



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:21 pm GMT

PDB ID : 3JCS
EMDB ID: : EMD-6583
Title : 2.8 Angstrom cryo-EM structure of the large ribosomal subunit from the eukaryotic parasite Leishmania
Authors : Shalev-Benami, M.; Zhang, Y.; Matzov, D.; Halfon, Y.; Zackay, A.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on : 2016-01-21
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

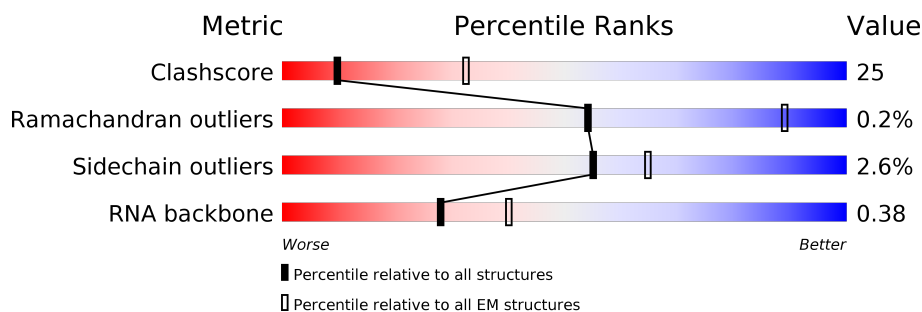
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.







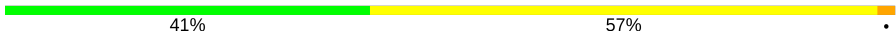
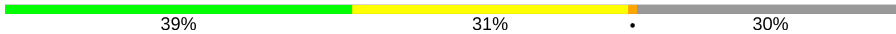
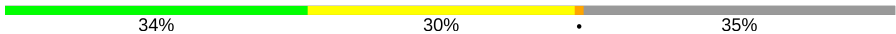
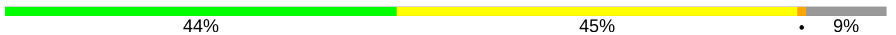
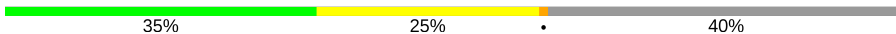

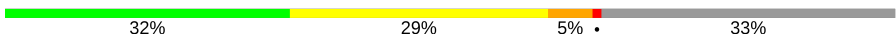





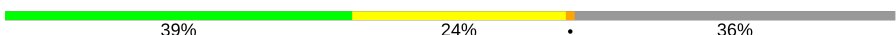








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	1	1782	26% 39% 22% • 13%
2	2	1527	21% 34% 18% 27%
3	3	213	23% 39% 24% 14%
4	4	183	28% 36% 18% 19%
5	5	133	17% 28% 14% • 40%
6	6	76	• 20% 54% • 20%
7	7	171	28% 45% 16% • 10%
8	8	121	13% 47% 38% •

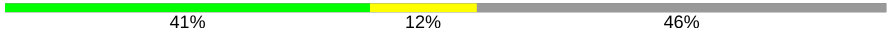














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Mol	Chain	Length	Quality of chain
9	A	260	
10	B	419	
11	C	373	
12	D	188	
13	E	190	
14	F	195	
15	G	348	
16	H	222	
17	I	220	
18	J	139	
19	K	233	
20	L	145	
21	M	204	
22	N	213	
23	O	305	
24	P	198	
25	Q	245	
26	R	179	
27	S	159	
28	T	166	
29	U	129	
30	V	145	
31	W	143	
32	X	124	
33	Y	134	

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Mol	Chain	Length	Quality of chain
34	Z	147	
35	a	127	
36	b	70	
37	c	252	
38	d	104	
39	e	183	
40	f	133	
41	g	144	
42	h	168	
43	i	105	
44	j	83	
45	k	83	
46	l	51	
47	m	92	
48	n	106	

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
1	OMU	1	36	-	-	X	-
1	OMG	1	959	-	-	X	-
2	OMU	2	1078	-	-	X	-
2	OMG	2	1079	-	-	X	-
2	OMG	2	1254	-	-	X	-
2	OMC	2	1318	-	-	X	-
2	OMC	2	443	-	-	X	-
2	A2M	2	527	-	-	X	-
2	OMG	2	71	-	-	X	-
7	OMU	7	7	-	-	X	-

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 117257 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 26S alpha ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1554	Total	C	N	O	P	0	0
			33313	14886	6081	10792	1554		

- Molecule 2 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1119	Total	C	N	O	P	0	0
			23926	10702	4308	7797	1119		

- Molecule 3 is a RNA chain called 26S gamma ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	184	Total	C	N	O	P	0	0
			3893	1740	662	1307	184		

- Molecule 4 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	149	Total	C	N	O	P	0	0
			3177	1418	570	1040	149		

- Molecule 5 is a RNA chain called 26S epsilon ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	80	Total	C	N	O	P	0	0
			1708	763	310	555	80		

- Molecule 6 is a RNA chain called 26S zeta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	61	Total	C	N	O	P	0	0
			1288	577	225	425	61		

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	154	Total	C	N	O	P	0	0
			3280	1469	584	1074	153		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	119	Total	C	N	O	P	0	0
			2531	1132	450	830	119		

- Molecule 9 is a protein called ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	245	Total	C	N	O	S	2	0
			1859	1158	384	307	10		

- Molecule 10 is a protein called ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	396	Total	C	N	O	S	2	0
			3020	1908	592	508	12		

- Molecule 11 is a protein called ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	301	Total	C	N	O	S	1	0
			2237	1413	428	384	12		

- Molecule 12 is a protein called ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	D	161	Total	C	N	O	0	0
			799	476	161	162		

- Molecule 13 is a protein called ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	190	Total	C	N	O	S	0	0
			1509	953	276	272	8		

- Molecule 14 is a protein called ribosomal protein L6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	137	Total	C	N	O	S	1	0
			1002	641	192	167	2		

- Molecule 15 is a protein called ribosomal protein L8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	226	Total	C	N	O	S	1	0
			1772	1113	353	299	7		

- Molecule 16 is a protein called ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	202	Total	C	N	O	S	0	0
			1596	1019	307	263	7		

- Molecule 17 is a protein called ribosomal protein L13e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	132	Total	C	N	O	S	0	0
			1061	666	221	169	5		

- Molecule 18 is a protein called ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	128	Total	C	N	O	S	0	0
			924	588	171	160	5		

- Molecule 19 is a protein called ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	156	Total	C	N	O	S	0	0
			1061	661	212	184	4		

- Molecule 20 is a protein called ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	144	Total	C	N	O	S	0	0
			1096	691	223	177	5		

- Molecule 21 is a protein called ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	203	Total	C	N	O	S	0	0
			1714	1080	362	264	8		

- Molecule 22 is a protein called ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	213	Total	C	N	O	S	0	0
			1714	1077	340	281	16		

- Molecule 23 is a protein called ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	235	Total	C	N	O	S	0	0
			1557	986	300	268	3		

- Molecule 24 is a protein called ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	195	Total	C	N	O	S	1	0
			1494	942	299	247	6		

- Molecule 25 is a protein called ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	156	Total	C	N	O	S	0	0
			1162	730	243	186	3		

- Molecule 26 is a protein called ribosomal protein L20e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	131	Total	C	N	O	S	1	0
			1019	651	197	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	158	ILE	LEU	VARIANT	UNP E9BRT7

- Molecule 27 is a protein called ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	149	Total	C	N	O	S	2	0
			1112	704	218	187	3		

- Molecule 28 is a protein called ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	154	Total	C	N	O	S	2	0
			1221	763	241	206	11		

- Molecule 29 is a protein called ribosomal protein L22e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	100	Total	C	N	O		0	0
			541	331	101	109			

- Molecule 30 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	118	Total	C	N	O	S	0	0
			892	566	171	153	2		

- Molecule 31 is a protein called ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	117	Total	C	N	O	S	1	0
			896	562	187	144	3		

- Molecule 32 is a protein called ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	64	Total	C	N	O	S	0	0
			508	333	96	76	3		

- Molecule 33 is a protein called ribosomal protein L27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	132	Total	C	N	O		0	0
			914	589	174	151			

- Molecule 34 is a protein called ribosomal protein L28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	79	Total	C	N	O	S	0	0
			538	329	111	95	3		

- Molecule 35 is a protein called ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	124	Total	C	N	O	S	0	0
			982	613	203	163	3		

- Molecule 36 is a protein called ribosomal protein L29e.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	65	Total	C	N	O	S	0	0
			503	309	113	80	1		

- Molecule 37 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	222	Total	C	N	O	S	0	0
			1732	1105	327	289	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	49	ALA	GLY	VARIANT	UNP E9BI29

- Molecule 38 is a protein called ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	75	Total	C	N	O	S	0	0
			518	325	93	97	3		

- Molecule 39 is a protein called ribosomal protein L31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	112	Total	C	N	O	S	1	0
			824	531	155	136	2		

- Molecule 40 is a protein called ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	126	Total	C	N	O	S	0	0
			982	616	195	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	105	LYS	THR	VARIANT	UNP E9BFJ5

- Molecule 41 is a protein called ribosomal protein L33e.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	125	Total	C	N	O	S	0	0
			983	612	205	161	5		

- Molecule 42 is a protein called ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	109	Total	C	N	O	S	0	0
			856	529	182	140	5		

- Molecule 43 is a protein called ribosomal protein L36e.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	63	Total	C	N	O	S	1	0
			494	316	100	76	2		

- Molecule 44 is a protein called ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	78	Total	C	N	O	S	0	0
			639	385	149	99	6		

- Molecule 45 is a protein called ribosomal protein L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	58	Total	C	N	O	S	0	0
			373	234	71	66	2		

- Molecule 46 is a protein called ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	50	Total	C	N	O	S	1	0
			457	294	98	64	1		

- Molecule 47 is a protein called ribosomal protein L43e.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	90	Total	C	N	O	S	0	0
			668	414	135	113	6		

- Molecule 48 is a protein called ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	86	Total	C	N	O	S	0	0
			659	418	129	110	2		

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	g	1	Total	Mg	0
			1	1	
49	j	4	Total	Mg	0
			4	4	
49	l	51	Total	Mg	0
			51	51	
49	K	1	Total	Mg	0
			1	1	
49	h	1	Total	Mg	0
			1	1	
49	C	1	Total	Mg	0
			1	1	
49	V	1	Total	Mg	0
			1	1	
49	7	9	Total	Mg	0
			9	9	
49	a	1	Total	Mg	0
			1	1	
49	4	2	Total	Mg	0
			2	2	
49	5	4	Total	Mg	0
			4	4	
49	2	25	Total	Mg	0
			25	25	

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Mol	Chain	Residues	Atoms		AltConf
49	3	3	Total 3	Mg 3	0
49	f	2	Total 2	Mg 2	0
49	M	3	Total 3	Mg 3	0

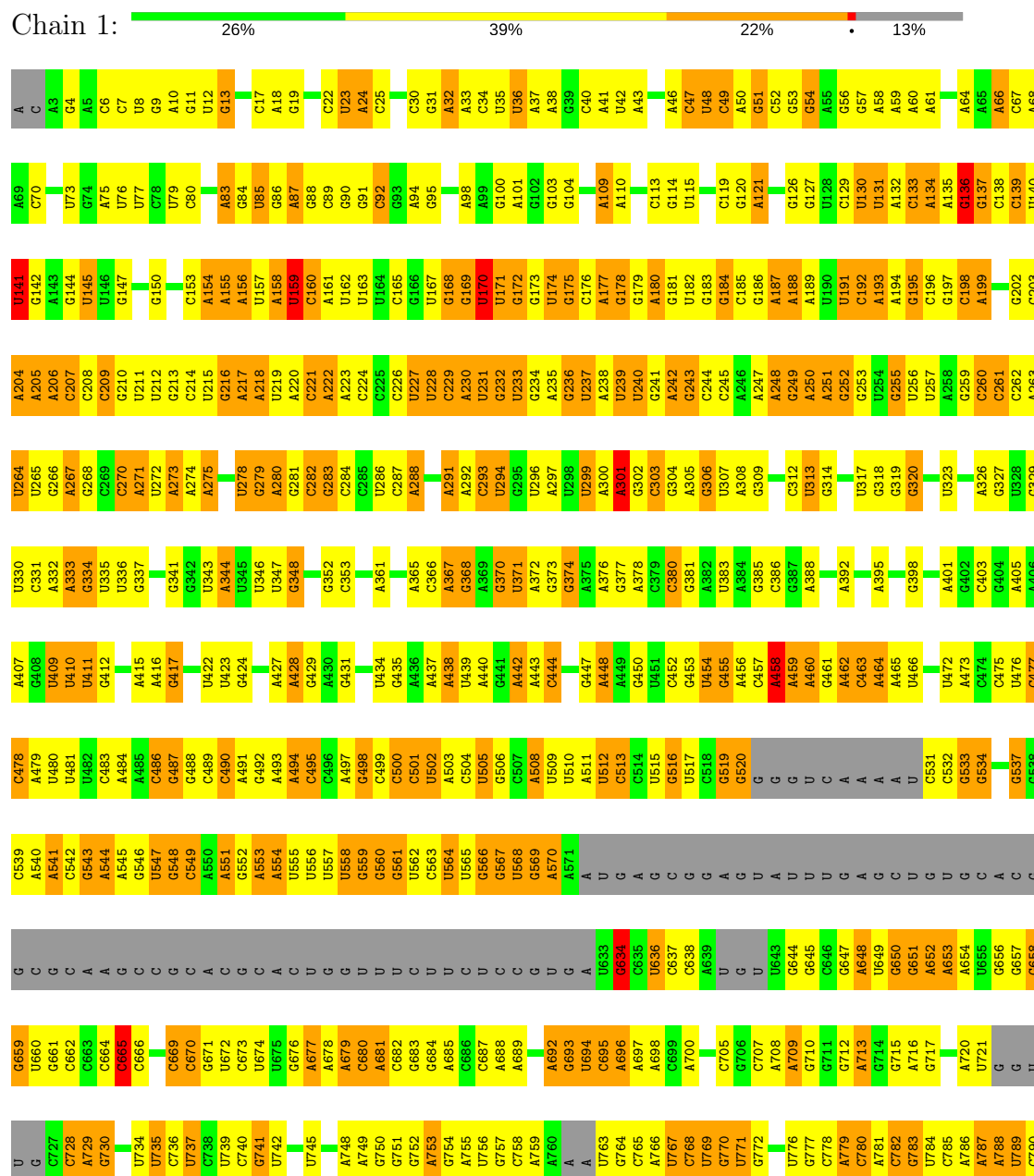
- Molecule 50 is water.

Mol	Chain	Residues	Atoms		AltConf
50	1	72	Total 72	O 72	0
50	2	40	Total 40	O 40	0
50	4	4	Total 4	O 4	0
50	5	4	Total 4	O 4	0
50	7	16	Total 16	O 16	0
50	8	1	Total 1	O 1	0
50	A	2	Total 2	O 2	0
50	G	1	Total 1	O 1	0
50	M	2	Total 2	O 2	0
50	i	1	Total 1	O 1	0
50	j	1	Total 1	O 1	0

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: 26S alpha ribosomal RNA

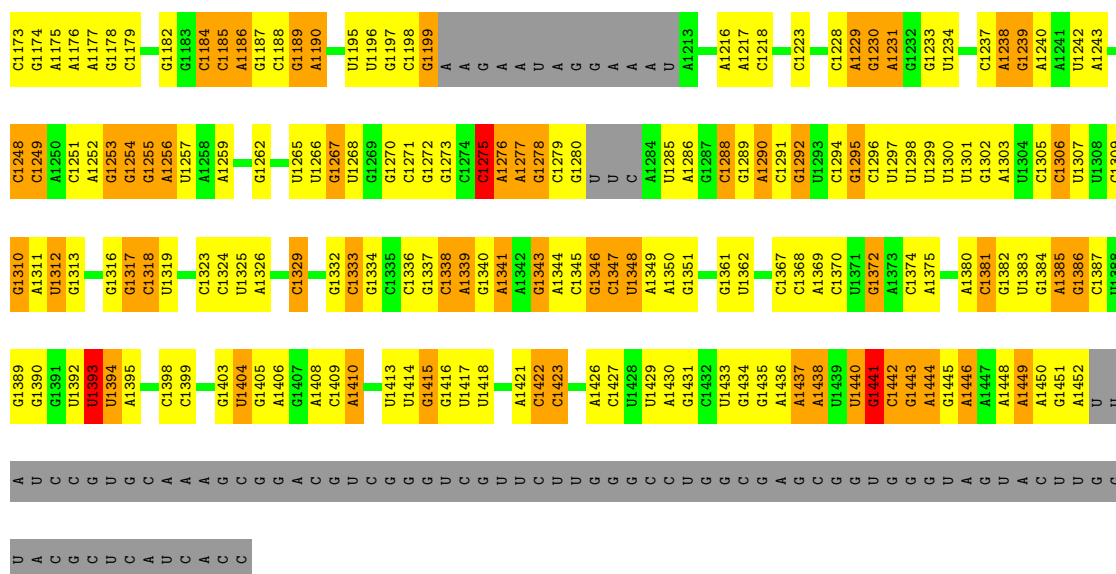


U1749	C1617	G1555	C1482	A1414	G	A1287	U1225	G	U1090	U1021	A933	C854	C791
G1750	U1618	G1556	G1483	A1415	U	G	G1228	U	A1091	G1025	A934	C855	G792
G1751	C1619	A1557	U1484	G1416	U	U	G1229	U	U1092	C1026	C939	G856	U793
G1752	G1620	G1558	A1485	G1417	U	U	C1230	G	U1093	U1027	U940	A857	U794
A	U1621	U	U1489	C1418	G	G	G1231	G	C1094	A1028	U845	G860	U795
U1754	A1622	A	U1490	C1419	G	A	A1234	A	U1095	G1029	U846	G867	U796
U1755	U1623	U	A1491	G1420	C	C	A1235	C	C1096	U1030	G946	A868	U797
A1756	G1626	U	U1492	G1421	C	U	A1236	C	A	A1031	A947	A	U798
U1757	U1627	U	G1493	A1422	G	G	A1237	G	A	U1032	U799	U800	U799
U1758	G1628	C	U1494	A1423	U	U	U1238	U	U1101	G951	G951	G801	G801
U1759	U1629	U	C1495	A1424	G	G	U1239	G	U1102	G952	U872	U872	C802
U1760	G1630	C	A	C	G	G	U1240	G	U1103	U954	C874	C874	A806
C1761	G1631	A	A	A	C	C	U1241	C	A1104	U955	C875	C875	C807
U1762	U1632	A	U1498	A	C	C	A1242	C	A1105	U956	C876	C876	A808
U1763	U1633	C	A1504	A	A	A	G1243	U	U1108	C957	G877	G877	C809
A1764	G1634	U	U1505	C	U	U	G1244	G	U1109	G958	A878	A878	C810
A1765	U1635	U	U1506	U1432	G	G	U1245	G	U1110	G959	A882	A882	C811
A1766	C1640	G	U1507	U1433	A	A	G1246	A	U1111	G960	G883	G883	C814
A1767	U1644	A	G1508	U1434	U	U	U1247	U	C1112	U1046	G884	G884	G815
G1768	A1648	U	U1509	U1435	G	G	C1248	G	A1113	C962	G887	G887	G816
A1769	A1649	C	C1510	G1436	U	U	U1249	U	A1114	A1048	A888	A888	C817
U1770	U1650	U	C1511	G1437	U	U	U1250	C	C1115	A1049	A889	A889	C818
U1771	G1651	U	C1512	G1438	G	G	U	C	C1116	G1050	A890	A890	C819
U1772	U1578	U	U1518	A1439	G	G	C	C	A1117	C1051	G957	G957	U820
U1773	G1581	U	G1582	A1440	C	C	U1253	C	A1118	A	C892	C892	C821
G1774	U1583	C	U1584	A1441	A	A	C1254	A	C1119	A1054	G893	G893	C822
U1777	C1576	U	U1585	U1442	U	U	G1255	C	C1120	U1055	G894	G894	G823
U1778	G1586	U	C1587	U1443	C	C	A1256	C	G	G1056	G895	G895	U824
U1779	U1587	U	U1588	U1444	C	C	U1257	C	U1122	A1057	Q	Q	G825
U1780	G1658	U	G1589	U1445	C	C	A1258	C	G1123	U1058	A	A	G826
G1781	U1659	U	U1590	U1446	U	U	C1259	C	C1124	A1059	A898	A898	G827
U	U1660	U	U1591	G1447	U	U	U1260	U	C1125	A1060	G976	G976	U828
U	U1661	U	U1592	C1448	A	A	U1261	A	U1126	G1061	A977	A977	U829
U	U1662	U	U1593	C1449	A	A	G1262	A	U1127	A1062	C901	C901	G830
U	U1663	U	U1594	U1450	G	G	A1263	C	A1128	G1063	C902	C902	G831
U	U1664	U	U1595	U1451	G	G	A1264	C	G1129	C1064	A903	A903	G832
U	U1665	U	G1532	U1452	A	A	A1265	C	C1130	C	G904	G904	U833
U	U1666	U	U1533	U1453	G	G	G1266	C	U1131	A	G905	G905	U834
U	U1667	U	U1534	G1458	U	U	G1267	C	A	G906	U906	U906	G835
U	U1668	U	U1535	U1461	U	U	G1268	C	A	G907	G907	G907	A836
U	U1669	U	U1536	G1461	U	U	U1269	C	C	U908	G908	G908	A837
U	U1670	U	G1537	U1462	U	U	A1270	C	U1073	A909	U922	U922	G838
U	A1671	U	U1538	U1463	U	U	G1271	C	U1074	G910	G923	G923	U839
U	A1672	U	U1539	G1466	A	A	U1272	C	U	G911	U924	U924	G840
U	A1673	U	U1540	G1467	A	A	G1273	C	U	C912	C912	C912	U841
U	G1674	U	C1541	C1468	C	C	G1274	C	U	G1000	G1001	G1001	U842
U	G1675	U	G1542	C1469	A	A	U1275	C	G1142	U925	U925	U925	G843
U	A1676	U	C1543	U1470	A	A	U1276	C	C1143	G1012	G1012	G1012	U844
U	U1677	U	A1544	G1471	C	C	G1277	C	C1144	A1081	U926	U926	U845
U	G1678	U	G1547	U1472	U	U	U1278	C	G1145	U1082	G1004	G1004	U846
U	G1679	U	U1548	G1475	C	C	A1279	C	A1146	A1083	C1010	C1010	U847
U	U1680	U	U1549	U1476	A	A	U1280	C	A1147	U1084	U927	U927	U848
U	G1681	U	C1550	U1477	C	C	A1281	C	G1148	C1085	A1013	A1013	U849
U	U1682	U	U1551	U1478	C	C	U	C	A1150	G1086	G1014	G1014	G850
U	G1683	U	U1552	A1479	A	A	G	C	A	A1087	U930	U930	G851
U	U	U	A1553	G1480	C	C	G1285	C	A	C1088	G931	G931	A852
U	G	U	C1554	U1413	C	C	C1286	C	A	C1089	C932	C932	C853

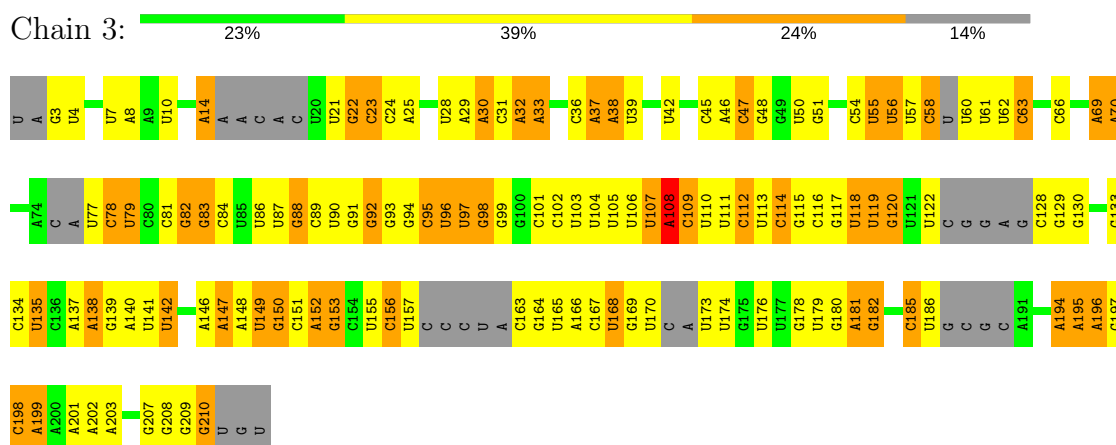
• Molecule 2: 26S delta ribosomal RNA

Chain 2: 21% 34% 18% 27%

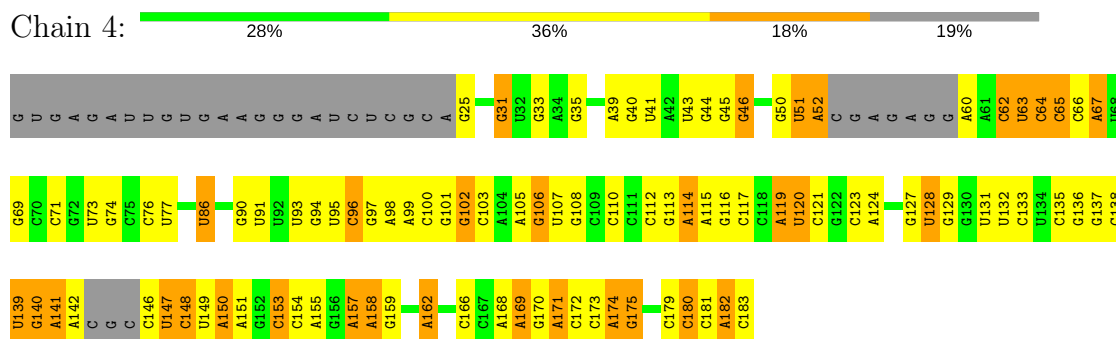
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	U78	G83	G89	G90	C91	A93	A94	A95	U96	A97	G98	A99	U100	G101	C102	U103	A104	U109	C110	G111	A112	C113	A114	G115	A116	A117	C118	C119	U120	A121	C122	G123	C125	U126	C127	A130	U131	G132	A133	C134	A135	A136	U	U	A	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U



• Molecule 3: 26S gamma ribosomal RNA

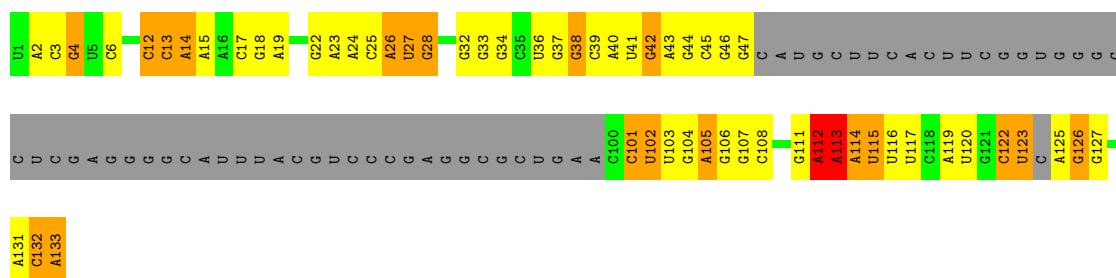


• Molecule 4: 26S delta ribosomal RNA



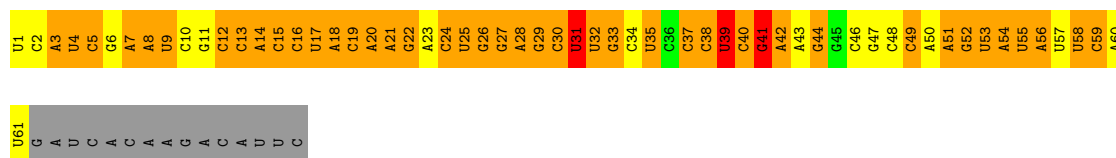
• Molecule 5: 26S epsilon ribosomal RNA





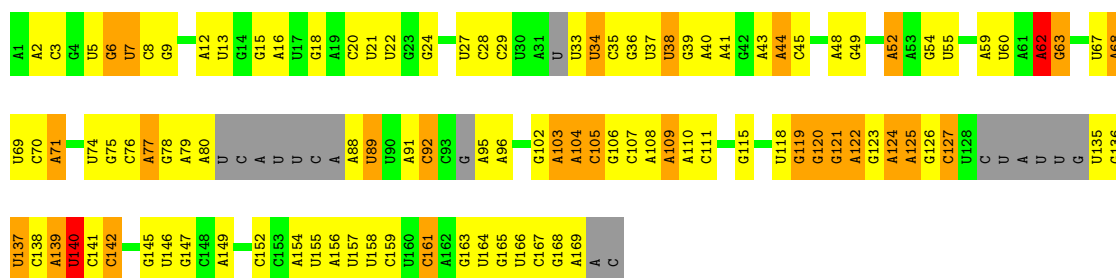
• Molecule 6: 26S zeta ribosomal RNA

Chain 6: 20% 54% 20%



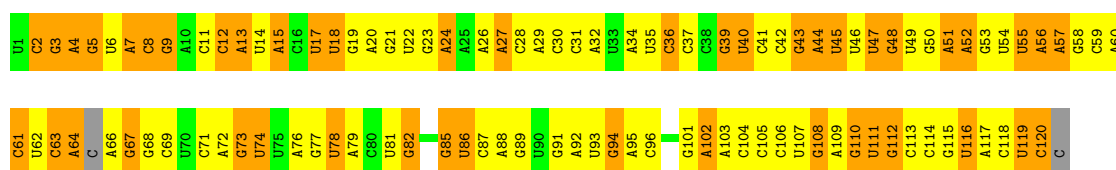
• Molecule 7: 5.8S ribosomal RNA

Chain 7: 28% 45% 16% 10%



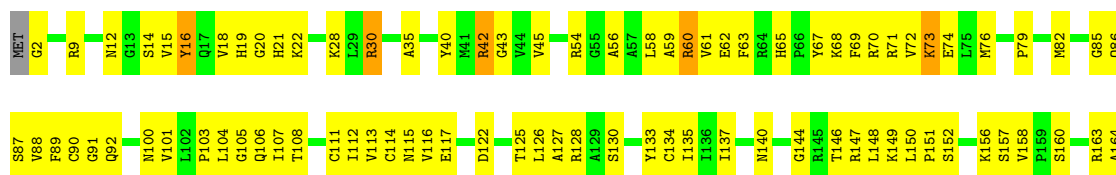
• Molecule 8: 5S ribosomal RNA

Chain 8: 13% 47% 38%



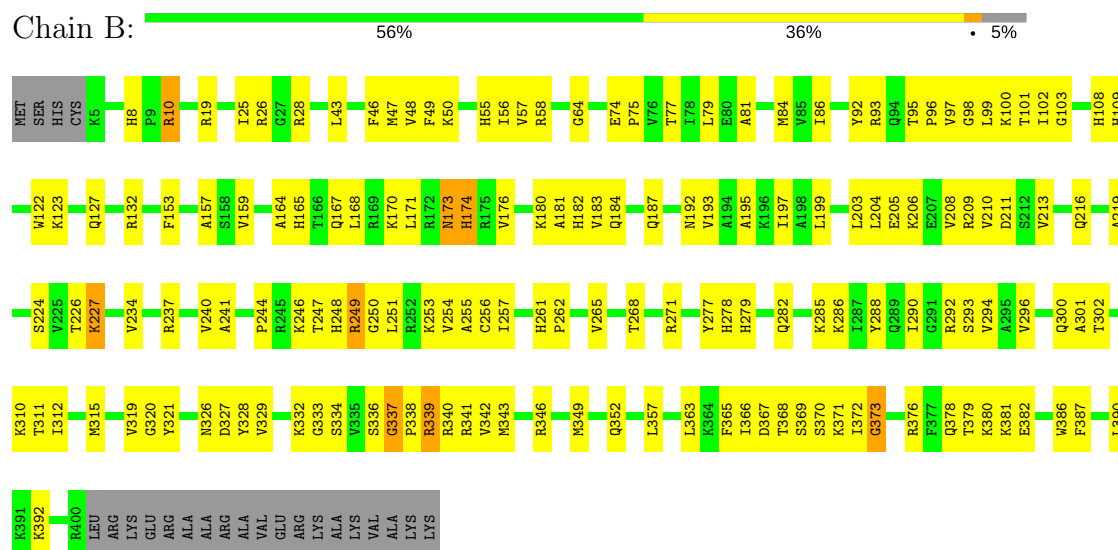
• Molecule 9: ribosomal protein L2

Chain A: 47% 45% 6%

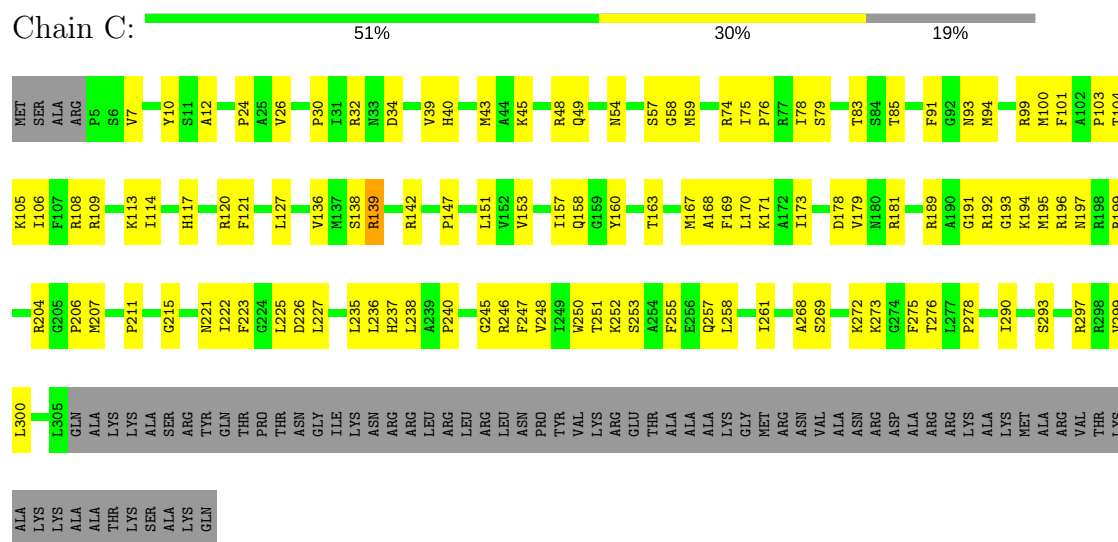




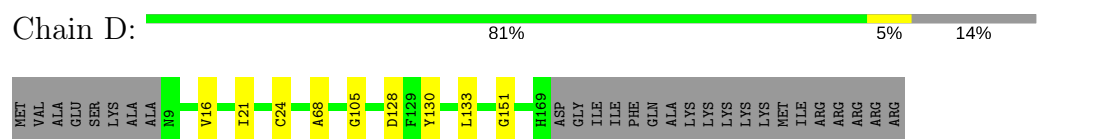
• Molecule 10: ribosomal protein L3



• Molecule 11: ribosomal protein L4

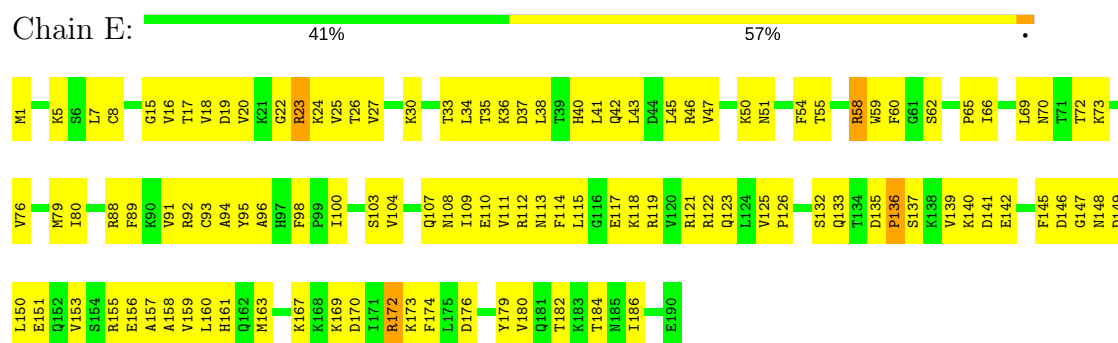


• Molecule 12: ribosomal protein L5



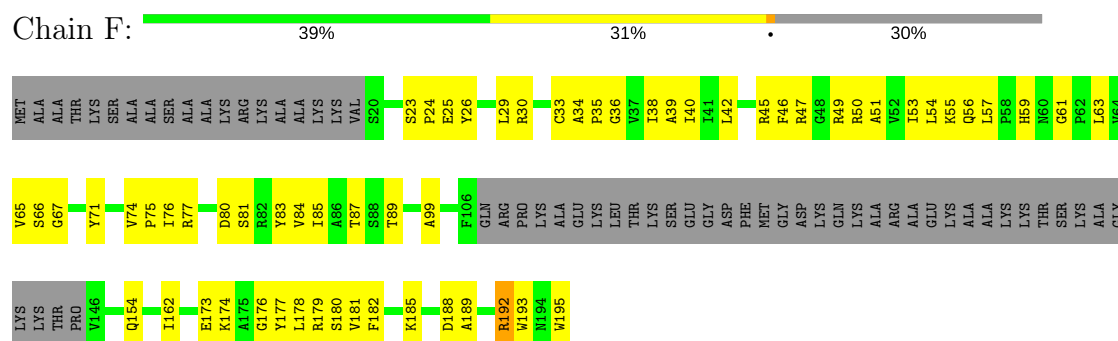
• Molecule 13: ribosomal protein L6

Chain E:



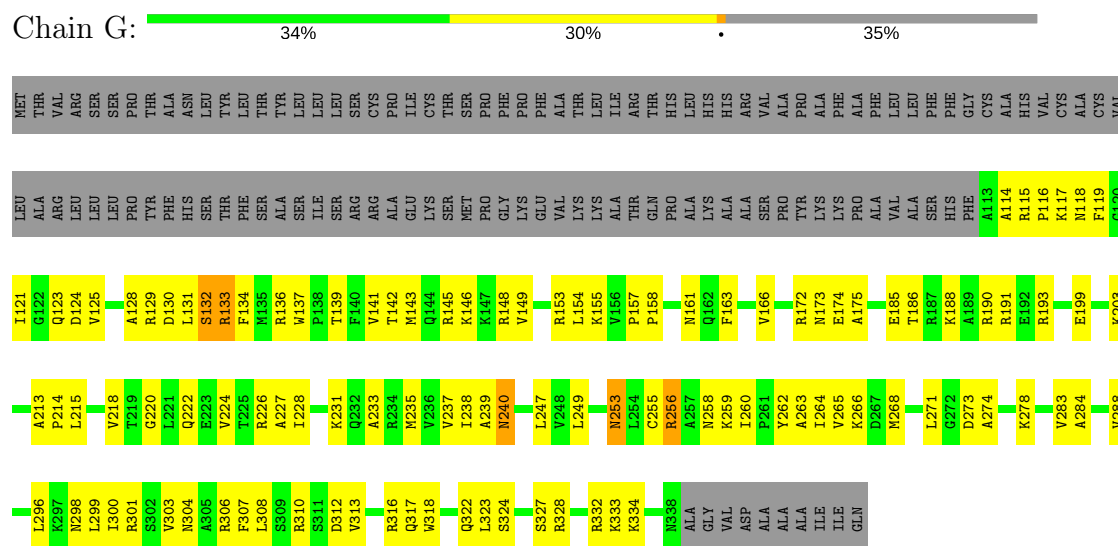
- Molecule 14: ribosomal protein L6e

Chain F:



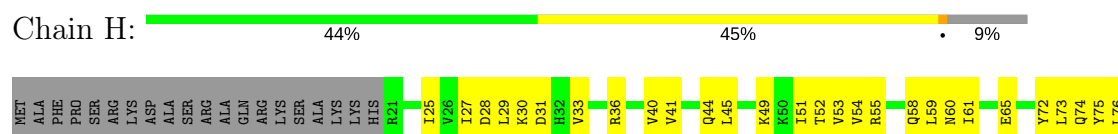
- Molecule 15: ribosomal protein L8e

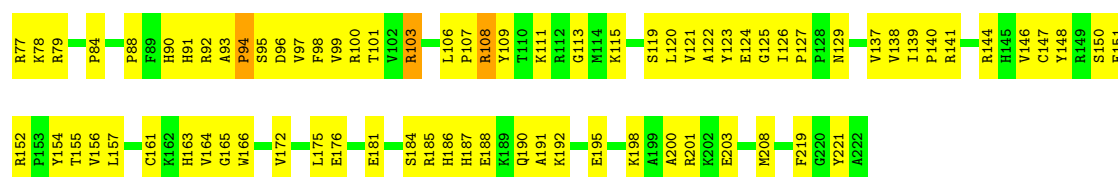
Chain G:



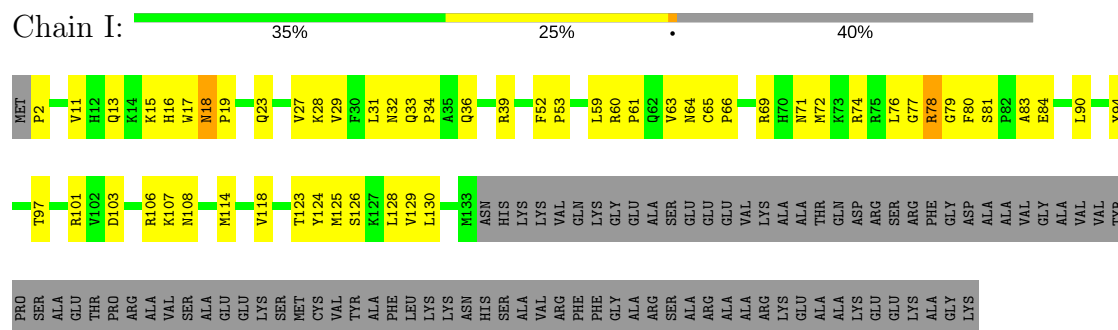
- Molecule 16: ribosomal protein L13

Chain H:

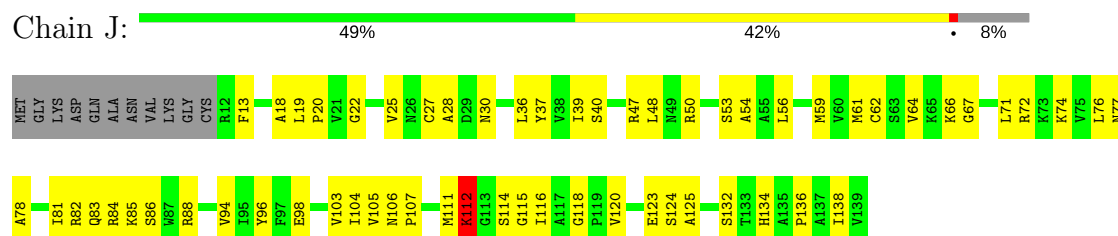




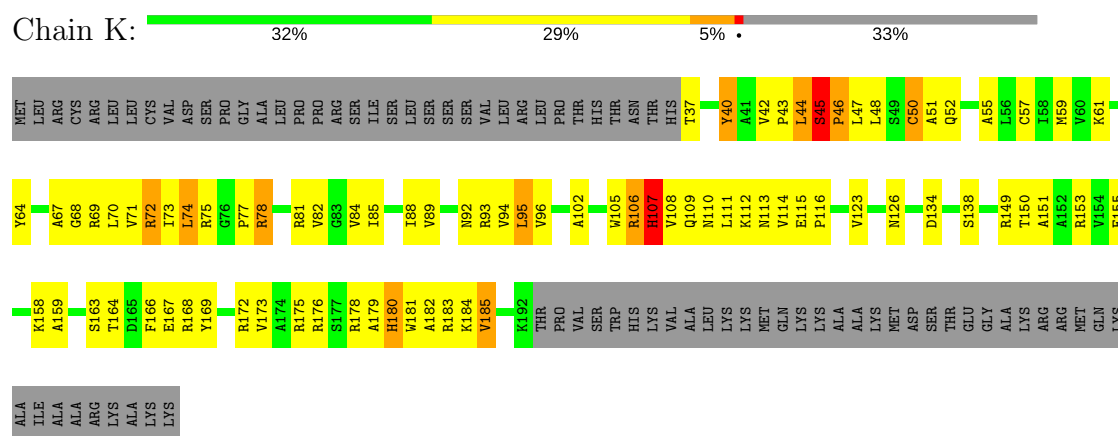
• Molecule 17: ribosomal protein L13e



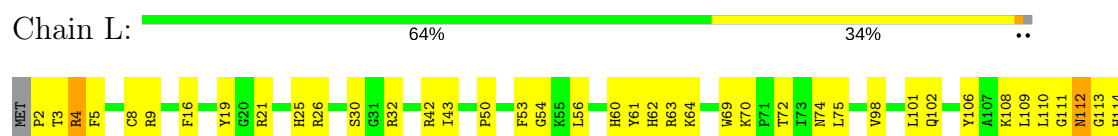
• Molecule 18: ribosomal protein L14



• Molecule 19: ribosomal protein L14e



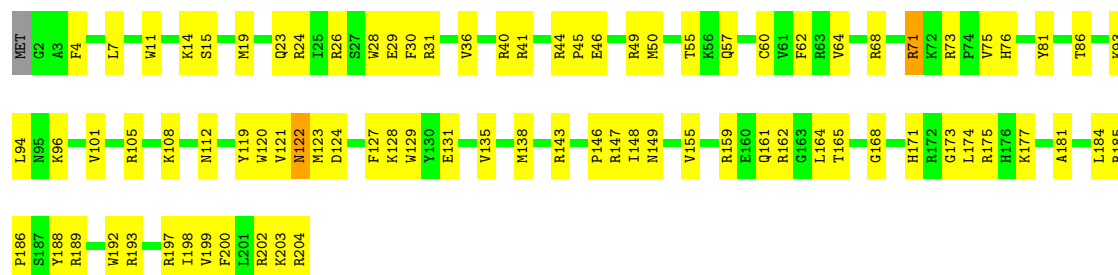
• Molecule 20: ribosomal protein L15





• Molecule 21: ribosomal protein L15e

Chain M: 58% 40%



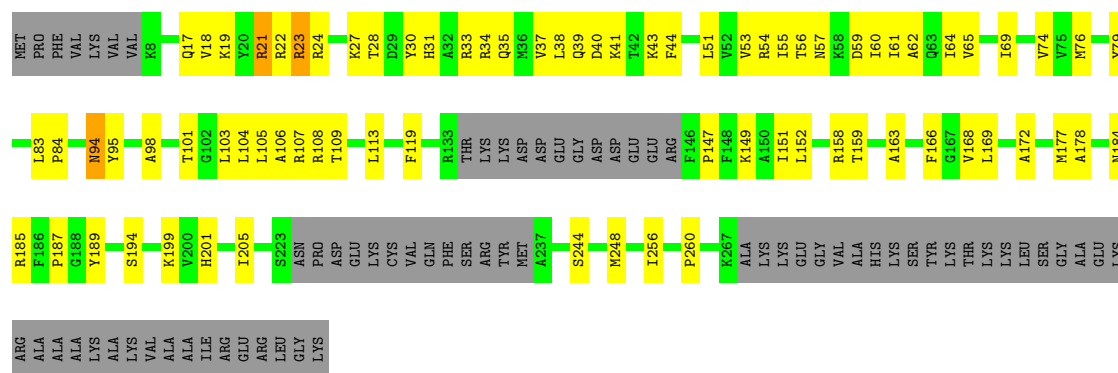
• Molecule 22: ribosomal protein L16

Chain N: 46% 53%



• Molecule 23: ribosomal protein L18

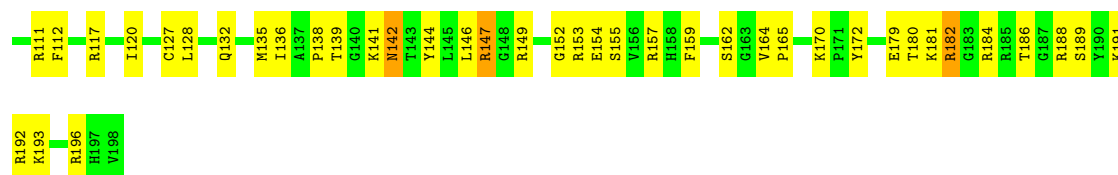
Chain O: 52% 24% 23%



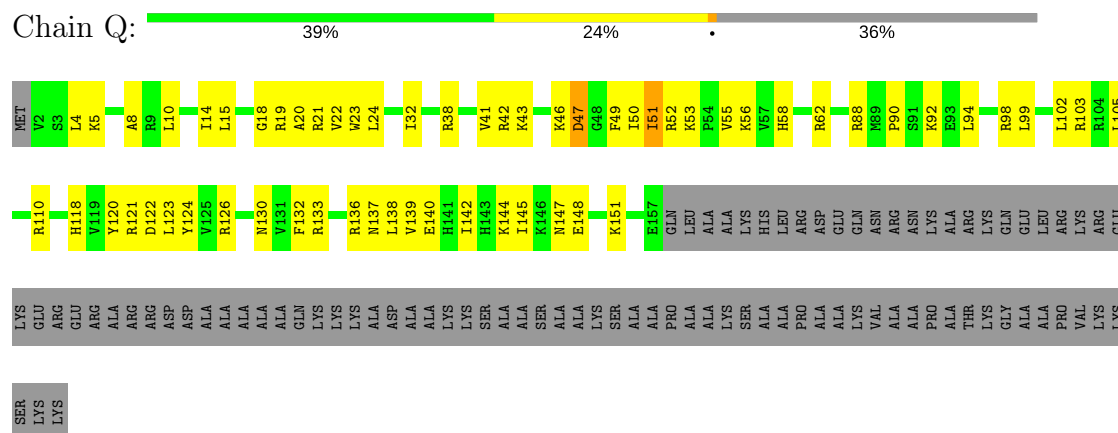
• Molecule 24: ribosomal protein L18e

Chain P: 61% 36%

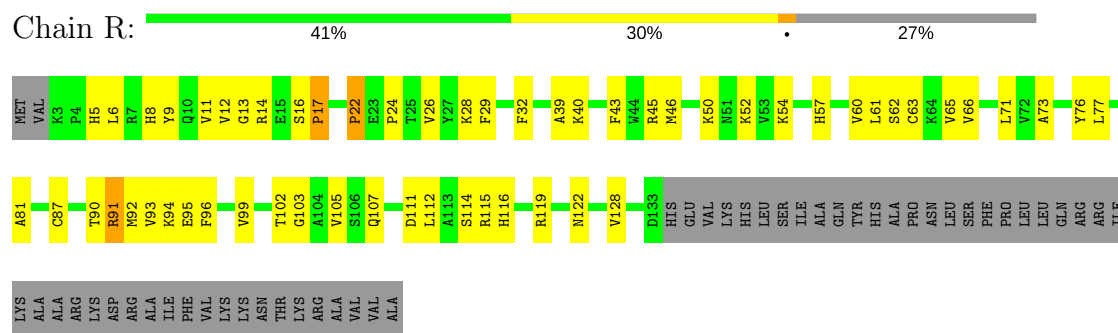




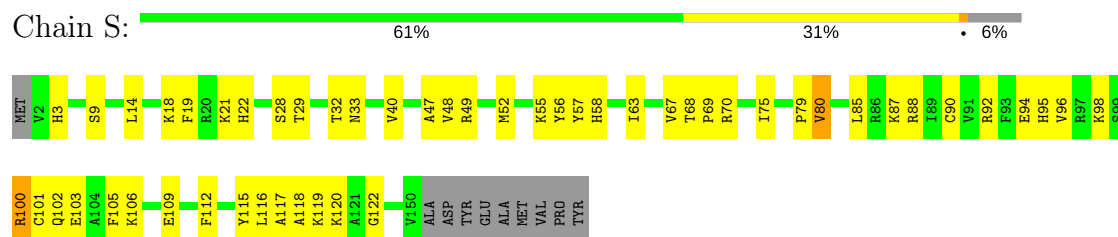
- Molecule 25: ribosomal protein L19e



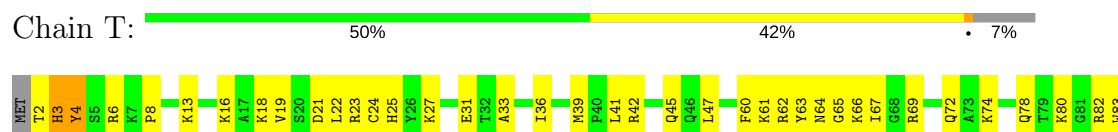
- Molecule 26: ribosomal protein L20e

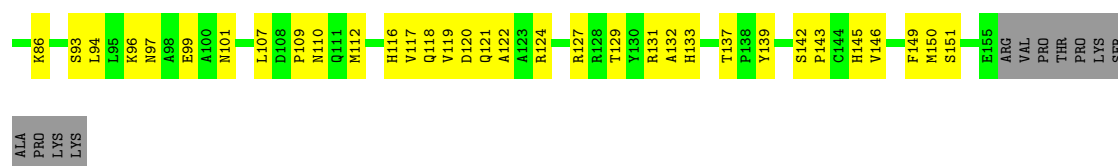


- Molecule 27: ribosomal protein L21e

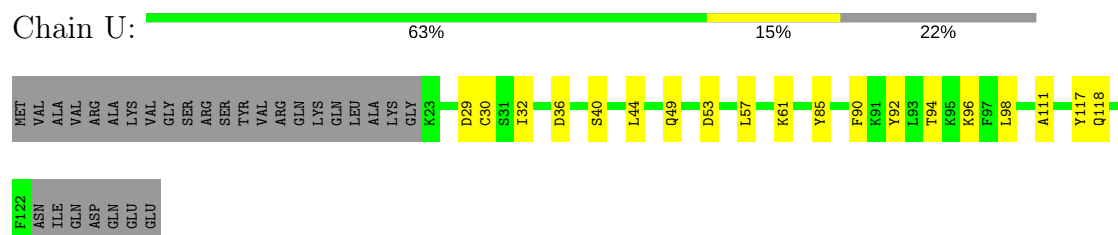


- Molecule 28: ribosomal protein L22

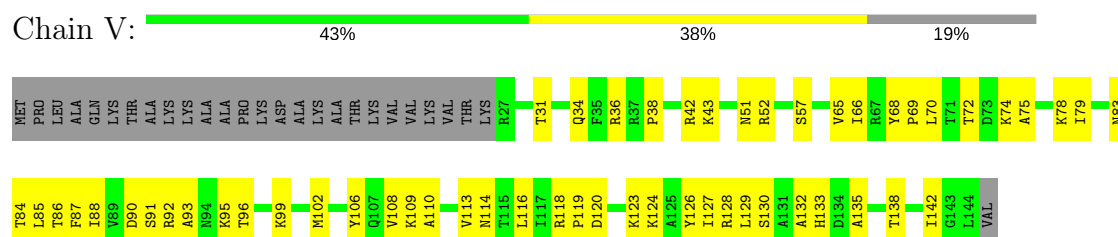




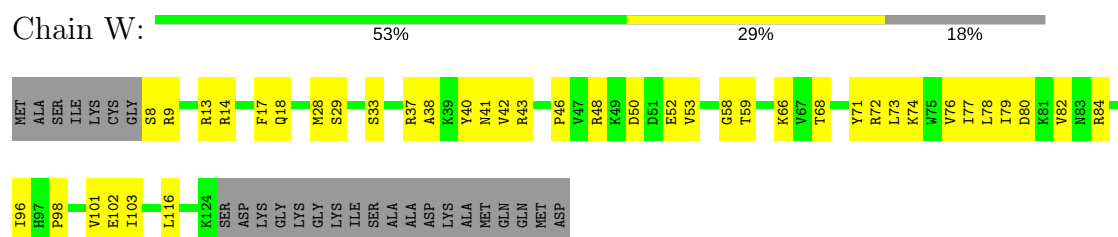
- Molecule 29: ribosomal protein L22e



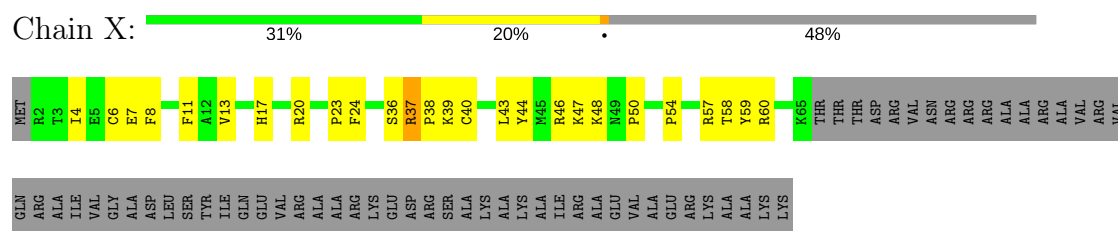
- Molecule 30: ribosomal protein L23



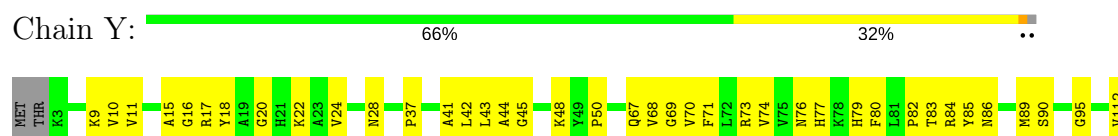
- Molecule 31: ribosomal protein L24



- Molecule 32: ribosomal protein L24e

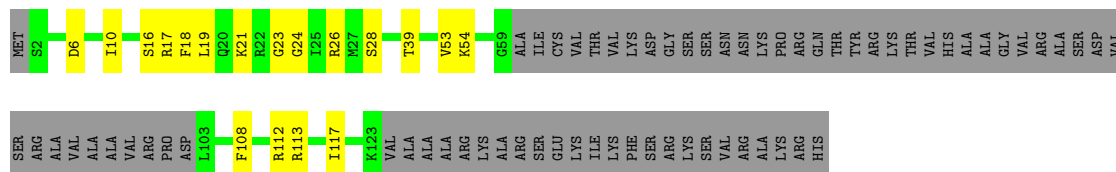


- Molecule 33: ribosomal protein L27e





- Molecule 34: ribosomal protein L28e



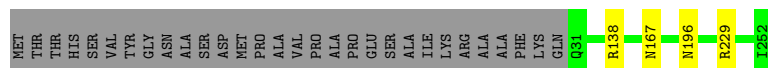
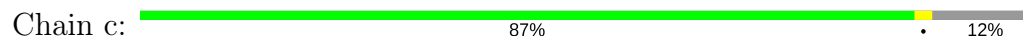
- Molecule 35: ribosomal protein L29



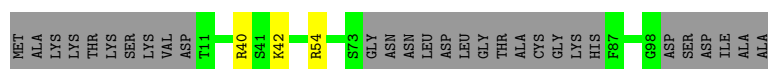
- Molecule 36: ribosomal protein L29e



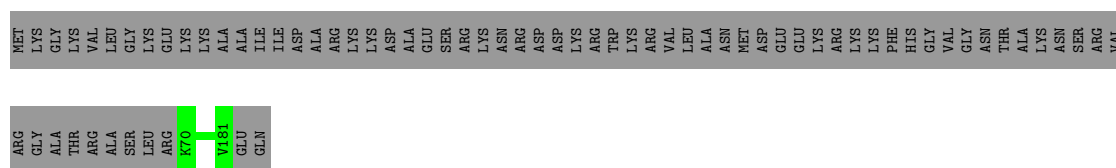
- Molecule 37: ribosomal protein L30




- Molecule 38: ribosomal protein L30e



- Molecule 39: ribosomal protein L31e




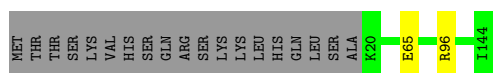
- Molecule 40: ribosomal protein L32e

Chain f:  92% • 5%



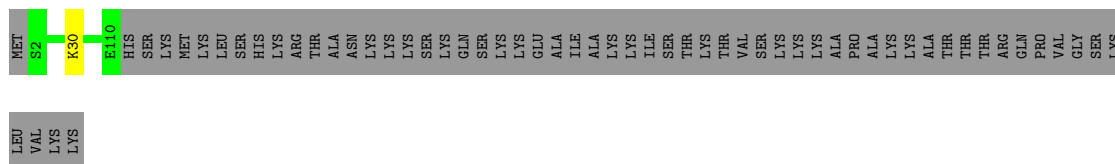
- Molecule 41: ribosomal protein L33e

Chain g:  85% • 13%



- Molecule 42: ribosomal protein L34e

Chain h:  64% • 35%



- Molecule 43: ribosomal protein L36e

Chain i:  57% • 40%



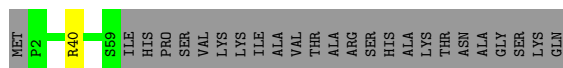
- Molecule 44: ribosomal protein L37e

Chain j:  90% • 6%



- Molecule 45: ribosomal protein L38e

Chain k:  69% • 30%

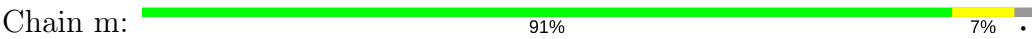


- Molecule 46: ribosomal protein L39e

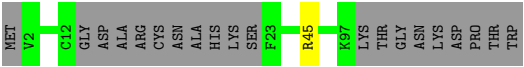
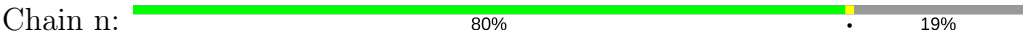
Chain l:  92% • 6%



- Molecule 47: ribosomal protein L43e



• Molecule 48: ribosomal protein L44e



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	107134	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	25000	Depositor
Image detector	K2 Summit direct electron detector	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, MG, OMG, H2U, OMU, A2M

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	1	0.75	8/36881 (0.0%)	0.90	48/57466 (0.1%)
10	B	0.44	0/3086	0.55	0/4176
11	C	0.45	0/2284	0.60	0/3092
12	D	0.25	0/800	0.49	0/1111
13	E	0.29	0/1529	0.56	0/2056
14	F	0.40	0/1023	0.56	0/1390
15	G	0.38	0/1798	0.59	1/2423 (0.0%)
16	H	0.42	0/1628	0.60	0/2194
17	I	0.40	0/1084	0.57	0/1454
18	J	0.39	0/941	0.61	2/1277 (0.2%)
19	K	0.27	0/1077	0.59	1/1475 (0.1%)
2	2	0.60	0/26109	0.86	28/40668 (0.1%)
20	L	0.43	0/1123	0.56	0/1505
21	M	0.49	0/1754	0.57	0/2342
22	N	0.27	0/1747	0.54	0/2338
23	O	0.32	0/1583	0.50	0/2157
24	P	0.42	0/1519	0.57	0/2040
25	Q	0.35	0/1179	0.53	0/1588
26	R	0.42	0/1044	0.59	1/1415 (0.1%)
27	S	0.43	0/1142	0.60	0/1547
28	T	0.45	0/1249	0.65	1/1679 (0.1%)
29	U	0.26	0/545	0.49	0/754
3	3	0.48	0/4337	0.84	1/6734 (0.0%)
30	V	0.42	0/907	0.51	0/1227
31	W	0.37	0/910	0.56	0/1224
32	X	0.40	0/527	0.53	0/716
33	Y	0.37	0/934	0.51	0/1274
34	Z	0.28	0/545	0.52	0/739
35	a	0.32	0/992	0.53	0/1326
36	b	0.34	0/514	0.50	0/690
37	c	0.42	0/1763	0.52	0/2374
38	d	0.31	0/525	0.50	0/719

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	e	0.37	0/838	0.57	0/1131
4	4	0.69	0/3549	0.88	3/5525 (0.1%)
40	f	0.46	0/1002	0.55	0/1346
41	g	0.49	0/1003	0.53	0/1352
42	h	0.38	0/868	0.55	0/1160
43	i	0.38	0/499	0.56	0/662
44	j	0.50	0/651	0.61	0/869
45	k	0.30	0/378	0.57	0/518
46	l	0.43	0/470	0.51	0/627
47	m	0.43	0/680	0.53	0/913
48	n	0.34	0/667	0.56	0/889
5	5	0.69	0/1908	0.91	3/2967 (0.1%)
6	6	0.39	2/1437 (0.1%)	0.79	4/2234 (0.2%)
7	7	0.76	0/3615	0.87	2/5622 (0.0%)
8	8	0.47	0/2828	0.82	0/4401
9	A	0.47	0/1903	0.56	0/2559
All	All	0.59	10/125375 (0.0%)	0.79	95/185945 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	B	0	2
13	E	0	1
15	G	0	1
16	H	0	1
19	K	0	3
26	R	0	1
27	S	0	1
28	T	0	1
40	f	0	1
9	A	0	1
All	All	0	13

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	634	G	C1'-N9	-6.69	1.37	1.46
1	1	159	U	C1'-N1	6.17	1.58	1.48
1	1	568	U	C1'-N1	6.06	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	564	U	C1'-N1	5.95	1.57	1.48
1	1	565	U	C1'-N1	5.91	1.57	1.48

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	45	SER	C-N-CD	-11.87	94.48	120.60
1	1	1575	A	OP1-P-O3'	-11.81	79.22	105.20
1	1	1757	U	C2-N1-C1'	8.96	128.45	117.70
2	2	776	C	N1-C2-O2	8.91	124.25	118.90
2	2	776	C	C2-N1-C1'	8.72	128.39	118.80

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	60[B]	ARG	Mainchain
10	B	337	GLY	Peptide
10	B	373	GLY	Peptide
13	E	136	PRO	Peptide
15	G	114	ALA	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	1	33313	0	16798	1118	0
2	2	23926	0	12113	740	0
3	3	3893	0	1971	147	0
4	4	3177	0	1611	112	0
5	5	1708	0	867	59	0
6	6	1288	0	657	184	0
7	7	3280	0	1664	103	0
8	8	2531	0	1281	155	0
9	A	1859	0	1901	128	0
10	B	3020	0	3003	172	0
11	C	2237	0	2231	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	799	0	374	5	0
13	E	1509	0	1595	122	0
14	F	1002	0	994	55	0
15	G	1772	0	1853	108	0
16	H	1596	0	1683	143	0
17	I	1061	0	1123	64	0
18	J	924	0	934	60	0
19	K	1061	0	939	196	0
20	L	1096	0	1096	52	0
21	M	1714	0	1793	95	0
22	N	1714	0	1786	111	0
23	O	1557	0	1351	84	0
24	P	1494	0	1554	83	0
25	Q	1162	0	1130	74	0
26	R	1019	0	981	52	0
27	S	1112	0	1051	57	0
28	T	1221	0	1230	98	0
29	U	541	0	295	10	0
30	V	892	0	903	48	0
31	W	896	0	915	36	0
32	X	508	0	477	25	0
33	Y	914	0	813	40	0
34	Z	538	0	479	18	0
35	a	982	0	1029	0	0
36	b	503	0	500	0	0
37	c	1732	0	1768	0	0
38	d	518	0	462	0	0
39	e	824	0	839	0	0
40	f	982	0	985	0	0
41	g	983	0	1006	0	0
42	h	856	0	873	0	0
43	i	494	0	535	0	0
44	j	639	0	641	0	0
45	k	373	0	302	0	0
46	l	457	0	484	0	0
47	m	668	0	648	0	0
48	n	659	0	672	0	0
49	1	51	0	0	0	0
49	2	25	0	0	0	0
49	3	3	0	0	0	0
49	4	2	0	0	0	0
49	5	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	7	9	0	0	0	0
49	C	1	0	0	0	0
49	K	1	0	0	0	0
49	M	3	0	0	0	0
49	V	1	0	0	0	0
49	a	1	0	0	0	0
49	f	2	0	0	0	0
49	g	1	0	0	0	0
49	h	1	0	0	0	0
49	j	4	0	0	0	0
50	1	72	0	0	18	0
50	2	40	0	0	17	0
50	4	4	0	0	1	0
50	5	4	0	0	0	0
50	7	16	0	0	2	0
50	8	1	0	0	1	0
50	A	2	0	0	1	0
50	G	1	0	0	0	0
50	M	2	0	0	0	0
50	i	1	0	0	0	0
50	j	1	0	0	0	0
All	All	117257	0	80190	3902	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 25.

The worst 5 of 3902 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)
3:3:57:U:H2'	3:3:58:C:C5	1.26	1.62
19:K:89:VAL:CG1	26:R:73:ALA:HB2	1.26	1.56
19:K:89:VAL:HG12	26:R:73:ALA:CB	1.38	1.50
24:P:17:HIS:CE1	24:P:18:HIS:HD1	1.29	1.50
25:Q:23:TRP:CE3	25:Q:51:ILE:CD1	2.02	1.42

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	
9	A	245/260 (94%)	220 (90%)	25 (10%)	0	100	100
10	B	396/419 (94%)	352 (89%)	43 (11%)	1 (0%)	44	77
11	C	300/373 (80%)	269 (90%)	31 (10%)	0	100	100
12	D	159/188 (85%)	136 (86%)	23 (14%)	0	100	100
13	E	188/190 (99%)	160 (85%)	28 (15%)	0	100	100
14	F	134/195 (69%)	112 (84%)	22 (16%)	0	100	100
15	G	225/348 (65%)	205 (91%)	18 (8%)	2 (1%)	20	52
16	H	200/222 (90%)	175 (88%)	24 (12%)	1 (0%)	32	67
17	I	130/220 (59%)	120 (92%)	10 (8%)	0	100	100
18	J	126/139 (91%)	115 (91%)	11 (9%)	0	100	100
19	K	154/233 (66%)	136 (88%)	17 (11%)	1 (1%)	28	62
20	L	142/145 (98%)	127 (89%)	15 (11%)	0	100	100
21	M	201/204 (98%)	187 (93%)	14 (7%)	0	100	100
22	N	211/213 (99%)	186 (88%)	25 (12%)	0	100	100
23	O	229/305 (75%)	205 (90%)	24 (10%)	0	100	100
24	P	194/198 (98%)	179 (92%)	15 (8%)	0	100	100
25	Q	154/245 (63%)	141 (92%)	13 (8%)	0	100	100
26	R	130/179 (73%)	104 (80%)	25 (19%)	1 (1%)	22	55
27	S	149/159 (94%)	125 (84%)	22 (15%)	2 (1%)	14	41
28	T	154/166 (93%)	127 (82%)	27 (18%)	0	100	100
29	U	98/129 (76%)	81 (83%)	17 (17%)	0	100	100
30	V	116/145 (80%)	99 (85%)	17 (15%)	0	100	100
31	W	116/143 (81%)	106 (91%)	10 (9%)	0	100	100
32	X	62/124 (50%)	59 (95%)	3 (5%)	0	100	100
33	Y	130/134 (97%)	111 (85%)	19 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Z	75/147 (51%)	65 (87%)	10 (13%)	0	100	100
35	a	122/127 (96%)	105 (86%)	17 (14%)	0	100	100
36	b	63/70 (90%)	53 (84%)	10 (16%)	0	100	100
37	c	220/252 (87%)	190 (86%)	30 (14%)	0	100	100
38	d	71/104 (68%)	63 (89%)	8 (11%)	0	100	100
39	e	111/183 (61%)	92 (83%)	19 (17%)	0	100	100
40	f	124/133 (93%)	110 (89%)	14 (11%)	0	100	100
41	g	123/144 (85%)	112 (91%)	11 (9%)	0	100	100
42	h	106/168 (63%)	91 (86%)	15 (14%)	0	100	100
43	i	62/105 (59%)	57 (92%)	5 (8%)	0	100	100
44	j	76/83 (92%)	68 (90%)	8 (10%)	0	100	100
45	k	56/83 (68%)	52 (93%)	4 (7%)	0	100	100
46	l	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	9	28
47	m	88/92 (96%)	71 (81%)	16 (18%)	1 (1%)	17	47
48	n	82/106 (77%)	66 (80%)	16 (20%)	0	100	100
All	All	5771/7124 (81%)	5078 (88%)	683 (12%)	10 (0%)	54	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	G	132	SER
26	R	22	PRO
27	S	101	CYS
47	m	40	SER
10	B	380	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	
9	A	188/204 (92%)	181 (96%)	7 (4%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	B	296/352 (84%)	288 (97%)	8 (3%)	50	83
11	C	222/302 (74%)	221 (100%)	1 (0%)	91	97
12	D	4/163 (2%)	4 (100%)	0	100	100
13	E	172/172 (100%)	169 (98%)	3 (2%)	66	90
14	F	92/154 (60%)	91 (99%)	1 (1%)	78	94
15	G	179/292 (61%)	173 (97%)	6 (3%)	42	76
16	H	166/188 (88%)	164 (99%)	2 (1%)	75	94
17	I	114/181 (63%)	110 (96%)	4 (4%)	41	75
18	J	91/111 (82%)	88 (97%)	3 (3%)	43	77
19	K	79/195 (40%)	68 (86%)	11 (14%)	4	12
20	L	105/115 (91%)	103 (98%)	2 (2%)	62	89
21	M	179/180 (99%)	176 (98%)	3 (2%)	66	90
22	N	178/179 (99%)	175 (98%)	3 (2%)	66	90
23	O	103/242 (43%)	100 (97%)	3 (3%)	48	81
24	P	149/164 (91%)	145 (97%)	4 (3%)	50	83
25	Q	100/196 (51%)	98 (98%)	2 (2%)	60	88
26	R	98/158 (62%)	96 (98%)	2 (2%)	60	88
27	S	100/133 (75%)	100 (100%)	0	100	100
28	T	125/144 (87%)	125 (100%)	0	100	100
29	U	13/114 (11%)	13 (100%)	0	100	100
30	V	86/124 (69%)	84 (98%)	2 (2%)	56	86
31	W	87/122 (71%)	87 (100%)	0	100	100
32	X	48/104 (46%)	46 (96%)	2 (4%)	34	68
33	Y	70/115 (61%)	69 (99%)	1 (1%)	71	92
34	Z	44/119 (37%)	44 (100%)	0	100	100
35	a	99/117 (85%)	92 (93%)	7 (7%)	17	44
36	b	48/58 (83%)	44 (92%)	4 (8%)	13	36
37	c	168/209 (80%)	164 (98%)	4 (2%)	54	85
38	d	47/90 (52%)	44 (94%)	3 (6%)	20	50
39	e	79/156 (51%)	79 (100%)	0	100	100
40	f	97/114 (85%)	95 (98%)	2 (2%)	59	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	g	98/121 (81%)	96 (98%)	2 (2%)	60	88
42	h	85/145 (59%)	84 (99%)	1 (1%)	75	94
43	i	47/89 (53%)	44 (94%)	3 (6%)	20	50
44	j	63/70 (90%)	60 (95%)	3 (5%)	30	63
45	k	26/74 (35%)	25 (96%)	1 (4%)	38	72
46	l	46/47 (98%)	44 (96%)	2 (4%)	33	67
47	m	63/74 (85%)	58 (92%)	5 (8%)	14	38
48	n	64/92 (70%)	63 (98%)	1 (2%)	68	91
All	All	4118/5979 (69%)	4010 (97%)	108 (3%)	55	83

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	M	60	CYS
24	P	182	ARG
45	k	40	ARG
21	M	122	ASN
23	O	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
22	N	71	GLN
25	Q	130	ASN
42	h	62	HIS
22	N	163	GLN
23	O	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1533/1782 (86%)	588 (38%)	0
2	2	1105/1527 (72%)	445 (40%)	0
3	3	176/213 (82%)	83 (47%)	0
4	4	146/183 (79%)	48 (32%)	0
5	5	77/133 (57%)	30 (38%)	0
6	6	60/76 (78%)	48 (80%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	7	149/171 (87%)	50 (33%)	0
8	8	117/121 (96%)	54 (46%)	0
All	All	3363/4206 (79%)	1346 (40%)	0

5 of 1346 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	10	A
1	1	13	G
1	1	23	U
1	1	24	A

There are no RNA pucker outliers to report.

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

44 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	OMG	1	1526	1	18,26,27	1.21	2 (11%)	22,38,41	2.15	6 (27%)
1	OMC	1	1529	1	15,22,23	0.98	0	19,31,34	1.00	1 (5%)
1	A2M	1	1541	1,2	18,25,26	1.05	1 (5%)	20,36,39	1.64	2 (10%)
1	OMG	1	1542	1,2	18,26,27	1.20	2 (11%)	22,38,41	2.17	6 (27%)
1	OMG	1	1628	1	18,26,27	1.24	2 (11%)	22,38,41	2.25	6 (27%)
1	OMU	1	36	1	14,22,23	1.03	1 (7%)	18,31,34	1.82	1 (5%)
1	OMU	1	48	1	14,22,23	1.17	2 (14%)	18,31,34	1.95	1 (5%)
1	A2M	1	678	1,2	18,25,26	1.06	1 (5%)	20,36,39	1.70	2 (10%)
1	A2M	1	681	1	18,25,26	1.01	1 (5%)	20,36,39	1.67	2 (10%)
1	OMC	1	695	1	15,22,23	1.07	1 (6%)	19,31,34	1.14	2 (10%)
1	OMU	1	845	1	14,22,23	1.10	1 (7%)	18,31,34	1.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1	847	1	14,22,23	1.02	1 (7%)	18,31,34	1.84	1 (5%)
1	OMG	1	856	1	18,26,27	1.17	2 (11%)	22,38,41	2.14	6 (27%)
1	A2M	1	927	1	18,25,26	1.10	1 (5%)	20,36,39	1.70	2 (10%)
1	A2M	1	955	1	18,25,26	1.08	1 (5%)	20,36,39	1.72	2 (10%)
1	OMG	1	959	1	18,26,27	1.30	2 (11%)	22,38,41	2.13	6 (27%)
2	OMU	2	1078	2	14,22,23	0.97	1 (7%)	18,31,34	1.90	1 (5%)
2	OMG	2	1079	2	18,26,27	1.28	2 (11%)	22,38,41	2.22	6 (27%)
2	OMU	2	1153	2	14,22,23	1.14	2 (14%)	18,31,34	1.95	1 (5%)
2	OMC	2	1160	2	15,22,23	0.91	0	19,31,34	0.84	0
2	A2M	2	1186	2	18,25,26	1.04	1 (5%)	20,36,39	1.68	2 (10%)
2	OMG	2	1230	2	18,26,27	1.23	2 (11%)	22,38,41	2.12	6 (27%)
2	OMC	2	1249	2	15,22,23	0.84	0	19,31,34	0.93	1 (5%)
2	OMG	2	1254	2	18,26,27	1.22	2 (11%)	22,38,41	2.09	6 (27%)
2	OMC	2	1318	2	15,22,23	0.95	0	19,31,34	1.05	2 (10%)
2	OMC	2	1398	2	15,22,23	0.91	0	19,31,34	0.80	0
2	H2U	2	1404	2	17,21,22	1.17	2 (11%)	21,30,33	1.72	2 (9%)
2	A2M	2	382	2	18,25,26	1.03	1 (5%)	20,36,39	1.59	2 (10%)
2	OMC	2	443	2	15,22,23	0.91	0	19,31,34	0.95	0
2	A2M	2	527	2	18,25,26	1.02	1 (5%)	20,36,39	1.73	2 (10%)
2	OMG	2	534	2	18,26,27	1.25	2 (11%)	22,38,41	2.17	6 (27%)
2	OMC	2	554	2	15,22,23	0.89	0	19,31,34	1.04	1 (5%)
2	OMG	2	571	2	18,26,27	1.23	2 (11%)	22,38,41	2.21	6 (27%)
2	A2M	2	572	2	18,25,26	1.07	1 (5%)	20,36,39	1.57	2 (10%)
2	OMC	2	583	2	15,22,23	0.98	0	19,31,34	0.84	0
2	A2M	2	591	2	18,25,26	1.10	1 (5%)	20,36,39	1.71	2 (10%)
2	A2M	2	628	2	18,25,26	1.02	1 (5%)	20,36,39	1.67	2 (10%)
2	OMG	2	641	2	18,26,27	1.23	2 (11%)	22,38,41	2.18	6 (27%)
2	OMG	2	655	2	18,26,27	1.22	2 (11%)	22,38,41	2.11	6 (27%)
2	OMU	2	656	2	14,22,23	1.01	1 (7%)	18,31,34	1.85	1 (5%)
2	OMU	2	667	2	14,22,23	1.00	1 (7%)	18,31,34	2.00	1 (5%)
2	OMG	2	71	2	18,26,27	1.22	2 (11%)	22,38,41	2.05	6 (27%)
7	A2M	7	162	1,7	18,25,26	1.14	1 (5%)	20,36,39	1.71	3 (15%)
7	OMU	7	7	1,7	14,22,23	1.07	1 (7%)	18,31,34	1.93	1 (5%)

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
1	OMG	1	1526	1	-	0/5/27/28	0/3/3/3
1	OMC	1	1529	1	-	0/5/27/28	0/2/2/2
1	A2M	1	1541	1,2	-	0/5/27/28	0/3/3/3
1	OMG	1	1542	1,2	-	0/5/27/28	0/3/3/3
1	OMG	1	1628	1	-	0/5/27/28	0/3/3/3
1	OMU	1	36	1	-	0/5/27/28	0/2/2/2
1	OMU	1	48	1	-	0/5/27/28	0/2/2/2
1	A2M	1	678	1,2	-	0/5/27/28	0/3/3/3
1	A2M	1	681	1	-	0/5/27/28	0/3/3/3
1	OMC	1	695	1	-	0/5/27/28	0/2/2/2
1	OMU	1	845	1	-	0/5/27/28	0/2/2/2
1	OMU	1	847	1	-	0/5/27/28	0/2/2/2
1	OMG	1	856	1	-	0/5/27/28	0/3/3/3
1	A2M	1	927	1	-	0/5/27/28	0/3/3/3
1	A2M	1	955	1	-	0/5/27/28	0/3/3/3
1	OMG	1	959	1	-	0/5/27/28	0/3/3/3
2	OMU	2	1078	2	-	0/5/27/28	0/2/2/2
2	OMG	2	1079	2	-	0/5/27/28	0/3/3/3
2	OMU	2	1153	2	-	0/5/27/28	0/2/2/2
2	OMC	2	1160	2	-	0/5/27/28	0/2/2/2
2	A2M	2	1186	2	-	0/5/27/28	0/3/3/3
2	OMG	2	1230	2	-	0/5/27/28	0/3/3/3
2	OMC	2	1249	2	-	0/5/27/28	0/2/2/2
2	OMG	2	1254	2	-	0/5/27/28	0/3/3/3
2	OMC	2	1318	2	-	0/5/27/28	0/2/2/2
2	OMC	2	1398	2	-	0/5/27/28	0/2/2/2
2	H2U	2	1404	2	-	0/7/38/39	0/2/2/2
2	A2M	2	382	2	-	0/5/27/28	0/3/3/3
2	OMC	2	443	2	-	0/5/27/28	0/2/2/2
2	A2M	2	527	2	-	0/5/27/28	0/3/3/3
2	OMG	2	534	2	-	0/5/27/28	0/3/3/3
2	OMC	2	554	2	-	0/5/27/28	0/2/2/2
2	OMG	2	571	2	-	0/5/27/28	0/3/3/3
2	A2M	2	572	2	-	0/5/27/28	0/3/3/3
2	OMC	2	583	2	-	0/5/27/28	0/2/2/2
2	A2M	2	591	2	-	0/5/27/28	0/3/3/3
2	A2M	2	628	2	-	0/5/27/28	0/3/3/3
2	OMG	2	641	2	-	0/5/27/28	0/3/3/3
2	OMG	2	655	2	-	0/5/27/28	0/3/3/3
2	OMU	2	656	2	-	0/5/27/28	0/2/2/2
2	OMU	2	667	2	-	0/5/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	71	2	-	0/5/27/28	0/3/3/3
7	A2M	7	162	1,7	-	0/5/27/28	0/3/3/3
7	OMU	7	7	1,7	-	0/5/27/28	0/2/2/2

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1404	H2U	C4-N3	-2.72	1.33	1.37
2	2	1404	H2U	C2-N3	-2.64	1.33	1.38
1	1	845	OMU	C2-N3	-2.49	1.33	1.38
1	1	48	OMU	C2-N3	-2.44	1.33	1.38
1	1	36	OMU	C2-N3	-2.32	1.33	1.38

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	927	A2M	N3-C2-N1	-6.30	123.37	128.86
1	1	678	A2M	N3-C2-N1	-6.23	123.43	128.86
1	1	955	A2M	N3-C2-N1	-6.19	123.47	128.86
2	2	628	A2M	N3-C2-N1	-6.15	123.50	128.86
2	2	591	A2M	N3-C2-N1	-6.05	123.59	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

41 monomers are involved in 186 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1526	OMG	2	0
1	1	1529	OMC	6	0
1	1	1541	A2M	3	0
1	1	1542	OMG	2	0
1	1	1628	OMG	1	0
1	1	36	OMU	14	0
1	1	48	OMU	4	0
1	1	678	A2M	2	0
1	1	681	A2M	2	0
1	1	695	OMC	3	0
1	1	845	OMU	2	0
1	1	847	OMU	3	0
1	1	856	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	927	A2M	3	0
1	1	955	A2M	2	0
1	1	959	OMG	9	0
2	2	1078	OMU	11	0
2	2	1079	OMG	9	0
2	2	1153	OMU	6	0
2	2	1160	OMC	3	0
2	2	1186	A2M	3	0
2	2	1230	OMG	2	0
2	2	1249	OMC	1	0
2	2	1254	OMG	10	0
2	2	1318	OMC	7	0
2	2	1398	OMC	4	0
2	2	1404	H2U	2	0
2	2	382	A2M	2	0
2	2	443	OMC	7	0
2	2	527	A2M	13	0
2	2	534	OMG	4	0
2	2	554	OMC	3	0
2	2	571	OMG	1	0
2	2	572	A2M	2	0
2	2	583	OMC	1	0
2	2	591	A2M	7	0
2	2	628	A2M	4	0
2	2	655	OMG	7	0
2	2	667	OMU	5	0
2	2	71	OMG	11	0
7	7	7	OMU	10	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 109 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.