



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 10:16 PM EST

PDB ID : 4V6T
EMDB ID: : EMD-5386
Title : Structure of the bacterial ribosome complexed by tmRNA-SmpB and EF-G during translocation and MLD-loading
Authors : Ramrath, D.J.F.; Yamamoto, H.; Rother, K.; Wittek, D.; Pech, M.; Mielke, T.; Loerke, J.; Scheerer, P.; Ivanov, P.; Teraoka, Y.; Shpanchenko, O.; Nierhaus, K.H.; Spahn, C.M.T.
Deposited on : 2012-01-27
Resolution : 8.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

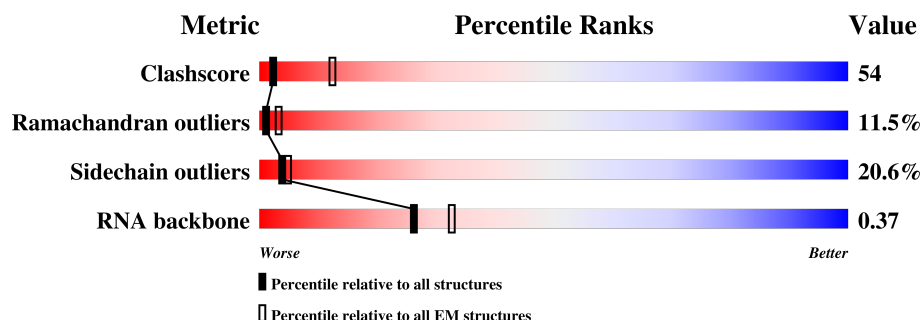
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.30 Å.

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




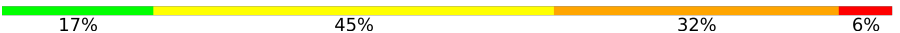
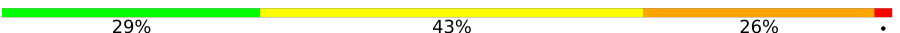

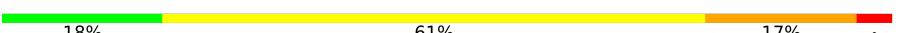
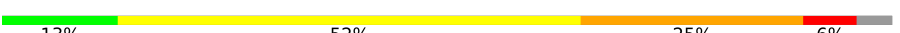
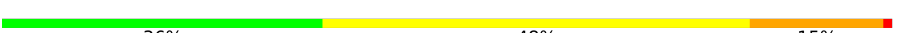




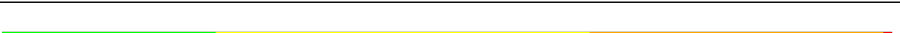





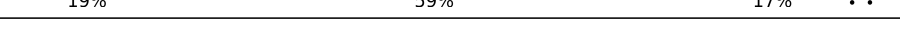




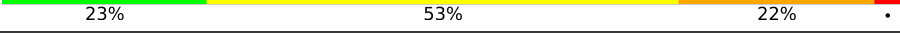

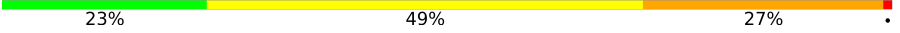
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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

Mol	Chain	Length	Quality of chain
1	AA	1539	13% 54% 29% .
2	AB	218	10% 46% 35% 9%
3	AC	206	20% 53% 21% 5%
4	AD	205	21% 45% 31% .
5	AE	150	17% 55% 23% 5%
6	AF	100	20% 50% 25% 5%
7	AG	151	27% 48% 23% .
8	AH	129	21% 58% 19% .





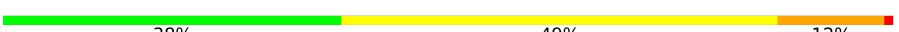
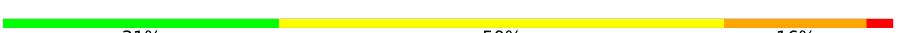
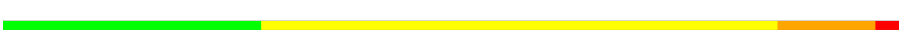





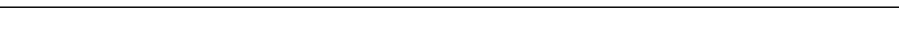



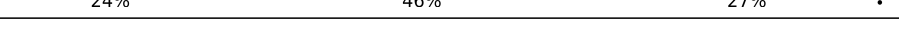






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Mol	Chain	Length	Quality of chain
9	AI	127	
10	AJ	98	
11	AK	117	
12	AL	123	
13	AM	114	
14	AN	100	
15	AO	88	
16	AP	82	
17	AQ	80	
18	AR	55	
19	AS	79	
20	AT	85	
21	AU	51	
22	AV	363	
23	AW	123	
24	AX	77	
25	AY	691	
26	BA	2903	
27	BC	271	
28	BD	209	
29	BE	201	
30	BF	177	
31	BG	176	
32	BH	149	
33	BI	141	

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Mol	Chain	Length	Quality of chain
34	BJ	142	 56% 33% 10% .
35	BK	122	 43% 39% 16% .
36	BL	143	 34% 46% 17% .
37	BM	136	 43% 40% 16% .
38	BN	120	 38% 49% 12% .
39	BO	116	 31% 50% 16% .
40	BP	114	 29% 58% 11% .
41	BQ	117	 47% 44% 8% .
42	BR	103	 45% 37% 17% .
43	BS	110	 56% 34% 9% .
44	BT	93	 34% 52% 13% .
45	BU	102	 36% 44% 18% .
46	BV	94	 46% 44% 11% .
47	BW	76	 54% 38% 8% .
48	BX	77	 40% 49% 10% .
49	BY	63	 24% 46% 27% .
50	BZ	58	 45% 50% 5% .
51	B0	56	 48% 38% 14% .
52	B1	50	 30% 54% 14% .
53	B2	46	 46% 46% 7% .
54	B3	64	 45% 52% .
55	B4	38	 32% 58% 8% .
56	BB	119	 18% 51% 28% .

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
22	PSU	AV	347	-	-	X	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 157519 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0
			32995	14716	6050	10691	1538		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 22 is a RNA chain called full length transfer messenger RNA (tmRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	334	Total	C	N	O	P	0	0
			7135	3185	1286	2330	334		

- Molecule 23 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	122	Total	C	N	O		0	0
			993	637	181	175			

- Molecule 24 is a RNA chain called formyl-methionine specific initiator transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 25 is a protein called elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	667	Total	C	N	O	S	0	1
			5215	3316	893	988	18		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	2903	Total	C	N	O	P	0	0
			62319	27801	11467	20149	2902		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BF	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BK	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	BO	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	BQ	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BT	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	102	Total	C	N	O	S	0	0
			780	492	146	142			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	B1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

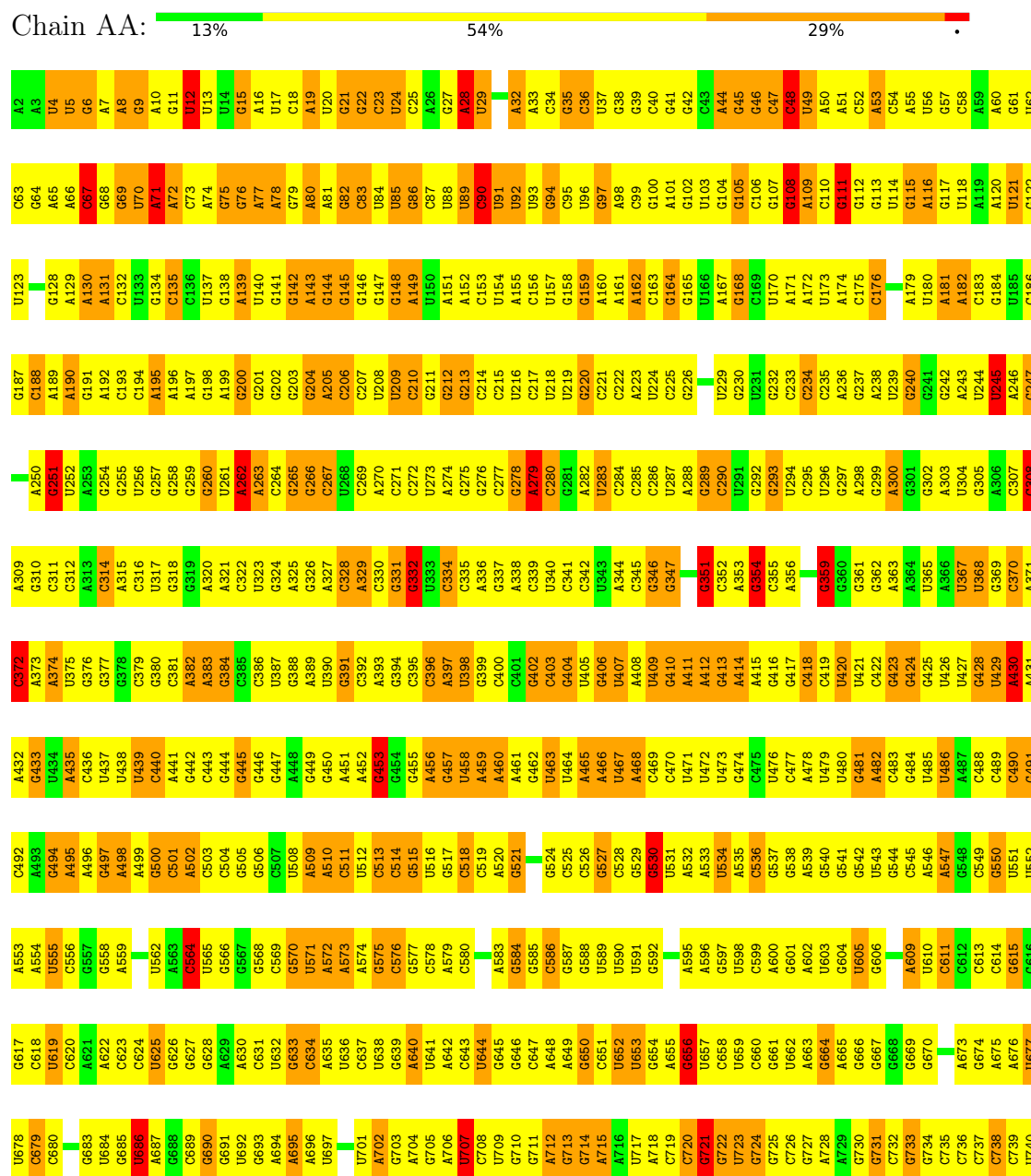
- Molecule 56 is a RNA chain called 5S ribosomal RNA.

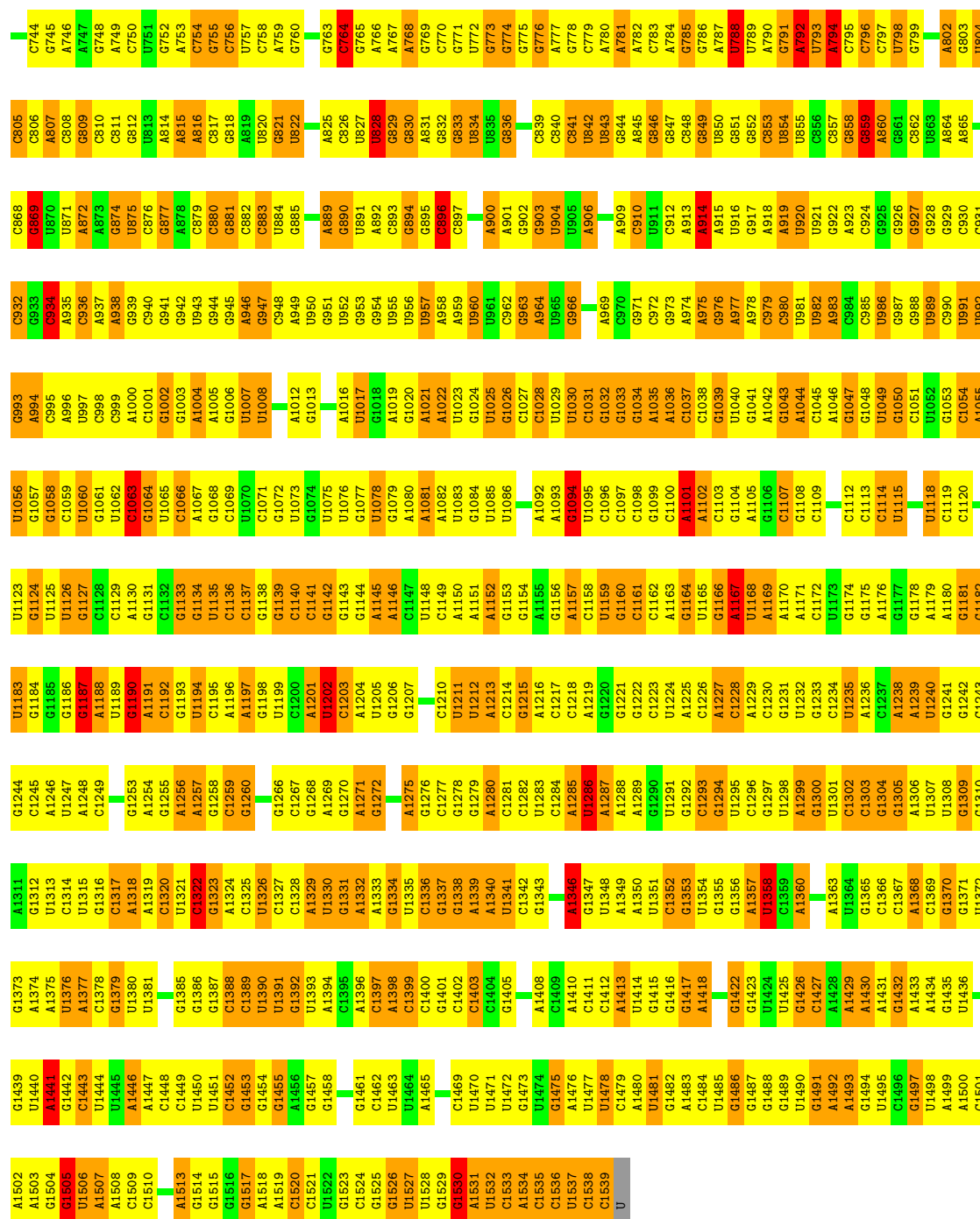
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	BB	119	2548	1135	466	829	118	0	0

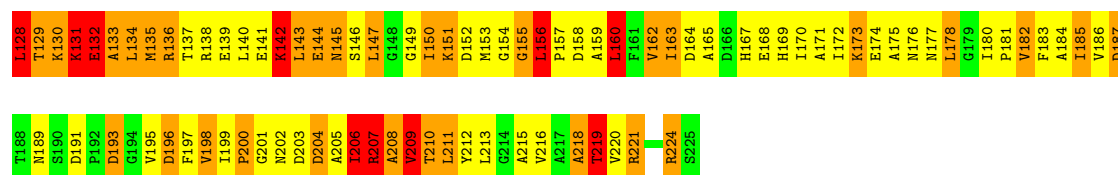
3 Residue-property plots

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: 16S ribosomal RNA

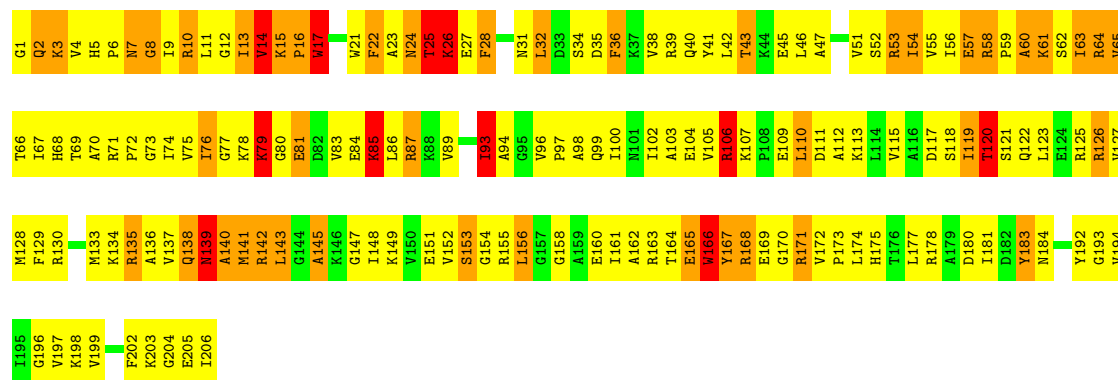






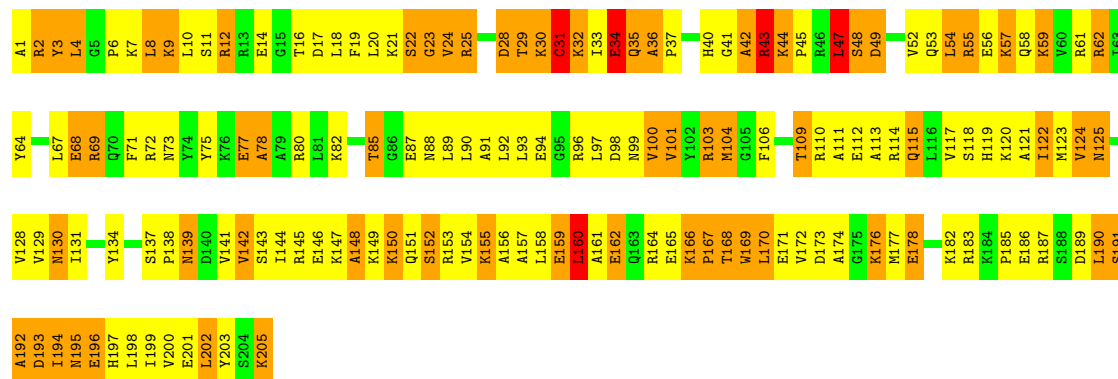
• Molecule 3: 30S ribosomal protein S3

Chain AC: 20% 53% 21% 5%



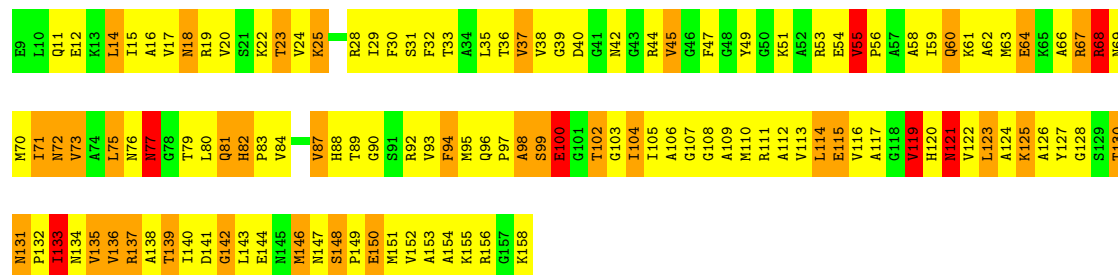
• Molecule 4: 30S ribosomal protein S4

Chain AD: 21% 45% 31% .



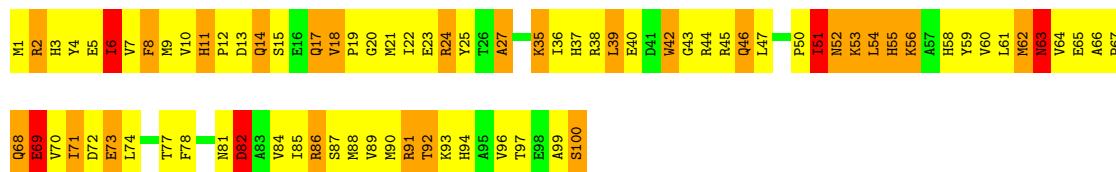
• Molecule 5: 30S ribosomal protein S5

Chain AE: 17% 55% 23% 5%



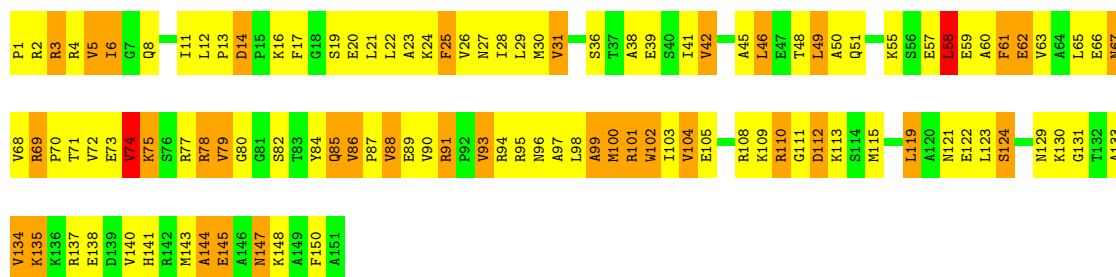
• Molecule 6: 30S ribosomal protein S6

Chain AF: 



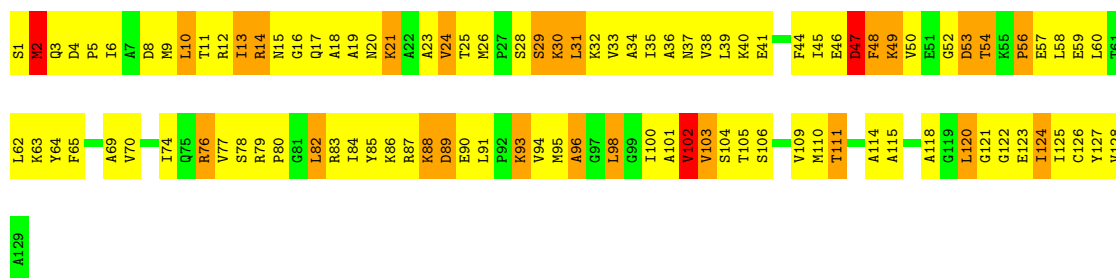
• Molecule 7: 30S ribosomal protein S7

Chain AG: 




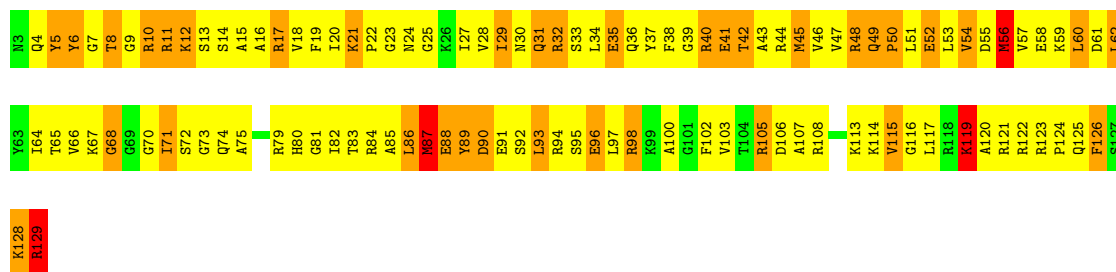
• Molecule 8: 30S ribosomal protein S8

Chain AH: 

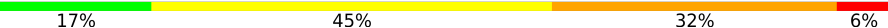


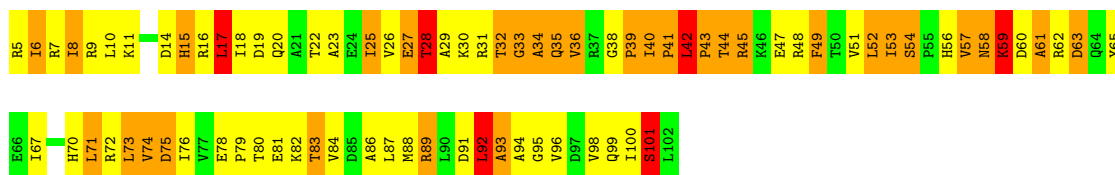
• Molecule 9: 30S ribosomal protein S9

Chain AI: 



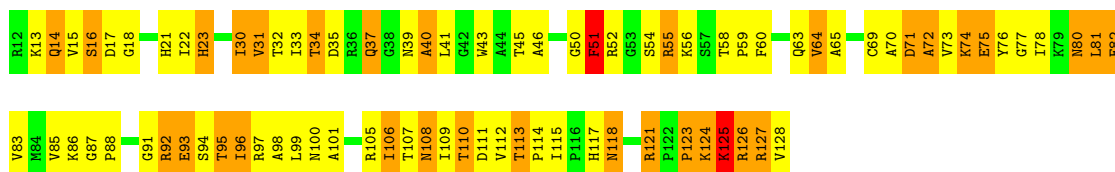
• Molecule 10: 30S ribosomal protein S10

Chain AJ: 



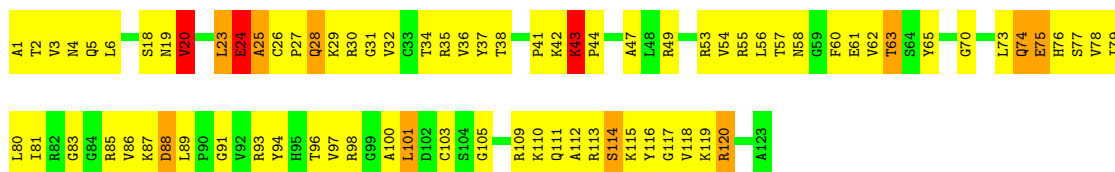
• Molecule 11: 30S ribosomal protein S11

Chain AK: 29% 43% 26% .



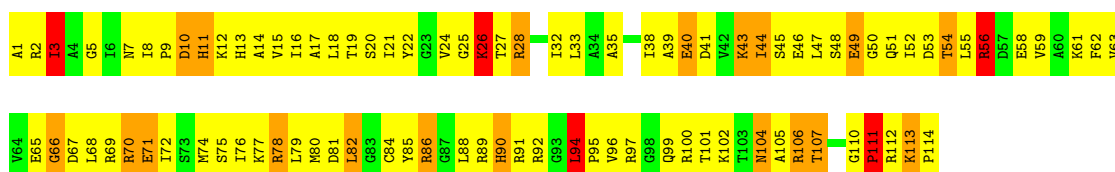
• Molecule 12: 30S ribosomal protein S12

Chain AL: 36% 54% 8% .



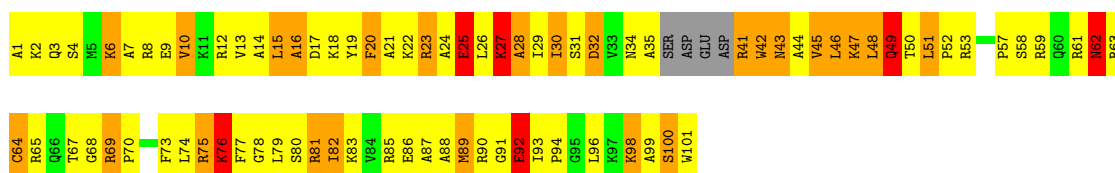
• Molecule 13: 30S ribosomal protein S13

Chain AM: 18% 61% 17% .



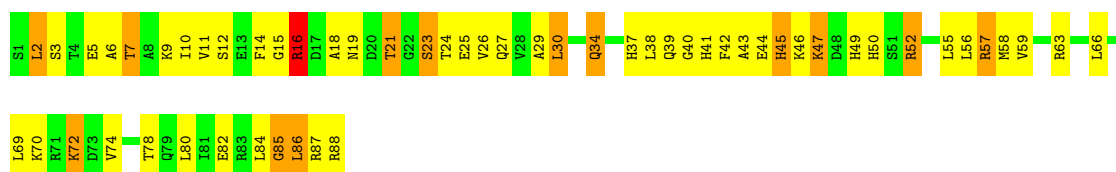
• Molecule 14: 30S ribosomal protein S14

Chain AN: 13% 52% 25% 6% .



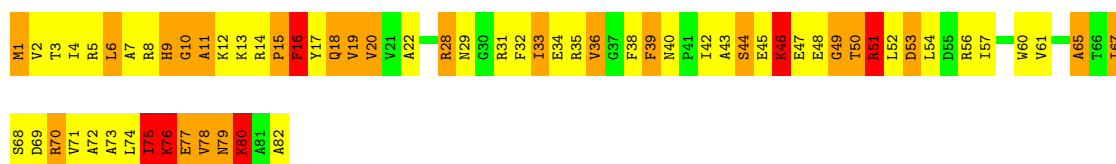
• Molecule 15: 30S ribosomal protein S15

Chain AO: 36% 48% 15% .



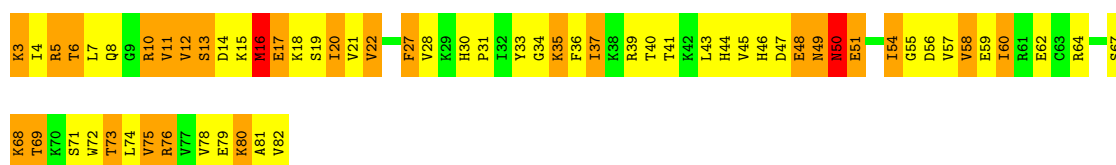
• Molecule 16: 30S ribosomal protein S16

Chain AP: 21% 44% 28% 7%



• Molecule 17: 30S ribosomal protein S17

Chain AQ: 21% 45% 31% .



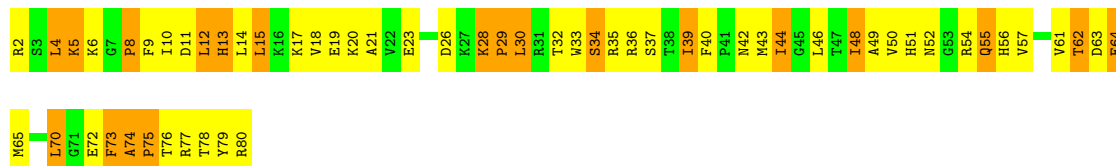
• Molecule 18: 30S ribosomal protein S18

Chain AR: 22% 64% 9% 5%



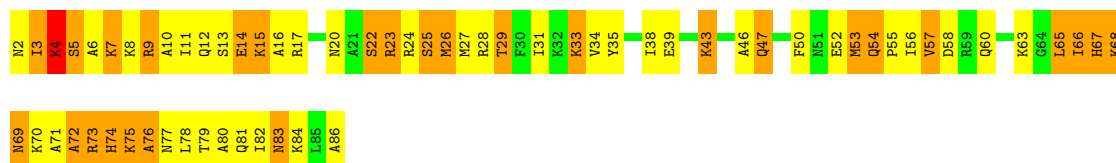
• Molecule 19: 30S ribosomal protein S19

Chain AS: 27% 48% 25%



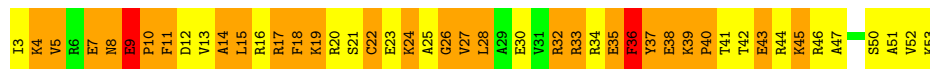
• Molecule 20: 30S ribosomal protein S20

Chain AT: 24% 42% 33% .



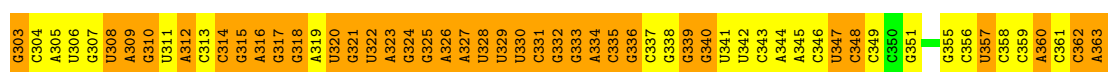
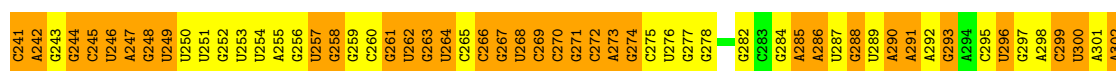
- Molecule 21: 30S ribosomal protein S21

Chain AU:  10% 37% 49%




- Molecule 22: full length transfer messenger RNA (tmRNA)

Chain AV:  30% 59% 8%



- Molecule 23: SsrA-binding protein

Chain AW:  11% 63% 19% 6%



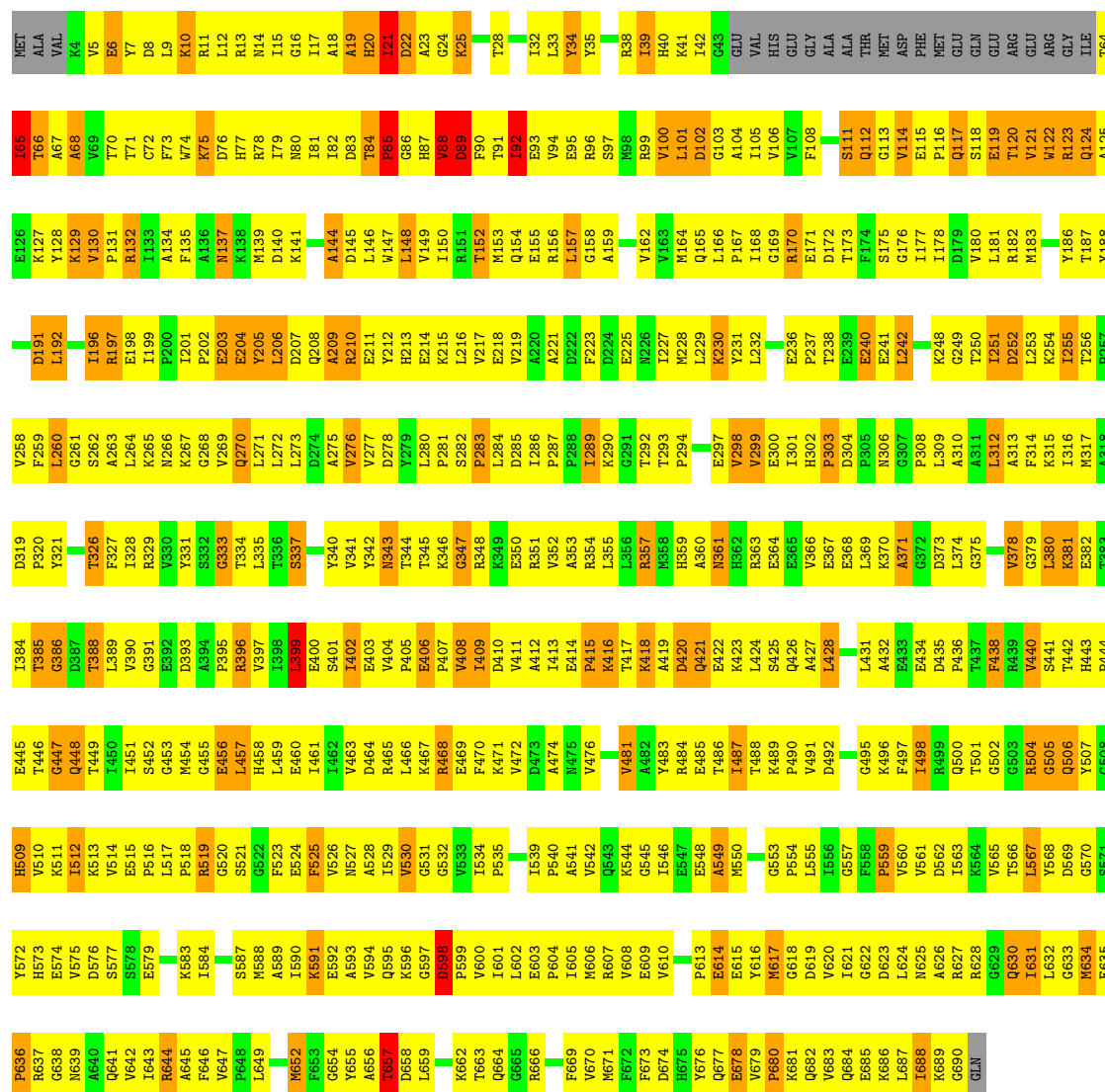
- Molecule 24: formyl-methionine specific initiator transfer RNA

Chain AX:  51% 48%




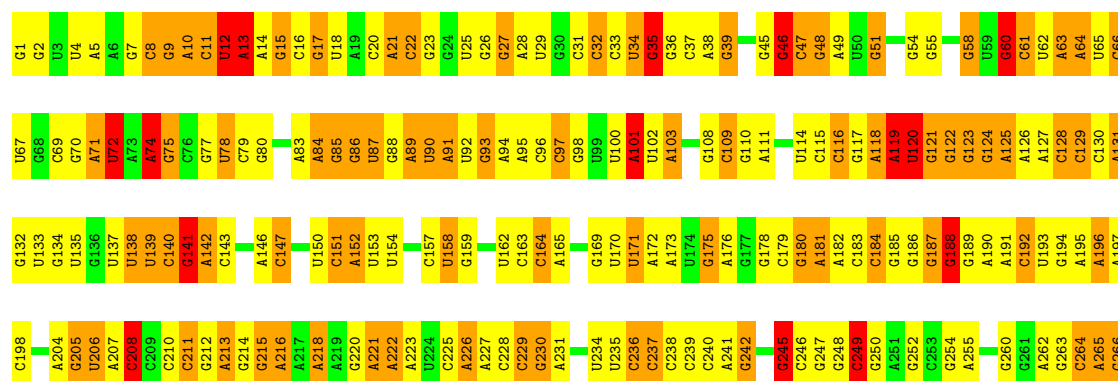
- Molecule 25: elongation factor G

Chain AY:  19% 59% 17% ..



• Molecule 26: 23S ribosomal RNA

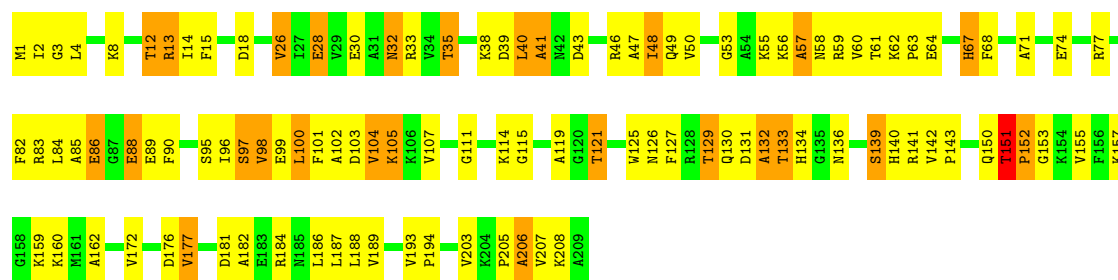
Chain BA:  18% 43% 32% 7%



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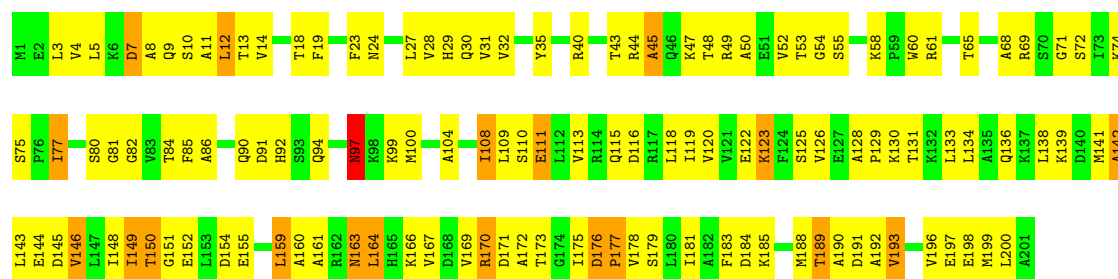
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A2284	G2223	A2101	U2039	A1977	G1910	A1847	U1782	A1722	C1658	A1596	A1532	A1469	U1409	
G2285	G2224	C2103	G2040	U1978	U1911		G1783	G1723	G1659	U1599	C1533	A1470	U1410	
G2286	A2225	C2164	U2041	A1979	A1912		A1784	G1724	G1660	U1541	U1411	G1471	C1350	
A2287	C2226	C2104	G2042	U1980	A1913	U1851	A1785	U1725	G1661	C1600	U1412	C1472	C1351	
A2288	U2106	U2105	A2043	A1981	G1914	U1852	G1786	C1726	U1662	G1601	G1473	U1476	U1352	
G2289	G2107	C2168	C2044	U1982	U1915	A1853	A1787	G1727	G1663	U1602	G1474	U1474	A1353	
G2290	A2108	A2108	G2045	G1983	A1916	A1854	C1788	C1728	A1664	A1603	G1475	G1475	A1354	
U2291	U2109	C2046	G2046	G1984	U1917	U1855	A1789	U1729	A1665	C1604	U1476	U1476	G1355	
U2292	A2171	A2110	C2047	C1985	A1918	U1856	G1790	G1730	G1666	C1605	U1542	A1477	C1356	
G2293	U2111	G2048	G2048		A1919	G1857	A1791	G1731	G1667	C1606	G1478	G1478	C1357	
G2294	C2173	A2173	G2049		C1920	A1858	G1792	G1732	A1667	C1607	G1479	G1479	C1357	
G2295	G2112	G2112	G2049	G1988	G1921	U1859	C1793	G1733	A1668	A1608	G1480	U1480	A1358	
G2296	U2114	A2114	A2051	C1989	U1922	G1860	A1794	G1734	C1670	A1605	G1546	U1481	G1360	
U2297	G2115	G2115	A2052	C1990	G1923	G1861	C1795	A1735	A1677	A1610	C1547	G1482	G1361	
A2298	C2116	G2053	G2053	C1999	U1924	U1862	U1796	G1736	U1678	C1611	G1483	G1422	G1362	
U2299	C2178	A2117	A2054	C2000	C1925	G1863	G1797	G1737	A1679	G1612	U1484	G1424	C1363	
C2300	C2239	U2118	C2055	C1994	U1926	U1864	U1798	G1738	G1674	G1613	U1485	G1425	C1364	
C2301	U2240	U2180	G2056		A1927	U1865	G1799	A1739	A1675	A1614	U1486	G1426	A1365	
U2302	A2241	U2181	G2057	C1997	U1928	A1866	G1800	G1740	A1676	C1615	A1627	U1487	A1366	
G2303	G2242	G2121	A2058	A1996	G1929	G1867	A1801	C1741	U1677	A1616	G1555	U1428	A1367	
G2304	U2243	A2183	A2059	C1999	U1930	C1868	A1802	U1742	C1556	C1617	G1429	G1429	G1368	
U2305	U2244	G2123	A2060	C2000	U1931	G1869	A1803	G1743	C1557	A1618	G1430	G1430	G1369	
C2306	U2245	U2185	G2061	C2001	A1932	C1870	C1804	A1744	U1680	G1619	G1431	G1431	C1370	
G2307	G2246	G2125	A2062	G2002	G1933	A1871	A1805	A1745	G1681	G1620	U1559	C1493	G1371	
G2308	A2247	A2126	C2063	A2003		A1872	C1806	A1746	C1682	U1621	G1560	A1494	U1372	
A2309	C2248	G2127	C2064	G2004	A1936	C1873	G1807	U1747	U1683	G1622	C1561	A1434	A1373	
C2310	U2249	U2189	C2065	A2005	A1937	C1874	A1808	C1748	G1684	G1623	U1562	A1435	G1374	
A2311	G2250	G2128	C2066	C2006	A1938	G1875	A1809	A1749	C1685	U1624	U1563	A1436	U1375	
G2312	G2251	A2191	G2067	U2007	U1939	A1876	A1810	G1750	C1686	C1564	C1437	C1376	G1376	
C2313	G2252	U2131	U2068	C2008		A1877	G1811	U1751	U1687	A1625	C1499	C1437	G1377	
G2314	G2253	G2193	G2069	A2009	U1943	G1878		C1752	U1688	G1627	G1500	U1438	A1378	
G2315	C2254	U2194	A2070	G2010	U1944	C1879	C1816	G1753	A1689	G1628	G1501	A1439	A1379	
G2316	A2134	G2134	A2071	U2011	G1945	U1880	G1817	A1754	C1567	A1502	A1502	U1440	U1379	
A2317	G2256	A2135	U2081	G2012	U1946	C1881	U1818	A1755	A1690	A1503	A1503	G1441	G1380	
G2318	U2257	U2197	A2013	A2013	C1947	U1882	A1819	G1756	C1691	A1630	A1569	G1442	G1381	
G2319	C2258	A2198	A2014	A2014	U1948	U1883	U1820	A1757	U1692	G1631	A1505	U1443	G1382	
U2320	U2075	U2139	U2076	A2015	G1949	G1884		U1758	U1693	A1632	U1506	G1444	A1383	
U2321	G2260	G2140	A2077	U2016	U1950	A1885	G1824	U1759	C1694	G1633	C1507	G1445	A1384	
	G2261	G2141	C2077	U2017	U1951		U1825	A1760		A1634	A1572	C1507	A1385	
	C2264	A2142	U2079	G2018	A1952	G1888	G1826	C1760	G1699	A1635	C1574	A1509	C1386	
U2325	U2265	C2143	A2080	A2019	A1953	A1889	U1827	G1761	U1700	A1636	C1575	A1509	A1387	
A2326	A2266	G2204	U2081	A2020	G1954	A1890	A1828	A1762	G1511	A1637	U1576	G1510	G1388	
G2327	A2267	C2145	A2082	C2021	U1955	G1891	A1829	G1763	A1701	C1638	C1577	G1512	G1389	
U2329	A2267	C2146	G2083	U2022	U1956	C1892	C1830	U1765	G1702	C1639	U1578	U1513	U1390	
G2330	A2268	C2207	C2084	C2023	C1957	C1893	G1831	U1766	C1704	A1640	A1579	G1514	G1451	
G2331	G2269	G2024	U2085	C2024	C1958	C1894	G1767	G1766		A1580	A1580	A1515	A1392	
C2332	A2270	U2149	U2086	C2025	G1959	C1895	C1833	C1768	G1707	G1642	C1582		A1393	





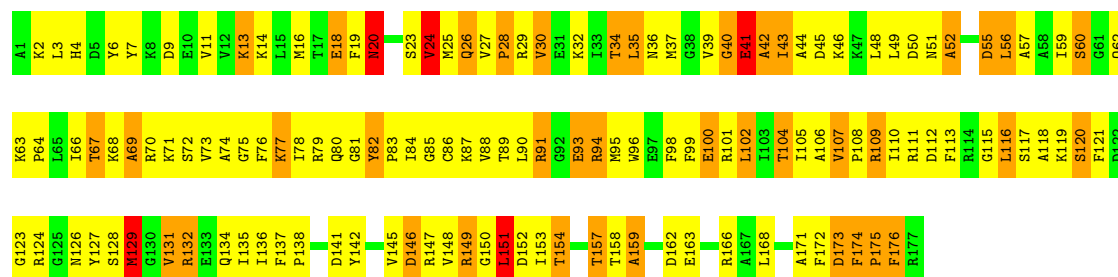
• Molecule 29: 50S ribosomal protein L4

Chain BE: 37% 53% 9%



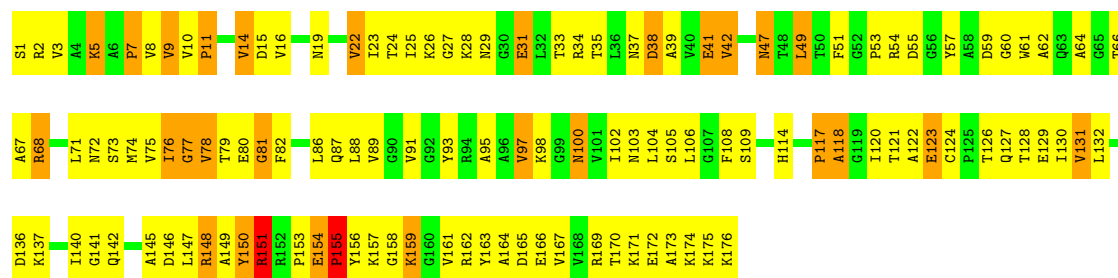
• Molecule 30: 50S ribosomal protein L5

Chain BF: 23% 53% 22%



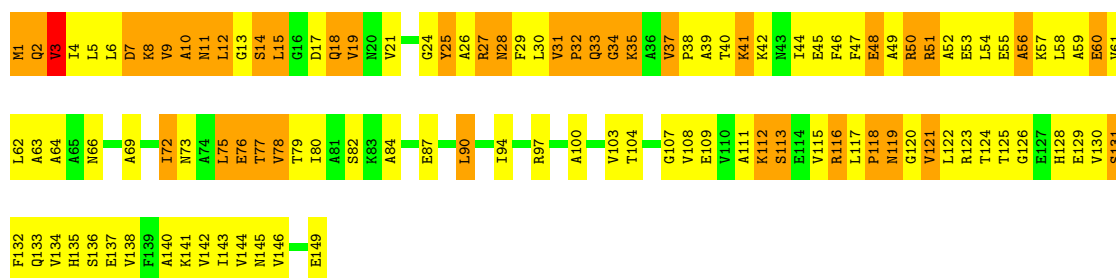
• Molecule 31: 50S ribosomal protein L6

Chain BG: 30% 53% 15%



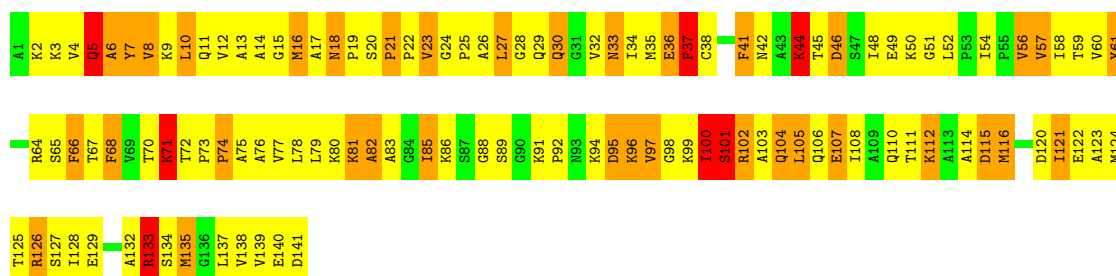
• Molecule 32: 50S ribosomal protein L9

Chain BH: 23% 49% 27%



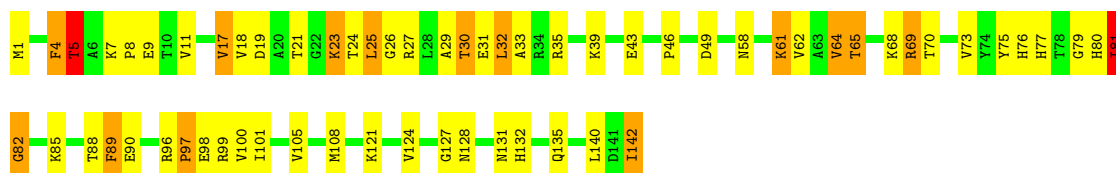
• Molecule 33: 50S ribosomal protein L11

Chain BI: 16% 53% 26% 5%



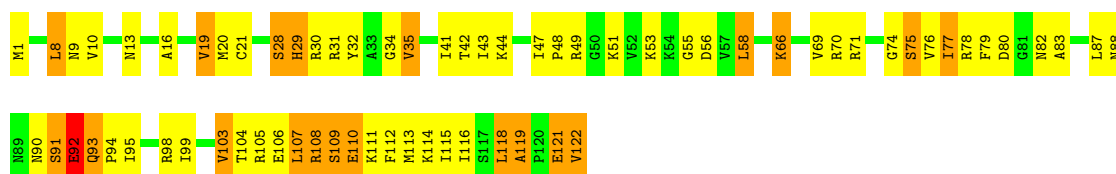
• Molecule 34: 50S ribosomal protein L13

Chain BJ: 56% 33% 10%



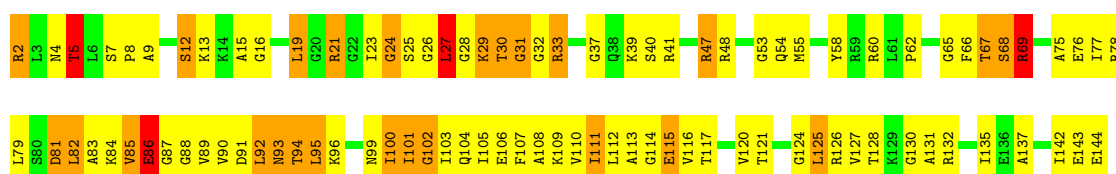
• Molecule 35: 50S ribosomal protein L14

Chain BK: 43% 39% 16%

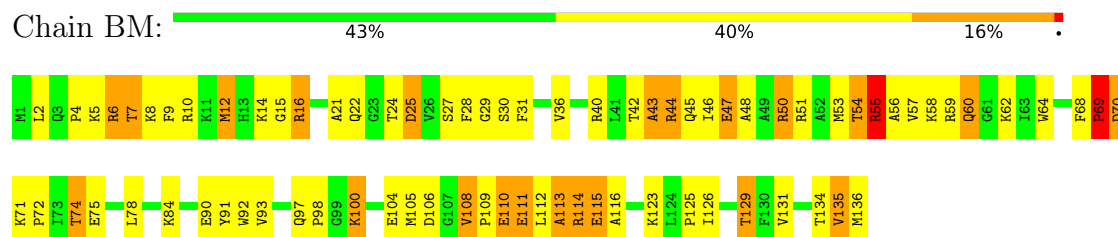


• Molecule 36: 50S ribosomal protein L15

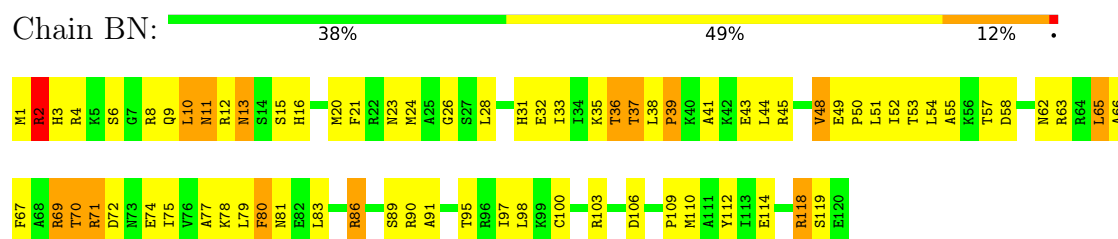
Chain BL: 34% 46% 17%



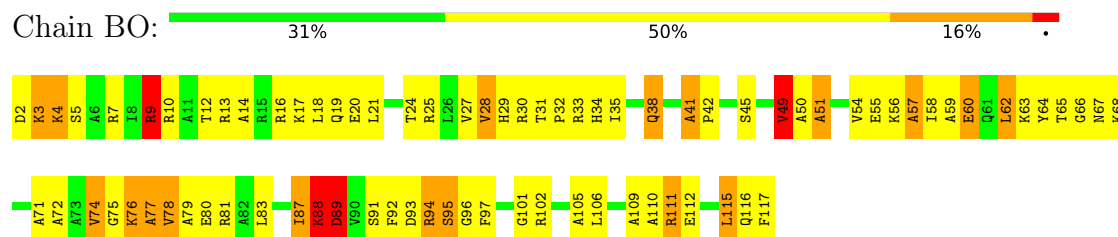
- Molecule 37: 50S ribosomal protein L16



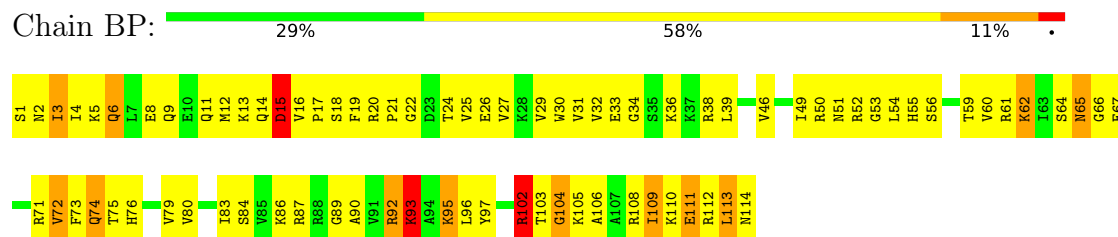
- Molecule 38: 50S ribosomal protein L17



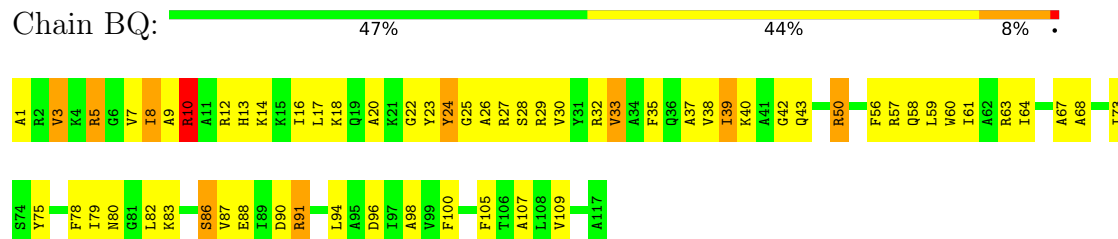
- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19

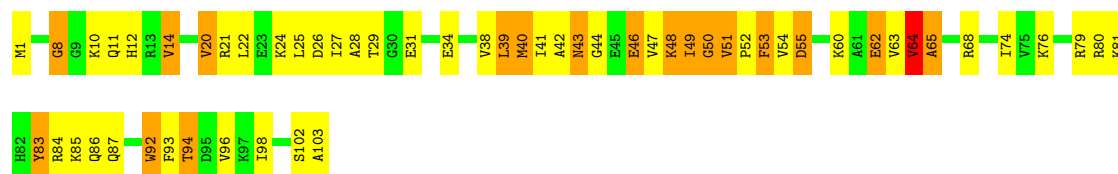


- Molecule 41: 50S ribosomal protein L20



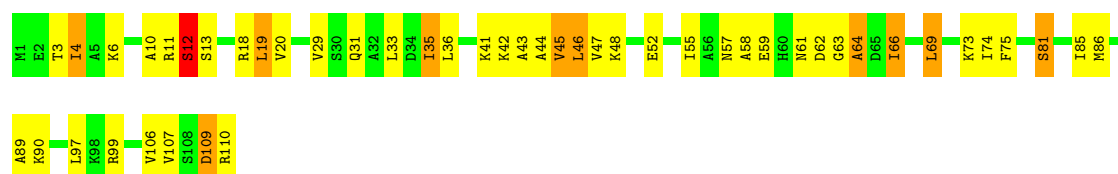
- Molecule 42: 50S ribosomal protein L21

Chain BR: 

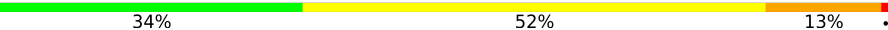


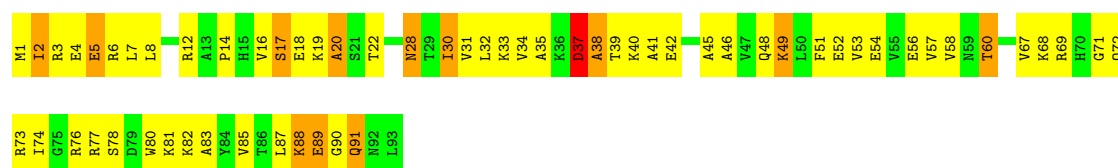
• Molecule 43: 50S ribosomal protein L22

Chain BS: 



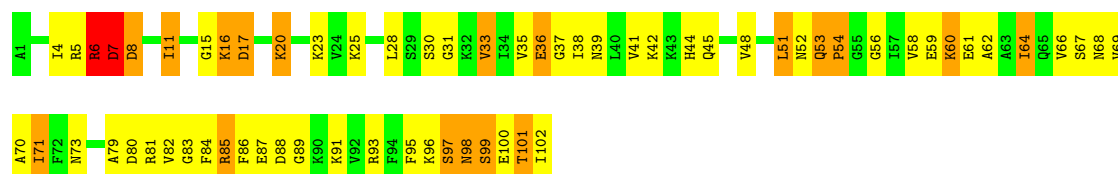
• Molecule 44: 50S ribosomal protein L23

Chain BT: 



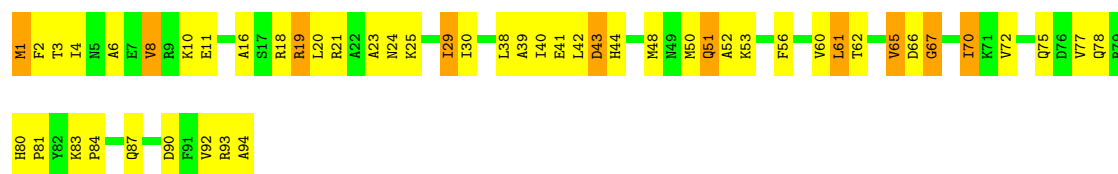
• Molecule 45: 50S ribosomal protein L24

Chain BU: 



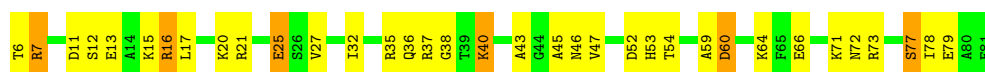
• Molecule 46: 50S ribosomal protein L25

Chain BV: 



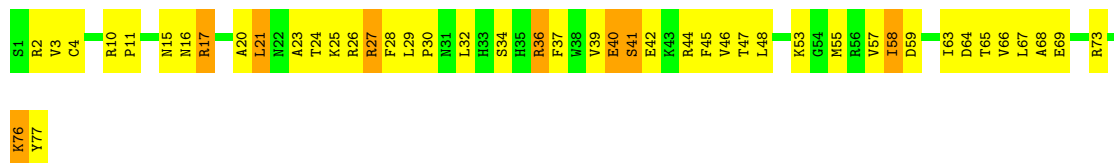
• Molecule 47: 50S ribosomal protein L27

Chain BW: 



- Molecule 48: 50S ribosomal protein L28

Chain BX: 40% 49% 10%



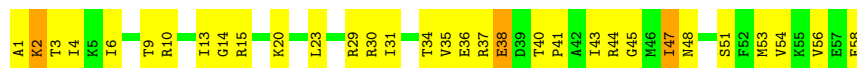
- Molecule 49: 50S ribosomal protein L29

Chain BY: 24% 46% 27%



- Molecule 50: 50S ribosomal protein L30

Chain BZ: 45% 50% 5%



- Molecule 51: 50S ribosomal protein L32

Chain B0: 48% 38% 14%



- Molecule 52: 50S ribosomal protein L33

Chain B1: 30% 54% 14%



- Molecule 53: 50S ribosomal protein L34

Chain B2: 46% 46% 7%



- Molecule 54: 50S ribosomal protein L35

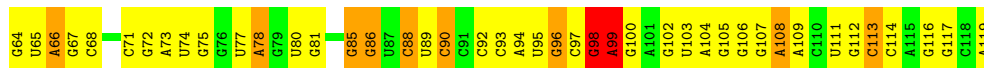
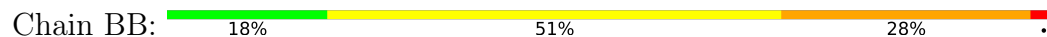
Chain B3: 45% 52% 3%



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 5S ribosomal RNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68843	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	The volumes were CTF-corrected in defocus groups, with an average of approximately 215 individual images per group	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU

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	AA	0.85	5/36944 (0.0%)	1.26	314/57632 (0.5%)
10	AJ	0.57	0/797	0.74	0/1077
11	AK	0.67	0/893	0.82	0/1205
12	AL	0.61	0/969	0.81	0/1300
13	AM	0.52	0/893	0.74	0/1193
14	AN	0.55	0/785	0.76	0/1043
15	AO	0.55	0/722	0.73	0/964
16	AP	0.54	0/659	0.82	1/884 (0.1%)
17	AQ	0.57	0/658	0.74	0/881
18	AR	0.61	0/463	0.70	0/621
19	AS	0.48	0/653	0.73	0/877
2	AB	0.60	0/1736	0.79	0/2338
20	AT	0.54	0/671	0.69	0/888
21	AU	0.93	0/431	0.97	0/570
22	AV	0.56	13/7912 (0.2%)	0.91	43/12332 (0.3%)
23	AW	0.79	1/1011 (0.1%)	0.96	1/1354 (0.1%)
24	AX	0.65	0/1832	0.81	0/2855
25	AY	0.40	0/5313	0.69	0/7195
26	BA	1.60	611/69795 (0.9%)	1.67	2068/108884 (1.9%)
27	BC	0.80	0/2122	0.90	1/2852 (0.0%)
28	BD	0.96	0/1586	0.92	1/2134 (0.0%)
29	BE	0.91	0/1571	0.89	1/2113 (0.0%)
3	AC	0.56	0/1652	0.71	0/2225
30	BF	0.65	0/1435	0.74	0/1926
31	BG	0.75	0/1343	0.85	1/1816 (0.1%)
32	BH	0.68	1/1121 (0.1%)	0.77	0/1515
33	BI	0.72	0/1046	0.74	0/1410
34	BJ	1.01	0/1152	0.84	1/1551 (0.1%)
35	BK	0.92	2/948 (0.2%)	0.94	1/1268 (0.1%)
36	BL	0.94	0/1054	1.01	0/1403
37	BM	0.94	0/1093	0.96	0/1460
38	BN	0.91	0/974	0.96	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BO	0.76	0/902	0.87	1/1209 (0.1%)
4	AD	0.59	0/1665	0.74	1/2227 (0.0%)
40	BP	0.89	0/929	0.88	1/1242 (0.1%)
41	BQ	1.14	0/960	0.96	1/1278 (0.1%)
42	BR	1.01	1/829 (0.1%)	0.98	0/1107
43	BS	1.08	1/864 (0.1%)	0.97	1/1156 (0.1%)
44	BT	0.82	0/745	0.86	0/994
45	BU	0.91	0/788	0.90	0/1051
46	BV	0.79	0/766	0.81	0/1025
47	BW	1.02	0/582	0.97	0/769
48	BX	0.79	0/635	0.84	0/848
49	BY	0.76	0/510	0.96	1/677 (0.1%)
5	AE	0.62	0/1119	0.85	0/1504
50	BZ	1.04	0/453	0.95	0/605
51	B0	0.96	0/450	0.98	2/599 (0.3%)
52	B1	0.75	0/417	0.76	0/554
53	B2	1.03	0/380	0.99	2/498 (0.4%)
54	B3	0.94	0/513	0.85	0/676
55	B4	0.92	0/303	0.99	0/397
56	BB	1.33	4/2847 (0.1%)	1.58	79/4440 (1.8%)
6	AF	0.65	0/836	0.82	1/1128 (0.1%)
7	AG	0.50	0/1196	0.67	0/1602
8	AH	0.60	0/989	0.78	0/1326
9	AI	0.52	1/1034 (0.1%)	0.71	0/1375
All	All	1.19	640/170946 (0.4%)	1.35	2524/255354 (1.0%)

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
11	AK	0	1
13	AM	0	1
14	AN	0	1
21	AU	0	2
23	AW	0	1
24	AX	0	4
27	BC	0	1
28	BD	0	2
33	BI	0	1
4	AD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	BR	0	1
45	BU	0	1
5	AE	0	1
50	BZ	0	1
9	AI	0	1
All	All	0	20

The worst 5 of 640 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1142	A	N9-C4	-18.15	1.26	1.37
26	BA	984	A	N9-C4	-13.41	1.29	1.37
26	BA	984	A	C5-C6	-10.40	1.31	1.41
26	BA	528	A	N7-C5	-10.33	1.33	1.39
26	BA	2250	G	N9-C4	-10.21	1.29	1.38

The worst 5 of 2524 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	984	A	C2-N3-C4	-18.77	101.21	110.60
26	BA	2250	G	N3-C4-C5	17.36	137.28	128.60
26	BA	1638	C	N1-C2-O2	-16.58	108.95	118.90
26	BA	1142	A	C2-N3-C4	-16.57	102.31	110.60
26	BA	1142	A	N3-C4-C5	16.05	138.03	126.80

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	47	LEU	Peptide
5	AE	100	GLU	Peptide
9	AI	5	TYR	Peptide
11	AK	125	LYS	Peptide
13	AM	111	PRO	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	AA	32995	0	16600	2522	0
2	AB	1705	0	1731	418	0
3	AC	1625	0	1695	268	0
4	AD	1643	0	1710	290	0
5	AE	1106	0	1147	238	0
6	AF	818	0	808	108	0
7	AG	1182	0	1238	130	0
8	AH	979	0	1034	159	0
9	AI	1022	0	1070	221	0
10	AJ	787	0	828	179	0
11	AK	877	0	887	162	0
12	AL	955	0	1019	110	0
13	AM	884	0	944	162	0
14	AN	774	0	827	134	0
15	AO	714	0	736	63	0
16	AP	649	0	666	105	0
17	AQ	649	0	691	118	0
18	AR	456	0	478	45	0
19	AS	638	0	665	77	0
20	AT	665	0	714	83	0
21	AU	426	0	449	138	0
22	AV	7135	0	3594	2248	0
23	AW	993	0	1030	330	0
24	AX	1640	0	835	262	0
25	AY	5215	0	5279	930	0
26	BA	62319	0	31328	3013	0
27	BC	2083	0	2157	231	0
28	BD	1565	0	1616	117	0
29	BE	1552	0	1619	139	0
30	BF	1411	0	1443	233	0
31	BG	1323	0	1374	154	0
32	BH	1110	0	1148	153	0
33	BI	1032	0	1086	289	0
34	BJ	1129	0	1162	61	0
35	BK	939	0	1012	77	0
36	BL	1045	0	1117	130	0
37	BM	1074	0	1157	125	0
38	BN	961	0	1000	90	0
39	BO	892	0	923	88	0
40	BP	917	0	965	96	0
41	BQ	947	0	1022	63	0
42	BR	816	0	839	84	0
43	BS	857	0	922	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BT	739	0	807	70	0
45	BU	780	0	834	63	0
46	BV	753	0	780	58	0
47	BW	575	0	589	29	0
48	BX	625	0	655	38	0
49	BY	509	0	543	88	0
50	BZ	449	0	491	28	0
51	B0	444	0	461	34	0
52	B1	410	0	440	36	0
53	B2	377	0	418	26	0
54	B3	504	0	574	41	0
55	B4	302	0	343	24	0
56	BB	2548	0	1292	102	0
All	All	157519	0	106792	14112	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 54.

The worst 5 of 14112 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)
23:AW:38:LYS:HE2	26:BA:1910:G:P	1.23	1.71
22:AV:172:U:H2'	22:AV:173:C:C6	1.25	1.65
25:AY:633:GLY:HA2	26:BA:1068:G:C8	1.19	1.62
22:AV:323:A:H2'	22:AV:324:G:C8	1.34	1.62
22:AV:48:C:C2'	22:AV:49:C:H5''	1.25	1.62

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	
2	AB	216/218 (99%)	109 (50%)	49 (23%)	58 (27%)	0	0
3	AC	204/206 (99%)	126 (62%)	48 (24%)	30 (15%)	0	4
4	AD	203/205 (99%)	123 (61%)	41 (20%)	39 (19%)	0	3
5	AE	148/150 (99%)	87 (59%)	38 (26%)	23 (16%)	0	4
6	AF	98/100 (98%)	62 (63%)	21 (21%)	15 (15%)	0	4
7	AG	149/151 (99%)	85 (57%)	42 (28%)	22 (15%)	0	4
8	AH	127/129 (98%)	79 (62%)	37 (29%)	11 (9%)	1	14
9	AI	125/127 (98%)	76 (61%)	34 (27%)	15 (12%)	0	7
10	AJ	96/98 (98%)	60 (62%)	14 (15%)	22 (23%)	0	1
11	AK	115/117 (98%)	84 (73%)	17 (15%)	14 (12%)	0	7
12	AL	121/123 (98%)	85 (70%)	29 (24%)	7 (6%)	2	23
13	AM	112/114 (98%)	78 (70%)	22 (20%)	12 (11%)	0	9
14	AN	92/100 (92%)	47 (51%)	27 (29%)	18 (20%)	0	2
15	AO	86/88 (98%)	57 (66%)	22 (26%)	7 (8%)	1	16
16	AP	80/82 (98%)	48 (60%)	11 (14%)	21 (26%)	0	1
17	AQ	78/80 (98%)	47 (60%)	18 (23%)	13 (17%)	0	4
18	AR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	0	8
19	AS	77/79 (98%)	37 (48%)	28 (36%)	12 (16%)	0	4
20	AT	83/85 (98%)	37 (45%)	31 (37%)	15 (18%)	0	3
21	AU	49/51 (96%)	20 (41%)	15 (31%)	14 (29%)	0	0
23	AW	120/123 (98%)	84 (70%)	24 (20%)	12 (10%)	0	12
25	AY	663/691 (96%)	436 (66%)	136 (20%)	91 (14%)	0	5
27	BC	269/271 (99%)	217 (81%)	31 (12%)	21 (8%)	1	17
28	BD	207/209 (99%)	166 (80%)	30 (14%)	11 (5%)	2	25
29	BE	199/201 (99%)	158 (79%)	32 (16%)	9 (4%)	3	28
30	BF	175/177 (99%)	118 (67%)	38 (22%)	19 (11%)	0	9
31	BG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	1	15
32	BH	147/149 (99%)	95 (65%)	29 (20%)	23 (16%)	0	4
33	BI	139/141 (99%)	65 (47%)	47 (34%)	27 (19%)	0	2
34	BJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	28
35	BK	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	20
36	BL	141/143 (99%)	99 (70%)	21 (15%)	21 (15%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BM	134/136 (98%)	111 (83%)	14 (10%)	9 (7%)	1	20
38	BN	118/120 (98%)	92 (78%)	20 (17%)	6 (5%)	2	25
39	BO	114/116 (98%)	83 (73%)	17 (15%)	14 (12%)	0	6
40	BP	112/114 (98%)	96 (86%)	12 (11%)	4 (4%)	4	32
41	BQ	115/117 (98%)	100 (87%)	13 (11%)	2 (2%)	10	49
42	BR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	16
43	BS	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	24
44	BT	91/93 (98%)	67 (74%)	13 (14%)	11 (12%)	0	7
45	BU	100/102 (98%)	75 (75%)	13 (13%)	12 (12%)	0	7
46	BV	92/94 (98%)	79 (86%)	11 (12%)	2 (2%)	7	42
47	BW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	5	38
48	BX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	5	38
49	BY	61/63 (97%)	34 (56%)	13 (21%)	14 (23%)	0	1
50	BZ	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
51	B0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	4	31
52	B1	48/50 (96%)	32 (67%)	12 (25%)	4 (8%)	1	15
53	B2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	7	41
54	B3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
55	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	37
All	All	6401/6536 (98%)	4452 (70%)	1212 (19%)	737 (12%)	1	7

5 of 737 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	PHE
2	AB	21	TYR
2	AB	33	ALA
2	AB	63	LYS
2	AB	67	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	114 (63%)	66 (37%)	0	1
3	AC	170/170 (100%)	125 (74%)	45 (26%)	0	4
4	AD	172/172 (100%)	132 (77%)	40 (23%)	1	5
5	AE	113/113 (100%)	80 (71%)	33 (29%)	0	3
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	2
7	AG	124/124 (100%)	90 (73%)	34 (27%)	0	4
8	AH	104/104 (100%)	78 (75%)	26 (25%)	0	4
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	3
10	AJ	86/86 (100%)	63 (73%)	23 (27%)	0	4
11	AK	90/90 (100%)	66 (73%)	24 (27%)	0	4
12	AL	103/103 (100%)	86 (84%)	17 (16%)	2	15
13	AM	92/92 (100%)	73 (79%)	19 (21%)	1	8
14	AN	79/83 (95%)	56 (71%)	23 (29%)	0	3
15	AO	76/76 (100%)	61 (80%)	15 (20%)	1	9
16	AP	65/65 (100%)	45 (69%)	20 (31%)	0	2
17	AQ	74/74 (100%)	54 (73%)	20 (27%)	0	4
18	AR	48/48 (100%)	40 (83%)	8 (17%)	2	15
19	AS	70/70 (100%)	56 (80%)	14 (20%)	1	9
20	AT	65/65 (100%)	45 (69%)	20 (31%)	0	2
21	AU	44/44 (100%)	23 (52%)	21 (48%)	0	0
23	AW	101/102 (99%)	76 (75%)	25 (25%)	0	5
25	AY	563/582 (97%)	489 (87%)	74 (13%)	4	22
27	BC	216/216 (100%)	182 (84%)	34 (16%)	3	17
28	BD	164/164 (100%)	143 (87%)	21 (13%)	5	22
29	BE	165/165 (100%)	143 (87%)	22 (13%)	4	22
30	BF	148/148 (100%)	112 (76%)	36 (24%)	1	5
31	BG	137/137 (100%)	114 (83%)	23 (17%)	2	15
32	BH	114/114 (100%)	89 (78%)	25 (22%)	1	7
33	BI	109/109 (100%)	78 (72%)	31 (28%)	0	3
34	BJ	116/116 (100%)	97 (84%)	19 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BK	103/103 (100%)	85 (82%)	18 (18%)	2	13
36	BL	102/102 (100%)	81 (79%)	21 (21%)	1	8
37	BM	109/109 (100%)	87 (80%)	22 (20%)	1	9
38	BN	100/100 (100%)	83 (83%)	17 (17%)	2	14
39	BO	86/86 (100%)	68 (79%)	18 (21%)	1	8
40	BP	99/99 (100%)	78 (79%)	21 (21%)	1	7
41	BQ	89/89 (100%)	76 (85%)	13 (15%)	3	19
42	BR	84/84 (100%)	70 (83%)	14 (17%)	2	15
43	BS	93/93 (100%)	83 (89%)	10 (11%)	7	28
44	BT	80/80 (100%)	69 (86%)	11 (14%)	4	21
45	BU	83/83 (100%)	64 (77%)	19 (23%)	1	6
46	BV	78/78 (100%)	63 (81%)	15 (19%)	1	10
47	BW	56/58 (97%)	50 (89%)	6 (11%)	7	28
48	BX	67/67 (100%)	56 (84%)	11 (16%)	2	15
49	BY	55/55 (100%)	46 (84%)	9 (16%)	2	15
50	BZ	48/48 (100%)	40 (83%)	8 (17%)	2	15
51	B0	47/47 (100%)	41 (87%)	6 (13%)	5	22
52	B1	45/45 (100%)	38 (84%)	7 (16%)	3	17
53	B2	38/38 (100%)	32 (84%)	6 (16%)	3	17
54	B3	51/51 (100%)	48 (94%)	3 (6%)	21	52
55	B4	34/34 (100%)	28 (82%)	6 (18%)	2	13
All	All	5327/5353 (100%)	4230 (79%)	1097 (21%)	4	8

5 of 1097 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	AT	47	GLN
25	AY	572	TYR
45	BU	60	LYS
21	AU	15	LEU
25	AY	88	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
25	AY	475	ASN
29	BE	90	GLN
49	BY	25	GLN
25	AY	573	HIS
27	BC	85	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	457 (29%)	27 (1%)
22	AV	332/363 (91%)	187 (56%)	32 (9%)
24	AX	76/77 (98%)	37 (48%)	3 (3%)
26	BA	2901/2903 (99%)	770 (26%)	58 (1%)
56	BB	118/119 (99%)	24 (20%)	1 (0%)
All	All	4964/5001 (99%)	1475 (29%)	121 (2%)

5 of 1475 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	9	G
1	AA	12	U

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	AV	308	U
26	BA	271	G
26	BA	2286	G
22	AV	320	U
24	AX	54	G

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

3 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
22	5MU	AV	341	22	13,22,23	1.46	1 (7%)	14,32,35	1.90	3 (21%)
22	PSU	AV	342	22	16,21,22	1.89	3 (18%)	20,30,33	5.41	7 (35%)
22	PSU	AV	347	22	16,21,22	1.68	3 (18%)	20,30,33	5.41	5 (25%)

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
22	5MU	AV	341	22	-	0/3/25/26	0/2/2/2
22	PSU	AV	342	22	-	1/7/25/26	0/2/2/2
22	PSU	AV	347	22	-	2/7/25/26	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	342	PSU	C5-C1'	-6.06	1.47	1.52
22	AV	347	PSU	C5-C1'	-5.13	1.47	1.52
22	AV	341	5MU	C4-N3	3.94	1.39	1.33
22	AV	347	PSU	C4-N3	2.66	1.37	1.33
22	AV	347	PSU	C2-N1	2.59	1.43	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	347	PSU	N1-C2-N3	-17.03	114.89	128.43
22	AV	342	PSU	N1-C2-N3	-16.47	115.34	128.43
22	AV	347	PSU	C4-N3-C2	14.16	127.10	115.14
22	AV	342	PSU	C4-N3-C2	13.97	126.93	115.14
22	AV	342	PSU	C5-C4-N3	-8.72	114.12	125.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AV	347	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
22	AV	342	PSU	O4'-C1'-C5-C4
22	AV	347	PSU	C2'-C1'-C5-C6

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	341	5MU	6	0
22	AV	342	PSU	3	0
22	AV	347	PSU	7	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.