 18%
66	SS	258	 71% 28%
67	ST	142	 68% 32%
68	SW	87	 98%
69	SX	360	 82% 18%
70	SY	190	 63% 34%
71	Sa	173	 93% 6%
72	Sb	205	 84% 16%
73	Sc	414	 8% 93% 7%
74	Sd	187	 51% 48%
75	Se	398	 87% 12%
76	Sg	395	 27% 73%
77	Si	106	 80% 19%
78	Sj	218	 92% 8%
79	Sk	323	 79% 21%
80	Sm	118	 95%
81	Sn	199	 35% 65%
82	So	689	 45% 89% 11%
83	S1	954	 74% 22%

## 2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 165243 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
			Total	C	N	O	P		
1	L1	1500	31847	14290	5750	10307	1500	0	0

- Molecule 2 is a RNA chain called Val tRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called Mitochondrial ribosomal protein L18, isoform CRA\_b.

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
28	Li	95	831	539	162	127	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
69	SX	295	2405	1530	413	454	8	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

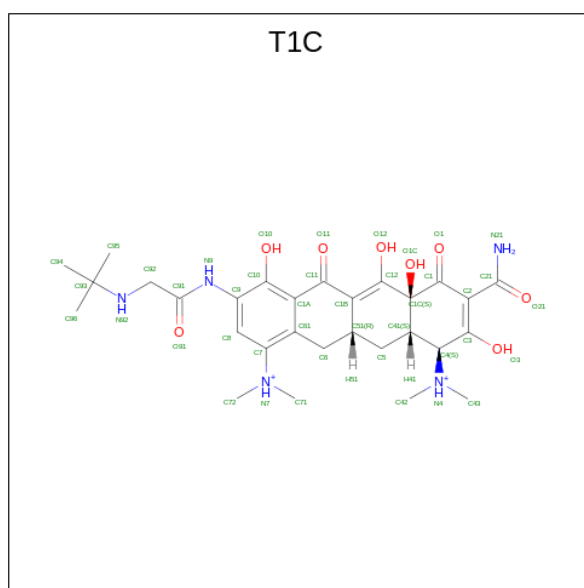
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	873	A	U	conflict	GB 587653923

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
84	L1	106	106	106	0
84	LB	3	3	3	0
84	LP	1	1	1	0
84	Lw	1	1	1	0
84	L6	1	1	1	0
84	S1	33	33	33	0

- Molecule 85 is TIGECYCLINE (three-letter code: T1C) (formula: C<sub>29</sub>H<sub>41</sub>N<sub>5</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).

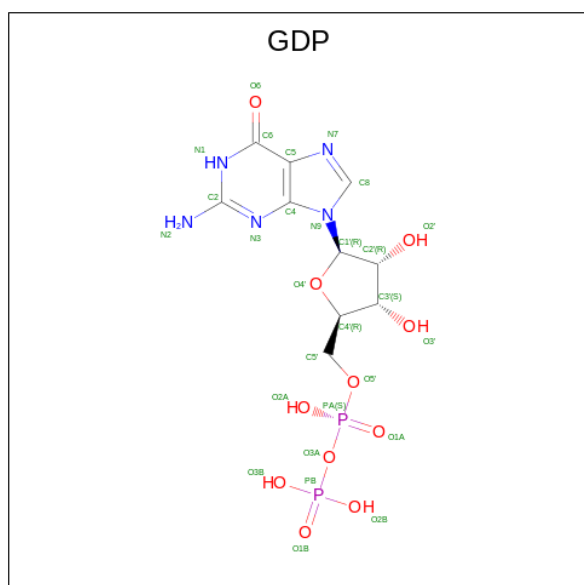


Mol	Chain	Residues	Atoms				AltConf
85	L1	1	Total	C	N	O	0
			42	29	5	8	
85	L1	1	Total	C	N	O	0
			42	29	5	8	
85	S1	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 86 is ZINC ION (three-letter code: 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 (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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





ILE THR ARG ALA TRP LEU GLY GLU TYR TRP CYS GLU VAL THR VAL THR VAL ASN GLY LEU ASP THR VAL ARG VAL ARG VAL PRO MET MET SER VAL VAL ASN PHE GLU LYS PRO LYS LYS ARG TYR LYS TYR TRP TRP ALA ALA GLN GLN ILE ALA ALA LYS MET ALA PRO THR THR SER PRO GLN ILE

- Molecule 7: Large ribosomal subunit protein uL10m



MET ALA ALA VAL ALA GLY MET LEU ARG GLY GLY LEU LEU PRO GLN ALA THR ARG LEU PRO HIS THR LEU LEU GLN VAL ARG THR TYR LEU GLN ILE G77 MET M123 D137 M164 V165 R166 D182 D183 K196 L197 PRO

PRO ASP SER

- Molecule 8: Large ribosomal subunit protein uL11m



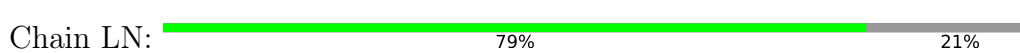
MET SER LYS LEU ARG ALA ALA ARG GLY LEU ARG LYS PRO GLU VAL G118 P31 D59 A121 D158 E188 A189 A190 K191 K192

- Molecule 9: Large ribosomal subunit protein uL13m



MET S2 L178

- Molecule 10: Large ribosomal subunit protein uL14m



MET ALA PHE THR LEU TRP GLY PRO PHE THR CYS VAL SER ARG LEU SER HIS CYS PHE SER THR THR SER A31 V145

- Molecule 11: Large ribosomal subunit protein uL15m




MET ALA GLY PRO LEU GLN GLY A10 R11 R39 S296

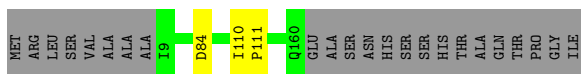
- Molecule 12: Large ribosomal subunit protein uL16m




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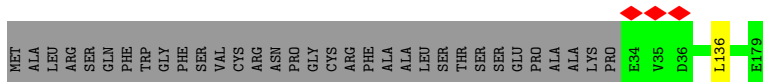
- Molecule 13: Large ribosomal subunit protein bL17m

Chain LQ:  85% 13%




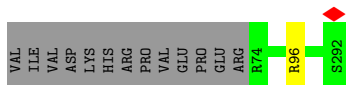
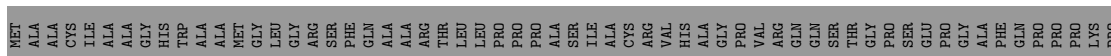
- Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA\_b

Chain LR:  81% 18%



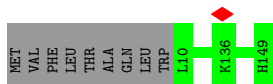
- Molecule 15: Large ribosomal subunit protein bL19m

Chain LS:  75% 25%




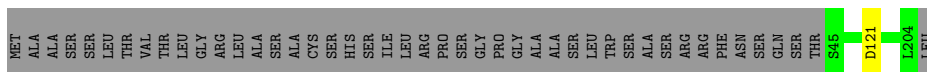
- Molecule 16: Large ribosomal subunit protein bL20m

Chain LT:  94% 6%




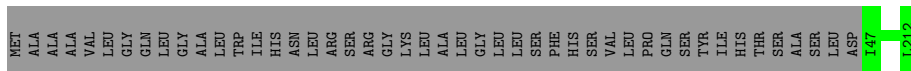
- Molecule 17: Large ribosomal subunit protein bL21m

Chain LU:  78% 22%



- Molecule 18: 39S ribosomal protein L22, mitochondrial

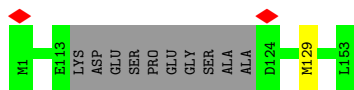
Chain LV:  78% 22%



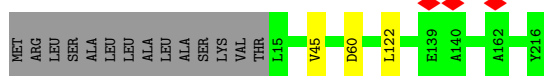
- Molecule 19: Large ribosomal subunit protein uL23m

Chain LW:  93% 7%

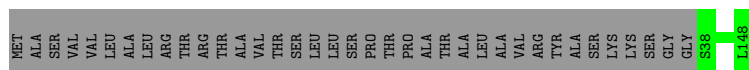




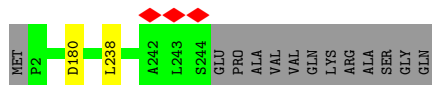
- Molecule 20: Large ribosomal subunit protein uL24m



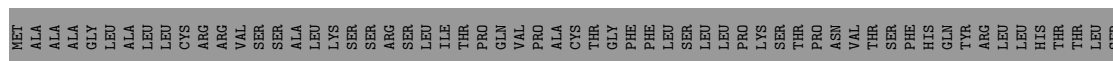
- Molecule 21: Large ribosomal subunit protein bL27m



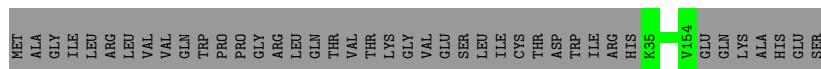
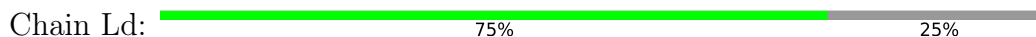
- Molecule 22: Large ribosomal subunit protein bL28m



- Molecule 23: Large ribosomal subunit protein uL29m



- Molecule 24: Large ribosomal subunit protein uL30m



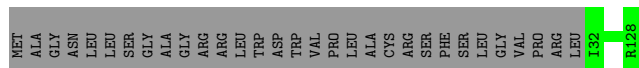
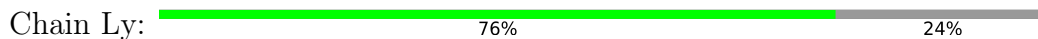
- Molecule 25: Large ribosomal subunit protein bL32m



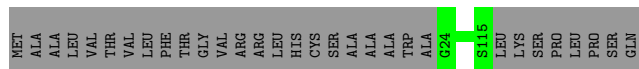
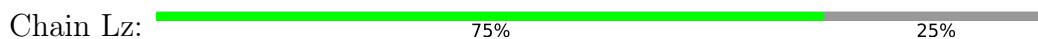




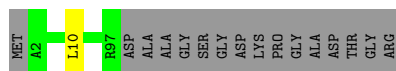
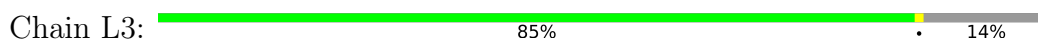




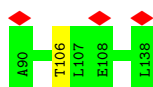
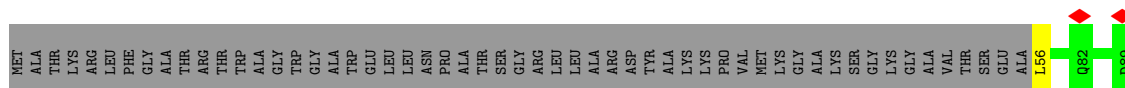
- Molecule 44: 39S ribosomal protein L52, mitochondrial



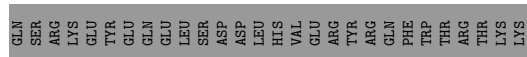
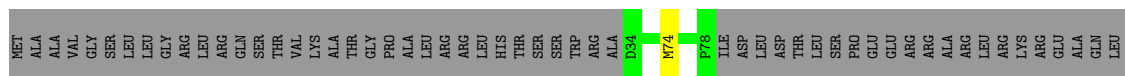
- Molecule 45: Large ribosomal subunit protein mL53



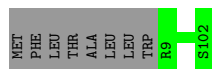
- Molecule 46: Large ribosomal subunit protein mL54



- Molecule 47: Large ribosomal subunit protein mL55



- Molecule 48: Large ribosomal subunit protein mL63

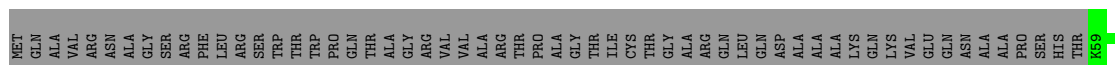


- Molecule 49: Large ribosomal subunit protein mL62

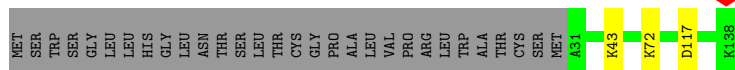
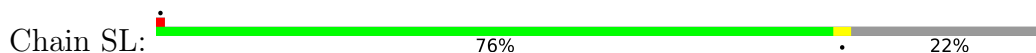




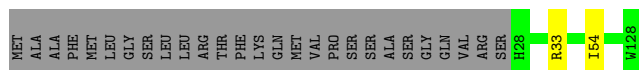
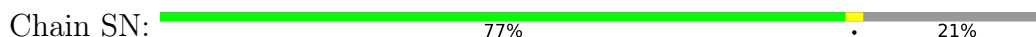




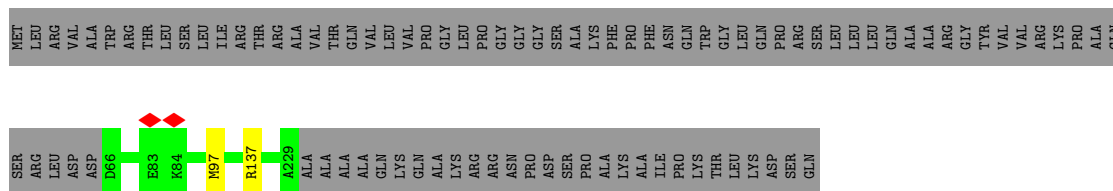
- Molecule 61: Small ribosomal subunit protein uS12m



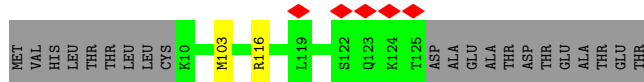
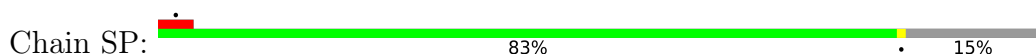
- Molecule 62: Small ribosomal subunit protein uS14m



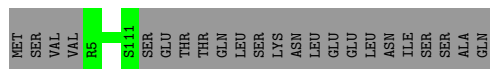
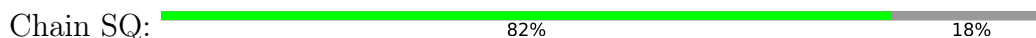
- Molecule 63: Small ribosomal subunit protein uS15m



- Molecule 64: Small ribosomal subunit protein bS16m



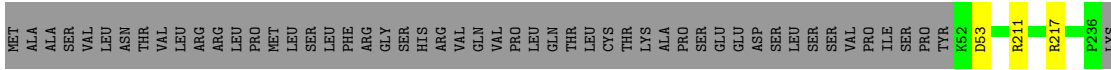
- Molecule 65: Small ribosomal subunit protein uS17m



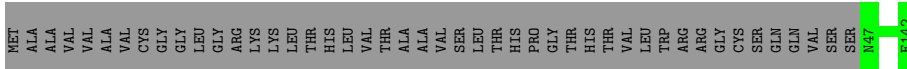
- Molecule 66: Small ribosomal subunit protein mS40



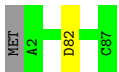




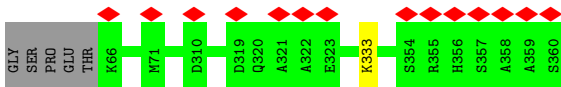
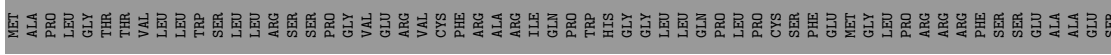
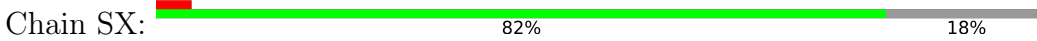
- Molecule 67: Small ribosomal subunit protein bS18m



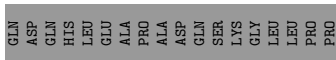
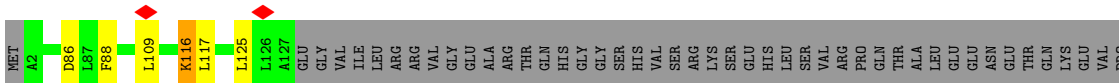
- Molecule 68: Small ribosomal subunit protein bS21m



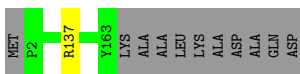
- Molecule 69: Small ribosomal subunit protein mS22



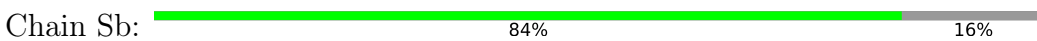
- Molecule 70: Small ribosomal subunit protein mS23



- Molecule 71: Small ribosomal subunit protein mS25

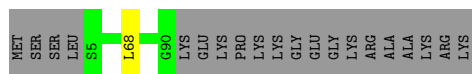
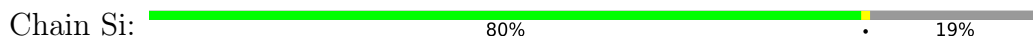


- Molecule 72: Small ribosomal subunit protein mS26

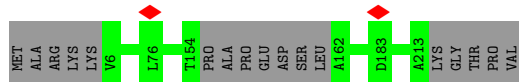




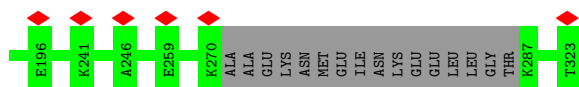
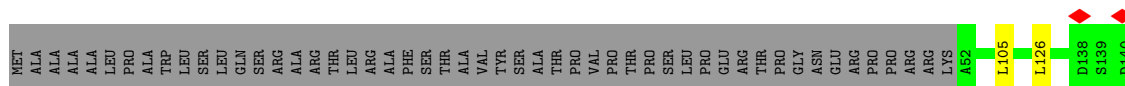
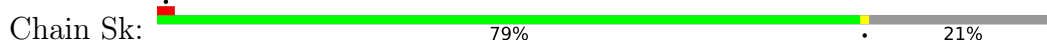
- Molecule 77: Small ribosomal subunit protein mS33



- Molecule 78: Small ribosomal subunit protein mS34



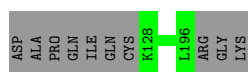
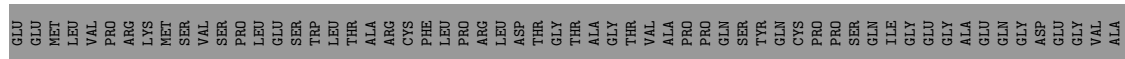
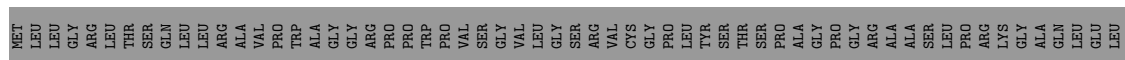
- Molecule 79: Small ribosomal subunit protein mS35



- Molecule 80: Small ribosomal subunit protein mS37

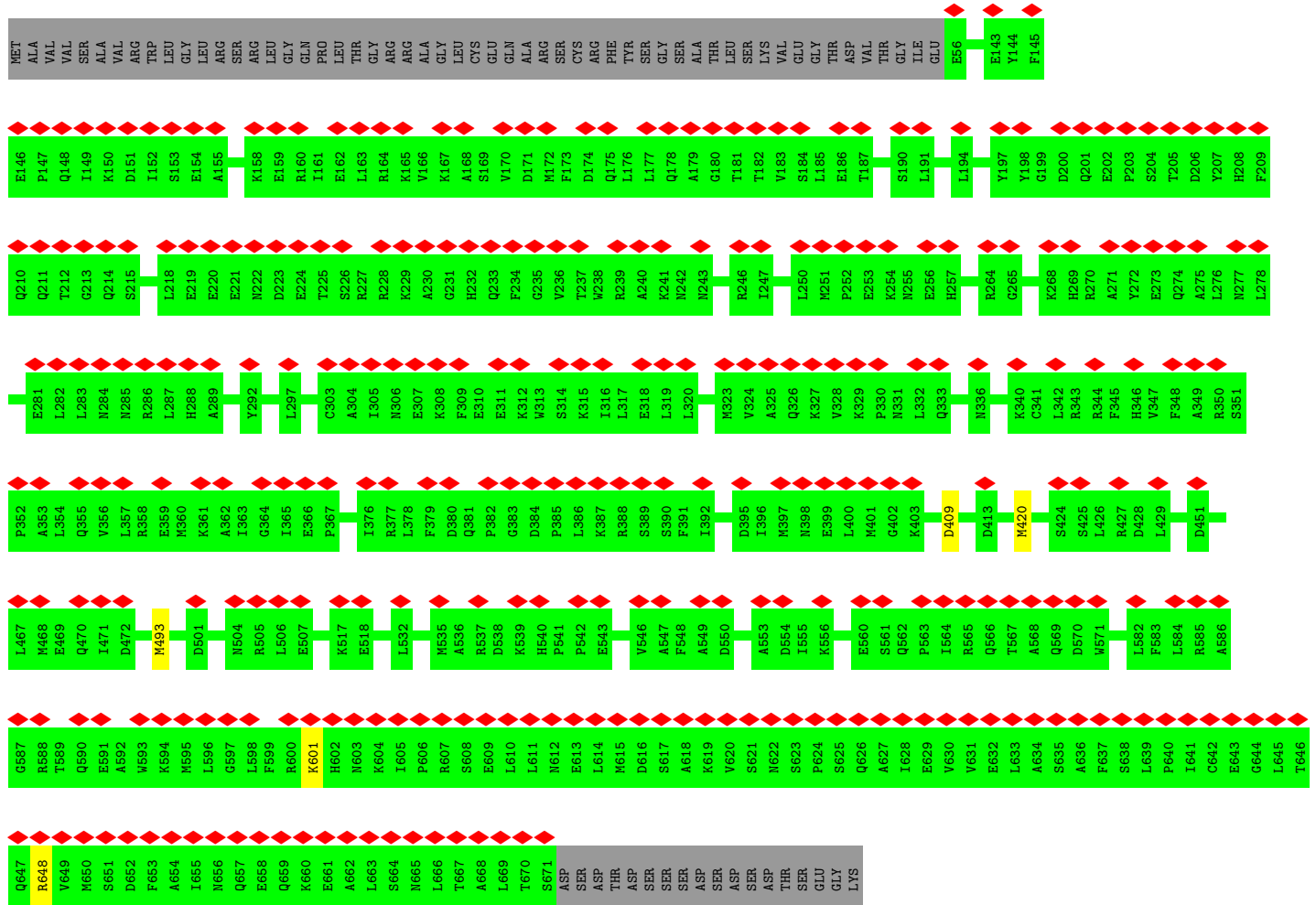


- Molecule 81: Small ribosomal subunit protein mS38



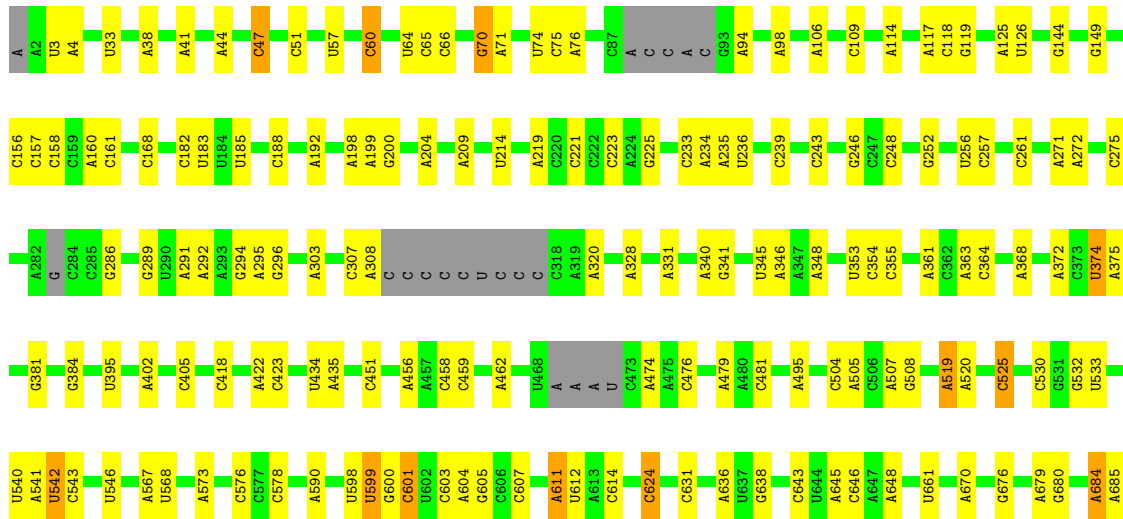
- Molecule 82: Small ribosomal subunit protein mS39

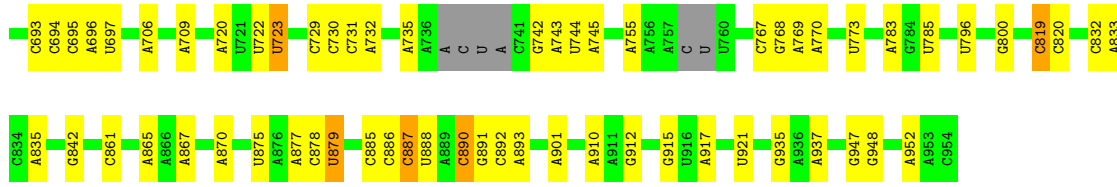




• Molecule 83: 12s rRNA

Chain S1: 74% 22%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112982	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	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	446.88, 446.88, 446.88	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	L1	0.85	1/35628 (0.0%)	1.05	131/55448 (0.2%)
2	L2	0.34	0/1328	0.96	0/2056
3	LB	0.43	0/1888	0.64	0/2538
4	LC	0.41	0/2462	0.59	0/3340
5	LD	0.44	0/2071	0.64	0/2817
6	LI	0.37	0/798	0.70	0/1073
7	LJ	0.47	0/1308	0.92	6/1761 (0.3%)
8	LK	0.33	0/1340	0.65	3/1802 (0.2%)
9	LM	0.41	0/1495	0.60	0/2029
10	LN	0.37	0/904	0.60	0/1218
11	LO	0.42	0/2359	0.61	0/3185
12	LP	0.39	0/1826	0.58	0/2458
13	LQ	0.40	0/1269	0.66	1/1708 (0.1%)
14	LR	0.38	0/1215	0.61	1/1645 (0.1%)
15	LS	0.39	0/1863	0.59	0/2509
16	LT	0.49	0/1174	0.64	0/1572
17	LU	0.41	0/1311	0.65	1/1778 (0.1%)
18	LV	0.44	0/1402	0.59	0/1886
19	LW	0.44	0/1217	0.68	1/1644 (0.1%)
20	LX	0.38	0/1697	0.70	3/2302 (0.1%)
21	La	0.47	0/893	0.59	0/1204
22	Lb	0.39	0/2090	0.63	3/2825 (0.1%)
23	Lu	0.43	1/1552 (0.1%)	0.64	2/2079 (0.1%)
24	Ld	0.43	0/1003	0.60	0/1354
25	Lf	0.41	0/895	0.59	0/1201
26	Lg	0.38	0/438	0.68	0/583
27	Lh	0.47	0/382	0.69	0/507
28	Li	0.45	0/852	0.62	0/1136
29	Lj	0.41	0/349	0.70	0/461
30	Lk	0.35	0/3305	0.58	2/4502 (0.0%)
31	Ll	0.36	0/3042	0.61	2/4140 (0.0%)
32	Lm	0.35	0/2439	0.57	0/3299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Ln	0.37	0/855	0.71	0/1152
34	Lo	0.41	0/1025	0.62	0/1379
35	Lp	0.40	0/839	0.64	1/1136 (0.1%)
36	Lq	0.41	0/1202	0.65	0/1626
37	Lr	0.35	0/2264	0.55	0/3059
38	Ls	0.35	0/1800	0.63	2/2436 (0.1%)
39	Lt	0.33	0/1797	0.65	1/2422 (0.0%)
40	Lv	0.44	1/1051 (0.1%)	0.81	2/1422 (0.1%)
41	Lw	0.41	0/1134	0.60	0/1547
42	Lx	0.40	0/918	0.77	1/1249 (0.1%)
43	Ly	0.46	0/849	0.64	0/1135
44	Lz	0.39	0/747	0.60	0/1005
45	L3	0.31	0/754	0.69	1/1017 (0.1%)
46	L4	0.32	0/722	0.69	1/978 (0.1%)
47	L5	0.39	0/379	0.96	1/510 (0.2%)
48	L6	0.43	0/818	0.65	0/1097
49	L7	0.34	0/1071	0.68	1/1433 (0.1%)
50	L8	0.32	0/1107	0.61	1/1498 (0.1%)
51	SR	0.42	0/1238	0.66	0/1676
52	Sf	0.38	0/3114	0.61	1/4225 (0.0%)
53	SB	0.38	0/1811	0.69	3/2451 (0.1%)
54	SZ	0.48	1/1112 (0.1%)	0.76	3/1505 (0.2%)
55	SE	0.36	0/2590	0.64	2/3477 (0.1%)
56	SF	0.37	0/989	0.66	0/1335
57	SG	0.38	1/1708 (0.1%)	0.68	3/2291 (0.1%)
58	SI	0.32	0/2555	0.65	1/3424 (0.0%)
59	SJ	0.43	0/1019	0.90	4/1379 (0.3%)
60	SK	0.34	0/1031	0.61	1/1390 (0.1%)
61	SL	0.42	0/854	0.73	1/1148 (0.1%)
62	SN	0.38	0/879	0.80	1/1182 (0.1%)
63	SO	0.38	0/1406	0.69	1/1878 (0.1%)
64	SP	0.31	0/941	0.70	1/1265 (0.1%)
65	SQ	0.33	0/864	0.58	0/1169
66	SS	0.35	0/1580	0.66	1/2150 (0.0%)
67	ST	0.43	0/791	0.61	0/1062
68	SW	0.39	0/752	0.70	1/1001 (0.1%)
69	SX	0.27	0/2452	0.56	0/3310
70	SY	0.49	1/1069 (0.1%)	0.87	7/1441 (0.5%)
71	Sa	0.33	0/1361	0.59	0/1829
72	Sb	0.30	0/1474	0.61	0/1976
73	Sc	0.27	0/3177	0.55	2/4292 (0.0%)
74	Sd	0.37	0/778	0.74	1/1048 (0.1%)
75	Se	0.32	1/2908 (0.0%)	0.58	2/3936 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	Sg	0.32	0/931	0.59	1/1259 (0.1%)
77	Si	0.36	0/748	0.69	1/1000 (0.1%)
78	Sj	0.29	0/1723	0.68	0/2334
79	Sk	0.31	0/2113	0.66	2/2863 (0.1%)
80	Sm	0.47	0/939	0.84	3/1256 (0.2%)
81	Sn	0.37	0/621	0.66	0/820
82	So	0.30	0/5093	0.63	3/6891 (0.0%)
83	S1	0.52	0/22053	0.98	68/34324 (0.2%)
All	All	0.53	7/173801 (0.0%)	0.81	282/246748 (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
5	LD	0	2
11	LO	0	1
12	LP	0	1
13	LQ	0	1
33	Ln	0	2
39	Lt	0	1
42	Lx	0	1
46	L4	0	1
59	SJ	0	1
63	SO	0	1
74	Sd	0	1
All	All	0	13

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	SZ	131	LYS	CG-CD	-7.13	1.28	1.52
70	SY	88	PHE	CD1-CE1	-6.07	1.27	1.39
23	Lu	116	GLU	CB-CG	-6.05	1.40	1.52
57	SG	234	ARG	CB-CG	-5.86	1.36	1.52
75	Se	397	TYR	CD1-CE1	-5.75	1.30	1.39

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	859	U	C5-C6-N1	14.20	129.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	So	493	MET	CG-SD-CE	-12.87	79.61	100.20
70	SY	117	LEU	CA-CB-CG	11.91	142.70	115.30
40	Lv	179	PRO	CA-N-CD	-11.69	95.14	111.50
1	L1	859	U	C6-N1-C2	-10.50	114.70	121.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LD	211	ARG	Sidechain
5	LD	234	THR	Peptide
11	LO	39	ARG	Sidechain
12	LP	73	ARG	Sidechain
13	LQ	110	ILE	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LB	235/305 (77%)	228 (97%)	6 (3%)	1 (0%)	30	64
4	LC	302/348 (87%)	283 (94%)	19 (6%)	0	100	100
5	LD	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
6	LI	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
7	LJ	154/261 (59%)	139 (90%)	15 (10%)	0	100	100
8	LK	173/192 (90%)	165 (95%)	8 (5%)	0	100	100
9	LM	175/178 (98%)	162 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	LN	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
11	LO	285/296 (96%)	274 (96%)	11 (4%)	0	100	100
12	LP	219/251 (87%)	214 (98%)	5 (2%)	0	100	100
13	LQ	150/175 (86%)	141 (94%)	8 (5%)	1 (1%)	19	54
14	LR	144/179 (80%)	143 (99%)	1 (1%)	0	100	100
15	LS	217/292 (74%)	205 (94%)	12 (6%)	0	100	100
16	LT	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	LU	158/205 (77%)	151 (96%)	7 (4%)	0	100	100
18	LV	164/212 (77%)	153 (93%)	11 (7%)	0	100	100
19	LW	139/153 (91%)	137 (99%)	2 (1%)	0	100	100
20	LX	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
21	La	109/148 (74%)	107 (98%)	2 (2%)	0	100	100
22	Lb	241/256 (94%)	232 (96%)	9 (4%)	0	100	100
23	Lu	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
24	Ld	118/161 (73%)	114 (97%)	4 (3%)	0	100	100
25	Lf	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
26	Lg	50/65 (77%)	50 (100%)	0	0	100	100
27	Lh	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	Li	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
29	Lj	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
30	Lk	392/423 (93%)	383 (98%)	9 (2%)	0	100	100
31	Ll	352/380 (93%)	327 (93%)	25 (7%)	0	100	100
32	Lm	291/338 (86%)	279 (96%)	12 (4%)	0	100	100
33	Ln	97/206 (47%)	85 (88%)	12 (12%)	0	100	100
34	Lo	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
35	Lp	93/142 (66%)	89 (96%)	4 (4%)	0	100	100
36	Lq	146/215 (68%)	135 (92%)	11 (8%)	0	100	100
37	Lr	271/332 (82%)	265 (98%)	6 (2%)	0	100	100
38	Ls	210/306 (69%)	200 (95%)	10 (5%)	0	100	100
39	Lt	211/279 (76%)	187 (89%)	23 (11%)	1 (0%)	25	60
40	Lv	125/212 (59%)	121 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Lw	130/166 (78%)	123 (95%)	7 (5%)	0	100	100
42	Lx	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
43	Ly	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
44	Lz	90/123 (73%)	86 (96%)	4 (4%)	0	100	100
45	L3	94/112 (84%)	85 (90%)	9 (10%)	0	100	100
46	L4	81/138 (59%)	75 (93%)	6 (7%)	0	100	100
47	L5	43/128 (34%)	40 (93%)	3 (7%)	0	100	100
48	L6	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
49	L7	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
50	L8	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
51	SR	140/196 (71%)	139 (99%)	1 (1%)	0	100	100
52	Sf	366/439 (83%)	351 (96%)	13 (4%)	2 (0%)	25	60
53	SB	215/296 (73%)	204 (95%)	11 (5%)	0	100	100
54	SZ	130/167 (78%)	117 (90%)	13 (10%)	0	100	100
55	SE	314/430 (73%)	295 (94%)	19 (6%)	0	100	100
56	SF	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
57	SG	197/242 (81%)	193 (98%)	4 (2%)	0	100	100
58	SI	300/396 (76%)	271 (90%)	29 (10%)	0	100	100
59	SJ	120/201 (60%)	103 (86%)	17 (14%)	0	100	100
60	SK	134/194 (69%)	123 (92%)	11 (8%)	0	100	100
61	SL	106/138 (77%)	96 (91%)	8 (8%)	2 (2%)	6	34
62	SN	99/128 (77%)	89 (90%)	10 (10%)	0	100	100
63	SO	162/257 (63%)	156 (96%)	6 (4%)	0	100	100
64	SP	114/137 (83%)	107 (94%)	7 (6%)	0	100	100
65	SQ	105/130 (81%)	95 (90%)	10 (10%)	0	100	100
66	SS	183/258 (71%)	167 (91%)	16 (9%)	0	100	100
67	ST	94/142 (66%)	88 (94%)	6 (6%)	0	100	100
68	SW	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
69	SX	293/360 (81%)	282 (96%)	11 (4%)	0	100	100
70	SY	124/190 (65%)	119 (96%)	5 (4%)	0	100	100
71	Sa	160/173 (92%)	150 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Sb	171/205 (83%)	167 (98%)	3 (2%)	1 (1%)	22	57
73	Sc	383/414 (92%)	374 (98%)	9 (2%)	0	100	100
74	Sd	95/187 (51%)	87 (92%)	8 (8%)	0	100	100
75	Se	348/398 (87%)	332 (95%)	16 (5%)	0	100	100
76	Sg	106/395 (27%)	98 (92%)	8 (8%)	0	100	100
77	Si	84/106 (79%)	82 (98%)	2 (2%)	0	100	100
78	Sj	197/218 (90%)	171 (87%)	26 (13%)	0	100	100
79	Sk	252/323 (78%)	226 (90%)	26 (10%)	0	100	100
80	Sm	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
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%)	12863 (95%)	686 (5%)	8 (0%)	50	80

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	Lt	266	PRO
61	SL	117	ASP
52	Sf	250	PHE
61	SL	72	LYS
52	Sf	260	GLU

### 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	
3	LB	191/245 (78%)	191 (100%)	0	100	100
4	LC	258/290 (89%)	258 (100%)	0	100	100
5	LD	217/262 (83%)	216 (100%)	1 (0%)	86	93
6	LI	86/228 (38%)	86 (100%)	0	100	100
7	LJ	145/232 (62%)	145 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	LK	137/150 (91%)	137 (100%)	0	100	100
9	LM	155/156 (99%)	155 (100%)	0	100	100
10	LN	98/124 (79%)	98 (100%)	0	100	100
11	LO	245/249 (98%)	244 (100%)	1 (0%)	89	94
12	LP	188/211 (89%)	188 (100%)	0	100	100
13	LQ	133/150 (89%)	133 (100%)	0	100	100
14	LR	128/154 (83%)	128 (100%)	0	100	100
15	LS	201/256 (78%)	200 (100%)	1 (0%)	86	93
16	LT	118/126 (94%)	118 (100%)	0	100	100
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%)	180 (100%)	0	100	100
21	La	91/119 (76%)	91 (100%)	0	100	100
22	Lb	219/229 (96%)	219 (100%)	0	100	100
23	Lu	159/223 (71%)	159 (100%)	0	100	100
24	Ld	111/147 (76%)	111 (100%)	0	100	100
25	Lf	97/164 (59%)	97 (100%)	0	100	100
26	Lg	49/60 (82%)	49 (100%)	0	100	100
27	Lh	40/72 (56%)	40 (100%)	0	100	100
28	Li	88/166 (53%)	87 (99%)	1 (1%)	70	86
29	Lj	37/89 (42%)	37 (100%)	0	100	100
30	Lk	353/368 (96%)	353 (100%)	0	100	100
31	Ll	313/332 (94%)	313 (100%)	0	100	100
32	Lm	269/303 (89%)	268 (100%)	1 (0%)	89	94
33	Ln	91/190 (48%)	90 (99%)	1 (1%)	70	86
34	Lo	104/112 (93%)	103 (99%)	1 (1%)	73	87
35	Lp	93/133 (70%)	91 (98%)	2 (2%)	47	73
36	Lq	130/186 (70%)	130 (100%)	0	100	100
37	Lr	241/288 (84%)	241 (100%)	0	100	100
38	Ls	196/274 (72%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Lt	188/236 (80%)	187 (100%)	1 (0%)	86	93
40	Lv	116/188 (62%)	115 (99%)	1 (1%)	75	89
41	Lw	122/148 (82%)	122 (100%)	0	100	100
42	Lx	104/148 (70%)	104 (100%)	0	100	100
43	Ly	86/110 (78%)	86 (100%)	0	100	100
44	Lz	73/97 (75%)	73 (100%)	0	100	100
45	L3	81/90 (90%)	81 (100%)	0	100	100
46	L4	78/116 (67%)	78 (100%)	0	100	100
47	L5	40/113 (35%)	40 (100%)	0	100	100
48	L6	80/87 (92%)	80 (100%)	0	100	100
49	L7	117/181 (65%)	116 (99%)	1 (1%)	75	89
50	L8	110/178 (62%)	110 (100%)	0	100	100
51	SR	133/169 (79%)	133 (100%)	0	100	100
52	Sf	326/381 (86%)	325 (100%)	1 (0%)	91	96
53	SB	191/249 (77%)	191 (100%)	0	100	100
54	SZ	115/143 (80%)	115 (100%)	0	100	100
55	SE	267/357 (75%)	267 (100%)	0	100	100
56	SF	104/107 (97%)	104 (100%)	0	100	100
57	SG	178/209 (85%)	178 (100%)	0	100	100
58	SI	263/342 (77%)	262 (100%)	1 (0%)	89	94
59	SJ	112/180 (62%)	111 (99%)	1 (1%)	75	89
60	SK	104/147 (71%)	104 (100%)	0	100	100
61	SL	93/118 (79%)	93 (100%)	0	100	100
62	SN	91/113 (80%)	90 (99%)	1 (1%)	70	86
63	SO	152/226 (67%)	152 (100%)	0	100	100
64	SP	95/113 (84%)	94 (99%)	1 (1%)	70	86
65	SQ	93/115 (81%)	93 (100%)	0	100	100
66	SS	166/230 (72%)	164 (99%)	2 (1%)	67	85
67	ST	87/123 (71%)	87 (100%)	0	100	100
68	SW	78/79 (99%)	78 (100%)	0	100	100
69	SX	263/318 (83%)	262 (100%)	1 (0%)	89	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	SY	109/164 (66%)	108 (99%)	1 (1%)	75	89
71	Sa	150/157 (96%)	149 (99%)	1 (1%)	81	92
72	Sb	148/174 (85%)	148 (100%)	0	100	100
73	Sc	338/364 (93%)	338 (100%)	0	100	100
74	Sd	84/158 (53%)	84 (100%)	0	100	100
75	Se	310/351 (88%)	309 (100%)	1 (0%)	91	96
76	Sg	97/357 (27%)	97 (100%)	0	100	100
77	Si	79/95 (83%)	79 (100%)	0	100	100
78	Sj	175/190 (92%)	175 (100%)	0	100	100
79	Sk	235/291 (81%)	235 (100%)	0	100	100
80	Sm	99/101 (98%)	98 (99%)	1 (1%)	73	87
81	Sn	63/166 (38%)	63 (100%)	0	100	100
82	So	548/609 (90%)	546 (100%)	2 (0%)	89	94
All	All	12121/15564 (78%)	12095 (100%)	26 (0%)	91	97

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	SJ	75	ARG
66	SS	211	ARG
82	So	601	LYS
64	SP	116	ARG
66	SS	217	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
56	SF	81	HIS
60	SK	129	GLN
76	Sg	303	GLN
59	SJ	179	GLN
62	SN	117	HIS

### 5.3.3 RNA [i](#)



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1491/1559 (95%)	358 (24%)	13 (0%)
2	L2	51/69 (73%)	14 (27%)	0
83	S1	921/954 (96%)	195 (21%)	10 (1%)
All	All	2463/2582 (95%)	567 (23%)	23 (0%)

5 of 567 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	A
1	L1	8	C
1	L1	9	U
1	L1	11	G
1	L1	19	C

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
83	S1	374	U
83	S1	599	U
83	S1	542	U
83	S1	611	A
1	L1	853	C

## 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 156 ligands modelled in this entry, 152 are monoatomic - leaving 4 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
87	GDP	Se	500	-	24,30,30	0.93	1 (4%)	30,47,47	1.37	5 (16%)
85	T1C	L1	1708	84	44,45,45	1.20	4 (9%)	53,72,72	0.75	1 (1%)
85	T1C	S1	1034	84	44,45,45	1.33	5 (11%)	53,72,72	1.31	5 (9%)
85	T1C	L1	1707	84	44,45,45	1.23	4 (9%)	53,72,72	1.18	4 (7%)

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
87	GDP	Se	500	-	-	1/12/32/32	0/3/3/3
85	T1C	L1	1708	84	-	15/22/80/80	0/4/4/4
85	T1C	S1	1034	84	-	15/22/80/80	0/4/4/4
85	T1C	L1	1707	84	-	11/22/80/80	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	L1	1707	T1C	C21-N21	5.63	1.48	1.33
85	L1	1708	T1C	C21-N21	5.44	1.47	1.33
85	S1	1034	T1C	C21-N21	5.04	1.46	1.33
85	S1	1034	T1C	C1C-C41	-3.47	1.50	1.53
85	L1	1707	T1C	C4-N4	2.52	1.53	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S1	1034	T1C	C1-C1C-C12	6.34	117.31	109.88
85	L1	1707	T1C	C1C-C41-C4	5.04	118.53	111.64
87	Se	500	GDP	C3'-C2'-C1'	3.58	106.37	100.98
87	Se	500	GDP	PA-O3A-PB	-3.54	120.69	132.83
85	S1	1034	T1C	C11-C1B-C12	3.16	121.30	118.80

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

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

*Continued on next page...*

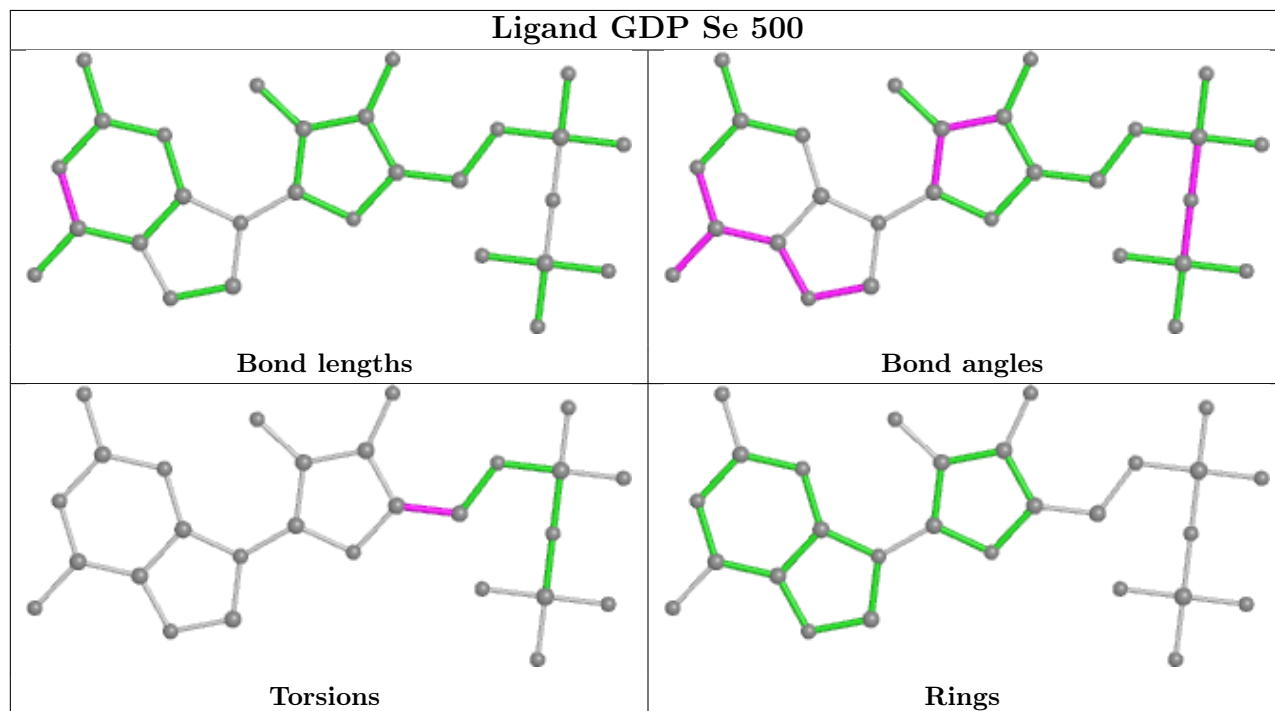
*Continued from previous page...*

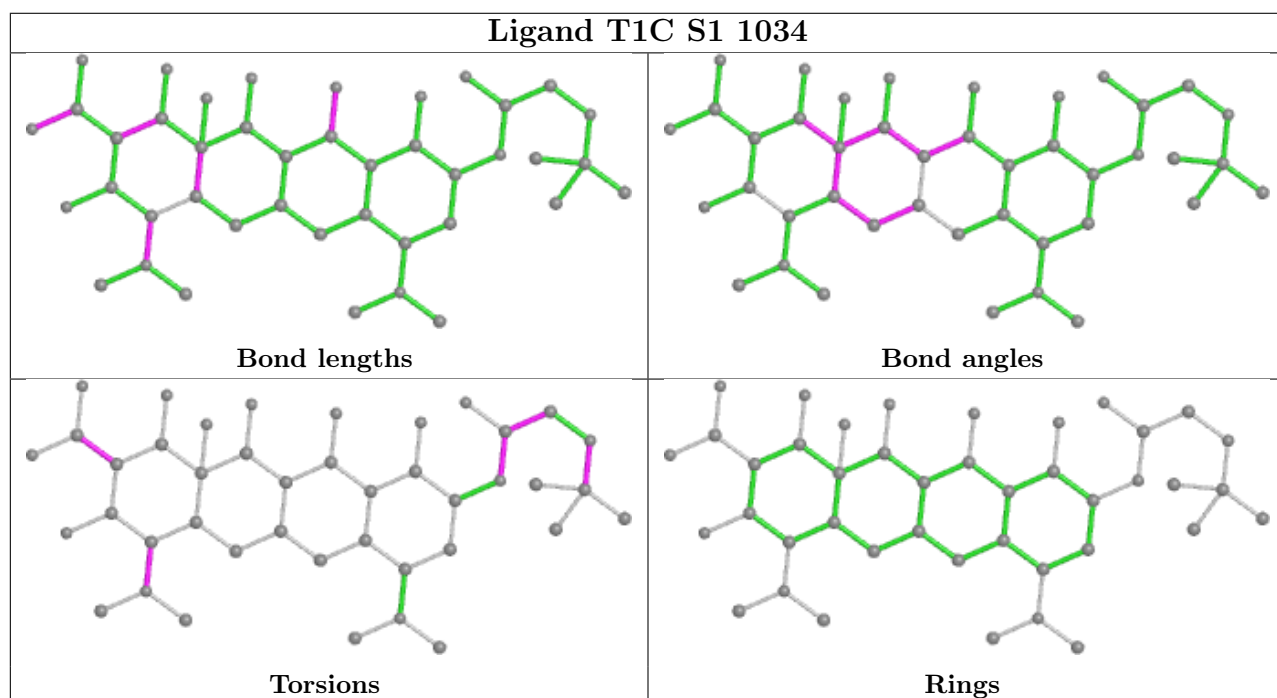
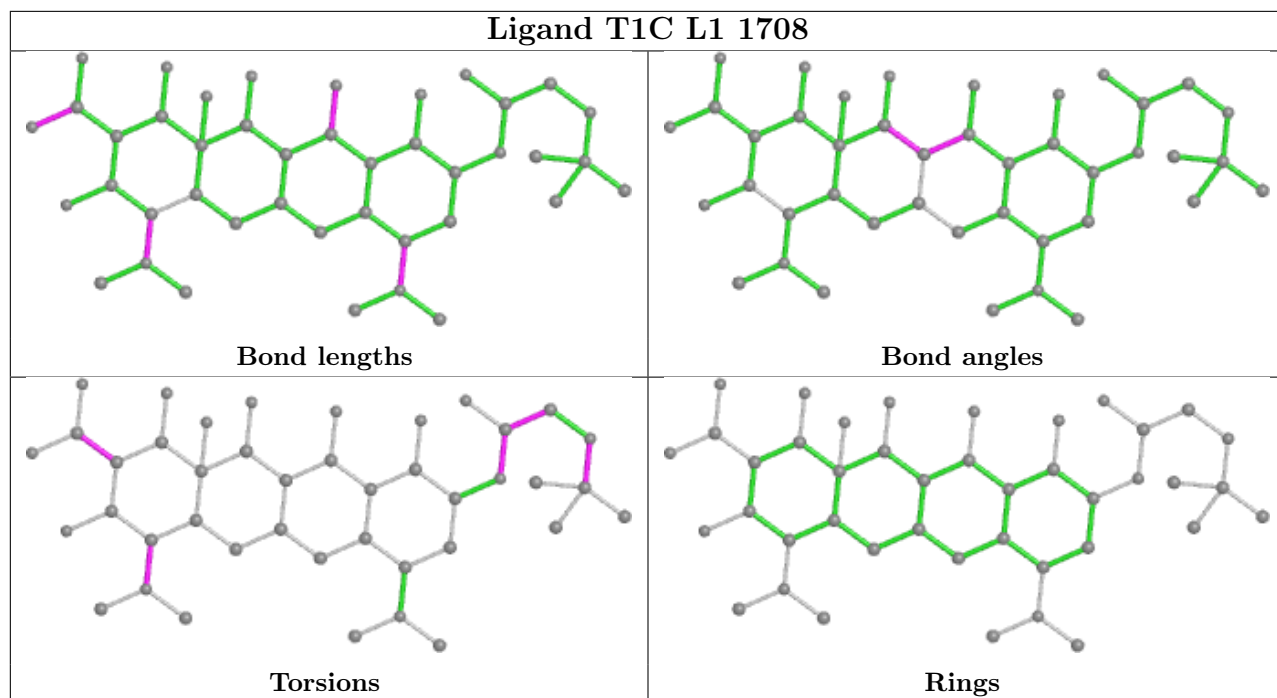
Mol	Chain	Res	Type	Atoms
85	L1	1707	T1C	C3-C4-N4-C42
85	L1	1707	T1C	C3-C2-C21-O21
85	L1	1708	T1C	C41-C4-N4-C43

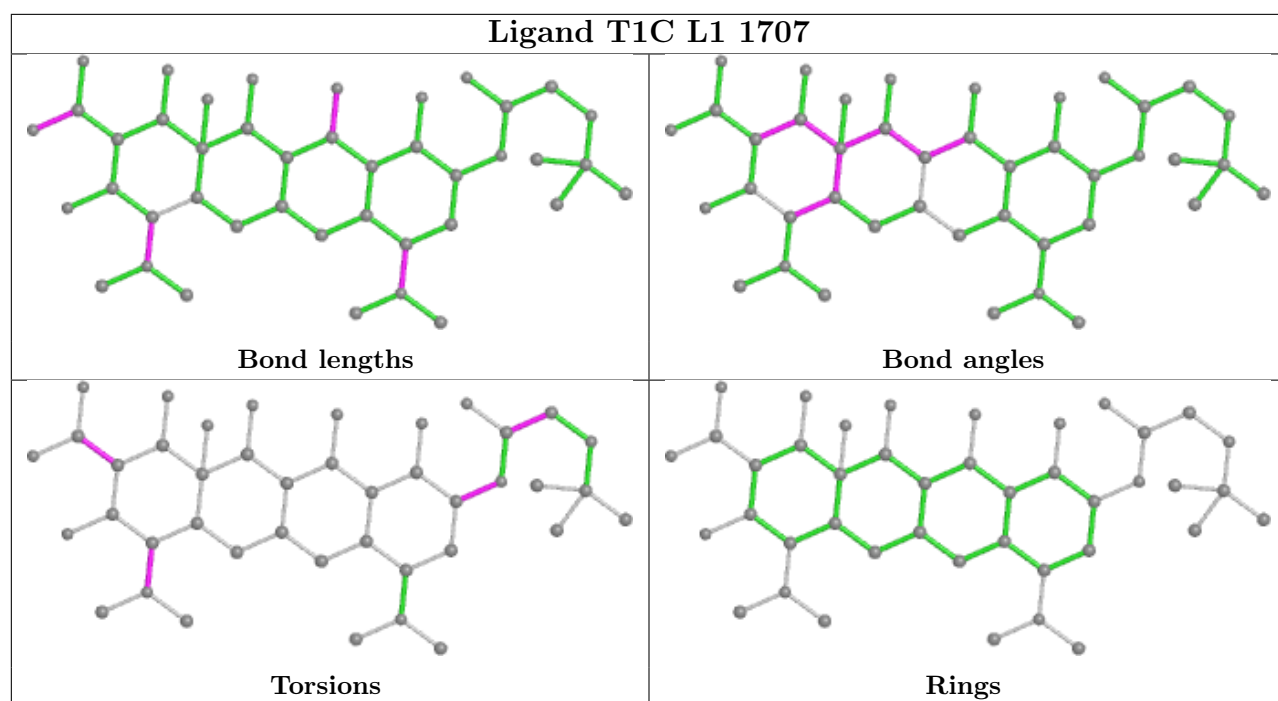
There are no ring outliers.

No monomer is involved in short contacts.

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.







## 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.

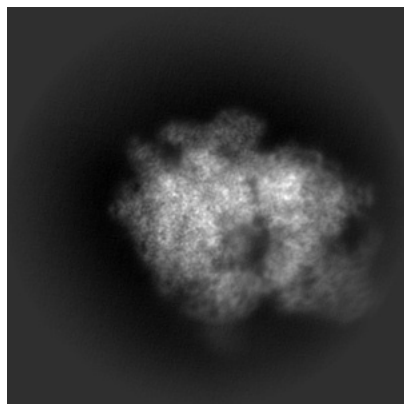
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38632. These allow visual inspection of the internal detail of the map and identification of artifacts.

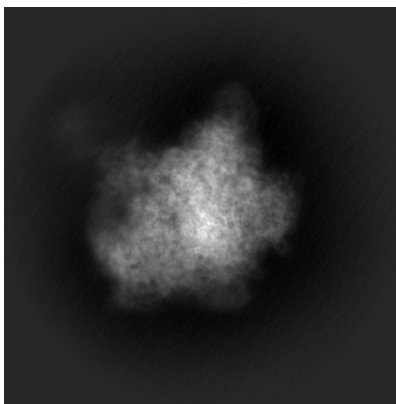
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

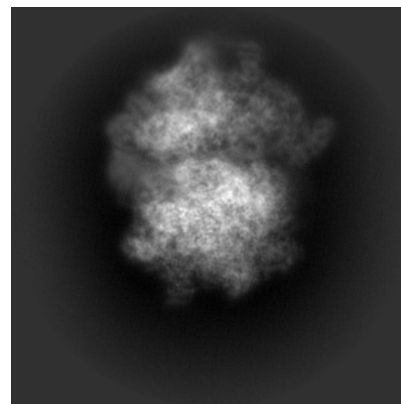
#### 6.1.1 Primary map



X

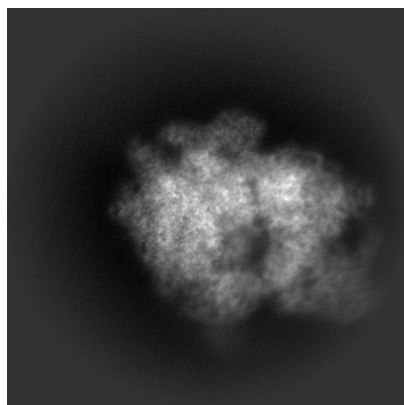


Y

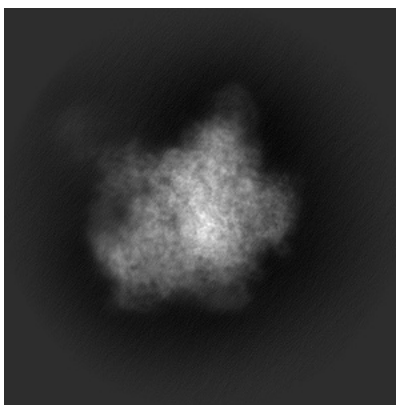


Z

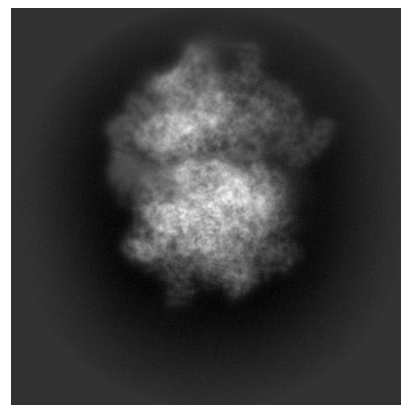
#### 6.1.2 Raw map



X



Y

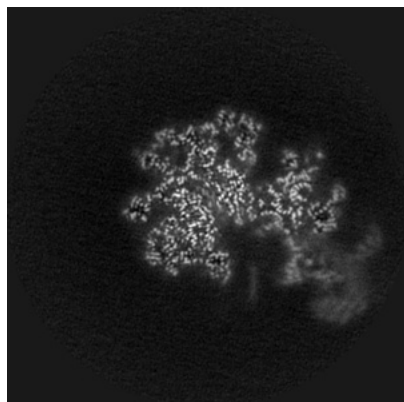


Z

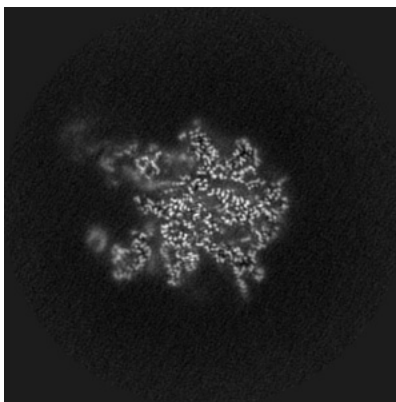
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

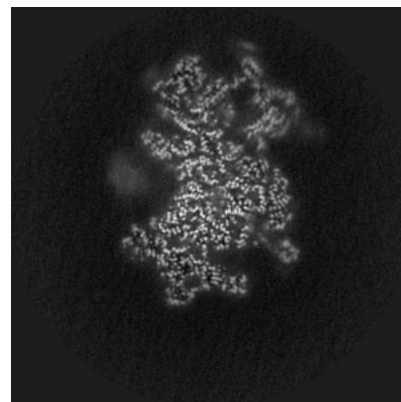
### 6.2.1 Primary map



X Index: 210

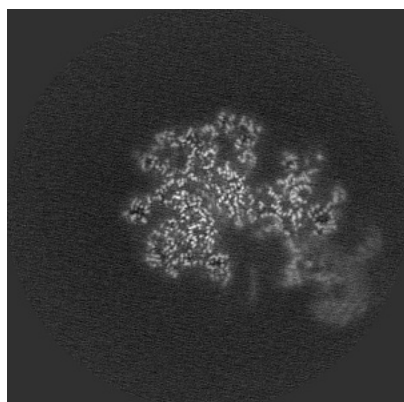


Y Index: 210

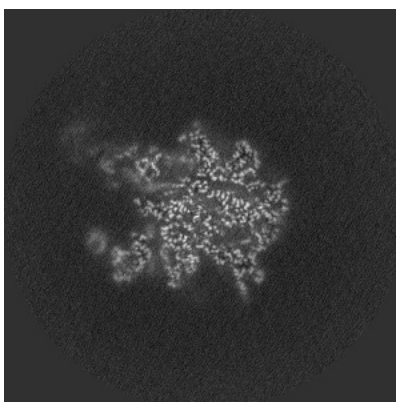


Z Index: 210

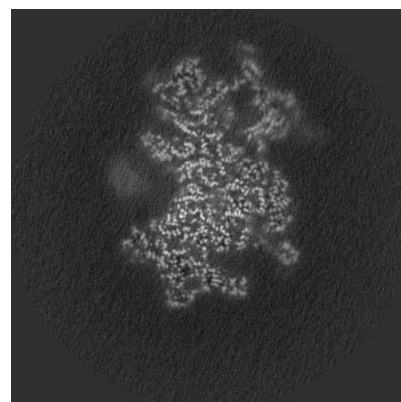
### 6.2.2 Raw map



X Index: 210



Y Index: 210



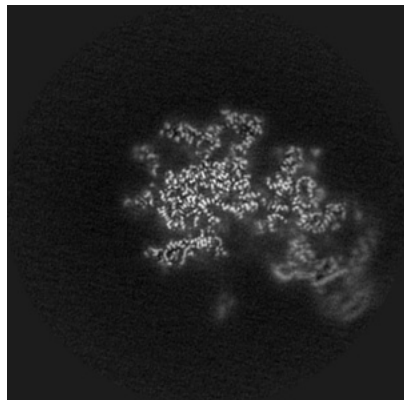
Z Index: 210

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

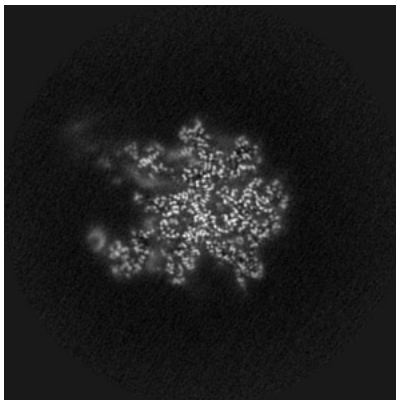


## 6.3 Largest variance slices [i](#)

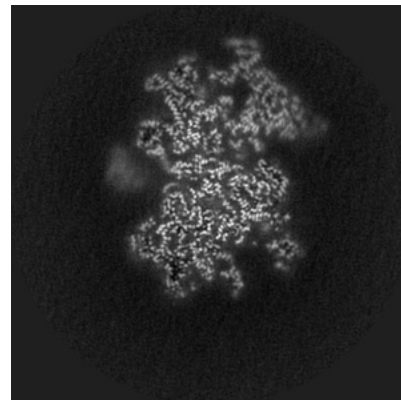
### 6.3.1 Primary map



X Index: 199

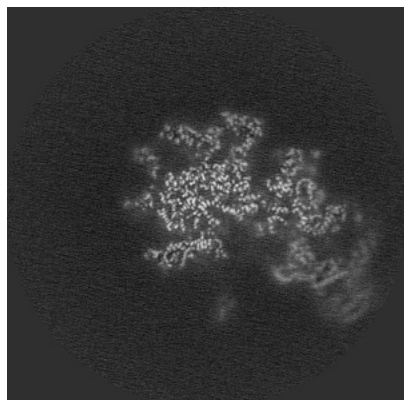


Y Index: 207

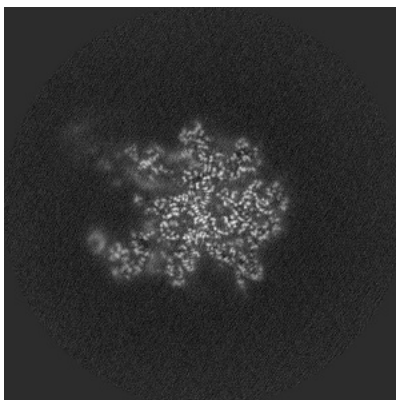


Z Index: 218

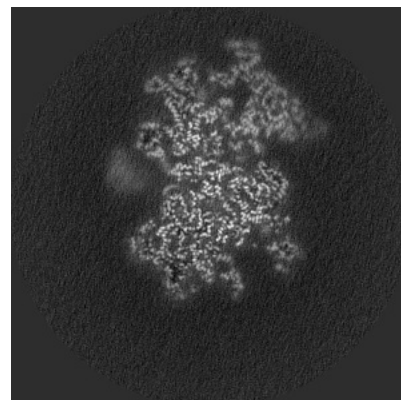
### 6.3.2 Raw map



X Index: 199



Y Index: 207



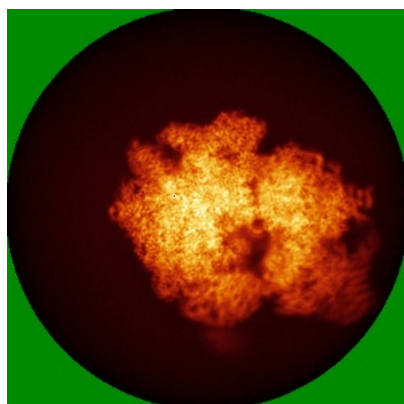
Z Index: 218

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

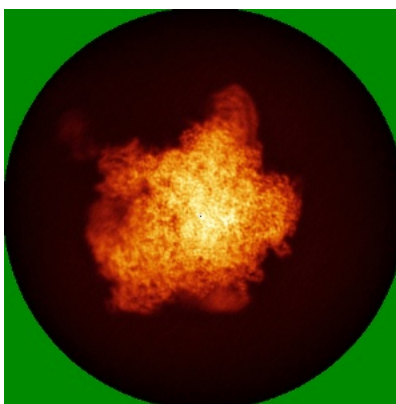


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

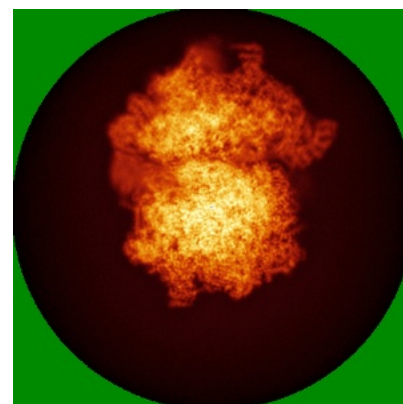
### 6.4.1 Primary map



X

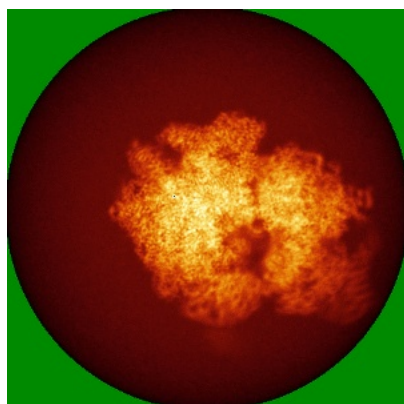


Y

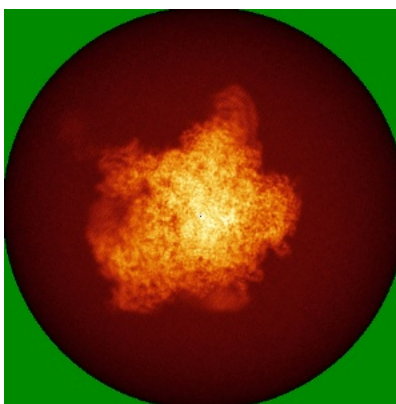


Z

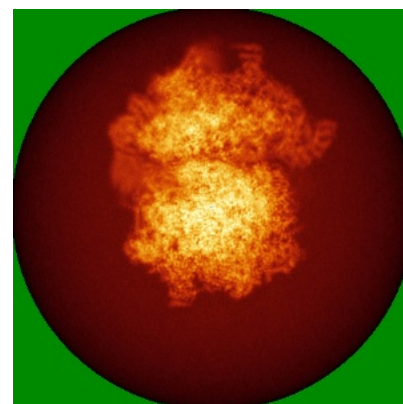
### 6.4.2 Raw map



X



Y

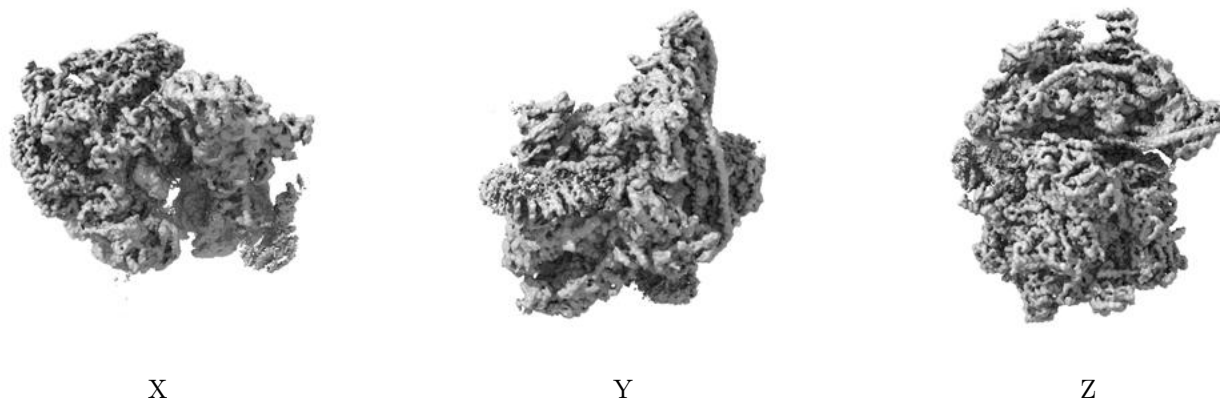


Z

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

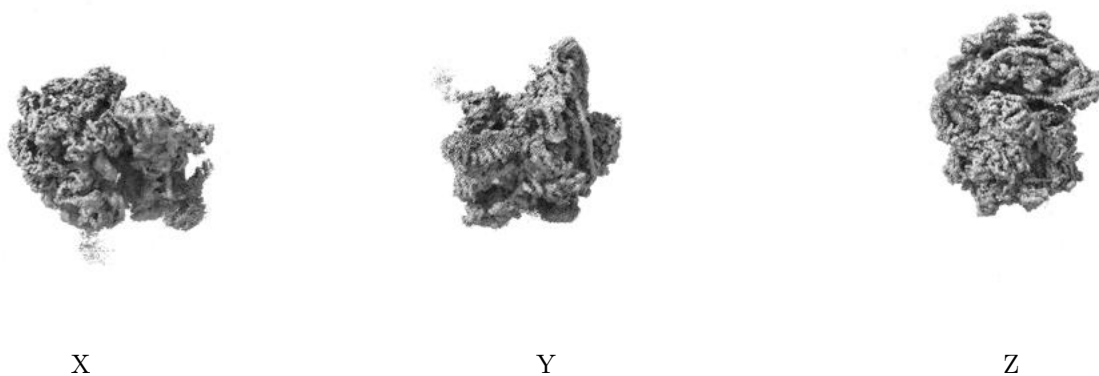
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

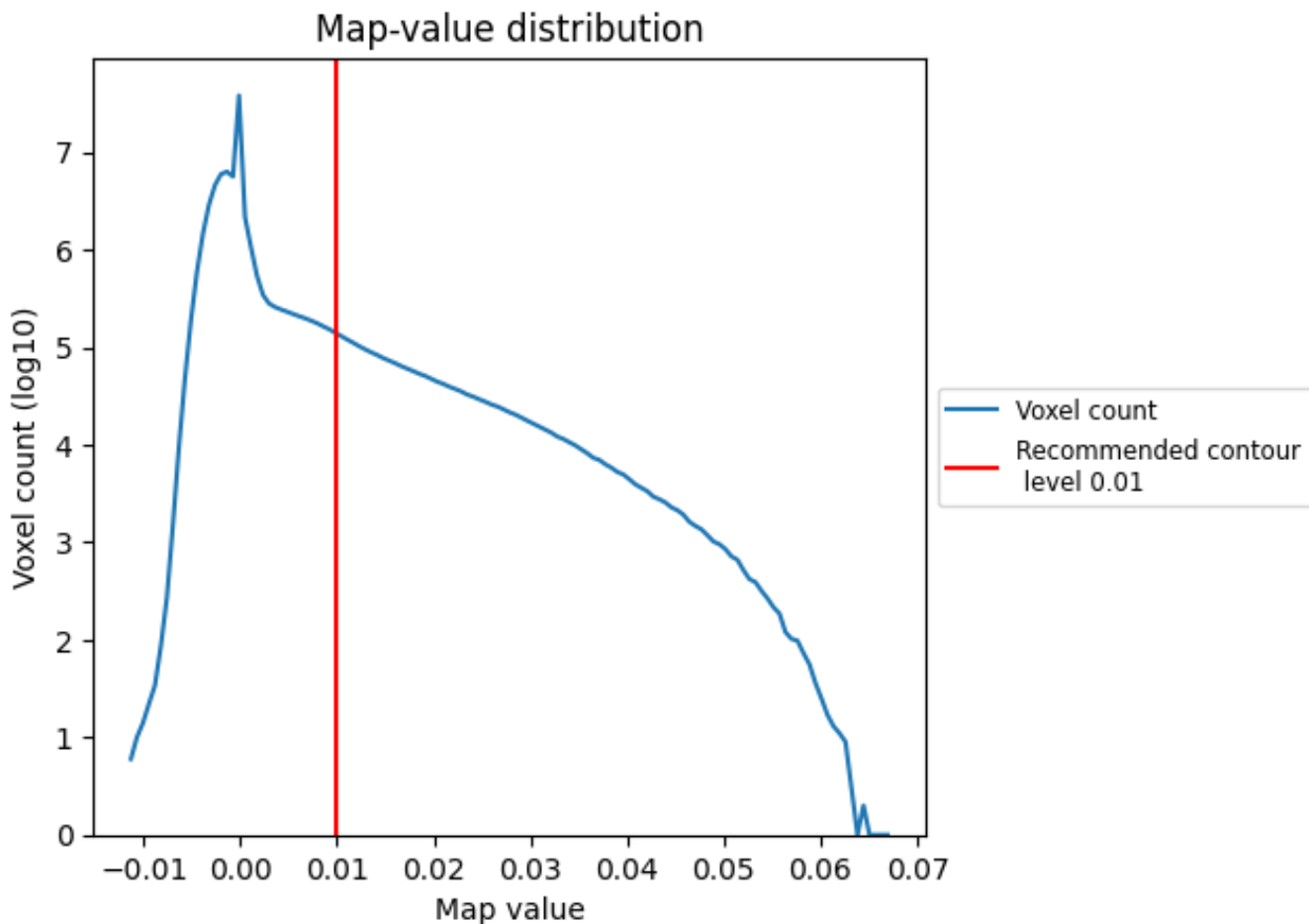
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

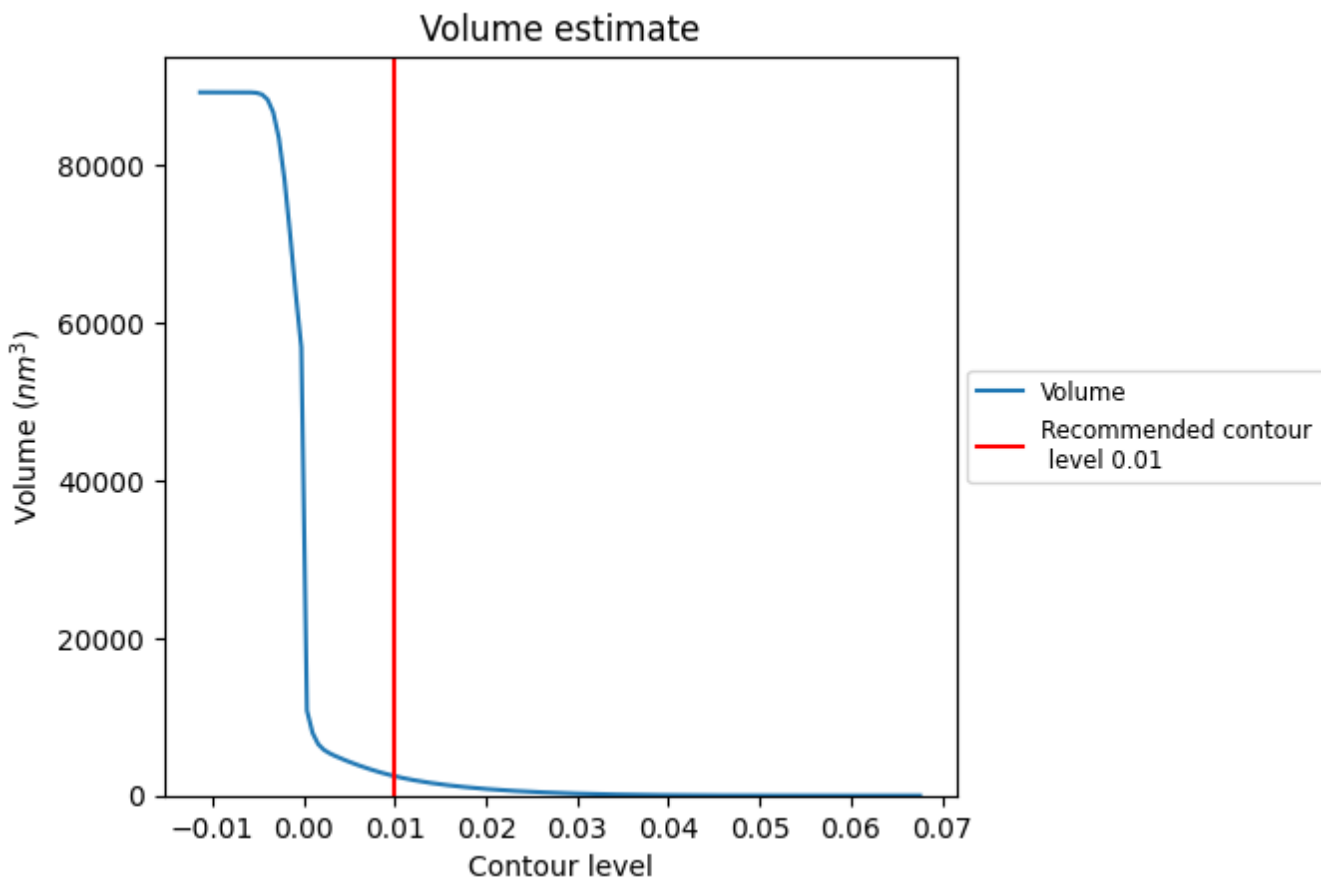
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

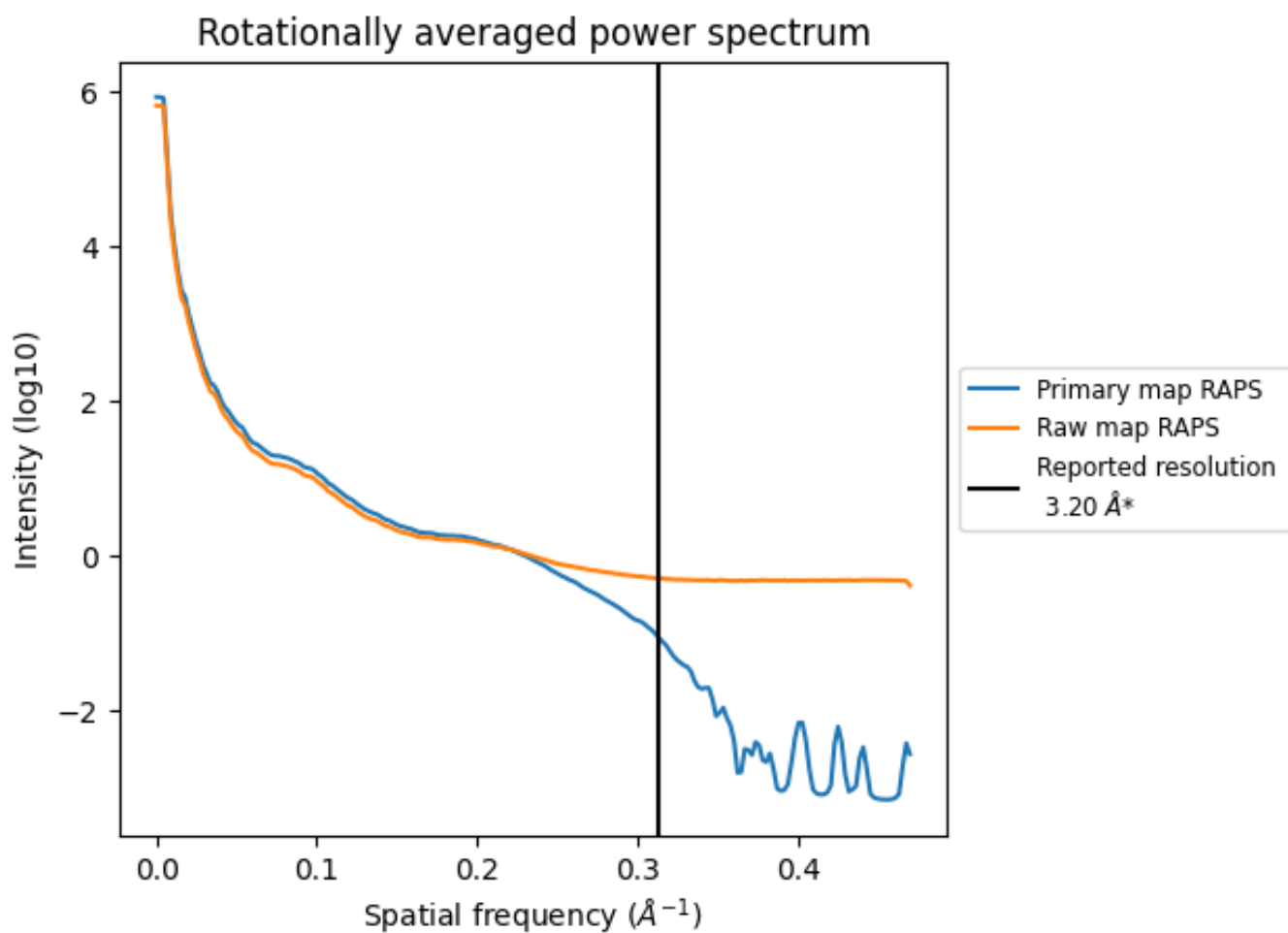
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2465  $\text{nm}^3$ ; this corresponds to an approximate mass of 2227 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](#)

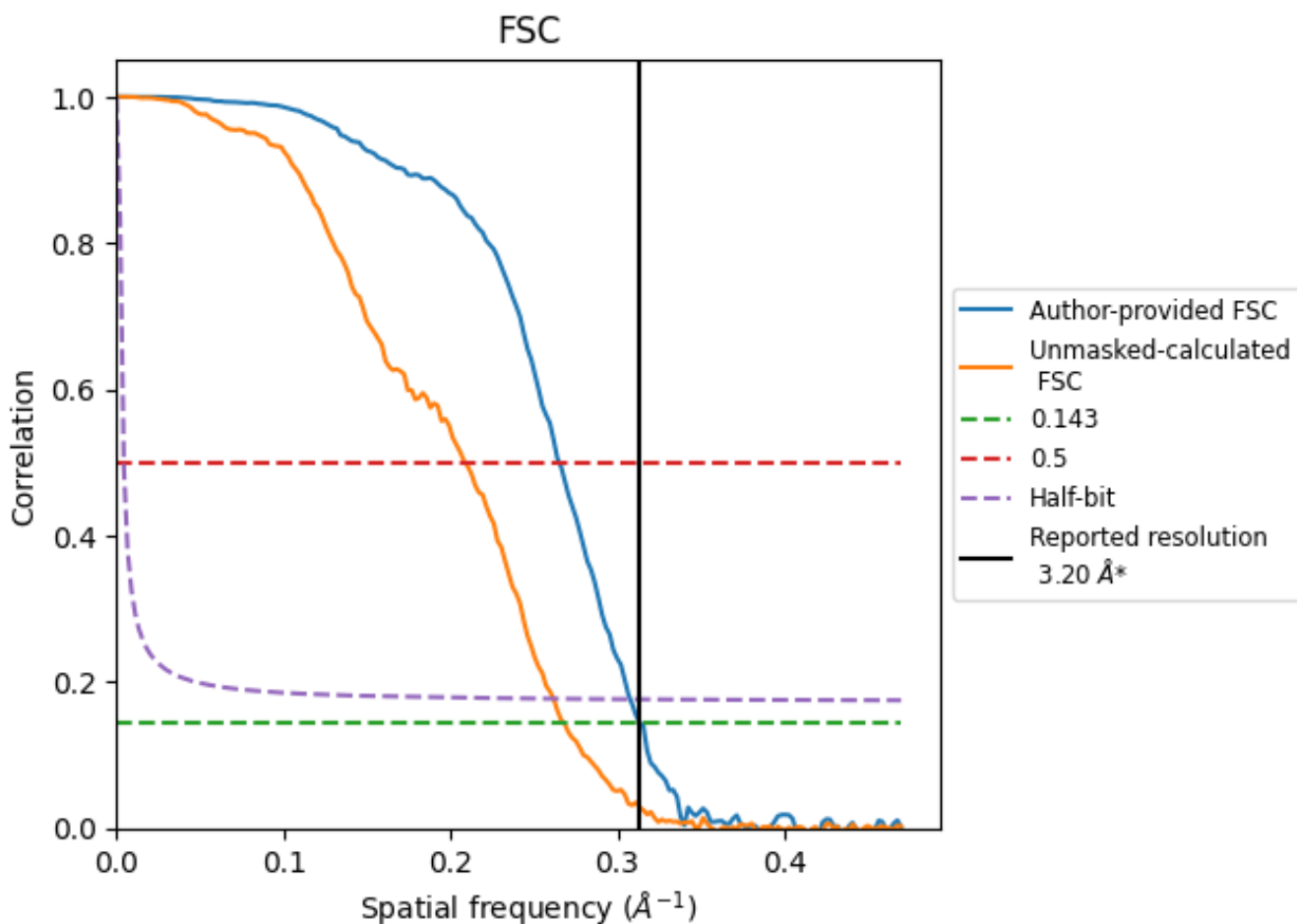


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

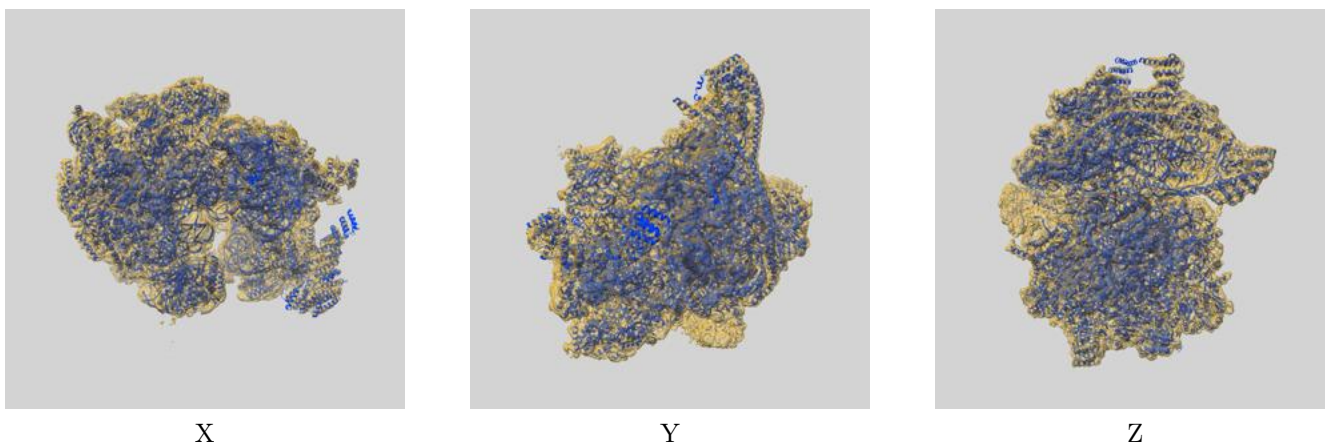
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.77	3.25
Unmasked-calculated*	3.73	4.79	3.82

\*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 3.73 differs from the reported value 3.2 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-38632 and PDB model 8XT0. Per-residue inclusion information can be found in section 3 on page 21.

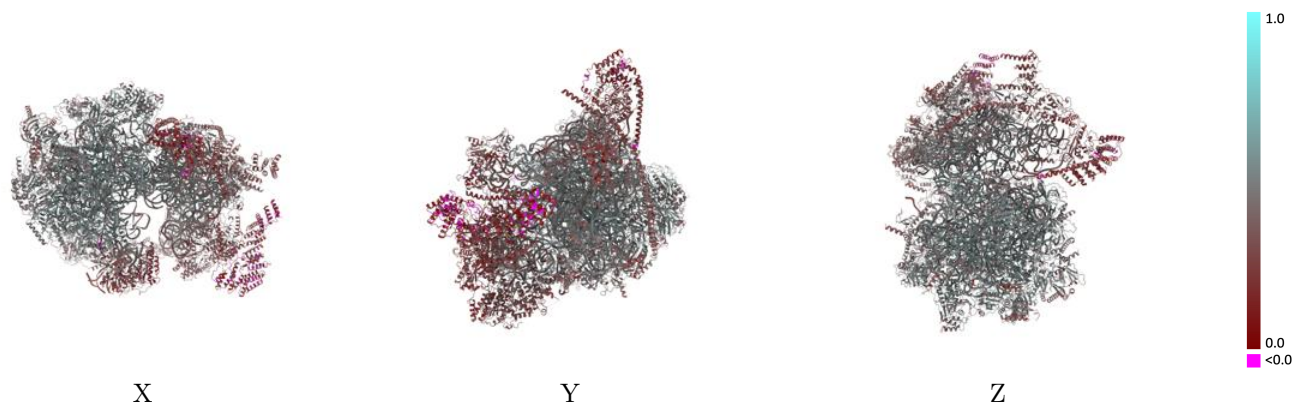
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

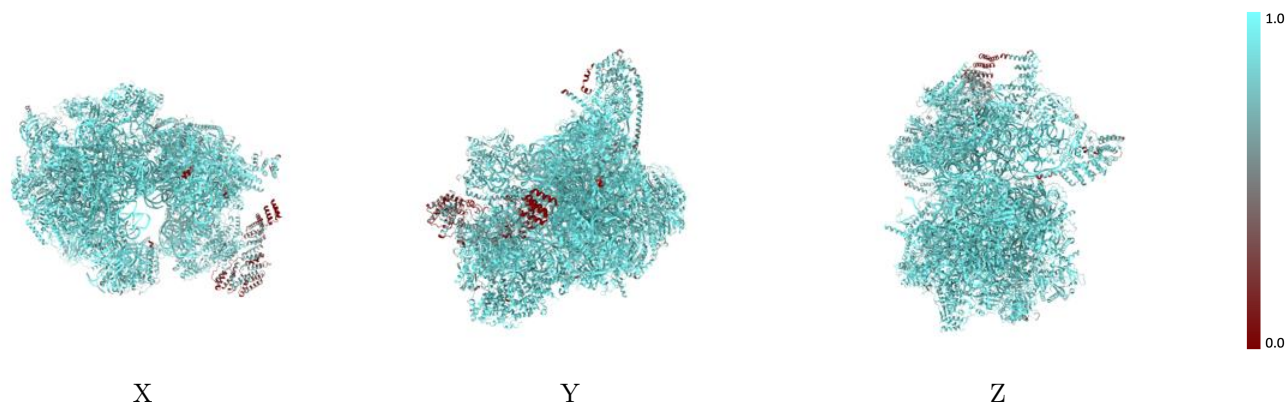


## 9.2 Q-score mapped to coordinate model [i](#)



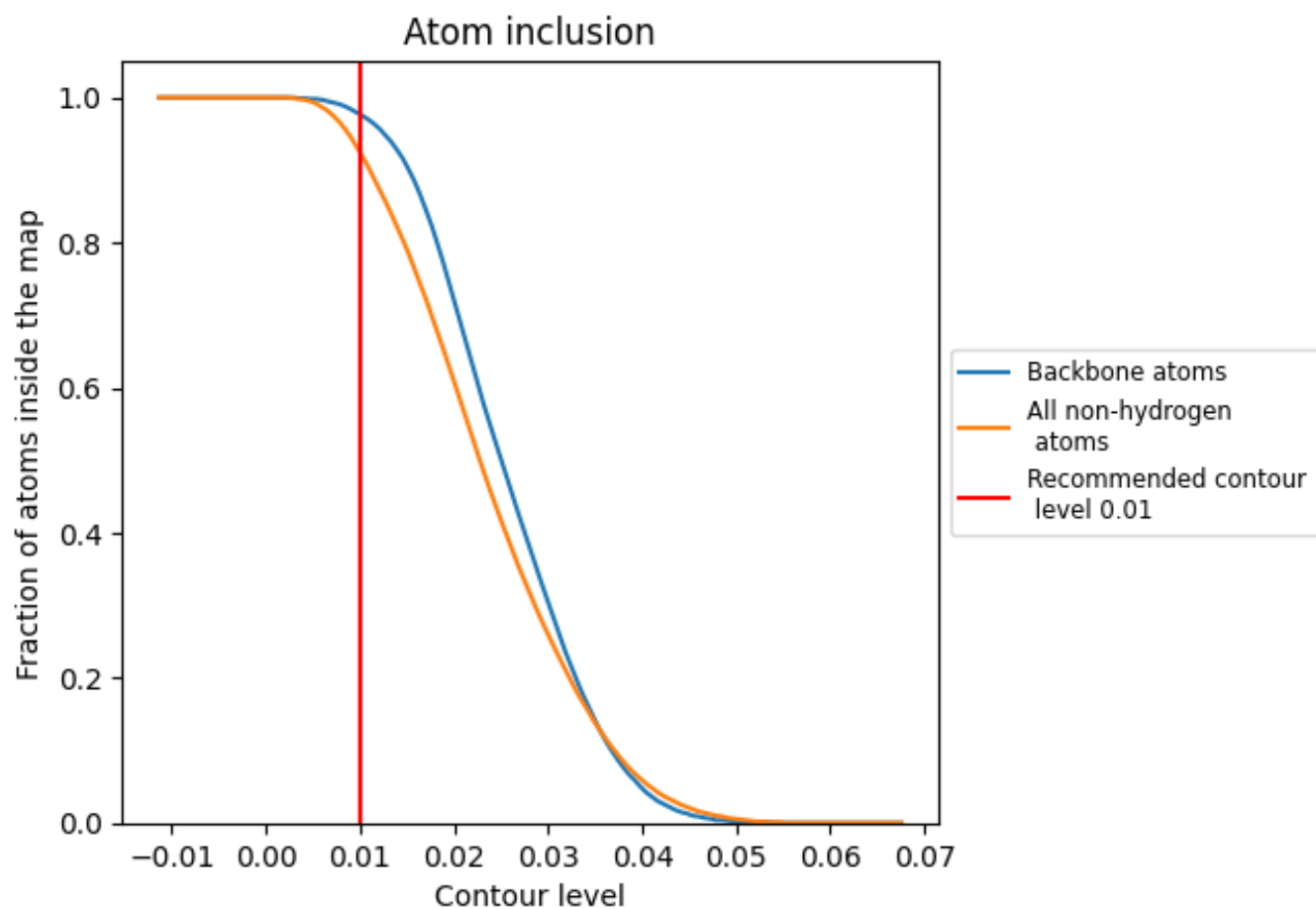
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.4340
L1	 0.9980	 0.5100
L2	 0.9790	 0.3420
L3	 0.8950	 0.3630
L4	 0.7860	 0.2920
L5	 0.9580	 0.3790
L6	 0.9690	 0.5140
L7	 0.9010	 0.4340
L8	 0.9100	 0.4230
LB	 0.9800	 0.5310
LC	 0.9580	 0.4980
LD	 0.9560	 0.5130
LI	 0.9080	 0.4410
LJ	 0.8450	 0.3500
LK	 0.7890	 0.2580
LM	 0.9710	 0.5100
LN	 0.9710	 0.5020
LO	 0.9530	 0.5040
LP	 0.9480	 0.4970
LQ	 0.9560	 0.4990
LR	 0.9320	 0.4640
LS	 0.9320	 0.4800
LT	 0.9590	 0.5140
LU	 0.9390	 0.5120
LV	 0.9590	 0.5170
LW	 0.9220	 0.4860
LX	 0.9020	 0.4410
La	 0.9730	 0.5290
Lb	 0.9240	 0.4730
Ld	 0.9550	 0.5180
Lf	 0.9400	 0.4900
Lg	 0.9740	 0.4920
Lh	 1.0000	 0.5440
Li	 0.9880	 0.5390
Lj	 0.9850	 0.5250

















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Chain	Atom inclusion	Q-score
Lk	 0.9390	 0.4810
Ll	 0.9140	 0.4310
Lm	 0.8820	 0.4270
Ln	 0.8630	 0.2960
Lo	 0.9170	 0.4650
Lp	 0.9200	 0.4780
Lq	 0.9570	 0.5170
Lr	 0.9150	 0.4690
Ls	 0.8360	 0.4150
Lt	 0.8240	 0.2640
Lu	 0.9450	 0.4820
Lv	 0.8910	 0.3720
Lw	 0.9450	 0.4940
Lx	 0.8950	 0.4390
Ly	 0.9700	 0.5270
Lz	 0.9210	 0.4670
S1	 0.9970	 0.4500
SB	 0.9360	 0.4410
SE	 0.9210	 0.4170
SF	 0.9160	 0.4640
SG	 0.9250	 0.3770
SI	 0.8940	 0.3450
SJ	 0.9160	 0.3130
SK	 0.9610	 0.4650
SL	 0.9550	 0.4570
SN	 0.9380	 0.3160
SO	 0.9110	 0.4250
SP	 0.9030	 0.3600
SQ	 0.9640	 0.4650
SR	 0.9720	 0.4930
SS	 0.9200	 0.3640
ST	 0.9240	 0.4580
SW	 0.9560	 0.4780
SX	 0.8340	 0.3130
SY	 0.8770	 0.3790
SZ	 0.8990	 0.3500
Sa	 0.9220	 0.4170
Sb	 0.8730	 0.3270
Sc	 0.7470	 0.2090
Sd	 0.8890	 0.4330
Se	 0.8770	 0.3180
Sf	 0.9530	 0.4910

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Chain	Atom inclusion	Q-score
Sg	 0.8000	 0.2380
Si	 0.9150	 0.2860
Sj	 0.8930	 0.3020
Sk	 0.8300	 0.2570
Sm	 0.9260	 0.4200
Sn	 0.9710	 0.4910
So	 0.4260	 0.1380