



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:10 PM BST

PDB ID : 3J5L
EMDB ID: : EMD-5771
Title : Structure of the E. coli 50S subunit with ErmBL nascent chain
Authors : Arenz, S.; Ramu, H.; Gupta, P.; Berninghausen, O.; Beckmann, R.; Vazquez-Laslop, N.; Mankin, A.S.; Wilson, D.N.
Deposited on : 2013-10-23
Resolution : 6.60 Å(reported)
Based on PDB ID : 3OFR

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

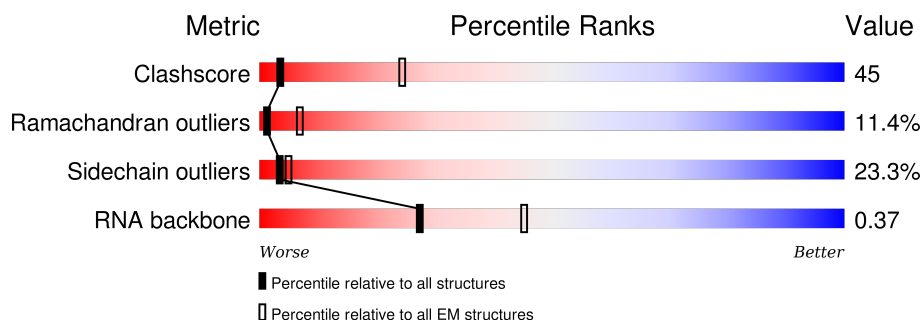
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 Å.

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







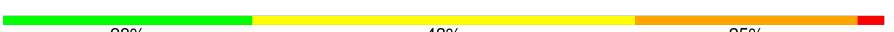
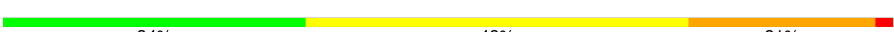
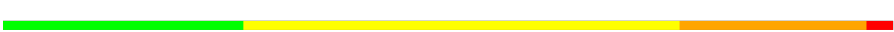





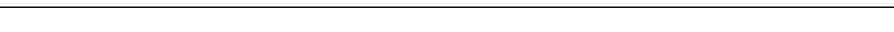

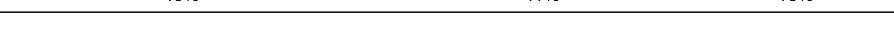

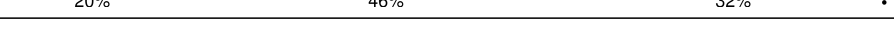

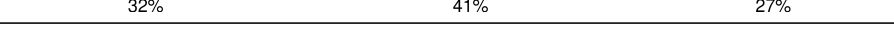


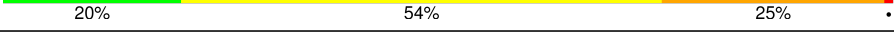


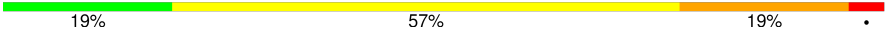
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	0	56	34% 48% 18%
2	1	50	32% 48% 20%
3	2	46	46% 33% 22%
4	3	64	36% 45% 17% .
5	4	38	32% 53% 13% .
6	5	2	100%
7	6	10	40% 40% 20%
8	7	3	33% 33% 33%

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Mol	Chain	Length	Quality of chain
9	A	2904	
10	B	118	
11	C	271	
12	D	209	
13	E	201	
14	F	177	
15	G	176	
16	H	56	
17	I	141	
18	J	142	
19	K	122	
20	L	143	
21	M	136	
22	N	120	
23	O	116	
24	P	114	
25	Q	117	
26	R	103	
27	S	110	
28	T	93	
29	U	102	
30	V	94	
31	W	79	
32	X	77	
33	Y	63	

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Mol	Chain	Length	Quality of chain
34	Z	58	<div><div></div><div>41%</div><div>34%</div><div>22%</div><div></div></div>

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 89382 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 protein called 50S ribosomal protein L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a RNA chain called 5'-R(*CP*(MA6))-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	2	Total	C	N	O	P	0	0
			41	21	8	11	1		

- Molecule 7 is a protein called Erythromycin resistance leader peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	6	8	Total C 8 8	0	8

- Molecule 8 is a RNA chain called 5'-R(*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	7	3	Total C N O P 59 28 11 18 2	0	0

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	A	2853	Total C N O P 61251 27324 11274 19800 2853	0	0

- Molecule 10 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	B	117	Total C N O P 2506 1116 459 814 117	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	56	Total	C	N	O	S	0	0
			431	275	77	78	1		

- Molecule 17 is a protein called 50S ribosomal protein L11.

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

- Molecule 18 is a protein called 50S ribosomal protein L13.

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

- Molecule 19 is a protein called 50S ribosomal protein L14.

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

- Molecule 20 is a protein called 50S ribosomal protein L15.

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

- Molecule 21 is a protein called 50S ribosomal protein L16.

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

- Molecule 22 is a protein called 50S ribosomal protein L17.

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

- Molecule 23 is a protein called 50S ribosomal protein L18.

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

- Molecule 24 is a protein called 50S ribosomal protein L19.

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

- Molecule 25 is a protein called 50S ribosomal protein L20.

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

- Molecule 26 is a protein called 50S ribosomal protein L21.

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

- Molecule 27 is a protein called 50S ribosomal protein L22.

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

- Molecule 28 is a protein called 50S ribosomal protein L23.

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

- Molecule 29 is a protein called 50S ribosomal protein L24.

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

- Molecule 30 is a protein called 50S ribosomal protein L25.

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

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 32 is a protein called 50S ribosomal protein L28.

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

- Molecule 33 is a protein called 50S ribosomal protein L29.

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

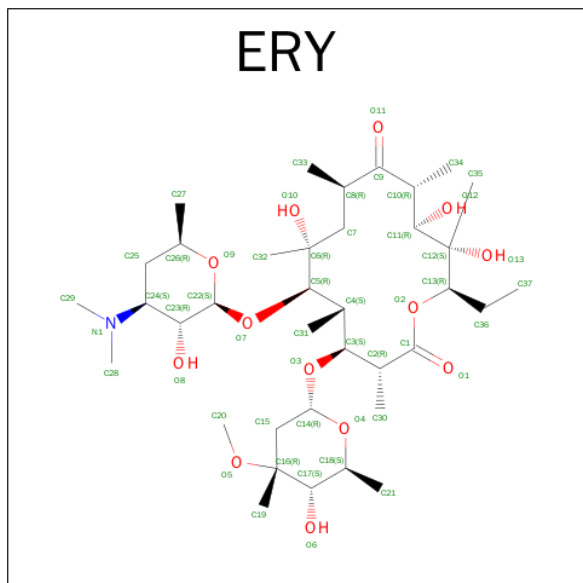
- Molecule 34 is a protein called 50S ribosomal protein L30.

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

- Molecule 35 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms				AltConf
35	5	1	Total	C	N	O	0
			4	2	1	1	

- Molecule 36 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).

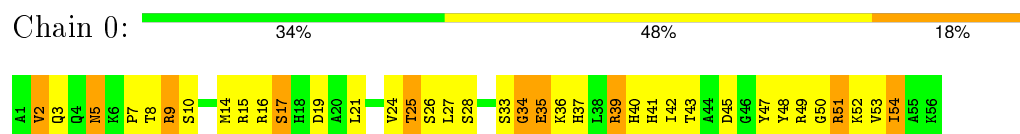


Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	N	O	0
			51	37	1	13	

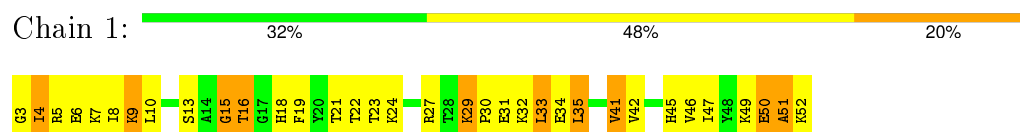
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

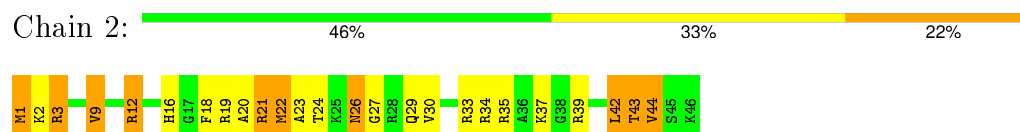
- Molecule 1: 50S ribosomal protein L32



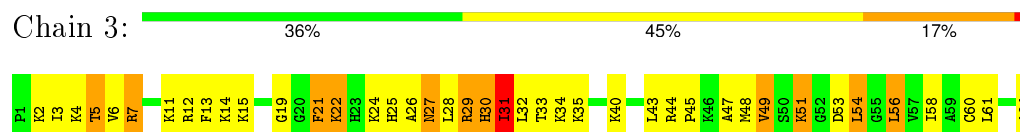
- Molecule 2: 50S ribosomal protein L33



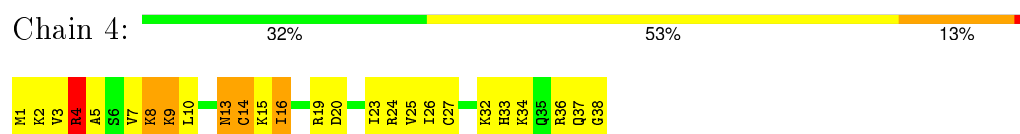
- Molecule 3: 50S ribosomal protein L34



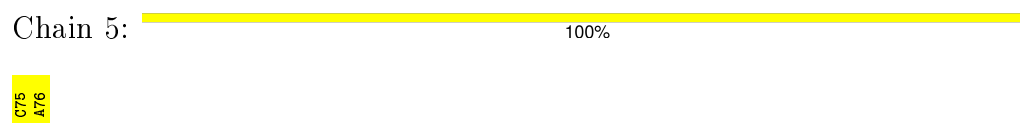
- Molecule 4: 50S ribosomal protein L35



- Molecule 5: 50S ribosomal protein L36



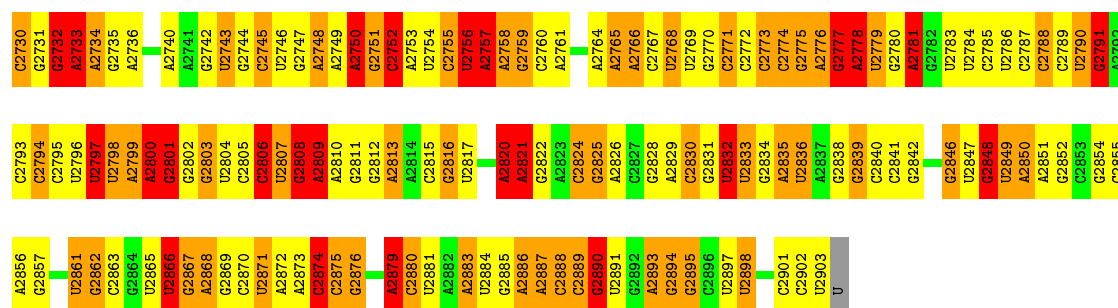
- Molecule 6: 5'-R(*CP*(MA6))-3'



WORLDWIDE
PDB
PROTEIN DATA BANK

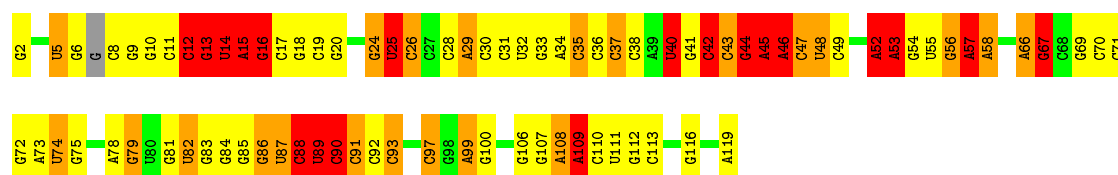
 **EMDataBank**
Unified Data Resource for 3DEM

C2666	A2602	C2540	U2479	C2417	C2350	G2290	A2237	U	G2107	A2042	A1977	A1916	G1850	A1785	U1720
C2667	G2603	A2541	C2480	A2418	G2351	U2291	G2228	G	A2108	A2043	A1978	U1917	U1851	A1786	G1721
G2668	U2604	A2542	G2481	U2419	A2352	U2292	U2230	A	U2109	C2043	U1979	A1918	C1852	A1787	A1722
G2669	U2605	G2543	A2482	C2420	G2353	G2293	G2230	A	G2110	C2044	G1980	A1919	A1853	C1788	
A2670	C2606	G2544	G2483	G2421	C2354	G2294	U2231	A	U		U1981	C1920	A1854	A1789	U1726
G2671	G2607	G2545	G2484	C2422	C2355	G2295	C2232	A	U	C2047	U1982	G1921	U1855	C1790	G1727
G2608	G2608	U2546	G2485	U2423	U2356	U2296	U2233	A	U	G2048	G1983	G1922	U1856	A1791	C1728
U2609	U2609	A2547	C2486	C2424	C2357	A2297	G2234	C	A	G2049	G1984	U1923	G1857	G1792	
C2610	C2610	U2548	G2487	A2425	A2358	A2298	G2235	C	U	C2050	G1985	C1924	U1858	C1793	
C2611	G2611	A2426	G2488	A2426		U2299	U2236	A	G	A2051	C1986	C1925	A1858	A1794	G1730
U2613	U2613	C2427	U2489	C2427	C2360	G2300	U2237	C	A	A2052	U1987	U1926	C1859	G1731	
A2614	A2614	G2428	G2490	G2428	C2362	U2302	G2238	C	A	G2053	G1988	A1927	U1860	G1732	
U2491	U2491	G2429	G2491	G2429	G2363	G2303	G2239	U	A	A2054	G1989	A1928	U1864	G1733	
U2492	U2492	A2430	U2492	A2430	C2364	G2303		G	U	C2055	C1990	G1929	U1865	G1734	
U2554	G2493	U2431	G2493	U2431	G2365	G2304	U2243	U2180	G	C2056	U1991	G1930	U1866	U1798	
U2555	G2494	A2432	A2494	A2432	A2366	U2305	U2244	U2181	U	G2057	G1992	U1931	G1867	A1799	U1736
C2556	G2495	A2433	G2495	C2367	G2367	C2306	U2245	A2183	G		U1993	A1932	C1868	C1800	
G2557	C2496	C2368	G2496	C2368	G2368	G2307	U2246	A2184	G	A2060	C1994	G1933	C1869	G1737	
A2497	A2497					G2308	A2247	U2185	U	G2061	U1995	C1934	C1870	G1738	
C2498	C2498	G2373	G2498	A2436		A2309	A2248	A2186	A	A2062	C1996	G1935	A1871	A1739	
C2499	C2499	G2374	G2437	U2437	G2374	C2310	U2249	U2187	G	C2063	C1997	A1936	A1872	G1740	
U2500	U2500	G2375	U2438	U2438	G2375	G2310	C2248	U2187	G	C2064	A1998	G1873	A1867	U1742	
C2501	C2501	A2439	A2439	A2439	G2380	U2312	G2250	U2188	G	C2065	A1999	A1938	C1867	G1743	
G2502	G2502	C2440	C2440	C2440	A2381	G2313	G2251	U2189	C	C2066	C2000	U1939	C1868	A1801	
A2503	A2503	U2441	U2441	U2441	C2382	A2314	G2252	G2190	U	G2067	C2001	U1940	C1876	G1738	
C2504	C2504	C2442	C2442	C2442	G2383	G2315		A2191	U	U2068	G2002	C1941	A1877	A1745	
G2505	G2505	G2443	G2443	G2444	U2384	G2316	G2255	U2192	U	G2069		C1942	A1878	A1746	
U2506	U2506	A2317	A2317	A2317	G2385	G2317	U2257	U2193	G	C2070	C2006	C1943	C1878	U1747	
C2507	C2507	G2386	G2386	G2386	U2387	G2318	G2258	U2195	A2135	C2071	U2007	U1944	C1879	C1748	
G2508	G2508	A2387	A2387	A2387	U2387	U2320	G2260	U2197	G2136	C2072	C2008	G1945	C1817	A1749	
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C2510	C2510	A2450	A2450	A2450	A2388	A2322	G2262	A2198	U2138	U2075	U2012	C1947	U1883	A1819	
G2511	G2511	C2451	C2451	C2451	U2389	G2323	G2263	A2199	U2139	U2076	G2013	G1950	G1884	A1754	
A2512	A2512	A2452	A2452	A2452	G2390	U2324	G2264	G2200	G2140	A2077	A2014	U1951	A1821	A1755	
C2513	C2513	G2453	G2453	G2453	G2391	G2325	U2265	G2201	G2141	C2078	A2015	A1952	A1822	G1756	
U2514	U2514	A2454	A2454	A2454	A2392	G2326	U2266	U2202	A2142	U2079	U2016	A1953	G1823	A1757	
C2515	C2515	G2455	G2455	G2455	U2393	A2327	A2267	U2203	G2143	A2080	U2017	G1954	G1824	A1758	
G2516	G2516	C2456	C2456	C2456	C2394	A2327	A2267	G2204	G2144	U2081	U2018	U1955	U1825	C1760	
C2517	C2517	U2457	U2457	U2457	C2395	A2328	A2268	A2205	C2145	A2082	G2019	U1956	G1826	C1761	
A2518	A2518	G2458	G2458	G2458	G2396	U2329	G2269	C2206	G2146	C2083	A2019	U1956	G1827	A1762	
U2519	U2519	C2459	C2459	C2459	G2397	G2330	A2270	C2207	A2147	C2084	A2020	C1957	G1828	G1763	
C2520	C2520	A2460	A2460	A2460	U2398	G2331	G2271	C2208	G2148	U2085	C2021	C1958	C1764	C1764	
G2521	G2521	U2461	U2461	U2461	G2399	C2332	U2272	C2209	U2149	U2086	U2022	G1959	U1765	U1765	
U2522	U2522	A2462	A2462	A2462	G2400	A2333	A2273	U2210	C2150	G2087	C2023	A1960	G1833	G1766	
G2523	G2523	C2463	C2463	C2463	U2401	U2334	A2274	A2211	U2151	A2088	G2024	C1961	U1898	G1767	
C2524	C2524	U2402	U2402	U2402	A2403	A2335	C2275	A2212	G2152	C2089	C2025	U1962	A1899	C1768	
G2525	G2525	G2404	G2404	G2404	U2404	A2336	G2276	U2213	C2153		U2026	U1963	A1900	U1769	
G2526	G2526	C2405	C2405	C2405	U2405	G2337	G2277	C2214	A2154	U2093	G2027	G1964	C1837		
C2527	C2527	A2406	A2406	A2406	G2406	C2338	A2278	C2215	U2155	U2094	U2028	G1965	C1838	A1773	
U2528	U2528	C2467	C2467	C2467	A2407	C2339	G2279	G2216	G2156	A2094	G2029	A1966	G1839	C1774	
G2529	G2529	A2468	A2468	A2468	U2407	A2340	G2280	G2217	G2157	A2095	A2030	C1967	G1840	U1775	
A2530	A2530	U2469	U2469	U2469	U2408	G2341	A2281	U2218	A	C2096	A2031	G1968	G1907	G1776	
C2531	C2531	G2470	G2470	G2470	G2409	C2342	G2282	U2219	G	A2097	G2032	A1969	C1908	U1777	
G2532	G2532	A2471	A2471	A2471	G2410	U2343	C2283	U2220	C	U2098	A2033	A1970	C1909	U1778	
U2533	U2533	A2411	A2411	A2411	G2411	G2345	A2284	G2221	U2099	U2099	U2034	U1971	G1910	U1779	
		U2473	U2473	U2473	A2412	G2346	C2285	G2222	C		G2035	G1972	U1911	A1780	
					G2413	A2346	G2286	G2223	A	C2103	C2036	G1973	A1912	U1781	
					G2414	G2347	A2287	G2224	C	C2104	A2037	C1974	A1913	U1782	
					G2415	G2348	A2288	G2225	C	U2105	G2038	G1975	A1848	A1783	
					G2416	G2349	G2289	G2226	U	U2106	U2039	U1976	G1849	A1784	



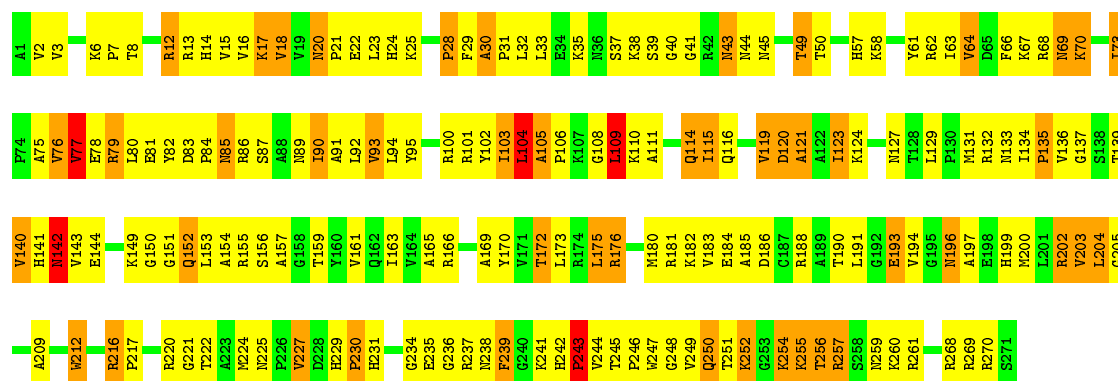
• Molecule 10: 5S ribosomal RNA

Chain B: 28% 36% 19% 16%



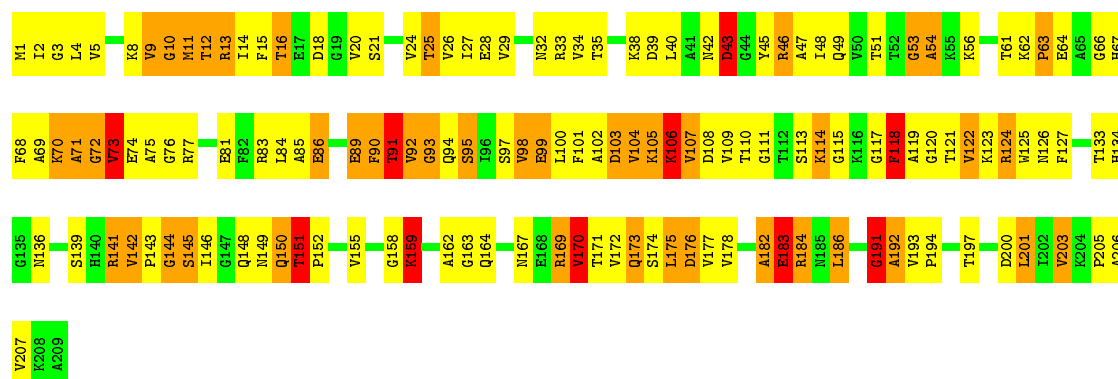
• Molecule 11: 50S ribosomal protein L2

Chain C: 33% 48% 17%

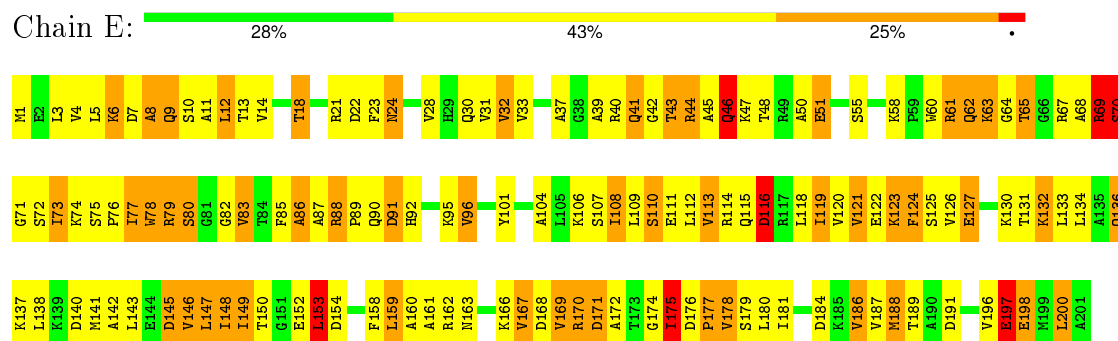


• Molecule 12: 50S ribosomal protein L3

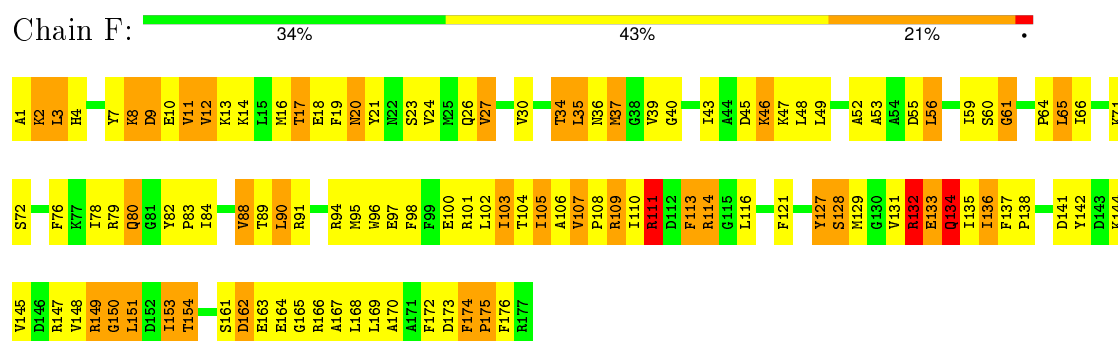
Chain D: 31% 44% 21% 5%



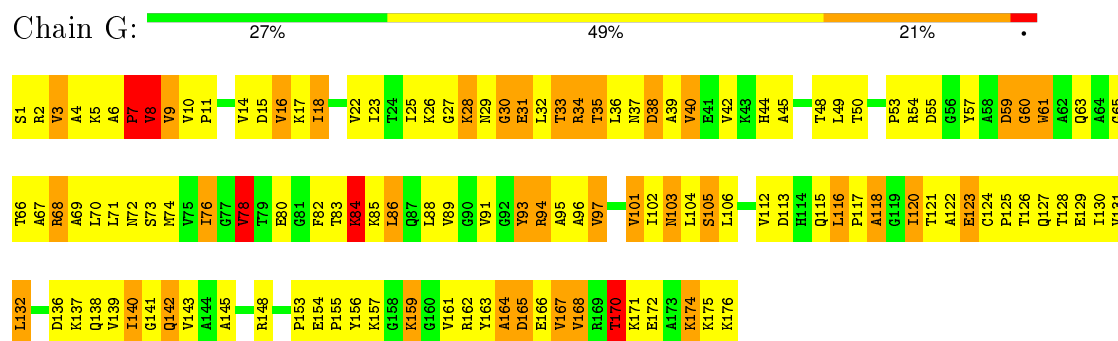
- Molecule 13: 50S ribosomal protein L4



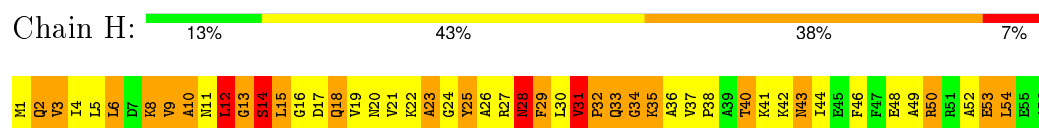
- Molecule 14: 50S ribosomal protein L5



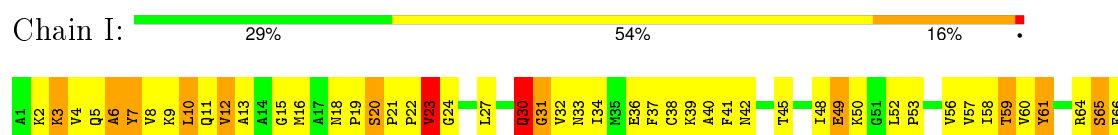
- Molecule 15: 50S ribosomal protein L6

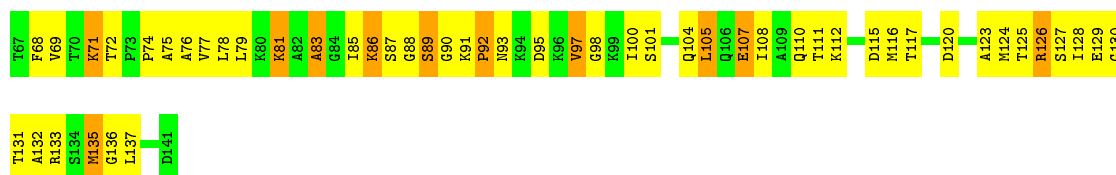


- Molecule 16: 50S ribosomal protein L9



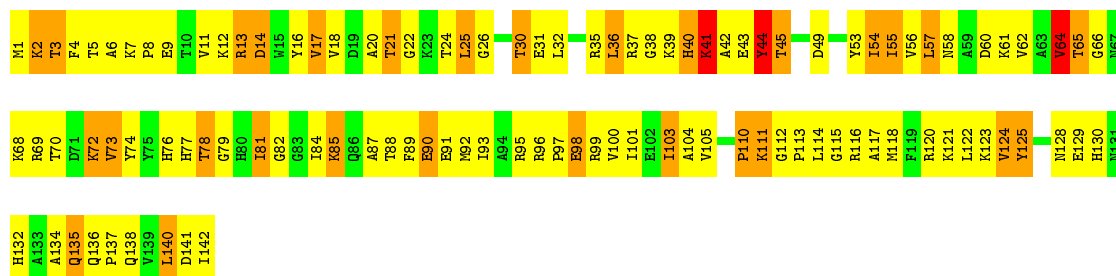
- Molecule 17: 50S ribosomal protein L11





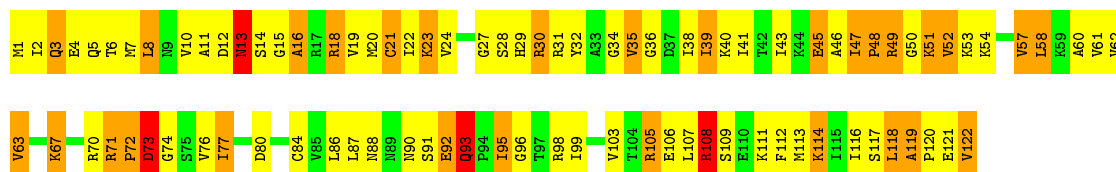
• Molecule 18: 50S ribosomal protein L13

Chain J: 25% 53% 20%



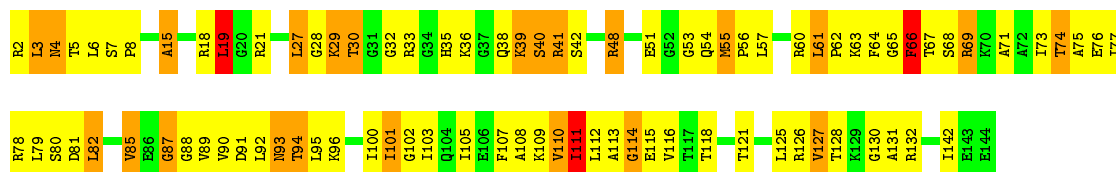
• Molecule 19: 50S ribosomal protein L14

Chain K: 26% 47% 24%



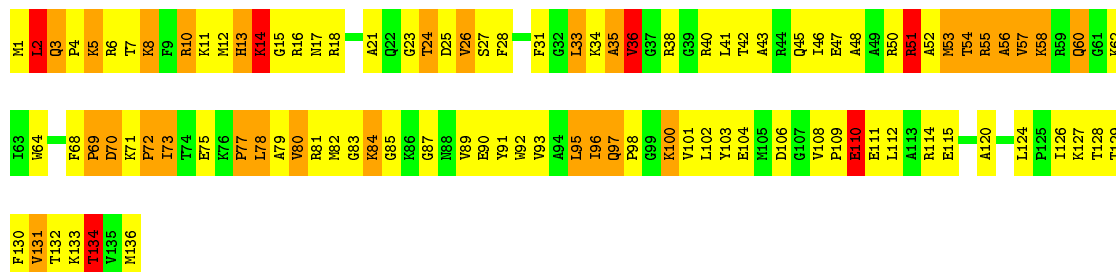
• Molecule 20: 50S ribosomal protein L15

Chain L: 38% 43% 16%

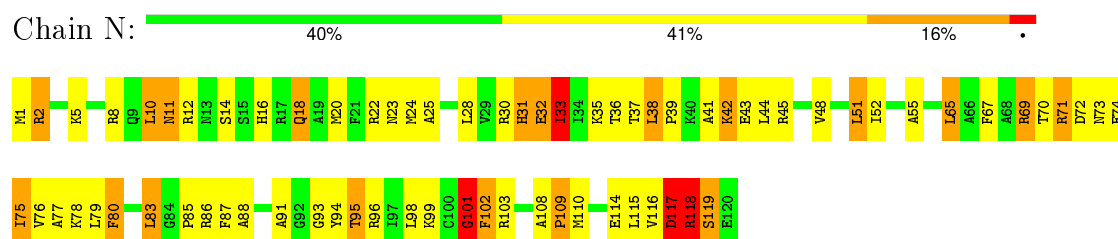


• Molecule 21: 50S ribosomal protein L16

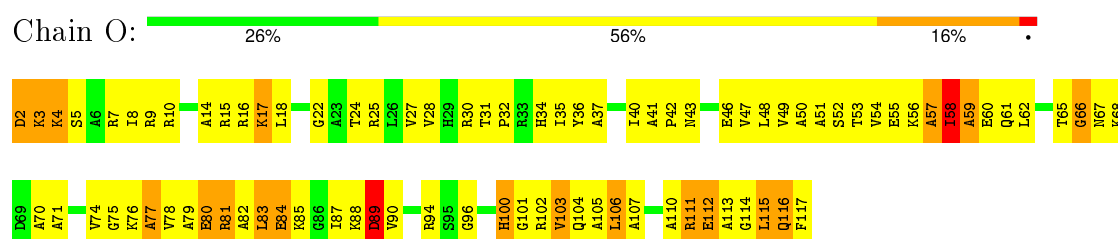
Chain M: 26% 49% 21%



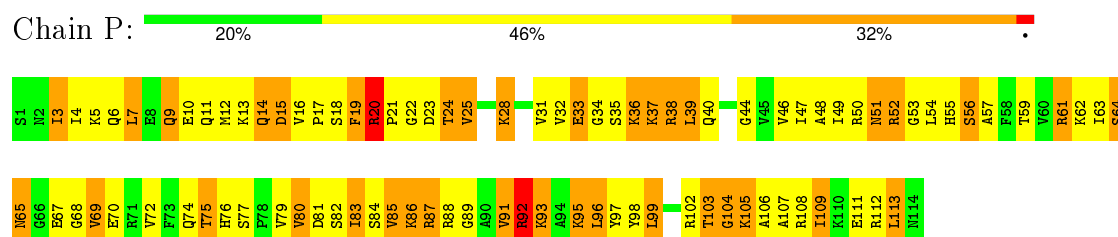
- Molecule 22: 50S ribosomal protein L17



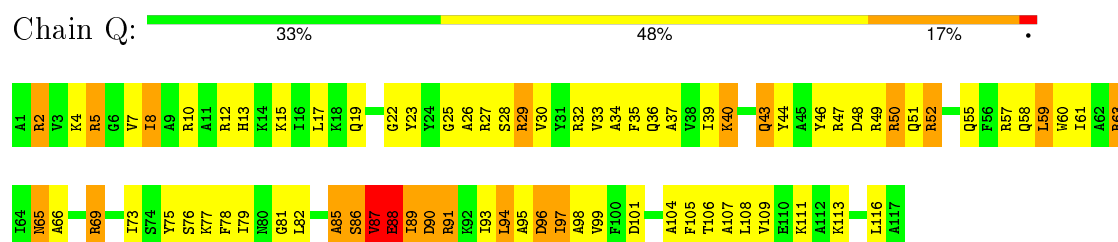
- Molecule 23: 50S ribosomal protein L18



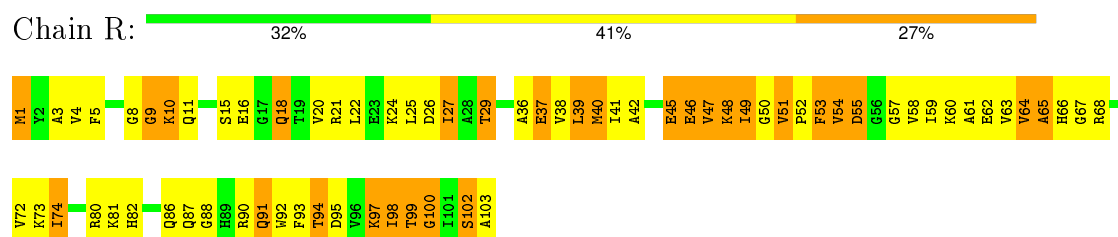
- Molecule 24: 50S ribosomal protein L19



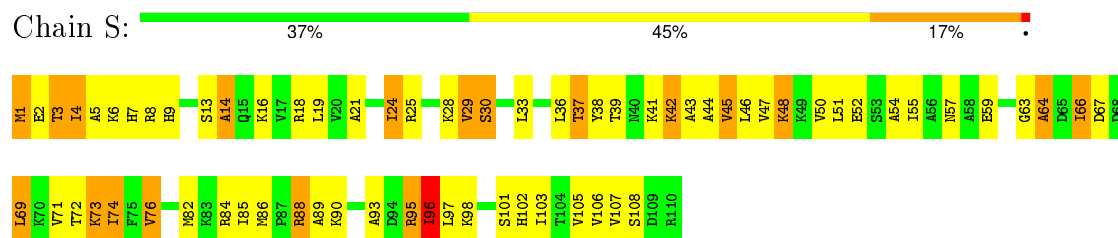
- Molecule 25: 50S ribosomal protein L20



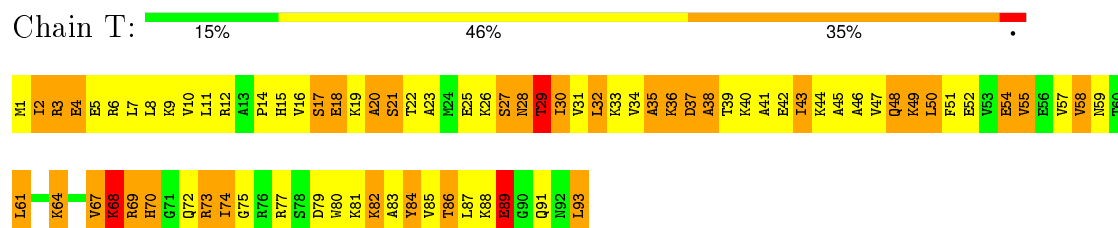
- Molecule 26: 50S ribosomal protein L21



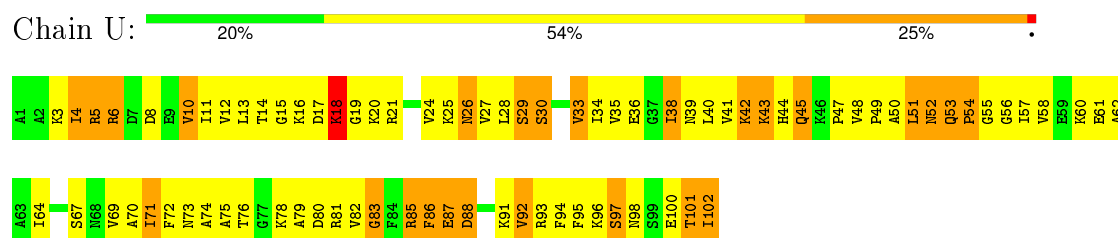
- Molecule 27: 50S ribosomal protein L22



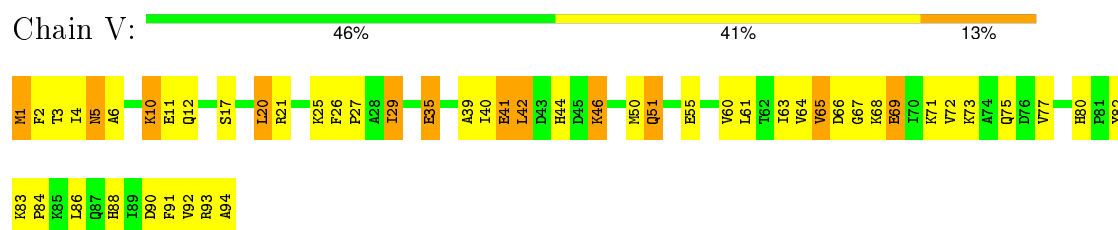
- Molecule 28: 50S ribosomal protein L23



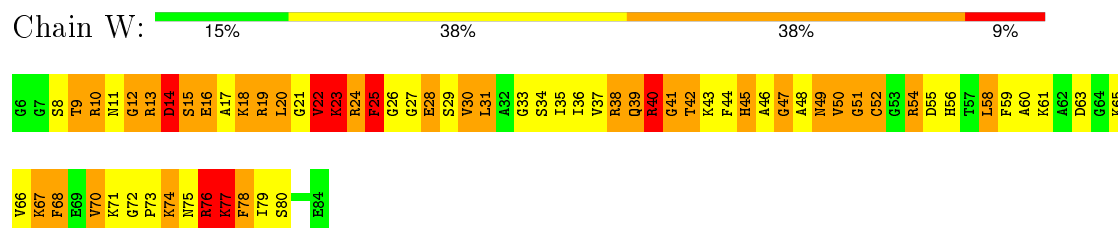
- Molecule 29: 50S ribosomal protein L24



- Molecule 30: 50S ribosomal protein L25

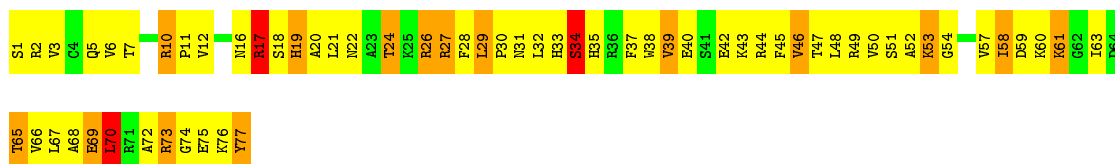


- Molecule 31: 50S ribosomal protein L27



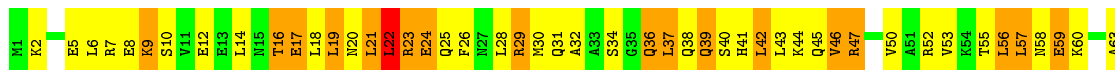
- Molecule 32: 50S ribosomal protein L28





- Molecule 33: 50S ribosomal protein L29

Chain Y: 24% 48% 27%



- Molecule 34: 50S ribosomal protein L30

Chain Z: 41% 34% 22%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	349744	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	148721	Depositor
Image detector	TemCam-F416 CMOS CCD camera	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, ERY, MA6

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	0	0.52	0/450	0.79	0/599
10	B	0.75	0/2801	1.57	48/4365 (1.1%)
11	C	0.48	0/2122	0.74	1/2852 (0.0%)
12	D	0.61	0/1586	0.80	2/2134 (0.1%)
13	E	0.51	0/1571	0.73	0/2113
14	F	0.33	0/1435	0.55	0/1926
15	G	0.38	0/1343	0.61	0/1816
16	H	0.32	0/436	0.57	0/586
17	I	0.23	0/1046	0.47	0/1410
18	J	0.60	0/1152	0.84	1/1551 (0.1%)
19	K	0.61	1/948 (0.1%)	0.83	0/1268
2	1	0.38	0/417	0.64	0/554
20	L	0.50	0/1054	0.80	2/1403 (0.1%)
21	M	0.55	0/1093	0.78	0/1460
22	N	0.55	0/974	0.82	2/1301 (0.2%)
23	O	0.42	0/902	0.66	0/1209
24	P	0.52	0/929	0.72	0/1242
25	Q	0.73	0/960	0.89	1/1278 (0.1%)
26	R	0.68	2/829 (0.2%)	0.85	1/1107 (0.1%)
27	S	0.63	0/864	0.84	0/1156
28	T	0.51	0/745	0.80	0/994
29	U	0.45	0/788	0.75	0/1051
3	2	0.52	0/380	0.71	0/498
30	V	0.47	0/766	0.65	0/1025
31	W	0.67	0/603	0.93	1/797 (0.1%)
32	X	0.43	0/635	0.75	1/848 (0.1%)
33	Y	0.39	0/510	0.63	0/677
34	Z	0.58	0/453	0.93	2/605 (0.3%)
4	3	0.50	0/513	0.70	1/676 (0.1%)
5	4	0.41	0/303	0.64	0/397
6	5	0.31	0/18	0.53	0/26
8	7	0.44	0/65	0.95	1/99 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
9	A	0.85	14/68599 (0.0%)	1.70	1689/107011 (1.6%)
All	All	0.77	17/97290 (0.0%)	1.52	1753/146034 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	D	0	1
18	J	0	1
22	N	0	1
All	All	0	3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1142	A	N9-C4	-8.37	1.32	1.37
9	A	984	A	C5-C6	-7.42	1.34	1.41
26	R	86	GLN	CB-CG	7.24	1.72	1.52
9	A	1783	A	N7-C5	-6.73	1.35	1.39
9	A	2606	C	N1-C6	-5.88	1.33	1.37

The worst 5 of 1753 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	571	U	O4'-C1'-N1	17.58	122.26	108.20
9	A	2848	G	P-O3'-C3'	17.00	140.11	119.70
9	A	627	A	P-O3'-C3'	16.26	139.22	119.70
9	A	984	A	N1-C6-N6	16.12	128.27	118.60
9	A	1603	A	P-O3'-C3'	-15.82	100.71	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	D	191	GLY	Peptide
18	J	110	PRO	Peptide
22	N	101	GLY	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	0	444	0	461	53	0
2	1	410	0	440	69	0
3	2	377	0	418	27	0
4	3	504	0	574	68	0
5	4	302	0	341	48	0
6	5	41	0	27	3	0
7	6	8	0	0	3	0
8	7	59	0	35	3	0
9	A	61251	0	30809	3080	0
10	B	2506	0	1271	108	0
11	C	2083	0	2157	319	0
12	D	1565	0	1616	271	0
13	E	1552	0	1619	199	0
14	F	1411	0	1447	207	0
15	G	1323	0	1374	223	0
16	H	431	0	451	83	0
17	I	1032	0	1088	132	0
18	J	1129	0	1162	214	0
19	K	939	0	1012	153	0
20	L	1045	0	1117	169	0
21	M	1074	0	1157	149	0
22	N	961	0	1000	121	0
23	O	892	0	923	113	0
24	P	917	0	965	185	0
25	Q	947	0	1022	191	0
26	R	816	0	839	145	0
27	S	857	0	922	91	0
28	T	739	0	807	153	0
29	U	780	0	834	100	0
30	V	753	0	780	60	0
31	W	596	0	610	284	0
32	X	625	0	655	109	0
33	Y	509	0	543	72	0
34	Z	449	0	491	45	0
35	5	4	0	0	0	0
36	A	51	0	67	4	0
All	All	89382	0	59034	6679	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 45.

The worst 5 of 6679 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)
24:P:50:ARG:CG	24:P:57:ALA:H	1.24	1.48
24:P:50:ARG:HD2	24:P:51:ASN:N	1.27	1.41
24:P:50:ARG:HG2	24:P:57:ALA:N	1.13	1.40
25:Q:63:ARG:NH1	25:Q:96:ASP:HA	1.37	1.35
12:D:114:LYS:HE3	12:D:114:LYS:N	1.41	1.33

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	
1	0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	21
2	1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	1	12
3	2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
4	3	62/64 (97%)	53 (86%)	5 (8%)	4 (6%)	1	25
5	4	36/38 (95%)	24 (67%)	9 (25%)	3 (8%)	1	18
11	C	269/271 (99%)	197 (73%)	47 (18%)	25 (9%)	1	16
12	D	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	5
13	E	199/201 (99%)	145 (73%)	34 (17%)	20 (10%)	1	14
14	F	175/177 (99%)	123 (70%)	36 (21%)	16 (9%)	1	17
15	G	174/176 (99%)	111 (64%)	38 (22%)	25 (14%)	0	6
16	H	54/56 (96%)	21 (39%)	13 (24%)	20 (37%)	0	0
17	I	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	J	140/142 (99%)	104 (74%)	24 (17%)	12 (9%)	1	17
19	K	120/122 (98%)	88 (73%)	18 (15%)	14 (12%)	0	9
20	L	141/143 (99%)	100 (71%)	30 (21%)	11 (8%)	1	20
21	M	134/136 (98%)	96 (72%)	18 (13%)	20 (15%)	0	5
22	N	118/120 (98%)	91 (77%)	16 (14%)	11 (9%)	1	16
23	O	114/116 (98%)	85 (75%)	18 (16%)	11 (10%)	1	15
24	P	112/114 (98%)	78 (70%)	20 (18%)	14 (12%)	0	8
25	Q	115/117 (98%)	100 (87%)	7 (6%)	8 (7%)	1	22
26	R	101/103 (98%)	76 (75%)	14 (14%)	11 (11%)	0	11
27	S	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	3	32
28	T	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	4
29	U	100/102 (98%)	66 (66%)	15 (15%)	19 (19%)	0	3
30	V	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	8	49
31	W	77/79 (98%)	31 (40%)	22 (29%)	24 (31%)	0	0
32	X	75/77 (97%)	58 (77%)	10 (13%)	7 (9%)	1	16
33	Y	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	7
34	Z	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	1	22
All	All	3216/3274 (98%)	2285 (71%)	564 (18%)	367 (11%)	1	10

5 of 367 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	51	ARG
1	0	54	ILE
2	1	16	THR
5	4	4	ARG
11	C	77	VAL

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	
1	0	47/47 (100%)	39 (83%)	8 (17%)	2	18
2	1	45/45 (100%)	37 (82%)	8 (18%)	2	16
3	2	38/38 (100%)	27 (71%)	11 (29%)	0	3
4	3	51/51 (100%)	42 (82%)	9 (18%)	2	16
5	4	34/34 (100%)	28 (82%)	6 (18%)	2	16
11	C	216/216 (100%)	170 (79%)	46 (21%)	1	9
12	D	164/164 (100%)	133 (81%)	31 (19%)	2	13
13	E	165/165 (100%)	110 (67%)	55 (33%)	0	2
14	F	148/148 (100%)	116 (78%)	32 (22%)	1	9
15	G	137/137 (100%)	106 (77%)	31 (23%)	1	8
16	H	44/44 (100%)	34 (77%)	10 (23%)	1	8
17	I	109/109 (100%)	91 (84%)	18 (16%)	3	19
18	J	116/116 (100%)	92 (79%)	24 (21%)	1	10
19	K	103/103 (100%)	77 (75%)	26 (25%)	1	6
20	L	102/102 (100%)	82 (80%)	20 (20%)	1	12
21	M	109/109 (100%)	81 (74%)	28 (26%)	0	6
22	N	100/100 (100%)	82 (82%)	18 (18%)	2	15
23	O	86/86 (100%)	67 (78%)	19 (22%)	1	9
24	P	99/99 (100%)	66 (67%)	33 (33%)	0	2
25	Q	89/89 (100%)	68 (76%)	21 (24%)	1	7
26	R	84/84 (100%)	66 (79%)	18 (21%)	1	9
27	S	93/93 (100%)	72 (77%)	21 (23%)	1	8
28	T	80/80 (100%)	53 (66%)	27 (34%)	0	2
29	U	83/83 (100%)	66 (80%)	17 (20%)	1	10
30	V	78/78 (100%)	62 (80%)	16 (20%)	1	10
31	W	59/59 (100%)	38 (64%)	21 (36%)	0	1
32	X	67/67 (100%)	51 (76%)	16 (24%)	1	7
33	Y	55/55 (100%)	42 (76%)	13 (24%)	1	7
34	Z	48/48 (100%)	35 (73%)	13 (27%)	0	4
All	All	2649/2649 (100%)	2033 (77%)	616 (23%)	3	7

5 of 616 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	J	57	LEU
21	M	33	LEU
31	W	54	ARG
18	J	129	GLU
19	K	111	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
17	I	30	GLN
20	L	54	GLN
30	V	88	HIS
17	I	110	GLN
18	J	130	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	115/118 (97%)	34 (29%)	17 (14%)
6	5	0/2	-	-
8	7	2/3 (66%)	0	0
9	A	2848/2904 (98%)	908 (31%)	423 (14%)
All	All	2965/3027 (97%)	942 (31%)	440 (14%)

5 of 942 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	10	A
9	A	13	A
9	A	14	A
9	A	15	G
9	A	23	G

5 of 440 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1329	U
9	A	1626	A
9	A	2777	G
9	A	1360	G
9	A	1459	G

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
6	MA6	5	76	9,35,6	18,26,27	0.70	0	15,38,41	1.35	1 (6%)

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
6	MA6	5	76	9,35,6	-	0/7/29/30	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	5	76	MA6	C2-N1-C6	3.09	118.94	111.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	5	76	MA6	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is unknown - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ERY	A	9000	-	53,53,53	0.78	1 (1%)	82,82,82	1.64	15 (18%)

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
36	ERY	A	9000	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	9000	ERY	C6-C5	2.19	1.59	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	9000	ERY	C25-C24-C23	-4.98	102.75	110.05
36	A	9000	ERY	O7-C5-C6	-4.65	100.45	106.45
36	A	9000	ERY	C3-C2-C1	-3.56	102.96	109.85
36	A	9000	ERY	O2-C1-O1	-3.40	117.30	123.88
36	A	9000	ERY	C15-C16-C17	-2.98	104.01	107.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	9000	ERY	4	0

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.