



wwPDB EM Map/Model Validation Report ⓘ

Jun 2, 2016 – 03:58 PM EDT

PDB ID : 4UJD
EMDB ID: : EMD-2682
Title : mammalian 80S HCV-IRES initiation complex with eIF5B PRE-like state
Authors : Yamamoto, H.; Unbehaun, A.; Loerke, J.; Behrmann, E.; Marianne, C.;
Burger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2014-06-18
Resolution : 8.90 Å(reported)
Based on PDB ID : 4CXC

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

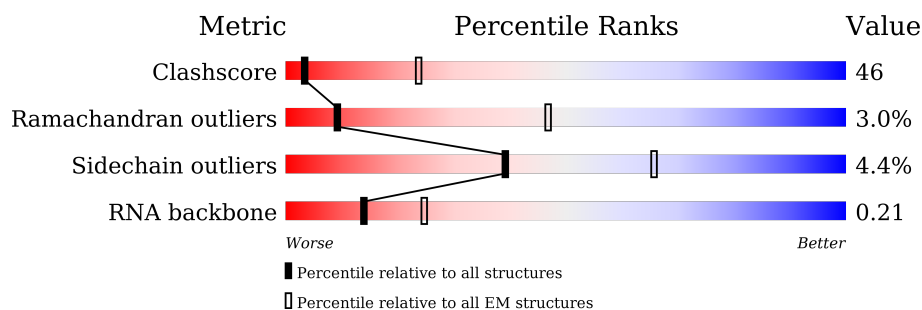
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.90 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.









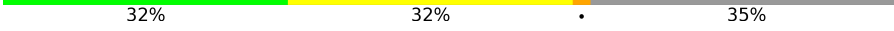




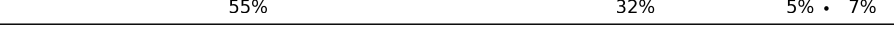







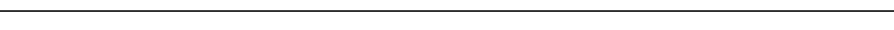

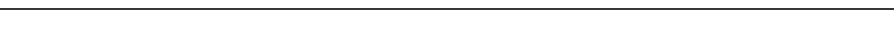
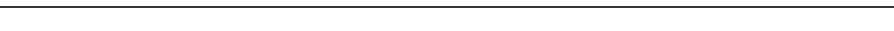


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A2	5025	7% 28% 36% . 28%
2	A3	194	8% 37% 35% . 19%
3	A4	121	12% 36% 49% . .
4	AA	257	56% 39% . .
5	AB	403	56% 37% 5% .
6	AC	427	46% 34% . . 15%
7	AD	297	57% 38% . .
8	AE	158	39% 54% 7%



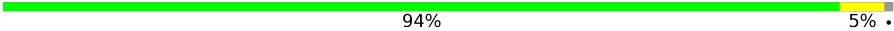


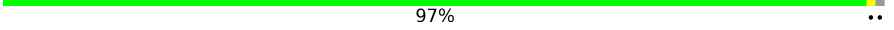
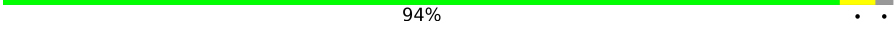

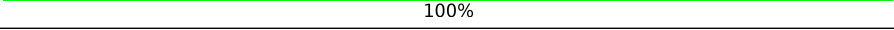
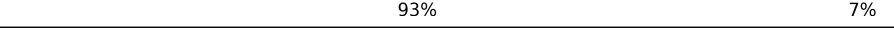
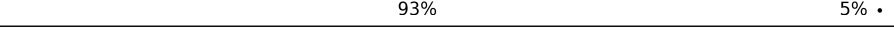
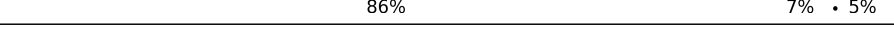
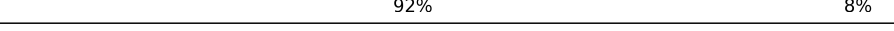





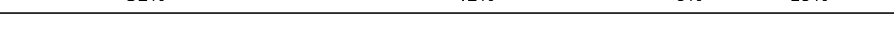
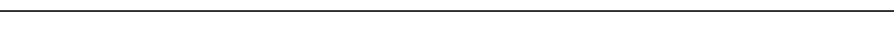

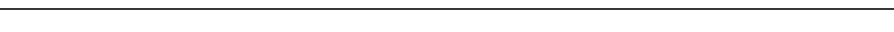
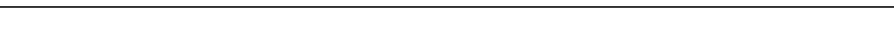


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Mol	Chain	Length	Quality of chain
9	AF	248	 53% 39% 6%
10	AG	266	 52% 33% 12%
11	AH	192	 56% 41% 1%
12	AI	214	 52% 37% 8%
13	AJ	178	 47% 41% 8%
14	AL	211	 51% 36% 7% 5%
15	AM	215	 32% 32% 35%
16	AN	204	 64% 35% 1%
17	AO	203	 54% 41% 5%
18	AP	184	 45% 35% 17%
19	AQ	188	 54% 39% 5%
20	AR	196	 55% 32% 5% 7%
21	AS	176	 56% 37% 6%
22	AT	160	 56% 40% 4%
23	AU	128	 52% 27% 20%
24	AV	140	 61% 29% 9%
25	AW	157	 27% 12% 59%
26	AX	156	 49% 27% 24%
27	AY	145	 43% 41% 12%
28	AZ	136	 53% 46% 1%
29	Aa	148	 94% 5%
30	Ab	159	 40% 57%
31	Ac	115	 88% 10%
32	Ad	125	 83% 13%
33	Ae	135	 90% 5%














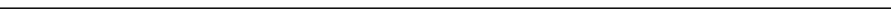











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Mol	Chain	Length	Quality of chain
34	Af	110	
35	Ag	117	
36	Ah	123	
37	Ai	105	
38	Aj	97	
39	Ak	70	
40	Al	51	
41	Am	128	
42	An	25	
43	Ao	106	
44	Ap	92	
45	At	137	
46	Au	210	
47	BA	76	
48	BB	627	
49	BC	504	
50	C1	1869	
51	CA	295	
52	CB	264	
53	CC	293	
54	CD	243	
55	CE	263	
56	CF	204	
57	CG	249	
58	CH	194	

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Mol	Chain	Length	Quality of chain
59	CI	208	
60	CJ	194	
61	CK	165	
62	CL	158	
63	CM	132	
64	CN	151	
65	CO	151	
66	CP	145	
67	CQ	146	
68	CR	135	
69	CS	152	
70	CT	145	
71	CU	119	
72	CV	83	
73	CW	130	
74	CX	143	
75	CY	133	
76	CZ	125	
77	Ca	115	
78	Cb	84	
79	Cc	69	
80	Cd	56	
81	Ce	59	
82	Cf	156	
83	Cg	317	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	GNP	BB	2435	-	-	X	-

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 223911 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 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	3616	Total	C	N	O	P	0	0
			77488	34508	14153	25212	3615		

- Molecule 2 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A3	157	Total	C	N	O	P	0	0
			3334	1489	587	1102	156		

- Molecule 3 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A4	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AA	247	Total	C	N	O	S	0	1
			1888	1183	388	311	6		

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AB	396	Total	C	N	O	S	0	1
			3190	2030	601	545	14		

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	364	Total	C	N	O	S	0	1
			2889	1817	578	480	14		

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AD	290	Total	C	N	O	S	0	0
			2362	1489	431	428	14		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AE	158	Total	C	N	O	S	0	0
			1287	834	238	215			

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	234	Total	C	N	O	S	0	0
			1950	1252	376	313	9		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AG	235	Total	C	N	O	S	0	1
			1881	1197	363	317	4		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	192	Total	C	N	O	S	0	0
			1536	965	286	279	6		

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	196	Total	C	N	O	S	0	0
			1605	1022	308	263	12		

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	170	Total	C	N	O	S	0	0
			1363	861	254	242	6		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AL	200	Total	C	N	O	S	0	1
			1617	1013	335	265	4		

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	140	Total	C	N	O	S	0	1
			1139	730	219	183	7		

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AN	204	Total	C	N	O	S	0	0
			1709	1077	360	267	5		

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN L13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AO	196	Total	C	N	O	S	0	1
			1607	1034	316	252	5		

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AP	153	Total	C	N	O	S	0	1
			1234	771	241	213	9		

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	184	Total	C	N	O	S	0	0
			1494	933	311	245	5		

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	183	Total	C	N	O	S	0	1
			1526	943	331	242	10		

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN L18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	173	Total	C	N	O	S	0	0
			1439	916	280	233	10		

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN L21.

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

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AU	102	Total	C	N	O	S	0	1
			827	529	146	150	2		

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AV	128	Total	C	N	O	S	0	0
			964	610	181	168	5		

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AW	64	Total	C	N	O	S	0	1
			529	337	104	85	3		

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	128	Total	C	N	O	S	0	1
			1065	668	217	177	3		

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AZ	136	Total	C	N	O	S	0	0
			1115	719	209	183	4		

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aa	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ab	69	Total	C	N	O	S	0	1
			560	344	123	90	3		

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	104	Total	C	N	O	S	0	1
			802	508	142	145	7		

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ad	109	Total	C	N	O	S	0	0
			905	570	174	159	2		

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ae	128	Total	C	N	O	S	0	1
			1053	664	219	165	5		

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Af	107	Total	C	N	O	S	0	0
			866	550	172	141	3		

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ag	115	Total	C	N	O	S	0	1
			907	566	188	147	6		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ah	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ai	97	Total	C	N	O	S	0	1
			783	488	168	122	5		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Aj	85	Total	C	N	O	S	0	1
			690	423	153	109	5		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L38.

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

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Al	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

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

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	An	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ao	106	Total	C	N	O	S	0	0
			871	547	176	141	7		

- Molecule 44 is a protein called 60S RIBOSOMAL PROTEIN L37A.

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

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	At	130	Total	C	N	O	S	0	1
			1043	646	220	172	5		

- Molecule 46 is a protein called 60S RIBOSOMAL PROTEIN L10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Au	210	Total	C	N	O	S	0	0
			1622	990	278	348	6		

- Molecule 47 is a RNA chain called TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BA	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 48 is a protein called EIF5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BB	611	Total	C	N	O	S	0	0
			4846	3084	834	906	22		

- Molecule 49 is a RNA chain called HCV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BC	261	Total	C	N	O	P	0	0
			5574	2485	1001	1828	260		

- Molecule 50 is a RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C1	1742	Total	C	N	O	P	0	0
			37159	16589	6665	12164	1741		

- Molecule 51 is a protein called 40S RIBOSOMAL PROTEIN US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	CA	218	Total	C	N	O	S	0	0
			1719	1091	301	319	8		

- Molecule 52 is a protein called 40S RIBOSOMAL PROTEIN ES1.

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

- Molecule 53 is a protein called 40S RIBOSOMAL PROTEIN US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CC	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 54 is a protein called 40S RIBOSOMAL PROTEIN US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CD	212	Total	C	N	O	S	0	0
			1646	1050	299	290	7		

- Molecule 55 is a protein called 40S RIBOSOMAL PROTEIN ES4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	CE	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 56 is a protein called 40S RIBOSOMAL PROTEIN US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CF	188	Total	C	N	O	S	0	0
			1486	930	283	266	7		

- Molecule 57 is a protein called 40S RIBOSOMAL PROTEIN ES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CG	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 58 is a protein called 40S RIBOSOMAL PROTEIN ES7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CH	191	Total	C	N	O	S	0	0
			1535	978	282	274	1		

- Molecule 59 is a protein called 40S RIBOSOMAL PROTEIN ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CI	207	Total	C	N	O	S	0	0
			1695	1064	334	292	5		

- Molecule 60 is a protein called 40S RIBOSOMAL PROTEIN US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CJ	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 61 is a protein called 40S RIBOSOMAL PROTEIN ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CK	94	Total	C	N	O	S	0	0
			791	519	138	129	5		

- Molecule 62 is a protein called 40S RIBOSOMAL PROTEIN US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	CL	146	Total	C	N	O	S	0	0
			1199	764	224	205	6		

- Molecule 63 is a protein called 40S RIBOSOMAL PROTEIN ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	CM	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 64 is a protein called 40S RIBOSOMAL PROTEIN ES15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	CN	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 65 is a protein called 40S RIBOSOMAL PROTEIN ES11.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	CO	137	Total	C	N	O	S	0	0
			1023	627	200	190	6		

- Molecule 66 is a protein called 40S RIBOSOMAL PROTEIN US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	CP	118	Total	C	N	O	S	0	0
			981	625	183	166	7		

- Molecule 67 is a protein called 40S RIBOSOMAL PROTEIN US9.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	CQ	139	Total	C	N	O	S	0	0
			1108	704	210	191	3		

- Molecule 68 is a protein called 40S RIBOSOMAL PROTEIN ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	CR	109	Total	C	N	O	S	0	0
			893	561	170	159	3		

- Molecule 69 is a protein called 40S RIBOSOMAL PROTEIN US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	CS	142	Total	C	N	O	S	0	0
			1172	736	236	199	1		

- Molecule 70 is a protein called 40S RIBOSOMAL PROTEIN ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	CT	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 71 is a protein called 40S RIBOSOMAL PROTEIN US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	CU	101	Total	C	N	O	S	0	0
			803	502	153	144	4		

- Molecule 72 is a protein called 40S RIBOSOMAL PROTEIN ES21.

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

- Molecule 73 is a protein called 40S RIBOSOMAL PROTEIN US8.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	CW	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 74 is a protein called 40S RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	CX	134	Total	C	N	O	S	0	0
			1046	663	205	176	2		

- Molecule 75 is a protein called 40S RIBOSOMAL PROTEIN ES24.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	CY	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 76 is a protein called 40S RIBOSOMAL PROTEIN ES25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	CZ	76	Total	C	N	O	S	0	0
			605	387	112	105	1		

- Molecule 77 is a protein called 40S RIBOSOMAL PROTEIN ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ca	96	Total	C	N	O	S	0	0
			767	476	159	127	5		

- Molecule 78 is a protein called 40S RIBOSOMAL PROTEIN ES27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Cb	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 79 is a protein called 40S RIBOSOMAL PROTEIN ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Cc	62	Total	C	N	O	S	0	0
			490	298	99	91	2		

- Molecule 80 is a protein called 40S RIBOSOMAL PROTEIN US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Cd	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 81 is a protein called 40S RIBOSOMAL PROTEIN ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ce	51	Total	C	N	O	S	0	0
			412	258	90	63	1		

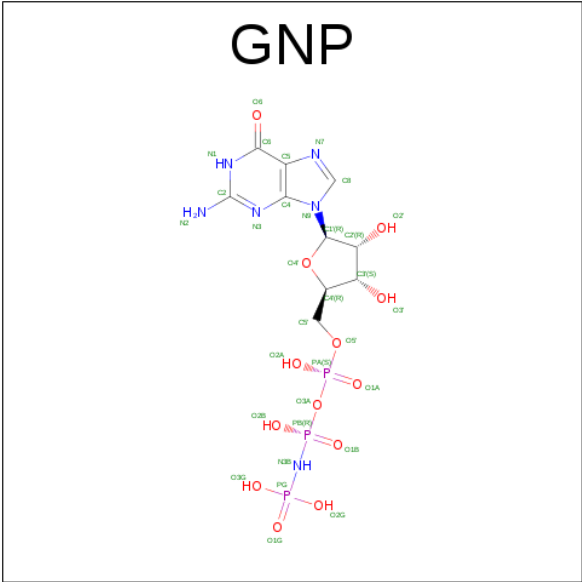
- Molecule 82 is a protein called 40S RIBOSOMAL PROTEIN ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Cf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 83 is a protein called 40S RIBOSOMAL PROTEIN RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Cg	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 84 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
84	BB	1	Total	C	N	O	P	0
			32	10	6	13	3	

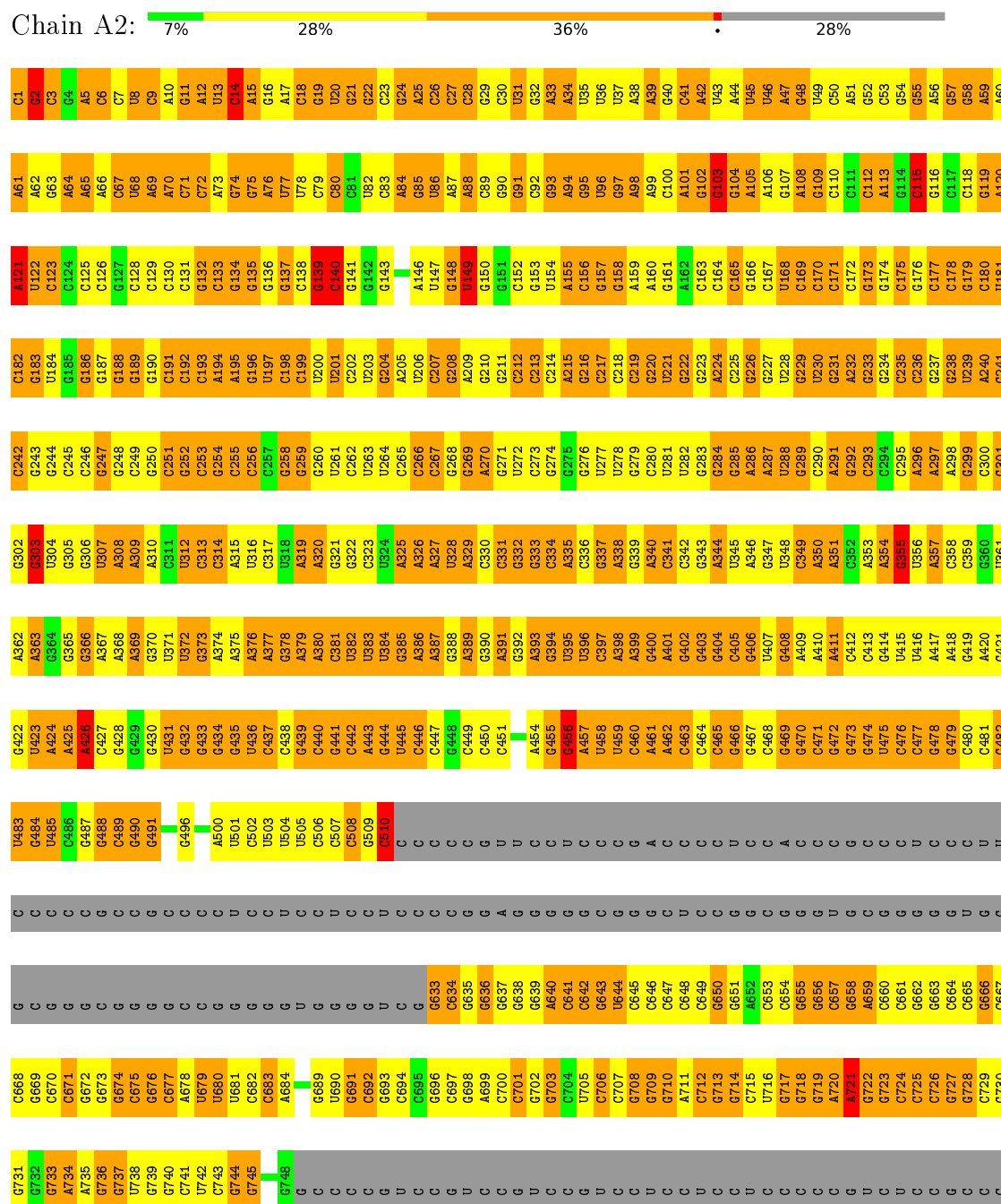
- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	BB	1	Total	Mg	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 errors 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: 28S Ribosomal RNA



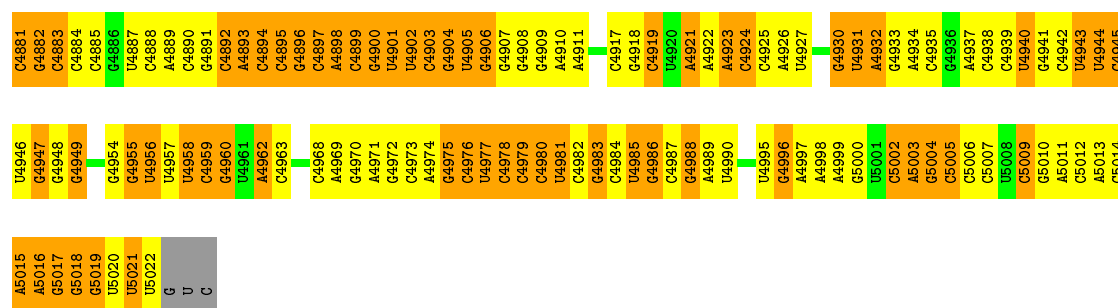
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A1708	A1648	G1587	C1525	G1463	U1403	G1342	G1279	C1219	G1158	C1096	U	G	C975	C915	G	C
U1709	G1649	U1588	A1526	C1464	G1404	C1343	G1280	G1220	U1159	C1097	C	C	C976	A916	G	C
C1710	U1650	C1589	G	C1465	G1405	U1344	U1281	G1221	C1160	C	U	G	C977	G917	C	G
G1711	U1651	G1590	C1529	G1466	G1406	G	U1282	G1222	C1161	G	C	C	G978	G918	G	G
G1712	U1652	C1591	G1530	G1467	A1407	C1347	A1283	G1223	C1162	C	C	C	G979	A919	G	G
G1713	C1653	A1592	G1531	A1468	U1408	A1348	C1284	G1224	C1163	G	U	U	G	C920	C	C
U1714	C1654	C1593	A1532	G	U1409	A1349	C1285	G1225	C1164	C	C	C	G	U921	C	C
A1715	C1655	C1594	A1533	G1471	C1410	C1349	C1286	G1226	C1165	C	G	G	C	C922	G	C
A1716	U1656	G1595	G1534	G1472	C1411	A1351	G1350	G1227	G1166	C	U	C	C	C923	G	C
A1717	C1657	C1596	G1535	U1473	G1412	A1352	C1288	C1228	U1167	C	C	A	C	C924	C	C
G1718	A1658	G1597	C1536	G1474	A1413	A1353	C1289	G1229	G	C	C	G1044	C	G925	G	C
G1719	G1659	A1537	G1537	G1475	G1414	G1354	C1290	C1230	C1170	G	C	G1045	C	G926	C	U
G1720	G1660	U1599	G1538	A1476	G1415	C1355	G1291	C1231	C1171	C	C	G1046	C	G927	G	C
A1721	A1661	A1600	A1539	G1477	C1416	C1356	A1292	C1232	C1172	C	C	G1047	C	A927	G	C
G	U1662	G	G1540	C1478	C1417	C1357	C1293	G	C1173	C	C	G1048	C	U928	G	U
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A1725	G1664	G1604	A1542	A1480	C1419	C1359	C1295	A	G1175	C	C	G1050	C	G930	G	C
U1726	C1665	G1605	A1543	G1481	U1420	G1360	G1296	G	G1176	C	C	G1051	C	C931	C	C
U1727	U1666	G1606	A1544	A1482	C1421	U1361	G1297	A	C1177	C	C	G1052	C	C932	C	C
A1728	G1667	C1607	C1545	A1483	C1422	G1362	C1298	G1238	C1178	G	C	G1053	C	G933	C	U
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U1733	U1672	G1612	G1550	C1488	C1427	A1367	A1303	A1243	G1183	C	C	G1058	C	C938	G	A
G1734	C1673	A1613	U1551	C1489	G1428	A1368	A1304	A1244	C1184	G	C	G1059	C	C939	A	G
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U1736	C	U1615	G1553	G1491	A1430	G1370	A1306	G1246	C1186	C	C	G1061	C	G941	C	G
G1737	G	G1616	A1554	U1492	G1431	A1371	C1307	G1247	C1187	C	C	G1062	G	G942	C	C
G1738	C	G1617	U1555	U1493	A1432	A1372	G1308	G1248	C1188	C	C	G1063	C	G943	A	C
G1739	A	U1618	G1556	A1494	G1433	G1373	G	A1249	U1189	U	C	G1064	A	A944	A	C
G1740	G	C1619	U1557	G1495	G1434	G1374	C1312	C1249	U1190	C	C	G1065	A	C945	A	C
C1741	A	G1620	C1558	G1496	G1435	U1375	A1313	A1250	C1191	C	C	G1066	G	C946	A	C
C1742	C	A1621	C1559	A1497	G1436	G1376	A1314	C1251	G1192	C	C	A1067	G	G947	C	C
G1743	C	A1622	G1560	C1498	C1437	A1377	G1315	C1252	G1193	C	C	G1068	G	A948	C	G
A1744	C	G1623	U1561	C1499	A1438	A1378	G1316	G1253	G1194	C	C	G1069	G	G949	C	G
A1745	G	C1624	A1562	C1500	C1439	G1379	A1317	A1254	C1194	C	C	G1070	G	A950	U	C
A1746	A	A1625	G1563	G1501	A1440	G1380	G1318	G1255	C1195	C	C	C1071	G	C951	C	C
C1747	C	U1626	C1564	A1502	A1441	C1381	U1319	C1256	C1196	C	C	G	U	C952	G	C
G1748	G	G1627	G1565	A1503	C1442	C1382	G	C1257	C1197	C	C	G1074	C	C953	C	C
A1749	C	U1628	G1566	A1504	C1443	G1383	A1322	C1258	G1198	C	C	A1075	U	C954	G	C
U1750	C	A1629	U1567	G1505	G1444	G1384	A1323	A1259	G1199	C	C	C1076	C1015	U955	A893	G
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U1752	C	U1631	C1569	U1507	C1446	G1386	A1325	G1261	G1201	C	C	G1078	C1017	C957	U895	C
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A1755	C	C1634	A1572	G1510	G1449	C1389	U1328	G1264	G1204	C	C	G1081	G1020	G960	U898	C
G1756	G	U1635	G1573	G	U1450	U1390	G1329	U1265	U1205	C	C	U1082	G	C961	A899	C
C1757	C	G1636	G1574	A1513	C1451	C1391	C1330	G1266	G1207	C	C	U1083	C	G962	C900	C
U1758	C	G1637	U1575	C1514	U1452	G1392	G1331	G1267	U1208	C	C	C1084	C	C963	A901	C
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U1760	C	U1639	A1516	U1517	G1454	C1394	G1333	C1269	U1210	C	C	G1146	C	U965	C903	C
U1761	G	C1640	U1517	U1517	C1455	G1395	A1334	G1270	C1211	C	C	C1147	G	C966	C904	C
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A1766	C	C1582	C1520	G1458	G1458	C1398	C1337	G1273	G1214	C	C	G1150	C	C969	C970	C
A1767	C	G1583	U1521	C1459	C1459	G1399	C1337	A1274	U1091	C	C	G	C	C971	G910	C
U1705	C	G1584	G1522	C1460	A1400	G1399	G1338	C1275	C1092	C	C	G1154	C	C972	G911	C
C1768	C	G1523	G1461	G1461	G1401	G1401	G1340	G1276	C1093	C	C	C1155	C	U973	C912	C
																A913





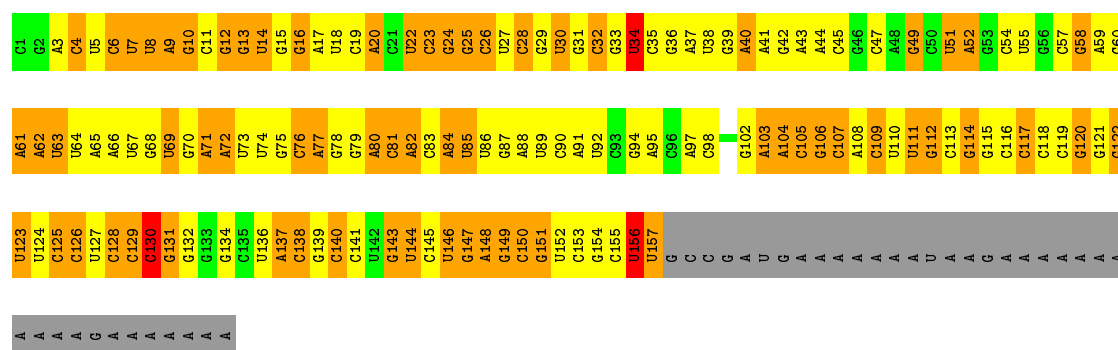




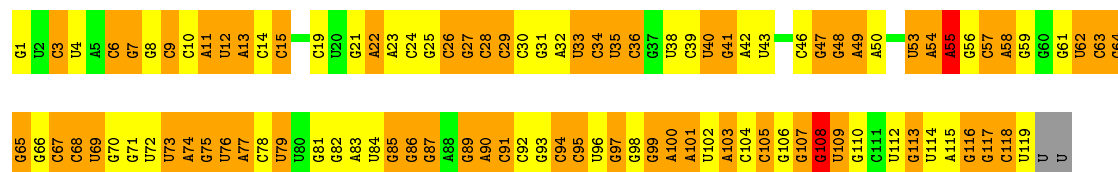
- Molecule 2: 5.8S Ribosomal RNA

Chain A3: 8% 37% 35% 19%



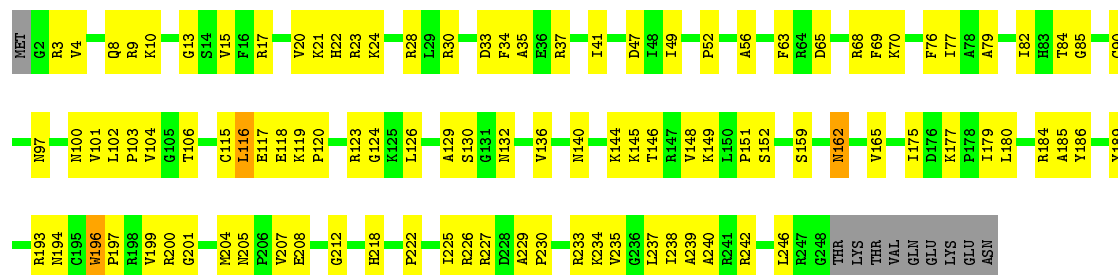
- Molecule 3: 5S Ribosomal RNA

Chain A4: 12% 36% 49%



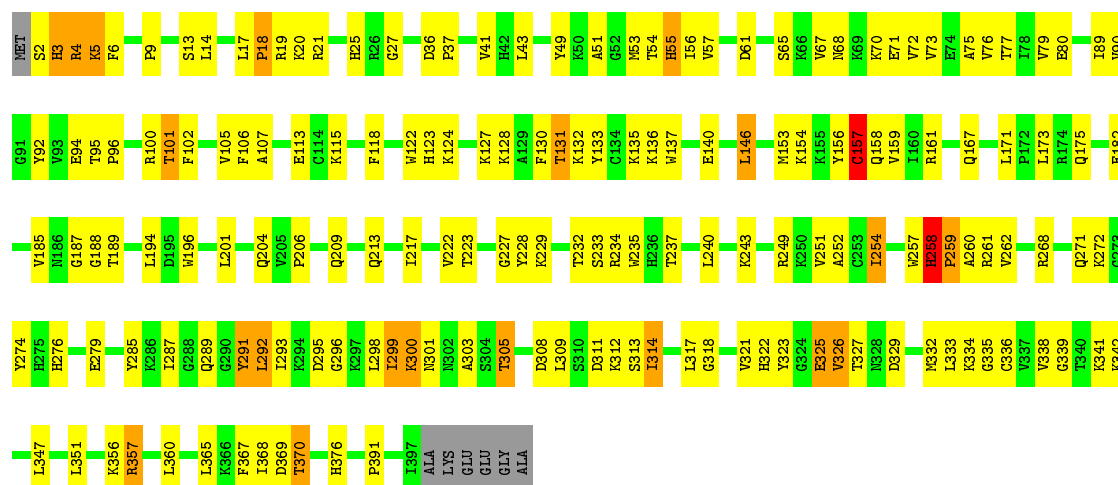
- Molecule 4: 60S RIBOSOMAL PROTEIN L8

Chain AA: 56% 39%



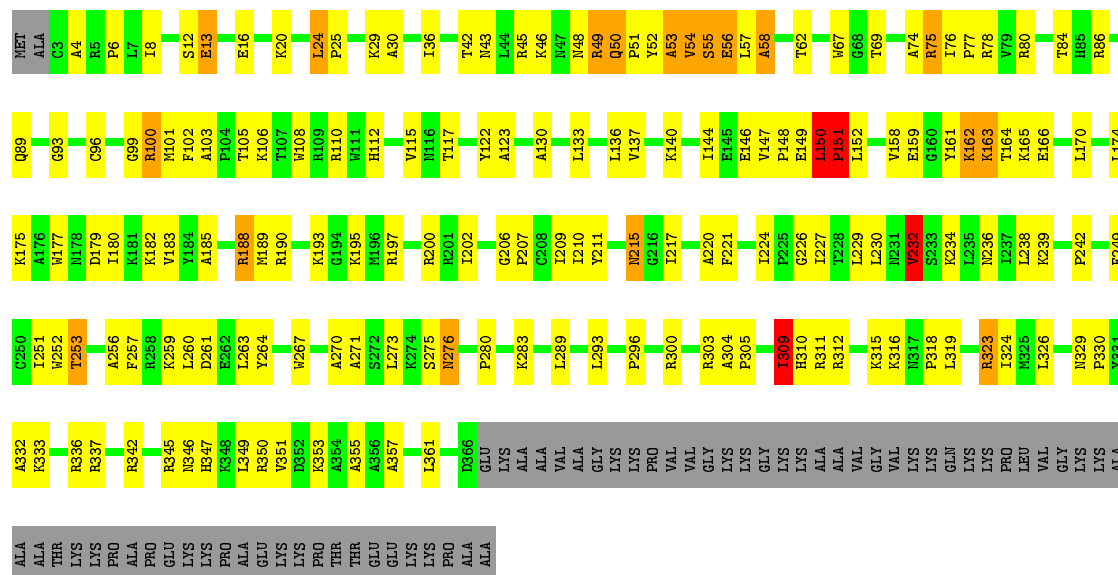
- Molecule 5: 60S RIBOSOMAL PROTEIN L3

Chain AB: 56% 37% 5%



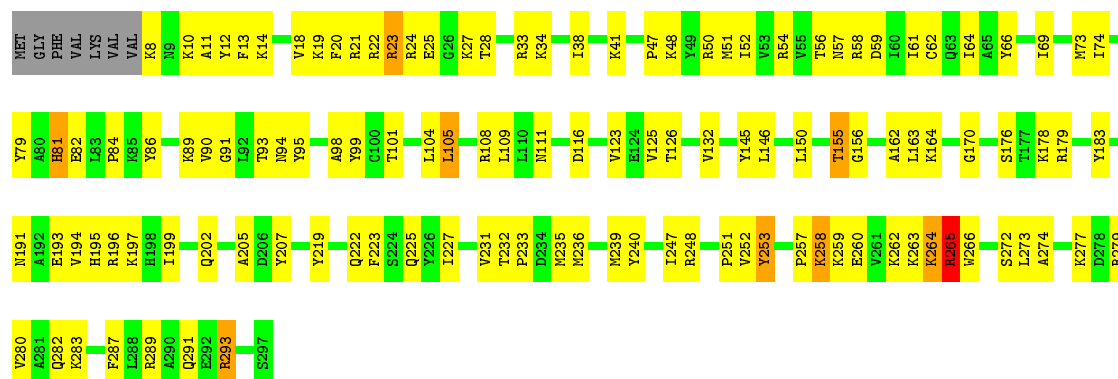
• Molecule 6: 60S RIBOSOMAL PROTEIN L4

Chain AC: 46% 34% 15%



• Molecule 7: 60S RIBOSOMAL PROTEIN L5

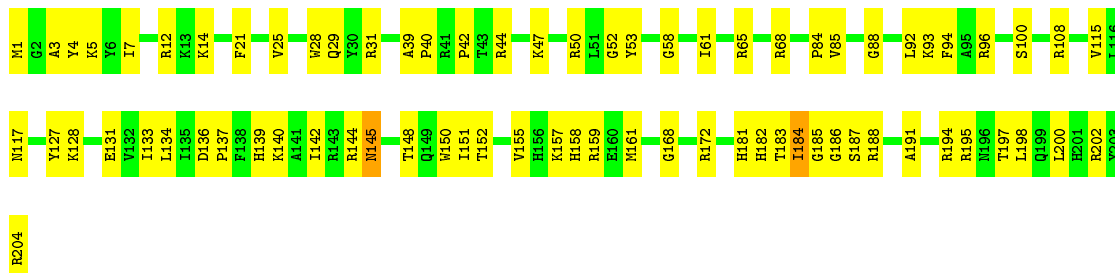
Chain AD: 57% 38% 5%



GLY
LYS
LYS
ALA

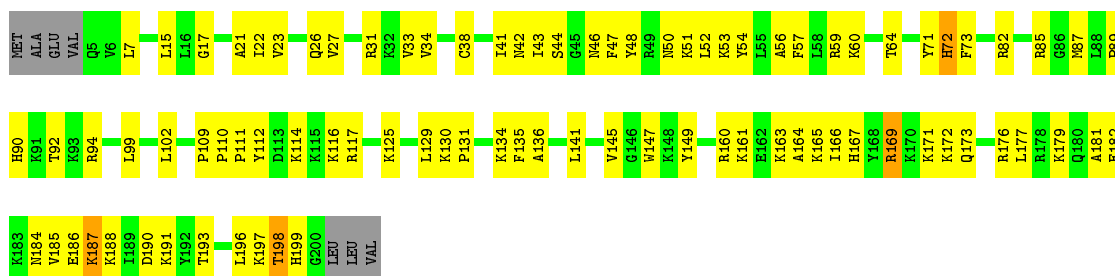
• Molecule 16: 60S RIBOSOMAL PROTEIN L15

Chain AN:  64% 35%



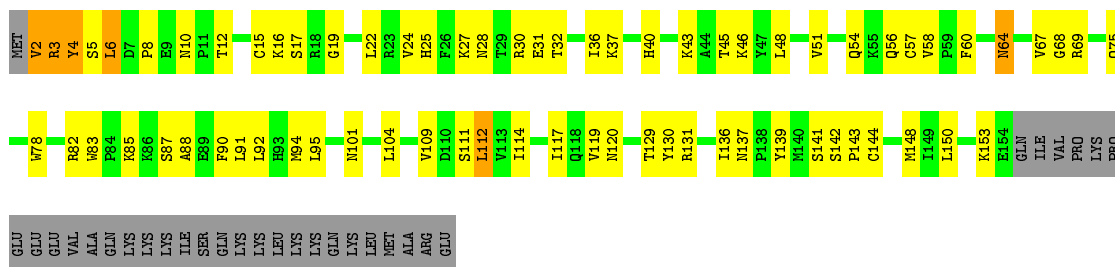
• Molecule 17: 60S RIBOSOMAL PROTEIN L13A

Chain AO:  54% 41%



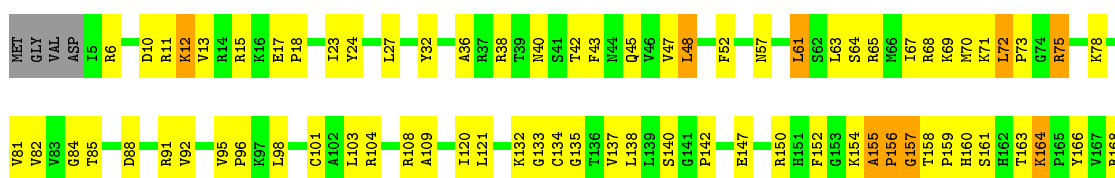
• Molecule 18: 60S RIBOSOMAL PROTEIN L17

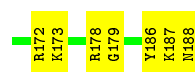
Chain AP:  45% 35% 17%



• Molecule 19: 60S RIBOSOMAL PROTEIN L18

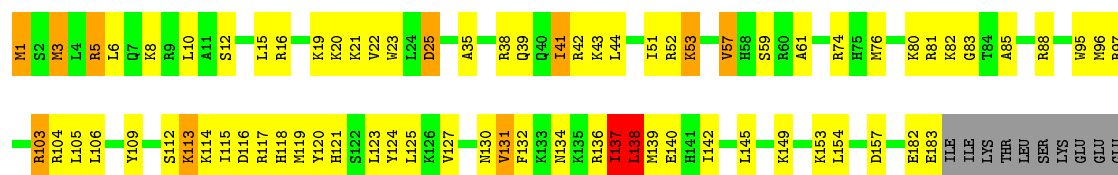
Chain AQ:  54% 39% 5%





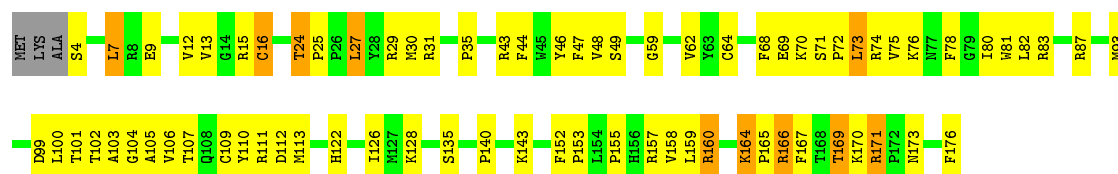
• Molecule 20: 60S RIBOSOMAL PROTEIN L19

Chain AR: 55% 32% 5% 7%



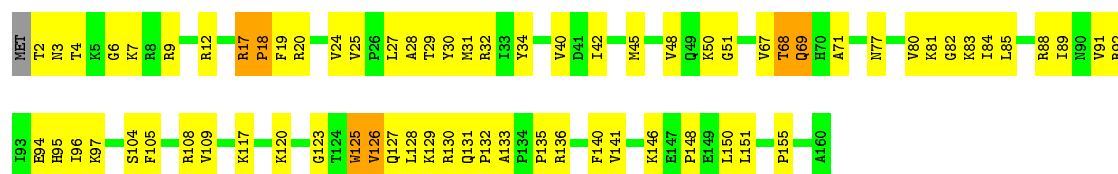
• Molecule 21: 60S RIBOSOMAL PROTEIN L18A

Chain AS: 56% 37% 6%



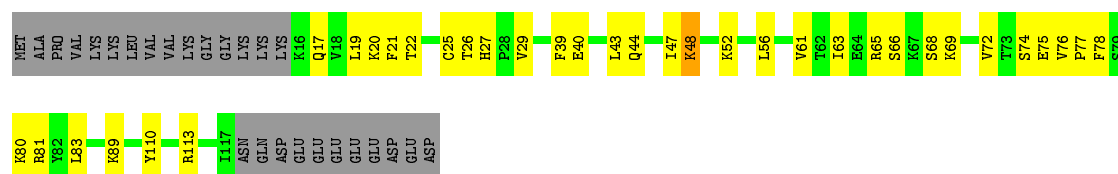
• Molecule 22: 60S RIBOSOMAL PROTEIN L21

Chain AT: 56% 40% 2%



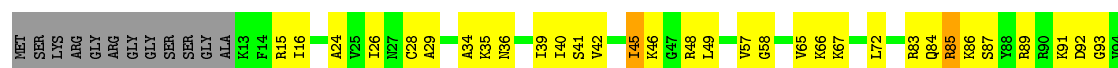
• Molecule 23: 60S RIBOSOMAL PROTEIN L22

Chain AU: 52% 27% 20%



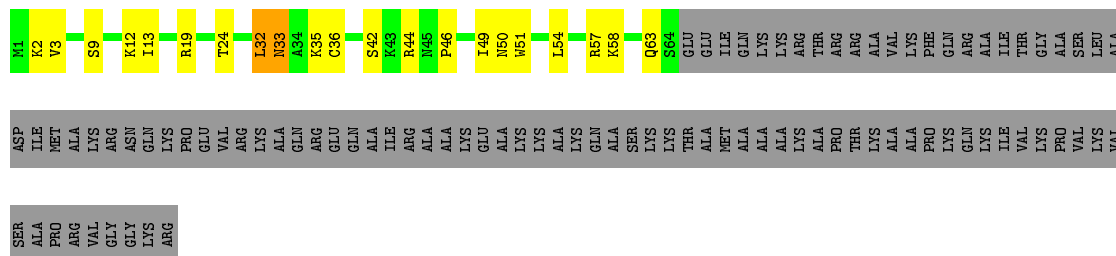
• Molecule 24: 60S RIBOSOMAL PROTEIN L23

Chain AV: 61% 29% 9%

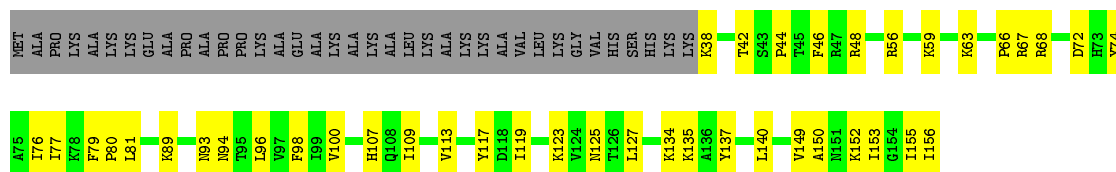




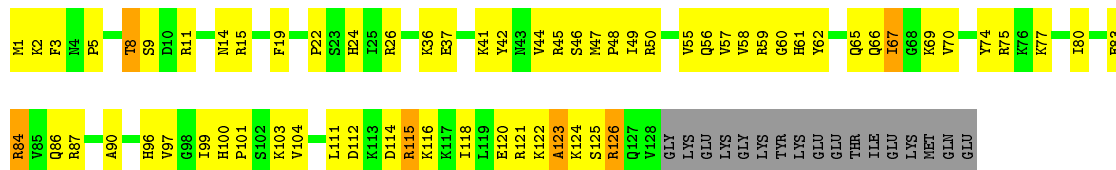
• Molecule 25: 60S RIBOSOMAL PROTEIN L24



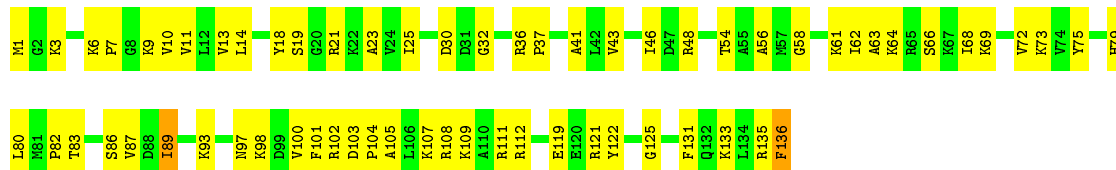
• Molecule 26: 60S RIBOSOMAL PROTEIN L23A



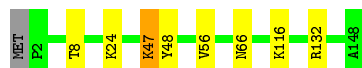
• Molecule 27: 60S RIBOSOMAL PROTEIN L26



● Molecule 28: 60S RIBOSOMAL PROTEIN L27

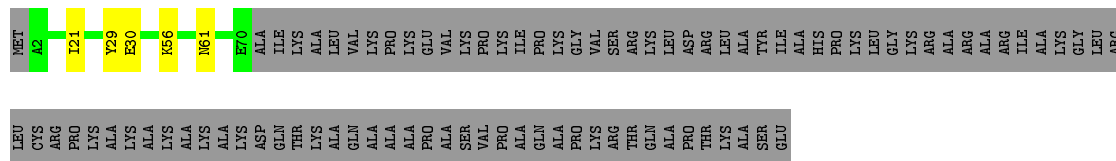


● Molecule 29: 60S RIBOSOMAL PROTEIN L27A




- Molecule 30: 60S RIBOSOMAL PROTEIN L29

Chain Ab:  40% 57%




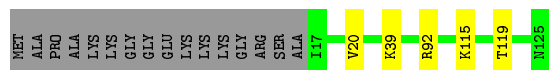
- Molecule 31: 60S RIBOSOMAL PROTEIN L30

Chain Ac:  88% 10%



- Molecule 32: 60S RIBOSOMAL PROTEIN L31

Chain Ad:  83% 13%




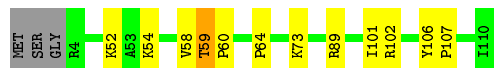
- Molecule 33: 60S RIBOSOMAL PROTEIN L32

Chain Ae:  90% 5%




- Molecule 34: 60S RIBOSOMAL PROTEIN L35A

Chain Af:  86% 10%



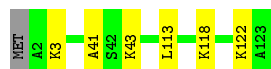
- Molecule 35: 60S RIBOSOMAL PROTEIN L34

Chain Ag:  87% 10%




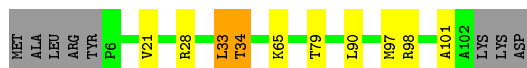
- Molecule 36: 60S RIBOSOMAL PROTEIN L35

Chain Ah:  94% 5%




- Molecule 37: 60S RIBOSOMAL PROTEIN L36

Chain Ai:  83% 8% 8%



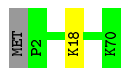
- Molecule 38: 60S RIBOSOMAL PROTEIN L37

Chain Aj:  84% 12%



- Molecule 39: 60S RIBOSOMAL PROTEIN L38

Chain Ak:  97% ..



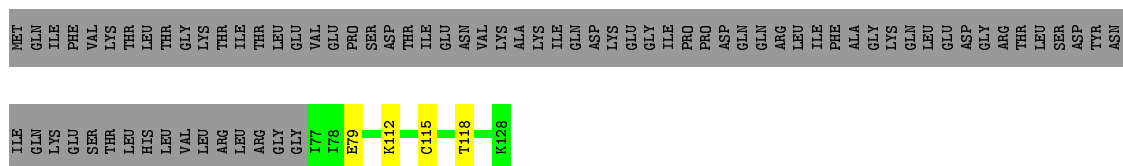
- Molecule 40: 60S RIBOSOMAL PROTEIN L39

Chain Al:  94% . .



- Molecule 41: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

Chain Am:  38% . 59%



- Molecule 42: 60S RIBOSOMAL PROTEIN L41

Chain An:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 60S RIBOSOMAL PROTEIN L36A

Chain Ao:  93% 7%



- Molecule 44: 60S RIBOSOMAL PROTEIN L37A

Chain Ap:  93% 5% .



- Molecule 45: 60S RIBOSOMAL PROTEIN L28

Chain At: 86% 7% 5%



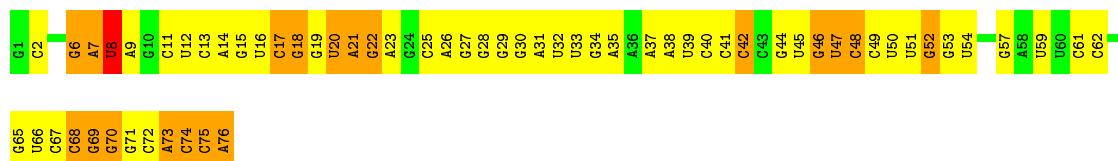
- Molecule 46: 60S RIBOSOMAL PROTEIN L10A

Chain Au: 92% 8%



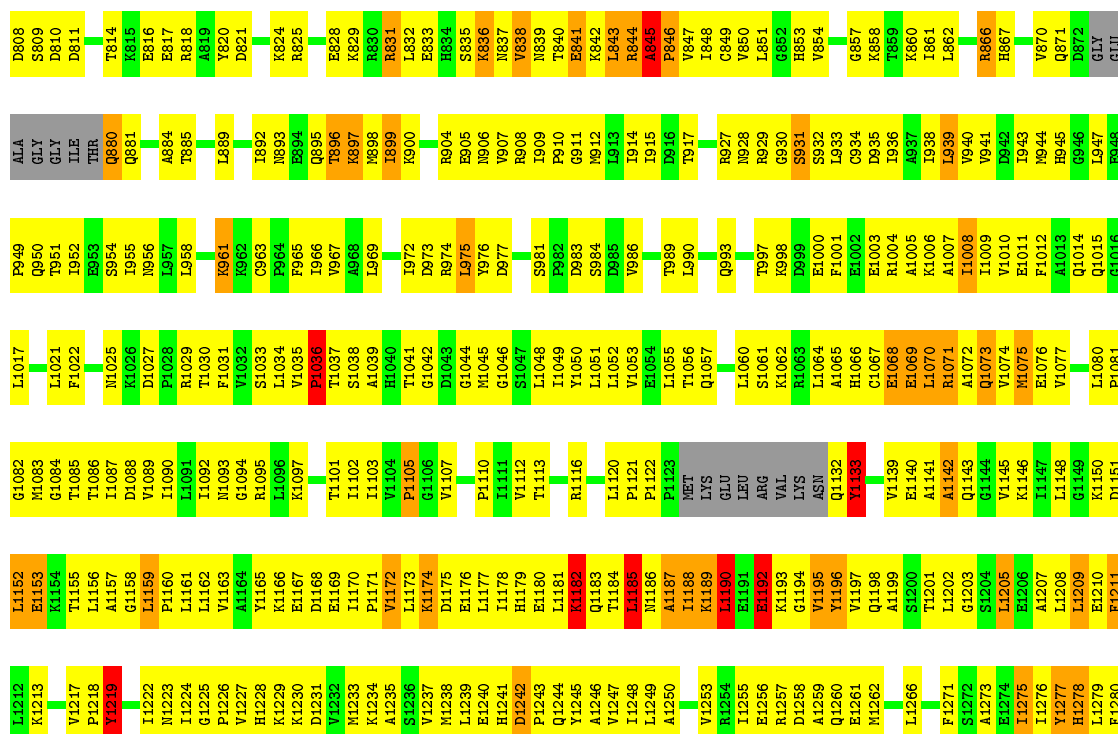
- Molecule 47: TRNA

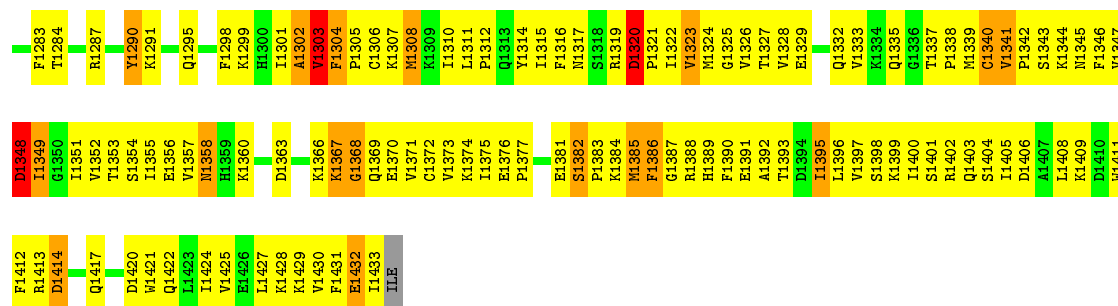
Chain BA: 18% 55% 25%



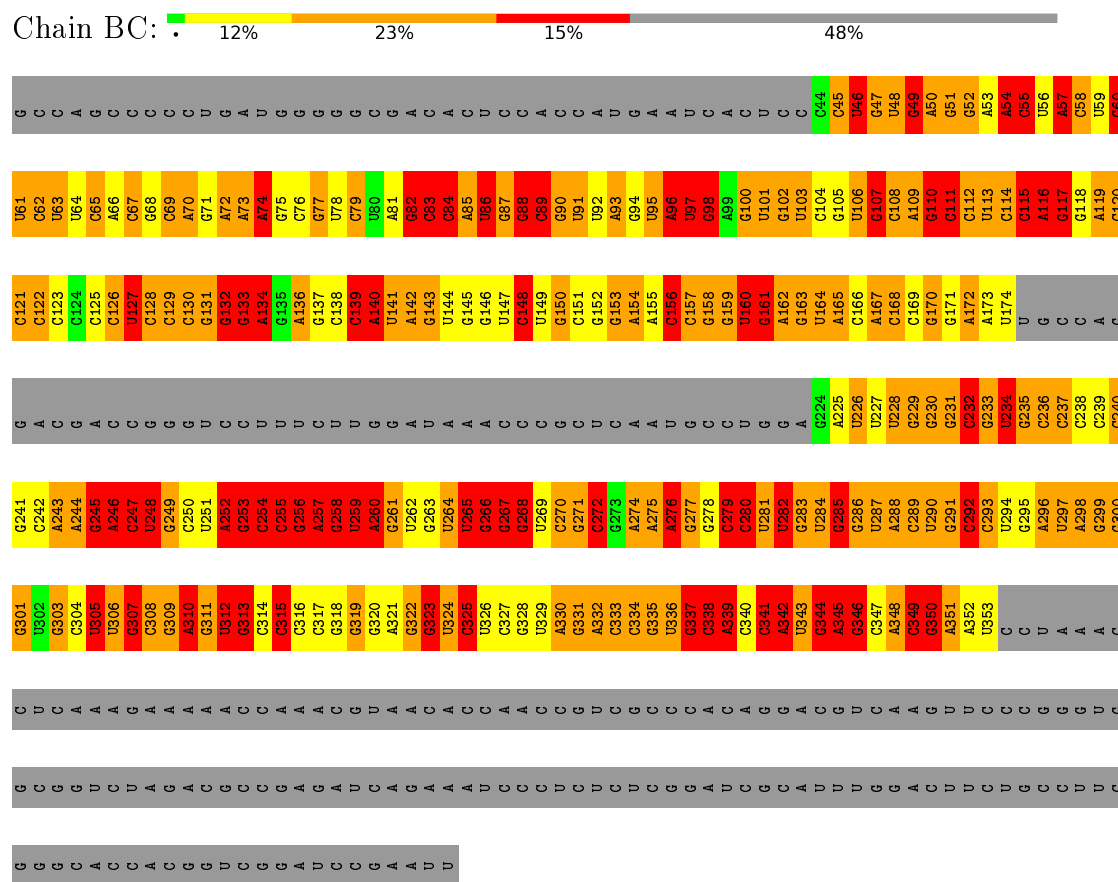
- Molecule 48: EIF5B

Chain BB: 28% 58% 9%

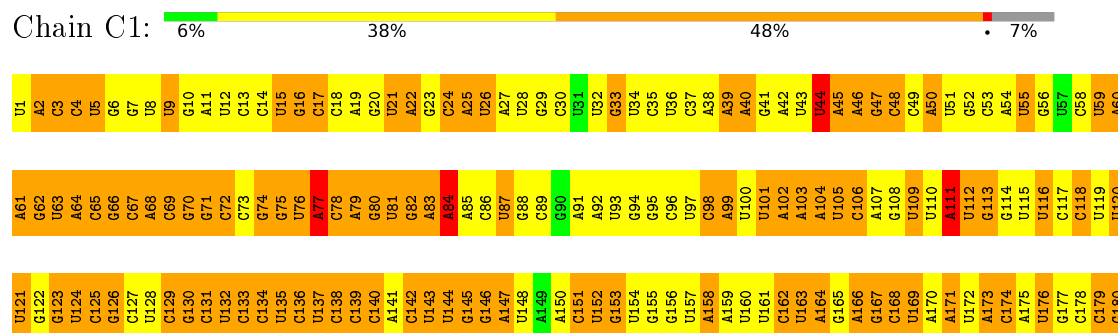




• Molecule 49: HCV-IRES

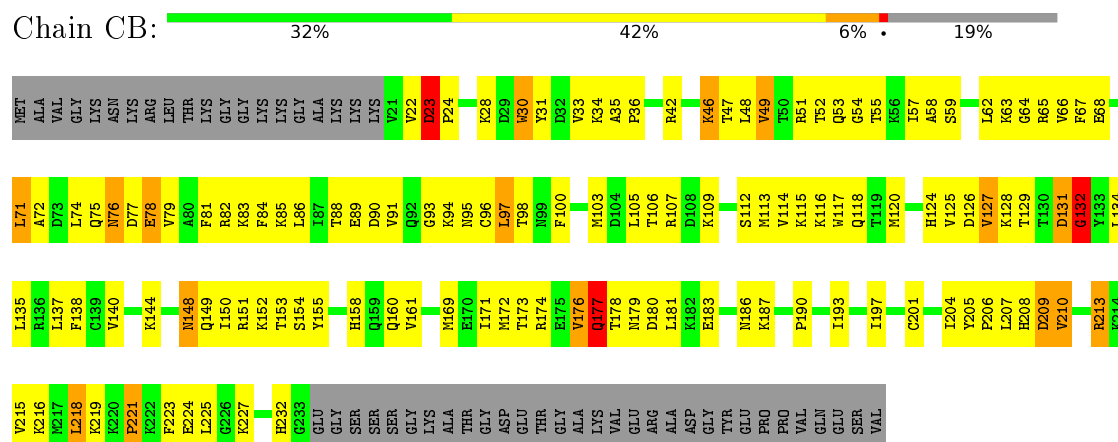


• Molecule 50: 18S Ribosomal RNA

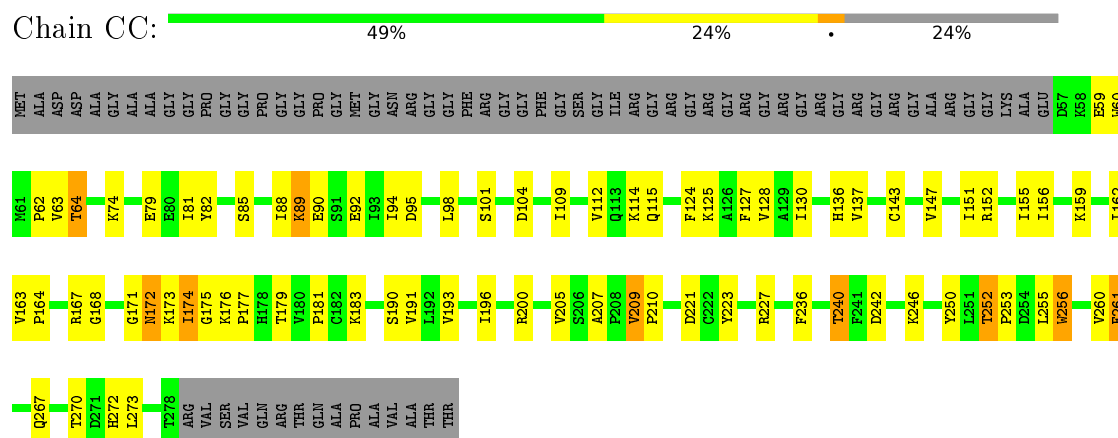


U1152	G1092	A1030	U968	G907	G846	G	C	U666	G606	G546	A486	A426	A363	A301	A181
C1183	A1093	A1031	U969	A908	A847	G	G	U667	U607	G547	U467	U427	A364	A302	C182
U1154	C1094	C1032	G970	C	U848	G	C	A668	C608	C548	U468	U428	C303	C304	G183
U1155	C1095	G1033	G971	C911	A849	G789	C	A669	U609	C549	A469	C429	U366	C305	G184
U1156	G1096	A1034	A972	C912	C850	C790	C	A670	G610	C550	C430	C430	U367	U305	G185
G1157	G1097	A1035	C973	A913	C851	C791	G	A671	G611	C551	C431	C431	U368	C306	C186
G1158	C1098	A1036	C974	U914	G852	C792	U	A672	U612	C552	C432	C432	C369	G307	G187
G1159	G1099	G1037	G975	G915	C853	C793	C	G673	G613	U553	A433	A433	G370	G308	C188
U1160	A1100	U1038	G976	A916	A854	A794	C	C674	C614	A554	G434	G434	A371	G309	C189
U1161	U1101	C1039	G977	U917	G855	A795	C	U675	G615	A555	U435	U435	U372	C310	G190
C1162	G1102	G1040	G978	U918	C856	G796	C	C676	A616	A556	G436	G436	G373	C311	A191
G1163	C1103	G1041	C979	A919	U857	G797	C	G677	G617	U557	G437	G437	U374	G312	C192
G1164	G1104	A1042	A980	A920	A858	G798	C	U678	C618	G558	G438	G438	U375	A313	C193
G1165	G1105	G1043	A981	G921	G859	U799	C	A679	A619	G559	A439	A439	A376	U314	C194
G1166	C1106	G1044	G982	A922	G860	U800	C	G680	G620	A560	A500	G440	G377	C315	C195
G1167	G1107	U1045	A983	G923	A861	U801	C	U681	C621	A561	C441	C441	U378	C316	C196
G1168	G1108	U1046	C984	G924	A862	A902	C	U682	C622	U562	C502	C442	C379	C317	U197
G1169	C1109	C1047	G985	G925	U863	C903	C	G683	G623	G563	C503	U443	G380	A318	C198
U1170	G1110	G1048	G986	A926	A864	U904	C	G684	C624	A564	G504	G444	C381	C319	C199
G1171	U1111	A1049	A987	C927	A865	U905	C	U685	G625	G565	G505	A445	C382	G320	G200
U1172	U1112	A1050	C988	G928	U866	U906	C	A686	U626	U566	G506	G446	G383	G321	G201
A1173	A1113	G1051	C989	G929	G867	G907	C	U687	U627	C567	A447	A447	U384	C322	G202
U1174	U1114	A1052	A990	C930	G868	A908	C	U688	U628	C568	A448	A448	G385	C323	G203
G1175	C1115	C1053	G991	C931	A869	A909	C	U689	A629	A569	G509	A449	C386	G324	G204
G1176	U1116	G1054	A992	G932	A870	A810	C	G690	U630	C570	G510	C450	C387	G325	G205
U1177	C1117	A1055	G993	G933	U871	A811	C	G691	U631	U571	U511	G451	U388	G326	G206
U1178	C1118	U1056	C994	G934	A872	A812	C	G692	C632	U572	A512	G452	A389	G329	G207
G1179	A1119	G1057	G995	G935	G873	A813	C	A693	C633	U573	G513	C453	C390	G330	G208
C1180	U1120	A1058	C996	G936	G874	U814	C	G694	A634	A574	U514	U454	C391	A209	G209
A1181	G1121	G1059	G999	C937	A875	U815	C	C695	G635	A575	G515	A455	U393	G332	G210
A1182	A1122	A1060	C1000	A938	C876	A816	C	G696	C636	A576	A516	C456	G394	G333	G211
A1183	C1123	U1061	U1001	U939	C877	G817	C	G	U637	U577	C457	C457	G395	G334	C212
C1184	G1124	A1062	U1002	U940	G878	A818	C	G	C638	C578	A458	A458	U396	G335	G213
C1185	C1125	C1063	U1003	C941	C879	G819	C	C	C639	C579	A459	C459	G397	A336	G214
U1186	G1126	G1064	U1004	G942	G880	U820	U	G	A640	U580	A460	A460	C398	G337	G215
G1187	C1127	G1065	G1005	U943	G881	G821	C	G	A641	U581	A521	U461	C399	G338	C216
A1188	C1128	U1066	G1006	A944	U883	U822	C	G	U642	U582	A522	C462	C400	A339	A217
A1189	G1129	C1067	C1007	U945	C884	U823	A	C	A643	A583	A523	C463	A401	C340	U218
A1190	U1130	G1068	A1008	U946	U885	C824	U	G	C644	A584	U524	A464	C402	G341	U219
C1191	G1131	U1069	A1009	U947	A886	A825	G	G	C645	C585	A525	A465	C	G342	U220
U1192	C1132	A1070	G1010	C948	U887	A826	C	U	G466	G586	A526	G466	U406	A343	C221
U1193	A1133	G1071	A1011	G949	U888	A827	U	C	U647	A587	C527	G467	G407	U344	U222
A1194	G1134	C1074	A1012	C950	U889	G828	C	C	A648	G588	A528	A468	A408	U345	C223
A1195	C1135	C1075	U1013	C951	U890	C829	U	C	U649	G589	A529	A469	C409	C346	A224
A1196	U1136	G1076	G1014	G952	G891	A830	U	C	A650	U590	U530	G470	G410	G347	G225
G1197	U1137	U1015	U1015	C953	U892	G831	A	C	U651	U591	A531	G471	G411	A348	A226
G1198	C1138	U1016	U1016	U954	U893	G832	G	G	U652	C592	C532	C472	G412	A349	U227
A1199	G1139	U1017	A955	G954	G894	C833	U	C	A653	C593	A533	A473	G413	C350	C228
A1200	G1140	G956	G956	G956	G895	C834	U	G	A654	A594	G534	G474	A414	G351	A229
U1201	G1141	U1019	A957	U957	U896	C835	G	A	A655	U595	G535	C475	A415	U352	A230
U1202	G1142	A1020	C897	G958	C897	G836	A	G	G656	U596	A536	A476	U416	C353	A231
G1203	A1143	U1021	U898	G959	U898	A837	G	G	U657	C597	C537	G477	C417	U354	A232
A1204	A1144	U1022	U899	G960	G899	G838	U	C	U658	G598	U538	G478	A418	C355	C233
C1205	A1145	C1023	C900	G961	C900	C839	G	C	G659	A599	C539	C479	G419	C356	C234
G1206	G1066	A1024	G901	A962	G901	G840	U	C	C660	G600	U540	G480	A420	C357	A235
G1207	A1087	U1025	G902	A963	G902	G841	C	C	U661	G601	U541	C481	G421	C358	A236
A1208	U1088	C1026	A903	A964	A903	C842	C	C	G662	G602	U542	G482	U422	U359	C237
A1209	G1089	A1027	A904	U965	A904	C843	C	C	C663	C603	C543	G483	U423	A360	G238
G1210	A1150	U1028	C905	U966	A944	C844	G	A	A664	A604	G544	A484	C424	U361	A239
G1211	G1151	C1091	U906	C967	U906	G845	C	C	G665	A605	A545	A485	G425	C362	G240

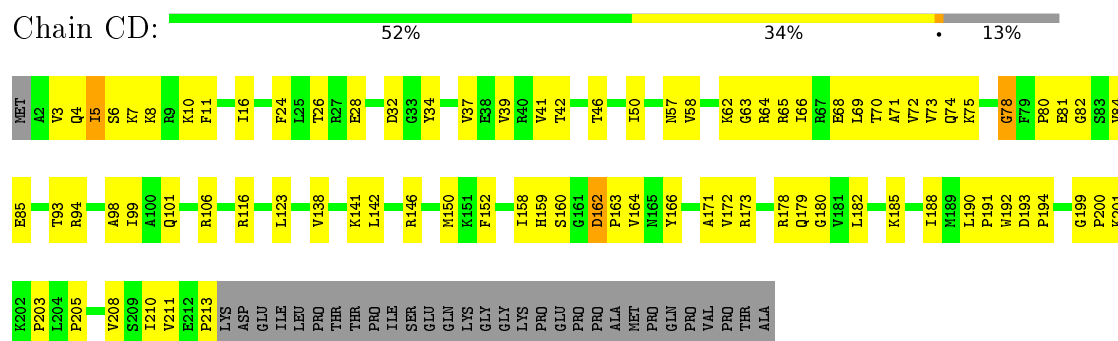
- Molecule 52: 40S RIBOSOMAL PROTEIN ES1



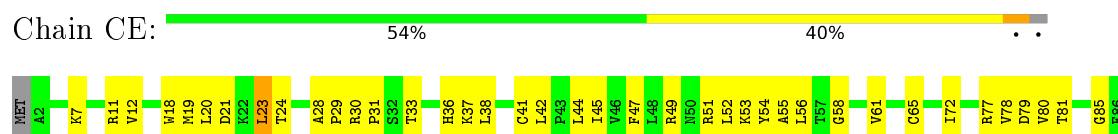
- Molecule 53: 40S RIBOSOMAL PROTEIN US5

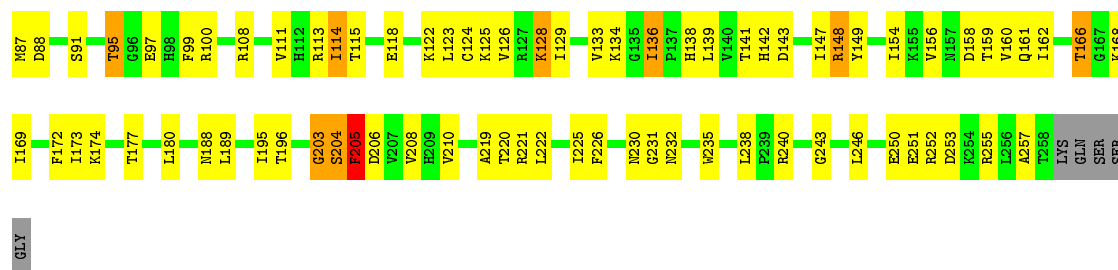


- Molecule 54: 40S RIBOSOMAL PROTEIN US3



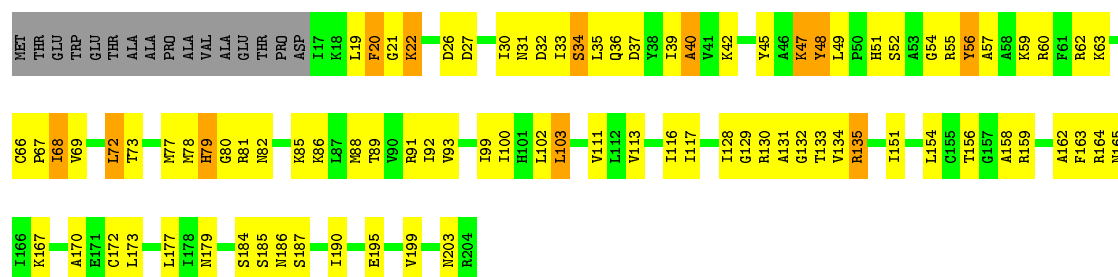
- Molecule 55: 40S RIBOSOMAL PROTEIN ES4





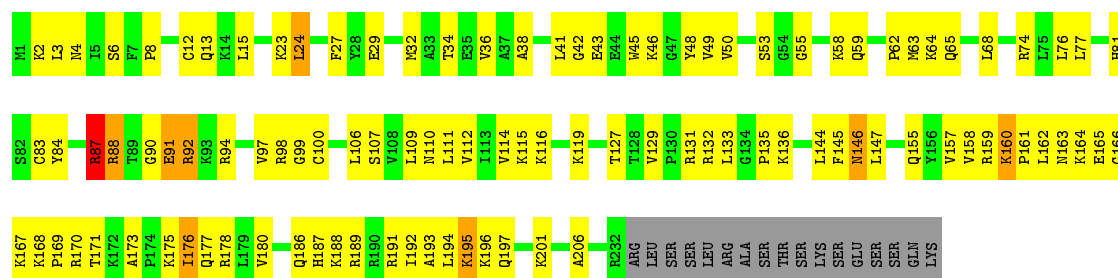
- Molecule 56: 40S RIBOSOMAL PROTEIN US7

Chain CF: 49% 38% 6% 8%



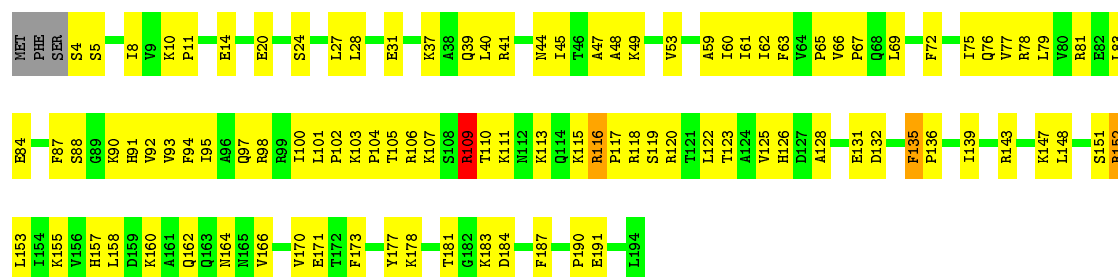
- Molecule 57: 40S RIBOSOMAL PROTEIN ES6

Chain CG: 51% 39% 7%



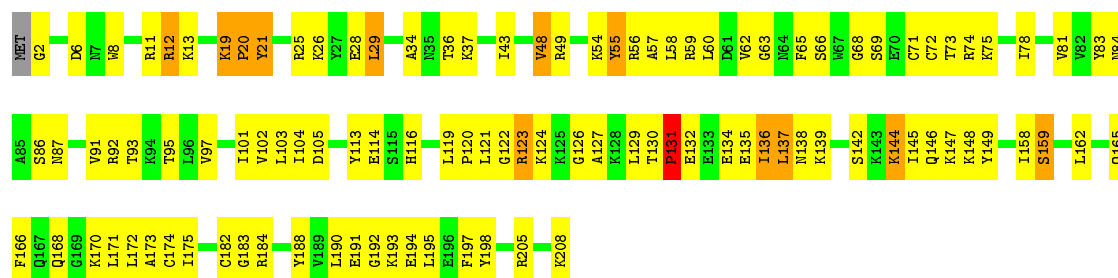
- Molecule 58: 40S RIBOSOMAL PROTEIN ES7

Chain CH: 46% 50% 4%



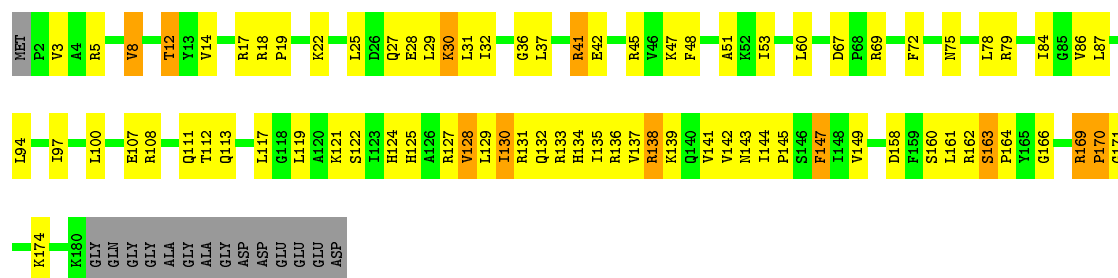
- Molecule 59: 40S RIBOSOMAL PROTEIN ES8

Chain CI: 48% 45% 6%



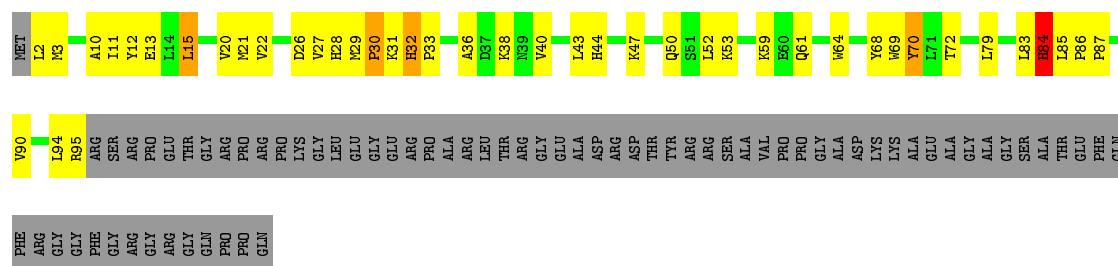
• Molecule 60: 40S RIBOSOMAL PROTEIN US4

Chain CJ: 51% 36% 6% 8%



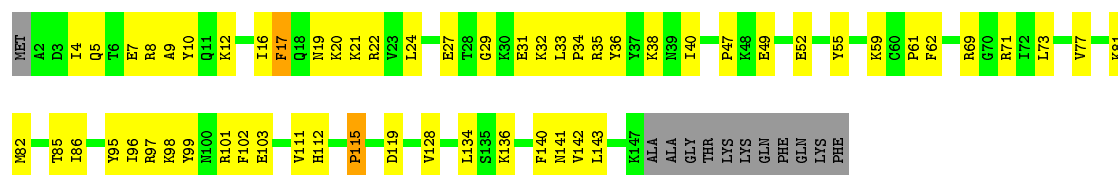
• Molecule 61: 40S RIBOSOMAL PROTEIN ES10

Chain CK: 31% 23% 43%



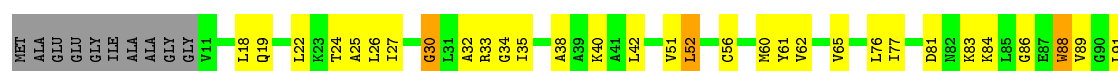
• Molecule 62: 40S RIBOSOMAL PROTEIN US17

Chain CL: 56% 35% 8%



• Molecule 63: 40S RIBOSOMAL PROTEIN ES12

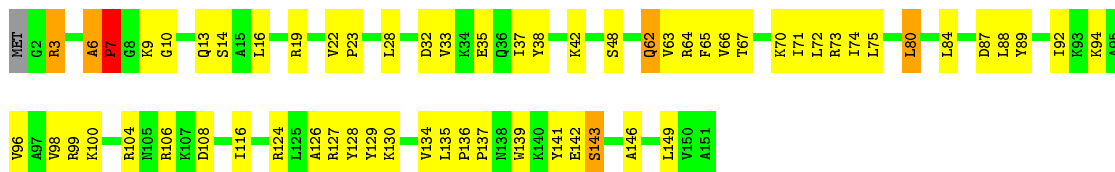
Chain CM: 55% 32% 9%





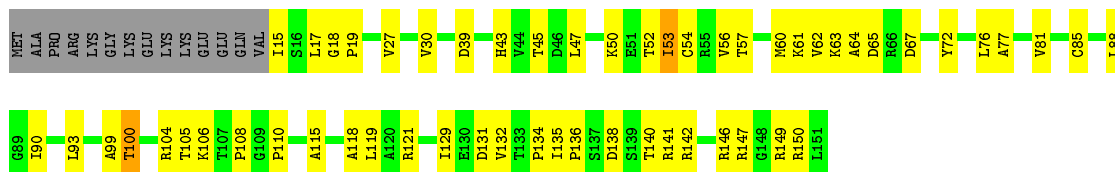
• Molecule 64: 40S RIBOSOMAL PROTEIN ES15

Chain CN: 58% 37% . .



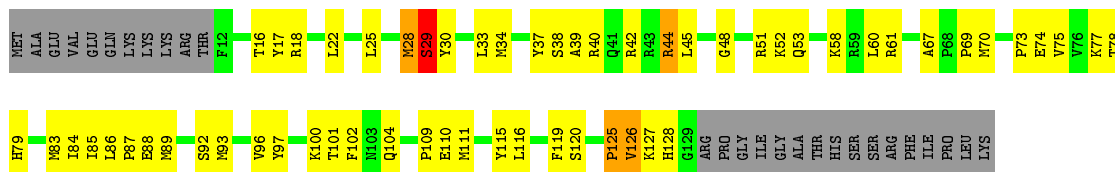
• Molecule 65: 40S RIBOSOMAL PROTEIN ES11

Chain CO: 54% 36% . 9%



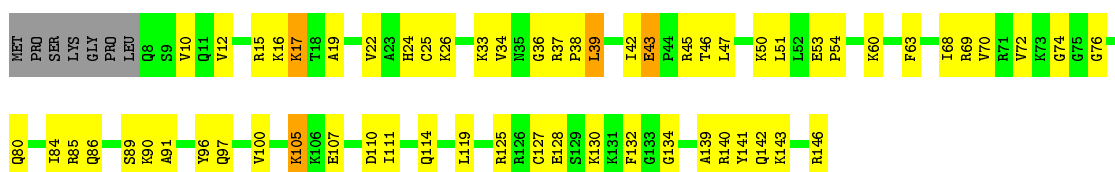
• Molecule 66: 40S RIBOSOMAL PROTEIN US19

Chain CP: 41% 37% . . 19%



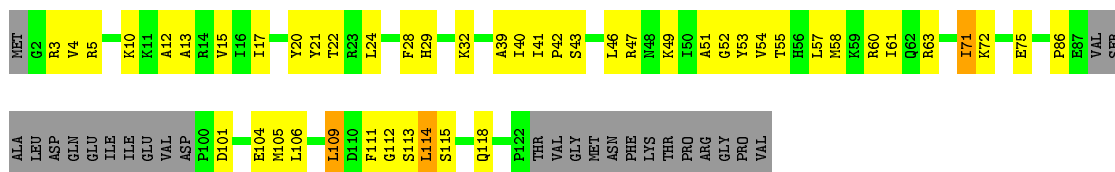
• Molecule 67: 40S RIBOSOMAL PROTEIN US9

Chain CQ: 53% 39% . 5%

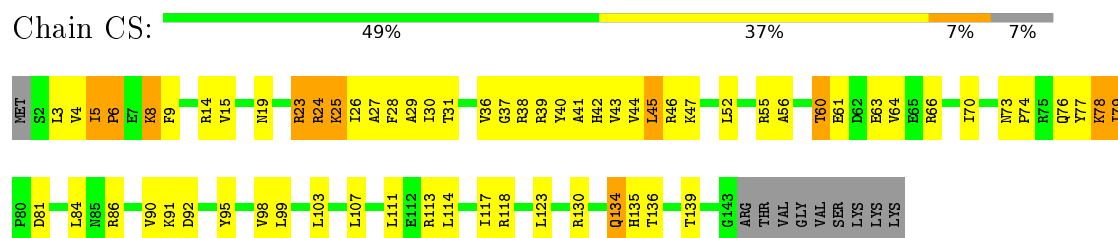


• Molecule 68: 40S RIBOSOMAL PROTEIN ES17

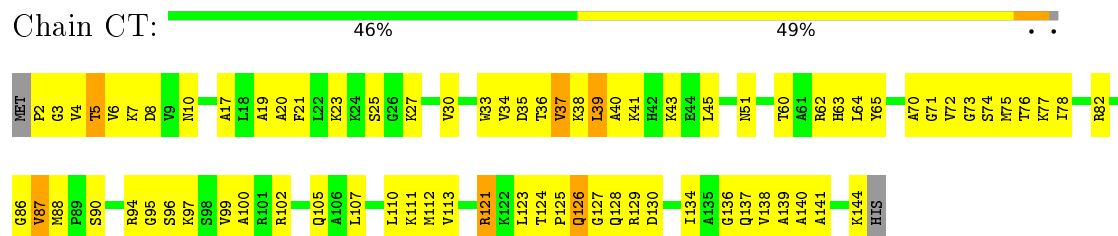
Chain CR: 45% 33% . 19%



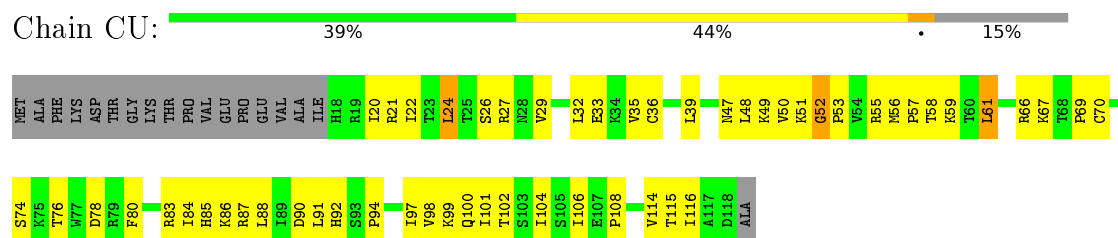
- Molecule 69: 40S RIBOSOMAL PROTEIN US13



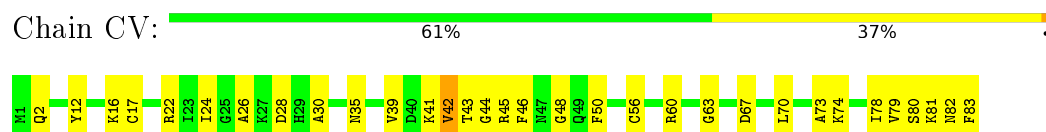
- Molecule 70: 40S RIBOSOMAL PROTEIN ES19



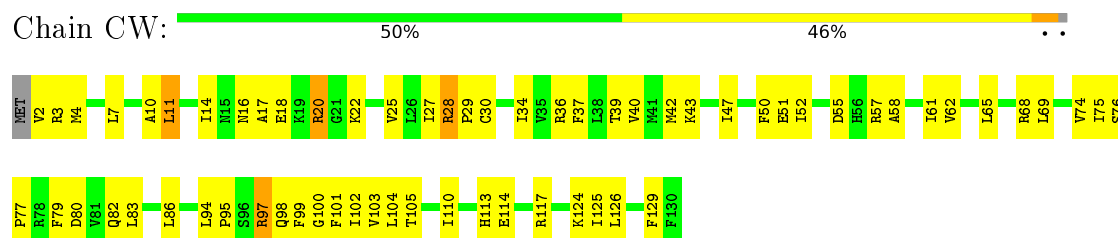
- Molecule 71: 40S RIBOSOMAL PROTEIN US10



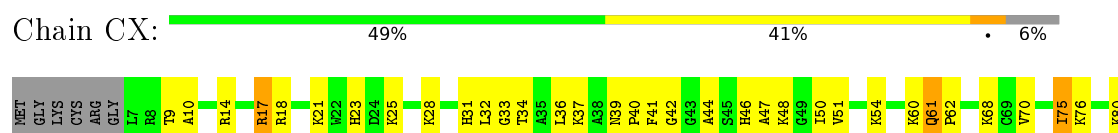
- Molecule 72: 40S RIBOSOMAL PROTEIN ES21



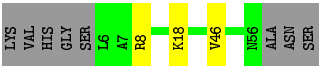
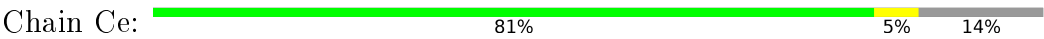
- Molecule 73: 40S RIBOSOMAL PROTEIN US8



- Molecule 74: 40S RIBOSOMAL PROTEIN US12







● Molecule 82: 40S RIBOSOMAL PROTEIN ES31



● Molecule 83: 40S RIBOSOMAL PROTEIN RACK1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	115000	Depositor
Image detector	TVIPS TEMCAM-F416 (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: GNP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A2	0.43	33/86671 (0.0%)	0.83	82/135194 (0.1%)
10	AG	0.46	0/1914	0.72	0/2578
11	AH	0.43	0/1555	0.69	0/2089
12	AI	0.42	0/1643	0.67	0/2194
13	AJ	0.49	0/1386	0.71	0/1852
14	AL	0.53	2/1647 (0.1%)	0.73	3/2205 (0.1%)
15	AM	0.49	0/1162	0.70	0/1556
16	AN	0.43	0/1754	0.65	0/2348
17	AO	0.44	0/1639	0.69	0/2193
18	AP	0.44	0/1260	0.70	0/1691
19	AQ	0.45	0/1518	0.74	0/2026
2	A3	0.36	0/3723	0.79	1/5800 (0.0%)
20	AR	0.39	0/1541	0.64	0/2035
21	AS	0.45	0/1479	0.73	0/1985
22	AT	0.46	0/1326	0.71	0/1770
23	AU	0.47	0/841	0.71	0/1128
24	AV	0.44	0/978	0.63	0/1312
25	AW	0.43	0/542	0.60	0/722
26	AX	0.42	0/993	0.67	0/1334
27	AY	0.47	0/1082	0.72	1/1441 (0.1%)
28	AZ	0.47	0/1138	0.79	0/1517
29	Aa	0.45	0/1191	0.71	0/1591
3	A4	0.38	0/2836	0.82	3/4421 (0.1%)
30	Ab	0.45	0/570	0.72	0/752
31	Ac	0.46	0/813	0.70	0/1091
32	Ad	0.45	0/920	0.67	0/1238
33	Ae	0.46	0/1071	0.68	0/1428
34	Af	0.50	0/885	0.81	0/1185
35	Ag	0.48	0/917	0.74	0/1222
36	Ah	0.38	0/1023	0.64	0/1351
37	Ai	0.43	0/793	0.75	0/1048
38	Aj	0.50	0/704	0.76	0/931

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	Ak	0.43	0/575	0.73	0/761
4	AA	0.44	0/1926	0.67	0/2583
40	Al	0.41	0/454	0.61	0/599
41	Am	0.42	0/435	0.70	0/575
42	An	0.40	0/241	0.51	0/305
43	Ao	0.45	0/885	0.74	0/1166
44	Ap	0.40	0/718	0.61	0/953
45	At	0.48	0/1058	0.75	0/1416
46	Au	0.45	0/1639	0.69	1/2222 (0.0%)
47	BA	0.53	0/1809	1.02	17/2819 (0.6%)
48	BB	0.65	1/4926 (0.0%)	1.15	29/6641 (0.4%)
49	BC	1.53	11/6230 (0.2%)	2.37	540/9712 (5.6%)
5	AB	0.45	0/3258	0.73	2/4361 (0.0%)
50	C1	0.37	2/41550 (0.0%)	0.80	6/64763 (0.0%)
51	CA	0.51	0/1756	0.68	0/2386
52	CB	0.51	0/1756	0.75	1/2350 (0.0%)
53	CC	0.42	0/1761	0.65	0/2379
54	CD	0.40	0/1672	0.66	0/2250
55	CE	0.47	0/2072	0.70	0/2793
56	CF	0.43	0/1507	0.74	0/2026
57	CG	0.48	0/1907	0.74	0/2538
58	CH	0.46	0/1558	0.74	1/2087 (0.0%)
59	CI	0.47	0/1724	0.72	0/2298
6	AC	0.47	0/2943	0.73	0/3953
60	CJ	0.45	0/1520	0.77	0/2030
61	CK	0.48	0/815	0.68	0/1101
62	CL	0.45	0/1220	0.72	0/1633
63	CM	0.48	0/941	0.72	0/1264
64	CN	0.43	0/1231	0.73	1/1656 (0.1%)
65	CO	0.46	0/1036	0.71	0/1391
66	CP	0.43	0/1000	0.67	0/1335
67	CQ	0.43	0/1125	0.66	0/1506
68	CR	0.42	0/904	0.67	0/1208
69	CS	0.42	0/1190	0.68	0/1594
7	AD	0.49	2/2407 (0.1%)	0.70	1/3221 (0.0%)
70	CT	0.44	0/1131	0.69	0/1515
71	CU	0.50	0/813	0.70	0/1092
72	CV	0.47	0/643	0.71	0/860
73	CW	0.44	0/1050	0.69	0/1406
74	CX	0.46	0/1063	0.70	0/1421
75	CY	0.45	0/1019	0.70	0/1354
76	CZ	0.46	0/611	0.71	0/820
77	Ca	0.48	0/778	0.75	1/1041 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	Cb	0.48	0/637	0.68	0/854
79	Cc	0.46	0/492	0.74	0/657
8	AE	0.52	0/1312	0.73	0/1763
80	Cd	0.51	0/454	0.77	0/603
81	Ce	0.45	0/417	0.69	0/548
82	Cf	0.53	0/507	0.84	1/673 (0.1%)
83	Cg	0.45	0/2497	0.67	0/3399
9	AF	0.44	0/1986	0.68	0/2644
All	All	0.49	51/240674 (0.0%)	0.87	691/353753 (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
1	A2	0	35
2	A3	0	2
48	BB	0	12
49	BC	0	105
50	C1	0	23
All	All	0	177

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1701	C	C5'-C4'	18.41	1.73	1.51
1	A2	1673	C	C3'-O3'	15.36	1.63	1.42
1	A2	1701	C	O5'-C5'	14.50	1.67	1.44
1	A2	1673	C	O3'-P	14.08	1.78	1.61
1	A2	1701	C	P-O5'	13.46	1.73	1.59

The worst 5 of 691 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	3919	U	N1-C2-O2	-33.15	99.59	122.80
1	A2	3919	U	N3-C2-O2	32.84	145.19	122.20
1	A2	1701	C	O4'-C4'-C3'	-15.18	88.82	104.00
1	A2	3914	A	O4'-C1'-N9	15.11	120.28	108.20
48	BB	1133	TYR	CB-CG-CD2	-14.74	112.15	121.00

There are no chirality outliers.

5 of 177 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A2	1	C	Sidechain
1	A2	115	C	Sidechain
1	A2	121	A	Sidechain
1	A2	140	C	Sidechain
1	A2	2	G	Sidechain

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	A2	77488	0	39156	7452	0
2	A3	3334	0	1693	288	0
3	A4	2538	0	1286	245	0
4	AA	1888	0	1983	130	0
5	AB	3190	0	3327	184	0
6	AC	2889	0	3064	238	0
7	AD	2362	0	2385	140	0
8	AE	1287	0	1398	154	0
9	AF	1950	0	2093	140	0
10	AG	1881	0	2018	121	0
11	AH	1536	0	1611	117	0
12	AI	1605	0	1652	69	0
13	AJ	1363	0	1398	107	0
14	AL	1617	0	1725	102	0
15	AM	1139	0	1204	130	0
16	AN	1709	0	1761	92	0
17	AO	1607	0	1745	124	0
18	AP	1234	0	1263	72	0
19	AQ	1494	0	1612	96	0
20	AR	1526	0	1682	86	0
21	AS	1439	0	1472	84	0
22	AT	1298	0	1366	106	0
23	AU	827	0	852	27	0
24	AV	964	0	1026	43	0
25	AW	529	0	541	32	0
26	AX	976	0	1053	43	0
27	AY	1065	0	1145	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AZ	1115	0	1194	74	0
29	Aa	1162	0	1213	0	0
30	Ab	560	0	590	0	0
31	Ac	802	0	845	0	0
32	Ad	905	0	947	0	0
33	Ae	1053	0	1144	0	0
34	Af	866	0	904	0	0
35	Ag	907	0	1002	0	0
36	Ah	1015	0	1148	0	0
37	Ai	783	0	862	0	0
38	Aj	690	0	719	0	0
39	Ak	569	0	637	0	0
40	Al	444	0	483	0	0
41	Am	429	0	466	0	0
42	An	240	0	287	0	0
43	Ao	871	0	940	0	0
44	Ap	708	0	760	0	0
45	At	1043	0	1120	0	0
46	Au	1622	0	1563	0	0
47	BA	1619	0	816	332	0
48	BB	4846	0	4954	1412	0
49	BC	5574	0	2803	272	0
50	C1	37159	0	18772	3847	0
51	CA	1719	0	1717	129	0
52	CB	1729	0	1803	143	0
53	CC	1724	0	1808	93	0
54	CD	1646	0	1737	110	0
55	CE	2031	0	2138	116	0
56	CF	1486	0	1543	102	0
57	CG	1884	0	2044	151	0
58	CH	1535	0	1632	129	0
59	CI	1695	0	1774	135	0
60	CJ	1495	0	1615	91	0
61	CK	791	0	811	48	0
62	CL	1199	0	1269	67	0
63	CM	931	0	961	40	0
64	CN	1207	0	1294	77	0
65	CO	1023	0	1050	57	0
66	CP	981	0	1026	56	0
67	CQ	1108	0	1172	93	0
68	CR	893	0	946	57	0
69	CS	1172	0	1229	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	CT	1112	0	1146	115	0
71	CU	803	0	866	68	0
72	CV	636	0	637	43	0
73	CW	1033	0	1080	64	0
74	CX	1046	0	1110	86	0
75	CY	1002	0	1075	64	0
76	CZ	605	0	665	69	0
77	Ca	767	0	816	0	0
78	Cb	625	0	642	0	0
79	Cc	490	0	519	0	0
80	Cd	444	0	442	0	0
81	Ce	412	0	463	0	0
82	Cf	497	0	497	0	0
83	Cg	2440	0	2396	0	0
84	BB	32	0	13	10	0
85	BB	1	0	0	0	0
All	All	223911	0	165616	16484	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 46.

The worst 5 of 16484 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)
48:BB:1116:ARG:HB3	50:C1:488:U:C6	1.22	1.65
47:BA:75:C:H5	48:BB:1316:PHE:CD2	1.14	1.64
47:BA:34:G:H4'	50:C1:1248:U:C1'	1.19	1.63
48:BB:1116:ARG:HB3	50:C1:488:U:C5	1.20	1.60
47:BA:75:C:C5	48:BB:1316:PHE:CD2	1.87	1.60

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AA	245/257 (95%)	236 (96%)	6 (2%)	3 (1%)	16	61
5	AB	394/403 (98%)	369 (94%)	11 (3%)	14 (4%)	4	38
6	AC	362/427 (85%)	338 (93%)	9 (2%)	15 (4%)	3	35
7	AD	288/297 (97%)	279 (97%)	4 (1%)	5 (2%)	11	55
8	AE	156/158 (99%)	141 (90%)	8 (5%)	7 (4%)	3	33
9	AF	232/248 (94%)	225 (97%)	3 (1%)	4 (2%)	11	55
10	AG	233/266 (88%)	216 (93%)	8 (3%)	9 (4%)	4	36
11	AH	190/192 (99%)	184 (97%)	3 (2%)	3 (2%)	12	56
12	AI	192/214 (90%)	187 (97%)	2 (1%)	3 (2%)	12	56
13	AJ	168/178 (94%)	153 (91%)	3 (2%)	12 (7%)	1	22
14	AL	198/211 (94%)	178 (90%)	9 (4%)	11 (6%)	2	28
15	AM	138/215 (64%)	132 (96%)	4 (3%)	2 (1%)	14	58
16	AN	202/204 (99%)	193 (96%)	6 (3%)	3 (2%)	13	57
17	AO	194/203 (96%)	187 (96%)	4 (2%)	3 (2%)	13	57
18	AP	151/184 (82%)	141 (93%)	7 (5%)	3 (2%)	9	51
19	AQ	182/188 (97%)	169 (93%)	7 (4%)	6 (3%)	5	40
20	AR	180/196 (92%)	172 (96%)	3 (2%)	5 (3%)	6	44
21	AS	171/176 (97%)	158 (92%)	7 (4%)	6 (4%)	4	39
22	AT	157/160 (98%)	150 (96%)	4 (2%)	3 (2%)	10	52
23	AU	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
24	AV	126/140 (90%)	119 (94%)	5 (4%)	2 (2%)	12	56
25	AW	62/157 (40%)	61 (98%)	1 (2%)	0	100	100
26	AX	117/156 (75%)	113 (97%)	4 (3%)	0	100	100
27	AY	126/145 (87%)	119 (94%)	4 (3%)	3 (2%)	7	47
28	AZ	134/136 (98%)	125 (93%)	5 (4%)	4 (3%)	5	42
29	Aa	145/148 (98%)	134 (92%)	6 (4%)	5 (3%)	5	40
30	Ab	67/159 (42%)	60 (90%)	3 (4%)	4 (6%)	2	26
31	Ac	102/115 (89%)	99 (97%)	1 (1%)	2 (2%)	9	51
32	Ad	107/125 (86%)	103 (96%)	3 (3%)	1 (1%)	21	67
33	Ae	126/135 (93%)	117 (93%)	6 (5%)	3 (2%)	7	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Af	105/110 (96%)	96 (91%)	4 (4%)	5 (5%)	3	32
35	Ag	113/117 (97%)	103 (91%)	6 (5%)	4 (4%)	4	39
36	Ah	120/123 (98%)	112 (93%)	5 (4%)	3 (2%)	7	46
37	Ai	95/105 (90%)	85 (90%)	4 (4%)	6 (6%)	2	25
38	Aj	83/97 (86%)	75 (90%)	6 (7%)	2 (2%)	7	47
39	Ak	67/70 (96%)	64 (96%)	2 (3%)	1 (2%)	13	57
40	Al	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	9	50
41	Am	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	9	51
42	An	23/25 (92%)	23 (100%)	0	0	100	100
43	Ao	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	10	52
44	Ap	89/92 (97%)	83 (93%)	3 (3%)	3 (3%)	5	40
45	At	128/137 (93%)	112 (88%)	9 (7%)	7 (6%)	2	29
46	Au	208/210 (99%)	199 (96%)	6 (3%)	3 (1%)	14	58
48	BB	605/627 (96%)	523 (86%)	51 (8%)	31 (5%)	2	30
51	CA	216/295 (73%)	209 (97%)	5 (2%)	2 (1%)	21	67
52	CB	211/264 (80%)	176 (83%)	18 (8%)	17 (8%)	1	19
53	CC	220/293 (75%)	213 (97%)	2 (1%)	5 (2%)	8	48
54	CD	210/243 (86%)	201 (96%)	4 (2%)	5 (2%)	7	47
55	CE	255/263 (97%)	237 (93%)	13 (5%)	5 (2%)	9	51
56	CF	186/204 (91%)	163 (88%)	13 (7%)	10 (5%)	2	29
57	CG	230/249 (92%)	216 (94%)	5 (2%)	9 (4%)	4	36
58	CH	189/194 (97%)	178 (94%)	7 (4%)	4 (2%)	9	50
59	CI	205/208 (99%)	184 (90%)	14 (7%)	7 (3%)	5	40
60	CJ	177/194 (91%)	169 (96%)	5 (3%)	3 (2%)	11	55
61	CK	92/165 (56%)	84 (91%)	1 (1%)	7 (8%)	1	20
62	CL	144/158 (91%)	133 (92%)	5 (4%)	6 (4%)	3	34
63	CM	118/132 (89%)	111 (94%)	1 (1%)	6 (5%)	2	30
64	CN	148/151 (98%)	138 (93%)	5 (3%)	5 (3%)	5	40
65	CO	135/151 (89%)	129 (96%)	3 (2%)	3 (2%)	8	49
66	CP	116/145 (80%)	106 (91%)	5 (4%)	5 (4%)	3	34
67	CQ	137/146 (94%)	129 (94%)	6 (4%)	2 (2%)	13	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	CR	105/135 (78%)	99 (94%)	4 (4%)	2 (2%)	10	52
69	CS	140/152 (92%)	125 (89%)	7 (5%)	8 (6%)	2	28
70	CT	141/145 (97%)	135 (96%)	4 (3%)	2 (1%)	14	58
71	CU	99/119 (83%)	95 (96%)	3 (3%)	1 (1%)	19	65
72	CV	81/83 (98%)	78 (96%)	1 (1%)	2 (2%)	7	46
73	CW	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	12	56
74	CX	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	2	29
75	CY	120/133 (90%)	114 (95%)	2 (2%)	4 (3%)	5	40
76	CZ	74/125 (59%)	71 (96%)	0	3 (4%)	3	35
77	Ca	94/115 (82%)	85 (90%)	5 (5%)	4 (4%)	3	34
78	Cb	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
79	Cc	60/69 (87%)	57 (95%)	1 (2%)	2 (3%)	5	40
80	Cd	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
81	Ce	49/59 (83%)	43 (88%)	5 (10%)	1 (2%)	9	51
82	Cf	59/156 (38%)	53 (90%)	6 (10%)	0	100	100
83	Cg	312/317 (98%)	291 (93%)	14 (4%)	7 (2%)	8	49
All	All	11794/13395 (88%)	10996 (93%)	442 (4%)	356 (3%)	9	42

5 of 356 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AA	144	LYS
4	AA	196	TRP
5	AB	4	ARG
5	AB	5	LYS
5	AB	157	CYS

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	
4	AA	189/199 (95%)	185 (98%)	4 (2%)	61	84
5	AB	344/349 (99%)	326 (95%)	18 (5%)	29	65
6	AC	302/348 (87%)	284 (94%)	18 (6%)	24	60
7	AD	244/250 (98%)	237 (97%)	7 (3%)	50	78
8	AE	143/143 (100%)	135 (94%)	8 (6%)	26	62
9	AF	203/215 (94%)	196 (97%)	7 (3%)	44	75
10	AG	199/223 (89%)	192 (96%)	7 (4%)	43	74
11	AH	171/171 (100%)	164 (96%)	7 (4%)	37	71
12	AI	170/181 (94%)	161 (95%)	9 (5%)	28	64
13	AJ	143/149 (96%)	137 (96%)	6 (4%)	36	70
14	AL	167/177 (94%)	156 (93%)	11 (7%)	21	57
15	AM	118/161 (73%)	114 (97%)	4 (3%)	44	75
16	AN	172/172 (100%)	170 (99%)	2 (1%)	78	90
17	AO	168/174 (97%)	166 (99%)	2 (1%)	78	90
18	AP	133/163 (82%)	126 (95%)	7 (5%)	28	64
19	AQ	162/165 (98%)	157 (97%)	5 (3%)	47	77
20	AR	161/175 (92%)	149 (92%)	12 (8%)	17	53
21	AS	155/157 (99%)	148 (96%)	7 (4%)	34	69
22	AT	139/140 (99%)	134 (96%)	5 (4%)	42	74
23	AU	91/115 (79%)	88 (97%)	3 (3%)	45	76
24	AV	100/107 (94%)	99 (99%)	1 (1%)	82	92
25	AW	55/126 (44%)	52 (94%)	3 (6%)	27	63
26	AX	107/133 (80%)	105 (98%)	2 (2%)	65	86
27	AY	119/135 (88%)	115 (97%)	4 (3%)	44	75
28	AZ	118/118 (100%)	112 (95%)	6 (5%)	29	66
29	Aa	120/121 (99%)	116 (97%)	4 (3%)	45	76
30	Ab	58/126 (46%)	57 (98%)	1 (2%)	68	87
31	Ac	88/97 (91%)	87 (99%)	1 (1%)	80	91
32	Ad	100/110 (91%)	96 (96%)	4 (4%)	38	71
33	Ae	115/121 (95%)	112 (97%)	3 (3%)	54	80
34	Af	87/89 (98%)	79 (91%)	8 (9%)	11	43
35	Ag	98/100 (98%)	88 (90%)	10 (10%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Ah	109/110 (99%)	106 (97%)	3 (3%)	51	78
37	Ai	82/89 (92%)	76 (93%)	6 (7%)	17	54
38	Aj	71/80 (89%)	69 (97%)	2 (3%)	51	78
39	Ak	64/65 (98%)	64 (100%)	0	100	100
40	Al	47/48 (98%)	46 (98%)	1 (2%)	61	84
41	Am	48/116 (41%)	45 (94%)	3 (6%)	22	59
42	An	24/24 (100%)	24 (100%)	0	100	100
43	Ao	94/94 (100%)	89 (95%)	5 (5%)	28	64
44	Ap	74/75 (99%)	72 (97%)	2 (3%)	52	79
45	At	113/121 (93%)	106 (94%)	7 (6%)	23	60
46	Au	177/177 (100%)	163 (92%)	14 (8%)	15	51
48	BB	540/552 (98%)	519 (96%)	21 (4%)	39	72
51	CA	181/243 (74%)	176 (97%)	5 (3%)	51	78
52	CB	194/231 (84%)	183 (94%)	11 (6%)	25	62
53	CC	188/225 (84%)	181 (96%)	7 (4%)	41	73
54	CD	175/202 (87%)	166 (95%)	9 (5%)	29	66
55	CE	220/225 (98%)	208 (94%)	12 (6%)	27	63
56	CF	158/170 (93%)	151 (96%)	7 (4%)	35	69
57	CG	202/218 (93%)	195 (96%)	7 (4%)	43	74
58	CH	171/174 (98%)	167 (98%)	4 (2%)	58	83
59	CI	179/180 (99%)	167 (93%)	12 (7%)	20	57
60	CJ	160/168 (95%)	150 (94%)	10 (6%)	22	59
61	CK	85/136 (62%)	82 (96%)	3 (4%)	43	74
62	CL	133/142 (94%)	131 (98%)	2 (2%)	72	88
63	CM	102/108 (94%)	96 (94%)	6 (6%)	24	61
64	CN	130/131 (99%)	128 (98%)	2 (2%)	72	88
65	CO	107/119 (90%)	100 (94%)	7 (6%)	21	58
66	CP	107/130 (82%)	102 (95%)	5 (5%)	32	68
67	CQ	115/121 (95%)	111 (96%)	4 (4%)	43	74
68	CR	99/122 (81%)	94 (95%)	5 (5%)	29	66
69	CS	123/132 (93%)	114 (93%)	9 (7%)	17	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	CT	113/115 (98%)	106 (94%)	7 (6%)	23	60
71	CU	93/107 (87%)	89 (96%)	4 (4%)	35	70
72	CV	67/67 (100%)	66 (98%)	1 (2%)	72	88
73	CW	112/113 (99%)	107 (96%)	5 (4%)	34	69
74	CX	108/115 (94%)	103 (95%)	5 (5%)	33	68
75	CY	107/115 (93%)	101 (94%)	6 (6%)	26	62
76	CZ	67/103 (65%)	63 (94%)	4 (6%)	24	60
77	Ca	83/98 (85%)	76 (92%)	7 (8%)	14	48
78	Cb	72/76 (95%)	68 (94%)	4 (6%)	26	62
79	Cc	55/62 (89%)	52 (94%)	3 (6%)	27	63
80	Cd	47/49 (96%)	43 (92%)	4 (8%)	13	48
81	Ce	42/48 (88%)	40 (95%)	2 (5%)	31	67
82	Cf	54/140 (39%)	51 (94%)	3 (6%)	26	62
83	Cg	272/275 (99%)	260 (96%)	12 (4%)	35	69
All	All	10303/11421 (90%)	9849 (96%)	454 (4%)	39	69

5 of 454 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	Aj	19	CYS
48	BB	1188	ILE
77	Ca	21	ILE
43	Ao	32	SER
46	Au	60	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 228 such sidechains are listed below:

Mol	Chain	Res	Type
34	Af	21	GLN
48	BB	928	ASN
74	CX	97	ASN
35	Ag	100	GLN
41	Am	90	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	3604/5025 (71%)	2040 (56%)	324 (8%)
2	A3	156/194 (80%)	82 (52%)	6 (3%)
3	A4	118/121 (97%)	68 (57%)	9 (7%)
47	BA	75/76 (98%)	14 (18%)	1 (1%)
49	BC	259/504 (51%)	135 (52%)	40 (15%)
50	C1	1738/1869 (92%)	1038 (59%)	152 (8%)
All	All	5950/7789 (76%)	3377 (56%)	532 (8%)

5 of 3377 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	G
1	A2	3	C
1	A2	5	A
1	A2	6	C
1	A2	8	U

5 of 532 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	4044	G
1	A2	4717	U
50	C1	1411	G
1	A2	4105	C
1	A2	4454	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
84	GNP	BB	2435	85	29,34,34	2.75	9 (31%)	28,54,54	1.83	6 (21%)

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
84	GNP	BB	2435	85	-	0/16/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	BB	2435	GNP	C4-N9	-9.55	1.35	1.47
84	BB	2435	GNP	C5-C6	-4.96	1.44	1.53
84	BB	2435	GNP	C8-N9	-3.48	1.36	1.47
84	BB	2435	GNP	C2'-C1'	-3.01	1.44	1.53
84	BB	2435	GNP	PB-O3A	-2.73	1.55	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	BB	2435	GNP	O6-C6-N1	-2.76	119.18	122.80
84	BB	2435	GNP	O2G-PG-O1G	2.26	119.53	113.58
84	BB	2435	GNP	O2A-PA-O3A	2.41	115.58	105.27
84	BB	2435	GNP	O3A-PB-N3B	2.42	112.73	106.07
84	BB	2435	GNP	O6-C6-C5	3.84	127.04	119.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	BB	2435	GNP	10	0

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
20	AR	1
1	A2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AR	182:GLU	C	183:GLU	N	5.96
1	A2	4036:U	O3'	4037:U	P	4.57