Full wwPDB EM Validation Report

Oct 1, 2024 – 07:39 PM JST

PDB ID	:	8K2A
EMDB ID	:	EMD-36836
Title	:	Cryo-EM structure of the human 55S mitoribosome with Tigecycline
Authors	:	Li, X.; Wang, M.; Cheng, J.
Deposited on	:	2023-07-12
Resolution	:	2.90 Å(reported)

This is a 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:

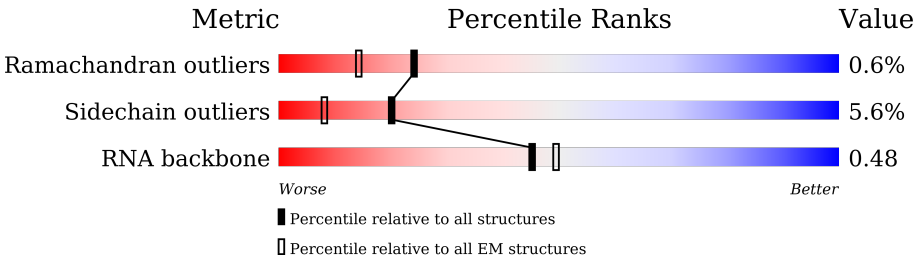
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	70% 25%
2	L2	69	64% 17% 19%
3	LB	305	75% 22%
4	LC	348	84% 13%
5	LD	311	78% 20%
6	LI	267	32% 64%
7	LJ	261	55% 6% 39%
8	LK	192	83% 7% 9%

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Mol	Chain	Length	Quality of chain
9	LM	178	98%
10	LN	145	77% 21%
11	LO	296	94%
12	LP	251	85% 12%
13	LQ	175	83% 13%
14	LR	179	80% 18%
15	LS	292	74% 25%
16	LT	149	91% 6%
17	LU	205	77% 22%
18	LV	212	77% 22%
19	LW	153	93% 7%
20	LX	216	88% 6% 6%
21	La	148	73% 25%
22	Lb	256	91% 5%
23	Lu	250	66% 30%
24	Ld	161	72% 25%
25	Lf	188	55% 43%
26	Lg	65	77% 20%
27	Lh	92	48% 50%
28	Li	188	49% 49%
29	Lj	103	34% 63%
30	Lk	423	90% 7%
31	Ll	380	89% 7%
32	Lm	338	83% 13%
33	Ln	206	42% 6% 52%

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Mol	Chain	Length	Quality of chain
34	Lo	137	88% 9%
35	Lp	142	61% 7% 32%
36	Lq	215	66% 31%
37	Lr	332	80% 17%
38	Ls	306	66% 30%
39	Lt	279	70% 8% 22%
40	Lv	212	55% 7% 38%
41	Lw	166	75% 5% 20%
42	Lx	158	63% 6% 30%
43	Ly	128	74% 24%
44	Lz	123	74% 25%
45	L3	112	79% 5% 14%
46	L4	138	53% 7% 40%
47	L5	128	30% 5% 65%
48	L6	102	89% 8%
49	L7	206	58% 38%
50	L8	222	55% 42%
51	SR	196	72% 26%
52	Sf	439	81% 16%
53	SB	296	70% 27%
54	SZ	167	69% 10% 21%
55	SE	430	71% 26%
56	SF	125	90% 8%
57	SG	242	77% 6% 17%
58	SI	396	70% 6% 23%

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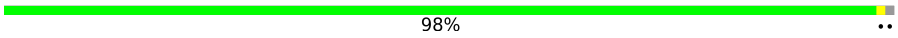
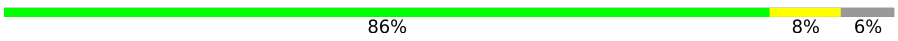
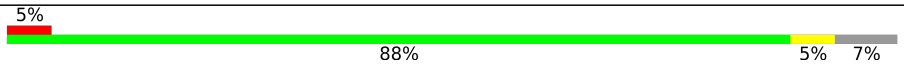
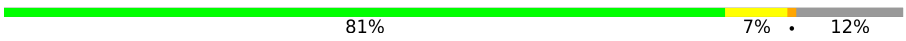
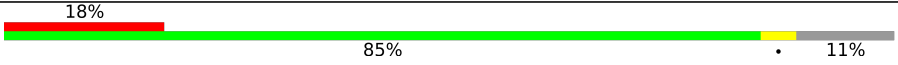
Mol	Chain	Length	Quality of chain
59	SJ	201	
60	SK	194	
61	SL	138	
62	SN	128	
63	SO	257	
64	SP	137	
65	SQ	130	
66	SS	258	
67	ST	142	
68	SW	87	
69	SX	360	
70	SY	190	
71	Sa	173	
72	Sb	205	
73	Sc	414	
74	Sd	187	
75	Se	398	
76	Sg	395	
77	Si	106	
78	Sj	218	
79	Sk	323	
80	Sm	118	
81	Sn	199	
82	So	689	
83	S1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

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 165285 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			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		

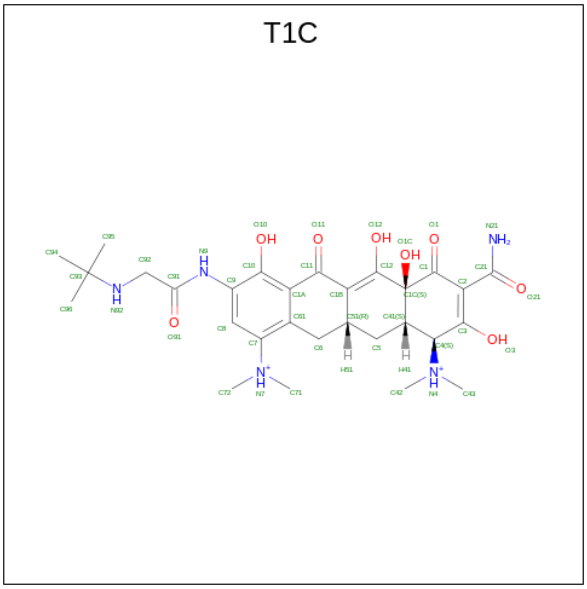
- Molecule 83 is a RNA chain called 12S rRNA.

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

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

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

- Molecule 85 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



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	

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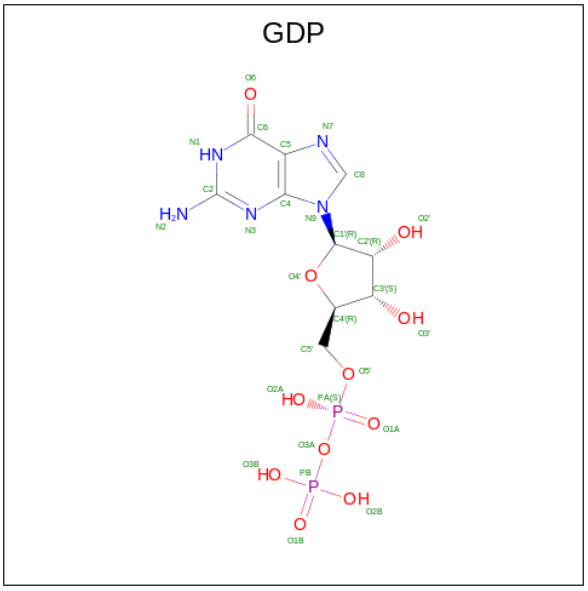
Mol	Chain	Residues	Atoms	AltConf
85	S1	1	Total C N O 42 29 5 8	0
85	S1	1	Total C N O 42 29 5 8	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



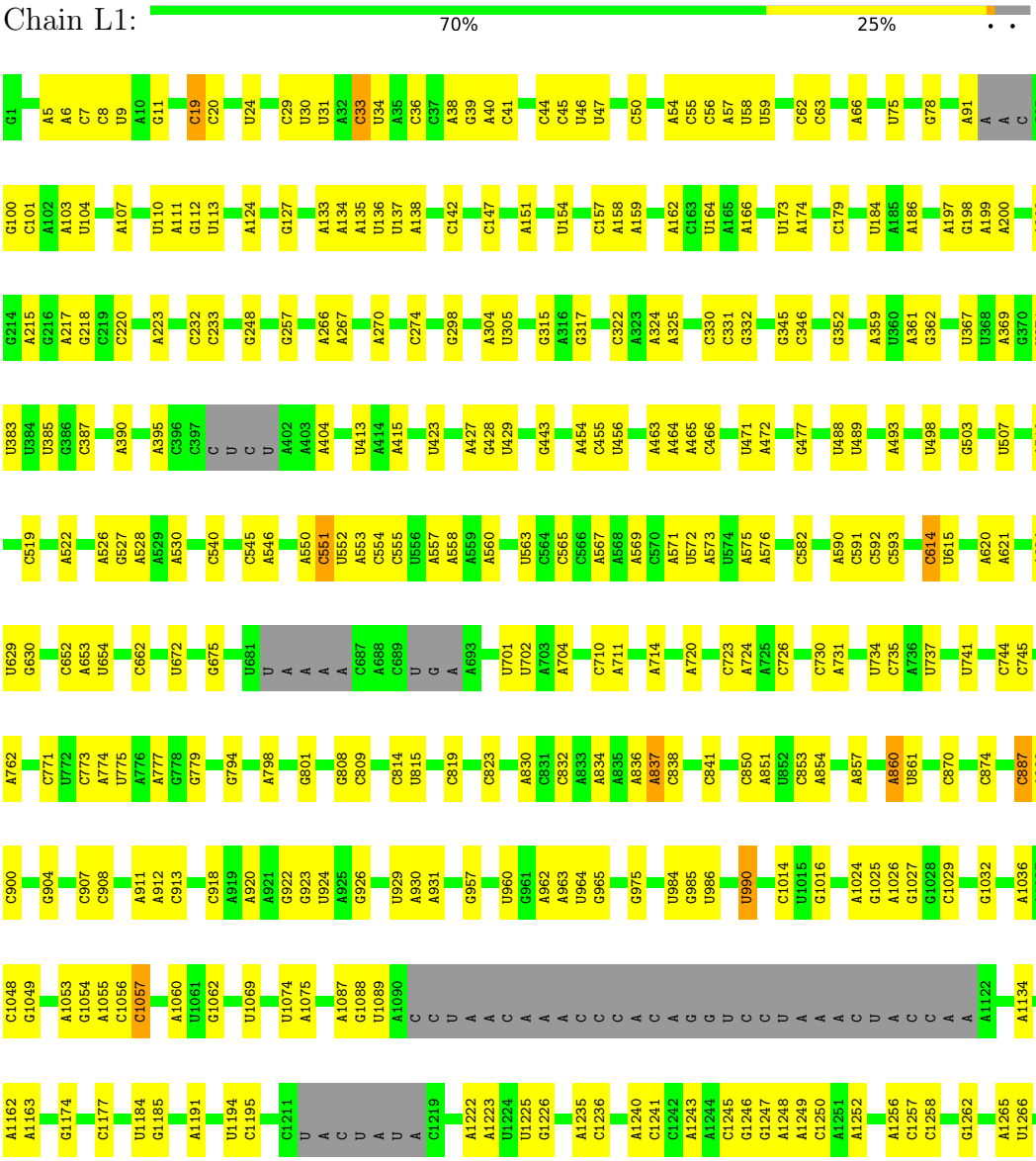
Mol	Chain	Residues	Atoms					AltConf
87	Se	1	Total	C	N	O	P	0
			28	10	5	11	2	

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.

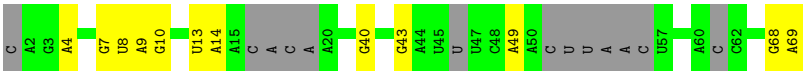
- Molecule 1: 16S rRNA

Chain L1:



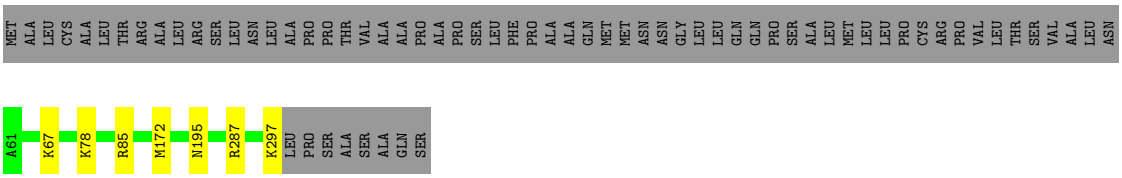
• Molecule 2: Val tRNA

Chain L2:



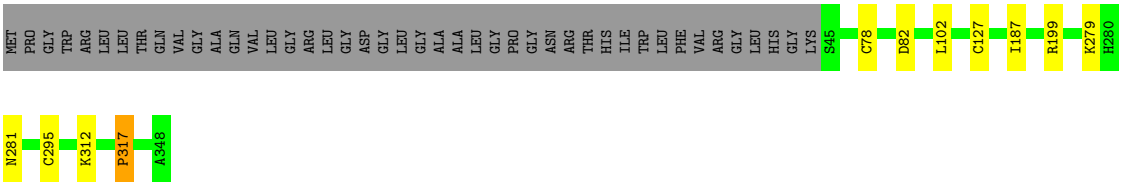
• Molecule 3: Large ribosomal subunit protein uL2m

Chain LB:



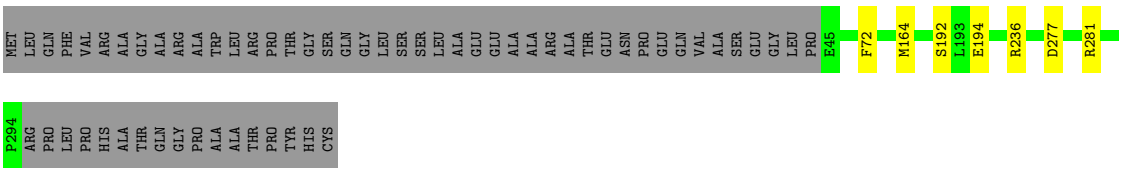
• Molecule 4: Large ribosomal subunit protein uL3m

Chain LC:



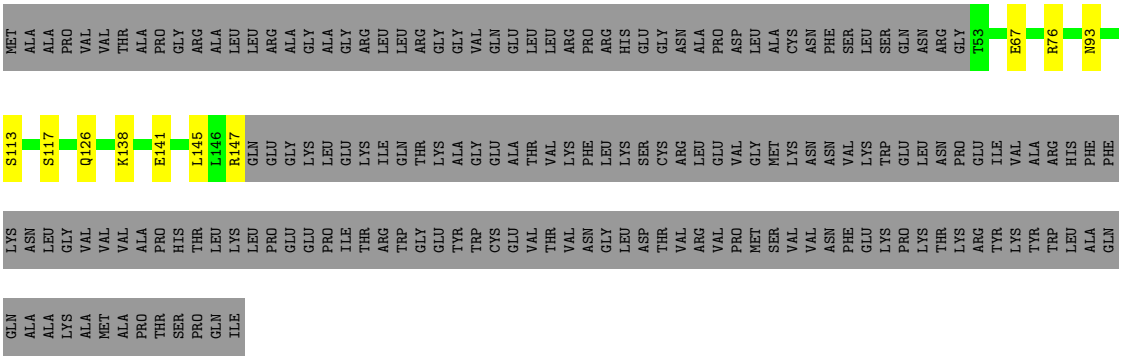
• Molecule 5: Large ribosomal subunit protein uL4m

Chain LD:



• Molecule 6: Large ribosomal subunit protein bL9m

Chain LI:

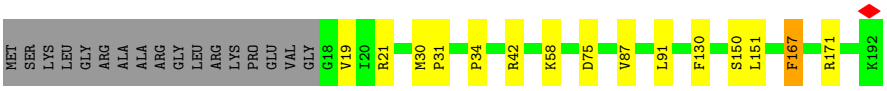


• Molecule 7: Large ribosomal subunit protein uL10m

Chain LJ:

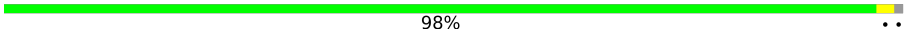
• Molecule 8: Large ribosomal subunit protein uL11m

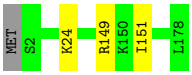
Chain LK:



• Molecule 9: Large ribosomal subunit protein uL13m

Chain LM:



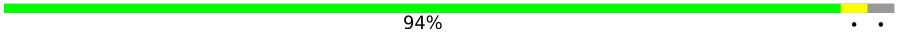


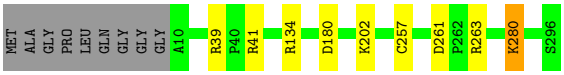
• Molecule 10: Large ribosomal subunit protein uL14m

Chain LN:

• Molecule 11: Large ribosomal subunit protein uL15m

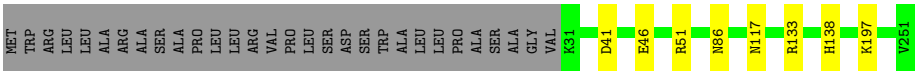
Chain LO:





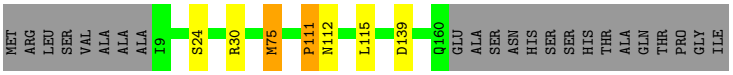
• Molecule 12: Large ribosomal subunit protein uL16m

Chain LP:



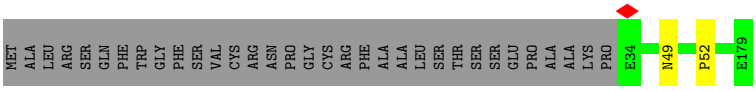
• Molecule 13: Large ribosomal subunit protein bL17m

Chain LQ:



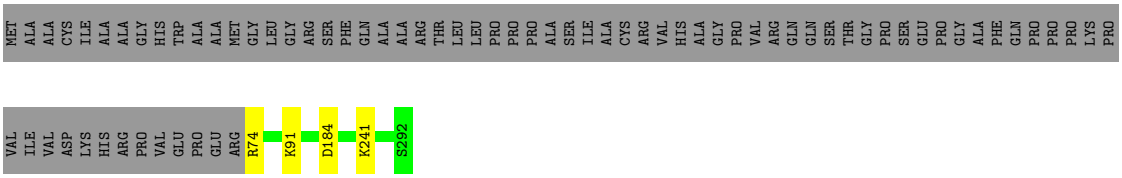
• Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain LR:



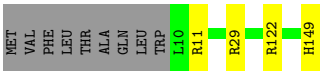
• Molecule 15: Large ribosomal subunit protein bL19m

Chain LS:



• Molecule 16: Large ribosomal subunit protein bL20m

Chain LT:

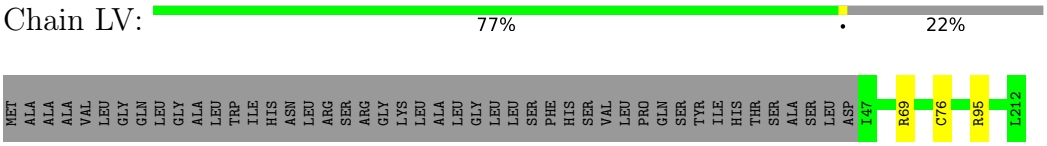


• Molecule 17: Large ribosomal subunit protein bL21m

Chain LU:

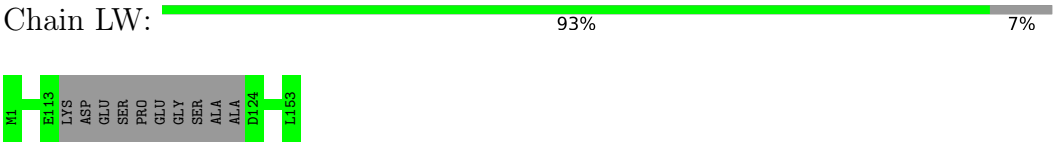
• Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain LV:



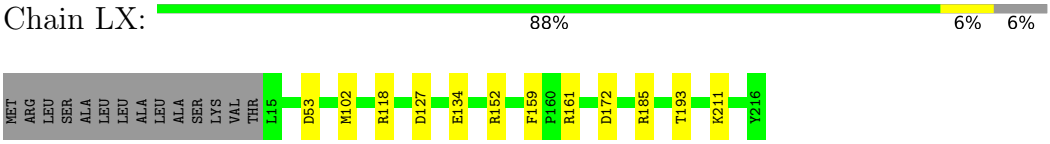
• Molecule 19: Large ribosomal subunit protein uL23m

Chain LW:



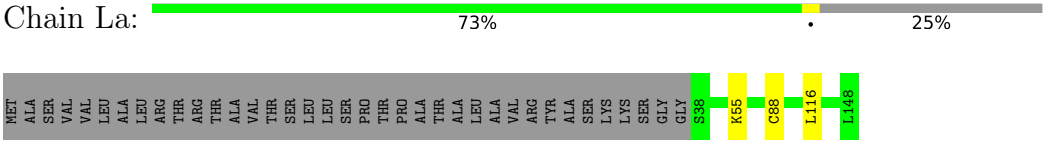
• Molecule 20: Large ribosomal subunit protein uL24m

Chain LX:



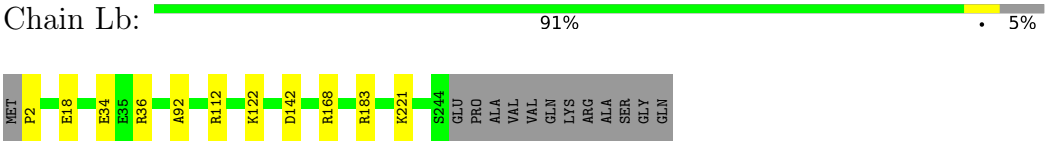
• Molecule 21: Large ribosomal subunit protein bL27m

Chain La:



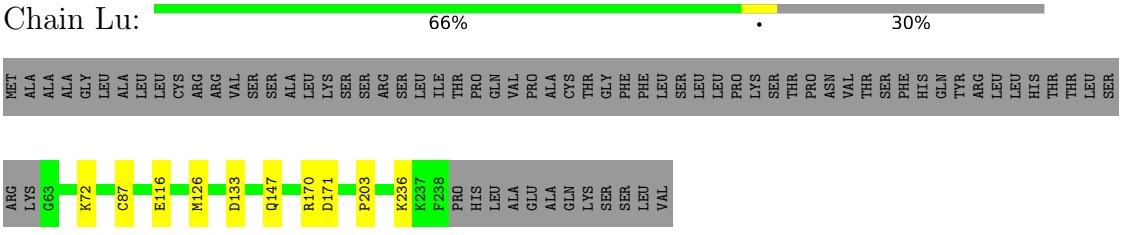
• Molecule 22: Large ribosomal subunit protein bL28m

Chain Lb:



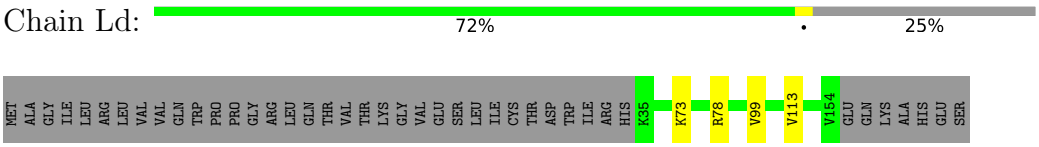
• Molecule 23: Large ribosomal subunit protein uL29m

Chain Lu:



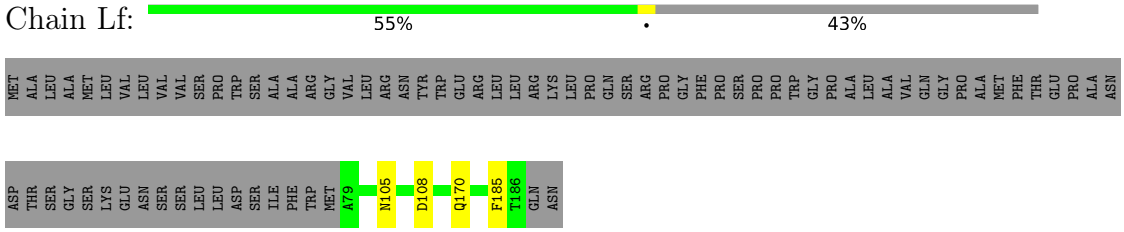
• Molecule 24: Large ribosomal subunit protein uL30m

Chain Ld:



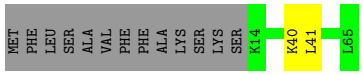
• Molecule 25: Large ribosomal subunit protein bL32m

Chain Lf:



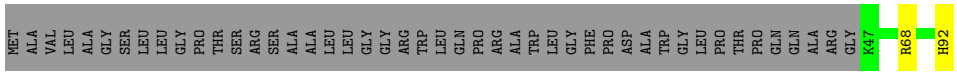
• Molecule 26: Large ribosomal subunit protein bL33m

Chain Lg:



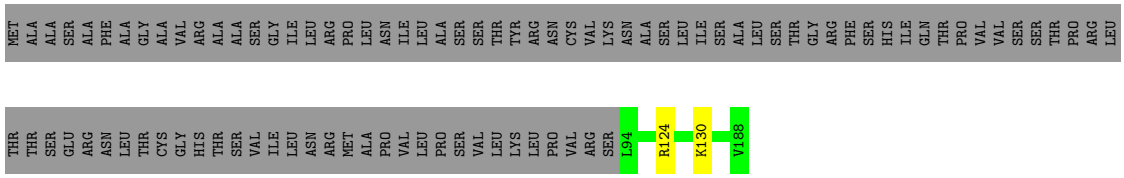
• Molecule 27: Large ribosomal subunit protein bL34m

Chain Lh:



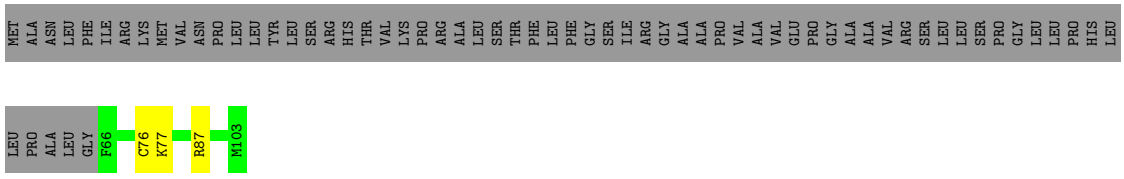
• Molecule 28: Large ribosomal subunit protein bL35m

Chain Li:



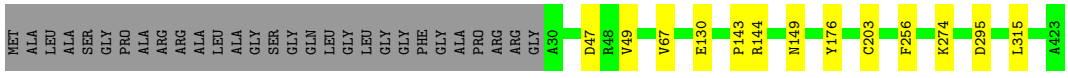
• Molecule 29: Large ribosomal subunit protein bL36m

Chain Lj:



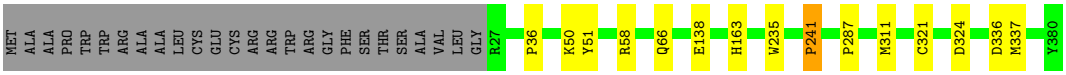
• Molecule 30: Large ribosomal subunit protein mL37

Chain Lk:



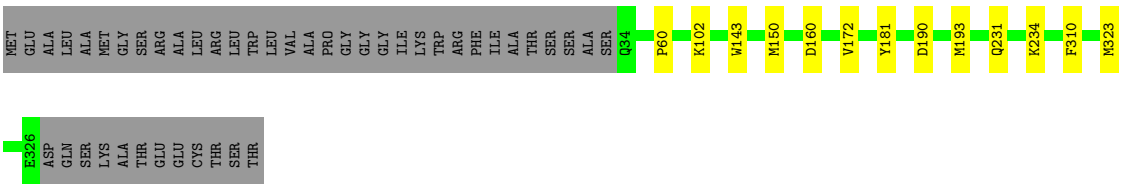
• Molecule 31: Large ribosomal subunit protein mL38

Chain Ll:



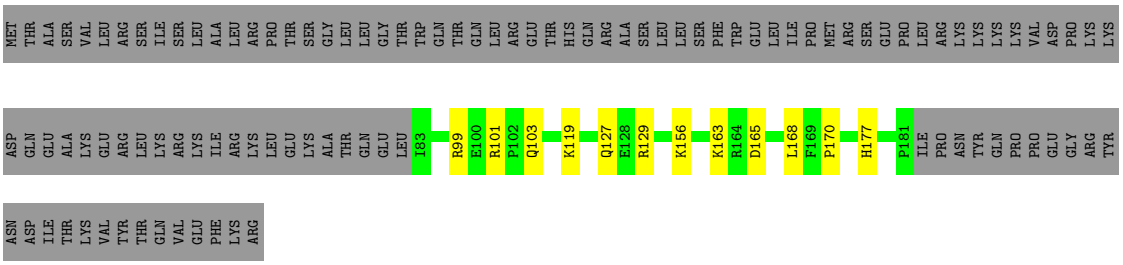
• Molecule 32: Large ribosomal subunit protein mL39

Chain Lm:



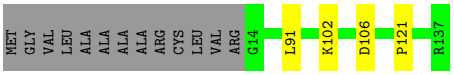
• Molecule 33: Large ribosomal subunit protein mL40

Chain Ln:



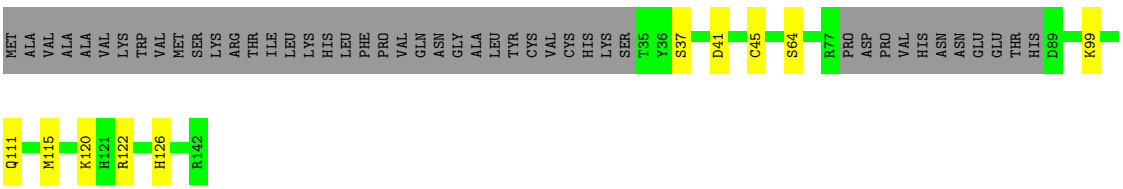
• Molecule 34: Large ribosomal subunit protein mL41

Chain Lo:



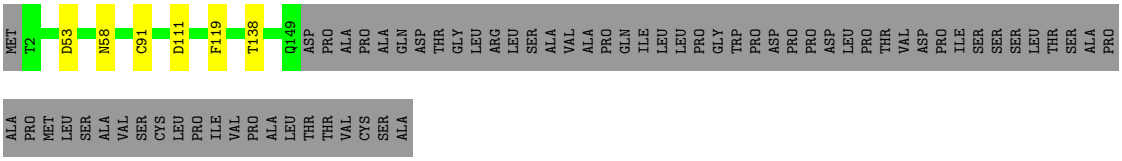
• Molecule 35: Large ribosomal subunit protein mL42

Chain Lp:



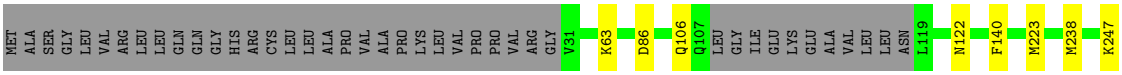
• Molecule 36: Large ribosomal subunit protein mL43

Chain Lq:



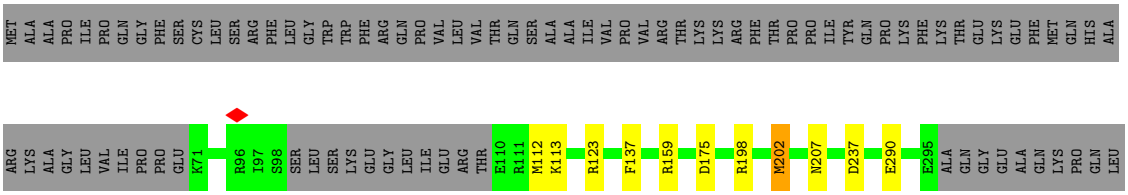
• Molecule 37: Large ribosomal subunit protein mL44

Chain Lr:



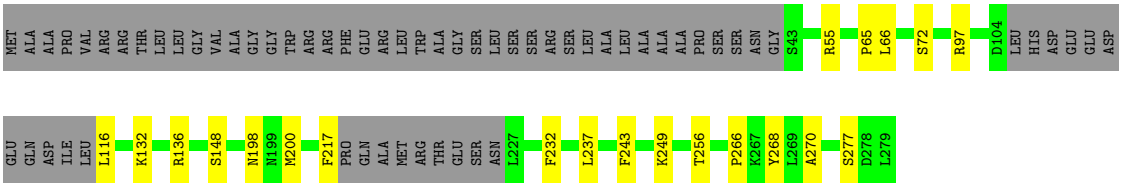
• Molecule 38: Large ribosomal subunit protein mL45

Chain Ls:



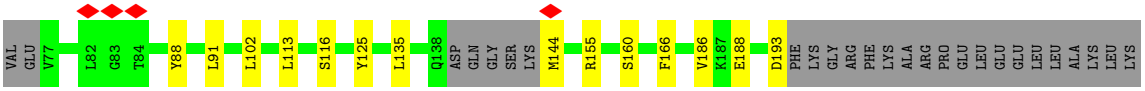
• Molecule 39: Large ribosomal subunit protein mL46

Chain Lt:



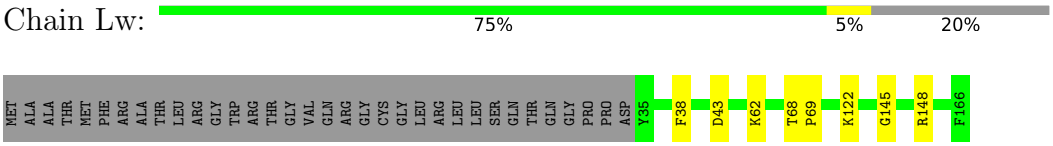
• Molecule 40: Large ribosomal subunit protein mL48

Chain Lv:



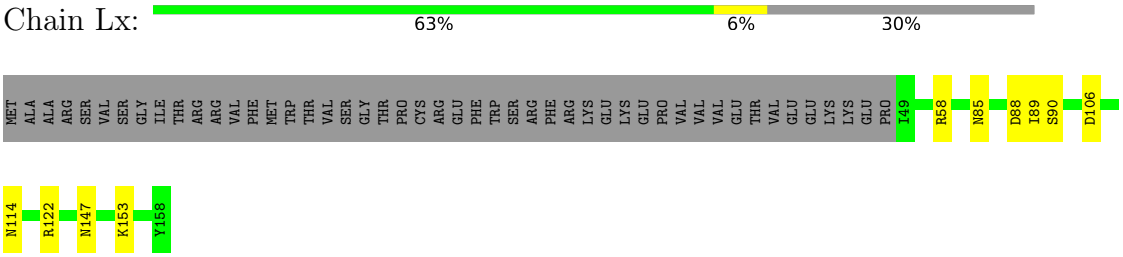
• Molecule 41: Large ribosomal subunit protein mL49

Chain Lw:



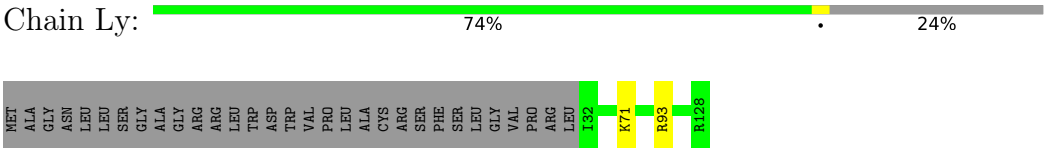
• Molecule 42: Large ribosomal subunit protein mL50

Chain Lx:



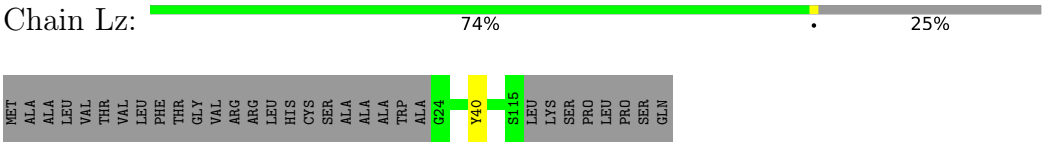
• Molecule 43: Large ribosomal subunit protein mL51

Chain Ly:



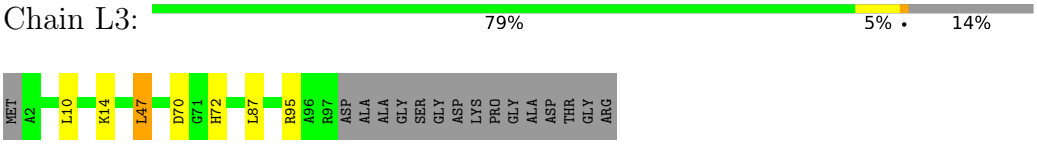
• Molecule 44: 39S ribosomal protein L52, mitochondrial

Chain Lz:



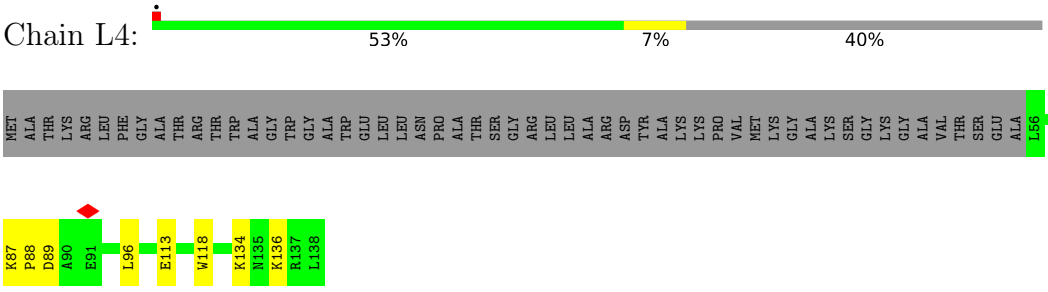
• Molecule 45: Large ribosomal subunit protein mL53

Chain L3:



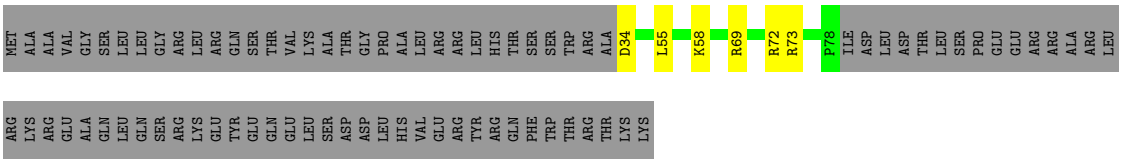
• Molecule 46: Large ribosomal subunit protein mL54

Chain L4:



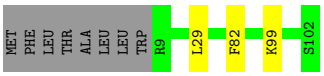
• Molecule 47: Large ribosomal subunit protein mL55

Chain L5:



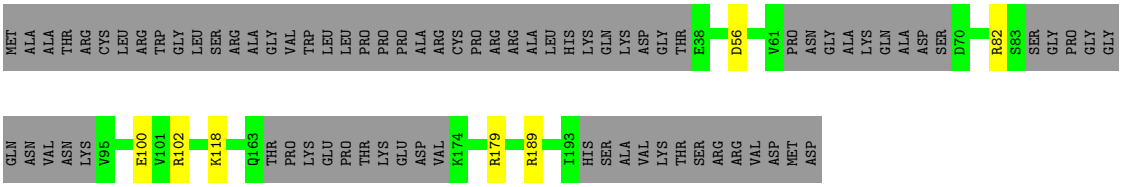
• Molecule 48: Large ribosomal subunit protein mL63

Chain L6:



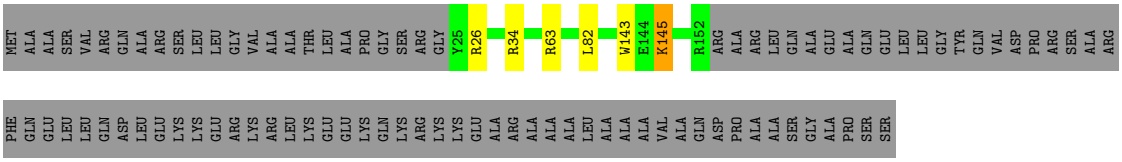
• Molecule 49: Large ribosomal subunit protein mL62

Chain L7:



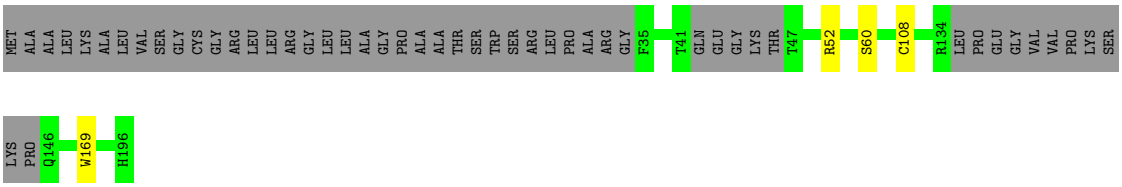
• Molecule 50: Large ribosomal subunit protein mL64

Chain L8:



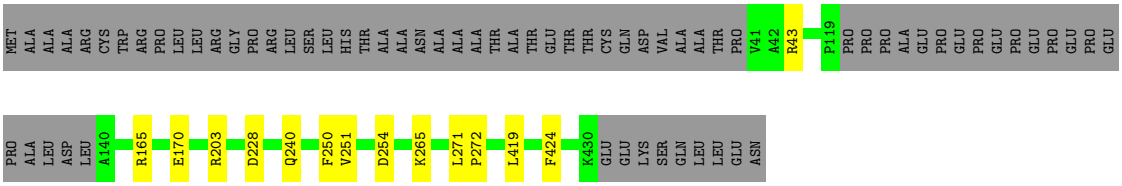
• Molecule 51: Large ribosomal subunit protein mL66

Chain SR:



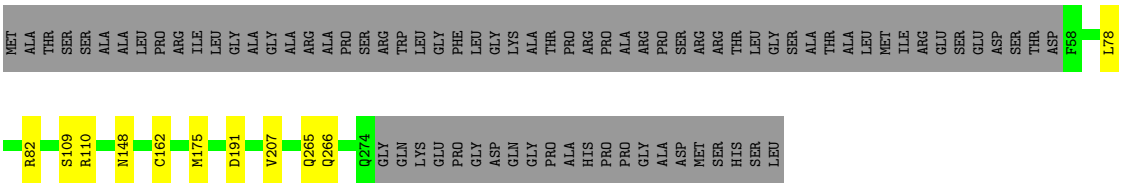
• Molecule 52: Large ribosomal subunit protein mL65

Chain Sf:



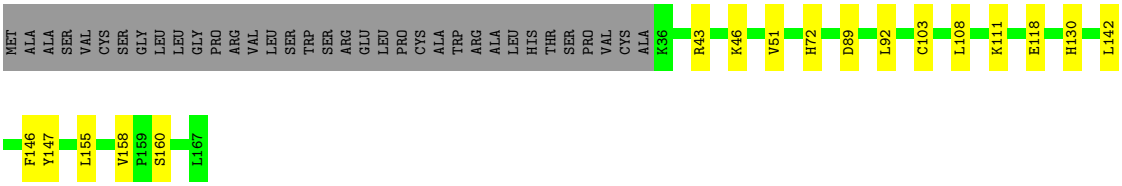
• Molecule 53: Small ribosomal subunit protein uS2m

Chain SB:



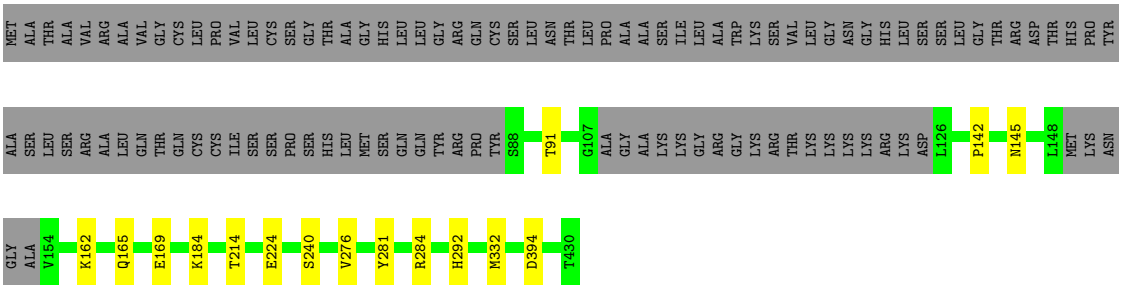
• Molecule 54: Small ribosomal subunit protein uS3m

Chain SZ:



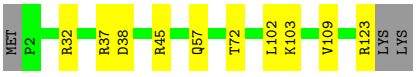
• Molecule 55: Small ribosomal subunit protein uS5m

Chain SE:



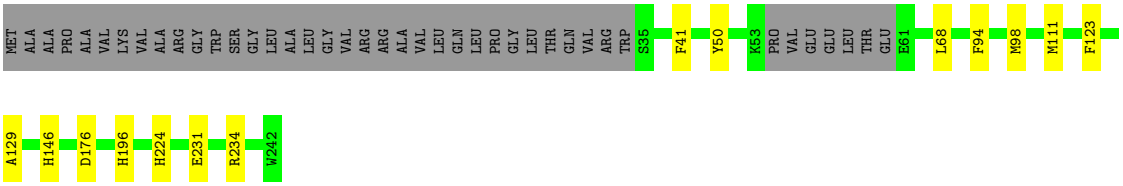
• Molecule 56: Small ribosomal subunit protein bS6m

Chain SF:



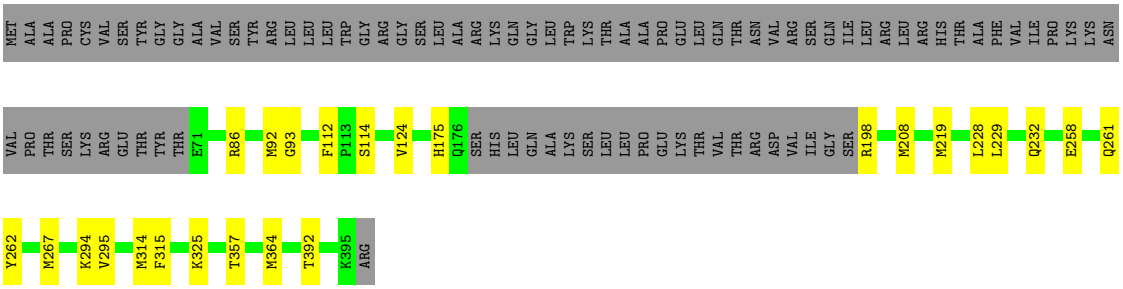
• Molecule 57: Small ribosomal subunit protein uS7m

Chain SG:



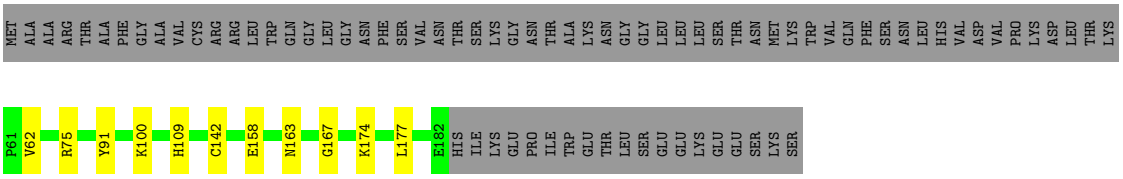
• Molecule 58: Small ribosomal subunit protein uS9m

Chain SI:



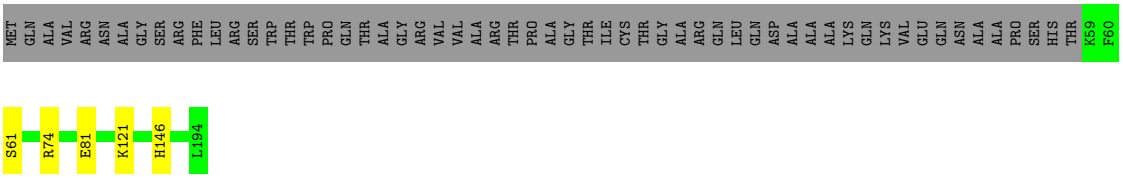
• Molecule 59: Small ribosomal subunit protein uS10m

Chain SJ:



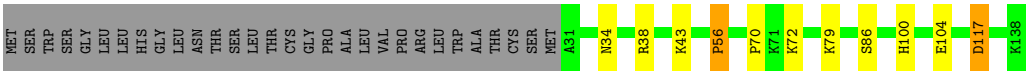
• Molecule 60: Small ribosomal subunit protein uS11m

Chain SK:



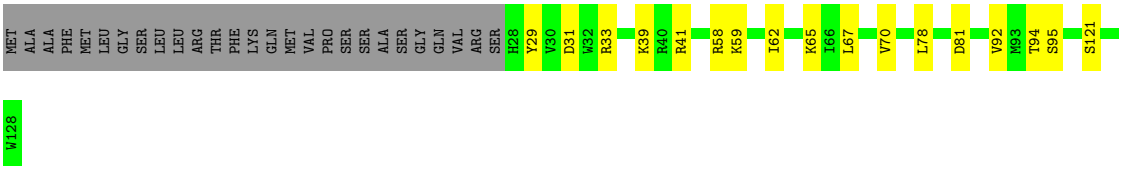
• Molecule 61: Small ribosomal subunit protein uS12m

Chain SL:



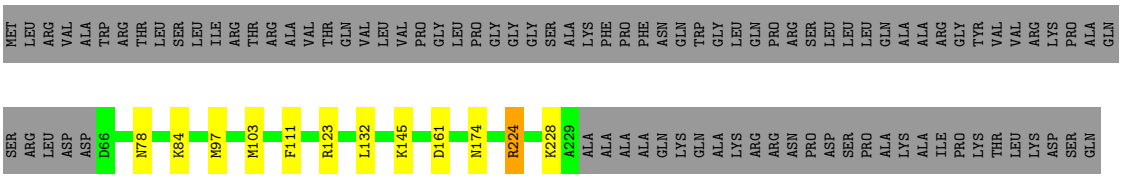
• Molecule 62: Small ribosomal subunit protein uS14m

Chain SN:



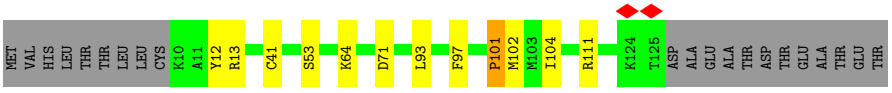
• Molecule 63: Small ribosomal subunit protein uS15m

Chain SO:



• Molecule 64: Small ribosomal subunit protein bS16m

Chain SP:

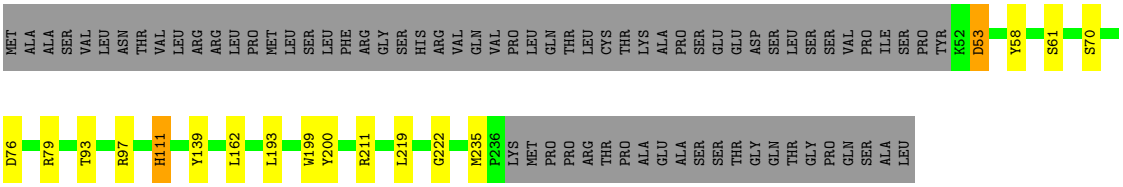


• Molecule 65: Small ribosomal subunit protein uS17m

Chain SQ:

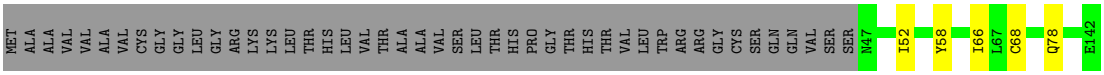
• Molecule 66: Small ribosomal subunit protein mS40

Chain SS:



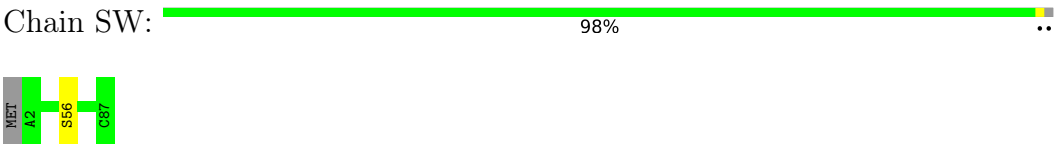
• Molecule 67: Small ribosomal subunit protein bS18m

Chain ST:



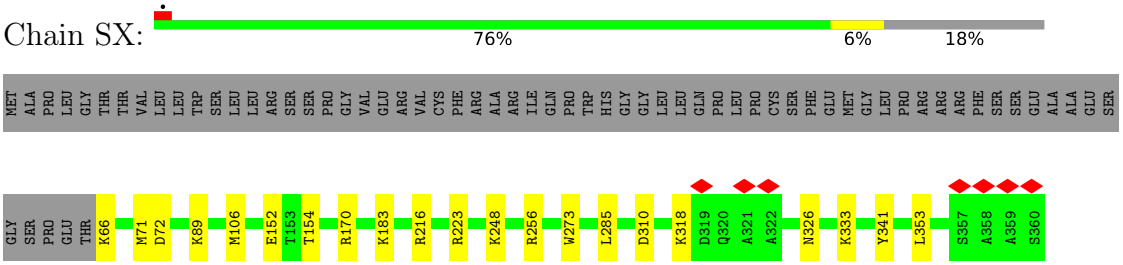
• Molecule 68: Small ribosomal subunit protein bS21m

Chain SW:



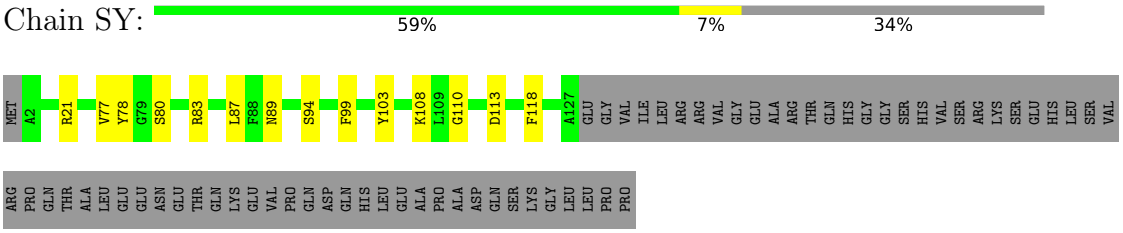
• Molecule 69: Small ribosomal subunit protein mS22

Chain SX:



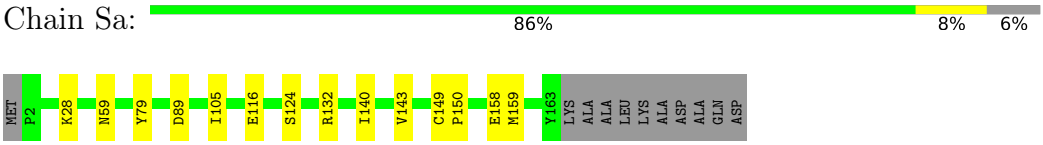
• Molecule 70: Small ribosomal subunit protein mS23

Chain SY:



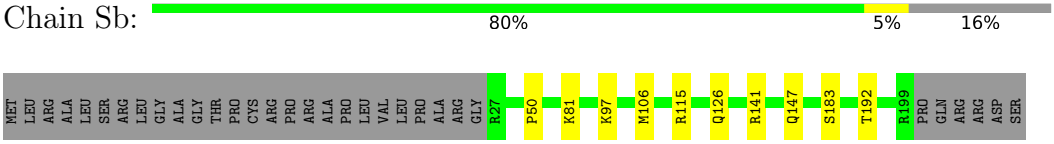
• Molecule 71: Small ribosomal subunit protein mS25

Chain Sa:



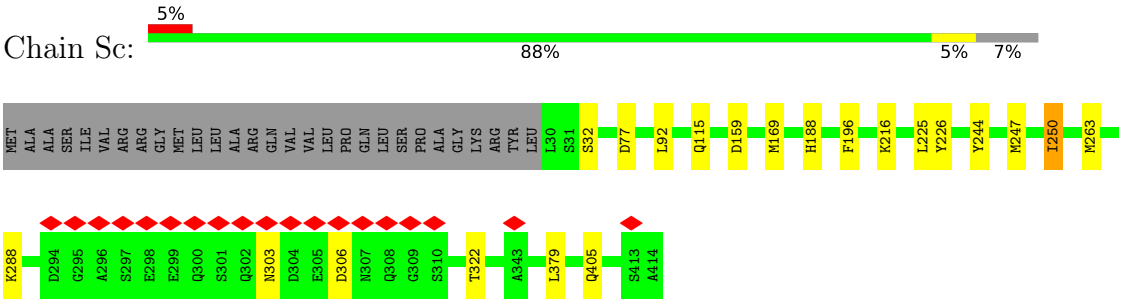
• Molecule 72: Small ribosomal subunit protein mS26

Chain Sb:



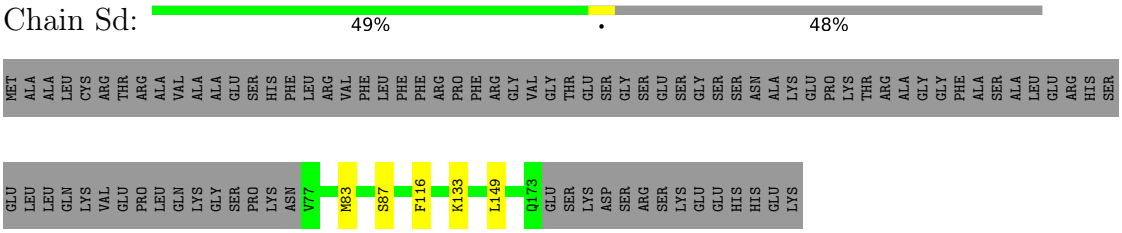
• Molecule 73: Small ribosomal subunit protein mS27

Chain Sc:



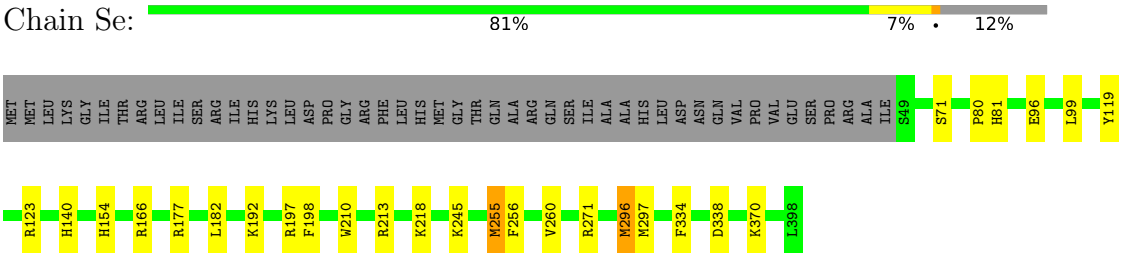
• Molecule 74: Small ribosomal subunit protein bS1m

Chain Sd:



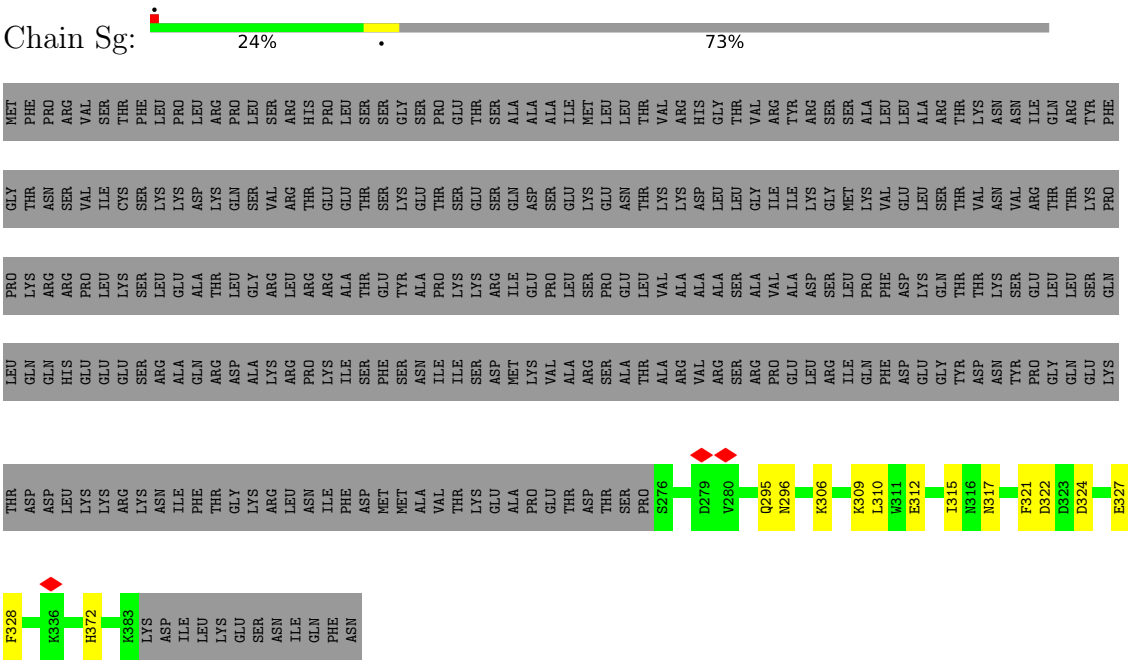
• Molecule 75: Small ribosomal subunit protein mS29

Chain Se:



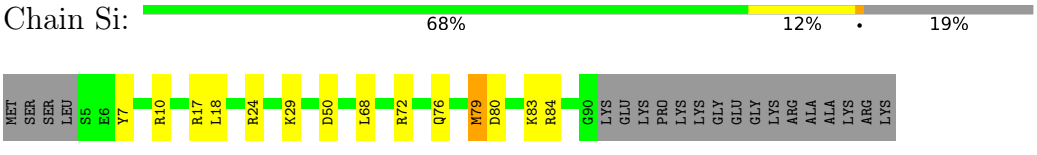
• Molecule 76: Small ribosomal subunit protein mS31

Chain Sg:



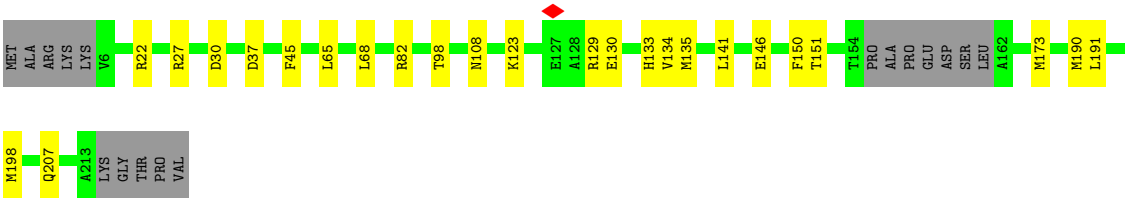
• Molecule 77: Small ribosomal subunit protein mS33

Chain Si:

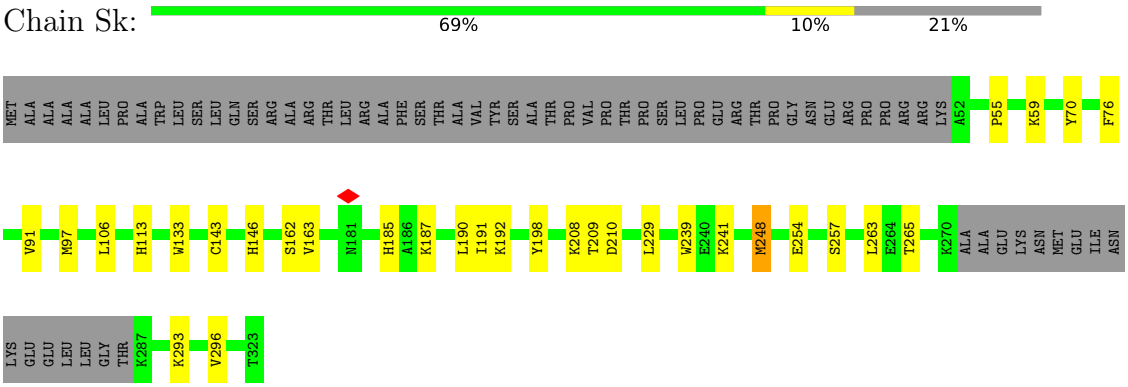


• Molecule 78: Small ribosomal subunit protein mS34

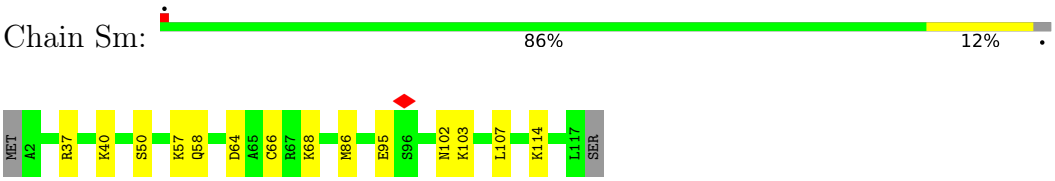
Chain Sj:



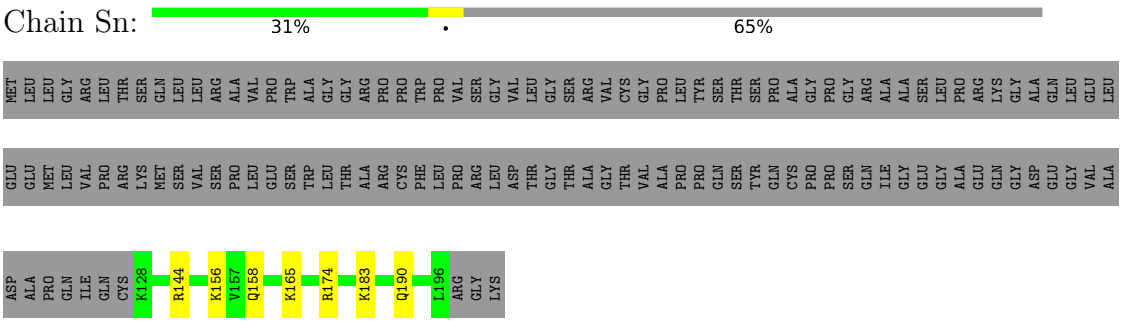
• Molecule 79: Small ribosomal subunit protein mS35



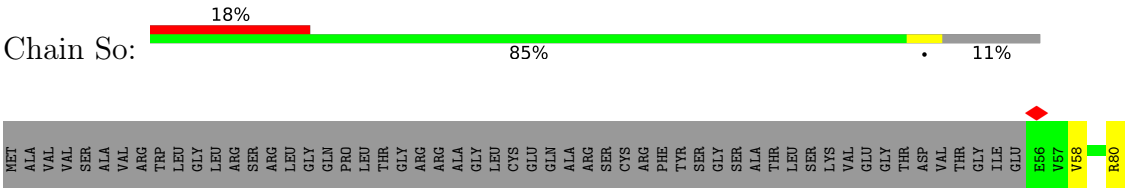
• Molecule 80: Small ribosomal subunit protein mS37

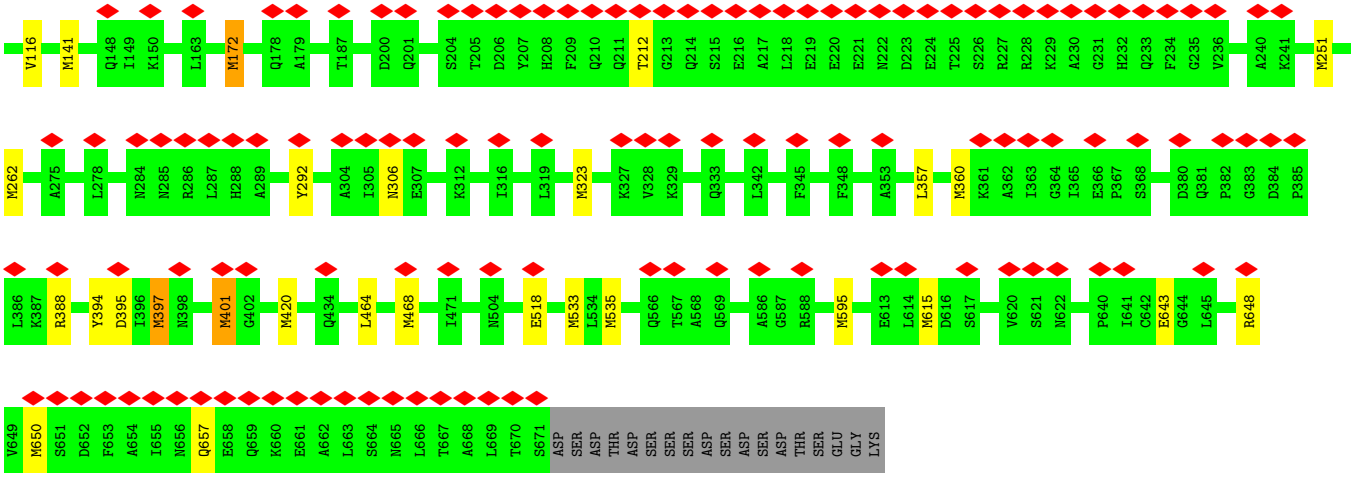


• Molecule 81: Small ribosomal subunit protein mS38



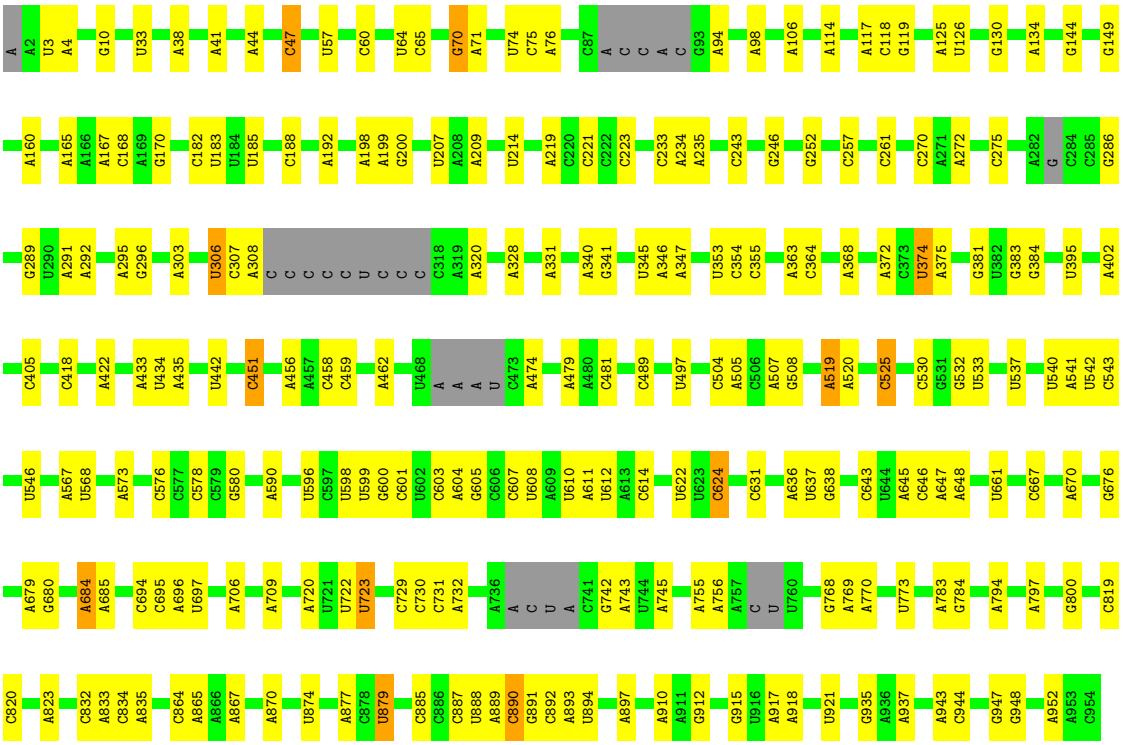
• Molecule 82: Small ribosomal subunit protein mS39





- Molecule 83: 12S rRNA

Chain S1: 73% 23%



4 Experimental information (i)

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.53	0/35628	0.96	43/55448 (0.1%)
2	L2	0.32	0/1328	0.99	0/2056
3	LB	0.41	0/1888	0.69	0/2538
4	LC	0.45	0/2462	0.71	2/3340 (0.1%)
5	LD	0.42	0/2071	0.70	0/2817
6	LI	0.41	0/798	0.80	1/1073 (0.1%)
7	LJ	0.48	0/1308	0.83	1/1761 (0.1%)
8	LK	0.37	0/1340	0.69	2/1802 (0.1%)
9	LM	0.41	0/1495	0.69	0/2029
10	LN	0.43	0/904	0.67	0/1218
11	LO	0.41	0/2359	0.69	1/3185 (0.0%)
12	LP	0.40	0/1826	0.66	0/2458
13	LQ	0.41	0/1269	0.73	1/1708 (0.1%)
14	LR	0.46	0/1215	0.73	0/1645
15	LS	0.35	0/1863	0.61	0/2509
16	LT	0.41	0/1174	0.65	0/1572
17	LU	0.42	0/1311	0.72	0/1778
18	LV	0.43	0/1402	0.65	0/1886
19	LW	0.35	0/1217	0.61	0/1644
20	LX	0.42	0/1697	0.72	1/2302 (0.0%)
21	La	0.44	0/893	0.64	0/1204
22	Lb	0.40	0/2090	0.68	1/2825 (0.0%)
23	Lu	0.39	0/1552	0.63	0/2079
24	Ld	0.44	0/1003	0.72	0/1354
25	Lf	0.44	0/895	0.68	0/1201
26	Lg	0.42	0/438	0.68	0/583
27	Lh	0.44	0/382	0.72	0/507
28	Li	0.34	0/852	0.66	0/1136
29	Lj	0.41	0/349	0.85	1/461 (0.2%)
30	Lk	0.37	0/3305	0.62	1/4502 (0.0%)
31	Ll	0.44	0/3042	0.72	1/4140 (0.0%)
32	Lm	0.36	0/2439	0.60	0/3299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ln	0.45	0/855	0.76	1/1152 (0.1%)
34	Lo	0.43	0/1025	0.68	1/1379 (0.1%)
35	Lp	0.36	0/839	0.68	0/1136
36	Lq	0.46	0/1202	0.70	0/1626
37	Lr	0.45	0/2264	0.68	2/3059 (0.1%)
38	Ls	0.41	0/1800	0.67	2/2436 (0.1%)
39	Lt	0.34	0/1797	0.69	2/2422 (0.1%)
40	Lv	0.46	0/1051	0.70	1/1422 (0.1%)
41	Lw	0.44	0/1134	0.72	0/1547
42	Lx	0.46	0/918	0.66	0/1249
43	Ly	0.41	0/849	0.71	0/1135
44	Lz	0.41	0/747	0.68	1/1005 (0.1%)
45	L3	0.45	0/754	0.86	1/1017 (0.1%)
46	L4	0.49	0/722	0.88	3/978 (0.3%)
47	L5	0.47	0/379	0.80	1/510 (0.2%)
48	L6	0.44	0/818	0.69	0/1097
49	L7	0.44	0/1071	0.74	1/1433 (0.1%)
50	L8	0.35	0/1107	0.68	1/1498 (0.1%)
51	SR	0.40	0/1238	0.70	0/1676
52	Sf	0.42	0/3114	0.70	1/4225 (0.0%)
53	SB	0.47	0/1811	0.75	1/2451 (0.0%)
54	SZ	0.43	0/1112	0.75	1/1505 (0.1%)
55	SE	0.38	0/2590	0.68	1/3477 (0.0%)
56	SF	0.33	0/989	0.66	0/1335
57	SG	0.39	0/1708	0.71	3/2291 (0.1%)
58	SI	0.38	0/2555	0.68	1/3424 (0.0%)
59	SJ	0.41	0/1019	0.91	0/1379
60	SK	0.38	0/1031	0.64	0/1390
61	SL	0.47	0/854	0.75	0/1148
62	SN	0.48	0/879	0.84	1/1182 (0.1%)
63	SO	0.47	0/1406	0.76	1/1878 (0.1%)
64	SP	0.43	0/941	0.75	2/1265 (0.2%)
65	SQ	0.48	0/864	0.74	0/1169
66	SS	0.44	0/1580	0.75	1/2150 (0.0%)
67	ST	0.48	0/791	0.76	0/1062
68	SW	0.44	0/752	0.76	0/1001
69	SX	0.38	0/2452	0.72	4/3310 (0.1%)
70	SY	0.44	0/1069	0.69	0/1441
71	Sa	0.45	0/1361	0.70	0/1829
72	Sb	0.38	0/1474	0.71	0/1976
73	Sc	0.33	0/3177	0.66	5/4292 (0.1%)
74	Sd	0.50	0/778	0.77	0/1048
75	Se	0.35	0/2908	0.63	4/3936 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Sg	0.42	0/931	0.73	2/1259 (0.2%)
77	Si	0.41	0/748	0.84	2/1000 (0.2%)
78	Sj	0.39	0/1723	0.80	1/2334 (0.0%)
79	Sk	0.45	0/2113	0.81	3/2863 (0.1%)
80	Sm	0.39	0/939	0.74	0/1256
81	Sn	0.40	0/621	0.76	0/820
82	So	0.33	0/5093	0.68	11/6891 (0.2%)
83	S1	0.41	0/22053	0.96	42/34324 (0.1%)
All	All	0.44	0/173801	0.81	160/246748 (0.1%)

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

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

There are no bond length outliers.

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	L3	70	ASP	CB-CG-OD1	8.78	126.20	118.30
29	Lj	76	CYS	CB-CA-C	-8.63	93.13	110.40
1	L1	554	C	N1-C2-O2	8.21	123.83	118.90
82	So	397	MET	CA-CB-CG	8.21	127.26	113.30
1	L1	554	C	C2-N1-C1'	7.90	127.49	118.80
53	SB	148	ASN	CB-CA-C	-7.70	94.99	110.40
69	SX	353	LEU	CA-CB-CG	7.62	132.83	115.30
52	Sf	254	ASP	CB-CG-OD1	7.60	125.14	118.30
1	L1	837	A	C2'-C3'-O3'	7.52	126.04	109.50
69	SX	285	LEU	CA-CB-CG	7.21	131.87	115.30
83	S1	819	C	N1-C2-O2	7.14	123.18	118.90
46	L4	89	ASP	CB-CG-OD1	7.08	124.67	118.30
82	So	401	MET	CG-SD-CE	-7.06	88.91	100.20
13	LQ	75	MET	CB-CG-SD	-7.01	91.38	112.40
77	Si	18	LEU	CB-CG-CD2	-6.95	99.19	111.00
75	Se	260	VAL	CG1-CB-CG2	-6.87	99.90	110.90
83	S1	661	U	C2-N1-C1'	6.85	125.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	SS	53	ASP	CB-CG-OD1	6.84	124.45	118.30
34	Lo	106	ASP	CB-CG-OD1	6.83	124.45	118.30
22	Lb	18	GLU	C-N-CA	-6.78	108.06	122.30
1	L1	428	G	O4'-C1'-N9	6.61	113.49	108.20
77	Si	79	MET	CA-CB-CG	6.58	124.49	113.30
1	L1	554	C	N3-C2-O2	-6.55	117.31	121.90
82	So	357	LEU	CA-CB-CG	6.53	130.31	115.30
83	S1	374	U	N3-C2-O2	-6.50	117.65	122.20
1	L1	887	C	N1-C2-O2	6.50	122.80	118.90
82	So	595	MET	CG-SD-CE	-6.47	89.84	100.20
82	So	397	MET	CB-CG-SD	6.43	131.68	112.40
40	Lv	188	GLU	CA-CB-CG	6.37	127.41	113.40
8	LK	167	PHE	CB-CG-CD1	6.36	125.25	120.80
83	S1	47	C	N3-C2-O2	-6.35	117.46	121.90
76	Sg	328	PHE	CB-CG-CD2	-6.32	116.38	120.80
83	S1	596	U	N3-C2-O2	-6.30	117.79	122.20
6	LI	145	LEU	CA-CB-CG	6.24	129.66	115.30
82	So	420	MET	CA-CB-CG	6.24	123.91	113.30
83	S1	784	G	C3'-C2'-C1'	-6.22	96.52	101.50
7	LJ	60	ILE	CG1-CB-CG2	-6.22	97.71	111.40
83	S1	624	C	C2-N1-C1'	6.16	125.58	118.80
83	S1	374	U	N1-C2-O2	6.13	127.09	122.80
82	So	172	MET	CA-CB-CG	6.11	123.69	113.30
37	Lr	63	LYS	CB-CA-C	6.09	122.58	110.40
37	Lr	122	ASN	CB-CA-C	-6.08	98.24	110.40
82	So	650	MET	CA-CB-CG	6.08	123.63	113.30
1	L1	50	C	N1-C2-O2	6.05	122.53	118.90
83	S1	637	U	N3-C2-O2	-6.05	117.97	122.20
1	L1	551	C	OP1-P-O3'	6.05	118.50	105.20
1	L1	428	G	C1'-O4'-C4'	-6.04	105.07	109.90
55	SE	281	TYR	CB-CA-C	-6.04	98.33	110.40
73	Sc	225	LEU	CA-CB-CG	6.03	129.17	115.30
46	L4	86	LEU	CA-CB-CG	5.99	129.08	115.30
39	Lt	116	LEU	CA-CB-CG	5.96	129.00	115.30
50	L8	145	LYS	CB-CG-CD	5.94	127.04	111.60
83	S1	723	U	N3-C2-O2	-5.92	118.06	122.20
83	S1	694	C	N3-C4-N4	-5.92	113.86	118.00
83	S1	661	U	N3-C2-O2	-5.89	118.07	122.20
75	Se	296	MET	CB-CG-SD	5.89	130.07	112.40
83	S1	374	U	P-O3'-C3'	5.88	126.75	119.70
83	S1	684	A	P-O3'-C3'	5.85	126.72	119.70
20	LX	102	MET	CA-CB-CG	5.85	123.24	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	S1	661	U	N1-C2-O2	5.85	126.89	122.80
47	L5	34	ASP	CB-CG-OD1	5.83	123.55	118.30
83	S1	519	A	P-O3'-C3'	5.82	126.68	119.70
78	Sj	68	LEU	CA-CB-CG	5.82	128.68	115.30
1	L1	554	C	C6-N1-C2	-5.78	117.99	120.30
83	S1	890	C	N3-C2-O2	-5.78	117.86	121.90
1	L1	908	C	N1-C2-O2	5.77	122.36	118.90
73	Sc	405	GLN	CA-CB-CG	5.76	126.06	113.40
64	SP	102	MET	CA-CB-CG	-5.75	103.53	113.30
62	SN	78	LEU	CA-CB-CG	5.73	128.47	115.30
83	S1	70	G	P-O3'-C3'	5.72	126.56	119.70
1	L1	19	C	N1-C2-O2	5.72	122.33	118.90
83	S1	608	U	N3-C2-O2	-5.71	118.20	122.20
83	S1	820	C	N1-C2-O2	5.69	122.31	118.90
83	S1	47	C	N1-C2-O2	5.67	122.30	118.90
83	S1	596	U	N1-C2-O2	5.67	126.77	122.80
4	LC	281	ASN	CB-CA-C	5.66	121.72	110.40
79	Sk	229	LEU	CB-CG-CD2	-5.65	101.39	111.00
83	S1	832	C	C2-N1-C1'	5.65	125.02	118.80
83	S1	832	C	C6-N1-C2	-5.62	118.05	120.30
1	L1	819	C	C2-N1-C1'	5.58	124.94	118.80
83	S1	890	C	P-O3'-C3'	5.58	126.40	119.70
1	L1	1532	U	C5-C6-N1	5.58	125.49	122.70
1	L1	889	U	P-O3'-C3'	5.55	126.36	119.70
64	SP	101	PRO	N-CA-CB	-5.55	96.50	102.60
1	L1	887	C	C2-N1-C1'	5.54	124.89	118.80
83	S1	624	C	N1-C2-O2	5.53	122.22	118.90
1	L1	33	C	C6-N1-C2	-5.50	118.10	120.30
79	Sk	263	LEU	CA-CB-CG	5.50	127.94	115.30
82	So	464	LEU	CA-CB-CG	5.46	127.85	115.30
1	L1	75	U	N3-C2-O2	-5.45	118.38	122.20
83	S1	944	C	C2-N1-C1'	5.45	124.80	118.80
73	Sc	169	MET	CA-CB-CG	5.43	122.54	113.30
1	L1	757	C	C2-N1-C1'	5.43	124.77	118.80
1	L1	113	U	N1-C2-O2	5.41	126.59	122.80
1	L1	55	C	N1-C2-O2	5.39	122.14	118.90
73	Sc	92	LEU	CA-CB-CG	5.38	127.68	115.30
83	S1	505	A	C4-N9-C1'	5.38	135.99	126.30
30	Lk	143	PRO	CA-N-CD	-5.38	103.97	111.50
83	S1	819	C	N3-C2-O2	-5.37	118.14	121.90
1	L1	75	U	N1-C2-O2	5.36	126.55	122.80
4	LC	317	PRO	N-CA-C	-5.36	98.17	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	Sc	379	LEU	CA-CB-CG	5.35	127.60	115.30
83	S1	608	U	N1-C2-O2	5.34	126.53	122.80
1	L1	614	C	N1-C2-O2	5.33	122.10	118.90
83	S1	605	G	C5-C6-O6	5.32	131.79	128.60
1	L1	614	C	C2-N1-C1'	5.31	124.65	118.80
1	L1	551	C	P-O3'-C3'	5.30	126.06	119.70
83	S1	694	C	C5-C4-N4	5.29	123.90	120.20
83	S1	890	C	C6-N1-C2	-5.29	118.18	120.30
69	SX	71	MET	CA-CB-CG	5.29	122.29	113.30
1	L1	113	U	N3-C2-O2	-5.28	118.50	122.20
8	LK	91	LEU	CA-CB-CG	5.28	127.45	115.30
82	So	535	MET	CA-CB-CG	5.28	122.28	113.30
1	L1	741	U	N1-C2-O2	5.28	126.49	122.80
1	L1	75	U	C2-N1-C1'	5.28	124.03	117.70
1	L1	860	A	P-O3'-C3'	5.27	126.03	119.70
57	SG	68	LEU	CA-CB-CG	5.27	127.43	115.30
75	Se	182	LEU	CA-CB-CG	5.26	127.41	115.30
38	Ls	202	MET	CB-CG-SD	5.24	128.13	112.40
1	L1	554	C	C6-N1-C1'	-5.24	114.52	120.80
44	Lz	40	TYR	CA-CB-CG	5.24	123.35	113.40
1	L1	990	U	N3-C2-O2	-5.23	118.54	122.20
1	L1	1482	C	C2-N1-C1'	5.22	124.55	118.80
83	S1	525	C	C2-N1-C1'	5.22	124.55	118.80
83	S1	530	C	C2-N1-C1'	5.22	124.54	118.80
1	L1	887	C	N3-C2-O2	-5.20	118.26	121.90
46	L4	96	LEU	CA-CB-CG	5.19	127.24	115.30
76	Sg	324	ASP	CB-CG-OD1	5.19	122.97	118.30
54	SZ	147	TYR	CA-CB-CG	5.19	123.26	113.40
1	L1	1558	U	N3-C2-O2	-5.19	118.57	122.20
1	L1	56	C	C6-N1-C2	-5.17	118.23	120.30
58	SI	267	MET	CA-CB-CG	5.16	122.08	113.30
1	L1	819	C	C6-N1-C2	-5.15	118.24	120.30
83	S1	433	A	O4'-C1'-N9	5.15	112.32	108.20
33	Ln	103	GLN	CA-CB-CG	5.15	124.72	113.40
57	SG	234	ARG	CB-CA-C	-5.15	100.11	110.40
63	SO	224	ARG	CB-CG-CD	5.15	124.98	111.60
79	Sk	248	MET	CA-CB-CG	5.14	122.05	113.30
39	Lt	237	LEU	CA-CB-CG	5.14	127.12	115.30
11	LO	180	ASP	CB-CG-OD1	5.11	122.90	118.30
82	So	58	VAL	CG1-CB-CG2	-5.11	102.72	110.90
69	SX	285	LEU	CB-CG-CD2	5.10	119.68	111.00
1	L1	1057	C	C6-N1-C2	-5.10	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L1	554	C	C5-C6-N1	5.10	123.55	121.00
83	S1	879	U	C2-N1-C1'	5.05	123.77	117.70
31	Ll	51	TYR	CB-CA-C	-5.05	100.30	110.40
83	S1	694	C	C2-N1-C1'	-5.05	113.25	118.80
57	SG	111	MET	CB-CG-SD	-5.04	97.27	112.40
1	L1	1487	C	C6-N1-C2	-5.04	118.28	120.30
1	L1	741	U	C2-N1-C1'	5.04	123.75	117.70
83	S1	442	U	N3-C2-O2	-5.03	118.68	122.20
1	L1	1542	C	O4'-C1'-N1	5.03	112.22	108.20
49	L7	56	ASP	CB-CG-OD1	5.03	122.83	118.30
83	S1	451	C	C2-N1-C1'	5.02	124.32	118.80
38	Ls	202	MET	CA-CB-CG	5.02	121.83	113.30
83	S1	306	U	C2-N1-C1'	5.02	123.72	117.70
75	Se	255	MET	CB-CG-SD	5.01	127.44	112.40
83	S1	637	U	N1-C2-O2	5.01	126.30	122.80
1	L1	59	U	N3-C2-O2	-5.00	118.70	122.20
1	L1	924	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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%)	224 (95%)	9 (4%)	2 (1%)	14 43
4	LC	302/348 (87%)	275 (91%)	25 (8%)	2 (1%)	19 49
5	LD	248/311 (80%)	233 (94%)	15 (6%)	0	100 100
6	LI	93/267 (35%)	83 (89%)	10 (11%)	0	100 100
7	LJ	154/261 (59%)	132 (86%)	19 (12%)	3 (2%)	6 24
8	LK	173/192 (90%)	156 (90%)	15 (9%)	2 (1%)	11 35
9	LM	175/178 (98%)	164 (94%)	10 (6%)	1 (1%)	22 52
10	LN	113/145 (78%)	103 (91%)	10 (9%)	0	100 100
11	LO	285/296 (96%)	274 (96%)	10 (4%)	1 (0%)	30 60
12	LP	219/251 (87%)	214 (98%)	4 (2%)	1 (0%)	25 56
13	LQ	150/175 (86%)	141 (94%)	8 (5%)	1 (1%)	19 49
14	LR	144/179 (80%)	138 (96%)	6 (4%)	0	100 100
15	LS	217/292 (74%)	206 (95%)	11 (5%)	0	100 100
16	LT	138/149 (93%)	135 (98%)	3 (2%)	0	100 100
17	LU	158/205 (77%)	150 (95%)	7 (4%)	1 (1%)	22 52
18	LV	164/212 (77%)	151 (92%)	12 (7%)	1 (1%)	22 52
19	LW	139/153 (91%)	138 (99%)	1 (1%)	0	100 100
20	LX	200/216 (93%)	184 (92%)	16 (8%)	0	100 100
21	La	109/148 (74%)	104 (95%)	5 (5%)	0	100 100
22	Lb	241/256 (94%)	225 (93%)	15 (6%)	1 (0%)	30 60
23	Lu	174/250 (70%)	167 (96%)	6 (3%)	1 (1%)	22 52
24	Ld	118/161 (73%)	111 (94%)	7 (6%)	0	100 100
25	Lf	106/188 (56%)	101 (95%)	5 (5%)	0	100 100
26	Lg	50/65 (77%)	49 (98%)	1 (2%)	0	100 100
27	Lh	44/92 (48%)	42 (96%)	2 (4%)	0	100 100
28	Li	93/188 (50%)	90 (97%)	3 (3%)	0	100 100
29	Lj	36/103 (35%)	36 (100%)	0	0	100 100
30	Lk	392/423 (93%)	375 (96%)	17 (4%)	0	100 100
31	Ll	352/380 (93%)	323 (92%)	26 (7%)	3 (1%)	14 43
32	Lm	291/338 (86%)	278 (96%)	12 (4%)	1 (0%)	37 66
33	Ln	97/206 (47%)	81 (84%)	14 (14%)	2 (2%)	5 22
34	Lo	122/137 (89%)	115 (94%)	6 (5%)	1 (1%)	16 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Lp	93/142 (66%)	89 (96%)	4 (4%)	0	100	100
36	Lq	146/215 (68%)	133 (91%)	13 (9%)	0	100	100
37	Lr	271/332 (82%)	261 (96%)	10 (4%)	0	100	100
38	Ls	210/306 (69%)	200 (95%)	10 (5%)	0	100	100
39	Lt	211/279 (76%)	186 (88%)	23 (11%)	2 (1%)	14	43
40	Lv	125/212 (59%)	114 (91%)	10 (8%)	1 (1%)	16	45
41	Lw	130/166 (78%)	121 (93%)	8 (6%)	1 (1%)	16	45
42	Lx	108/158 (68%)	103 (95%)	4 (4%)	1 (1%)	14	43
43	Ly	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
44	Lz	90/123 (73%)	84 (93%)	6 (7%)	0	100	100
45	L3	94/112 (84%)	79 (84%)	14 (15%)	1 (1%)	12	37
46	L4	81/138 (59%)	73 (90%)	6 (7%)	2 (2%)	4	18
47	L5	43/128 (34%)	38 (88%)	4 (9%)	1 (2%)	5	20
48	L6	92/102 (90%)	90 (98%)	2 (2%)	0	100	100
49	L7	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
50	L8	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
51	SR	140/196 (71%)	134 (96%)	6 (4%)	0	100	100
52	Sf	366/439 (83%)	345 (94%)	19 (5%)	2 (0%)	25	56
53	SB	215/296 (73%)	200 (93%)	15 (7%)	0	100	100
54	SZ	130/167 (78%)	111 (85%)	18 (14%)	1 (1%)	16	45
55	SE	314/430 (73%)	289 (92%)	24 (8%)	1 (0%)	37	66
56	SF	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
57	SG	197/242 (81%)	192 (98%)	4 (2%)	1 (0%)	25	56
58	SI	300/396 (76%)	267 (89%)	28 (9%)	5 (2%)	7	27
59	SJ	120/201 (60%)	101 (84%)	18 (15%)	1 (1%)	16	45
60	SK	134/194 (69%)	126 (94%)	8 (6%)	0	100	100
61	SL	106/138 (77%)	90 (85%)	12 (11%)	4 (4%)	2	11
62	SN	99/128 (77%)	86 (87%)	12 (12%)	1 (1%)	13	40
63	SO	162/257 (63%)	148 (91%)	12 (7%)	2 (1%)	11	35
64	SP	114/137 (83%)	105 (92%)	7 (6%)	2 (2%)	7	25
65	SQ	105/130 (81%)	91 (87%)	10 (10%)	4 (4%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
66	SS	183/258 (71%)	156 (85%)	24 (13%)	3 (2%)	8 28
67	ST	94/142 (66%)	89 (95%)	4 (4%)	1 (1%)	12 37
68	SW	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
69	SX	293/360 (81%)	274 (94%)	19 (6%)	0	100 100
70	SY	124/190 (65%)	115 (93%)	7 (6%)	2 (2%)	8 28
71	Sa	160/173 (92%)	143 (89%)	14 (9%)	3 (2%)	6 24
72	Sb	171/205 (83%)	168 (98%)	2 (1%)	1 (1%)	22 52
73	Sc	383/414 (92%)	364 (95%)	18 (5%)	1 (0%)	37 66
74	Sd	95/187 (51%)	85 (90%)	9 (10%)	1 (1%)	12 37
75	Se	348/398 (87%)	333 (96%)	13 (4%)	2 (1%)	22 52
76	Sg	106/395 (27%)	98 (92%)	7 (7%)	1 (1%)	14 43
77	Si	84/106 (79%)	78 (93%)	6 (7%)	0	100 100
78	Sj	197/218 (90%)	161 (82%)	31 (16%)	5 (2%)	4 18
79	Sk	252/323 (78%)	217 (86%)	33 (13%)	2 (1%)	16 45
80	Sm	114/118 (97%)	107 (94%)	6 (5%)	1 (1%)	14 43
81	Sn	67/199 (34%)	65 (97%)	2 (3%)	0	100 100
82	So	614/689 (89%)	595 (97%)	19 (3%)	0	100 100
All	All	13557/17977 (75%)	12631 (93%)	846 (6%)	80 (1%)	24 52

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	LC	82	ASP
13	LQ	111	PRO
22	Lb	92	ALA
39	Lt	266	PRO
39	Lt	270	ALA
46	L4	88	PRO
58	SI	92	MET
61	SL	56	PRO
63	SO	78	ASN
71	Sa	143	VAL
74	Sd	116	PHE
76	Sg	317	ASN
7	LJ	104	LEU
11	LO	280	LYS

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Mol	Chain	Res	Type
17	LU	179	ASN
31	Ll	241	PRO
42	Lx	147	ASN
45	L3	47	LEU
58	SI	114	SER
61	SL	117	ASP
62	SN	95	SER
65	SQ	88	VAL
65	SQ	101	ALA
78	Sj	45	PHE
78	Sj	151	THR
79	Sk	76	PHE
3	LB	195	ASN
8	LK	34	PRO
12	LP	46	GLU
32	Lm	60	PRO
47	L5	72	ARG
52	Sf	250	PHE
52	Sf	272	PRO
57	SG	129	ALA
61	SL	70	PRO
61	SL	72	LYS
63	SO	123	ARG
64	SP	12	TYR
66	SS	222	GLY
67	ST	78	GLN
72	Sb	50	PRO
75	Se	80	PRO
78	Sj	98	THR
80	Sm	64	ASP
9	LM	151	ILE
41	Lw	145	GLY
46	L4	136	LYS
54	SZ	155	LEU
58	SI	93	GLY
58	SI	392	THR
71	Sa	132	ARG
78	Sj	133	HIS
3	LB	67	LYS
4	LC	317	PRO
7	LJ	92	ASP
34	Lo	121	PRO

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Mol	Chain	Res	Type
40	Lv	59	TYR
31	Ll	287	PRO
33	Ln	165	ASP
33	Ln	170	PRO
64	SP	64	LYS
66	SS	111	HIS
31	Ll	36	PRO
65	SQ	97	GLY
66	SS	200	TYR
75	Se	338	ASP
8	LK	31	PRO
65	SQ	99	PRO
71	Sa	105	ILE
73	Sc	250	ILE
79	Sk	191	ILE
70	SY	110	GLY
7	LJ	175	PRO
18	LV	69	ARG
70	SY	77	VAL
78	Sj	134	VAL
23	Lu	203	PRO
55	SE	142	PRO
58	SI	295	VAL
59	SJ	167	GLY

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%)	186 (97%)	5 (3%)	41 74
4	LC	258/290 (89%)	250 (97%)	8 (3%)	35 70
5	LD	217/262 (83%)	210 (97%)	7 (3%)	34 69
6	LI	86/228 (38%)	77 (90%)	9 (10%)	5 18
7	LJ	145/232 (62%)	135 (93%)	10 (7%)	13 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	LK	137/150 (91%)	126 (92%)	11 (8%)	10 30
9	LM	155/156 (99%)	153 (99%)	2 (1%)	65 88
10	LN	98/124 (79%)	94 (96%)	4 (4%)	26 60
11	LO	245/249 (98%)	237 (97%)	8 (3%)	33 68
12	LP	188/211 (89%)	181 (96%)	7 (4%)	29 64
13	LQ	133/150 (89%)	126 (95%)	7 (5%)	19 49
14	LR	128/154 (83%)	126 (98%)	2 (2%)	58 84
15	LS	201/256 (78%)	197 (98%)	4 (2%)	50 79
16	LT	118/126 (94%)	114 (97%)	4 (3%)	32 67
17	LU	145/180 (81%)	143 (99%)	2 (1%)	62 86
18	LV	146/182 (80%)	144 (99%)	2 (1%)	62 86
19	LW	128/135 (95%)	128 (100%)	0	100 100
20	LX	180/191 (94%)	169 (94%)	11 (6%)	15 43
21	La	91/119 (76%)	88 (97%)	3 (3%)	33 68
22	Lb	219/229 (96%)	210 (96%)	9 (4%)	26 60
23	Lu	159/223 (71%)	150 (94%)	9 (6%)	17 47
24	Ld	111/147 (76%)	107 (96%)	4 (4%)	30 65
25	Lf	97/164 (59%)	93 (96%)	4 (4%)	26 60
26	Lg	49/60 (82%)	47 (96%)	2 (4%)	26 60
27	Lh	40/72 (56%)	38 (95%)	2 (5%)	20 52
28	Li	88/166 (53%)	86 (98%)	2 (2%)	45 77
29	Lj	37/89 (42%)	35 (95%)	2 (5%)	18 49
30	Lk	353/368 (96%)	341 (97%)	12 (3%)	32 67
31	Ll	313/332 (94%)	301 (96%)	12 (4%)	28 63
32	Lm	269/303 (89%)	257 (96%)	12 (4%)	23 56
33	Ln	91/190 (48%)	82 (90%)	9 (10%)	6 21
34	Lo	104/112 (93%)	102 (98%)	2 (2%)	52 81
35	Lp	93/133 (70%)	83 (89%)	10 (11%)	5 17
36	Lq	130/186 (70%)	124 (95%)	6 (5%)	23 55
37	Lr	241/288 (84%)	234 (97%)	7 (3%)	37 72
38	Ls	196/274 (72%)	185 (94%)	11 (6%)	17 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	Lt	188/236 (80%)	171 (91%)	17 (9%)	8 25
40	Lv	116/188 (62%)	103 (89%)	13 (11%)	5 16
41	Lw	122/148 (82%)	115 (94%)	7 (6%)	17 47
42	Lx	104/148 (70%)	95 (91%)	9 (9%)	8 27
43	Ly	86/110 (78%)	84 (98%)	2 (2%)	45 77
44	Lz	73/97 (75%)	73 (100%)	0	100 100
45	L3	81/90 (90%)	75 (93%)	6 (7%)	11 34
46	L4	78/116 (67%)	73 (94%)	5 (6%)	14 41
47	L5	40/113 (35%)	36 (90%)	4 (10%)	6 20
48	L6	80/87 (92%)	77 (96%)	3 (4%)	28 63
49	L7	117/181 (65%)	111 (95%)	6 (5%)	20 51
50	L8	110/178 (62%)	104 (94%)	6 (6%)	18 48
51	SR	133/169 (79%)	129 (97%)	4 (3%)	36 71
52	Sf	326/381 (86%)	315 (97%)	11 (3%)	32 67
53	SB	191/249 (77%)	181 (95%)	10 (5%)	19 50
54	SZ	115/143 (80%)	100 (87%)	15 (13%)	3 11
55	SE	267/357 (75%)	253 (95%)	14 (5%)	19 50
56	SF	104/107 (97%)	94 (90%)	10 (10%)	7 22
57	SG	178/209 (85%)	168 (94%)	10 (6%)	17 47
58	SI	263/342 (77%)	244 (93%)	19 (7%)	12 35
59	SJ	112/180 (62%)	102 (91%)	10 (9%)	8 26
60	SK	104/147 (71%)	99 (95%)	5 (5%)	21 54
61	SL	93/118 (79%)	84 (90%)	9 (10%)	6 22
62	SN	91/113 (80%)	76 (84%)	15 (16%)	2 6
63	SO	152/226 (67%)	142 (93%)	10 (7%)	14 39
64	SP	95/113 (84%)	86 (90%)	9 (10%)	7 22
65	SQ	93/115 (81%)	91 (98%)	2 (2%)	47 78
66	SS	166/230 (72%)	150 (90%)	16 (10%)	7 22
67	ST	87/123 (71%)	83 (95%)	4 (5%)	23 55
68	SW	78/79 (99%)	77 (99%)	1 (1%)	65 88
69	SX	263/318 (83%)	245 (93%)	18 (7%)	13 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
70	SY	109/164 (66%)	97 (89%)	12 (11%)	5 16
71	Sa	150/157 (96%)	139 (93%)	11 (7%)	11 34
72	Sb	148/174 (85%)	139 (94%)	9 (6%)	15 43
73	Sc	338/364 (93%)	322 (95%)	16 (5%)	22 55
74	Sd	84/158 (53%)	80 (95%)	4 (5%)	21 54
75	Se	310/351 (88%)	286 (92%)	24 (8%)	10 31
76	Sg	97/357 (27%)	87 (90%)	10 (10%)	6 19
77	Si	79/95 (83%)	66 (84%)	13 (16%)	2 6
78	Sj	175/190 (92%)	156 (89%)	19 (11%)	5 17
79	Sk	235/291 (81%)	207 (88%)	28 (12%)	4 13
80	Sm	99/101 (98%)	86 (87%)	13 (13%)	3 10
81	Sn	63/166 (38%)	56 (89%)	7 (11%)	5 16
82	So	548/609 (90%)	525 (96%)	23 (4%)	25 59
All	All	12121/15564 (78%)	11441 (94%)	680 (6%)	20 47

All (680) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LB	78	LYS
3	LB	85	ARG
3	LB	172	MET
3	LB	287	ARG
3	LB	297	LYS
4	LC	78	CYS
4	LC	102	LEU
4	LC	127	CYS
4	LC	187	ILE
4	LC	199	ARG
4	LC	279	LYS
4	LC	295	CYS
4	LC	312	LYS
5	LD	72	PHE
5	LD	164	MET
5	LD	192	SER
5	LD	194	GLU
5	LD	236	ARG
5	LD	277	ASP

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Mol	Chain	Res	Type
5	LD	281	ARG
6	LI	67	GLU
6	LI	76	ARG
6	LI	93	ASN
6	LI	113	SER
6	LI	117	SER
6	LI	126	GLN
6	LI	138	LYS
6	LI	141	GLU
6	LI	147	ARG
7	LJ	99	CYS
7	LJ	105	SER
7	LJ	116	LEU
7	LJ	140	TYR
7	LJ	165	VAL
7	LJ	171	VAL
7	LJ	183	ASP
7	LJ	185	ILE
7	LJ	188	ARG
7	LJ	197	LEU
8	LK	19	VAL
8	LK	21	ARG
8	LK	30	MET
8	LK	42	ARG
8	LK	75	ASP
8	LK	87	VAL
8	LK	130	PHE
8	LK	150	SER
8	LK	151	LEU
8	LK	167	PHE
8	LK	171	ARG
9	LM	24	LYS
9	LM	149	ARG
10	LN	101	ASP
10	LN	105	VAL
10	LN	121	THR
10	LN	131	GLU
11	LO	39	ARG
11	LO	41	ARG
11	LO	134	ARG
11	LO	202	LYS
11	LO	257	CYS

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Mol	Chain	Res	Type
11	LO	261	ASP
11	LO	263	ARG
11	LO	280	LYS
12	LP	41	ASP
12	LP	51	ARG
12	LP	86	ASN
12	LP	117	ASN
12	LP	133	ARG
12	LP	138	HIS
12	LP	197	LYS
13	LQ	24	SER
13	LQ	30	ARG
13	LQ	75	MET
13	LQ	111	PRO
13	LQ	112	ASN
13	LQ	115	LEU
13	LQ	139	ASP
14	LR	49	ASN
14	LR	52	PRO
15	LS	74	ARG
15	LS	91	LYS
15	LS	184	ASP
15	LS	241	LYS
16	LT	11	ARG
16	LT	29	ARG
16	LT	122	ARG
16	LT	149	HIS
17	LU	118	ASN
17	LU	155	ARG
18	LV	76	CYS
18	LV	95	ARG
20	LX	53	ASP
20	LX	118	ARG
20	LX	127	ASP
20	LX	134	GLU
20	LX	152	ARG
20	LX	159	PHE
20	LX	161	ARG
20	LX	172	ASP
20	LX	185	ARG
20	LX	193	THR
20	LX	211	LYS

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Mol	Chain	Res	Type
21	La	55	LYS
21	La	88	CYS
21	La	116	LEU
22	Lb	2	PRO
22	Lb	34	GLU
22	Lb	36	ARG
22	Lb	112	ARG
22	Lb	122	LYS
22	Lb	142	ASP
22	Lb	168	ARG
22	Lb	183	ARG
22	Lb	221	LYS
23	Lu	72	LYS
23	Lu	87	CYS
23	Lu	116	GLU
23	Lu	126	MET
23	Lu	133	ASP
23	Lu	147	GLN
23	Lu	170	ARG
23	Lu	171	ASP
23	Lu	236	LYS
24	Ld	73	LYS
24	Ld	78	ARG
24	Ld	99	VAL
24	Ld	113	VAL
25	Lf	105	ASN
25	Lf	108	ASP
25	Lf	170	GLN
25	Lf	185	PHE
26	Lg	40	LYS
26	Lg	41	LEU
27	Lh	68	ARG
27	Lh	92	HIS
28	Li	124	ARG
28	Li	130	LYS
29	Lj	77	LYS
29	Lj	87	ARG
30	Lk	47	ASP
30	Lk	49	VAL
30	Lk	67	VAL
30	Lk	130	GLU
30	Lk	144	ARG

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Mol	Chain	Res	Type
30	Lk	149	ASN
30	Lk	176	TYR
30	Lk	203	CYS
30	Lk	256	PHE
30	Lk	274	LYS
30	Lk	295	ASP
30	Lk	315	LEU
31	Ll	50	LYS
31	Ll	58	ARG
31	Ll	66	GLN
31	Ll	138	GLU
31	Ll	163	HIS
31	Ll	235	TRP
31	Ll	241	PRO
31	Ll	311	MET
31	Ll	321	CYS
31	Ll	324	ASP
31	Ll	336	ASP
31	Ll	337	MET
32	Lm	102	LYS
32	Lm	143	TRP
32	Lm	150	MET
32	Lm	160	ASP
32	Lm	172	VAL
32	Lm	181	TYR
32	Lm	190	ASP
32	Lm	193	MET
32	Lm	231	GLN
32	Lm	234	LYS
32	Lm	310	PHE
32	Lm	323	MET
33	Ln	99	ARG
33	Ln	101	ARG
33	Ln	119	LYS
33	Ln	127	GLN
33	Ln	129	ARG
33	Ln	156	LYS
33	Ln	163	LYS
33	Ln	168	LEU
33	Ln	177	HIS
34	Lo	91	LEU
34	Lo	102	LYS

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Mol	Chain	Res	Type
35	Lp	37	SER
35	Lp	41	ASP
35	Lp	45	CYS
35	Lp	64	SER
35	Lp	99	LYS
35	Lp	111	GLN
35	Lp	115	MET
35	Lp	120	LYS
35	Lp	122	ARG
35	Lp	126	HIS
36	Lq	53	ASP
36	Lq	58	ASN
36	Lq	91	CYS
36	Lq	111	ASP
36	Lq	119	PHE
36	Lq	138	THR
37	Lr	86	ASP
37	Lr	106	GLN
37	Lr	140	PHE
37	Lr	223	MET
37	Lr	238	MET
37	Lr	247	LYS
37	Lr	294	GLU
38	Ls	112	MET
38	Ls	113	LYS
38	Ls	123	ARG
38	Ls	137	PHE
38	Ls	159	ARG
38	Ls	175	ASP
38	Ls	198	ARG
38	Ls	202	MET
38	Ls	207	ASN
38	Ls	237	ASP
38	Ls	290	GLU
39	Lt	55	ARG
39	Lt	65	PRO
39	Lt	66	LEU
39	Lt	72	SER
39	Lt	97	ARG
39	Lt	132	LYS
39	Lt	136	ARG
39	Lt	148	SER

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Mol	Chain	Res	Type
39	Lt	198	ASN
39	Lt	200	MET
39	Lt	217	PHE
39	Lt	232	PHE
39	Lt	243	PHE
39	Lt	249	LYS
39	Lt	256	THR
39	Lt	268	TYR
39	Lt	277	SER
40	Lv	88	TYR
40	Lv	91	LEU
40	Lv	102	LEU
40	Lv	113	LEU
40	Lv	116	SER
40	Lv	125	TYR
40	Lv	135	LEU
40	Lv	144	MET
40	Lv	155	ARG
40	Lv	160	SER
40	Lv	166	PHE
40	Lv	186	VAL
40	Lv	193	ASP
41	Lw	38	PHE
41	Lw	43	ASP
41	Lw	62	LYS
41	Lw	68	THR
41	Lw	69	PRO
41	Lw	122	LYS
41	Lw	148	ARG
42	Lx	58	ARG
42	Lx	85	ASN
42	Lx	88	ASP
42	Lx	89	ILE
42	Lx	90	SER
42	Lx	106	ASP
42	Lx	114	ASN
42	Lx	122	ARG
42	Lx	153	LYS
43	Ly	71	LYS
43	Ly	93	ARG
45	L3	10	LEU
45	L3	14	LYS

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Mol	Chain	Res	Type
45	L3	47	LEU
45	L3	72	HIS
45	L3	87	LEU
45	L3	95	ARG
46	L4	73	MET
46	L4	87	LYS
46	L4	113	GLU
46	L4	118	TRP
46	L4	134	LYS
47	L5	55	LEU
47	L5	58	LYS
47	L5	69	ARG
47	L5	73	ARG
48	L6	29	LEU
48	L6	82	PHE
48	L6	99	LYS
49	L7	82	ARG
49	L7	100	GLU
49	L7	102	ARG
49	L7	118	LYS
49	L7	179	ARG
49	L7	189	ARG
50	L8	26	ARG
50	L8	34	ARG
50	L8	63	ARG
50	L8	82	LEU
50	L8	143	TRP
50	L8	145	LYS
51	SR	52	ARG
51	SR	60	SER
51	SR	108	CYS
51	SR	169	TRP
52	Sf	43	ARG
52	Sf	165	ARG
52	Sf	170	GLU
52	Sf	203	ARG
52	Sf	228	ASP
52	Sf	240	GLN
52	Sf	251	VAL
52	Sf	265	LYS
52	Sf	271	LEU
52	Sf	419	LEU

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Mol	Chain	Res	Type
52	Sf	424	PHE
53	SB	78	LEU
53	SB	82	ARG
53	SB	109	SER
53	SB	110	ARG
53	SB	162	CYS
53	SB	175	MET
53	SB	191	ASP
53	SB	207	VAL
53	SB	265	GLN
53	SB	266	GLN
54	SZ	43	ARG
54	SZ	46	LYS
54	SZ	51	VAL
54	SZ	72	HIS
54	SZ	89	ASP
54	SZ	92	LEU
54	SZ	103	CYS
54	SZ	108	LEU
54	SZ	111	LYS
54	SZ	118	GLU
54	SZ	130	HIS
54	SZ	142	LEU
54	SZ	146	PHE
54	SZ	158	VAL
54	SZ	160	SER
55	SE	91	THR
55	SE	145	ASN
55	SE	162	LYS
55	SE	165	GLN
55	SE	169	GLU
55	SE	184	LYS
55	SE	214	THR
55	SE	224	GLU
55	SE	240	SER
55	SE	276	VAL
55	SE	284	ARG
55	SE	292	HIS
55	SE	332	MET
55	SE	394	ASP
56	SF	32	ARG
56	SF	37	ARG

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Mol	Chain	Res	Type
56	SF	38	ASP
56	SF	45	ARG
56	SF	57	GLN
56	SF	72	THR
56	SF	102	LEU
56	SF	103	LYS
56	SF	109	VAL
56	SF	123	ARG
57	SG	41	PHE
57	SG	50	TYR
57	SG	94	PHE
57	SG	98	MET
57	SG	123	PHE
57	SG	146	HIS
57	SG	176	ASP
57	SG	196	HIS
57	SG	224	HIS
57	SG	231	GLU
58	SI	86	ARG
58	SI	112	PHE
58	SI	124	VAL
58	SI	175	HIS
58	SI	198	ARG
58	SI	208	MET
58	SI	219	MET
58	SI	228	LEU
58	SI	229	LEU
58	SI	232	GLN
58	SI	258	GLU
58	SI	261	GLN
58	SI	262	TYR
58	SI	294	LYS
58	SI	314	MET
58	SI	315	PHE
58	SI	325	LYS
58	SI	357	THR
58	SI	364	MET
59	SJ	62	VAL
59	SJ	75	ARG
59	SJ	91	TYR
59	SJ	100	LYS
59	SJ	109	HIS

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Mol	Chain	Res	Type
59	SJ	142	CYS
59	SJ	158	GLU
59	SJ	163	ASN
59	SJ	174	LYS
59	SJ	177	LEU
60	SK	61	SER
60	SK	74	ARG
60	SK	81	GLU
60	SK	121	LYS
60	SK	146	HIS
61	SL	34	ASN
61	SL	38	ARG
61	SL	43	LYS
61	SL	56	PRO
61	SL	79	LYS
61	SL	86	SER
61	SL	100	HIS
61	SL	104	GLU
61	SL	117	ASP
62	SN	29	TYR
62	SN	31	ASP
62	SN	33	ARG
62	SN	39	LYS
62	SN	41	ARG
62	SN	58	ARG
62	SN	59	LYS
62	SN	62	ILE
62	SN	65	LYS
62	SN	67	LEU
62	SN	70	VAL
62	SN	81	ASP
62	SN	92	VAL
62	SN	94	THR
62	SN	121	SER
63	SO	84	LYS
63	SO	97	MET
63	SO	103	MET
63	SO	111	PHE
63	SO	132	LEU
63	SO	145	LYS
63	SO	161	ASP
63	SO	174	ASN

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Mol	Chain	Res	Type
63	SO	224	ARG
63	SO	228	LYS
64	SP	13	ARG
64	SP	41	CYS
64	SP	53	SER
64	SP	71	ASP
64	SP	93	LEU
64	SP	97	PHE
64	SP	101	PRO
64	SP	104	ILE
64	SP	111	ARG
65	SQ	36	ASP
65	SQ	110	LEU
66	SS	53	ASP
66	SS	58	TYR
66	SS	61	SER
66	SS	70	SER
66	SS	76	ASP
66	SS	79	ARG
66	SS	93	THR
66	SS	97	ARG
66	SS	111	HIS
66	SS	139	TYR
66	SS	162	LEU
66	SS	193	LEU
66	SS	199	TRP
66	SS	211	ARG
66	SS	219	LEU
66	SS	235	MET
67	ST	52	ILE
67	ST	58	TYR
67	ST	66	ILE
67	ST	68	CYS
68	SW	56	SER
69	SX	66	LYS
69	SX	72	ASP
69	SX	89	LYS
69	SX	106	MET
69	SX	152	GLU
69	SX	154	THR
69	SX	170	ARG
69	SX	183	LYS

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Mol	Chain	Res	Type
69	SX	216	ARG
69	SX	223	ARG
69	SX	248	LYS
69	SX	256	ARG
69	SX	273	TRP
69	SX	310	ASP
69	SX	318	LYS
69	SX	326	ASN
69	SX	333	LYS
69	SX	341	TYR
70	SY	21	ARG
70	SY	78	TYR
70	SY	80	SER
70	SY	83	ARG
70	SY	87	LEU
70	SY	89	ASN
70	SY	94	SER
70	SY	99	PHE
70	SY	103	TYR
70	SY	108	LYS
70	SY	113	ASP
70	SY	118	PHE
71	Sa	28	LYS
71	Sa	59	ASN
71	Sa	79	TYR
71	Sa	89	ASP
71	Sa	116	GLU
71	Sa	124	SER
71	Sa	140	ILE
71	Sa	149	CYS
71	Sa	150	PRO
71	Sa	158	GLU
71	Sa	159	MET
72	Sb	81	LYS
72	Sb	97	LYS
72	Sb	106	MET
72	Sb	115	ARG
72	Sb	126	GLN
72	Sb	141	ARG
72	Sb	147	GLN
72	Sb	183	SER
72	Sb	192	THR

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Mol	Chain	Res	Type
73	Sc	32	SER
73	Sc	77	ASP
73	Sc	115	GLN
73	Sc	159	ASP
73	Sc	188	HIS
73	Sc	196	PHE
73	Sc	216	LYS
73	Sc	226	TYR
73	Sc	244	TYR
73	Sc	247	MET
73	Sc	250	ILE
73	Sc	263	MET
73	Sc	288	LYS
73	Sc	303	ASN
73	Sc	306	ASP
73	Sc	322	THR
74	Sd	83	MET
74	Sd	87	SER
74	Sd	133	LYS
74	Sd	149	LEU
75	Se	71	SER
75	Se	81	HIS
75	Se	96	GLU
75	Se	99	LEU
75	Se	119	TYR
75	Se	123	ARG
75	Se	140	HIS
75	Se	154	HIS
75	Se	166	ARG
75	Se	177	ARG
75	Se	192	LYS
75	Se	197	ARG
75	Se	198	PHE
75	Se	210	TRP
75	Se	213	ARG
75	Se	218	LYS
75	Se	245	LYS
75	Se	255	MET
75	Se	256	PHE
75	Se	271	ARG
75	Se	296	MET
75	Se	297	MET

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Mol	Chain	Res	Type
75	Se	334	PHE
75	Se	370	LYS
76	Sg	295	GLN
76	Sg	296	ASN
76	Sg	306	LYS
76	Sg	309	LYS
76	Sg	310	LEU
76	Sg	312	GLU
76	Sg	315	ILE
76	Sg	321	PHE
76	Sg	322	ASP
76	Sg	372	HIS
77	Si	7	TYR
77	Si	10	ARG
77	Si	17	ARG
77	Si	24	ARG
77	Si	29	LYS
77	Si	50	ASP
77	Si	68	LEU
77	Si	72	ARG
77	Si	76	GLN
77	Si	79	MET
77	Si	80	ASP
77	Si	83	LYS
77	Si	84	ARG
78	Sj	22	ARG
78	Sj	27	ARG
78	Sj	30	ASP
78	Sj	37	ASP
78	Sj	65	LEU
78	Sj	82	ARG
78	Sj	108	ASN
78	Sj	123	LYS
78	Sj	129	ARG
78	Sj	130	GLU
78	Sj	135	MET
78	Sj	141	LEU
78	Sj	146	GLU
78	Sj	150	PHE
78	Sj	173	MET
78	Sj	190	MET
78	Sj	191	LEU

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Mol	Chain	Res	Type
78	Sj	198	MET
78	Sj	207	GLN
79	Sk	55	PRO
79	Sk	59	LYS
79	Sk	70	TYR
79	Sk	91	VAL
79	Sk	97	MET
79	Sk	106	LEU
79	Sk	113	HIS
79	Sk	133	TRP
79	Sk	143	CYS
79	Sk	146	HIS
79	Sk	162	SER
79	Sk	163	VAL
79	Sk	185	HIS
79	Sk	187	LYS
79	Sk	190	LEU
79	Sk	192	LYS
79	Sk	198	TYR
79	Sk	208	LYS
79	Sk	209	THR
79	Sk	210	ASP
79	Sk	239	TRP
79	Sk	241	LYS
79	Sk	248	MET
79	Sk	254	GLU
79	Sk	257	SER
79	Sk	265	THR
79	Sk	293	LYS
79	Sk	296	VAL
80	Sm	37	ARG
80	Sm	40	LYS
80	Sm	50	SER
80	Sm	57	LYS
80	Sm	58	GLN
80	Sm	66	CYS
80	Sm	68	LYS
80	Sm	86	MET
80	Sm	95	GLU
80	Sm	102	ASN
80	Sm	103	LYS
80	Sm	107	LEU

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Mol	Chain	Res	Type
80	Sm	114	LYS
81	Sn	144	ARG
81	Sn	156	LYS
81	Sn	158	GLN
81	Sn	165	LYS
81	Sn	174	ARG
81	Sn	183	LYS
81	Sn	190	GLN
82	So	80	ARG
82	So	116	VAL
82	So	141	MET
82	So	172	MET
82	So	212	THR
82	So	251	MET
82	So	262	MET
82	So	292	TYR
82	So	306	ASN
82	So	323	MET
82	So	360	MET
82	So	388	ARG
82	So	394	TYR
82	So	395	ASP
82	So	397	MET
82	So	401	MET
82	So	468	MET
82	So	518	GLU
82	So	533	MET
82	So	615	MET
82	So	643	GLU
82	So	648	ARG
82	So	657	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
5	LD	241	ASN
7	LJ	93	ASN
7	LJ	115	GLN
7	LJ	119	HIS
7	LJ	193	ASN
8	LK	168	GLN
9	LM	140	ASN

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Mol	Chain	Res	Type
10	LN	113	ASN
14	LR	49	ASN
14	LR	146	GLN
15	LS	239	ASN
33	Ln	158	HIS
35	Lp	111	GLN
38	Ls	119	GLN
38	Ls	196	GLN
38	Ls	205	GLN
38	Ls	251	GLN
39	Lt	67	GLN
40	Lv	92	ASN
45	L3	46	ASN
46	L4	76	ASN
52	Sf	420	GLN
53	SB	64	ASN
53	SB	126	GLN
56	SF	81	HIS
57	SG	151	ASN
57	SG	215	ASN
59	SJ	161	GLN
59	SJ	179	GLN
60	SK	146	HIS
62	SN	117	HIS
62	SN	124	GLN
63	SO	174	ASN
65	SQ	44	ASN
66	SS	147	HIS
68	SW	79	ASN
69	SX	246	HIS
71	Sa	63	GLN
72	Sb	43	ASN
72	Sb	161	GLN
73	Sc	405	GLN
75	Se	90	GLN
75	Se	159	HIS
75	Se	367	GLN
76	Sg	331	HIS
76	Sg	372	HIS
77	Si	55	HIS
78	Sj	137	HIS
79	Sk	64	GLN

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Mol	Chain	Res	Type
79	Sk	255	ASN
79	Sk	311	GLN
81	Sn	141	HIS
82	So	285	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1491/1559 (95%)	382 (25%)	27 (1%)
2	L2	51/69 (73%)	12 (23%)	0
83	S1	921/954 (96%)	207 (22%)	16 (1%)
All	All	2463/2582 (95%)	601 (24%)	43 (1%)

All (601) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	5	A
1	L1	6	A
1	L1	7	C
1	L1	8	C
1	L1	9	U
1	L1	11	G
1	L1	19	C
1	L1	20	C
1	L1	24	U
1	L1	29	C
1	L1	30	U
1	L1	31	U
1	L1	34	U
1	L1	36	C
1	L1	38	A
1	L1	39	G
1	L1	40	A
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

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Mol	Chain	Res	Type
1	L1	62	C
1	L1	63	C
1	L1	66	A
1	L1	78	G
1	L1	91	A
1	L1	98	G
1	L1	100	G
1	L1	101	C
1	L1	103	A
1	L1	104	U
1	L1	107	A
1	L1	110	U
1	L1	111	A
1	L1	112	G
1	L1	124	A
1	L1	127	G
1	L1	134	A
1	L1	135	A
1	L1	136	U
1	L1	137	U
1	L1	138	A
1	L1	142	C
1	L1	147	C
1	L1	151	A
1	L1	154	U
1	L1	157	C
1	L1	158	A
1	L1	159	A
1	L1	162	A
1	L1	164	U
1	L1	166	A
1	L1	173	U
1	L1	174	A
1	L1	179	C
1	L1	184	U
1	L1	186	A
1	L1	197	A
1	L1	198	G
1	L1	199	A
1	L1	200	A
1	L1	203	A
1	L1	212	A

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Mol	Chain	Res	Type
1	L1	213	G
1	L1	215	A
1	L1	217	A
1	L1	218	G
1	L1	220	C
1	L1	223	A
1	L1	232	C
1	L1	233	C
1	L1	248	G
1	L1	257	G
1	L1	266	A
1	L1	267	A
1	L1	270	A
1	L1	274	C
1	L1	298	G
1	L1	304	A
1	L1	305	U
1	L1	315	G
1	L1	317	G
1	L1	322	C
1	L1	324	A
1	L1	325	A
1	L1	330	C
1	L1	331	C
1	L1	332	G
1	L1	345	G
1	L1	346	C
1	L1	352	G
1	L1	359	A
1	L1	361	A
1	L1	362	G
1	L1	367	U
1	L1	369	A
1	L1	371	U
1	L1	375	A
1	L1	383	U
1	L1	385	U
1	L1	387	C
1	L1	390	A
1	L1	395	A
1	L1	404	A
1	L1	413	U

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Mol	Chain	Res	Type
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	488	U
1	L1	489	U
1	L1	493	A
1	L1	498	U
1	L1	503	G
1	L1	507	U
1	L1	510	A
1	L1	511	A
1	L1	512	G
1	L1	513	C
1	L1	519	C
1	L1	522	A
1	L1	527	G
1	L1	528	A
1	L1	530	A
1	L1	540	C
1	L1	545	C
1	L1	546	A
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	560	A
1	L1	563	U

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Mol	Chain	Res	Type
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	590	A
1	L1	591	C
1	L1	592	C
1	L1	593	C
1	L1	614	C
1	L1	615	U
1	L1	620	A
1	L1	621	A
1	L1	624	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
1	L1	701	U
1	L1	702	U
1	L1	704	A
1	L1	711	A
1	L1	714	A
1	L1	720	A
1	L1	723	C
1	L1	724	A
1	L1	726	C
1	L1	730	C
1	L1	731	A
1	L1	734	U
1	L1	735	C
1	L1	737	U
1	L1	744	C

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Mol	Chain	Res	Type
1	L1	745	C
1	L1	756	C
1	L1	762	A
1	L1	771	C
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	798	A
1	L1	801	G
1	L1	808	G
1	L1	809	C
1	L1	814	C
1	L1	815	U
1	L1	823	C
1	L1	830	A
1	L1	832	C
1	L1	834	A
1	L1	836	A
1	L1	838	C
1	L1	841	C
1	L1	850	C
1	L1	851	A
1	L1	853	C
1	L1	854	A
1	L1	857	A
1	L1	860	A
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

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Mol	Chain	Res	Type
1	L1	918	C
1	L1	920	A
1	L1	922	G
1	L1	923	G
1	L1	926	G
1	L1	929	U
1	L1	930	A
1	L1	931	A
1	L1	957	G
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	1014	C
1	L1	1016	G
1	L1	1024	A
1	L1	1025	G
1	L1	1026	A
1	L1	1027	G
1	L1	1029	C
1	L1	1032	G
1	L1	1036	A
1	L1	1038	C
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	1057	C
1	L1	1060	A
1	L1	1062	G
1	L1	1069	U
1	L1	1074	U
1	L1	1075	A

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Mol	Chain	Res	Type
1	L1	1087	A
1	L1	1088	G
1	L1	1089	U
1	L1	1134	A
1	L1	1140	G
1	L1	1161	G
1	L1	1162	A
1	L1	1163	A
1	L1	1174	G
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	1243	A
1	L1	1245	C
1	L1	1246	G
1	L1	1247	G
1	L1	1248	A
1	L1	1249	A
1	L1	1250	C
1	L1	1252	A
1	L1	1256	A
1	L1	1257	C
1	L1	1258	C
1	L1	1262	G
1	L1	1265	A
1	L1	1266	U
1	L1	1286	A
1	L1	1292	C
1	L1	1293	A
1	L1	1304	A
1	L1	1305	G
1	L1	1307	G

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Mol	Chain	Res	Type
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	1321	U
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	1372	U
1	L1	1379	U
1	L1	1383	A
1	L1	1384	G
1	L1	1386	C
1	L1	1390	C
1	L1	1393	G
1	L1	1402	U
1	L1	1403	C
1	L1	1416	U
1	L1	1419	A
1	L1	1426	U
1	L1	1430	U
1	L1	1432	U
1	L1	1438	U
1	L1	1439	U
1	L1	1442	A
1	L1	1443	A
1	L1	1444	U
1	L1	1452	U
1	L1	1461	G
1	L1	1465	A
1	L1	1469	G
1	L1	1479	C
1	L1	1480	U
1	L1	1482	C
1	L1	1485	C

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Mol	Chain	Res	Type
1	L1	1487	C
1	L1	1488	A
1	L1	1490	A
1	L1	1491	G
1	L1	1492	C
1	L1	1498	C
1	L1	1499	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	1534	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	1550	A
2	L2	4	A
2	L2	7	G
2	L2	8	U
2	L2	9	A
2	L2	10	G
2	L2	13	U
2	L2	14	A
2	L2	40	G
2	L2	43	G
2	L2	49	A
2	L2	68	G
2	L2	69	A
83	S1	3	U
83	S1	4	A
83	S1	10	G
83	S1	33	U
83	S1	38	A
83	S1	41	A
83	S1	44	A
83	S1	47	C
83	S1	57	U

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Mol	Chain	Res	Type
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	118	C
83	S1	119	G
83	S1	125	A
83	S1	126	U
83	S1	130	G
83	S1	134	A
83	S1	144	G
83	S1	149	G
83	S1	160	A
83	S1	165	A
83	S1	167	A
83	S1	168	C
83	S1	170	G
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	207	U
83	S1	209	A
83	S1	214	U
83	S1	219	A
83	S1	221	C
83	S1	223	C
83	S1	233	C
83	S1	234	A
83	S1	235	A

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Mol	Chain	Res	Type
83	S1	243	C
83	S1	246	G
83	S1	252	G
83	S1	257	C
83	S1	261	C
83	S1	270	C
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	306	U
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	347	A
83	S1	353	U
83	S1	354	C
83	S1	355	C
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	434	U

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Mol	Chain	Res	Type
83	S1	435	A
83	S1	451	C
83	S1	456	A
83	S1	458	C
83	S1	459	C
83	S1	462	A
83	S1	474	A
83	S1	479	A
83	S1	481	C
83	S1	489	C
83	S1	497	U
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	537	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	580	G
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	610	U
83	S1	611	A
83	S1	612	U

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Mol	Chain	Res	Type
83	S1	614	C
83	S1	622	U
83	S1	624	C
83	S1	631	C
83	S1	636	A
83	S1	638	G
83	S1	643	C
83	S1	645	A
83	S1	646	C
83	S1	647	A
83	S1	648	A
83	S1	667	C
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	742	G
83	S1	743	A
83	S1	745	A
83	S1	755	A
83	S1	756	A
83	S1	768	G
83	S1	769	A
83	S1	770	A
83	S1	773	U
83	S1	783	A
83	S1	794	A
83	S1	797	A
83	S1	800	G
83	S1	823	A

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Mol	Chain	Res	Type
83	S1	833	A
83	S1	834	C
83	S1	835	A
83	S1	865	A
83	S1	867	A
83	S1	870	A
83	S1	874	U
83	S1	877	A
83	S1	879	U
83	S1	885	C
83	S1	888	U
83	S1	889	A
83	S1	890	C
83	S1	891	G
83	S1	892	C
83	S1	893	A
83	S1	894	U
83	S1	897	A
83	S1	910	A
83	S1	912	G
83	S1	915	G
83	S1	917	A
83	S1	918	A
83	S1	921	U
83	S1	935	G
83	S1	937	A
83	S1	943	A
83	S1	947	G
83	S1	948	G
83	S1	952	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	33	C
1	L1	133	A
1	L1	200	A
1	L1	304	A
1	L1	324	A
1	L1	395	A
1	L1	427	A
1	L1	465	A

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Mol	Chain	Res	Type
1	L1	510	A
1	L1	511	A
1	L1	526	A
1	L1	528	A
1	L1	551	C
1	L1	575	A
1	L1	592	C
1	L1	710	C
1	L1	773	C
1	L1	814	C
1	L1	837	A
1	L1	853	C
1	L1	860	A
1	L1	889	U
1	L1	929	U
1	L1	1055	A
1	L1	1235	A
1	L1	1319	G
1	L1	1371	U
83	S1	70	G
83	S1	117	A
83	S1	374	U
83	S1	383	G
83	S1	507	A
83	S1	519	A
83	S1	542	U
83	S1	599	U
83	S1	600	G
83	S1	611	A
83	S1	684	A
83	S1	722	U
83	S1	768	G
83	S1	864	C
83	S1	887	C
83	S1	890	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	T1C	L1	1707	84	44,45,45	1.19	4 (9%)	53,72,72	1.01	4 (7%)
85	T1C	S1	1035	-	44,45,45	1.17	4 (9%)	53,72,72	1.10	4 (7%)
87	GDP	Se	500	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)
85	T1C	L1	1706	84	44,45,45	1.17	4 (9%)	53,72,72	0.88	2 (3%)
85	T1C	S1	1034	84	44,45,45	1.22	4 (9%)	53,72,72	1.02	2 (3%)

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	1707	84	-	9/22/80/80	0/4/4/4
85	T1C	S1	1035	-	-	7/22/80/80	0/4/4/4
87	GDP	Se	500	-	-	1/12/32/32	0/3/3/3
85	T1C	L1	1706	84	-	10/22/80/80	0/4/4/4
85	T1C	S1	1034	84	-	10/22/80/80	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	S1	1034	T1C	C21-N21	5.45	1.47	1.33
85	L1	1707	T1C	C21-N21	5.42	1.47	1.33
85	S1	1035	T1C	C21-N21	5.42	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	L1	1706	T1C	C21-N21	5.31	1.47	1.33
87	Se	500	GDP	C6-N1	-2.48	1.34	1.37
85	S1	1034	T1C	C4-N4	2.36	1.52	1.47
85	S1	1034	T1C	O11-C11	2.27	1.28	1.23
85	S1	1035	T1C	O11-C11	2.25	1.28	1.23
85	L1	1706	T1C	O11-C11	2.22	1.27	1.23
85	L1	1707	T1C	C4-N4	2.16	1.52	1.47
85	L1	1707	T1C	O11-C11	2.11	1.27	1.23
85	S1	1035	T1C	C4-N4	2.10	1.52	1.47
85	S1	1035	T1C	C7-N7	2.09	1.48	1.42
85	L1	1706	T1C	C4-N4	2.08	1.52	1.47
85	S1	1034	T1C	C7-N7	2.07	1.48	1.42
85	L1	1706	T1C	C7-N7	2.07	1.48	1.42
85	L1	1707	T1C	C7-N7	2.06	1.48	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	S1	1035	T1C	C11-C1B-C12	4.06	122.01	118.80
85	S1	1034	T1C	C1-C1C-C12	3.83	114.37	109.88
87	Se	500	GDP	PA-O3A-PB	-3.70	120.14	132.83
85	S1	1034	T1C	C11-C1B-C12	3.48	121.56	118.80
87	Se	500	GDP	C3'-C2'-C1'	3.43	106.14	100.98
85	S1	1035	T1C	C1-C1C-C12	3.42	113.90	109.88
85	L1	1707	T1C	C1C-C1-C2	2.87	120.31	115.75
85	L1	1707	T1C	O1C-C1C-C12	-2.75	105.74	110.14
85	L1	1707	T1C	C11-C1B-C12	2.74	120.96	118.80
85	L1	1706	T1C	C11-C1B-C12	2.73	120.96	118.80
87	Se	500	GDP	C5-C6-N1	2.39	118.18	113.95
85	S1	1035	T1C	C1C-C41-C4	2.37	114.88	111.64
87	Se	500	GDP	C8-N7-C5	2.31	107.39	102.99
85	S1	1035	T1C	O1C-C1C-C12	-2.23	106.57	110.14
85	L1	1706	T1C	C1C-C1-C2	2.23	119.29	115.75
85	L1	1707	T1C	C1C-C41-C4	2.07	114.47	111.64

There are no chirality outliers.

All (37) torsion outliers are listed below:

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

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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	S1	1034	T1C	C92-C91-N9-C9
85	S1	1035	T1C	C3-C2-C21-O21
85	L1	1707	T1C	C92-C91-N9-C9
85	S1	1035	T1C	C92-C91-N9-C9
85	S1	1034	T1C	O91-C91-N9-C9
85	L1	1707	T1C	O91-C91-N9-C9
85	S1	1035	T1C	O91-C91-N9-C9
85	L1	1706	T1C	O91-C91-C92-N92
85	L1	1706	T1C	N9-C91-C92-N92
85	L1	1707	T1C	N9-C91-C92-N92
85	L1	1707	T1C	O91-C91-C92-N92
85	L1	1706	T1C	C41-C4-N4-C42
85	L1	1706	T1C	C3-C2-C21-N21
85	L1	1707	T1C	C3-C2-C21-N21
85	S1	1034	T1C	C3-C2-C21-N21
85	S1	1035	T1C	C3-C2-C21-N21
85	L1	1706	T1C	C3-C2-C21-O21
85	S1	1034	T1C	C3-C2-C21-O21
85	L1	1706	T1C	C1-C2-C21-N21
85	L1	1707	T1C	C1-C2-C21-N21
85	S1	1034	T1C	C1-C2-C21-N21
85	S1	1035	T1C	C1-C2-C21-N21
85	S1	1034	T1C	N9-C91-C92-N92
85	S1	1035	T1C	N9-C91-C92-N92
87	Se	500	GDP	O4'-C4'-C5'-O5'
85	S1	1035	T1C	O91-C91-C92-N92
85	S1	1034	T1C	O91-C91-C92-N92
85	L1	1706	T1C	C10-C9-N9-C91
85	S1	1034	T1C	C61-C7-N7-C72
85	S1	1034	T1C	C41-C4-N4-C42
85	S1	1034	T1C	C61-C7-N7-C71

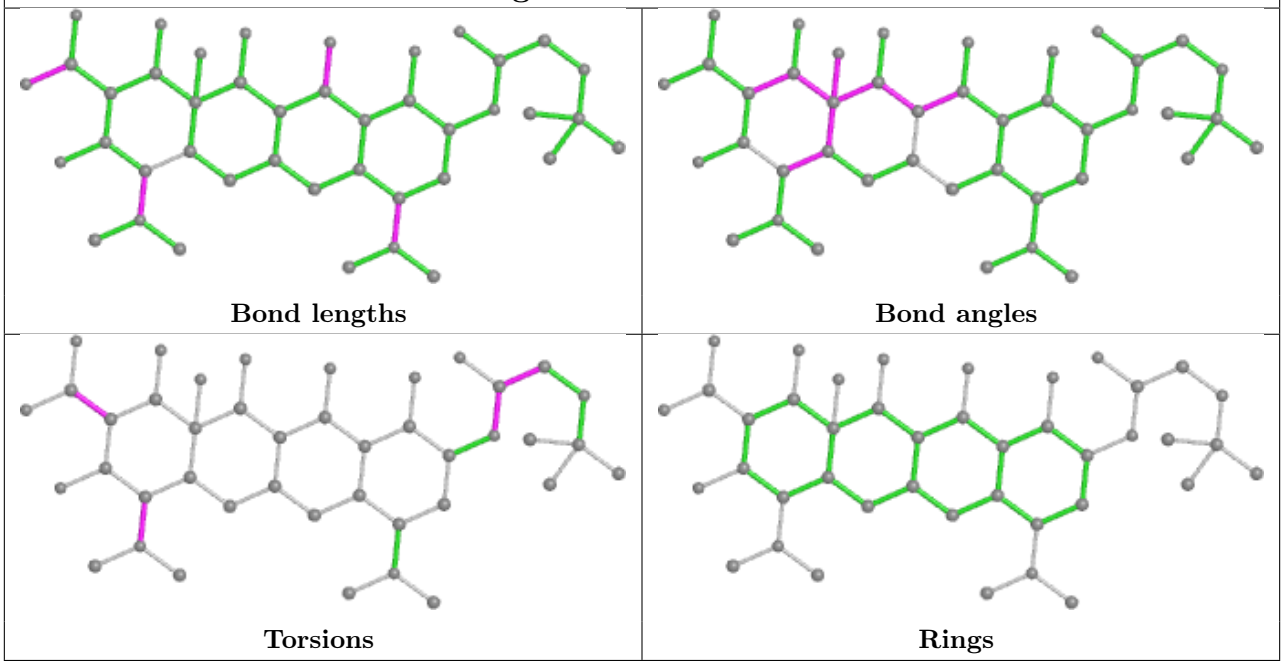
There are no ring outliers.

No monomer is involved in short contacts.

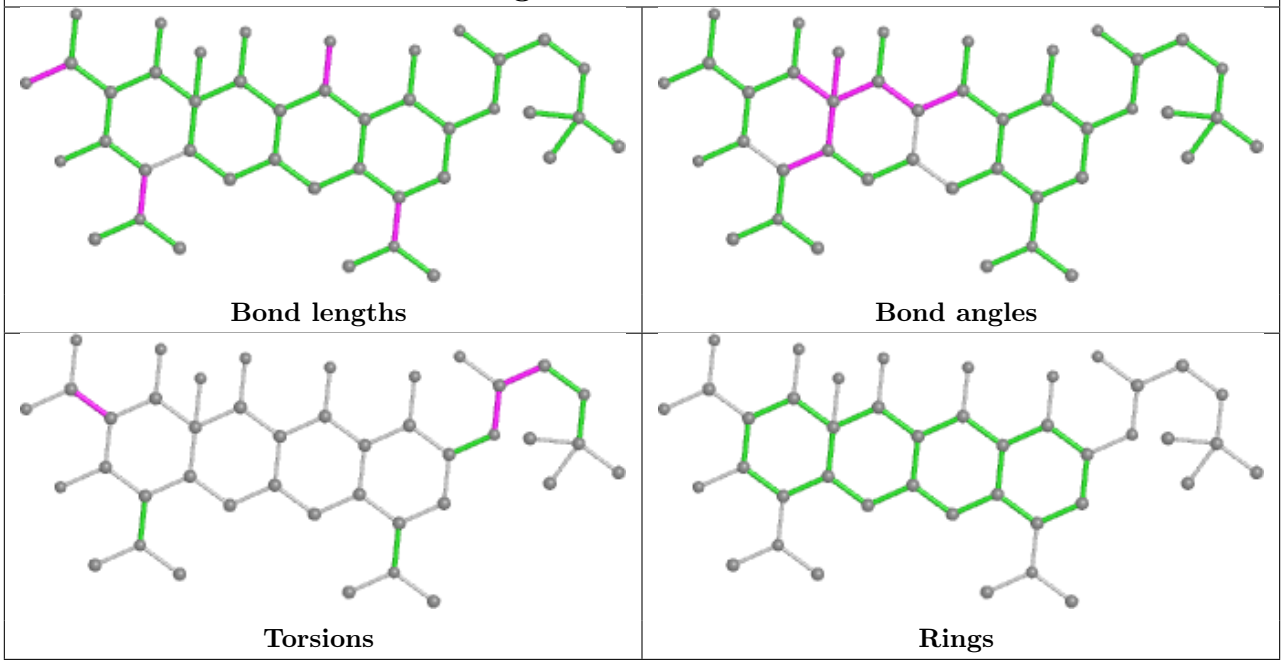
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

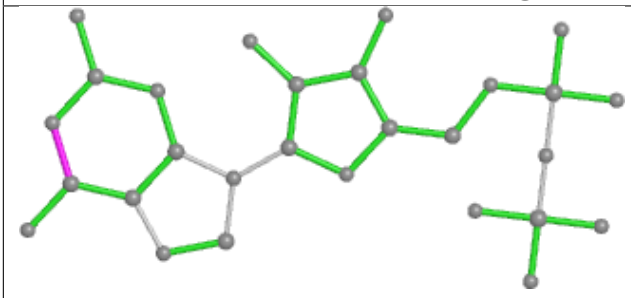
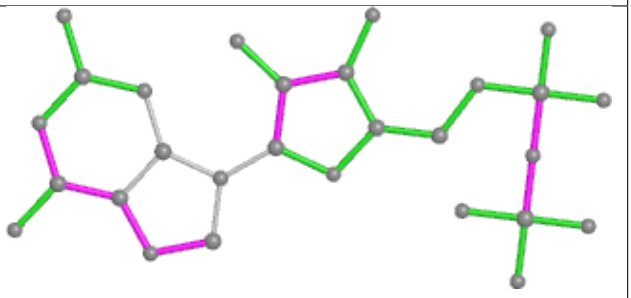
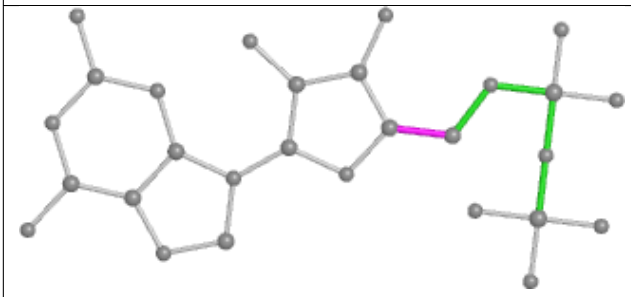
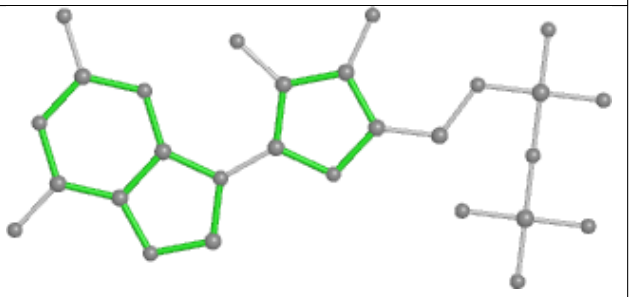
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

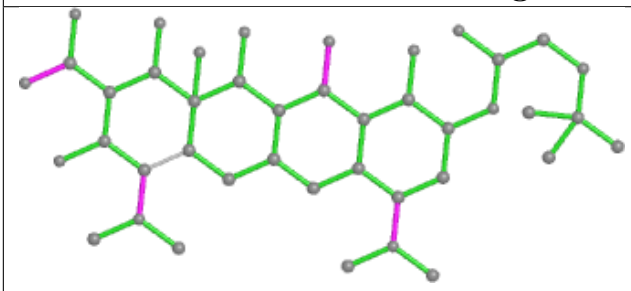
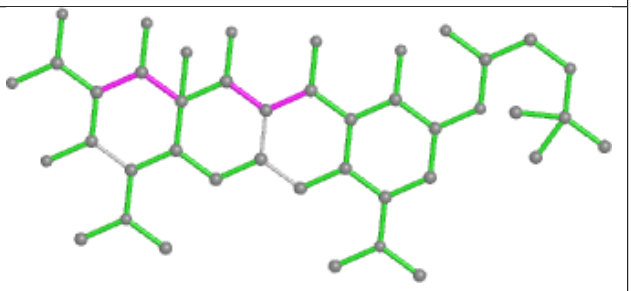
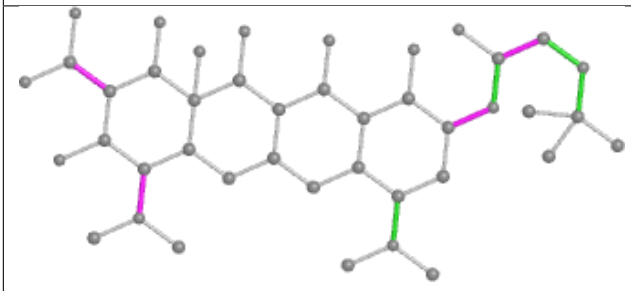
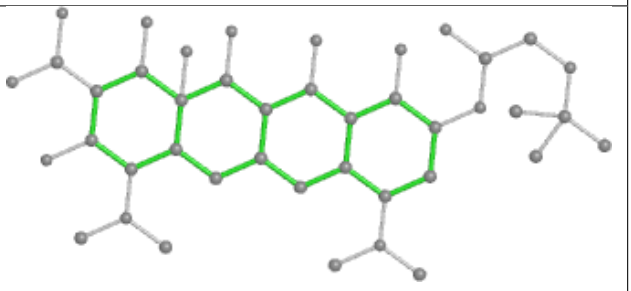
Ligand T1C L1 1707



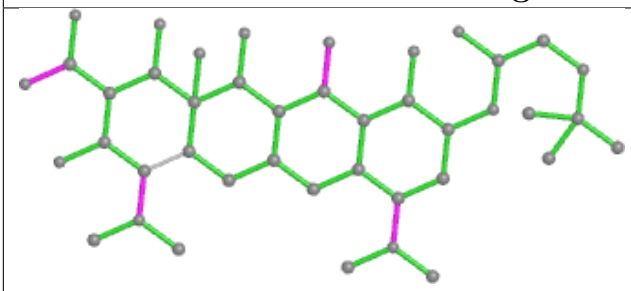
Ligand T1C S1 1035



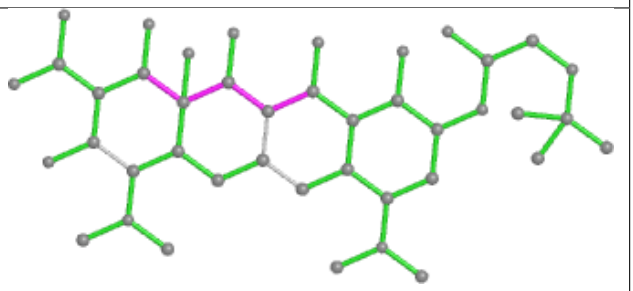
Ligand GDP Se 500	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand T1C L1 1706	
	
Bond lengths	Bond angles
	
Torsions	Rings

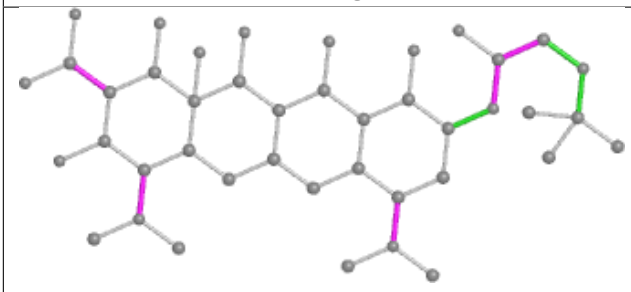
Ligand T1C S1 1034



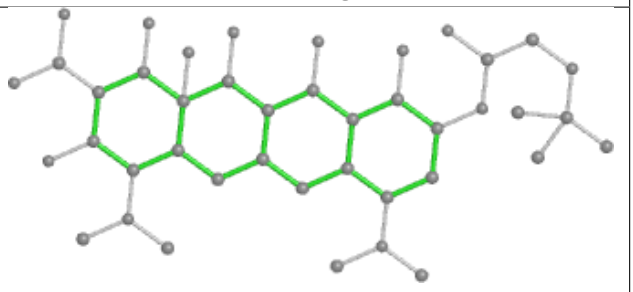
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

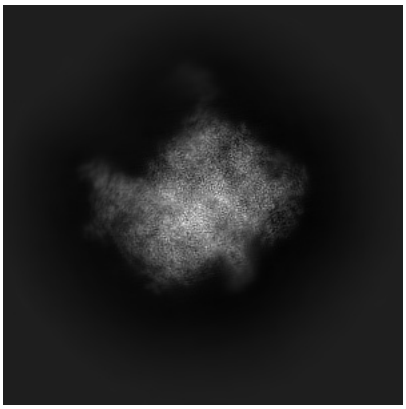
6 Map visualisation

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

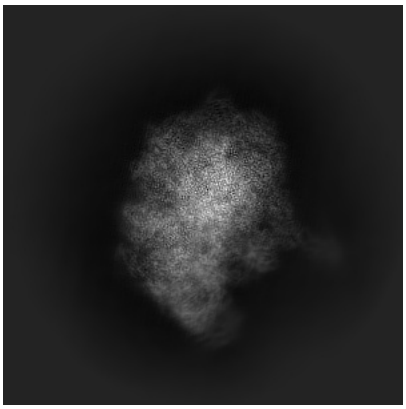
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

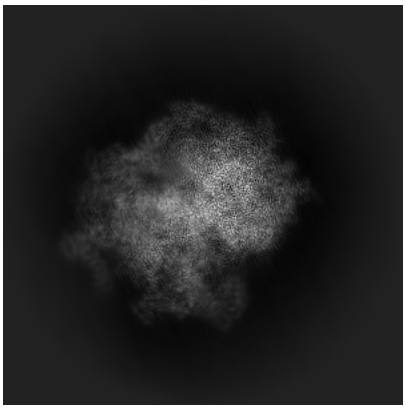
6.1.1 Primary map



X

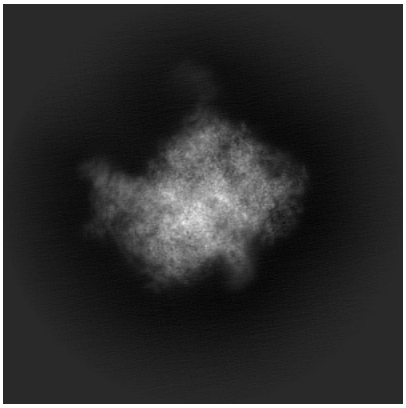


Y

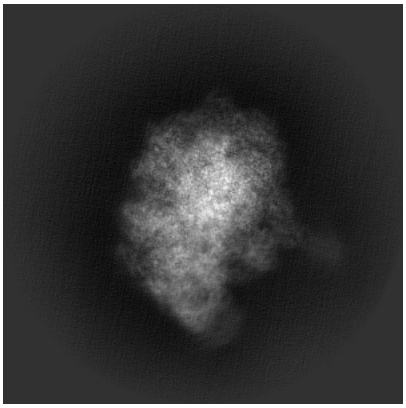


Z

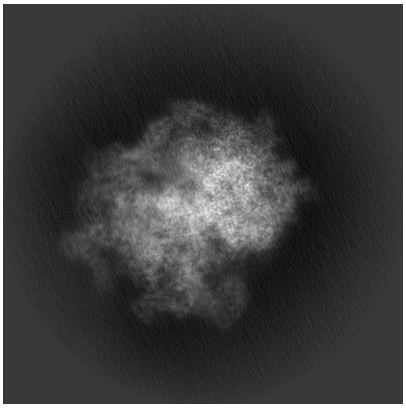
6.1.2 Raw map



X



Y



Z

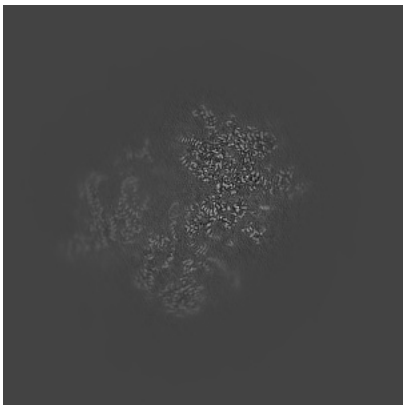
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

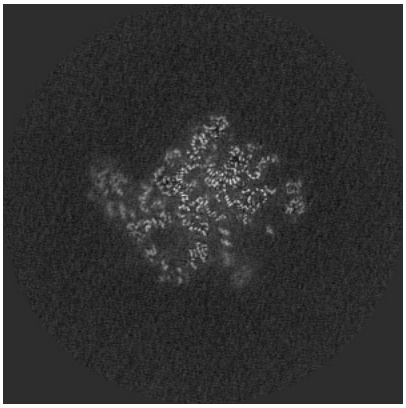
X Index: 210

Y Index: 210

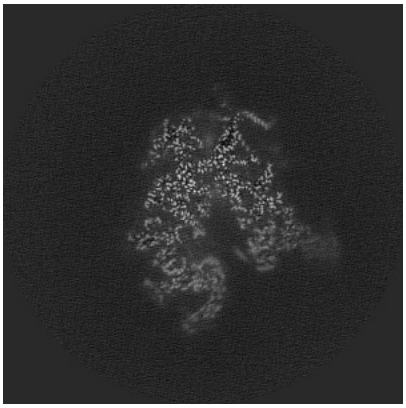


Z Index: 210

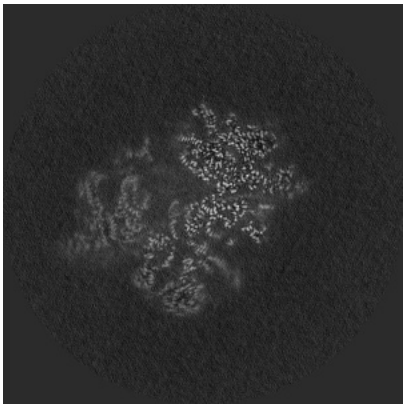
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

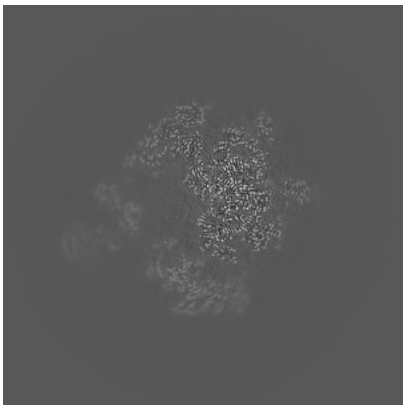
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

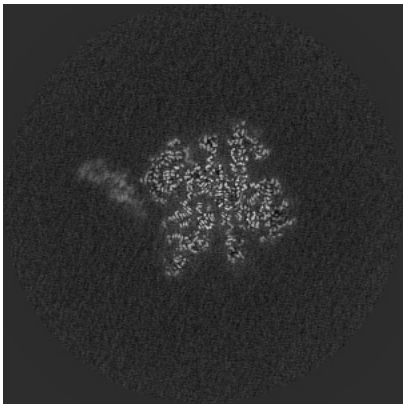
X Index: 236

Y Index: 206

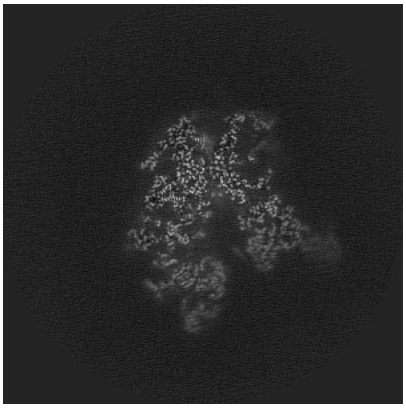


Z Index: 230

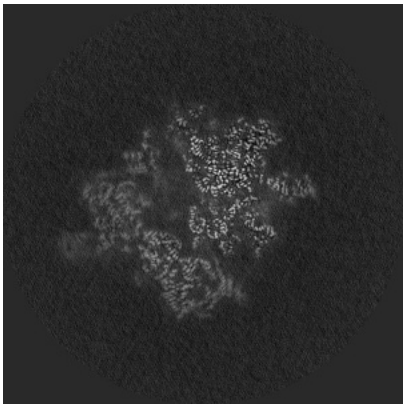
6.3.2 Raw map



X Index: 236



Y Index: 207

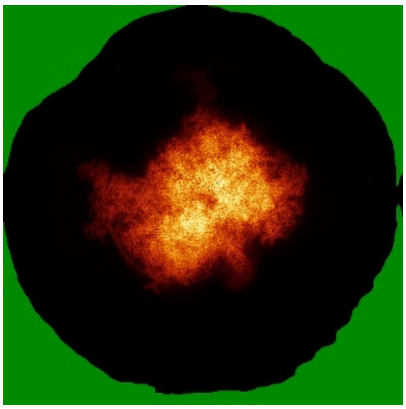


Z Index: 218

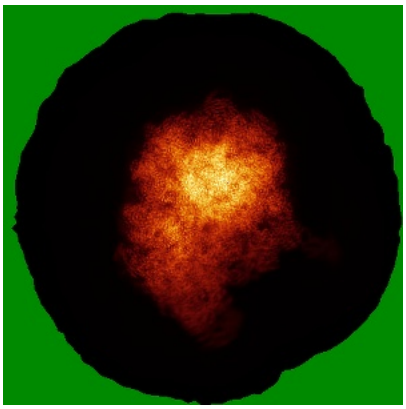
The images above show the largest variance slices of the map in three orthogonal directions.

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

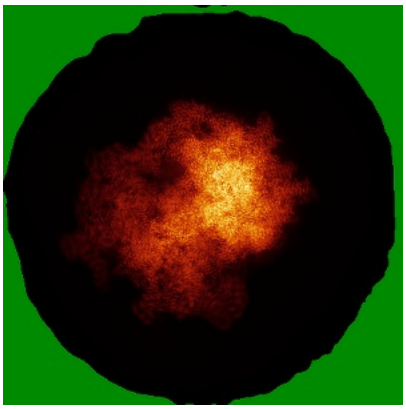
6.4.1 Primary map



X

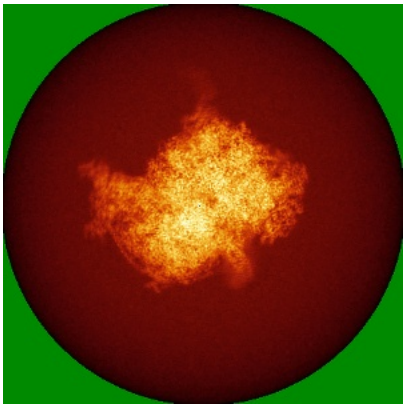


Y

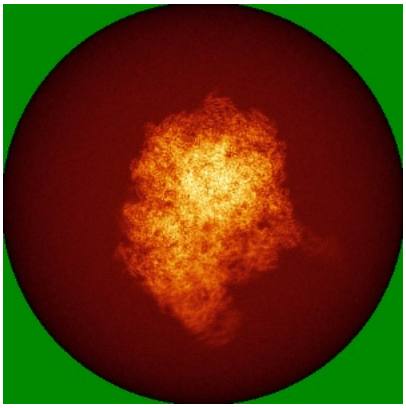


Z

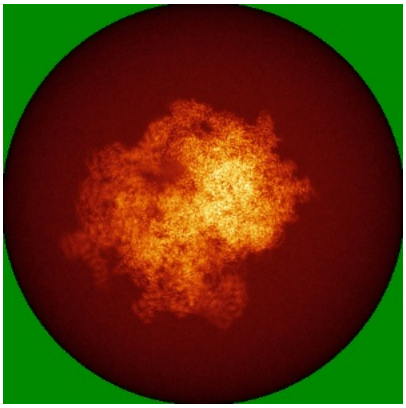
6.4.2 Raw map



X



Y

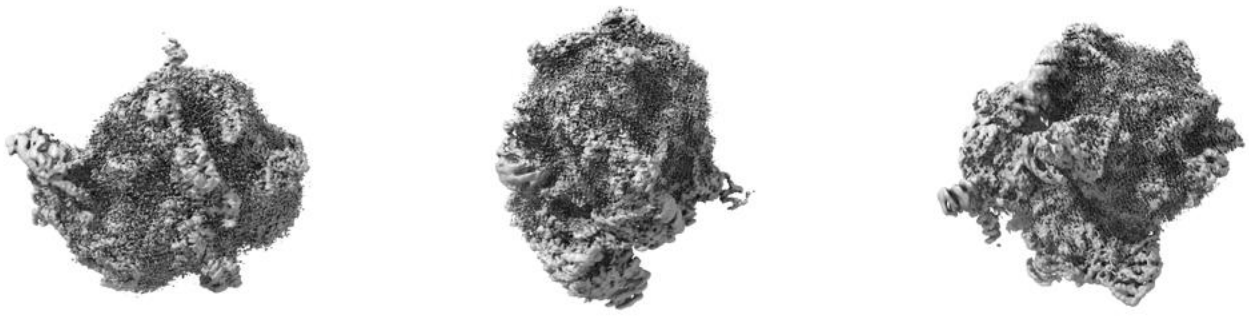


Z

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)

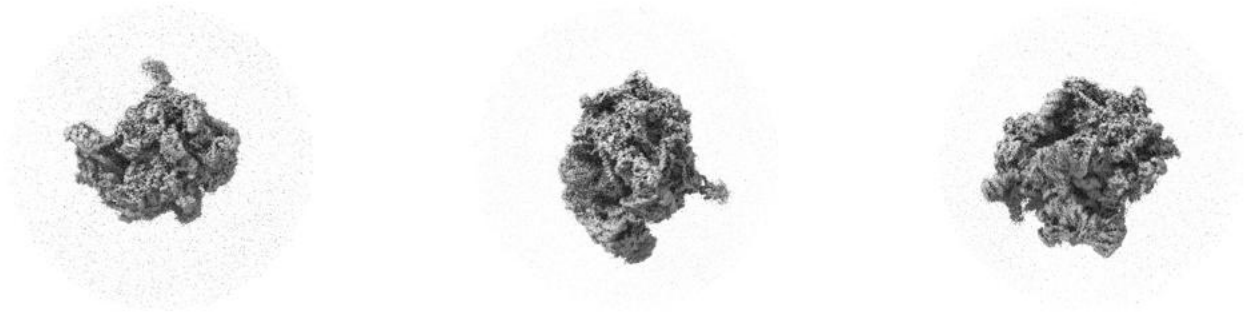
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

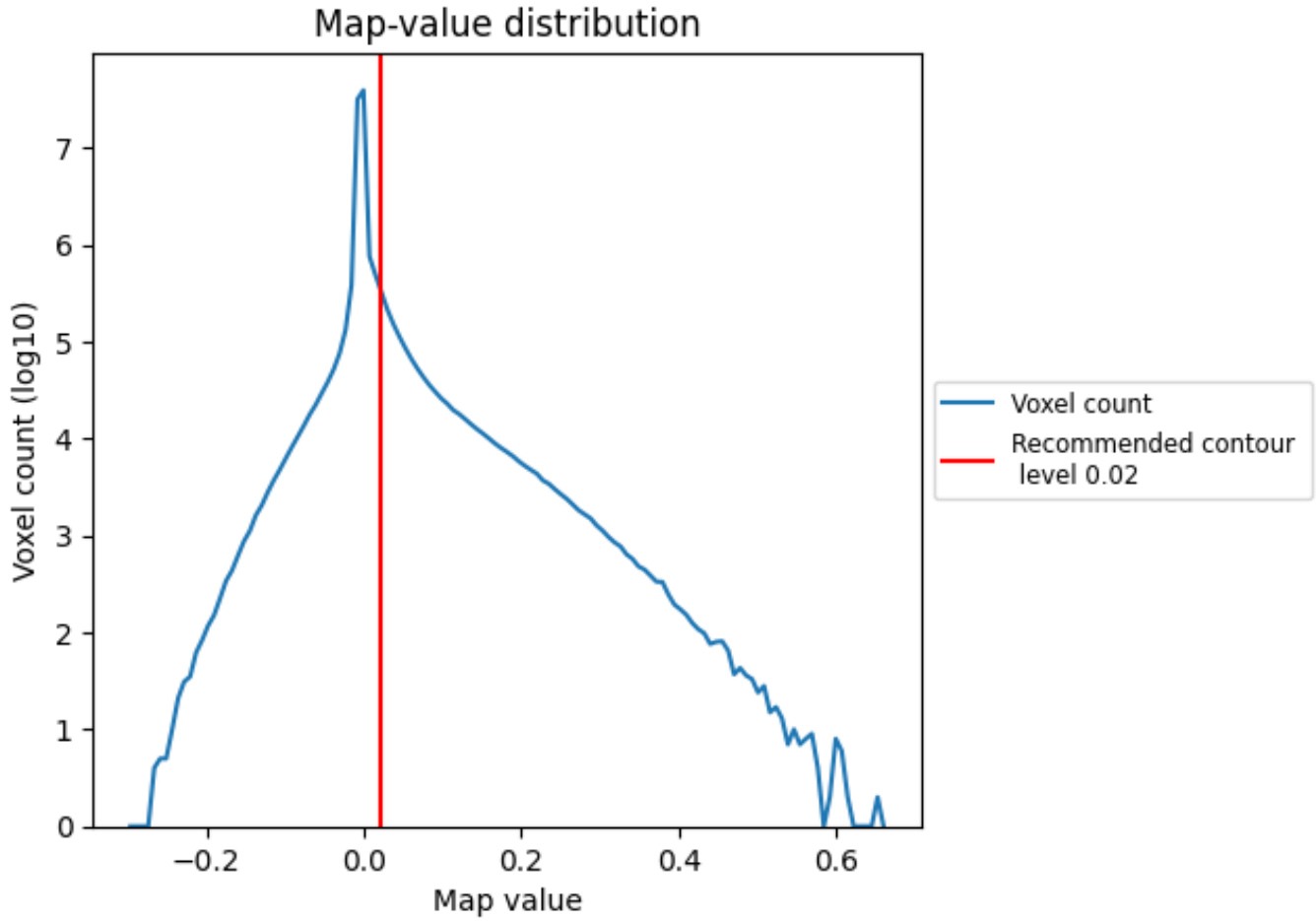
6.6 Mask visualisation (i)

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

7 Map analysis

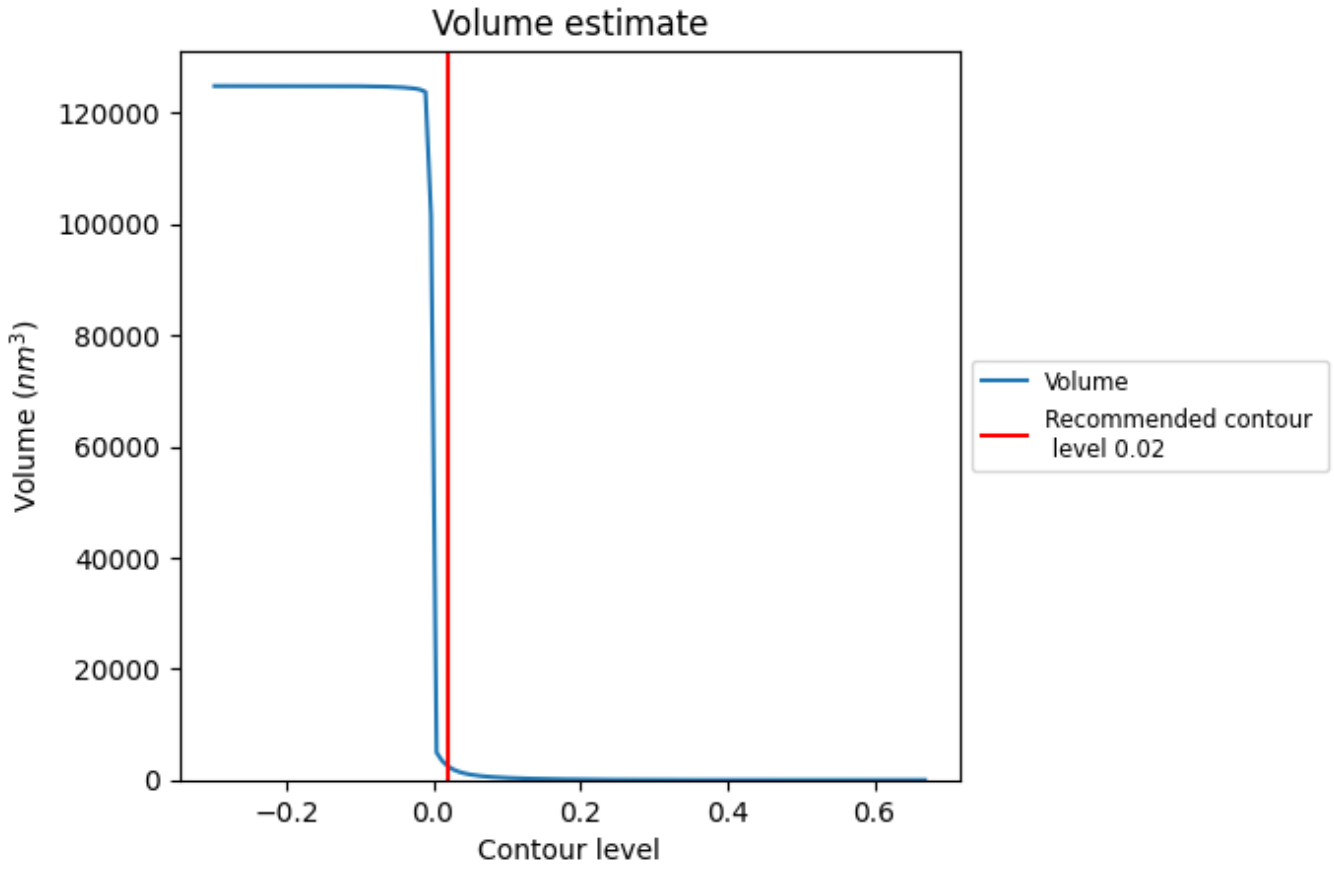
This section contains the results of statistical analysis of the map.

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.

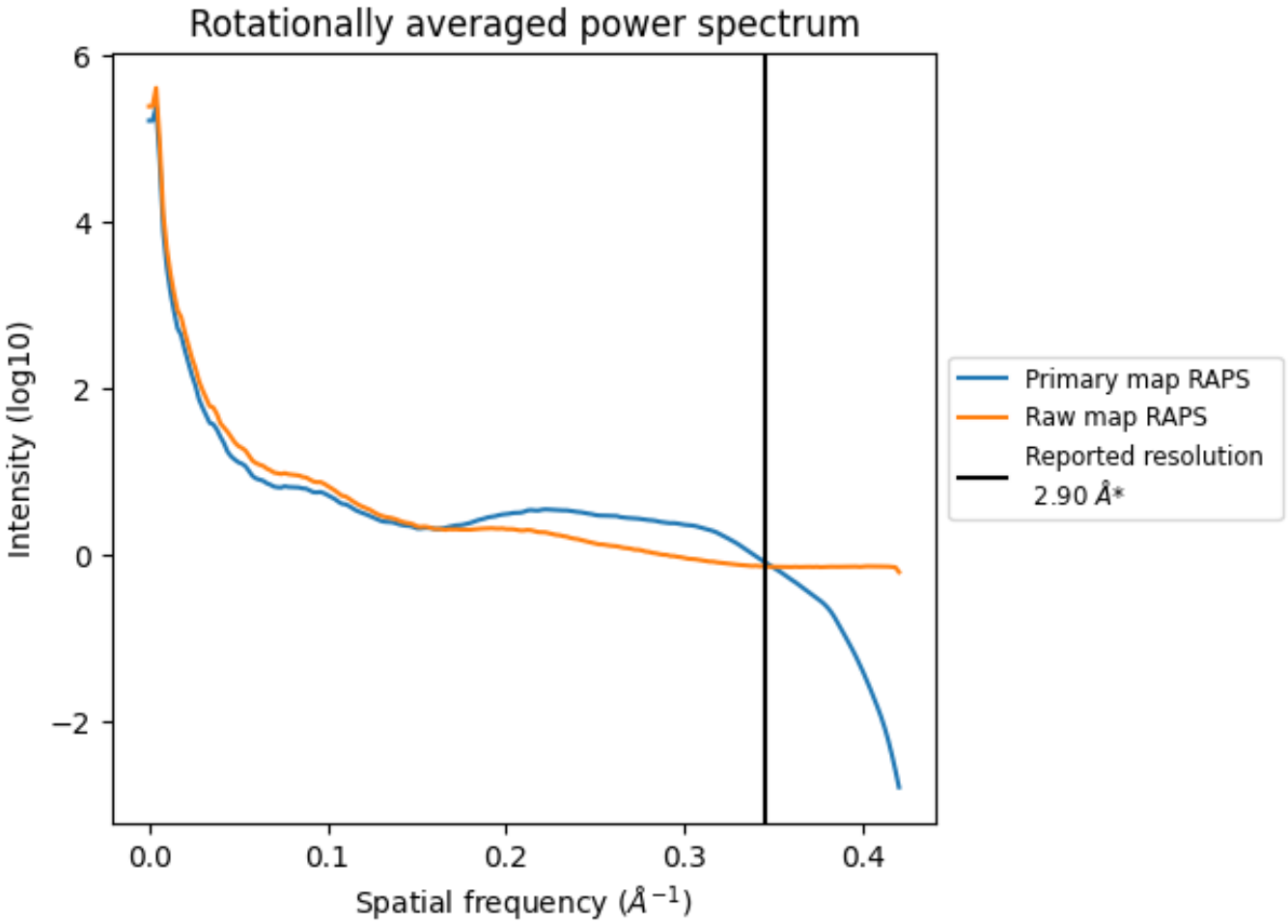
7.2 Volume estimate



The volume at the recommended contour level is 2486 nm^3; this corresponds to an approximate mass of 2246 kDa.

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

7.3 Rotationally averaged power spectrum (i)

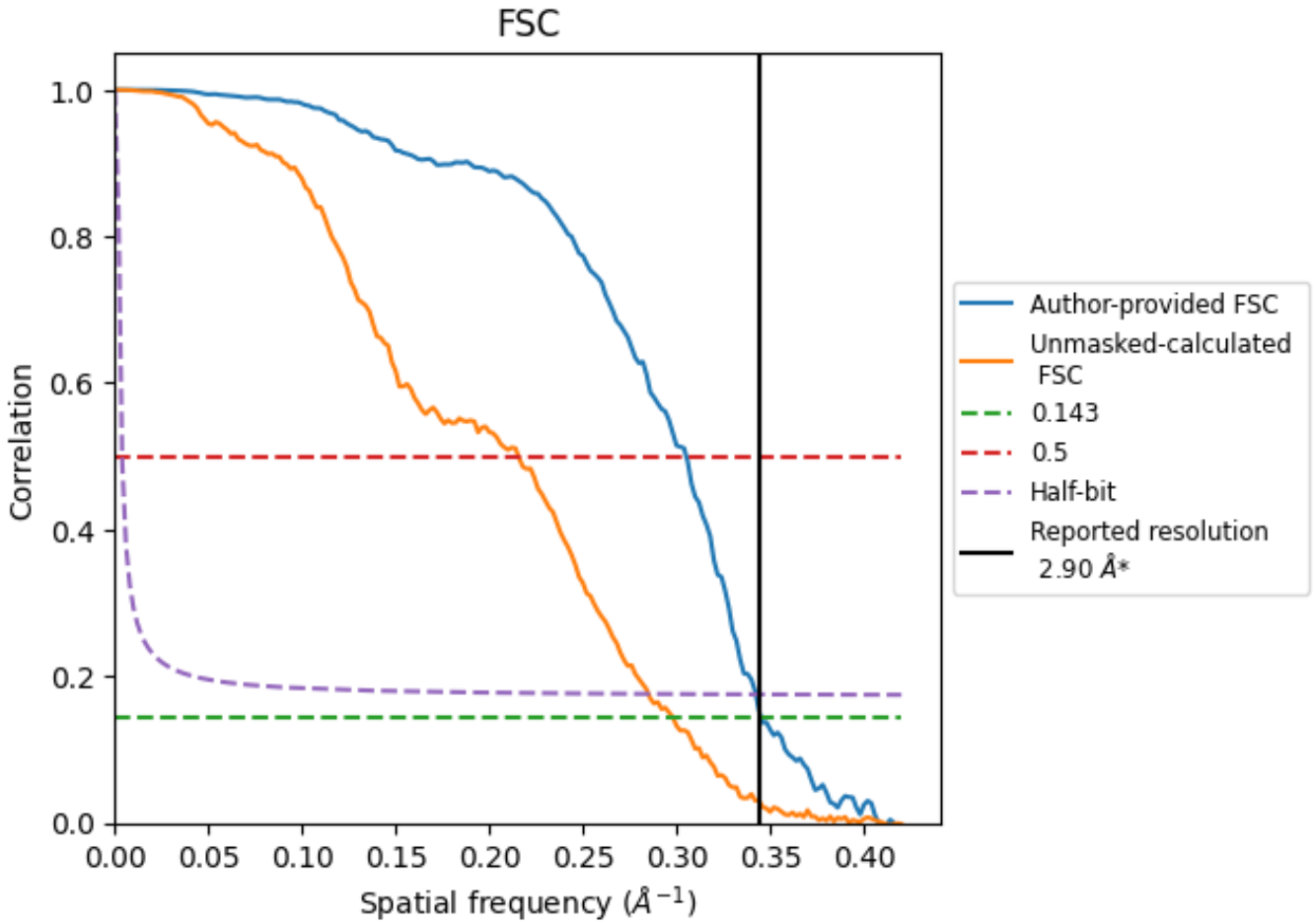


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

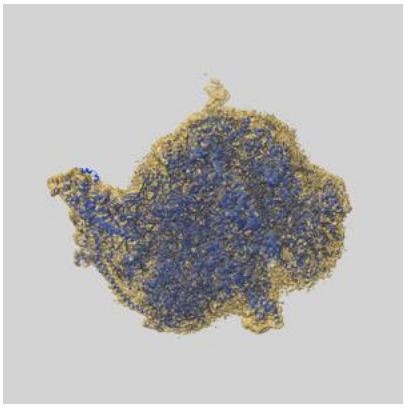
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.28	2.92
Unmasked-calculated*	3.35	4.64	3.51

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

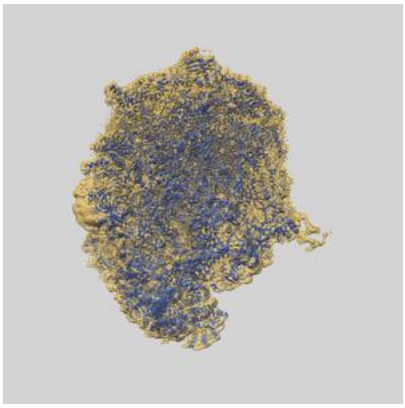
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36836 and PDB model 8K2A. Per-residue inclusion information can be found in section 3 on page 21.

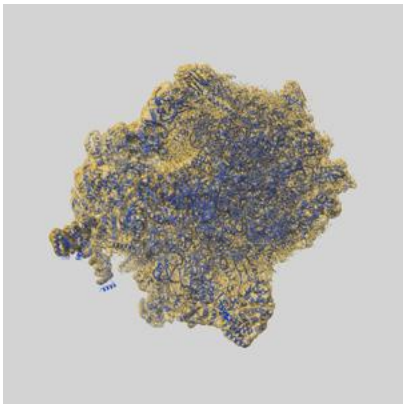
9.1 Map-model overlay



X



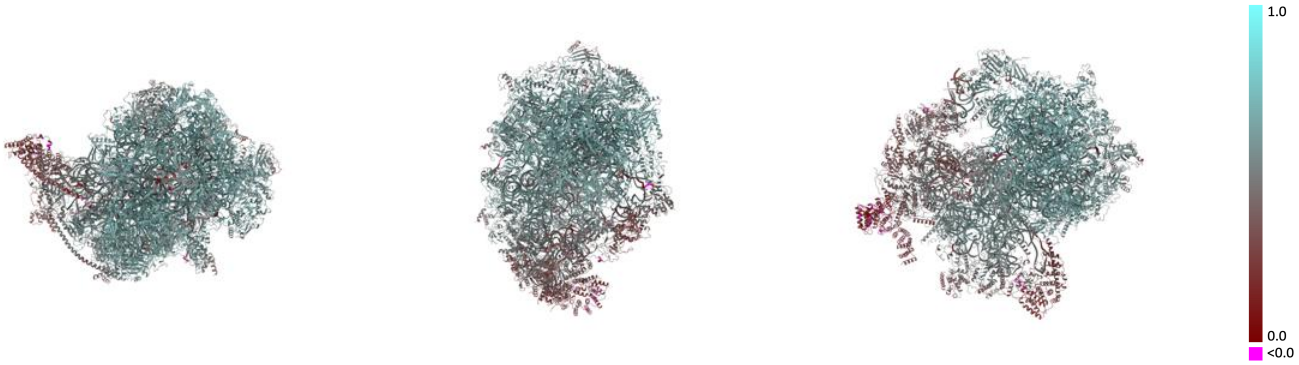
Y



Z

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

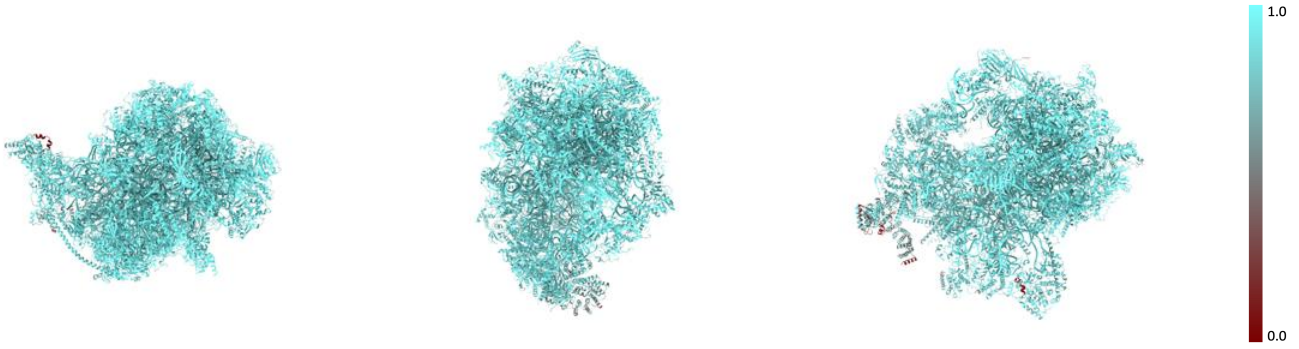
9.2 Q-score mapped to coordinate model (i)



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.

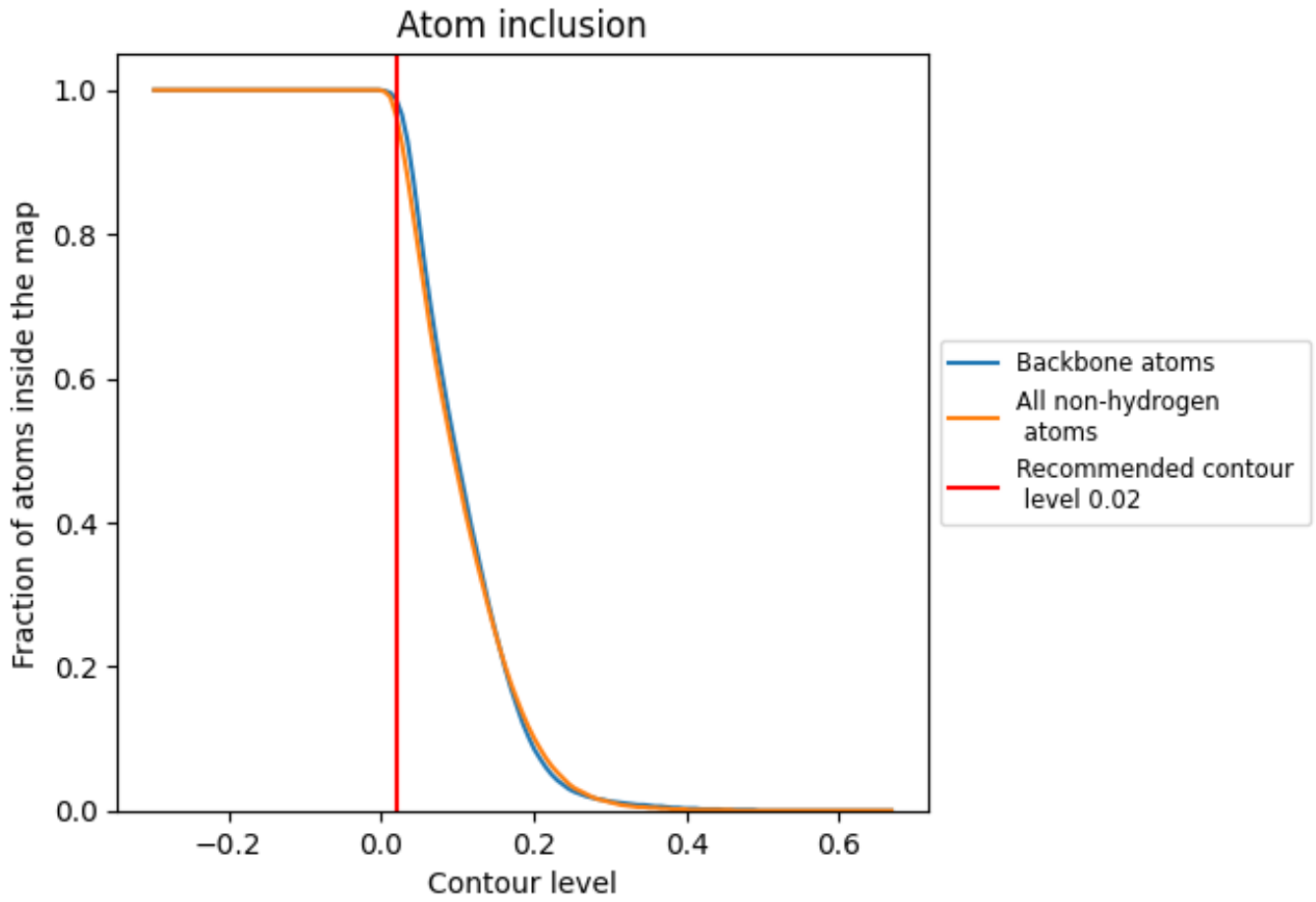
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

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

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

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

Continued on next page...

Continued from previous page...

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