Full wwPDB EM Validation Report ⓘ

Jul 2, 2024 – 03:21 PM 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

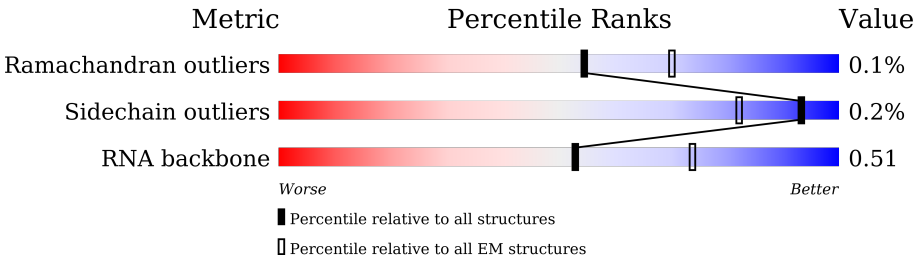
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	L1	1559	71% 23%
2	L2	69	61% 20% 19%
3	LB	305	77% 22%
4	LC	348	87% 13%
5	LD	311	79% 20%
6	LI	267	36% 64%
7	LJ	261	58% 39%
8	LK	192	90% 9%

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Mol	Chain	Length	Quality of chain
9	LM	178	99%
10	LN	145	79% 21%
11	LO	296	96%
12	LP	251	88% 12%
13	LQ	175	85% 13%
14	LR	179	81% 18%
15	LS	292	75% 25%
16	LT	149	94% 6%
17	LU	205	78% 22%
18	LV	212	78% 22%
19	LW	153	93% 7%
20	LX	216	92% 6%
21	La	148	75% 25%
22	Lb	256	94% 5%
23	Lu	250	70% 30%
24	Ld	161	75% 25%
25	Lf	188	57% 43%
26	Lg	65	80% 20%
27	Lh	92	50% 50%
28	Li	188	50% 49%
29	Lj	103	37% 63%
30	Lk	423	93% 7%
31	Ll	380	93% 7%
32	Lm	338	86% 13%
33	Ln	206	47% 52%

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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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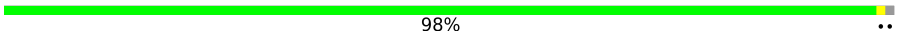
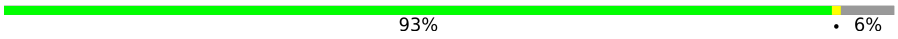
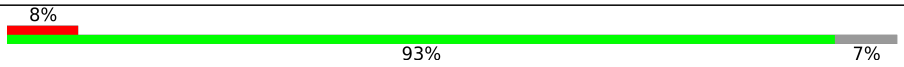
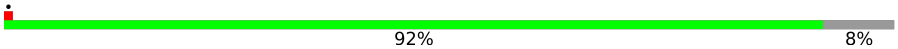
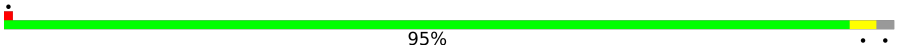
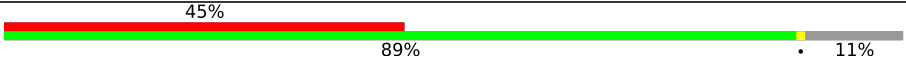
Mol	Chain	Length	Quality of chain
59	SJ	201	
60	SK	194	
61	SL	138	
62	SN	128	
63	SO	257	
64	SP	137	
65	SQ	130	
66	SS	258	
67	ST	142	
68	SW	87	
69	SX	360	
70	SY	190	
71	Sa	173	
72	Sb	205	
73	Sc	414	
74	Sd	187	
75	Se	398	
76	Sg	395	
77	Si	106	
78	Sj	218	
79	Sk	323	
80	Sm	118	
81	Sn	199	
82	So	689	
83	S1	954	

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
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		

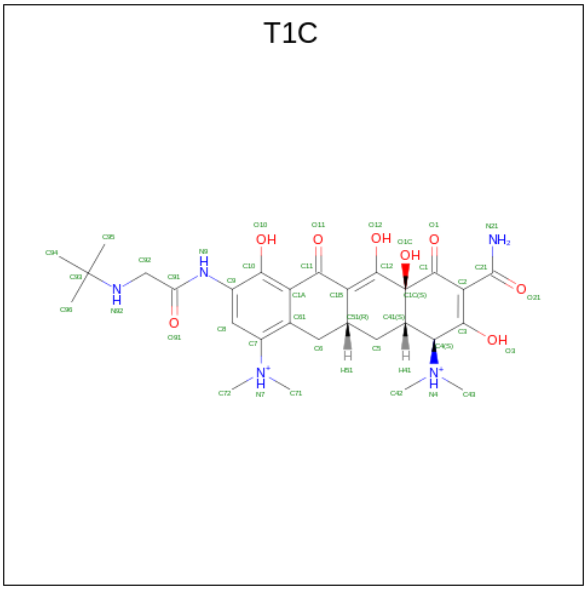
There is a discrepancy between the modelled and reference sequences:

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
84	L1	106	Total	Mg	0
			106	106	
84	LB	3	Total	Mg	0
			3	3	
84	LP	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 (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$) (labeled as "Ligand of Interest" by depositor).

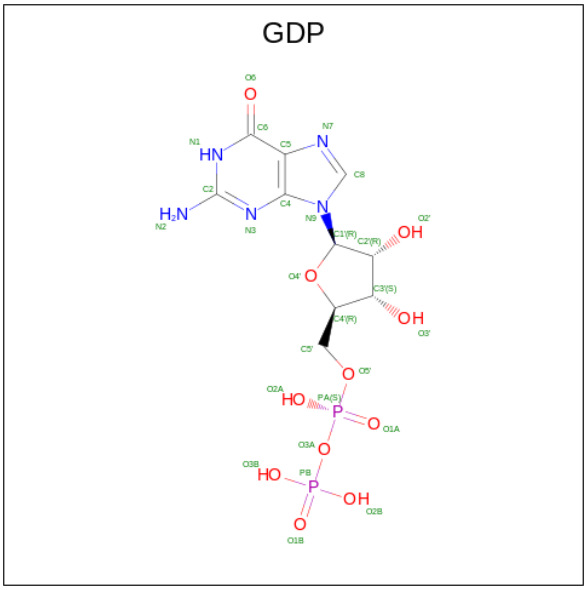


Mol	Chain	Residues	Atoms				AltConf
85	L1	1	Total	C	N	O	0
			42	29	5	8	
85	L1	1	Total	C	N	O	0
			42	29	5	8	
85	S1	1	Total	C	N	O	0
			42	29	5	8	

- 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: $C_{10}H_{15}N_5O_{11}P_2$).



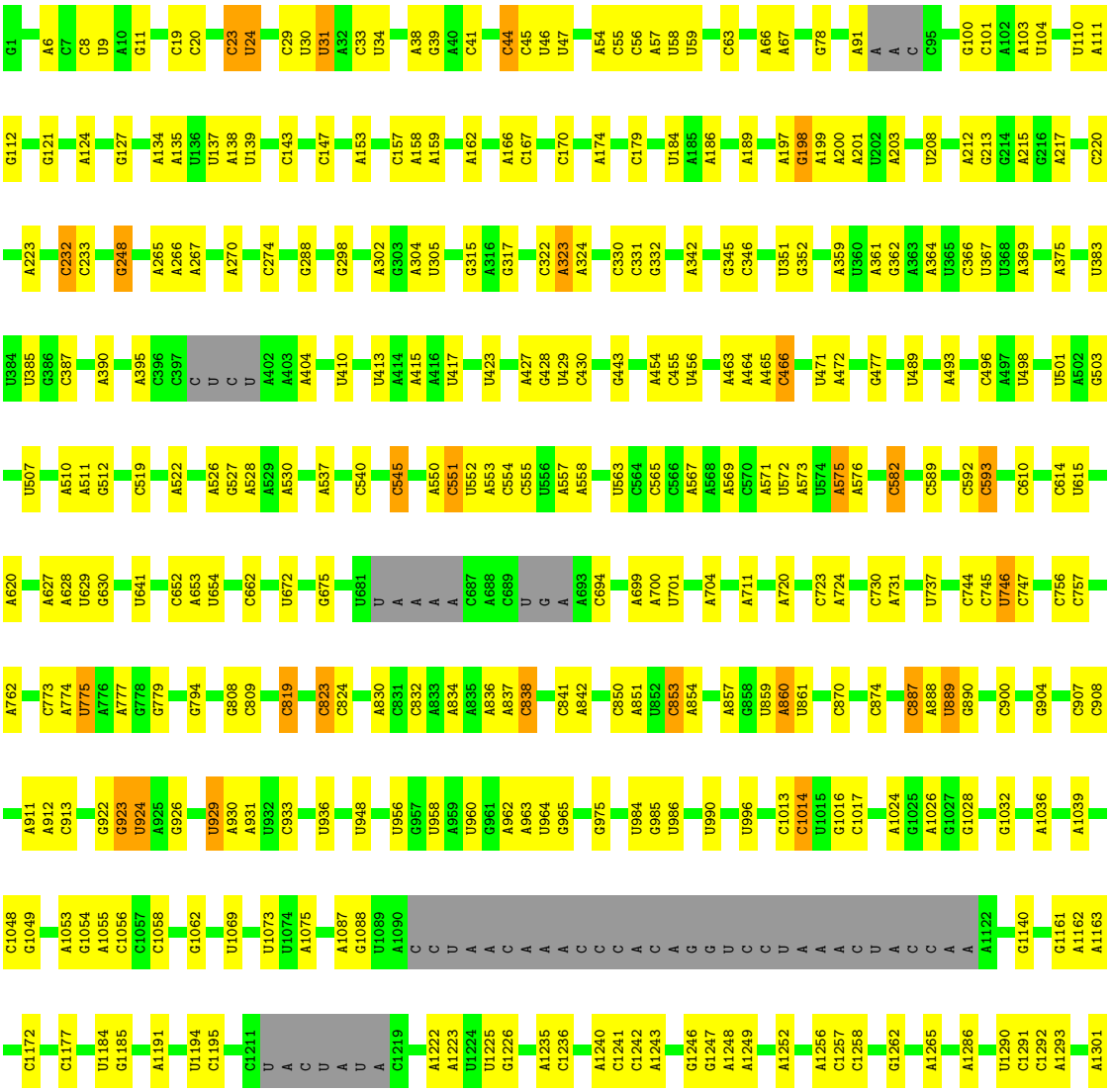
Mol	Chain	Residues	Atoms					AltConf
87	Se	1	Total	C	N	O	P	0
			28	10	5	11	2	

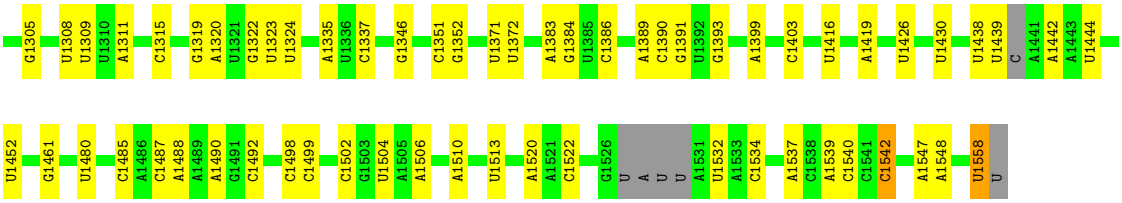
3 Residue-property plots (i)

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

- Molecule 1: 16s rRNA

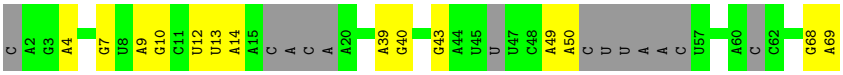
Chain L1:





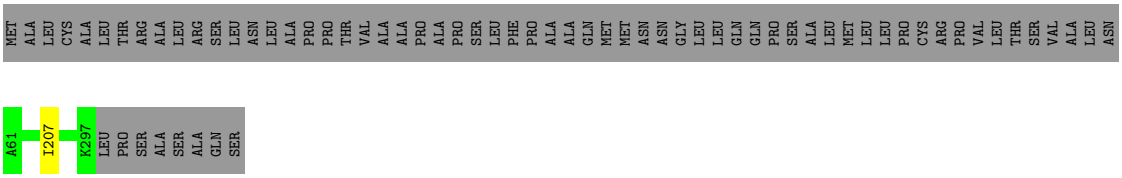
• Molecule 2: Val tRNA

Chain L2:



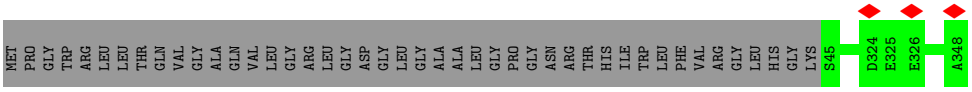
• Molecule 3: Large ribosomal subunit protein uL2m

Chain LB:



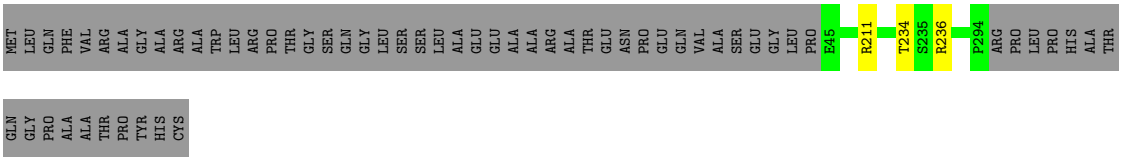
• Molecule 4: Large ribosomal subunit protein uL3m

Chain LC:



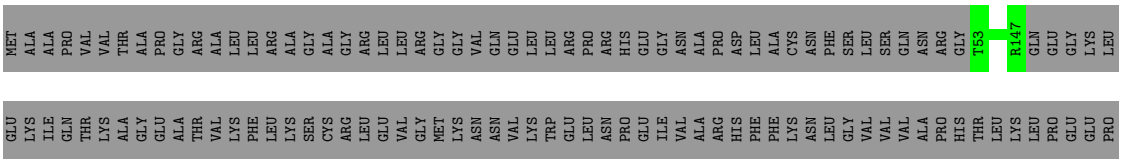
• Molecule 5: Large ribosomal subunit protein uL4m

Chain LD:



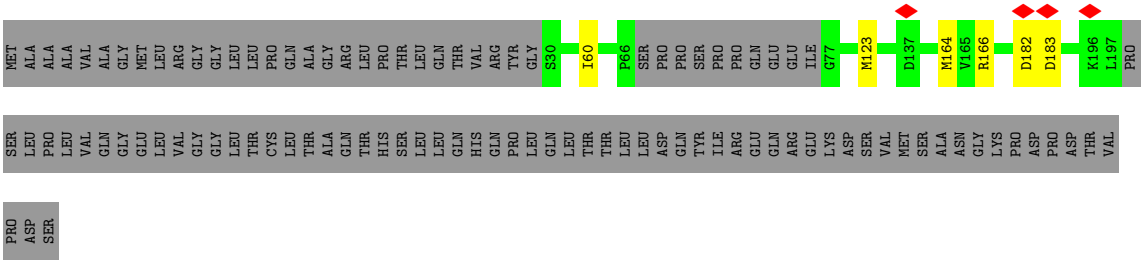
• Molecule 6: Large ribosomal subunit protein bL9m

Chain LI:



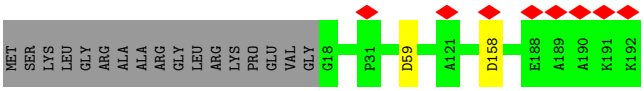
• Molecule 7: Large ribosomal subunit protein uL10m

Chain LJ:



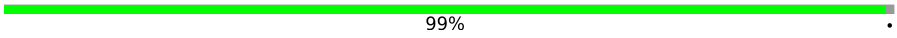
• Molecule 8: Large ribosomal subunit protein uL11m

Chain LK:



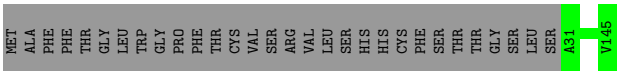
• Molecule 9: Large ribosomal subunit protein uL13m

Chain LM:



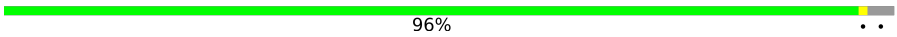
• Molecule 10: Large ribosomal subunit protein uL14m

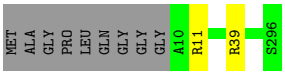
Chain LN:



• Molecule 11: Large ribosomal subunit protein uL15m

Chain LO:



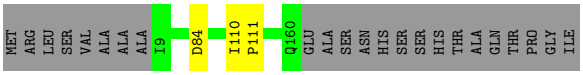


• Molecule 12: Large ribosomal subunit protein uL16m

Chain LP:

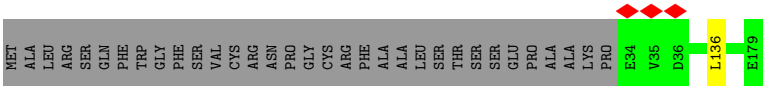
• Molecule 13: Large ribosomal subunit protein bL17m

Chain LQ:



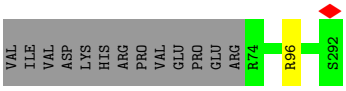
• Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain LR:



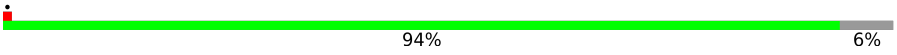
• Molecule 15: Large ribosomal subunit protein bL19m

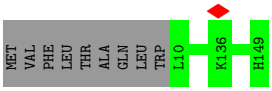
Chain LS:



• Molecule 16: Large ribosomal subunit protein bL20m

Chain LT:



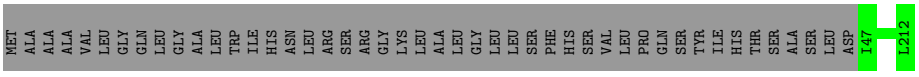


• Molecule 17: Large ribosomal subunit protein bL21m

Chain LU:

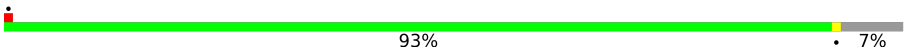
• Molecule 18: 39S ribosomal protein L22, mitochondrial

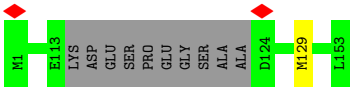
Chain LV:



• Molecule 19: Large ribosomal subunit protein uL23m

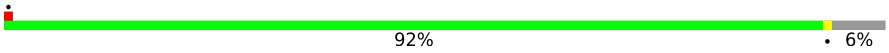
Chain LW:

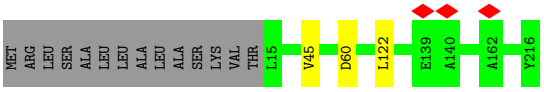




• Molecule 20: Large ribosomal subunit protein uL24m

Chain LX:



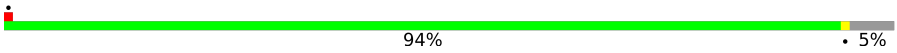


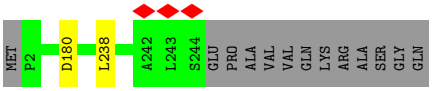
• Molecule 21: Large ribosomal subunit protein bL27m

Chain La:

• Molecule 22: Large ribosomal subunit protein bL28m

Chain Lb:



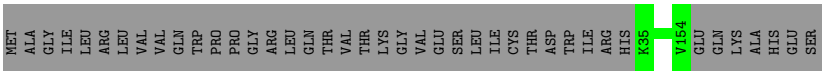


• Molecule 23: Large ribosomal subunit protein uL29m

Chain Lu:

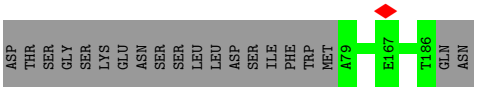
• Molecule 24: Large ribosomal subunit protein uL30m

Chain Ld:



• Molecule 25: Large ribosomal subunit protein bL32m

Chain Lf:

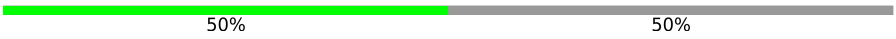


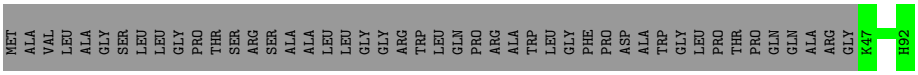
• Molecule 26: Large ribosomal subunit protein bL33m

Chain Lg:

• Molecule 27: Large ribosomal subunit protein bL34m

Chain Lh:



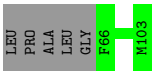


• Molecule 28: Large ribosomal subunit protein bL35m

Chain Li:

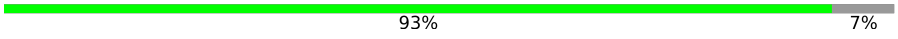
• Molecule 29: Large ribosomal subunit protein bL36m

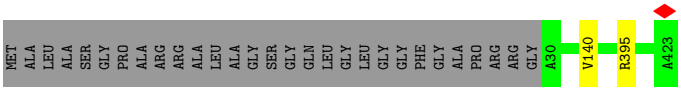
Chain Lj:



• Molecule 30: Large ribosomal subunit protein mL37

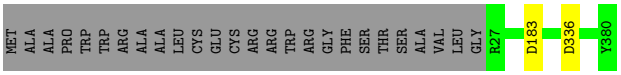
Chain Lk:





• Molecule 31: Large ribosomal subunit protein mL38

Chain Ll:



• Molecule 32: Large ribosomal subunit protein mL39

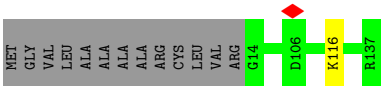
Chain Lm:

• Molecule 33: Large ribosomal subunit protein mL40

Chain Ln:

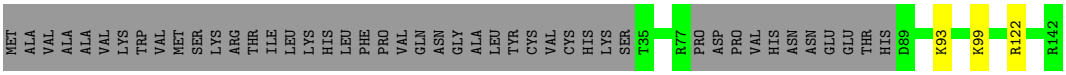
• Molecule 34: Large ribosomal subunit protein mL41

Chain Lo:



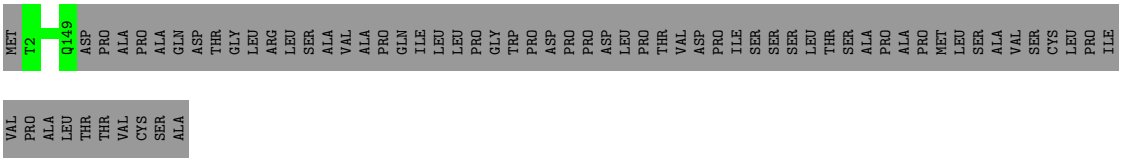
• Molecule 35: Large ribosomal subunit protein mL42

Chain Lp:



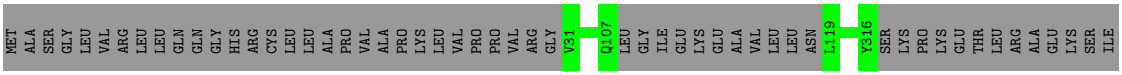
• Molecule 36: Large ribosomal subunit protein mL43

Chain Lq:



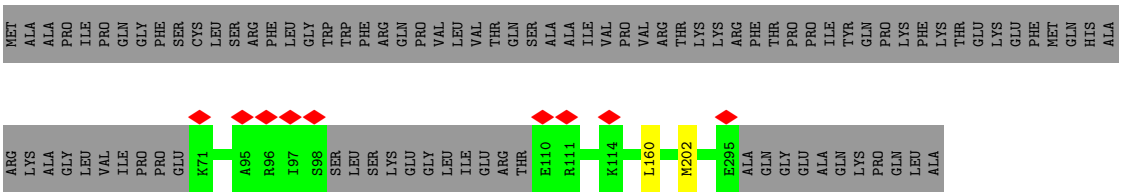
• Molecule 37: Large ribosomal subunit protein mL44

Chain Lr:



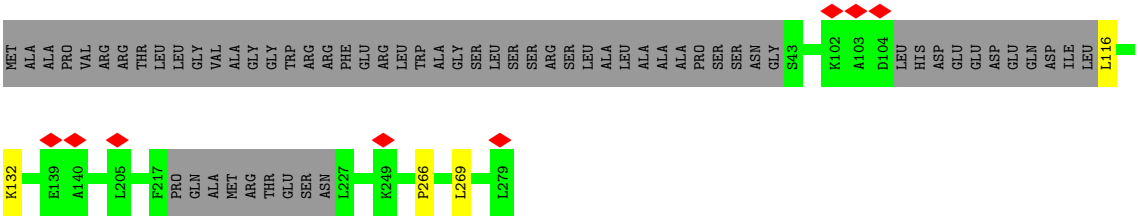
• Molecule 38: Large ribosomal subunit protein mL45

Chain Ls:



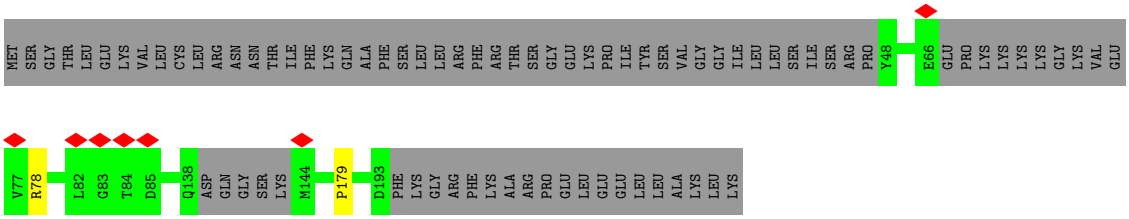
• Molecule 39: Large ribosomal subunit protein mL46

Chain Lt:



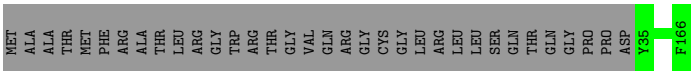
• Molecule 40: Large ribosomal subunit protein mL48

Chain Lv:



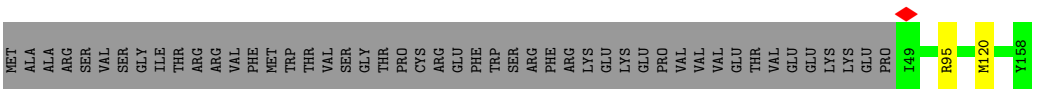
• Molecule 41: Large ribosomal subunit protein mL49

Chain Lw:



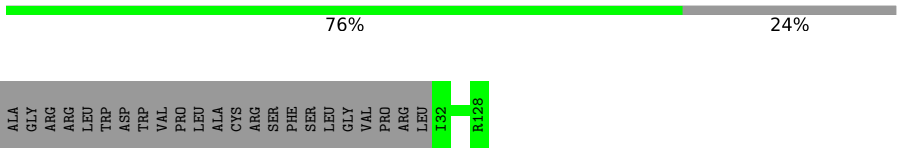
• Molecule 42: Large ribosomal subunit protein mL50

Chain Lx:



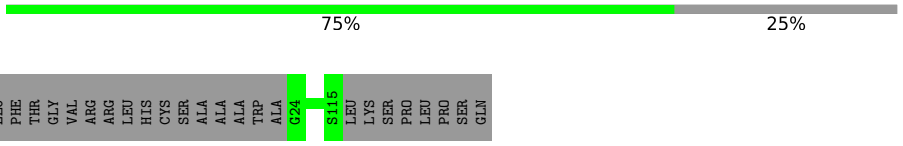
• Molecule 43: Large ribosomal subunit protein mL51

Chain Ly:



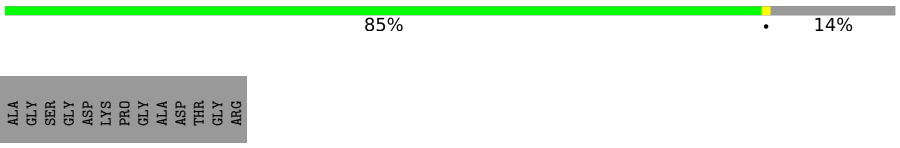
• Molecule 44: 39S ribosomal protein L52, mitochondrial

Chain Lz:



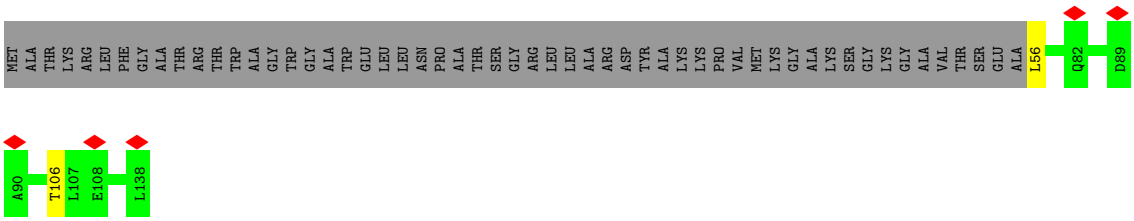
• Molecule 45: Large ribosomal subunit protein mL53

Chain L3:



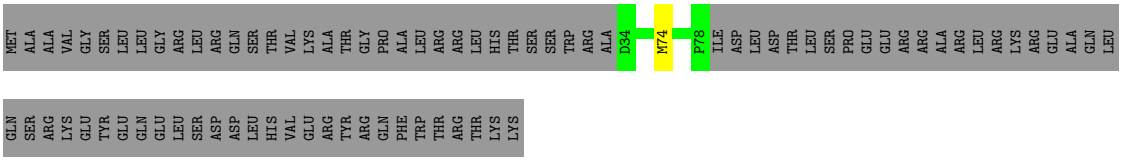
• Molecule 46: Large ribosomal subunit protein mL54

Chain L4:



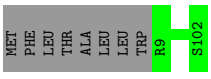
• Molecule 47: Large ribosomal subunit protein mL55

Chain L5:



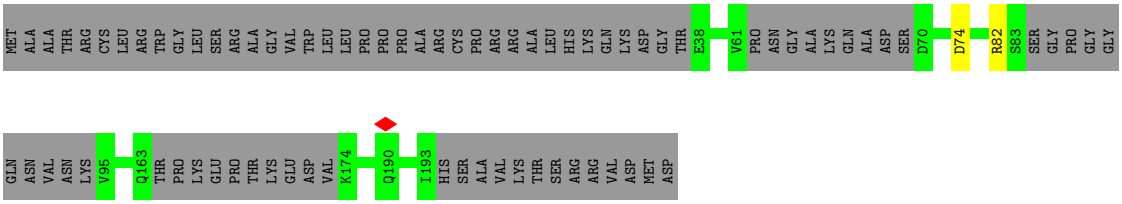
• Molecule 48: Large ribosomal subunit protein mL63

Chain L6:



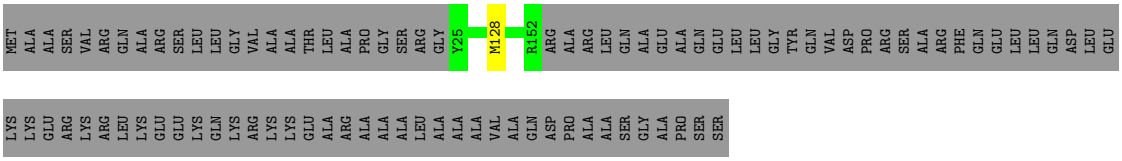
• Molecule 49: Large ribosomal subunit protein mL62

Chain L7:



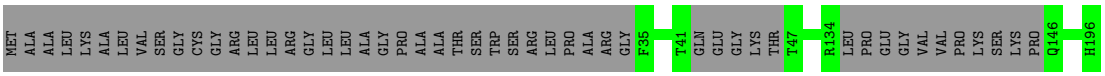
• Molecule 50: Large ribosomal subunit protein mL64

Chain L8:



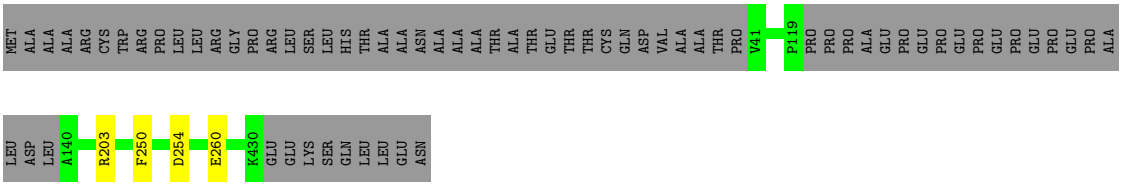
• Molecule 51: Large ribosomal subunit protein mL66

Chain SR:



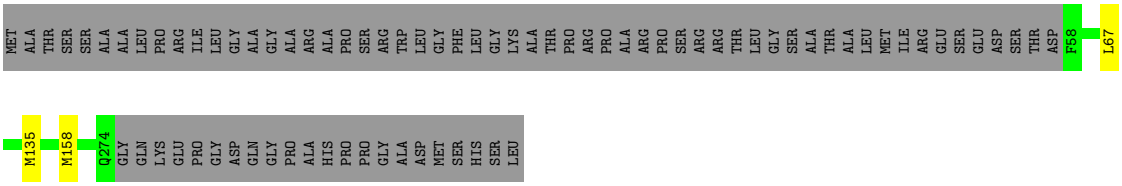
• Molecule 52: Large ribosomal subunit protein mL65

Chain Sf:



• Molecule 53: Small ribosomal subunit protein uS2m

Chain SB:

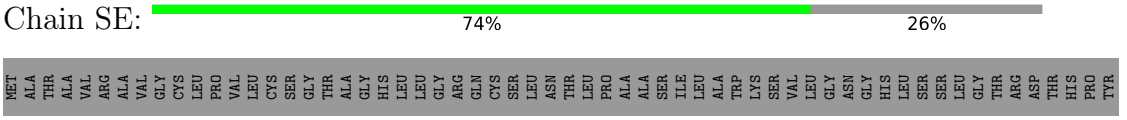


• Molecule 54: Small ribosomal subunit protein uS3m

Chain SZ:

• Molecule 55: Small ribosomal subunit protein uS5m

Chain SE:

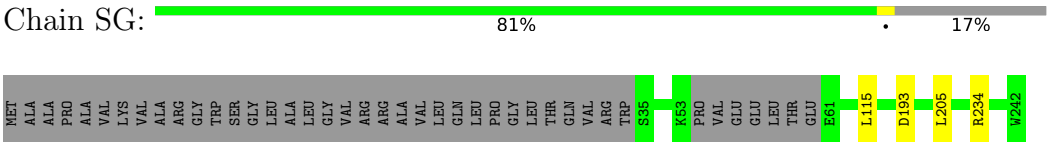


• Molecule 56: Small ribosomal subunit protein bS6m

Chain SF:

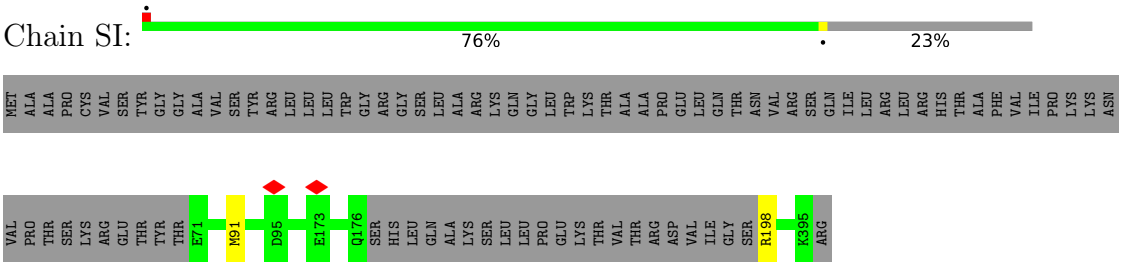
• Molecule 57: Small ribosomal subunit protein uS7m

Chain SG:



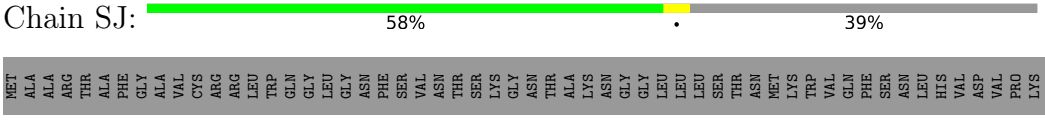
• Molecule 58: Small ribosomal subunit protein uS9m

Chain SI:



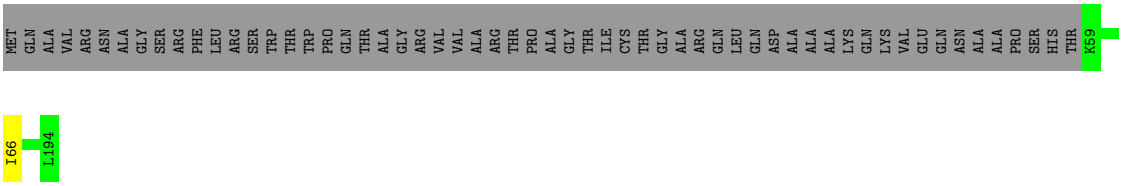
• Molecule 59: Small ribosomal subunit protein uS10m

Chain SJ:



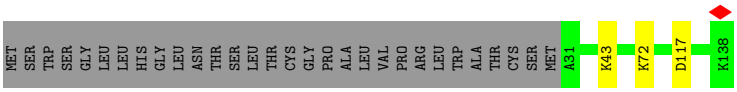
• Molecule 60: Small ribosomal subunit protein uS11m

Chain SK:



• Molecule 61: Small ribosomal subunit protein uS12m

Chain SL:

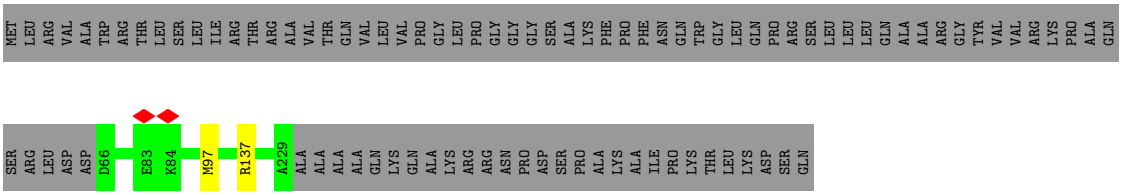


• Molecule 62: Small ribosomal subunit protein uS14m

Chain SN:

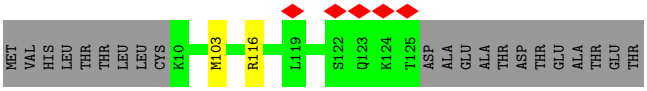
• Molecule 63: Small ribosomal subunit protein uS15m

Chain SO:



• Molecule 64: Small ribosomal subunit protein bS16m

Chain SP:

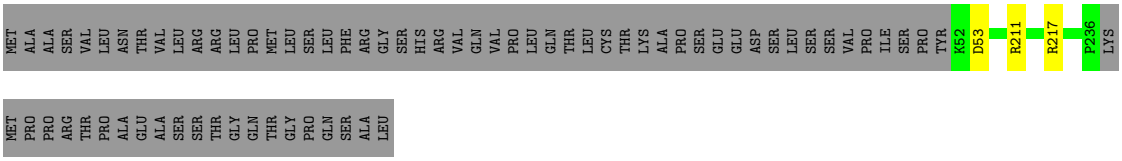


• Molecule 65: Small ribosomal subunit protein uS17m

Chain SQ:

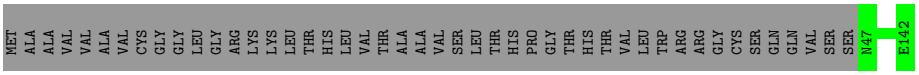
• Molecule 66: Small ribosomal subunit protein mS40

Chain SS:



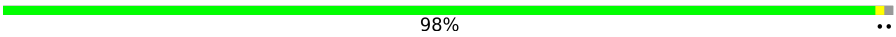
• Molecule 67: Small ribosomal subunit protein bS18m

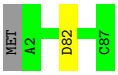
Chain ST:



• Molecule 68: Small ribosomal subunit protein bS21m

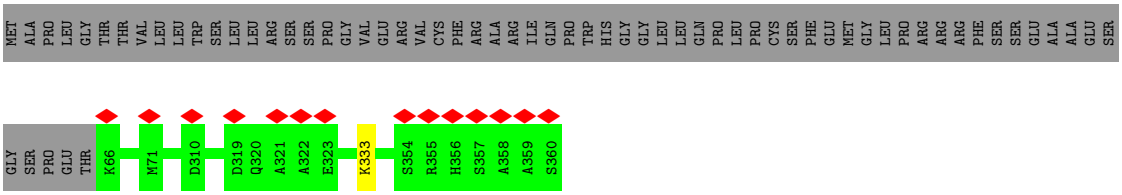
Chain SW:





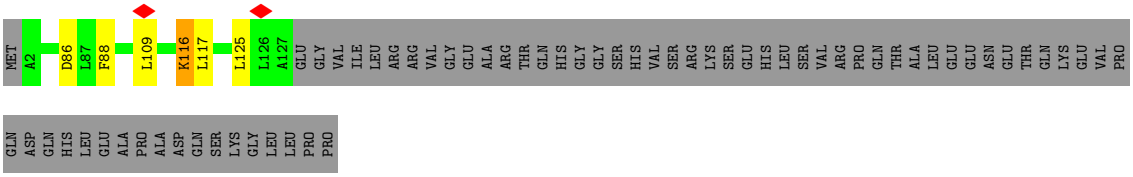
• Molecule 69: Small ribosomal subunit protein mS22

Chain SX:



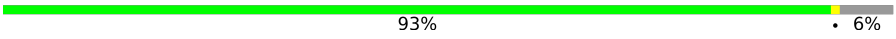
• Molecule 70: Small ribosomal subunit protein mS23

Chain SY:



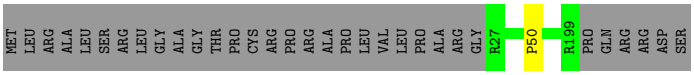
• Molecule 71: Small ribosomal subunit protein mS25

Chain Sa:



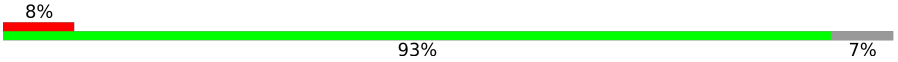
• Molecule 72: Small ribosomal subunit protein mS26

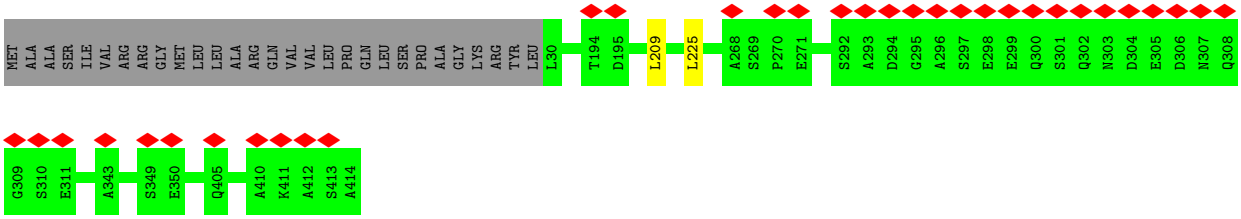
Chain Sb:



• Molecule 73: Small ribosomal subunit protein mS27

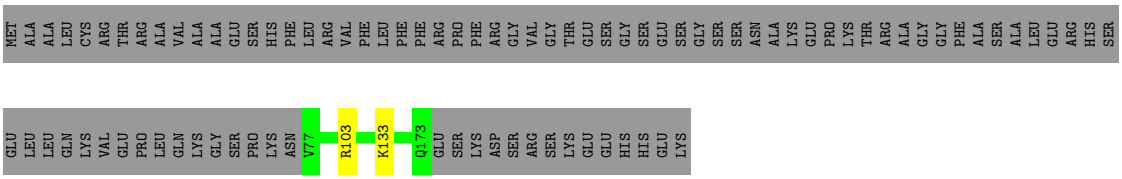
Chain Sc:





• Molecule 74: Small ribosomal subunit protein bS1m

Chain Sd:

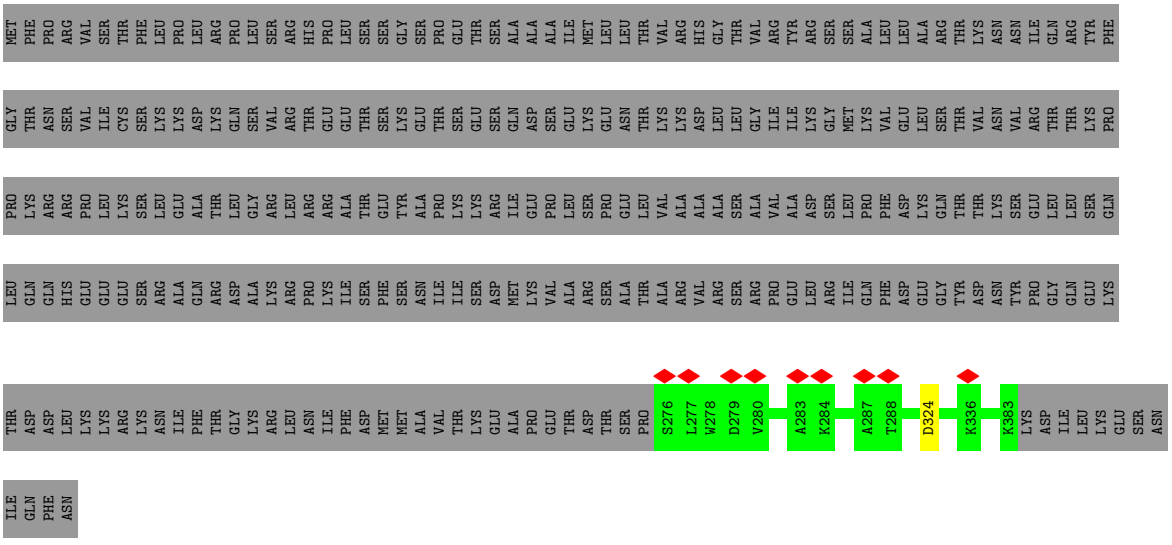


• Molecule 75: Small ribosomal subunit protein mS29

Chain Se:

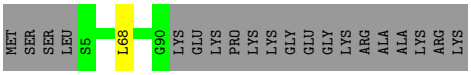
• Molecule 76: Small ribosomal subunit protein mS31

Chain Sg:



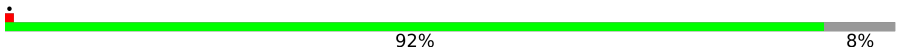
• Molecule 77: Small ribosomal subunit protein mS33

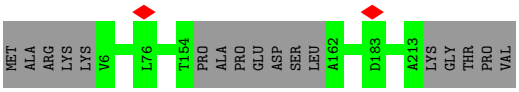
Chain Si:



• Molecule 78: Small ribosomal subunit protein mS34

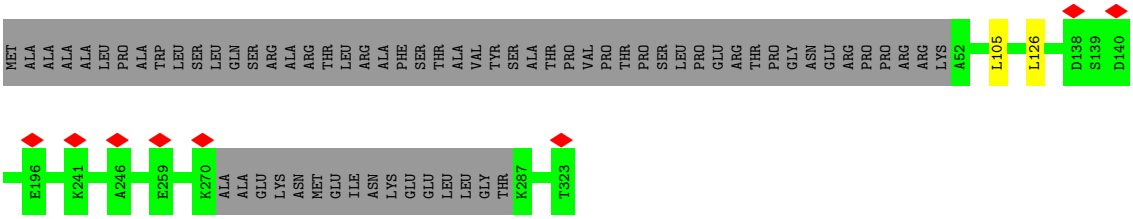
Chain Sj:





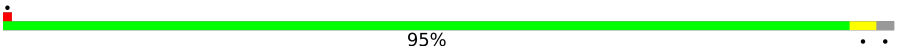
• Molecule 79: Small ribosomal subunit protein mS35

Chain Sk:



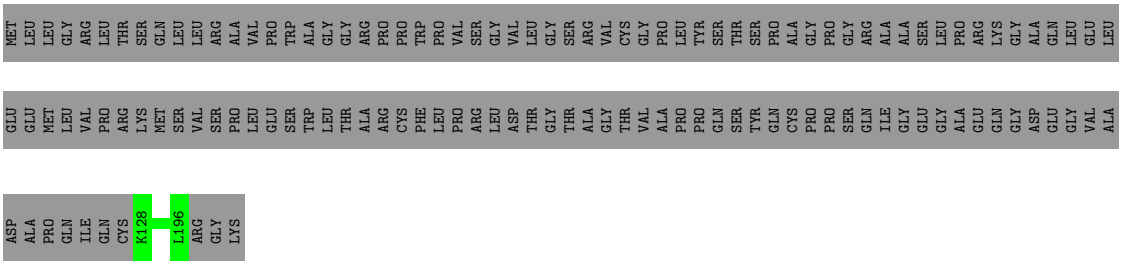
• Molecule 80: Small ribosomal subunit protein mS37

Chain Sm:



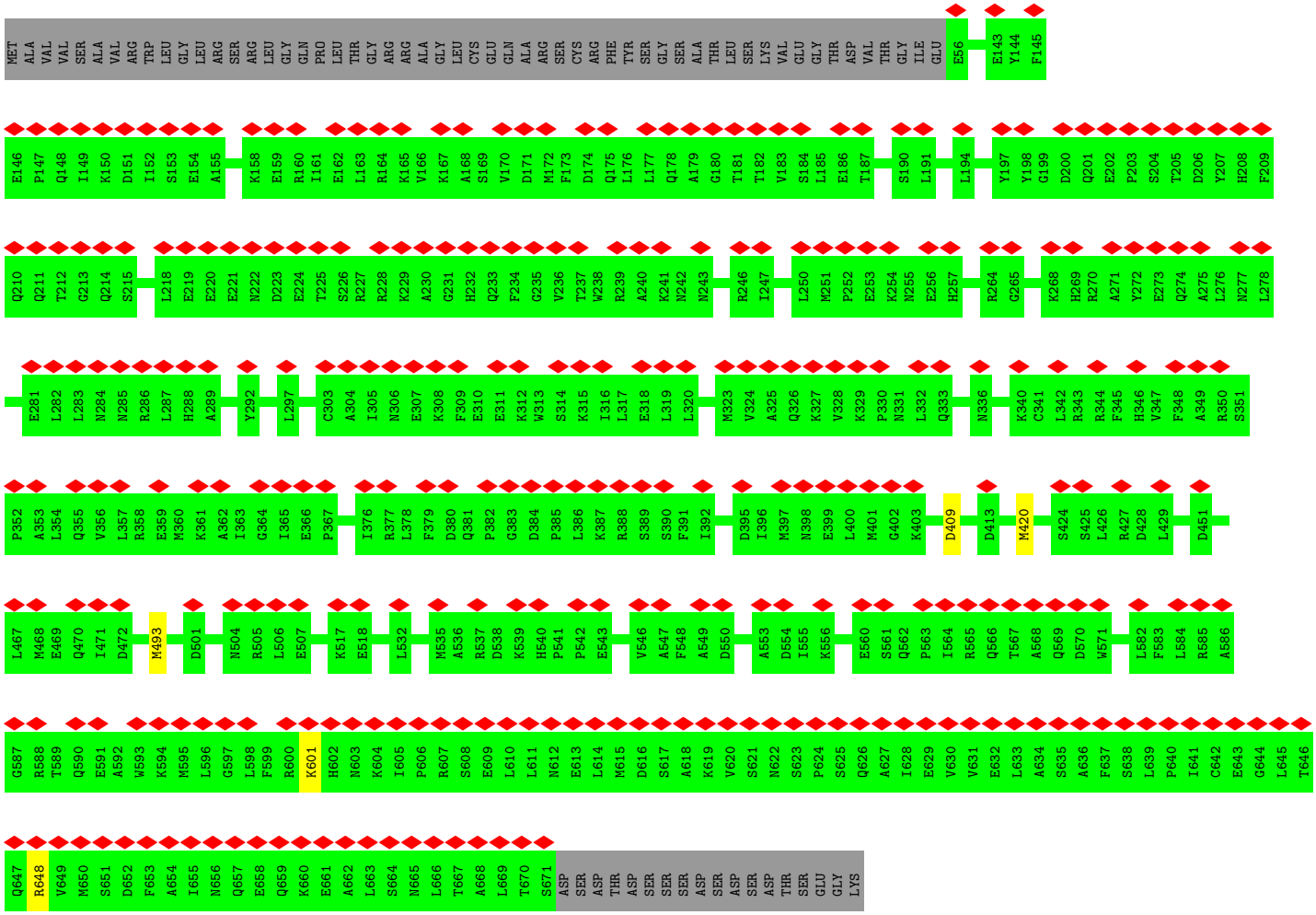
• Molecule 81: Small ribosomal subunit protein mS38

Chain Sn:



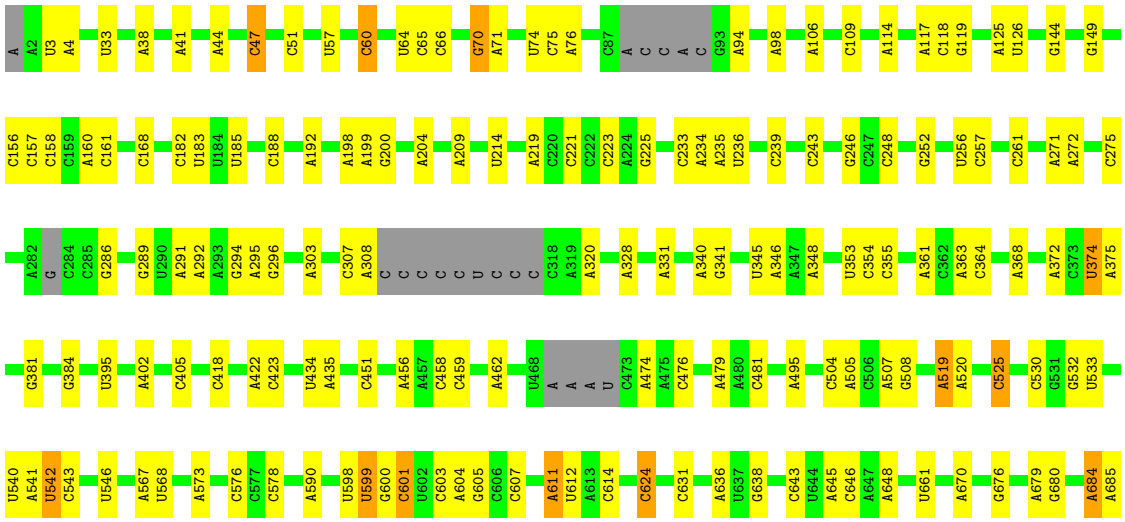
• Molecule 82: Small ribosomal subunit protein mS39

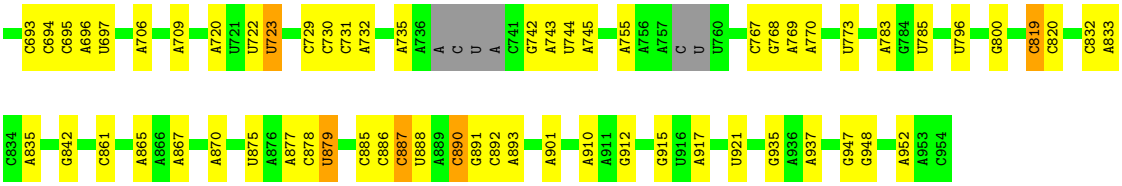
Chain So:



• Molecule 83: 12s rRNA

Chain S1:




C693 C694 C695 A696 U697 A706 A709 A720 U721 U722 U723 C729 C730 C731 A732 A735 A736 A C U A C741 G742 A743 U744 A745 A755 A756 A757 C U U760 C767 G768 A769 A770 U773 A783 G784 U785 U796 G800 C819 C820 C832 A833
C834 A835 G842 C861 A865 A866 A867 A870 U875 A876 A877 C878 U879 C885 C886 C887 U888 A889 C890 G891 C892 A893 A901 A910 A911 G912 G915 U916 A917 U921 G935 A936 A937 G947 G948 A952 A953 C954

4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

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

All (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
40	Lv	179	PRO	CG-CD	-5.54	1.32	1.50
1	L1	859	U	N1-C6	-5.50	1.32	1.38

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	859	U	C5-C6-N1	14.20	129.80	122.70
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
82	So	420	MET	CG-SD-CE	-10.49	83.41	100.20
63	SO	97	MET	CG-SD-CE	-10.04	84.13	100.20
42	Lx	120	MET	CG-SD-CE	-9.87	84.41	100.20
53	SB	135	MET	CG-SD-CE	-9.72	84.65	100.20
70	SY	86	ASP	CB-CG-OD1	9.31	126.68	118.30
83	S1	118	C	C2-N1-C1'	9.21	128.93	118.80
59	SJ	81	LYS	CD-CE-NZ	-9.16	90.63	111.70
1	L1	554	C	N1-C2-O2	9.08	124.35	118.90
49	L7	74	ASP	CB-CG-OD1	9.06	126.46	118.30
1	L1	428	G	O4'-C1'-N9	9.06	115.45	108.20
77	Si	68	LEU	CA-CB-CG	8.81	135.57	115.30
83	S1	248	C	C6-N1-C2	-8.51	116.90	120.30
40	Lv	179	PRO	N-CD-CG	-8.44	90.53	103.20
1	L1	1542	C	C2-N1-C1'	8.43	128.07	118.80
52	Sf	254	ASP	CB-CG-OD1	8.29	125.76	118.30
1	L1	1534	C	N1-C2-O2	8.29	123.87	118.90
57	SG	115	LEU	CA-CB-CG	8.24	134.24	115.30
1	L1	859	U	N3-C4-O4	8.11	125.08	119.40
1	L1	232	C	C2-N1-C1'	8.11	127.72	118.80
19	LW	129	MET	CA-CB-CG	8.03	126.95	113.30
47	L5	74	MET	CB-CG-SD	-7.93	88.62	112.40
1	L1	554	C	C2-N1-C1'	7.83	127.41	118.80
1	L1	232	C	N1-C2-O2	7.81	123.59	118.90
54	SZ	131	LYS	CD-CE-NZ	-7.77	93.84	111.70
1	L1	823	C	C2-N1-C1'	7.76	127.33	118.80
57	SG	205	LEU	CB-CG-CD2	7.71	124.11	111.00
66	SS	53	ASP	CB-CG-OD1	7.71	125.23	118.30
55	SE	144	LEU	CB-CG-CD1	7.67	124.05	111.00
1	L1	887	C	N1-C2-O2	7.61	123.46	118.90
22	Lb	180	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	L1	823	C	N1-C2-O2	7.57	123.44	118.90
1	L1	232	C	N3-C2-O2	-7.56	116.61	121.90
1	L1	853	C	C2-N1-C1'	7.54	127.10	118.80
1	L1	1290	U	N1-C2-O2	7.51	128.06	122.80
70	SY	116	LYS	CD-CE-NZ	-7.44	94.58	111.70
1	L1	1291	C	N1-C2-O2	7.33	123.30	118.90
8	LK	158	ASP	CB-CG-OD1	7.31	124.88	118.30
1	L1	853	C	N1-C2-O2	7.31	123.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	410	U	N3-C2-O2	-7.31	117.08	122.20
1	L1	323	A	C8-N9-C4	-7.31	102.88	105.80
1	L1	824	C	N3-C2-O2	-7.28	116.81	121.90
1	L1	554	C	N3-C2-O2	-7.26	116.82	121.90
1	L1	1542	C	C6-N1-C2	-7.23	117.41	120.30
1	L1	823	C	N3-C2-O2	-7.21	116.85	121.90
83	S1	767	C	N1-C2-O2	7.21	123.23	118.90
83	S1	66	C	N1-C2-O2	7.18	123.21	118.90
20	LX	60	ASP	CB-CG-OD2	-7.16	111.86	118.30
83	S1	693	C	N3-C2-O2	-7.13	116.91	121.90
1	L1	198	G	C5-C6-O6	7.13	132.88	128.60
58	SI	91	MET	CG-SD-CE	-7.10	88.85	100.20
1	L1	1534	C	C2-N1-C1'	7.01	126.51	118.80
57	SG	193	ASP	CB-CG-OD1	7.01	124.61	118.30
80	Sm	52	MET	CA-CB-CG	7.01	125.21	113.30
59	SJ	84	ASP	CB-CG-OD1	6.99	124.59	118.30
1	L1	908	C	N1-C2-O2	6.97	123.08	118.90
1	L1	1542	C	N1-C2-O2	6.96	123.08	118.90
1	L1	430	C	C5-C6-N1	6.95	124.48	121.00
80	Sm	53	MET	CG-SD-CE	-6.92	89.13	100.20
14	LR	136	LEU	CB-CG-CD1	-6.91	99.25	111.00
1	L1	1534	C	C6-N1-C2	-6.90	117.54	120.30
1	L1	323	A	C2-N3-C4	6.89	114.05	110.60
1	L1	1290	U	N3-C2-O2	-6.87	117.39	122.20
1	L1	887	C	C2-N1-C1'	6.85	126.33	118.80
83	S1	60	C	N1-C2-O2	6.84	123.00	118.90
83	S1	118	C	C6-N1-C2	-6.83	117.57	120.30
1	L1	63	C	C2-N1-C1'	6.83	126.31	118.80
83	S1	661	U	C2-N1-C1'	6.79	125.85	117.70
38	Ls	160	LEU	CB-CG-CD2	6.76	122.50	111.00
1	L1	1058	C	C5-C6-N1	6.76	124.38	121.00
31	Ll	183	ASP	CB-CG-OD1	-6.75	112.22	118.30
7	LJ	183	ASP	CB-CG-OD1	6.73	124.36	118.30
83	S1	158	C	O4'-C1'-N1	6.72	113.57	108.20
1	L1	410	U	C2-N1-C1'	6.68	125.71	117.70
83	S1	158	C	C2-N1-C1'	6.64	126.10	118.80
1	L1	59	U	N3-C2-O2	-6.64	117.55	122.20
83	S1	542	U	P-O3'-C3'	6.61	127.63	119.70
83	S1	109	C	O5'-P-OP1	-6.59	99.77	105.70
1	L1	55	C	N1-C2-O2	6.57	122.84	118.90
83	S1	157	C	N3-C2-O2	-6.55	117.32	121.90
8	LK	59	ASP	CB-CG-OD1	-6.52	112.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	SW	82	ASP	CB-CG-OD1	6.52	124.17	118.30
80	Sm	63	ASP	CB-CG-OD1	6.50	124.15	118.30
1	L1	23	C	C2-N1-C1'	6.48	125.92	118.80
1	L1	775	U	C2-N1-C1'	6.47	125.47	117.70
61	SL	43	LYS	CD-CE-NZ	-6.46	96.85	111.70
1	L1	410	U	N1-C2-O2	6.45	127.31	122.80
1	L1	1058	C	C6-N1-C2	-6.44	117.72	120.30
13	LQ	84	ASP	CB-CG-OD1	6.43	124.09	118.30
1	L1	853	C	OP1-P-O3'	6.42	119.31	105.20
1	L1	1534	C	N3-C2-O2	-6.41	117.41	121.90
83	S1	819	C	N1-C2-O2	6.40	122.74	118.90
54	SZ	77	ASP	CB-CG-OD1	6.40	124.06	118.30
1	L1	593	C	N1-C2-O2	6.38	122.73	118.90
59	SJ	126	ILE	CG1-CB-CG2	-6.35	97.43	111.40
1	L1	554	C	C6-N1-C2	-6.30	117.78	120.30
1	L1	1290	U	C2-N1-C1'	6.30	125.26	117.70
83	S1	661	U	N3-C2-O2	-6.29	117.80	122.20
1	L1	1534	C	C5-C6-N1	6.26	124.13	121.00
1	L1	824	C	N1-C2-O2	6.23	122.64	118.90
82	So	409	ASP	CB-CG-OD1	6.22	123.90	118.30
83	S1	374	U	P-O3'-C3'	6.22	127.17	119.70
83	S1	661	U	N1-C2-O2	6.22	127.15	122.80
20	LX	122	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	L1	112	G	C5-C6-N1	6.19	114.60	111.50
1	L1	589	C	N1-C2-O2	6.18	122.61	118.90
83	S1	601	C	N1-C2-O2	6.17	122.60	118.90
1	L1	1291	C	N3-C2-O2	-6.16	117.58	121.90
1	L1	859	U	N3-C4-C5	-6.15	110.91	114.60
83	S1	66	C	C2-N1-C1'	6.08	125.49	118.80
83	S1	118	C	C6-N1-C1'	-6.08	113.50	120.80
83	S1	611	A	P-O3'-C3'	6.07	126.99	119.70
83	S1	451	C	C2-N1-C1'	6.07	125.48	118.80
1	L1	387	C	C2-N1-C1'	6.06	125.46	118.80
83	S1	684	A	P-O3'-C3'	6.04	126.95	119.70
1	L1	593	C	N3-C2-O2	-6.02	117.69	121.90
1	L1	610	C	N1-C2-O2	5.99	122.49	118.90
83	S1	605	G	C5-C6-O6	5.98	132.19	128.60
1	L1	1291	C	C2-N1-C1'	5.98	125.38	118.80
39	Lt	116	LEU	CA-CB-CG	5.97	129.02	115.30
83	S1	519	A	P-O3'-C3'	5.97	126.86	119.70
83	S1	767	C	C2-N1-C1'	5.96	125.35	118.80
7	LJ	166	ARG	CB-CG-CD	5.95	127.07	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	LK	59	ASP	CB-CG-OD2	5.93	123.64	118.30
60	SK	66	ILE	CG1-CB-CG2	-5.93	98.36	111.40
79	Sk	126	LEU	CA-CB-CG	5.93	128.93	115.30
83	S1	70	G	P-O3'-C3'	5.92	126.81	119.70
59	SJ	148	LEU	CB-CG-CD2	-5.91	100.96	111.00
83	S1	767	C	N3-C2-O2	-5.90	117.77	121.90
1	L1	1542	C	N3-C2-O2	-5.90	117.77	121.90
83	S1	239	C	C2-N1-C1'	5.89	125.28	118.80
7	LJ	60	ILE	CG1-CB-CG2	-5.89	98.44	111.40
83	S1	723	U	N3-C2-O2	-5.88	118.08	122.20
83	S1	832	C	C2-N1-C1'	5.88	125.26	118.80
1	L1	929	U	P-O3'-C3'	5.87	126.75	119.70
1	L1	232	C	C6-N1-C1'	-5.86	113.77	120.80
1	L1	1542	C	C5-C6-N1	5.85	123.93	121.00
1	L1	55	C	N3-C2-O2	-5.84	117.81	121.90
1	L1	1403	C	C6-N1-C2	-5.84	117.97	120.30
74	Sd	133	LYS	CD-CE-NZ	5.81	125.06	111.70
46	L4	56	LEU	CA-CB-CG	5.80	128.65	115.30
1	L1	198	G	N1-C6-O6	-5.80	116.42	119.90
45	L3	10	LEU	CA-CB-CG	5.80	128.63	115.30
70	SY	117	LEU	CB-CG-CD2	5.78	120.83	111.00
1	L1	63	C	N1-C2-O2	5.78	122.37	118.90
1	L1	838	C	C6-N1-C2	-5.78	117.99	120.30
50	L8	128	MET	CB-CG-SD	-5.78	95.08	112.40
1	L1	775	U	N1-C2-O2	5.77	126.84	122.80
79	Sk	105	LEU	CB-CG-CD2	-5.76	101.20	111.00
83	S1	887	C	N3-C2-O2	-5.76	117.87	121.90
1	L1	55	C	C2-N1-C1'	5.76	125.14	118.80
1	L1	551	C	OP1-P-O3'	5.74	117.82	105.20
54	SZ	76	LEU	CA-CB-CG	5.73	128.48	115.30
83	S1	605	G	N1-C6-O6	-5.73	116.46	119.90
62	SN	54	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	L1	775	U	N3-C2-O2	-5.72	118.19	122.20
70	SY	125	LEU	CA-CB-CG	5.72	128.46	115.30
1	L1	610	C	C2-N1-C1'	5.72	125.09	118.80
1	L1	889	U	P-O3'-C3'	5.71	126.55	119.70
1	L1	593	C	C2-N1-C1'	5.71	125.08	118.80
83	S1	157	C	C6-N1-C2	-5.71	118.02	120.30
30	Lk	395	ARG	CG-CD-NE	5.70	123.77	111.80
1	L1	265	A	O4'-C1'-N9	5.69	112.75	108.20
1	L1	887	C	N3-C2-O2	-5.65	117.94	121.90
1	L1	1014	C	N1-C2-O2	5.65	122.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	610	C	N3-C2-O2	-5.64	117.95	121.90
1	L1	56	C	C6-N1-C2	-5.63	118.05	120.30
83	S1	694	C	C2-N1-C1'	-5.63	112.61	118.80
1	L1	31	U	N3-C2-O2	-5.62	118.27	122.20
83	S1	875	U	N3-C2-O2	-5.61	118.27	122.20
35	Lp	93	LYS	CA-CB-CG	5.61	125.74	113.40
1	L1	582	C	C2-N1-C1'	5.59	124.95	118.80
1	L1	859	U	N1-C2-O2	-5.59	118.89	122.80
1	L1	24	U	N1-C2-O2	5.59	126.71	122.80
83	S1	60	C	C2-N1-C1'	5.58	124.94	118.80
83	S1	158	C	N1-C2-O2	5.58	122.25	118.90
83	S1	542	U	OP1-P-O3'	5.58	117.48	105.20
1	L1	1532	U	C5-C6-N1	5.57	125.49	122.70
1	L1	908	C	N3-C2-O2	-5.57	118.00	121.90
83	S1	525	C	C2-N1-C1'	5.57	124.92	118.80
83	S1	694	C	C6-N1-C1'	5.56	127.47	120.80
1	L1	417	U	C5-C6-N1	5.55	125.48	122.70
1	L1	23	C	N1-C2-O2	5.55	122.23	118.90
1	L1	323	A	N1-C6-N6	-5.55	115.27	118.60
1	L1	853	C	N3-C2-O2	-5.54	118.02	121.90
23	Lu	132	LEU	CA-CB-CG	-5.54	102.56	115.30
1	L1	44	C	N1-C2-O2	5.54	122.22	118.90
83	S1	601	C	C2-N1-C1'	5.53	124.88	118.80
1	L1	628	A	C5-C6-N6	-5.53	119.28	123.70
83	S1	60	C	N3-C2-O2	-5.52	118.03	121.90
83	S1	722	U	C2-N1-C1'	5.52	124.32	117.70
83	S1	156	C	N1-C2-O2	5.49	122.19	118.90
20	LX	45	VAL	CG1-CB-CG2	-5.47	102.15	110.90
76	Sg	324	ASP	CB-CG-OD1	5.47	123.22	118.30
83	S1	248	C	C5-C6-N1	5.46	123.73	121.00
83	S1	832	C	C6-N1-C2	-5.46	118.12	120.30
22	Lb	180	ASP	CB-CG-OD1	5.46	123.21	118.30
1	L1	323	A	N3-C4-C5	-5.45	122.98	126.80
83	S1	890	C	P-O3'-C3'	5.45	126.24	119.70
1	L1	63	C	C6-N1-C2	-5.45	118.12	120.30
1	L1	23	C	C6-N1-C2	-5.45	118.12	120.30
7	LJ	164	MET	CG-SD-CE	-5.44	91.49	100.20
1	L1	545	C	N1-C2-O2	5.42	122.15	118.90
23	Lu	132	LEU	CB-CG-CD2	5.41	120.19	111.00
1	L1	1017	C	C6-N1-C2	-5.40	118.14	120.30
70	SY	109	LEU	CA-CB-CG	5.40	127.72	115.30
83	S1	158	C	C6-N1-C1'	-5.39	114.33	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	LJ	123	MET	CB-CG-SD	5.39	128.56	112.40
1	L1	551	C	P-O3'-C3'	5.38	126.16	119.70
1	L1	823	C	C6-N1-C1'	-5.38	114.34	120.80
64	SP	103	MET	CG-SD-CE	-5.38	91.59	100.20
30	Lk	140	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	L1	170	C	C5-C6-N1	5.37	123.69	121.00
1	L1	853	C	C6-N1-C1'	-5.37	114.36	120.80
1	L1	545	C	C2-N1-C1'	5.37	124.70	118.80
1	L1	860	A	P-O3'-C3'	5.37	126.14	119.70
83	S1	294	G	N3-C4-N9	-5.37	122.78	126.00
83	S1	66	C	N3-C2-O2	-5.36	118.15	121.90
83	S1	693	C	N1-C2-O2	5.36	122.11	118.90
31	Ll	336	ASP	CB-CG-OD1	5.35	123.11	118.30
83	S1	47	C	N3-C2-O2	-5.34	118.16	121.90
1	L1	1558	U	N3-C2-O2	-5.33	118.47	122.20
1	L1	59	U	N1-C2-O2	5.32	126.53	122.80
73	Sc	225	LEU	CA-CB-CG	5.32	127.53	115.30
38	Ls	202	MET	CA-CB-CG	5.31	122.32	113.30
1	L1	628	A	N1-C6-N6	5.29	121.78	118.60
75	Se	397	TYR	CB-CG-CD1	-5.29	117.83	121.00
83	S1	879	U	C2-N1-C1'	5.28	124.03	117.70
1	L1	996	U	N3-C2-O2	-5.25	118.52	122.20
1	L1	1542	C	C6-N1-C1'	-5.25	114.50	120.80
70	SY	86	ASP	CB-CG-OD2	-5.25	113.58	118.30
83	S1	505	A	C4-N9-C1'	5.25	135.74	126.30
1	L1	248	G	N3-C4-N9	5.24	129.14	126.00
1	L1	288	G	O4'-C1'-N9	5.23	112.39	108.20
1	L1	582	C	C5-C6-N1	5.22	123.61	121.00
83	S1	601	C	N3-C2-O2	-5.21	118.25	121.90
1	L1	554	C	C5-C6-N1	5.20	123.60	121.00
83	S1	624	C	C2-N1-C1'	5.20	124.52	118.80
1	L1	747	C	C2-N1-C1'	5.19	124.51	118.80
1	L1	23	C	C5-C6-N1	5.18	123.59	121.00
1	L1	887	C	C6-N1-C1'	-5.18	114.59	120.80
1	L1	1291	C	C6-N1-C2	-5.17	118.23	120.30
83	S1	374	U	N3-C2-O2	-5.16	118.59	122.20
83	S1	820	C	N1-C2-O2	5.16	121.99	118.90
1	L1	819	C	C6-N1-C2	-5.15	118.24	120.30
1	L1	746	U	C4-C5-C6	5.15	122.79	119.70
1	L1	610	C	C6-N1-C2	-5.15	118.24	120.30
1	L1	628	A	N9-C4-C5	-5.14	103.74	105.80
83	S1	722	U	N1-C2-O2	5.14	126.40	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	SB	158	MET	CA-CB-CG	5.13	122.03	113.30
83	S1	796	U	C2-N1-C1'	5.13	123.86	117.70
1	L1	1014	C	C2-N1-C1'	5.13	124.44	118.80
83	S1	599	U	P-O3'-C3'	5.13	125.85	119.70
1	L1	641	U	N3-C2-O2	-5.12	118.61	122.20
53	SB	67	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	L1	323	A	C4-N9-C1'	5.11	135.49	126.30
83	S1	530	C	C2-N1-C1'	5.11	124.42	118.80
1	L1	55	C	C6-N1-C2	-5.10	118.26	120.30
1	L1	924	U	N1-C2-O2	5.10	126.37	122.80
83	S1	118	C	C5-C6-N1	5.09	123.55	121.00
83	S1	294	G	C4-N9-C1'	-5.08	119.89	126.50
1	L1	575	A	P-O3'-C3'	5.07	125.78	119.70
1	L1	1542	C	O4'-C1'-N1	5.07	112.25	108.20
22	Lb	238	LEU	CA-CB-CG	5.07	126.95	115.30
1	L1	1058	C	C2-N1-C1'	5.06	124.37	118.80
17	LU	121	ASP	CB-CG-OD1	5.06	122.86	118.30
83	S1	887	C	N1-C2-O2	5.06	121.94	118.90
1	L1	323	A	N7-C8-N9	5.05	116.33	113.80
1	L1	923	G	O4'-C1'-N9	5.05	112.24	108.20
55	SE	137	TYR	CA-CB-CG	5.05	122.99	113.40
83	S1	530	C	C6-N1-C2	-5.03	118.29	120.30
1	L1	143	C	C6-N1-C2	-5.02	118.29	120.30
7	LJ	182	ASP	CB-CG-OD1	5.02	122.81	118.30
75	Se	397	TYR	CA-CB-CG	-5.02	103.87	113.40
1	L1	466	C	C2-N1-C1'	5.01	124.31	118.80
1	L1	823	C	C6-N1-C2	-5.01	118.30	120.30
83	S1	861	C	N1-C2-O2	5.01	121.91	118.90
73	Sc	209	LEU	CB-CG-CD1	-5.00	102.49	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	L4	106	THR	Peptide
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
33	Ln	101	ARG	Sidechain
33	Ln	99	ARG	Sidechain

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Mol	Chain	Res	Type	Group
39	Lt	269	LEU	Peptide
42	Lx	95	ARG	Sidechain
59	SJ	169	ALA	Peptide
63	SO	137	ARG	Sidechain
74	Sd	103	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LB	235/305 (77%)	228 (97%)	6 (3%)	1 (0%)	34	69
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
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%)	22	61
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	67
40	Lv	125/212 (59%)	121 (97%)	4 (3%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	29	67
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%)	8	39
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
72	Sb	171/205 (83%)	167 (98%)	3 (2%)	1 (1%)	25	64
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	54	83

All (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
13	LQ	111	PRO
72	Sb	50	PRO
3	LB	207	ILE

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%)	88	95
6	LI	86/228 (38%)	86 (100%)	0	100	100
7	LJ	145/232 (62%)	145 (100%)	0	100	100
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%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	88	95
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%)	73	88
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%)	91	95
33	Ln	91/190 (48%)	90 (99%)	1 (1%)	73	88
34	Lo	104/112 (93%)	103 (99%)	1 (1%)	76	90
35	Lp	93/133 (70%)	91 (98%)	2 (2%)	52	79
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
39	Lt	188/236 (80%)	187 (100%)	1 (0%)	88	95
40	Lv	116/188 (62%)	115 (99%)	1 (1%)	78	91
41	Lw	122/148 (82%)	122 (100%)	0	100	100
42	Lx	104/148 (70%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	78	91
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%)	92	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%)	91	95
59	SJ	112/180 (62%)	111 (99%)	1 (1%)	78	91
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%)	73	88
63	SO	152/226 (67%)	152 (100%)	0	100	100
64	SP	95/113 (84%)	94 (99%)	1 (1%)	73	88
65	SQ	93/115 (81%)	93 (100%)	0	100	100
66	SS	166/230 (72%)	164 (99%)	2 (1%)	71	88
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%)	91	95
70	SY	109/164 (66%)	108 (99%)	1 (1%)	78	91
71	Sa	150/157 (96%)	149 (99%)	1 (1%)	84	94
72	Sb	148/174 (85%)	148 (100%)	0	100	100
73	Sc	338/364 (93%)	338 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
74	Sd	84/158 (53%)	84 (100%)	0	100 100
75	Se	310/351 (88%)	309 (100%)	1 (0%)	92 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%)	76 90
81	Sn	63/166 (38%)	63 (100%)	0	100 100
82	So	548/609 (90%)	546 (100%)	2 (0%)	91 95
All	All	12121/15564 (78%)	12095 (100%)	26 (0%)	93 98

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LD	236	ARG
11	LO	11	ARG
15	LS	96	ARG
28	Li	124	ARG
32	Lm	61	ARG
33	Ln	97	LYS
34	Lo	116	LYS
35	Lp	99	LYS
35	Lp	122	ARG
39	Lt	132	LYS
40	Lv	78	ARG
49	L7	82	ARG
52	Sf	203	ARG
58	SI	198	ARG
59	SJ	75	ARG
62	SN	33	ARG
64	SP	116	ARG
66	SS	211	ARG
66	SS	217	ARG
69	SX	333	LYS
70	SY	116	LYS
71	Sa	137	ARG
75	Se	370	LYS
80	Sm	37	ARG
82	So	601	LYS

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Mol	Chain	Res	Type
82	So	648	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
4	LC	202	GLN
6	LI	100	GLN
14	LR	96	GLN
17	LU	118	ASN
22	Lb	240	GLN
22	Lb	241	GLN
30	Lk	191	GLN
31	Ll	275	GLN
32	Lm	69	HIS
40	Lv	175	GLN
46	L4	76	ASN
52	Sf	96	GLN
53	SB	265	GLN
54	SZ	75	ASN
56	SF	81	HIS
59	SJ	83	HIS
59	SJ	179	GLN
60	SK	129	GLN
62	SN	117	HIS
66	SS	125	GLN
69	SX	299	ASN
73	Sc	388	GLN
73	Sc	391	GLN
75	Se	143	HIS
76	Sg	303	GLN

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%)

All (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
1	L1	20	C
1	L1	23	C
1	L1	24	U
1	L1	29	C
1	L1	30	U
1	L1	31	U
1	L1	34	U
1	L1	38	A
1	L1	39	G
1	L1	41	C
1	L1	44	C
1	L1	45	C
1	L1	46	U
1	L1	47	U
1	L1	54	A
1	L1	57	A
1	L1	58	U
1	L1	66	A
1	L1	67	A
1	L1	78	G
1	L1	91	A
1	L1	100	G
1	L1	101	C
1	L1	103	A
1	L1	104	U
1	L1	110	U
1	L1	111	A
1	L1	121	G
1	L1	124	A
1	L1	127	G
1	L1	134	A
1	L1	135	A
1	L1	137	U
1	L1	138	A
1	L1	139	U
1	L1	147	C
1	L1	153	A
1	L1	157	C

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Mol	Chain	Res	Type
1	L1	158	A
1	L1	159	A
1	L1	162	A
1	L1	166	A
1	L1	167	C
1	L1	174	A
1	L1	179	C
1	L1	184	U
1	L1	186	A
1	L1	189	A
1	L1	197	A
1	L1	198	G
1	L1	199	A
1	L1	200	A
1	L1	201	A
1	L1	203	A
1	L1	208	U
1	L1	212	A
1	L1	213	G
1	L1	215	A
1	L1	217	A
1	L1	220	C
1	L1	223	A
1	L1	232	C
1	L1	233	C
1	L1	248	G
1	L1	266	A
1	L1	267	A
1	L1	270	A
1	L1	274	C
1	L1	298	G
1	L1	302	A
1	L1	304	A
1	L1	305	U
1	L1	315	G
1	L1	317	G
1	L1	322	C
1	L1	323	A
1	L1	324	A
1	L1	330	C
1	L1	331	C
1	L1	332	G

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Mol	Chain	Res	Type
1	L1	342	A
1	L1	345	G
1	L1	346	C
1	L1	351	U
1	L1	352	G
1	L1	359	A
1	L1	361	A
1	L1	362	G
1	L1	364	A
1	L1	366	C
1	L1	367	U
1	L1	369	A
1	L1	375	A
1	L1	383	U
1	L1	385	U
1	L1	390	A
1	L1	395	A
1	L1	404	A
1	L1	413	U
1	L1	415	A
1	L1	423	U
1	L1	427	A
1	L1	429	U
1	L1	443	G
1	L1	454	A
1	L1	455	C
1	L1	456	U
1	L1	463	A
1	L1	464	A
1	L1	465	A
1	L1	466	C
1	L1	471	U
1	L1	472	A
1	L1	477	G
1	L1	489	U
1	L1	493	A
1	L1	496	C
1	L1	498	U
1	L1	501	U
1	L1	503	G
1	L1	507	U
1	L1	510	A

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Mol	Chain	Res	Type
1	L1	511	A
1	L1	512	G
1	L1	519	C
1	L1	522	A
1	L1	526	A
1	L1	527	G
1	L1	528	A
1	L1	530	A
1	L1	537	A
1	L1	540	C
1	L1	545	C
1	L1	550	A
1	L1	551	C
1	L1	552	U
1	L1	553	A
1	L1	555	C
1	L1	557	A
1	L1	558	A
1	L1	563	U
1	L1	565	C
1	L1	567	A
1	L1	569	A
1	L1	571	A
1	L1	572	U
1	L1	573	A
1	L1	575	A
1	L1	576	A
1	L1	582	C
1	L1	592	C
1	L1	593	C
1	L1	614	C
1	L1	615	U
1	L1	620	A
1	L1	627	A
1	L1	629	U
1	L1	630	G
1	L1	652	C
1	L1	653	A
1	L1	654	U
1	L1	662	C
1	L1	672	U
1	L1	675	G

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Mol	Chain	Res	Type
1	L1	694	C
1	L1	699	A
1	L1	700	A
1	L1	701	U
1	L1	704	A
1	L1	711	A
1	L1	720	A
1	L1	723	C
1	L1	724	A
1	L1	730	C
1	L1	731	A
1	L1	737	U
1	L1	744	C
1	L1	745	C
1	L1	746	U
1	L1	756	C
1	L1	757	C
1	L1	762	A
1	L1	773	C
1	L1	774	A
1	L1	775	U
1	L1	777	A
1	L1	779	G
1	L1	794	G
1	L1	808	G
1	L1	809	C
1	L1	819	C
1	L1	823	C
1	L1	830	A
1	L1	832	C
1	L1	834	A
1	L1	836	A
1	L1	837	A
1	L1	838	C
1	L1	841	C
1	L1	842	A
1	L1	850	C
1	L1	851	A
1	L1	853	C
1	L1	854	A
1	L1	857	A
1	L1	860	A

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Mol	Chain	Res	Type
1	L1	861	U
1	L1	870	C
1	L1	874	C
1	L1	887	C
1	L1	888	A
1	L1	889	U
1	L1	890	G
1	L1	900	C
1	L1	904	G
1	L1	907	C
1	L1	911	A
1	L1	912	A
1	L1	913	C
1	L1	922	G
1	L1	923	G
1	L1	924	U
1	L1	926	G
1	L1	929	U
1	L1	930	A
1	L1	931	A
1	L1	933	C
1	L1	936	U
1	L1	948	U
1	L1	956	U
1	L1	958	U
1	L1	960	U
1	L1	962	A
1	L1	963	A
1	L1	964	U
1	L1	965	G
1	L1	975	G
1	L1	984	U
1	L1	985	G
1	L1	986	U
1	L1	990	U
1	L1	1013	C
1	L1	1014	C
1	L1	1016	G
1	L1	1024	A
1	L1	1026	A
1	L1	1028	G
1	L1	1032	G

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Mol	Chain	Res	Type
1	L1	1036	A
1	L1	1039	A
1	L1	1048	C
1	L1	1049	G
1	L1	1053	A
1	L1	1054	G
1	L1	1055	A
1	L1	1056	C
1	L1	1062	G
1	L1	1069	U
1	L1	1073	U
1	L1	1075	A
1	L1	1087	A
1	L1	1088	G
1	L1	1140	G
1	L1	1161	G
1	L1	1162	A
1	L1	1163	A
1	L1	1172	C
1	L1	1177	C
1	L1	1184	U
1	L1	1185	G
1	L1	1191	A
1	L1	1194	U
1	L1	1195	C
1	L1	1222	A
1	L1	1223	A
1	L1	1225	U
1	L1	1226	G
1	L1	1236	C
1	L1	1240	A
1	L1	1241	C
1	L1	1242	C
1	L1	1243	A
1	L1	1246	G
1	L1	1247	G
1	L1	1248	A
1	L1	1249	A
1	L1	1252	A
1	L1	1256	A
1	L1	1257	C
1	L1	1258	C

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Mol	Chain	Res	Type
1	L1	1262	G
1	L1	1265	A
1	L1	1286	A
1	L1	1292	C
1	L1	1293	A
1	L1	1301	A
1	L1	1305	G
1	L1	1308	U
1	L1	1309	U
1	L1	1311	A
1	L1	1315	C
1	L1	1319	G
1	L1	1320	A
1	L1	1322	G
1	L1	1323	U
1	L1	1324	U
1	L1	1335	A
1	L1	1337	C
1	L1	1346	G
1	L1	1351	C
1	L1	1352	G
1	L1	1371	U
1	L1	1372	U
1	L1	1383	A
1	L1	1384	G
1	L1	1386	C
1	L1	1389	A
1	L1	1390	C
1	L1	1391	G
1	L1	1393	G
1	L1	1399	A
1	L1	1416	U
1	L1	1419	A
1	L1	1426	U
1	L1	1430	U
1	L1	1438	U
1	L1	1439	U
1	L1	1442	A
1	L1	1444	U
1	L1	1452	U
1	L1	1461	G
1	L1	1480	U

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Mol	Chain	Res	Type
1	L1	1485	C
1	L1	1487	C
1	L1	1488	A
1	L1	1490	A
1	L1	1492	C
1	L1	1498	C
1	L1	1499	C
1	L1	1502	C
1	L1	1504	U
1	L1	1506	A
1	L1	1510	A
1	L1	1513	U
1	L1	1520	A
1	L1	1522	C
1	L1	1537	A
1	L1	1539	A
1	L1	1540	C
1	L1	1542	C
1	L1	1547	A
1	L1	1548	A
1	L1	1558	U
2	L2	4	A
2	L2	7	G
2	L2	9	A
2	L2	10	G
2	L2	12	U
2	L2	13	U
2	L2	14	A
2	L2	39	A
2	L2	40	G
2	L2	43	G
2	L2	49	A
2	L2	50	A
2	L2	68	G
2	L2	69	A
83	S1	3	U
83	S1	4	A
83	S1	33	U
83	S1	38	A
83	S1	41	A
83	S1	44	A
83	S1	47	C

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Mol	Chain	Res	Type
83	S1	51	C
83	S1	57	U
83	S1	60	C
83	S1	64	U
83	S1	65	C
83	S1	71	A
83	S1	74	U
83	S1	75	C
83	S1	76	A
83	S1	94	A
83	S1	98	A
83	S1	106	A
83	S1	114	A
83	S1	117	A
83	S1	119	G
83	S1	125	A
83	S1	126	U
83	S1	144	G
83	S1	149	G
83	S1	160	A
83	S1	161	C
83	S1	168	C
83	S1	182	C
83	S1	183	U
83	S1	185	U
83	S1	188	C
83	S1	192	A
83	S1	198	A
83	S1	199	A
83	S1	200	G
83	S1	204	A
83	S1	209	A
83	S1	214	U
83	S1	219	A
83	S1	221	C
83	S1	223	C
83	S1	225	G
83	S1	233	C
83	S1	234	A
83	S1	235	A
83	S1	236	U
83	S1	243	C

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Mol	Chain	Res	Type
83	S1	246	G
83	S1	252	G
83	S1	256	U
83	S1	257	C
83	S1	261	C
83	S1	271	A
83	S1	272	A
83	S1	275	C
83	S1	286	G
83	S1	289	G
83	S1	291	A
83	S1	292	A
83	S1	295	A
83	S1	296	G
83	S1	303	A
83	S1	307	C
83	S1	308	A
83	S1	320	A
83	S1	328	A
83	S1	331	A
83	S1	340	A
83	S1	341	G
83	S1	345	U
83	S1	346	A
83	S1	348	A
83	S1	353	U
83	S1	354	C
83	S1	355	C
83	S1	361	A
83	S1	363	A
83	S1	364	C
83	S1	368	A
83	S1	372	A
83	S1	375	A
83	S1	381	G
83	S1	384	G
83	S1	395	U
83	S1	402	A
83	S1	405	C
83	S1	418	C
83	S1	422	A
83	S1	423	C

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Mol	Chain	Res	Type
83	S1	434	U
83	S1	435	A
83	S1	456	A
83	S1	458	C
83	S1	459	C
83	S1	462	A
83	S1	474	A
83	S1	476	C
83	S1	479	A
83	S1	481	C
83	S1	495	A
83	S1	504	C
83	S1	507	A
83	S1	508	G
83	S1	519	A
83	S1	520	A
83	S1	525	C
83	S1	532	G
83	S1	533	U
83	S1	540	U
83	S1	541	A
83	S1	542	U
83	S1	543	C
83	S1	546	U
83	S1	567	A
83	S1	568	U
83	S1	573	A
83	S1	576	C
83	S1	578	C
83	S1	590	A
83	S1	598	U
83	S1	599	U
83	S1	600	G
83	S1	601	C
83	S1	603	C
83	S1	604	A
83	S1	607	C
83	S1	612	U
83	S1	614	C
83	S1	624	C
83	S1	631	C
83	S1	636	A

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Mol	Chain	Res	Type
83	S1	638	G
83	S1	643	C
83	S1	645	A
83	S1	646	C
83	S1	648	A
83	S1	670	A
83	S1	676	G
83	S1	679	A
83	S1	680	G
83	S1	685	A
83	S1	695	C
83	S1	696	A
83	S1	697	U
83	S1	706	A
83	S1	709	A
83	S1	720	A
83	S1	723	U
83	S1	729	C
83	S1	730	C
83	S1	731	C
83	S1	732	A
83	S1	735	A
83	S1	742	G
83	S1	743	A
83	S1	744	U
83	S1	745	A
83	S1	755	A
83	S1	768	G
83	S1	769	A
83	S1	770	A
83	S1	773	U
83	S1	783	A
83	S1	785	U
83	S1	800	G
83	S1	819	C
83	S1	833	A
83	S1	835	A
83	S1	842	G
83	S1	865	A
83	S1	867	A
83	S1	870	A
83	S1	877	A

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Mol	Chain	Res	Type
83	S1	878	C
83	S1	879	U
83	S1	885	C
83	S1	886	C
83	S1	888	U
83	S1	890	C
83	S1	891	G
83	S1	892	C
83	S1	893	A
83	S1	901	A
83	S1	910	A
83	S1	912	G
83	S1	915	G
83	S1	917	A
83	S1	921	U
83	S1	935	G
83	S1	937	A
83	S1	947	G
83	S1	948	G
83	S1	952	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	33	C
1	L1	304	A
1	L1	324	A
1	L1	551	C
1	L1	575	A
1	L1	837	A
1	L1	853	C
1	L1	860	A
1	L1	889	U
1	L1	929	U
1	L1	1235	A
1	L1	1319	G
1	L1	1371	U
83	S1	70	G
83	S1	374	U
83	S1	519	A
83	S1	542	U
83	S1	599	U

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Mol	Chain	Res	Type
83	S1	611	A
83	S1	684	A
83	S1	768	G
83	S1	887	C
83	S1	890	C

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
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%)
87	GDP	Se	500	-	24,30,30	0.93	1 (4%)	30,47,47	1.37	5 (16%)

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	1708	84	-	15/22/80/80	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
87	GDP	Se	500	-	-	1/12/32/32	0/3/3/3

All (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
87	Se	500	GDP	C6-N1	-2.50	1.34	1.37
85	S1	1034	T1C	C4-N4	2.26	1.52	1.47
85	L1	1708	T1C	C4-N4	2.23	1.52	1.47
85	L1	1708	T1C	O11-C11	2.23	1.27	1.23
85	L1	1707	T1C	O11-C11	2.18	1.27	1.23
85	L1	1707	T1C	C7-N7	2.14	1.48	1.42
85	S1	1034	T1C	O11-C11	2.10	1.27	1.23
85	L1	1708	T1C	C7-N7	2.09	1.48	1.42
85	S1	1034	T1C	C2-C1	-2.05	1.40	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
85	L1	1707	T1C	C1-C1C-C12	3.06	113.47	109.88
85	S1	1034	T1C	C41-C1C-C1	-2.59	108.08	111.05
87	Se	500	GDP	C5-C6-N1	2.53	118.41	113.95
85	S1	1034	T1C	C51-C5-C41	-2.46	106.17	110.49
85	L1	1707	T1C	C11-C1B-C12	2.44	120.73	118.80
87	Se	500	GDP	C8-N7-C5	2.24	107.25	102.99
87	Se	500	GDP	O6-C6-C5	-2.22	120.04	124.37
85	L1	1707	T1C	C1C-C1-C2	2.21	119.26	115.75
85	L1	1708	T1C	C11-C1B-C12	2.08	120.44	118.80
85	S1	1034	T1C	C1C-C12-C1B	-2.05	120.98	123.06

There are no chirality outliers.

All (42) torsion outliers are listed below:

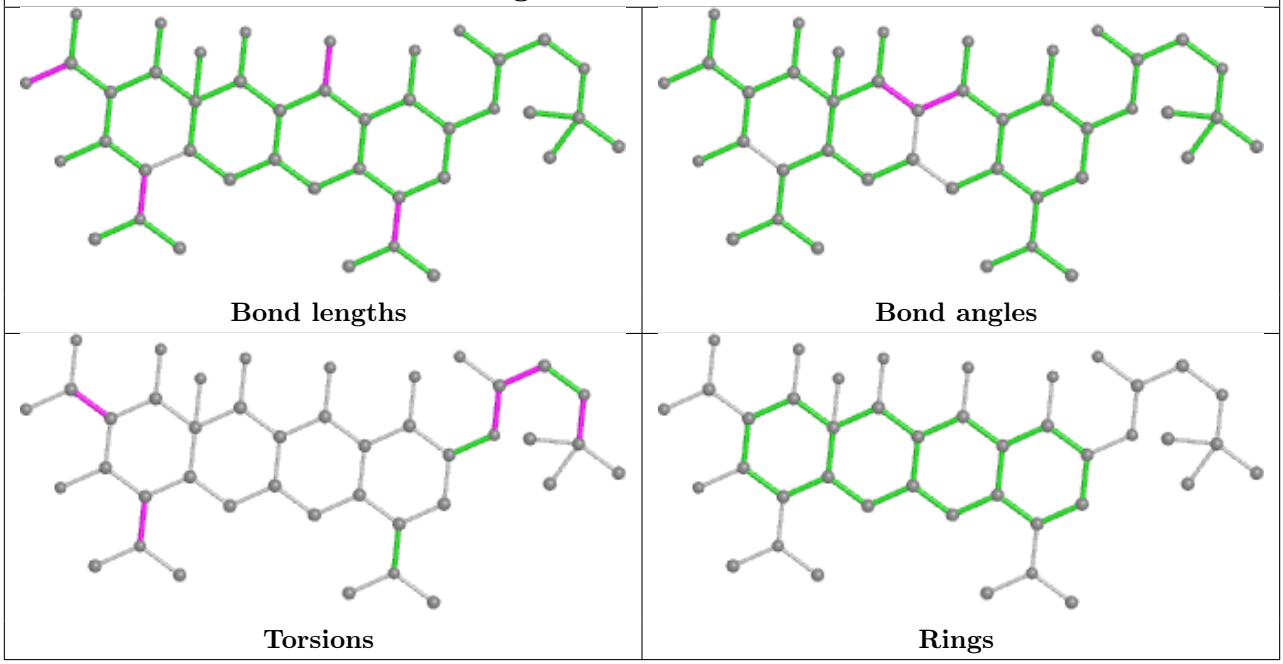
Mol	Chain	Res	Type	Atoms
85	L1	1707	T1C	C41-C4-N4-C43
85	L1	1707	T1C	C3-C4-N4-C43
85	L1	1707	T1C	C3-C4-N4-C42
85	L1	1707	T1C	C3-C2-C21-O21
85	L1	1708	T1C	C41-C4-N4-C43
85	L1	1708	T1C	C3-C4-N4-C43
85	L1	1708	T1C	C3-C4-N4-C42
85	L1	1708	T1C	C3-C2-C21-O21
85	L1	1708	T1C	C3-C2-C21-N21
85	L1	1708	T1C	C1-C2-C21-O21
85	L1	1708	T1C	C1-C2-C21-N21
85	S1	1034	T1C	C94-C93-N92-C92
85	S1	1034	T1C	C95-C93-N92-C92
85	S1	1034	T1C	C92-C91-N9-C9
85	S1	1034	T1C	C41-C4-N4-C43
85	S1	1034	T1C	C3-C4-N4-C43
85	S1	1034	T1C	C3-C4-N4-C42
85	S1	1034	T1C	C3-C2-C21-O21
85	S1	1034	T1C	C3-C2-C21-N21
85	S1	1034	T1C	C1-C2-C21-O21
85	S1	1034	T1C	O91-C91-N9-C9
85	L1	1708	T1C	C96-C93-N92-C92
85	S1	1034	T1C	C96-C93-N92-C92
85	L1	1708	T1C	C92-C91-N9-C9
85	L1	1707	T1C	O91-C91-C92-N92
85	L1	1707	T1C	N9-C91-C92-N92
85	L1	1708	T1C	C95-C93-N92-C92
85	L1	1708	T1C	O91-C91-N9-C9
85	S1	1034	T1C	N9-C91-C92-N92
85	S1	1034	T1C	O91-C91-C92-N92
85	L1	1707	T1C	C10-C9-N9-C91
85	L1	1707	T1C	C41-C4-N4-C42
85	L1	1708	T1C	C41-C4-N4-C42
85	S1	1034	T1C	C41-C4-N4-C42
85	L1	1707	T1C	C3-C2-C21-N21
85	L1	1707	T1C	C1-C2-C21-N21
85	S1	1034	T1C	C1-C2-C21-N21
85	L1	1708	T1C	C94-C93-N92-C92
85	L1	1708	T1C	N9-C91-C92-N92
85	L1	1707	T1C	C8-C9-N9-C91
85	L1	1708	T1C	O91-C91-C92-N92
87	Se	500	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

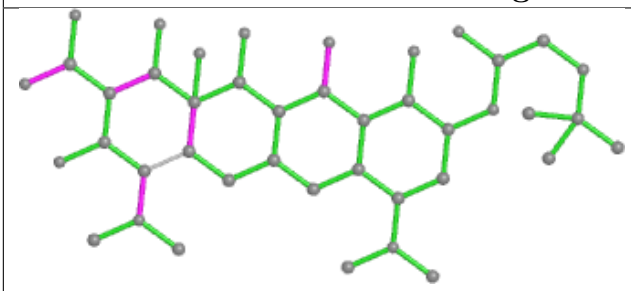
No monomer is involved in short contacts.

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 then 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.

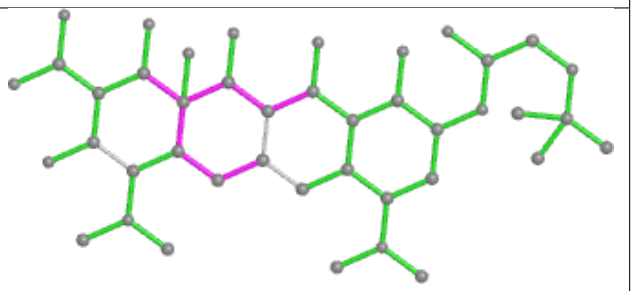
Ligand T1C L1 1708



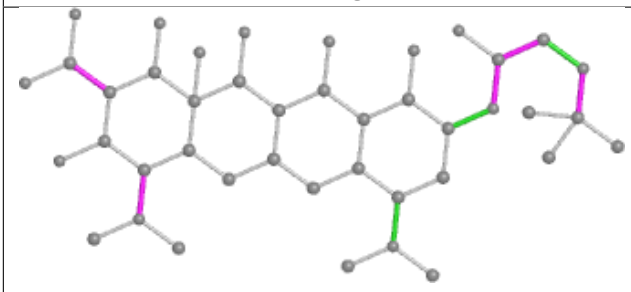
Ligand T1C S1 1034



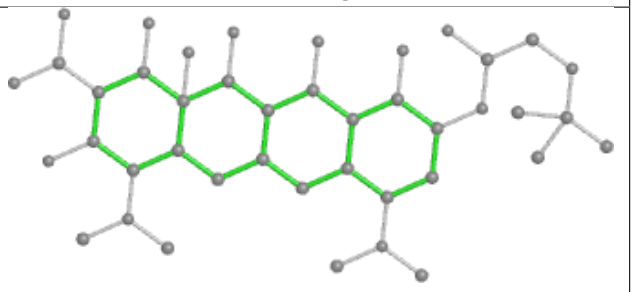
Bond lengths



Bond angles

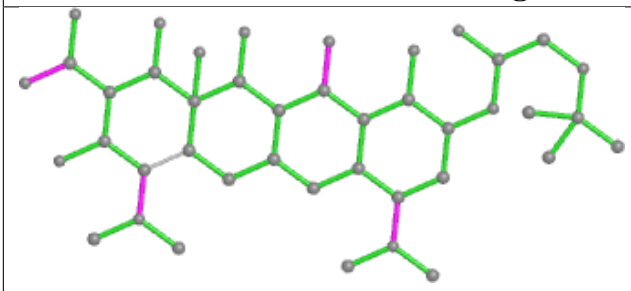


Torsions

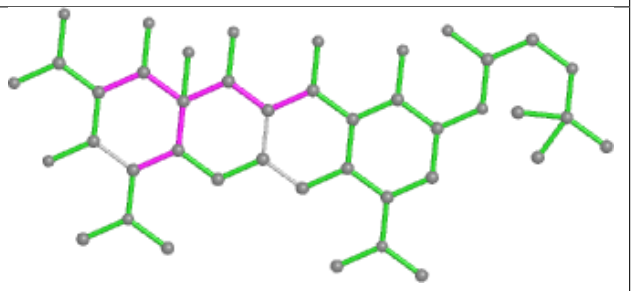


Rings

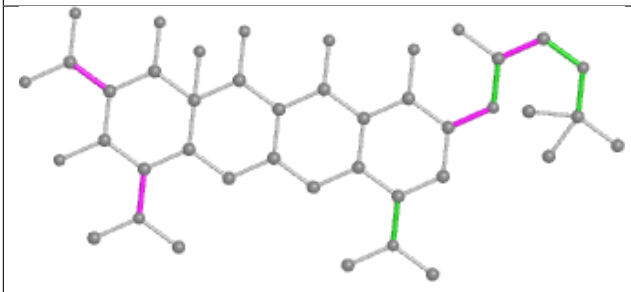
Ligand T1C L1 1707



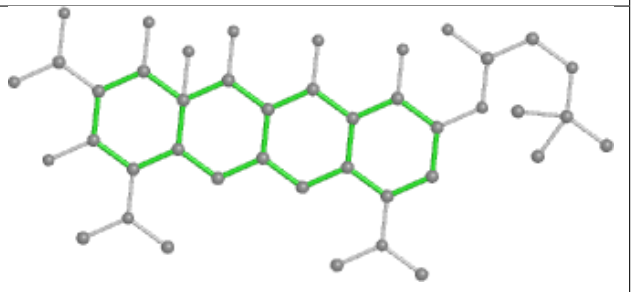
Bond lengths



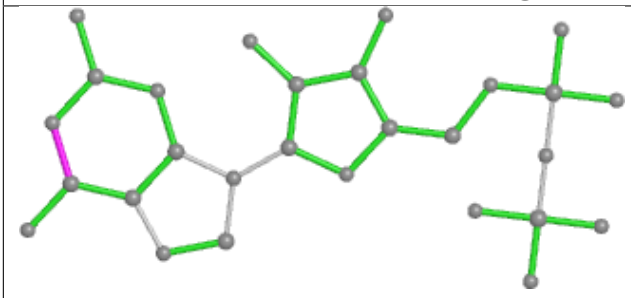
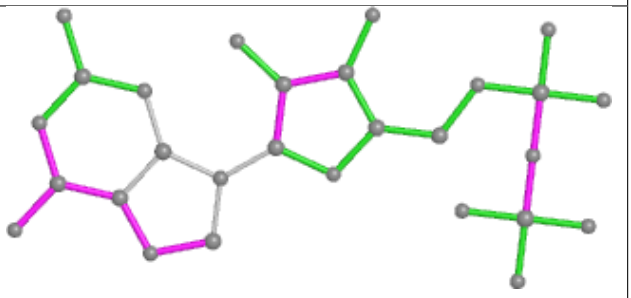
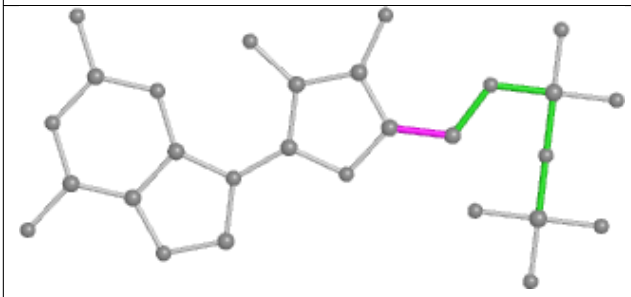
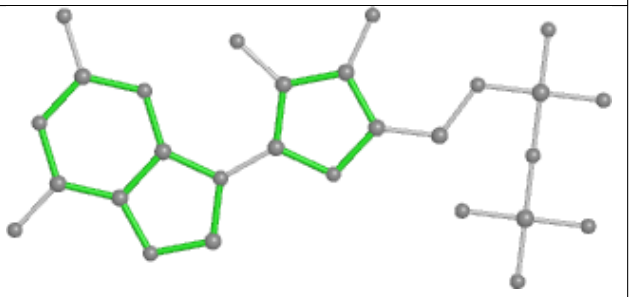
Bond angles



Torsions



Rings

Ligand GDP Se 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

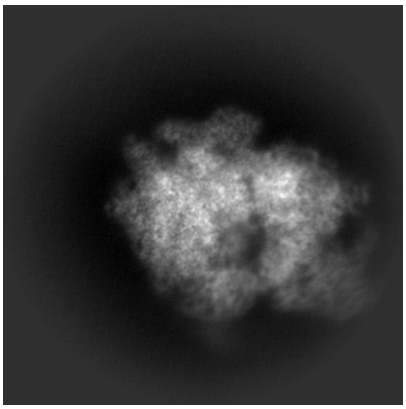
6 Map visualisation

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.

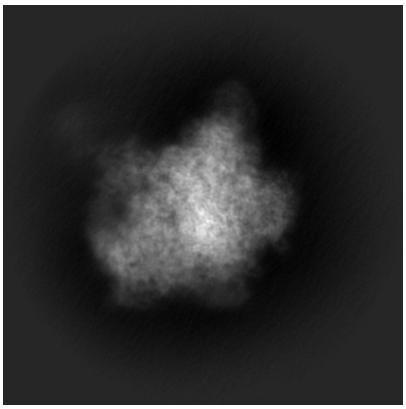
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

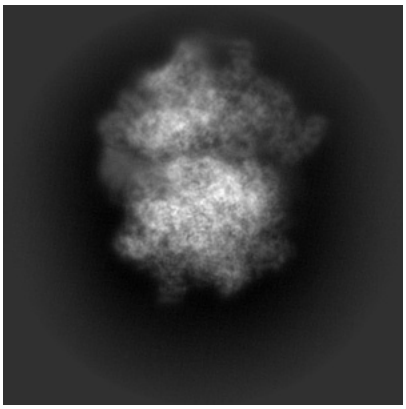
6.1.1 Primary map



X

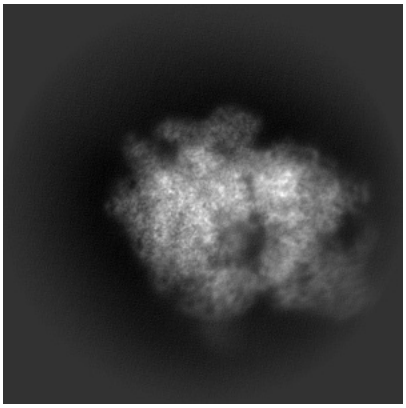


Y

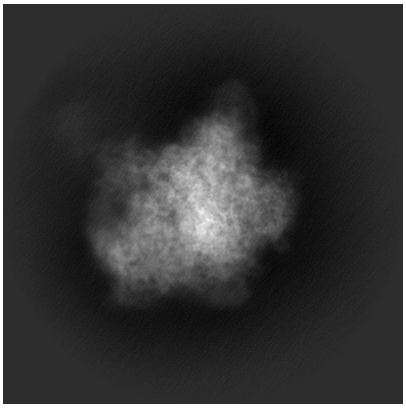


Z

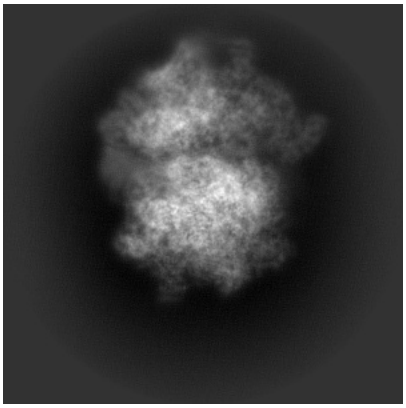
6.1.2 Raw map



X



Y

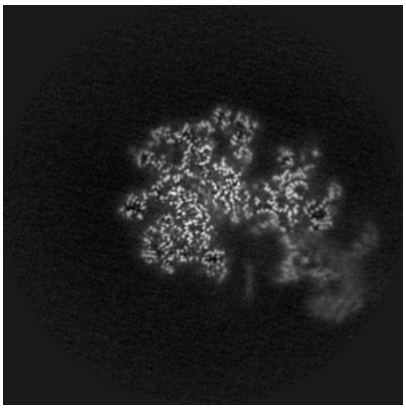


Z

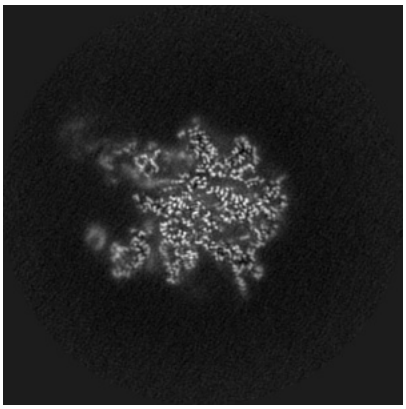
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

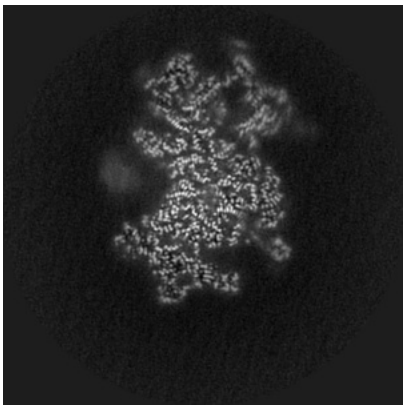
6.2.1 Primary map



X Index: 210

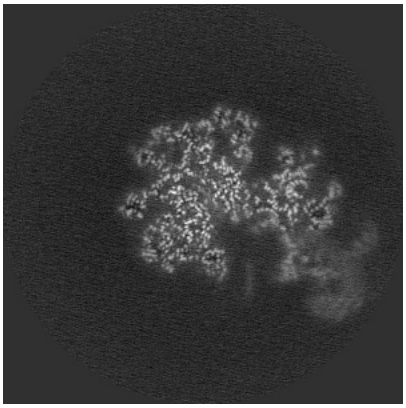


Y Index: 210

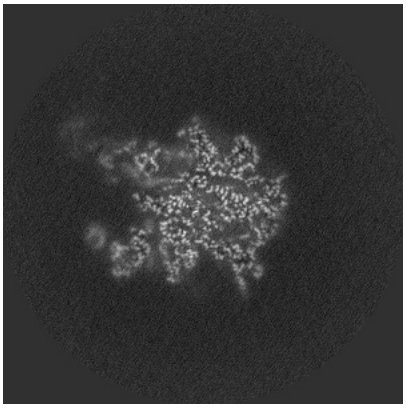


Z Index: 210

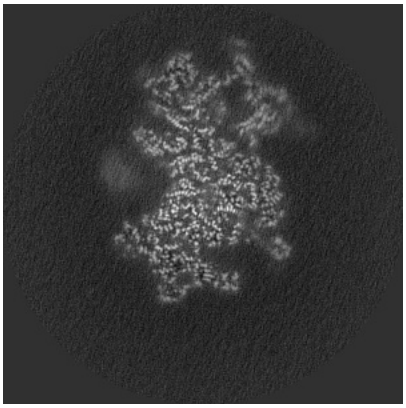
6.2.2 Raw map



X Index: 210



Y Index: 210

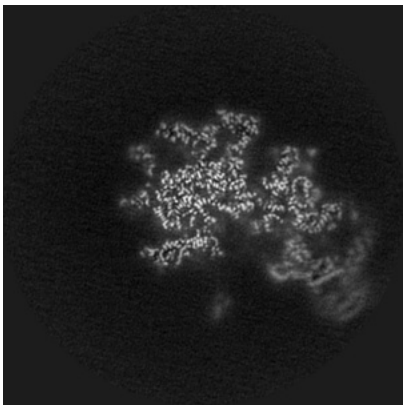


Z Index: 210

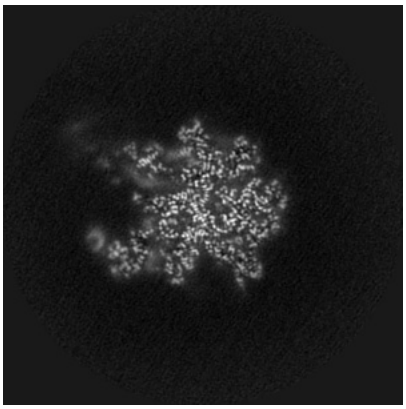
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

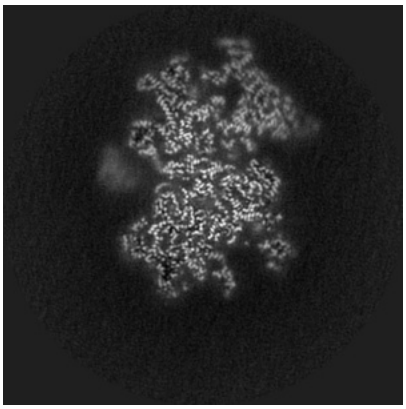
6.3.1 Primary map



X Index: 199

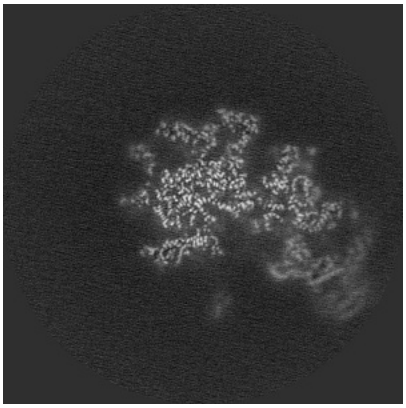


Y Index: 207

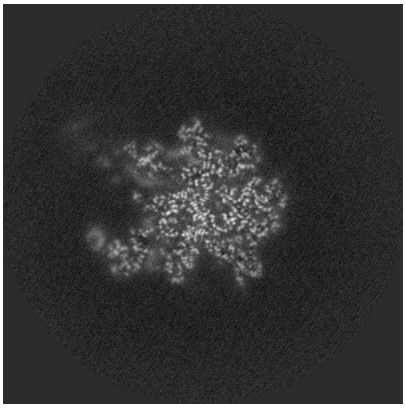


Z Index: 218

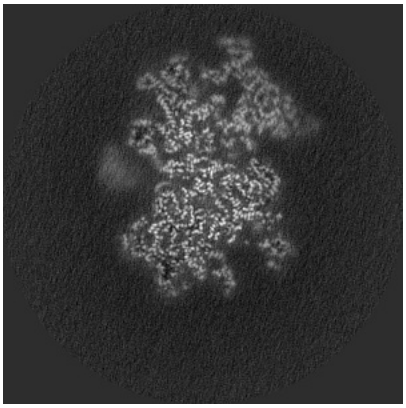
6.3.2 Raw map



X Index: 199



Y Index: 207

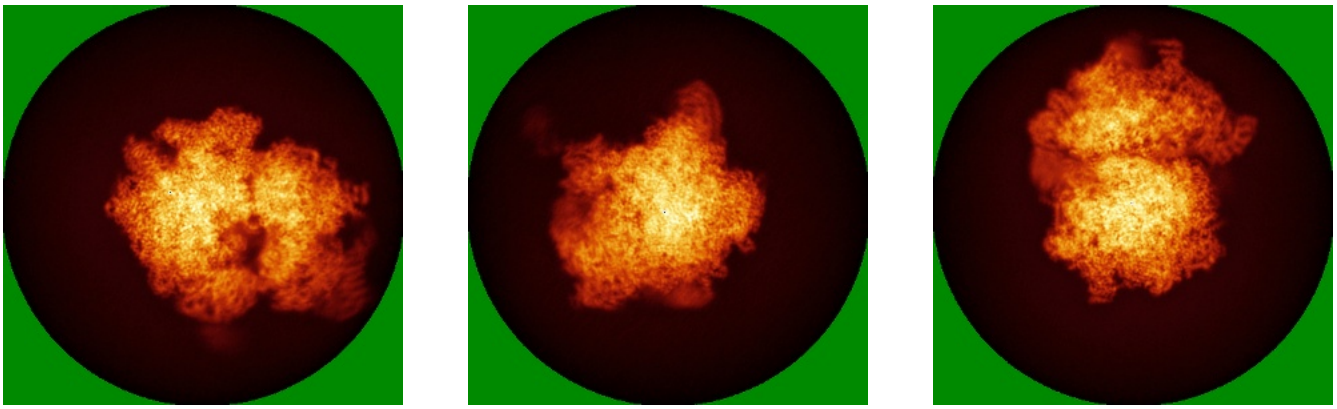


Z Index: 218

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

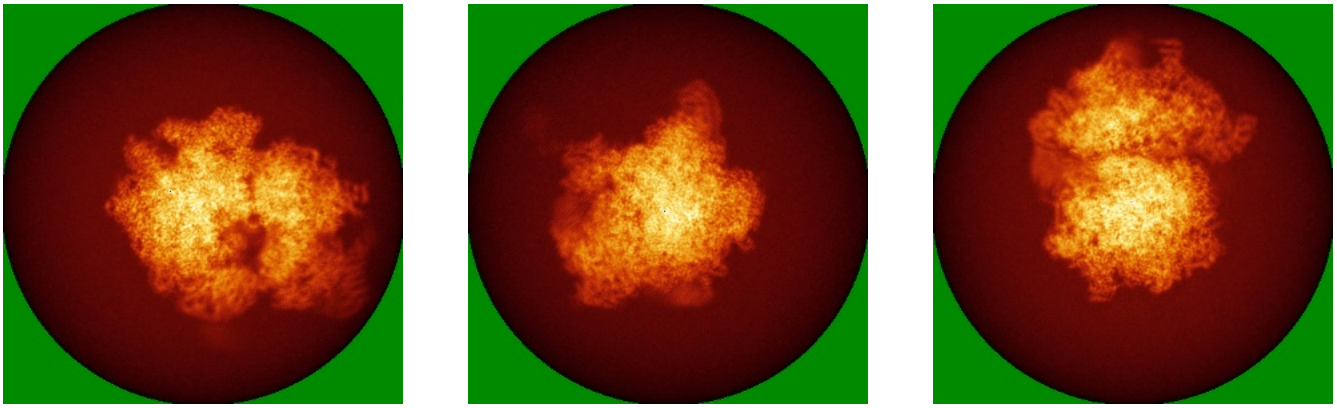
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

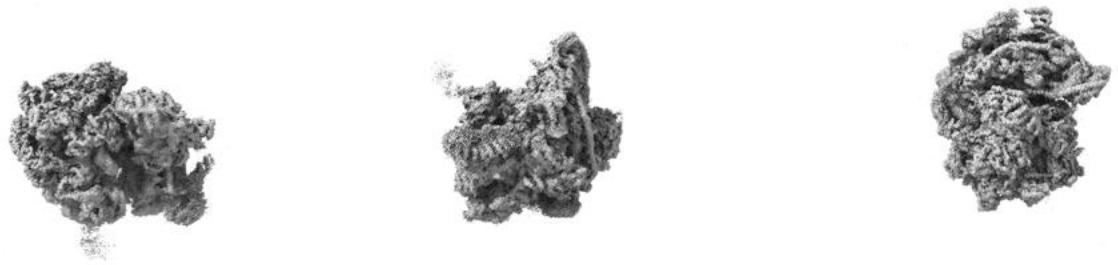
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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



X Y Z

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

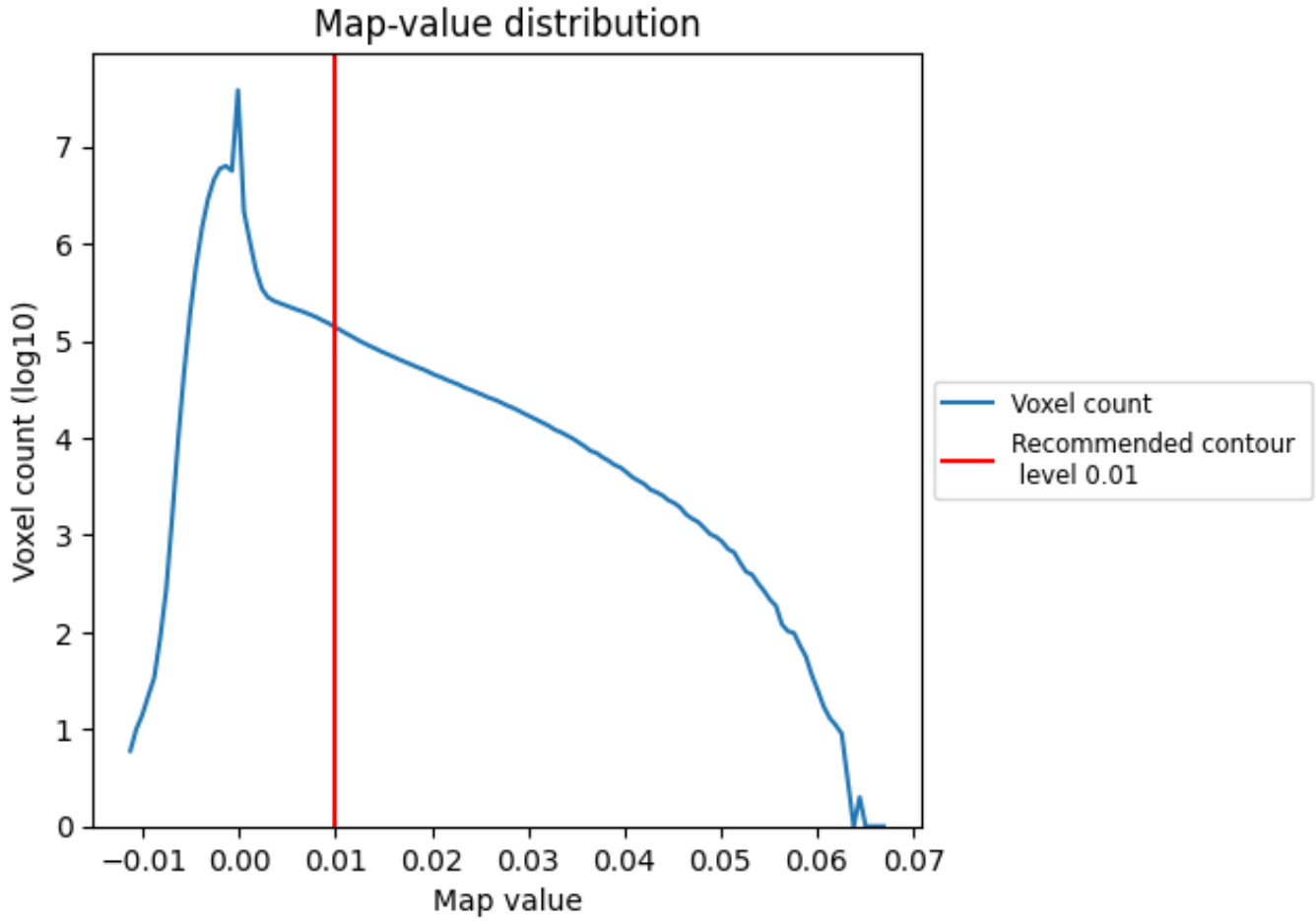
6.6 Mask visualisation (i)

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

7 Map analysis

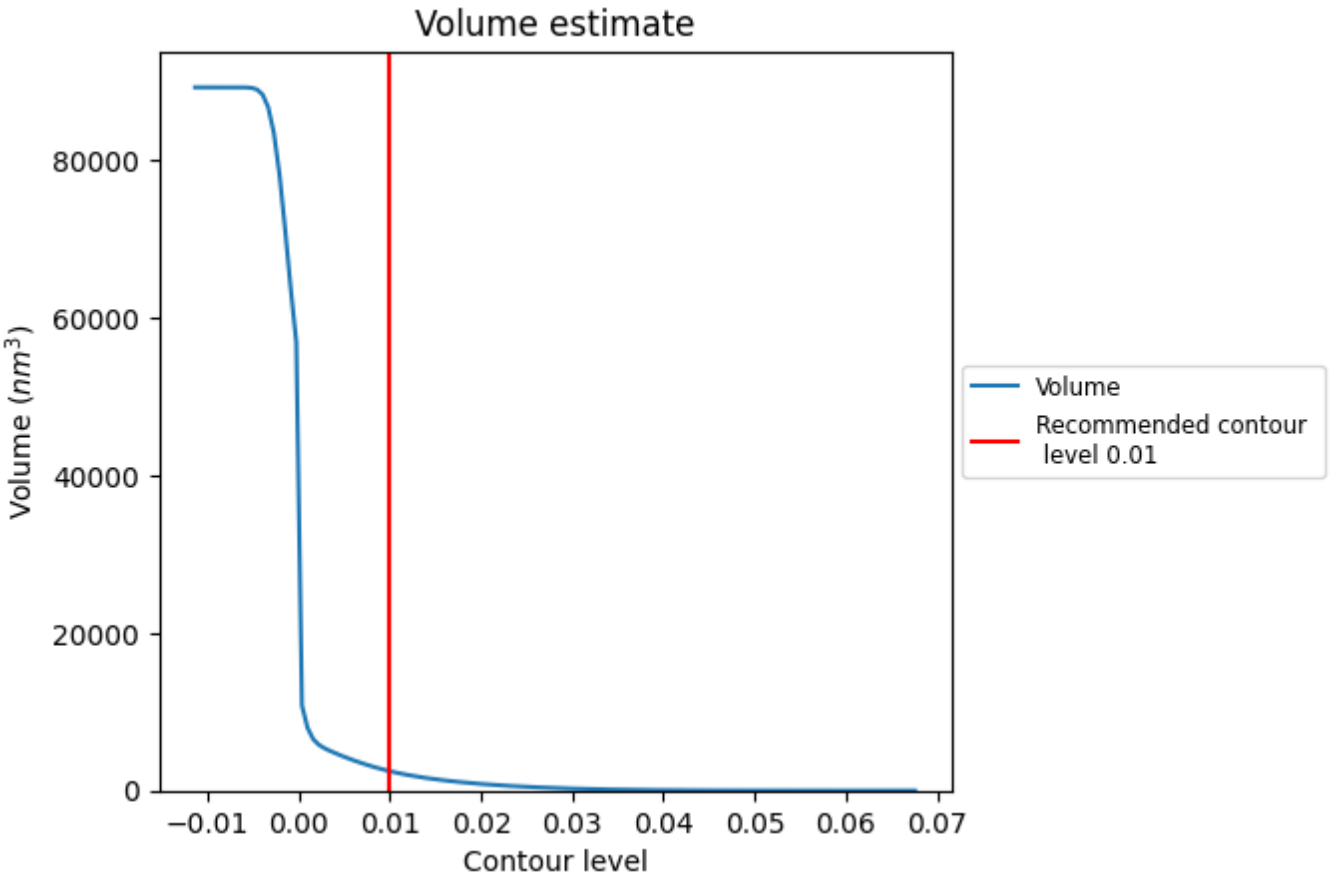
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

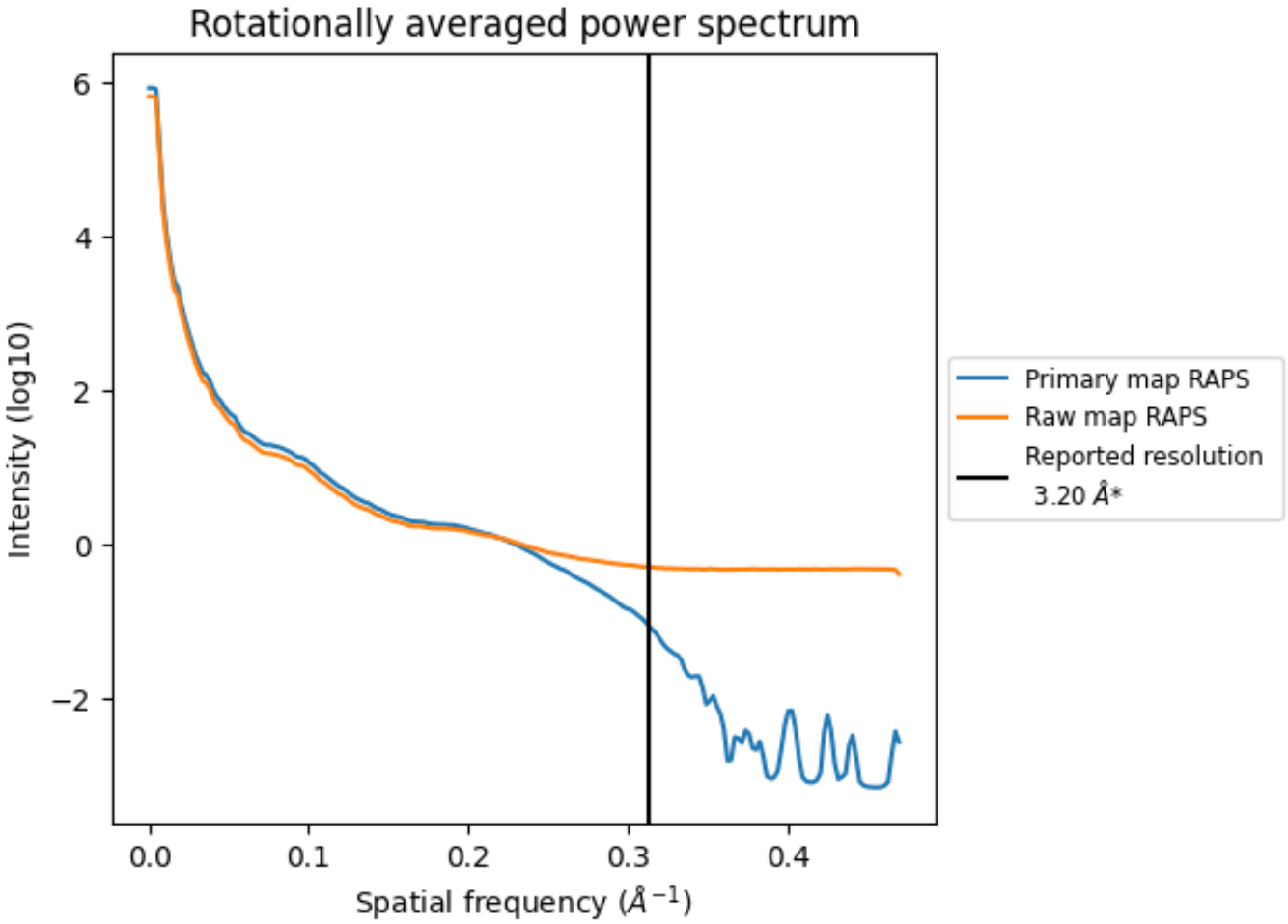
7.2 Volume estimate



The volume at the recommended contour level is 2465 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)

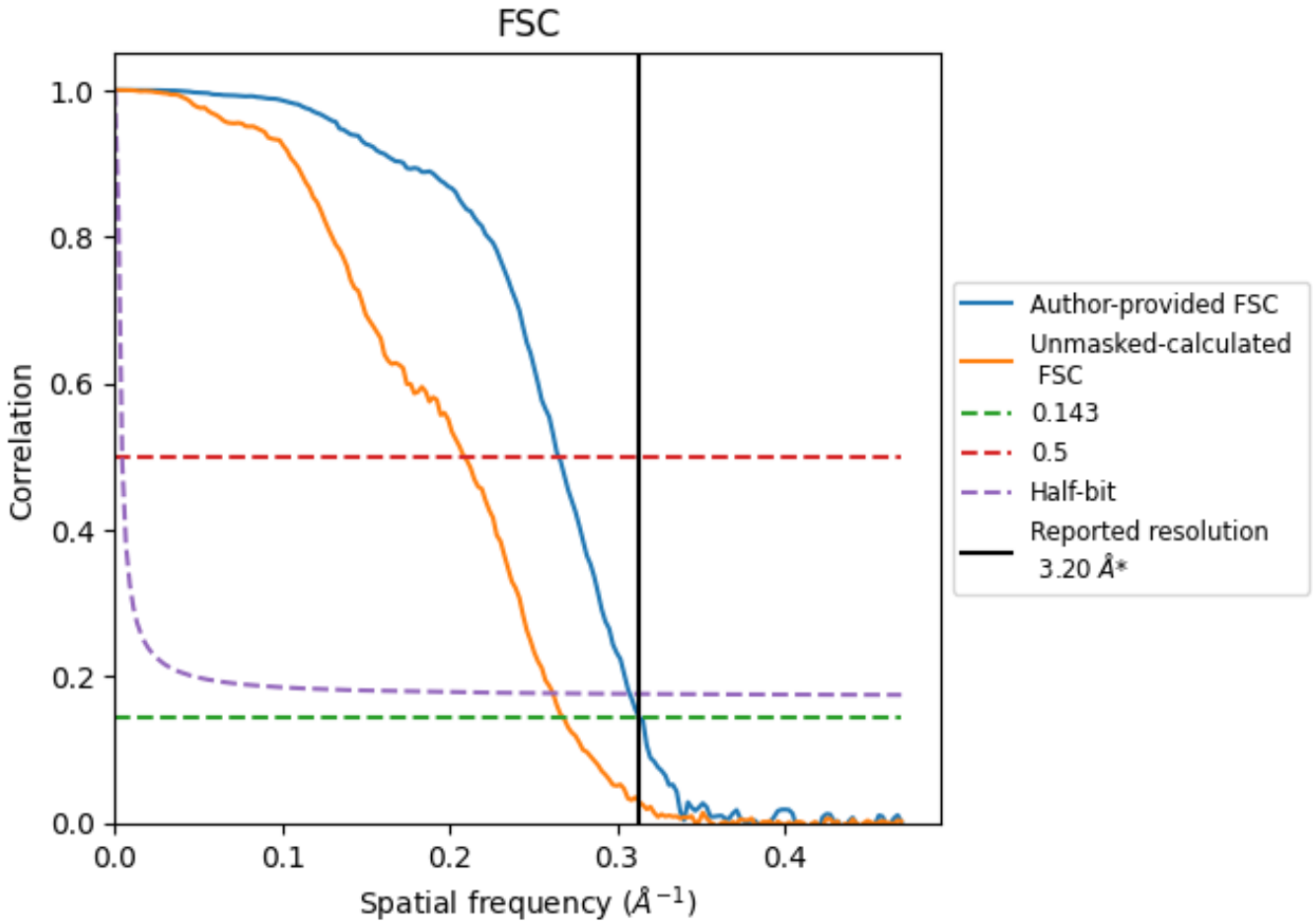


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

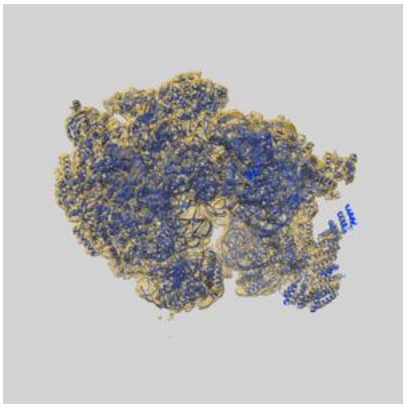
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.77	3.25
Unmasked-calculated*	3.73	4.79	3.82

*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 %

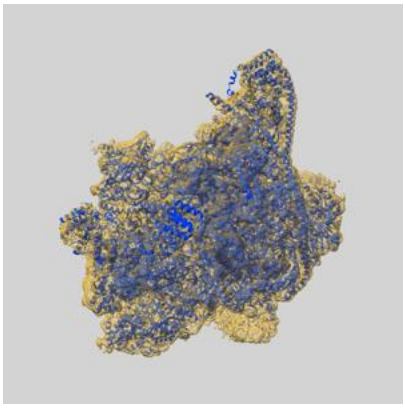
9 Map-model fit

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.

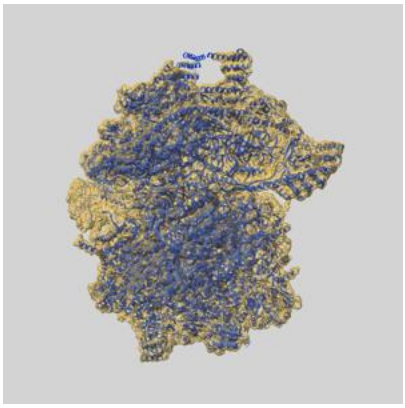
9.1 Map-model overlay



X



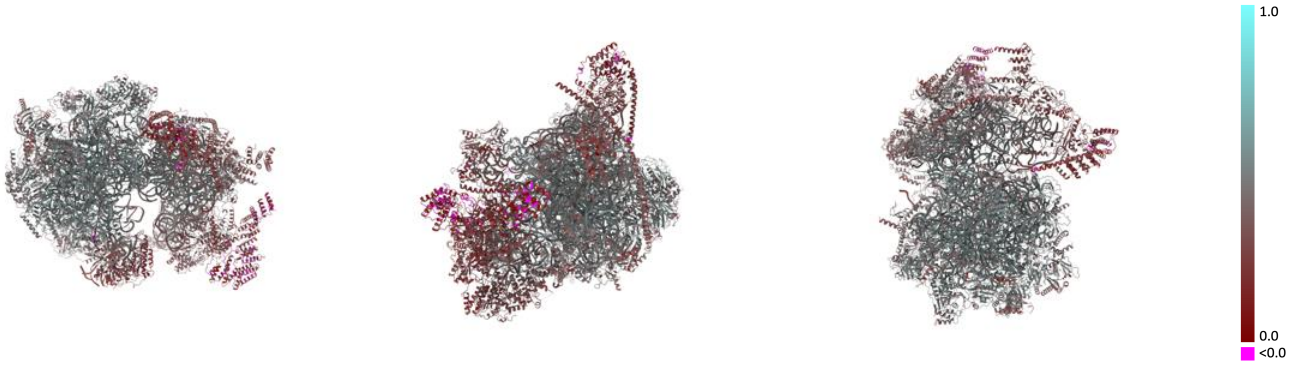
Y



Z

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.

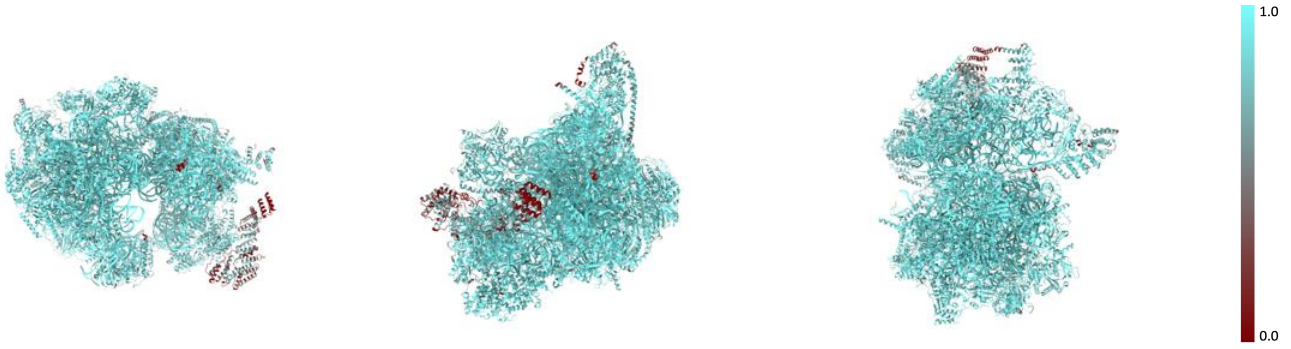
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

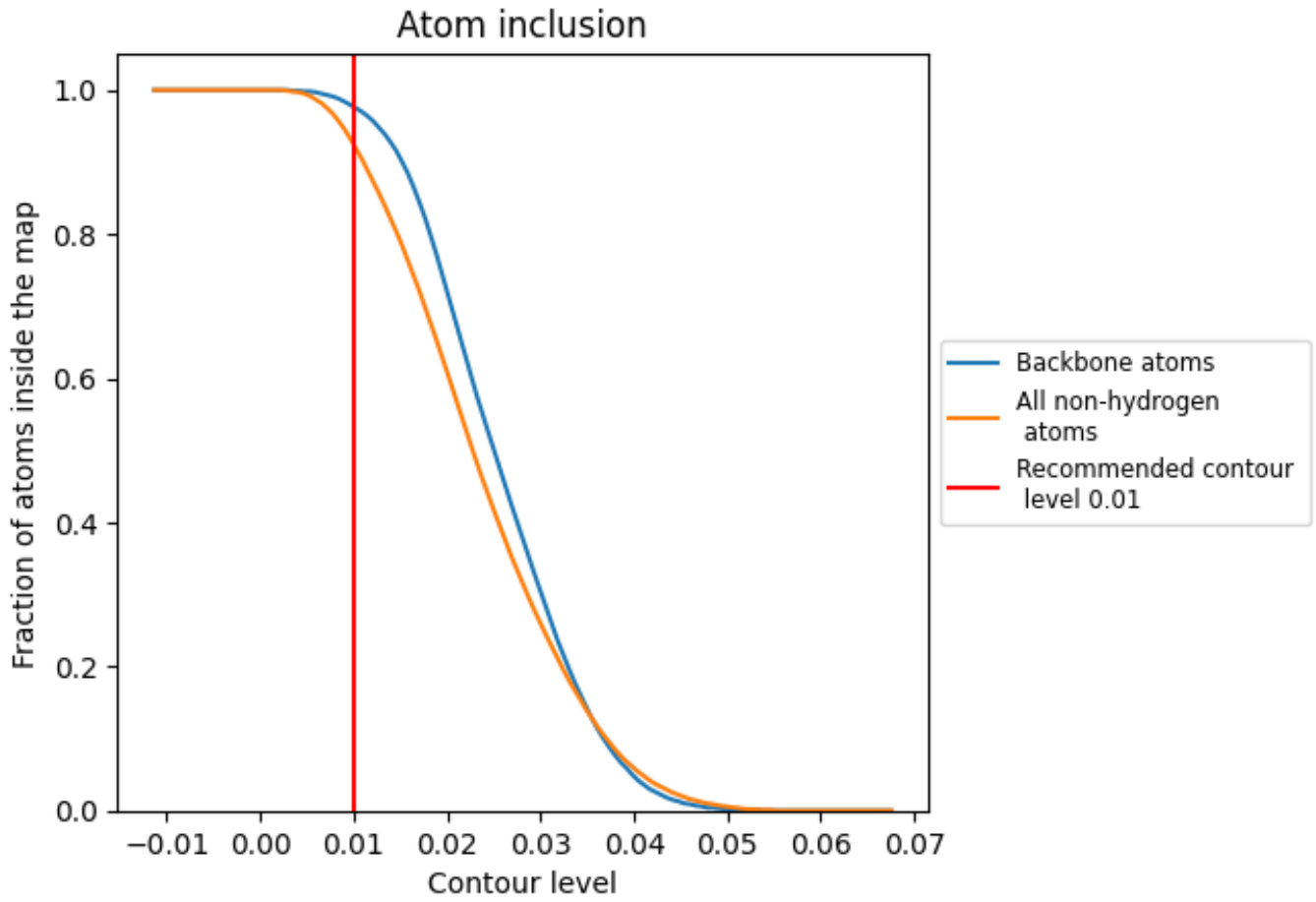
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

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