



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 17, 2019 – 08:08 AM EST

PDB ID : 6HCF
EMDB ID: : EMD-0192
Title : Structure of the rabbit 80S ribosome stalled on globin mRNA at the stop codon
Authors : Juszkievicz, S.; Chandrasekaran, V.; Lin, Z.; Kraatz, S.; Ramakrishnan, V.;
Hegde, R.S.
Deposited on : 2018-08-14
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

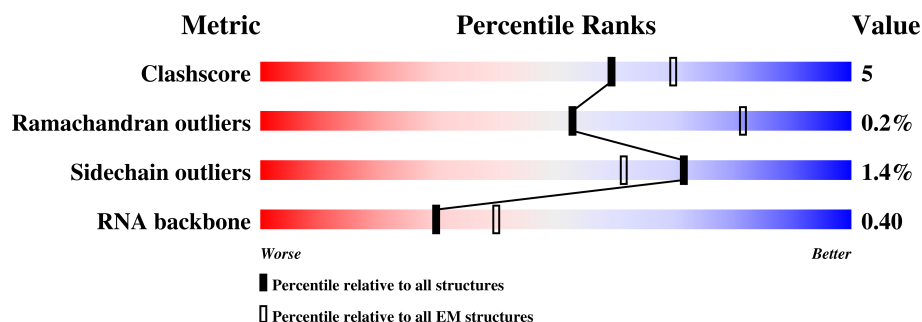
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.
















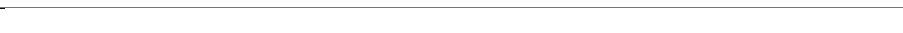

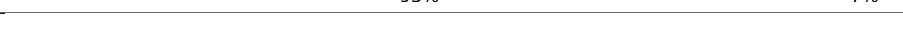
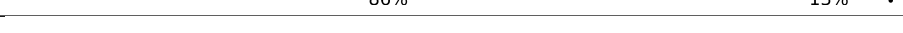
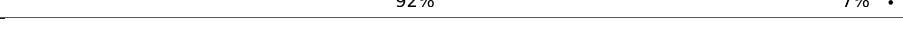



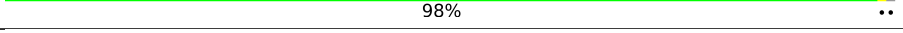

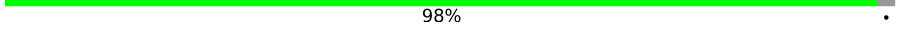

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A1	1869	56% 31% 5% • 7%
2	B1	295	65% 8% 26%
3	C1	264	67% 13% 19%
4	D1	293	68% 8% 25%
5	E1	243	78% 16% 6%
6	F1	263	90% 10%
7	G1	204	83% 7% 9%
8	H1	249	78% 18% 5%

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Mol	Chain	Length	Quality of chain
9	I1	194	 90% 6% 5%
10	J1	208	 86% 13% .
11	K1	194	 85% 9% . 5%
12	L1	165	 53% 5% 42%
13	M1	158	 78% 12% 9%
14	N1	132	 67% 20% . 11%
15	O1	151	 92% 7% .
16	P1	168	 70% 10% . 19%
17	Q1	145	 73% 9% . 17%
18	R1	146	 87% 9% . .
19	S1	135	 85% 13% .
20	T1	152	 88% 7% 5%
21	U1	145	 87% 10% . .
22	V1	119	 76% 8% 16%
23	W1	83	 93% 7%
24	X1	130	 86% 13% .
25	Y1	143	 92% 7% .
26	Z1	130	 83% 12% 5%
27	a1	125	 60% 40%
28	b1	115	 88% 12%
29	c1	84	 98% . .
30	d1	69	 90% 10%
31	e1	56	 98% .
32	f1	133	 40% . 59%
33	g1	156	 43% . 56%



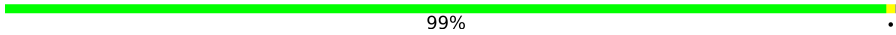



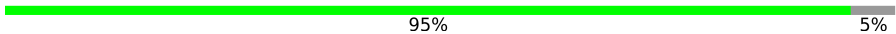
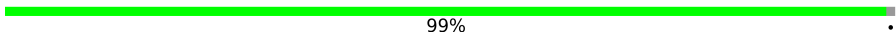

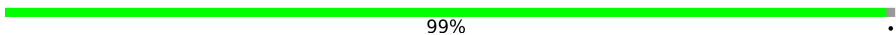
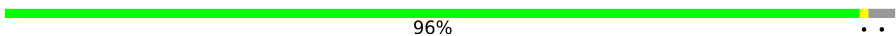


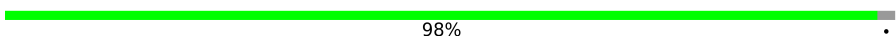

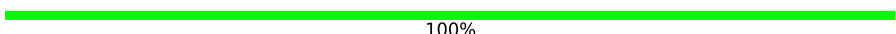
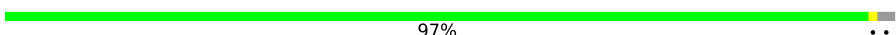
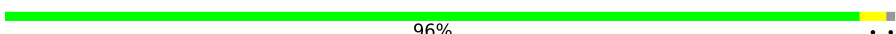


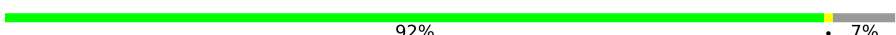




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Mol	Chain	Length	Quality of chain
34	h1	317	98% ..
35	j1	439	94% • 5%
36	k1	599	95% • •
37	52	3634	56% 34% 8% •
38	72	120	56% 38% • •
39	82	156	58% 34% • •
40	A3	257	69% 23% • • •
41	B3	403	83% 15% •
42	C3	425	79% 6% 15%
43	E3	291	64% 9% • 26%
44	F3	247	81% 11% 9%
45	H3	192	90% 9% •
46	L3	211	91% 8%
47	M3	218	56% 7% 37%
48	N3	204	81% 18%
49	O3	203	91% 6% •
50	P3	184	78% 5% 17%
51	Q3	188	91% 8% • •
52	R3	196	72% 17% • 8%
53	S3	176	89% 10% •
54	T3	160	89% 11% •
55	U3	128	63% 13% • 23%
56	V3	140	80% 13% • 6%
57	W3	157	55% 11% • 32%
58	X3	156	69% 6% 24%




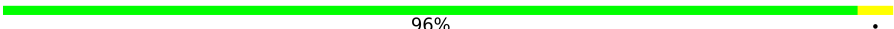
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Mol	Chain	Length	Quality of chain
59	Y3	145	 78%14%8%
60	Z3	136	 72%25%...
61	a3	148	 99%..
62	b3	226	 45%54%
63	c3	115	 83%15%
64	d3	125	 84%14%
65	e3	135	 95%5%
66	f3	110	 99%.
67	g3	117	 89%5%..
68	h3	123	 99%.
69	i3	105	 96%..
70	j3	97	 88%11%
71	k3	70	 94%..
72	l3	51	 98%.
73	m3	102	 50%49%
74	n3	25	 100%
75	o3	106	 97%..
76	p3	92	 96%..
77	r3	137	 89%9%
78	s3	318	 58%38%
79	t3	165	 92%7%
80	23	76	 66%26%8%
81	w3	23	 52%43%.
82	J3	178	 86%10%.
83	G3	319	 61%10%27%

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Mol	Chain	Length	Quality of chain
84	D3	297	 84%14%..
85	I3	214	 83%11%..
86	1	22	 68%9%23%
87	u3	217	 96%.

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226754 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	1732	Total	C	N	O	P	0	0
			36969	16502	6637	12099	1731		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 33 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g1	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called eRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j1	419	Total	C	N	O	S	0	0
			3309	2106	562	629	12		

- Molecule 36 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k1	577	Total	C	N	O	S	0	0
			4555	2914	780	830	31		

- Molecule 37 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	52	3634	Total	C	N	O	P	0	0
			77819	34651	14241	25293	3634		

- Molecule 38 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	72	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 39 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	82	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 40 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A3	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 41 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B3	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 42 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C3	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	E3	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 44 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	F3	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	61	ARG	GLY	conflict	UNP G1TUB1
F3	93	ARG	GLY	conflict	UNP G1TUB1
F3	131	MET	VAL	conflict	UNP G1TUB1
F3	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 45 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H3	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 46 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L3	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 47 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M3	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N3	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 49 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O3	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 50 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P3	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q3	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 52 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R3	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 53 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 54 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T3	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 55 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U3	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 56 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V3	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 57 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W3	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 58 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X3	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 59 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y3	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z3	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 61 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a3	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 62 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b3	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 63 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c3	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 64 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d3	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 65 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	e3	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 66 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f3	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 67 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g3	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 68 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h3	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 69 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i3	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j3	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 71 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k3	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 72 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l3	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 73 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m3	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 74 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n3	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 75 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o3	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 76 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p3	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 77 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	r3	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 78 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	s3	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 79 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t3	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 80 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	23	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w3	23	Total	C	N	O	P	0	0
			493	222	94	154	23		

- Molecule 82 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	J3	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 83 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	G3	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

- Molecule 84 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	D3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 85 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	I3	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 86 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	1	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 87 is a protein called uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	u3	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

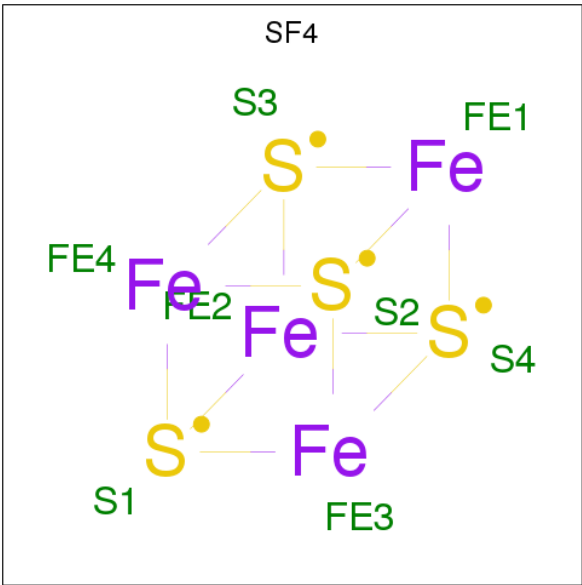
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	G1	1	Total 1	Mg 1	0
88	A1	77	Total 77	Mg 77	0
88	g3	1	Total 1	Mg 1	0
88	w3	1	Total 1	Mg 1	0
88	P3	1	Total 1	Mg 1	0
88	72	7	Total 7	Mg 7	0
88	52	204	Total 204	Mg 204	0
88	M1	1	Total 1	Mg 1	0
88	V3	1	Total 1	Mg 1	0
88	82	5	Total 5	Mg 5	0
88	a3	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	g1	1	Total 1	Zn 1	0
89	g3	1	Total 1	Zn 1	0
89	e1	1	Total 1	Zn 1	0
89	p3	1	Total 1	Zn 1	0
89	m3	1	Total 1	Zn 1	0
89	b1	1	Total 1	Zn 1	0
89	j3	1	Total 1	Zn 1	0
89	o3	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
90	k1	1	Total	Fe	S	0
			16	8	8	
90	k1	1	Total	Fe	S	0
			16	8	8	

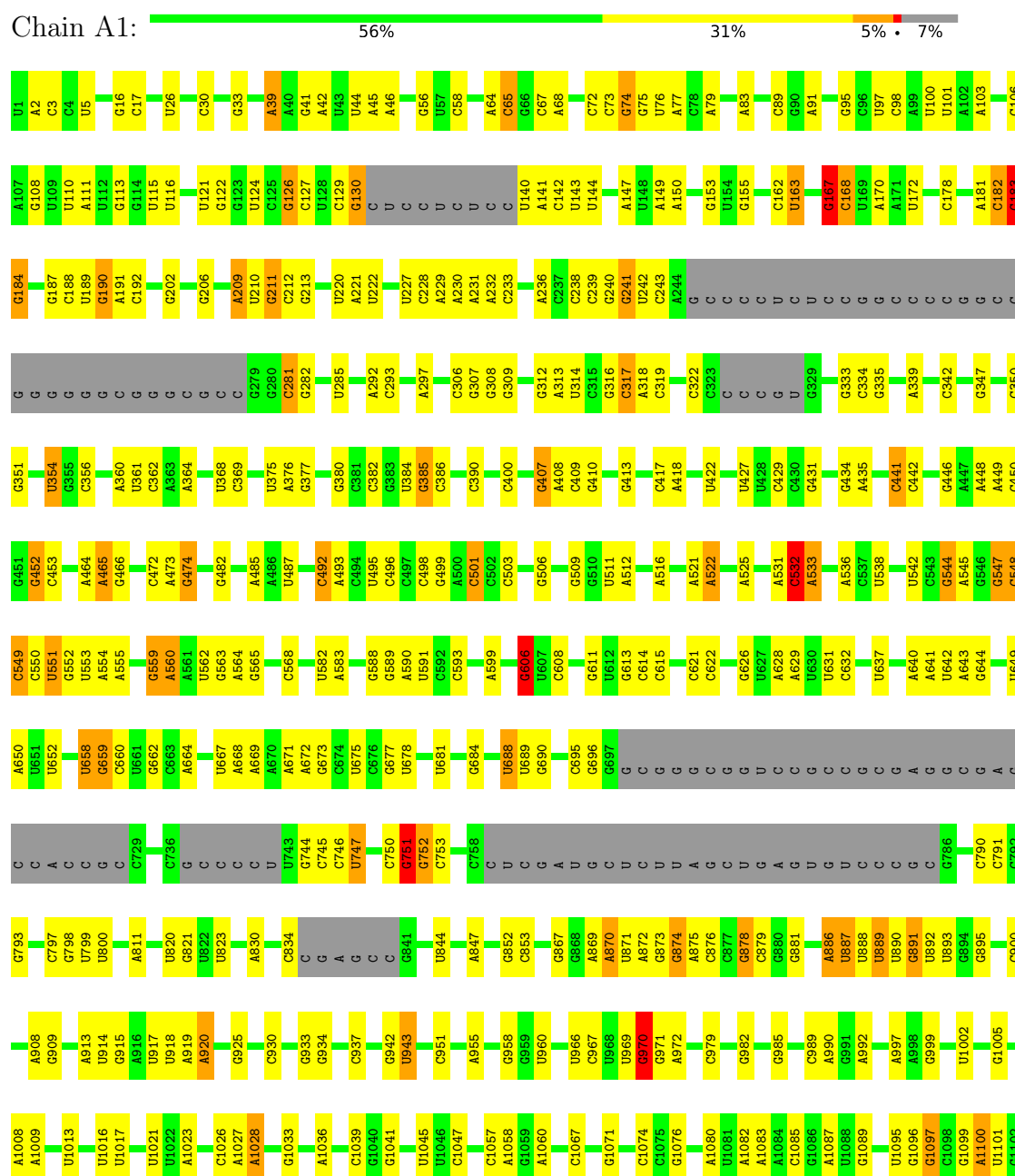
- Molecule 91 is water.

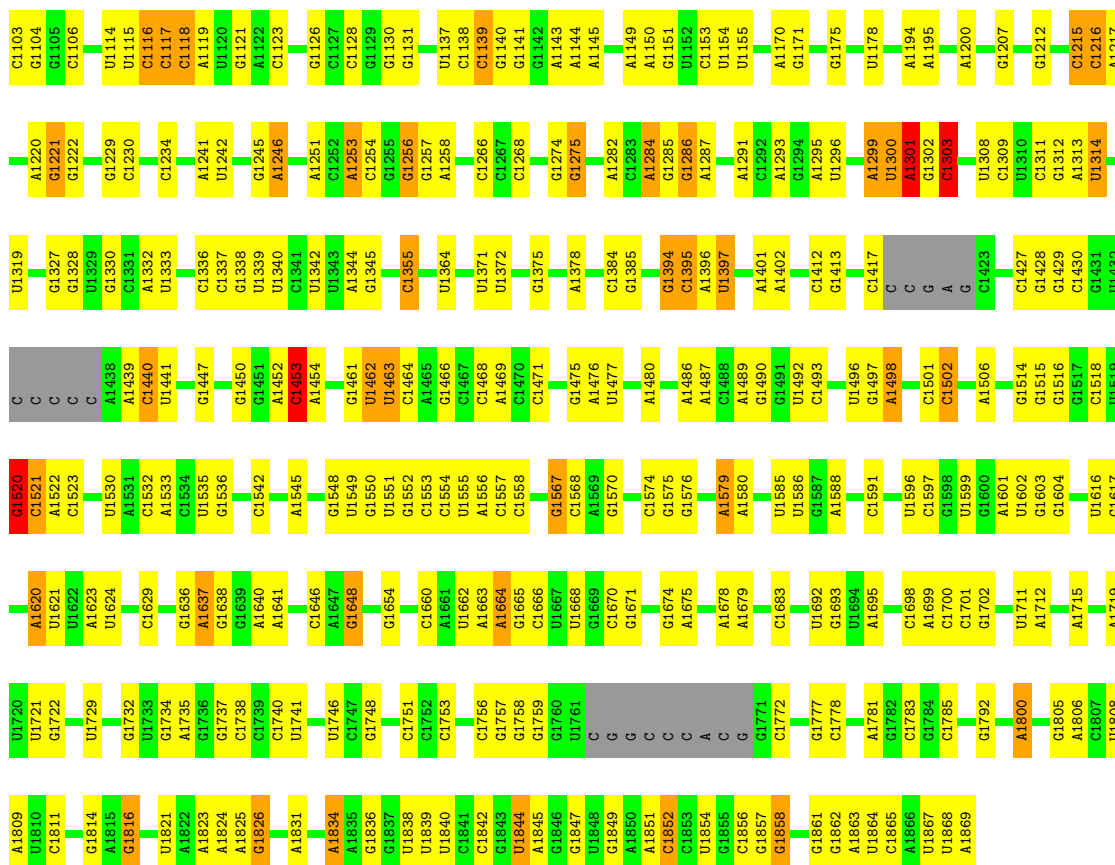
Mol	Chain	Residues	Atoms		AltConf
91	52	3	Total	O	0
			3	3	
91	1	1	Total	O	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

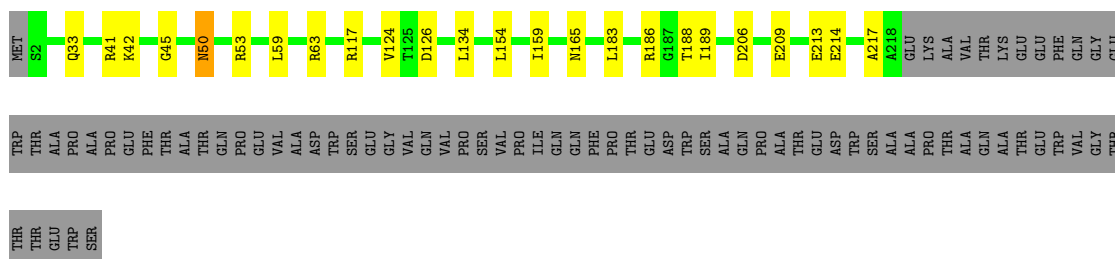
• Molecule 1: 18S ribosomal RNA





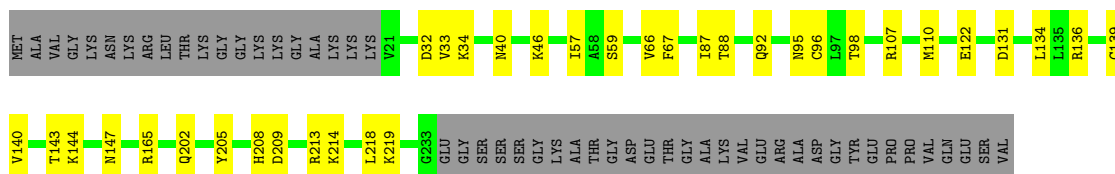
- Molecule 2: uS2

Chain B1:



- Molecule 3: 40S ribosomal protein S3a

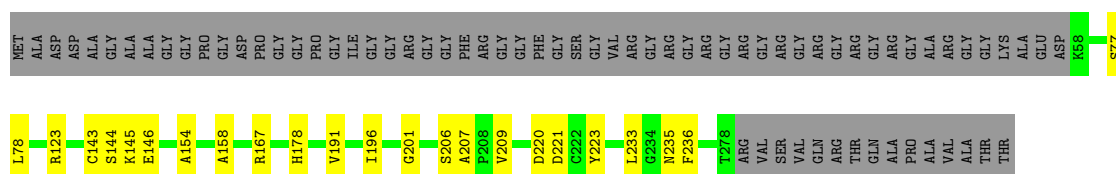
Chain C1:



- Molecule 4: uS5

Chain D1:





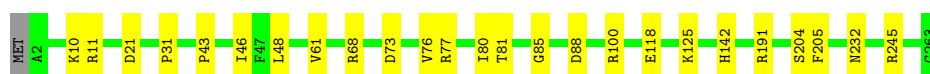
- Molecule 5: uS3

Chain E1: 78% 16% 6%



- Molecule 6: eS4

Chain F1: 90% 10%



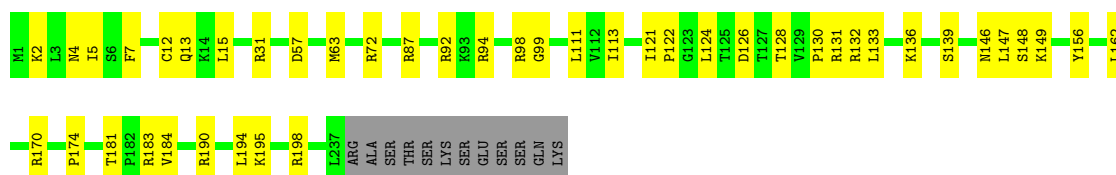
- Molecule 7: Ribosomal protein S5

Chain G1: 83% 7% 9%



- Molecule 8: 40S ribosomal protein S6

Chain H1: 78% 18% 5%



- Molecule 9: 40S ribosomal protein S7

Chain I1: 90% 6% 5%



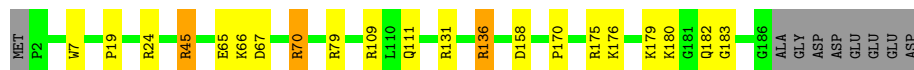
- Molecule 10: eS8

Chain J1: 86% 13% 1%



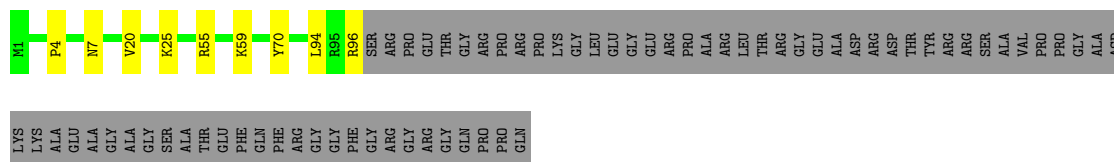
- Molecule 11: Ribosomal protein S9 (Predicted)

Chain K1: 85% 9% 5%



- Molecule 12: eS10

Chain L1: 53% 5% 42%



- Molecule 13: Ribosomal protein S11

Chain M1: 78% 12% 9%



- Molecule 14: 40S ribosomal protein S12

Chain N1: 67% 20% 11%



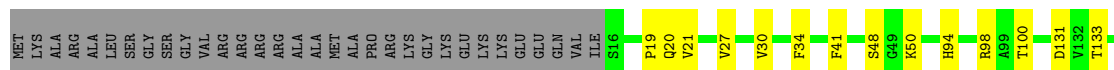
- Molecule 15: uS15

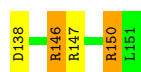
Chain O1: 92% 7% 1%



- Molecule 16: uS11

Chain P1: 70% 10% 19%





- Molecule 17: uS19

Chain Q1: 73% 9% 17%



- Molecule 18: Ribosomal protein S16

Chain R1: 87% 9% ..



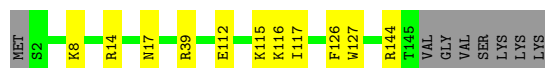
- Molecule 19: eS17

Chain S1: 85% 13% .



- Molecule 20: uS13

Chain T1: 88% 7% 5%



- Molecule 21: eS19

Chain U1: 87% 10% ..



- Molecule 22: uS10

Chain V1: 76% 8% 16%

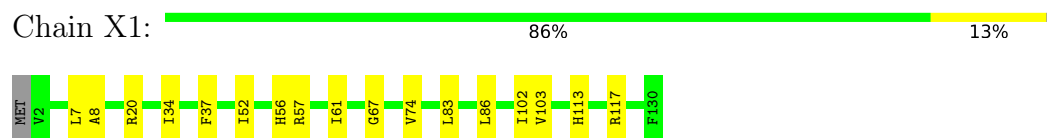


- Molecule 23: eS21

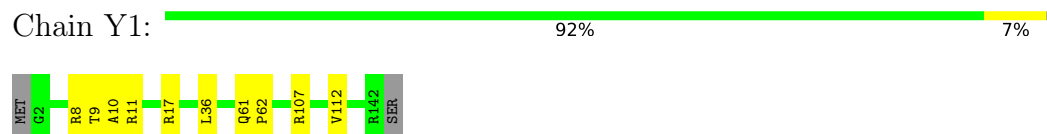
Chain W1: 93% 7%



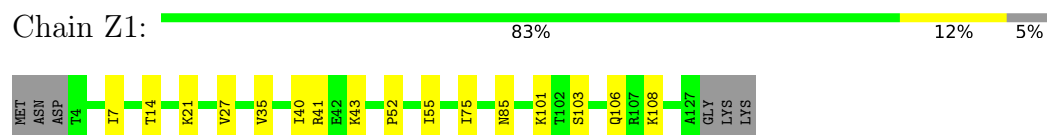
- Molecule 24: Ribosomal protein S15a



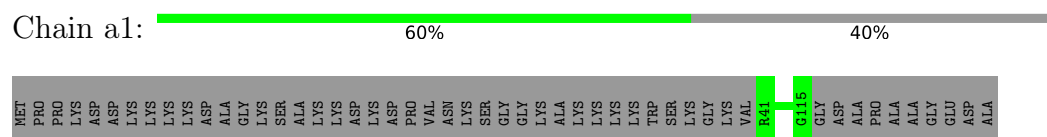
- Molecule 25: uS12



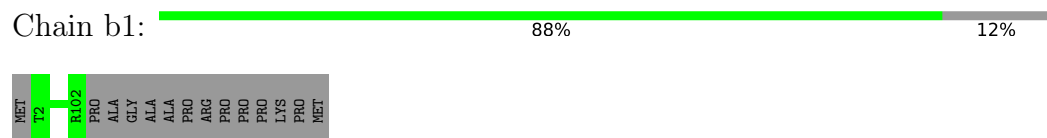
- Molecule 26: eS24



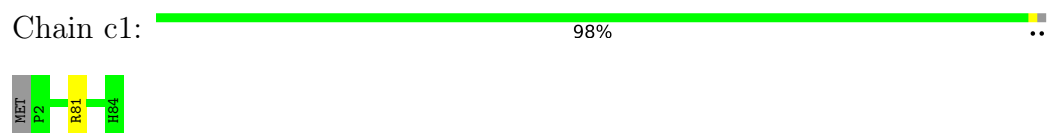
- Molecule 27: eS25



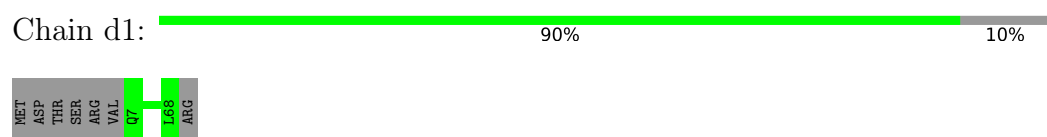
- Molecule 28: eS26



- Molecule 29: 40S ribosomal protein S27



- Molecule 30: Ribosomal protein S28



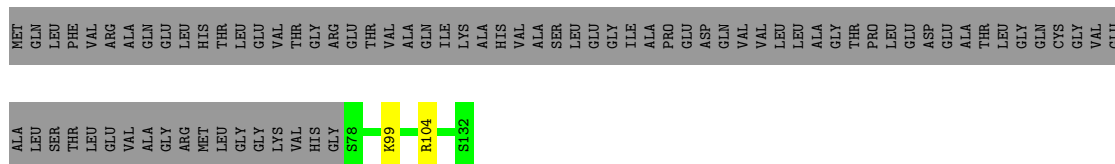
- Molecule 31: uS14





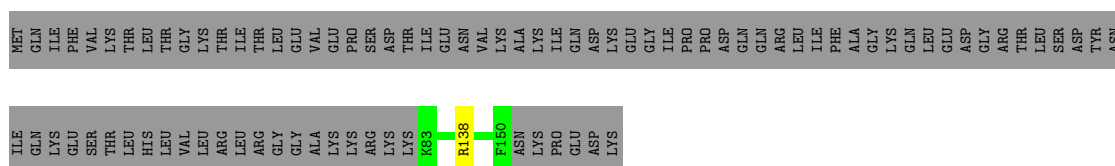
- Molecule 32: 40S ribosomal protein S30

Chain f1: 40% 59%



- Molecule 33: Ribosomal protein S27a

Chain g1: 43% 56%



- Molecule 34: RACK1

Chain h1: 98% ..



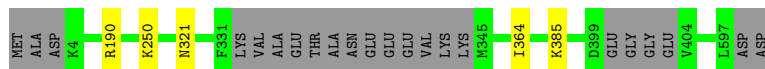
- Molecule 35: eRF1(AAQ)

Chain j1: 94% 5%



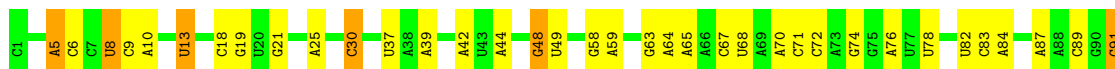
- Molecule 36: ATP binding cassette subfamily E member 1

Chain k1: 95% ..



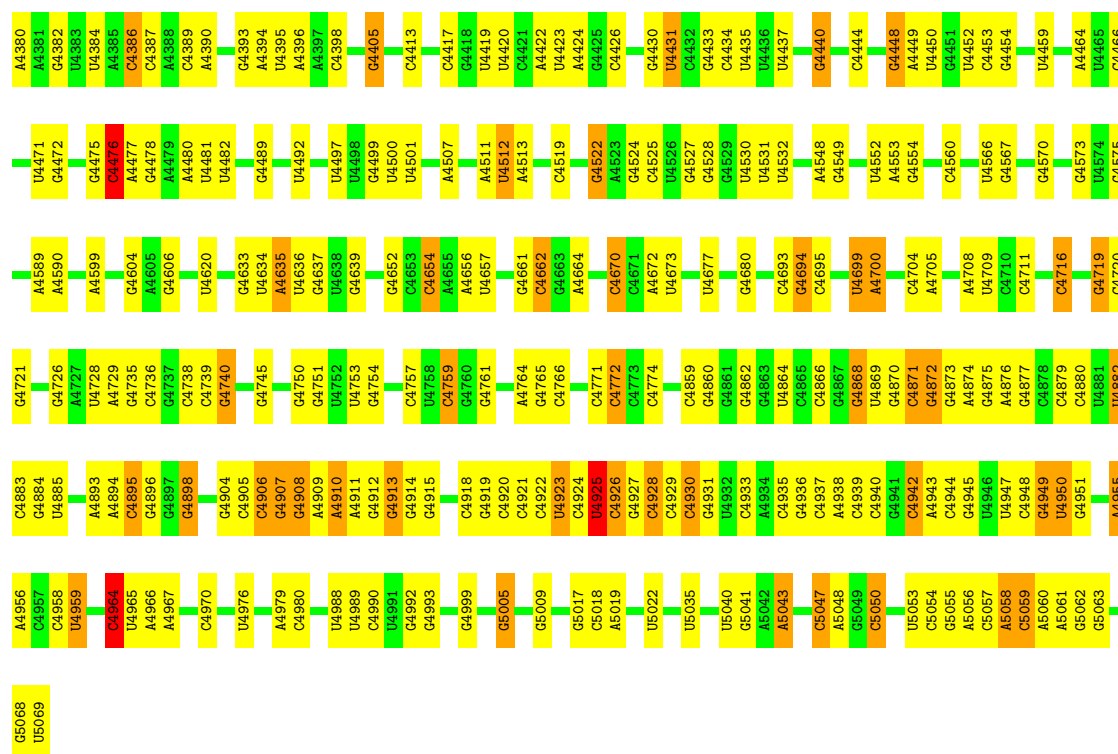
- Molecule 37: 28S ribosomal RNA

Chain 52: 56% 34% 8%



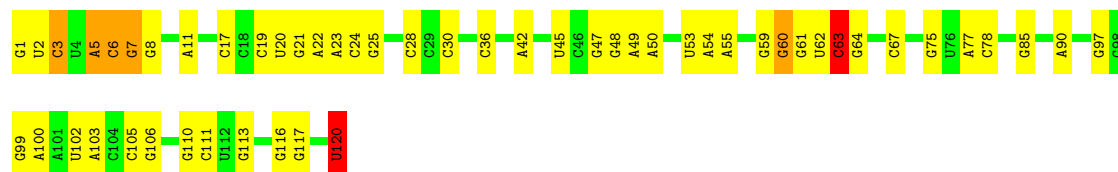
C1920	G1818	G1731	C1614	G1517	G1426	G1338	G1234	G1094	C941	C719	G497	C390	C276	C172	C92
C1921	G1819	G1734	G1624	A1518	C1429	U1341	G1235	A1095	G942	G720	C498	C390	G277	C173	G93
G1922	G1820	G1735	G1625	A1518	C1429	U1341	G1236	A1095	A943	G721	G499	A395	G280	C174	A94
C1924	G1821	G1736	G1626	C1521	G1434	C1346	G1237	U1100	A945	G722	G500	A396	G280	C175	G95
G1928	U1822	C1740	G1627	G1522	G1435	C1347	A1238	U1101	U946	G729	G504	A407	G292	G176	U96
A1929	G1823	G1741	A1631	A1523	C1436	C1352	G1239	U1102	C947	G730	G505	A407	G293	G179	C100
U1930	G1824	A1742	A1632	A1524	C1437	G1353	G1244	C1103	G948	G731	G506	A410	G294	C180	A101
C1931	C1828	A1746	A1633	U1531	U1440	A1354	G1245	C1104	G949	G732	U510	G411	U297	C181	G102
A1932	G1829	G1750	G1634	U1531	C1441	G1355	G1246	C1105	G950	A733	C515	G412	G301	G182	G104
G1933	U1834	G1751	C1635	A1534	U1356	U1357	G1272	C1106	G951	G737	C516	G413	A300	G191	A105
A1934	G1835	G1752	A1636	C1535	U1357	G1358	G1273	C1107	G855	C737	C517	G417	C302	A197	G107
C1935	A1837	G1753	A1637	U1538	U1445	C1446	G1276	C1108	A856	C738	C518	G417	C303	U200	A108
A1939	G1842	C1754	U1638	G1539	U1445	C1446	G1277	C1109	G857	C739	G641	G423	A306	C201	G109
G1940	G1843	U1756	U1639	G1540	G1453	G1360	G1278	G1161	G959	G740	G642	G423	A307	U204	G114
A1941	U1757	U1756	A1643	C1540	G1454	G1361	G1279	G1162	A960	G741	G643	G441	C309	G214	C115
G1942	G1844	G1758	G1455	G1543	G1455	G1362	A1279	G1164	G961	G743	G648	U440	G310	C216	G119
A1943	G1847	G1759	C1456	G1547	C1457	G1370	G1280	G1165	G962	G747	A649	U440	G311	C217	U122
A1944	C1847	G1760	G1457	C1458	C1457	G1371	G1281	G1167	G965	A747	G661	C446	G312	C218	G126
G1948	G1853	C1762	G1458	A1547	C1458	A1371	G1282	C1168	A966	G748	G661	C447	G312	C219	C126
G1951	G1854	G1763	A1652	G1548	G1459	A1372	G1283	G1169	C967	G749	G662	C448	G312	C220	C133
G1952	G1855	G1764	G1654	G1549	A1459	A1373	G1284	G1171	C968	G750	G664	C449	G312	C221	G134
A1956	C1857	A1767	G1658	G1550	G1466	G1377	G1285	U1177	C969	G751	G665	C450	G315	C222	G135
U1957	G1858	G1768	U1659	G1551	C1467	G1378	G1286	U1178	G970	G752	G666	C451	G315	C223	G136
A1958	U1866	C1772	U1660	G1552	C1467	C1378	G1287	G1181	G971	G753	A667	A452	G321	C224	G137
U1959	U1867	U1773	C1661	G1553	C1468	C1379	G1291	C1182	G971A	G754	G668	G453	G322	C225	G142
A1960	A1868	G1774	G1662	G1554	C1469	U1381	G1292	C1183	C972	G755	G669	U454	G322	C226	G143
G1961	G1869	U1775	C1663	A1558	G1472	U1381	G1293	C1184	G978	G756	G670	U454	G323	C227	G144
A1962	C1870	C1777	G1664	G1566	G1473	A1387	G1294	C1185	G978	G757	G671	U463	G324	C228	G145
C1963	G1878	G1767	U1665	G1567	G1474	U1388	G1295	C1186	U982	G758	G672	U464	G324	C229	G146
A1964	U1882	A1767	G1666	G1570	G1475	U1389	G1296	C1187	C983	G759	G673	U465	G325	C230	G147
G1968	U1889	U1790	C1673	G1571	G1476	A1391	G1297	C1193	C984	G760	G674	U467	G326	C231	G148
G1969	U1890	U1791	C1674	G1572	G1477	A1392	G1298	C1194	C985	G761	G675	U468	G327	C232	G149
A1970	U1891	U1792	C1675	G1573	G1478	G1393	G1299	C1195	C986	G762	G676	U469	G327	C233	G150
U1971	U1892	U1793	C1676	G1574	G1479	G1394	G1300	C1196	U989	G763	G677	C474	G327	C234	U152
G1976	A1891	U1796	U1679	G1575	G1480	G1395	G1301	C1199	U990	G764	G678	C475	G327	C235	G153
C1978	C1893	U1800	A1694	U1590	C1481	G1396	U1302	G1200	G1064	G765	G679	C475	G327	C236	G154
U1979	A1897	A1801	U1687	U1591	G1482	G1397	A1303	G1201	A915	G766	G680	C475	G327	C237	U155
A1980	G1898	U1802	U1688	G1592	G1483	A1397	C1304	G1202	G916	G767	G681	C475	G327	C238	G156
G1981	G1899	G1803	G1688	G1593	G1484	A1398	C1305	G1203	A917	G768	G682	C475	G327	C239	U157
A1983	U1906	A1804	G1689	U1596	G1485	G1399	C1306	G1204	G918	G769	G683	C475	G327	C240	A158
A1984	U1907	G1806	G1690	G1597	G1486	G1400	C1307	G1205	C922B	G770	G684	C475	G327	C241	C159
A1990	G1910	C1807	G1691	U1602	G1487	G1401	C1308	G1206	C923	G771	G685	C475	G327	C242	G160
A1991	C1911	C1808	C1720	U1603	G1488	C1411	C1309	G1207	A929	G772	G686	C475	G327	C243	G161
U1992	G1912	G1809	G1724	G1605	G1489	C1412	C1310	G1208	G930	G773	G687	C475	G327	C244	G162
C1993	G1913	G1810	G1725	U1609	G1490	C1413	C1311	G1209	G931	G774	G688	C475	G327	C245	G163
C1994	G1914	G1811	U1726	U1610	G1491	C1414	C1312	U1210	A932	G775	G689	C475	G327	C246	G164
G1995	U1918	C1812	A1729	G1612	G1492	C1415	C1313	G1211	A933	G776	G690	C475	G327	C247	C165
U1997	G1919	G1815	U1730	A1613	U1514	G1425	C1314	G1212	A934	G777	G691	C475	G327	C248	C166

G4276	G4277	A4280	A4281	A4282	U4285	U4290	U4291	A4292	A4293	U4293	U4300	U4301	U4302	U4303	A4304	A4305	U4306	A4313	A4317	A4318	U4321	A4322	A4323	G4330	G4331	G4332	U4334	U4335	A4336	A4339	A4348	A4349	C4350	U4351	G4355	U4359	A4366	U4374	G4377	A4378	A4379											
C4171	A4172	G4173	G4180	G4183	G4184	G4191	U4194	G4195	G4196	G4201	U4202	A4203	C4204	A4205	A4206	C4207	U4208	G4209	A4212	C4215	C4223	A4224	U4229	U4232	A4233	A4234	C4237	G4240	C4243	A4251	G4254	A4255	A4256	U4257	U4265	G4266	A4268	A4271	G4272	A4273	A4274	A4275										
U4068	U4069	U4070	U4071	G4076	U4077	G4078	G4084	A4085	G4086	G4091	G4092	G4093	G4094	G4099	C4100	G4108	U4111	C4112	U4113	C4114	G4115	U4116	U4117	U4118	C4119	U4120	G4121	C4122	C4123	G4124	A4127	A4128	G4129	C4130	G4131	C4132	C4133	C4138	G4156	A4157	C4158	C4159										
U3925	C3926	U3927	A3928	C3937	C3938	U3939	U3940	G3941	A3942	A3943	G3944	A3947	C3948	U3957	C3958	U3959	A3960	A3961	A3962	A3963	U3964	A3965	A3966	U3967	U3968	G3969	C3970	G3971	U3972	C3973	G4034	G4035	G4036	C4037	C4038	G4039	U4044	U4045	U4046	A4047	A4048	U4049	A4050	C4051	C4052	A4053	G4061	A4062	G4065	U4066	U4067	
U3822	A3825	C3834	C3837	U3838	U3839	U3840	C3841	C3842	C3843	C3844	C3845	U3853	G3857	C3858	A3865	C3866	A3867	C3868	C3869	C3870	A3871	A3872	A3873	C3874	C3875	C3876	C3877	C3878	C3879	G3880	C3881	C3882	G3888	C3889	U3892	C3893	A3894	C3895	C3896	C3897	A3901	A3902	A3905	A3906	U3907	A3908	C3909	U3915	C3919	U3920	U3921	
C3716	A3717	U3729	U3730	C3731	A3732	C3733	U3734	C3735	A3736	G3743	G3744	G3753	U3758	A3759	A3760	A3763	A3766	C3767	U3774	A3775	C3776	C3777	A3783	A3784	C3787	C3788	C3789	U3793	U3796	C3797	U3798	U3802	A3807	C3808	C3809	C3810	C3811	C3812	C3813	U3814	C3815	C3816	A3817	U3818	C3823	A3824	C3825					
G3626	A3635	C3636	U3637	G3638	A3642	A3643	U3644	A3645	A3646	A3649	C3650	A3651	G3654	C3660	A3661	A3662	A3663	G3664	C3667	C3668	C3673	C3674	C3675	C3676	C3677	C3678	U3679	A3680	A3682	C3683	G3684	C3685	U3688	C3689	C3690	C3691	A3692	C3696	G3705	C3706	U3707	C3708	U3709	A3711	A3712	U3713	A3714	U3715				
U2826	G2827	U2837	G2838	G2842	G2847	G2848	G2849	A2850	G2851	G2854	G2855	G2856	A2857	A2858	G2862	G2863	A2864	C2872	U2873	C2875	C2876	G2889	C2890	U2891	A2895	C2896	G2897	G2898	C3598	A3599	G3600	G3603	A3604	C3605	U3606	G3615	C3617	C3618	C3619	G3620	A3621	C3622	C3623	A3624	G3625							
A2743	A2744	U2747	C2748	C2749	G2750	G2751	G2752	G2753	A2754	A2755	G2756	A2757	G2758	G2759	G2760	U2761	G2762	A2763	A2764	A2765	G2766	U2767	C2768	U2769	G2778	C2779	A2787	U2788	A2789	U2790	C2794	A2795	G2796	C2797	A2798	U2799	G2800	U2801	C2804	C2805	A2806	A2807	C2808	U2809	U2810	G2811	A2812	A2813	C2817	U2821	G2822	G2823
G2664	U2665	U2666	G2667	G2668	C2669	C2670	A2674	G2675	A2676	G2677	C2683	C2684	C2685	G2686	G2687	G2688	C2689	G2693	A2694	A2695	A2696	A2697	U2701	C2702	G2703	G2706	U2707	U2708	C2709	G2710	G2711	G2712	C2713	G2714	C2715	C2716	C2719	G2722	U2723	G2724	A2725	G2726	G2732	G2735	C2738	C2739	U2740	G2742				
U2575	G2576	C2577	G2578	U2580	A2581	A2582	C2583	A2587	C2588	C2589	G2590	A2591	U2592	C2593	C2594	C2595	C2596	C2597	A2598	C2599	A2600	A2601	C2604	C2607	C2608	C2609	G2610	U2611	G2620	A2621	G2622	A2623	G2624	C2627	U2631	U2633	U2639	G2655	G2656	C2657	C2658	A2659	G2662	C2663								
U2494	U2495	G2496	C2499	U2500	C2501	A2502	G2503	C2504	C2505	C2506	A2507	U2508	A2511	A2512	A2513	G2516	G2521	G2528	A2529	C2532	C2533	C2534	C2535	A2536	A2537	U2538	C2539	G2542	A2543	G2544	U2545	G2549	C2550	A2551	G2552	G2555	G2556	C2561	G2562	C2563	U2485	G2566	U2570	C2571	C2572	C2573	C2574					
A2420	G2421	C2422	A2423	G2424	U2425	U2426	G2427	A2428	C2429	C2430	A2431	U2432	G2433	C2437	A2438	C2439	U2440	C2441	G2450	A2451	C2452	A2453	U2454	C2455	G2456	U2457	C2458	A2459	A2460	G2461	U2468	C2469	G2470	C2471	A2472	G2473	G2474	G2475	G2479	G2480	G2481	A2484	U2485	C2488	U2489	C2491	C2492	C2493				
C2078	C2081	U2084	G2085	A2088	C2089	U2090	C2091	G2092	C2093	A2010	C2011	C2014	U2015	C2016	C2019	U2020	C2021	C2022	G2023	A2024	A2025	A2026	G2112	G2113	C2158	C2159	C2160	G2261	G2262	A2263	U2267	A2268	C2269	G2270	C2274	G2275	C2276	G2277	G2278	C2279	G2280	U2281	G2284	A2285	G2286	C2289	G2294	C2295	A2300	G2301		
C2302	C2303	G2306	A2307	A2308	A2313	G2314	G2328	G2333	C2334	C2335	G2345	C2346	A2347	G2348	C2351	U2352	U2353	A2360	A2363	C2364	U2365	A2374	G2376	A2379	C2380	A2381	U2385	A2389	C2390	C2393	C2394	A2395	U2396	G2397	C2398	C2399	G2400	G2407	C2411	U2412	G2413	G2414	U2415	G2416								



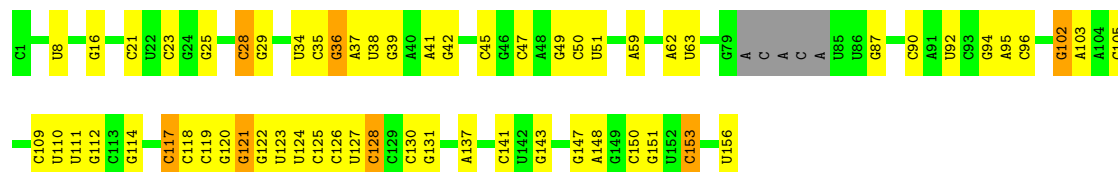
• Molecule 38: 5S ribosomal RNA

Chain 72: 56% 38%



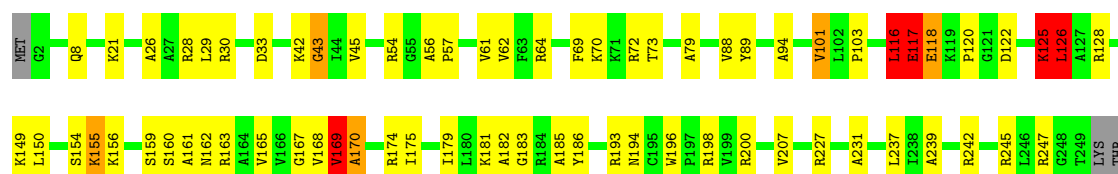
• Molecule 39: 5.8S ribosomal RNA

Chain 82: 58% 34%



• Molecule 40: Ribosomal protein L8

Chain A3: 69% 23%



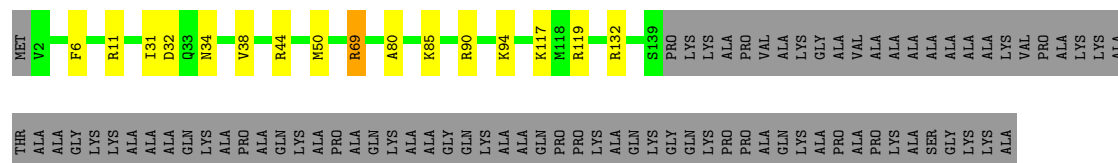
- Molecule 46: eL13

Chain L3:  91% 8%




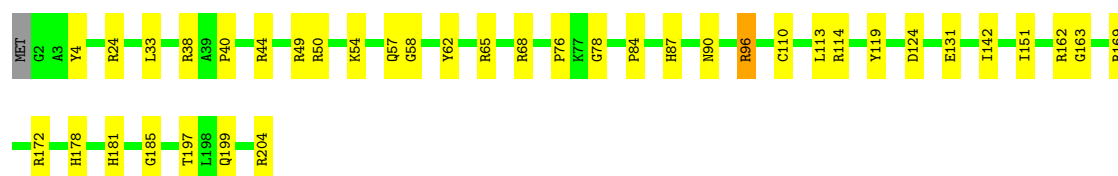
- Molecule 47: Ribosomal protein L14

Chain M3: 56% 7% 37%



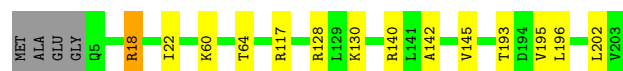
- Molecule 48: Ribosomal protein L15

Chain N3:  81% 18%




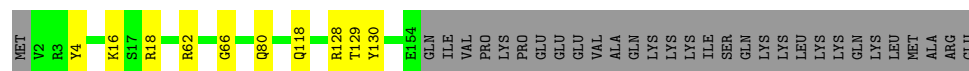
- Molecule 49: uL13

Chain O3: 91% 6%



- Molecule 50: uL22

Chain P3:  78% 5% 17%



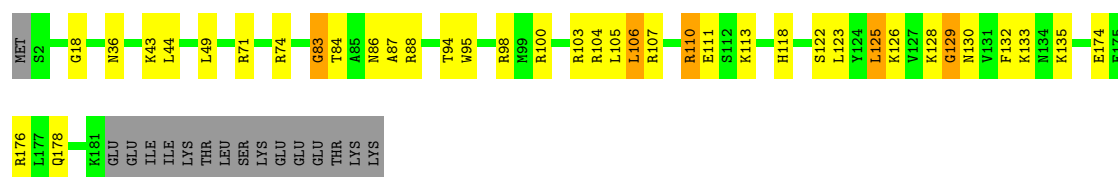
- Molecule 51: eL18

Chain Q3:  91% 8% ..



- Molecule 52: eL19

Chain R3: 72% 17% 1% 8%



- Molecule 53: eL20

Chain S3: 89% 10% .



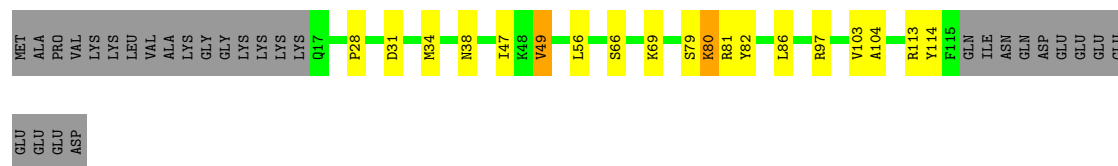
- Molecule 54: eL21

Chain T3: 89% 11% .



- Molecule 55: eL22

Chain U3: 63% 13% 23% .



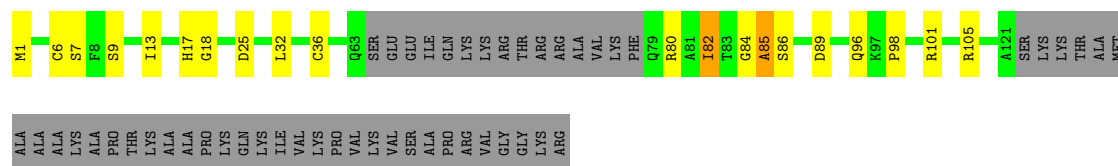
- Molecule 56: Ribosomal protein L23

Chain V3: 80% 13% 6% .



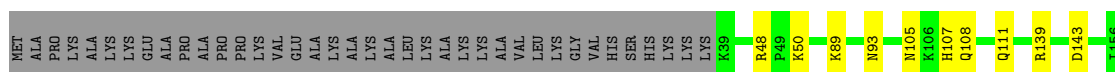
- Molecule 57: eL24

Chain W3: 55% 11% 32% .

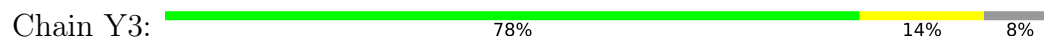


- Molecule 58: uL23

Chain X3: 69% 6% 24% .



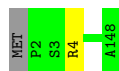
- Molecule 59: Ribosomal protein L26



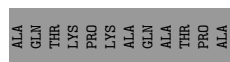
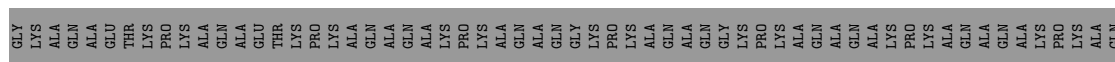
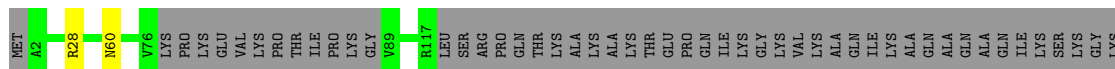
- Molecule 60: 60S ribosomal protein L27



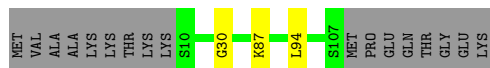
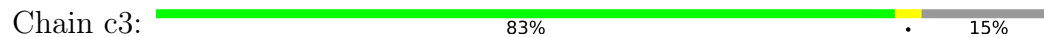
- Molecule 61: uL15



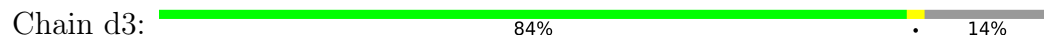
- Molecule 62: eL29

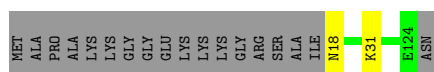


- Molecule 63: eL30



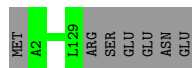
- Molecule 64: eL31





- Molecule 65: eL32

Chain e3: 95% 5%



- Molecule 66: eL33

Chain f3: 99% .



- Molecule 67: eL34

Chain g3: 89% 5% . .



- Molecule 68: uL29

Chain h3: 99% .



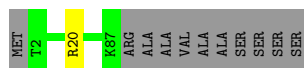
- Molecule 69: 60S ribosomal protein L36

Chain i3: 96% . .



- Molecule 70: Ribosomal protein L37

Chain j3: 88% . 11%



- Molecule 71: eL38

Chain k3: 94% . .



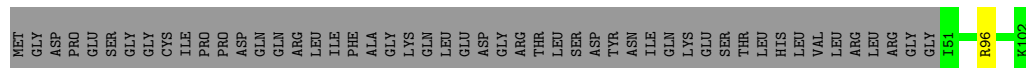
- Molecule 72: eL39

Chain 13: 98%



- Molecule 73: eL40

Chain m3: 50% 49%



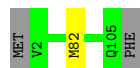
- Molecule 74: eL41

Chain n3: 100%

There are no outlier residues recorded for this chain.

- Molecule 75: eL42

Chain 03: 97% ..



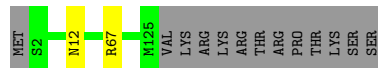
- Molecule 76: eL43

Chain p3:  96%



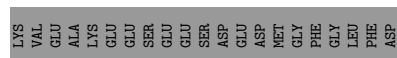
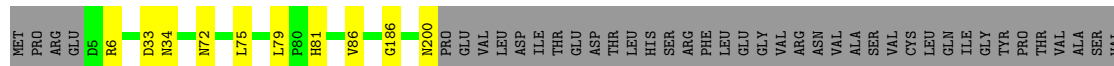
- Molecule 77: eL28

Chain r3: 89% 9%



- Molecule 78: uL10

Chain s3:  58% . 38%



- Molecule 79: Ribosomal protein L12

Chain t3: 92% . 7%



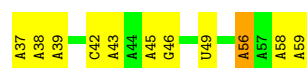
- Molecule 80: P-site tRNA

Chain 23: 66% 26% 8%



- Molecule 81: mRNA

Chain w3:  52% 43% .



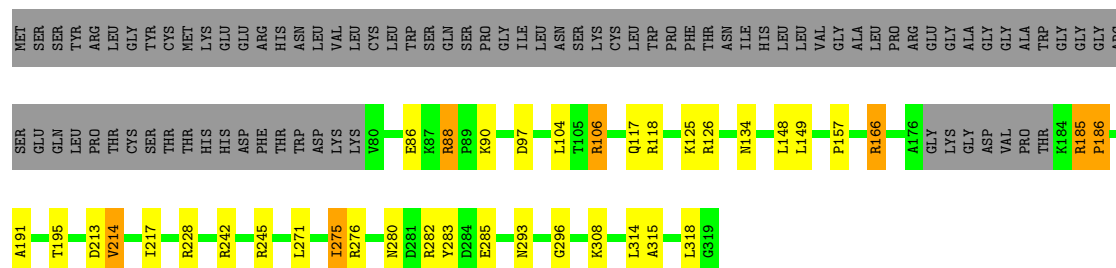
- Molecule 82: Ribosomal protein L11

Chain J3: 86% 10% .

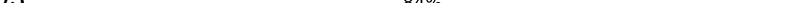


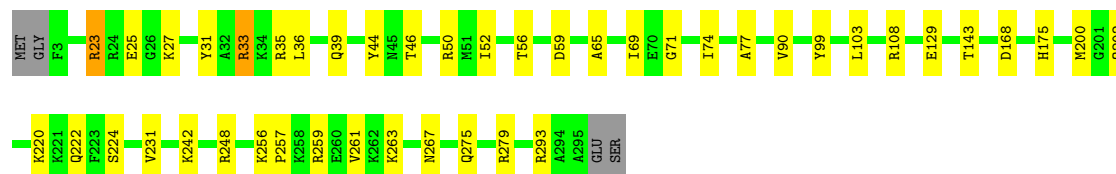
- Molecule 83: eL8

Chain G3:  61% 10% 27%

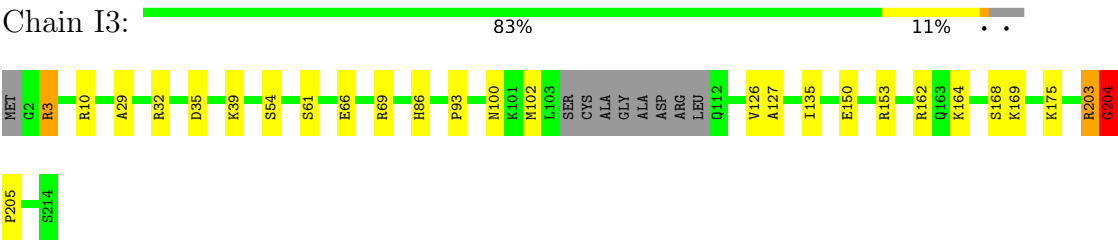


- Molecule 84: 60S ribosomal protein L5

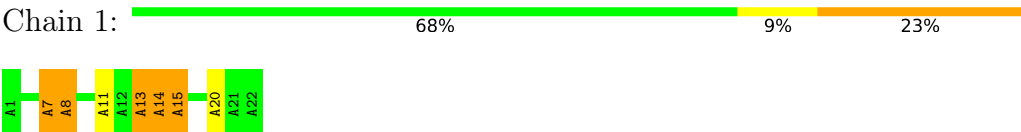
Chain D3:  84% 14%



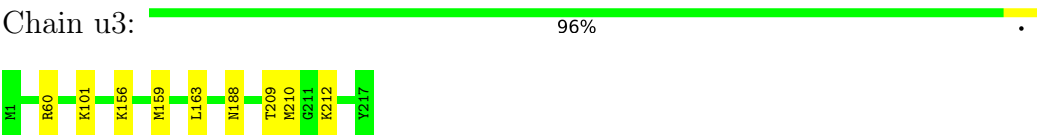
- Molecule 85: 60S ribosomal protein L10



● Molecule 86: nascent chain



● Molecule 87: uL1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.79	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A1	1.76	9/41324 (0.0%)	1.12	170/64370 (0.3%)
10	J1	0.42	0/1715	0.57	0/2287
11	K1	0.38	0/1550	0.60	0/2069
12	L1	0.37	0/834	0.59	0/1125
13	M1	0.45	0/1195	0.57	0/1597
14	N1	0.32	0/918	0.65	1/1233 (0.1%)
15	O1	0.39	0/1226	0.55	0/1649
16	P1	0.39	0/1029	0.57	0/1380
17	Q1	0.42	0/1017	0.60	0/1358
18	R1	0.41	0/1146	0.59	0/1534
19	S1	0.35	0/1082	0.55	0/1452
2	B1	0.39	0/1747	0.57	0/2374
20	T1	0.39	0/1208	0.59	0/1618
21	U1	0.39	0/1115	0.57	0/1493
22	V1	0.33	0/805	0.54	0/1081
23	W1	0.40	0/643	0.59	0/860
24	X1	0.42	0/1051	0.58	0/1406
25	Y1	0.43	0/1116	0.59	0/1490
26	Z1	0.36	0/1028	0.53	0/1366
27	a1	0.37	0/604	0.67	0/810
28	b1	0.42	0/828	0.54	0/1109
29	c1	0.36	0/665	0.57	0/891
3	C1	0.38	0/1756	0.58	1/2350 (0.0%)
30	d1	0.38	0/490	0.55	0/656
31	e1	0.44	0/470	0.57	0/623
32	f1	0.35	0/447	0.51	0/587
33	g1	0.28	0/567	0.57	0/753
34	h1	0.34	0/2493	0.58	0/3394
35	j1	0.35	0/3363	0.57	1/4523 (0.0%)
36	k1	0.36	0/4640	0.57	0/6264
37	52	2.86	72/87026 (0.1%)	1.46	556/135683 (0.4%)
38	72	5.70	7/2858 (0.2%)	1.28	21/4455 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	82	1.02	0/3581	1.12	14/5577 (0.3%)
4	D1	0.44	0/1753	0.58	0/2369
40	A3	0.56	2/1936 (0.1%)	0.85	7/2596 (0.3%)
41	B3	0.51	0/3240	0.63	3/4339 (0.1%)
42	C3	0.53	0/2937	0.63	1/3946 (0.0%)
43	E3	2.24	3/1762 (0.2%)	0.69	3/2362 (0.1%)
44	F3	0.57	0/1911	0.61	0/2549
45	H3	0.47	0/1535	0.60	0/2063
46	L3	0.50	0/1733	0.62	0/2316
47	M3	0.52	0/1158	0.59	0/1547
48	N3	0.58	0/1746	0.64	0/2338
49	O3	0.53	0/1662	0.65	1/2222 (0.0%)
5	E1	0.38	0/1796	0.59	0/2417
50	P3	0.55	0/1268	0.59	0/1700
51	Q3	1.98	2/1539 (0.1%)	0.95	4/2054 (0.2%)
52	R3	0.46	0/1524	0.71	1/2013 (0.0%)
53	S3	1.00	1/1501 (0.1%)	0.82	5/2012 (0.2%)
54	T3	0.53	0/1326	0.56	0/1770
55	U3	1.95	3/823 (0.4%)	1.37	7/1104 (0.6%)
56	V3	0.49	0/993	0.60	0/1332
57	W3	0.43	0/873	0.60	0/1158
58	X3	0.45	0/984	0.55	0/1323
59	Y3	0.51	0/1132	0.60	0/1504
6	F1	0.39	0/2118	0.57	1/2849 (0.0%)
60	Z3	0.61	0/1130	0.99	4/1507 (0.3%)
61	a3	0.52	0/1191	0.59	0/1590
62	b3	1.83	2/861 (0.2%)	0.84	4/1138 (0.4%)
63	c3	0.46	0/771	0.84	3/1034 (0.3%)
64	d3	0.51	0/903	0.62	0/1216
65	e3	0.52	0/1071	0.60	0/1429
66	f3	0.59	0/895	0.63	0/1198
67	g3	5.33	4/916 (0.4%)	1.34	7/1220 (0.6%)
68	h3	0.47	0/1021	0.59	0/1348
69	i3	0.43	0/841	0.59	0/1112
7	G1	0.38	0/1492	0.56	0/2005
70	j3	0.54	0/720	0.61	0/952
71	k3	0.42	0/575	0.80	1/761 (0.1%)
72	l3	0.47	0/459	0.58	0/608
73	m3	0.46	0/435	0.55	0/575
74	n3	0.40	0/240	0.66	0/305
75	o3	0.45	0/864	0.58	0/1140
76	p3	0.55	0/718	0.74	0/953
77	r3	0.53	0/1010	0.63	0/1354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	s3	0.50	1/1530 (0.1%)	0.89	5/2064 (0.2%)
79	t3	0.31	0/1174	0.64	0/1582
8	H1	0.36	0/1946	0.62	0/2590
80	23	0.61	0/1805	1.13	10/2809 (0.4%)
81	w3	0.62	0/553	1.24	3/859 (0.3%)
82	J3	0.41	0/1385	0.58	0/1852
83	G3	1.53	2/1910 (0.1%)	0.98	6/2569 (0.2%)
84	D3	0.48	0/2437	0.61	0/3264
85	I3	1.09	2/1702 (0.1%)	0.76	4/2272 (0.2%)
86	1	0.45	0/109	0.65	0/151
87	u3	0.29	0/1769	0.64	1/2371 (0.0%)
9	I1	0.34	0/1510	0.60	1/2022 (0.0%)
All	All	2.04	110/242730 (0.0%)	1.12	846/355150 (0.2%)

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
14	N1	0	1
16	P1	0	1
17	Q1	0	2
2	B1	0	1
25	Y1	0	1
35	j1	0	1
36	k1	0	1
40	A3	0	5
42	C3	0	1
47	M3	0	1
48	N3	0	2
52	R3	0	5
53	S3	0	1
55	U3	0	1
57	W3	0	1
60	Z3	0	3
63	c3	0	1
67	g3	0	8
71	k3	0	1
76	p3	0	2
78	s3	0	4
79	t3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
83	G3	0	3
85	I3	0	1
87	u3	0	2
All	All	0	51

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	52	732	A	N3-C4	183.88	2.45	1.34
37	52	1805	A	N3-C4	177.26	2.41	1.34
37	52	732	A	C6-N1	163.87	2.50	1.35
1	A1	970	G	C6-N1	162.13	2.53	1.39
37	52	2631	U	C2-N3	160.48	2.50	1.37

The worst 5 of 846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	3712	A	N1-C2-N3	-240.10	9.25	129.30
37	52	3712	A	C2-N3-C4	88.07	154.63	110.60
37	52	3712	A	C6-N1-C2	69.39	160.23	118.60
37	52	3712	A	C4-C5-C6	-48.11	92.95	117.00
1	A1	970	G	C4-C5-N7	-38.17	95.53	110.80

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B1	42	LYS	Peptide
14	N1	37	GLU	Peptide
16	P1	21	VAL	Peptide
17	Q1	17	TYR	Peptide
17	Q1	37	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	36969	0	18687	184	0
2	B1	1710	0	1708	13	0
3	C1	1729	0	1803	19	0
4	D1	1716	0	1806	12	0
5	E1	1768	0	1866	21	0
6	F1	2076	0	2177	13	0
7	G1	1471	0	1522	8	0
8	H1	1923	0	2089	36	0
9	I1	1488	0	1582	6	0
10	J1	1686	0	1772	18	0
11	K1	1525	0	1640	13	0
12	L1	810	0	836	5	0
13	M1	1175	0	1249	12	0
14	N1	908	0	939	16	0
15	O1	1202	0	1289	7	0
16	P1	1016	0	1039	15	0
17	Q1	997	0	1044	8	0
18	R1	1128	0	1195	9	0
19	S1	1068	0	1121	11	0
20	T1	1190	0	1249	6	0
21	U1	1097	0	1132	9	0
22	V1	795	0	862	4	0
23	W1	636	0	637	3	0
24	X1	1034	0	1080	12	0
25	Y1	1098	0	1167	7	0
26	Z1	1011	0	1083	9	0
27	a1	598	0	656	0	0
28	b1	814	0	865	0	0
29	c1	651	0	672	0	0
30	d1	488	0	514	0	0
31	e1	459	0	449	0	0
32	f1	443	0	492	0	0
33	g1	555	0	564	0	0
34	h1	2436	0	2393	0	0
35	j1	3309	0	3350	0	0
36	k1	4555	0	4696	0	0
37	52	77819	0	39310	602	0
38	72	2558	0	1296	36	0
39	82	3208	0	1629	12	0
40	A3	1898	0	1993	46	0
41	B3	3172	0	3310	37	0
42	C3	2883	0	3053	14	0
43	E3	1729	0	1887	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	F3	1875	0	1995	21	0
45	H3	1516	0	1597	8	0
46	L3	1702	0	1820	14	0
47	M3	1137	0	1211	12	0
48	N3	1701	0	1749	26	0
49	O3	1630	0	1778	12	0
50	P3	1242	0	1274	7	0
51	Q3	1515	0	1634	29	0
52	R3	1508	0	1664	30	0
53	S3	1462	0	1508	37	0
54	T3	1298	0	1366	12	0
55	U3	809	0	833	41	0
56	V3	979	0	1039	9	0
57	W3	860	0	903	20	0
58	X3	967	0	1040	8	0
59	Y3	1115	0	1205	12	0
60	Z3	1107	0	1182	41	0
61	a3	1162	0	1209	0	0
62	b3	848	0	920	0	0
63	c3	761	0	794	0	0
64	d3	888	0	930	0	0
65	e3	1053	0	1147	0	0
66	f3	876	0	912	0	0
67	g3	906	0	1001	0	0
68	h3	1013	0	1147	0	0
69	i3	830	0	916	0	0
70	j3	705	0	737	0	0
71	k3	569	0	637	0	0
72	l3	447	0	480	0	0
73	m3	429	0	465	0	0
74	n3	239	0	289	0	0
75	o3	851	0	922	0	0
76	p3	708	0	757	0	0
77	r3	994	0	1051	0	0
78	s3	1507	0	1564	0	0
79	t3	1160	0	1218	0	0
80	23	1616	0	824	7	0
81	w3	493	0	249	0	0
82	J3	1362	0	1399	9	0
83	G3	1879	0	2027	37	0
84	D3	2391	0	2424	27	0
85	I3	1664	0	1711	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	1	110	0	112	9	0
87	u3	1741	0	1854	0	0
88	52	204	0	0	0	0
88	72	7	0	0	0	0
88	82	5	0	0	0	0
88	A1	77	0	0	0	0
88	G1	1	0	0	0	0
88	M1	1	0	0	0	0
88	P3	1	0	0	0	0
88	V3	1	0	0	0	0
88	a3	1	0	0	0	0
88	g3	1	0	0	0	0
88	w3	1	0	0	0	0
89	b1	1	0	0	0	0
89	e1	1	0	0	0	0
89	g1	1	0	0	0	0
89	g3	1	0	0	0	0
89	j3	1	0	0	0	0
89	m3	1	0	0	0	0
89	o3	1	0	0	0	0
89	p3	1	0	0	0	0
90	k1	16	0	0	0	0
91	1	1	0	0	0	0
91	52	3	0	0	0	0
All	All	226754	0	171197	1304	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1304 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2395:A:C6	37:52:2395:A:C5	1.79	1.66
37:52:1239:C:C5	37:52:1239:C:C6	1.83	1.60
37:52:2395:A:N3	37:52:2395:A:C2	1.73	1.56
37:52:2395:A:C4	37:52:2395:A:N3	1.75	1.52
55:U3:49:VAL:CG2	55:U3:49:VAL:CB	1.82	1.51

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	B1	215/295 (73%)	199 (93%)	16 (7%)	0	100	100
3	C1	211/264 (80%)	191 (90%)	20 (10%)	0	100	100
4	D1	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
5	E1	226/243 (93%)	211 (93%)	15 (7%)	0	100	100
6	F1	260/263 (99%)	226 (87%)	34 (13%)	0	100	100
7	G1	181/204 (89%)	167 (92%)	14 (8%)	0	100	100
8	H1	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
9	I1	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	J1	204/208 (98%)	184 (90%)	20 (10%)	0	100	100
11	K1	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
12	L1	94/165 (57%)	83 (88%)	11 (12%)	0	100	100
13	M1	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
14	N1	115/132 (87%)	101 (88%)	14 (12%)	0	100	100
15	O1	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
16	P1	134/168 (80%)	123 (92%)	11 (8%)	0	100	100
17	Q1	118/145 (81%)	106 (90%)	12 (10%)	0	100	100
18	R1	140/146 (96%)	126 (90%)	14 (10%)	0	100	100
19	S1	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
20	T1	142/152 (93%)	129 (91%)	13 (9%)	0	100	100
21	U1	139/145 (96%)	128 (92%)	11 (8%)	0	100	100
22	V1	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
23	W1	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
24	X1	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
25	Y1	139/143 (97%)	124 (89%)	14 (10%)	1 (1%)	24	64
26	Z1	122/130 (94%)	109 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	a1	73/125 (58%)	65 (89%)	8 (11%)	0	100	100
28	b1	99/115 (86%)	92 (93%)	7 (7%)	0	100	100
29	c1	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
30	d1	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
31	e1	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
32	f1	53/133 (40%)	49 (92%)	4 (8%)	0	100	100
33	g1	66/156 (42%)	58 (88%)	8 (12%)	0	100	100
34	h1	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
35	j1	417/439 (95%)	388 (93%)	29 (7%)	0	100	100
36	k1	571/599 (95%)	517 (90%)	54 (10%)	0	100	100
40	A3	246/257 (96%)	185 (75%)	54 (22%)	7 (3%)	5	39
41	B3	392/403 (97%)	355 (91%)	37 (9%)	0	100	100
42	C3	360/425 (85%)	325 (90%)	35 (10%)	0	100	100
43	E3	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
44	F3	223/247 (90%)	204 (92%)	19 (8%)	0	100	100
45	H3	188/192 (98%)	174 (93%)	13 (7%)	1 (0%)	31	71
46	L3	208/211 (99%)	194 (93%)	12 (6%)	2 (1%)	17	57
47	M3	136/218 (62%)	121 (89%)	15 (11%)	0	100	100
48	N3	201/204 (98%)	181 (90%)	20 (10%)	0	100	100
49	O3	197/203 (97%)	185 (94%)	12 (6%)	0	100	100
50	P3	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
51	Q3	185/188 (98%)	167 (90%)	18 (10%)	0	100	100
52	R3	178/196 (91%)	161 (90%)	17 (10%)	0	100	100
53	S3	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
54	T3	157/160 (98%)	144 (92%)	12 (8%)	1 (1%)	27	67
55	U3	97/128 (76%)	79 (81%)	18 (19%)	0	100	100
56	V3	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
57	W3	102/157 (65%)	92 (90%)	10 (10%)	0	100	100
58	X3	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
59	Y3	132/145 (91%)	120 (91%)	12 (9%)	0	100	100
60	Z3	133/136 (98%)	105 (79%)	25 (19%)	3 (2%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	a3	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
62	b3	100/226 (44%)	94 (94%)	6 (6%)	0	100	100
63	c3	96/115 (84%)	82 (85%)	14 (15%)	0	100	100
64	d3	105/125 (84%)	90 (86%)	15 (14%)	0	100	100
65	e3	126/135 (93%)	115 (91%)	11 (9%)	0	100	100
66	f3	107/110 (97%)	96 (90%)	11 (10%)	0	100	100
67	g3	112/117 (96%)	98 (88%)	13 (12%)	1 (1%)	19	59
68	h3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
69	i3	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
70	j3	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
71	k3	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
72	l3	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
73	m3	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
74	n3	23/25 (92%)	23 (100%)	0	0	100	100
75	o3	102/106 (96%)	96 (94%)	6 (6%)	0	100	100
76	p3	89/92 (97%)	77 (86%)	12 (14%)	0	100	100
77	r3	122/137 (89%)	110 (90%)	12 (10%)	0	100	100
78	s3	194/318 (61%)	156 (80%)	37 (19%)	1 (0%)	31	71
79	t3	151/165 (92%)	126 (83%)	25 (17%)	0	100	100
82	J3	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
83	G3	229/319 (72%)	195 (85%)	34 (15%)	0	100	100
84	D3	291/297 (98%)	253 (87%)	38 (13%)	0	100	100
85	I3	201/214 (94%)	167 (83%)	33 (16%)	1 (0%)	31	71
86	1	20/22 (91%)	11 (55%)	4 (20%)	5 (25%)	0	1
87	u3	215/217 (99%)	183 (85%)	30 (14%)	2 (1%)	19	59
All	All	12742/14633 (87%)	11465 (90%)	1252 (10%)	25 (0%)	53	83

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	A3	116	LEU
40	A3	118	GLU
40	A3	126	LEU

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Mol	Chain	Res	Type
46	L3	64	VAL
60	Z3	73	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	180/245 (74%)	177 (98%)	3 (2%)	63	83
3	C1	194/231 (84%)	191 (98%)	3 (2%)	67	85
4	D1	187/225 (83%)	186 (100%)	1 (0%)	90	95
5	E1	190/202 (94%)	186 (98%)	4 (2%)	56	79
6	F1	224/225 (100%)	223 (100%)	1 (0%)	92	96
7	G1	158/170 (93%)	156 (99%)	2 (1%)	71	86
8	H1	207/218 (95%)	205 (99%)	2 (1%)	78	89
9	I1	165/174 (95%)	165 (100%)	0	100	100
10	J1	178/180 (99%)	174 (98%)	4 (2%)	55	78
11	K1	161/168 (96%)	157 (98%)	4 (2%)	50	75
12	L1	87/136 (64%)	85 (98%)	2 (2%)	53	77
13	M1	130/142 (92%)	128 (98%)	2 (2%)	67	85
14	N1	99/108 (92%)	98 (99%)	1 (1%)	78	89
15	O1	130/131 (99%)	128 (98%)	2 (2%)	67	85
16	P1	106/130 (82%)	104 (98%)	2 (2%)	60	81
17	Q1	109/130 (84%)	108 (99%)	1 (1%)	81	90
18	R1	117/121 (97%)	115 (98%)	2 (2%)	63	83
19	S1	119/121 (98%)	119 (100%)	0	100	100
20	T1	125/132 (95%)	124 (99%)	1 (1%)	83	91
21	U1	111/115 (96%)	110 (99%)	1 (1%)	81	90
22	V1	92/107 (86%)	90 (98%)	2 (2%)	55	78
23	W1	67/67 (100%)	66 (98%)	1 (2%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	X1	112/113 (99%)	112 (100%)	0	100	100
25	Y1	113/115 (98%)	113 (100%)	0	100	100
26	Z1	107/112 (96%)	106 (99%)	1 (1%)	81	90
27	a1	66/103 (64%)	66 (100%)	0	100	100
28	b1	88/98 (90%)	88 (100%)	0	100	100
29	c1	75/76 (99%)	74 (99%)	1 (1%)	71	86
30	d1	55/62 (89%)	55 (100%)	0	100	100
31	e1	48/49 (98%)	48 (100%)	0	100	100
32	f1	46/106 (43%)	44 (96%)	2 (4%)	32	64
33	g1	61/140 (44%)	60 (98%)	1 (2%)	65	84
34	h1	272/275 (99%)	269 (99%)	3 (1%)	76	88
35	j1	361/377 (96%)	356 (99%)	5 (1%)	69	86
36	k1	509/526 (97%)	505 (99%)	4 (1%)	83	91
40	A3	190/199 (96%)	185 (97%)	5 (3%)	49	75
41	B3	342/348 (98%)	340 (99%)	2 (1%)	87	94
42	C3	302/347 (87%)	295 (98%)	7 (2%)	53	77
43	E3	190/251 (76%)	188 (99%)	2 (1%)	76	88
44	F3	196/215 (91%)	194 (99%)	2 (1%)	78	89
45	H3	169/171 (99%)	164 (97%)	5 (3%)	44	71
46	L3	175/176 (99%)	174 (99%)	1 (1%)	87	94
47	M3	117/161 (73%)	117 (100%)	0	100	100
48	N3	171/172 (99%)	168 (98%)	3 (2%)	62	83
49	O3	171/173 (99%)	169 (99%)	2 (1%)	74	87
50	P3	134/163 (82%)	133 (99%)	1 (1%)	85	93
51	Q3	164/165 (99%)	161 (98%)	3 (2%)	62	83
52	R3	159/175 (91%)	154 (97%)	5 (3%)	43	71
53	S3	157/157 (100%)	157 (100%)	0	100	100
54	T3	139/140 (99%)	137 (99%)	2 (1%)	69	86
55	U3	89/114 (78%)	87 (98%)	2 (2%)	55	78
56	V3	101/107 (94%)	99 (98%)	2 (2%)	58	80
57	W3	86/126 (68%)	85 (99%)	1 (1%)	74	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	X3	106/134 (79%)	106 (100%)	0	100	100
59	Y3	124/135 (92%)	122 (98%)	2 (2%)	65	84
60	Z3	117/118 (99%)	115 (98%)	2 (2%)	63	83
61	a3	119/120 (99%)	118 (99%)	1 (1%)	83	91
62	b3	84/172 (49%)	83 (99%)	1 (1%)	74	87
63	c3	84/98 (86%)	84 (100%)	0	100	100
64	d3	98/110 (89%)	96 (98%)	2 (2%)	58	80
65	e3	114/121 (94%)	114 (100%)	0	100	100
66	f3	88/89 (99%)	88 (100%)	0	100	100
67	g3	98/100 (98%)	96 (98%)	2 (2%)	58	80
68	h3	109/110 (99%)	109 (100%)	0	100	100
69	i3	86/89 (97%)	85 (99%)	1 (1%)	74	87
70	j3	73/80 (91%)	72 (99%)	1 (1%)	69	86
71	k3	64/65 (98%)	63 (98%)	1 (2%)	65	84
72	l3	47/48 (98%)	47 (100%)	0	100	100
73	m3	48/90 (53%)	47 (98%)	1 (2%)	56	79
74	n3	24/24 (100%)	24 (100%)	0	100	100
75	o3	92/94 (98%)	91 (99%)	1 (1%)	76	88
76	p3	74/75 (99%)	73 (99%)	1 (1%)	69	86
77	r3	108/121 (89%)	106 (98%)	2 (2%)	60	81
78	s3	164/258 (64%)	162 (99%)	2 (1%)	74	87
79	t3	126/137 (92%)	126 (100%)	0	100	100
82	J3	143/149 (96%)	143 (100%)	0	100	100
83	G3	200/272 (74%)	191 (96%)	9 (4%)	30	63
84	D3	247/250 (99%)	240 (97%)	7 (3%)	47	73
85	I3	175/181 (97%)	167 (95%)	8 (5%)	29	62
87	u3	195/196 (100%)	191 (98%)	4 (2%)	56	79
All	All	11108/12426 (89%)	10957 (99%)	151 (1%)	71	86

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	C3	188	ARG

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Mol	Chain	Res	Type
48	N3	162	ARG
85	I3	3	ARG
42	C3	312	ARG
45	H3	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
35	j1	67	ASN
41	B3	245	HIS
84	D3	195	HIS
35	j1	380	ASN
36	k1	381	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1709/1869 (91%)	474 (27%)	23 (1%)
37	52	3591/3634 (98%)	1136 (31%)	45 (1%)
38	72	119/120 (99%)	34 (28%)	0
39	82	149/156 (95%)	43 (28%)	0
80	23	74/76 (97%)	18 (24%)	0
81	w3	22/23 (95%)	10 (45%)	0
All	All	5664/5878 (96%)	1715 (30%)	68 (1%)

5 of 1715 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	C
1	A1	5	U
1	A1	16	G
1	A1	17	C

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	52	504	G
37	52	1291	G
37	52	4699	U

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Mol	Chain	Res	Type
37	52	930	G
37	52	971(A)	G

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 308 are monoatomic - leaving 2 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	$\# Z > 2$
90	SF4	k1	600	-	0,12,12	0.00	-	0,24,24	0.00	-
90	SF4	k1	601	-	0,12,12	0.00	-	0,24,24	0.00	-

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
90	SF4	k1	600	-	-	0/0/48/48	0/6/5/5
90	SF4	k1	601	-	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	52	37
1	A1	12
78	s3	1
80	23	1
85	I3	1

The worst 5 of 52 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	2113:G	O3'	2258:C	P	42.99
1	52	1252:C	O3'	1271:G	P	36.84
1	52	1406(C):G	O3'	1411:C	P	19.25
1	52	1109:C	O3'	1161:G	P	17.69
1	52	3977:C	O3'	4034:G	P	16.37