



# wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 05:43 PM GMT

PDB ID : 2QAO  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with neomycin. This file contains the 50S subunit of the second 70S ribosome, with neomycin bound. The entire crystal structure contains two 70S ribosomes and is described in remark 400.  
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.  
Deposited on : 2007-06-15  
Resolution : 3.21 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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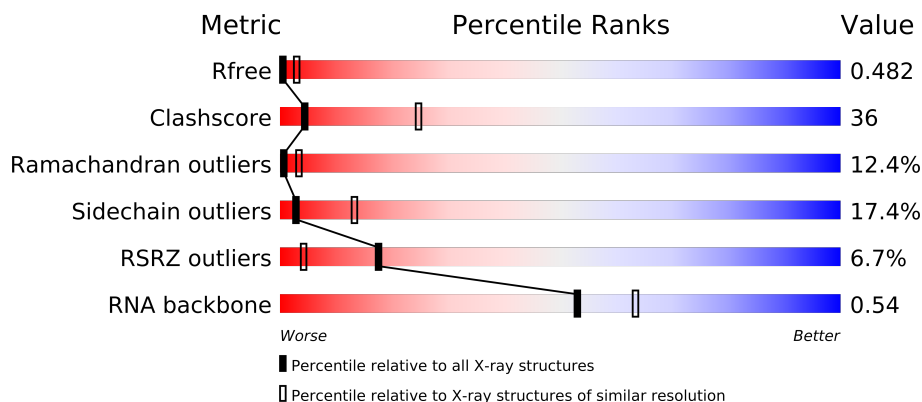
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.21 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	120	
2	B	2904	
3	I	141	
4	C	272	
5	D	209	
6	K	123	
7	P	114	
8	E	201	
9	Y	58	
10	0	56	
11	4	38	
12	1	54	

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Mol	Chain	Length	Quality of chain
13	3	64	
14	V	94	
15	2	46	
16	L	144	
17	M	136	
18	X	63	
19	H	149	
20	J	142	
21	N	127	
22	O	117	
23	Q	117	
24	S	110	
25	U	103	
26	F	178	
27	G	176	
28	R	103	
29	T	100	
30	Z	78	
31	W	84	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	NMY	B	2905	-	X
33	MG	B	3165	-	X
33	MG	B	3172	-	X
33	MG	B	3201	-	X
33	MG	B	3207	-	X
33	MG	B	3337	-	X
33	MG	B	3351	-	X
33	MG	B	3389	-	X
33	MG	B	3452	-	X
33	MG	B	3515	-	X
33	MG	B	3592	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 90305 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 3 is a protein called 50S ribosomal protein L11.

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

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 7 is a protein called 50S ribosomal protein L19.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Y	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 10 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 11 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 12 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 13 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 14 is a protein called 50S ribosomal protein L25.

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

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 16 is a protein called 50S ribosomal protein L15.

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

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 19 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 20 is a protein called 50S ribosomal protein L13.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L22.

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

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	U	102	Total	C	N	O		0	0	0
			779	492	146	141				

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 27 is a protein called 50S ribosomal protein L6.

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

- Molecule 28 is a protein called 50S ribosomal protein L21.

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

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

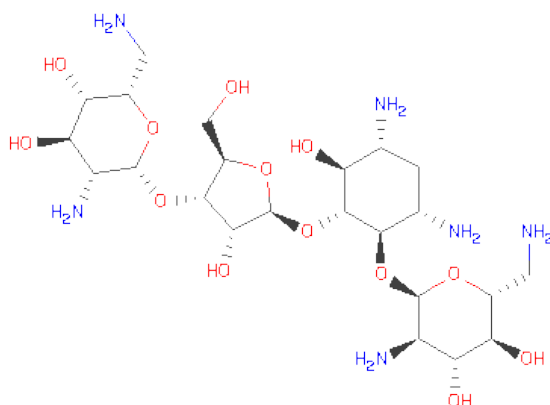
- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Z	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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

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

- Molecule 32 is NEOMYCIN (three-letter code: NMY) (formula:  $\text{C}_{23}\text{H}_{46}\text{N}_6\text{O}_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	N	O	0	0
			42	23	6	13		



- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	111	Total 111	Mg 111	0	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	4	1	Total 1	Zn 1	0	0

- Molecule 35 is water.

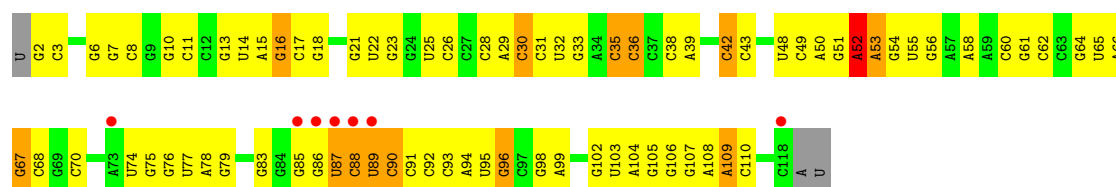
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	503	Total 503	O 503	0	0
35	C	6	Total 6	O 6	0	0
35	L	2	Total 2	O 2	0	0
35	R	1	Total 1	O 1	0	0

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

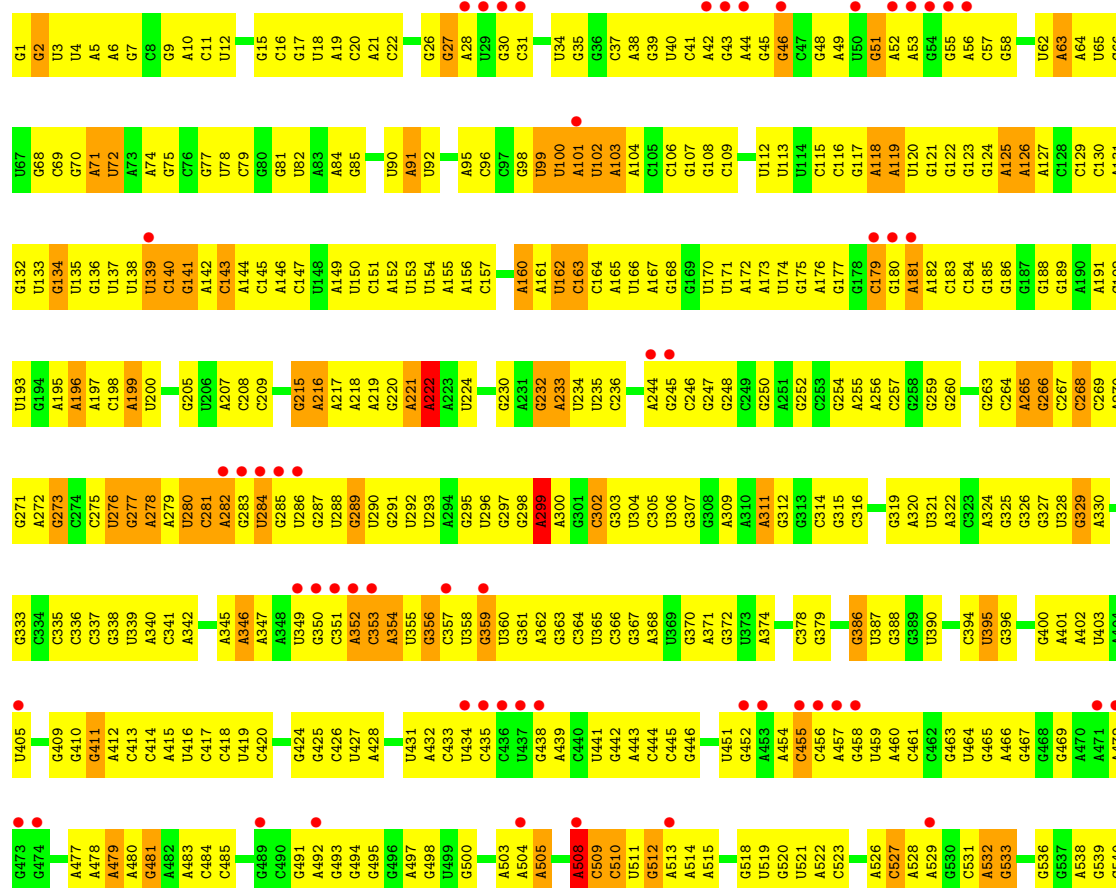
#### • Molecule 1: 5S rRNA

Chain A: 



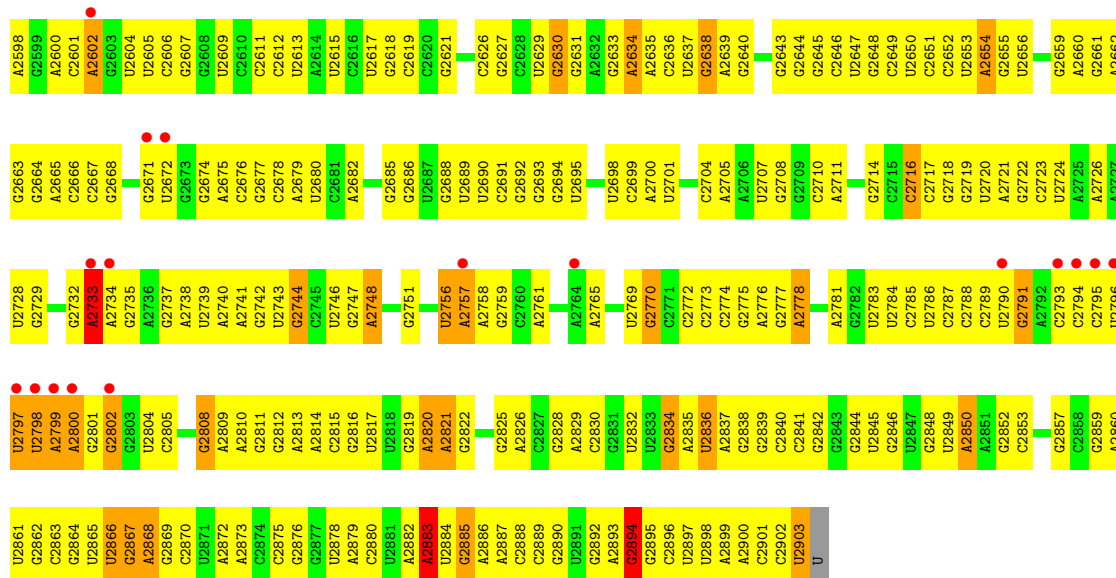
#### • Molecule 2: 23S rRNA

Chain B: 



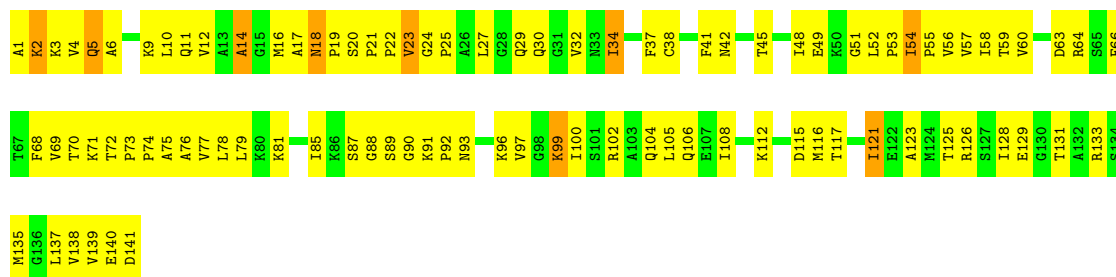


U2519	A2451	C2385	A2322	G2256	U2192	U	A2071	G2002	U1936	U1859	A1794	C1727	A1572
C2520	G2454	A2386	G2323	U2257	G2193	G2183	C2072	U2007	A1927	G1860	C1795	C1728	G1573
C2521	U2387	A2387	U2324	C2258	U2194	A2134	U2073	C2008	A1928	G1863	U1796	U1729	G1574
U2522	G2455	A2388	G2325	U2259	U2195	A2135	U2074	G2009	G1929	U1864	G1797	C1730	C1575
C2523	G2456	U2389	A2328	C2260	U2197	G2136	U2075	A2009	U1931	U1865	U1798	G1731	C1576
G2524	U2457	U2390	U2329	U2262	U2198	G2137	U2076	A2009	U1931	U1866	G1799	C1732	C1577
C2527	G2458	U2393	G2330	C2263	A2199	G2138	A2077	G2012	A1932	A1867	C1800	G1733	U1578
U2528	U2459	C2394	G2331	C2264	A2199	U2139	C2078	A2013	G1934	C1868	A1801	G1734	A1579
C2529	C2460	C2395	G2332	U2265	C2200	G2140	U2079	A2014	C1935	U1869	A1802	A1735	A1580
A2530	C2461	G2396	A2333	U2266	G2201	G2141	A2080	A2015	U1936	C1870	A1803	U1736	G1581
A2531	G2463	U2400	U2334	A2267	U2203	C2143	G2083	U2016	A1937	A1871	C1804	G1737	C1582
G2535	C2464	A2335	A2335	A2268	G2204	G2144	C2084	G2018	U1938	A1872	A1805	G1738	A1583
U2537	U2401	A2336	A2336	C2269	C2207	C2145	U2085	A2019	U1939	G1873	A1808	G1740	C1585
C2538	U2402	A2337	U2337	U2270	G2208	C2146	U2086	A2020	U1940	C1874	A1809	C1741	A1586
U2539	C2467	G2338	G2338	C2271	C2209	A2147	G2087	C2021	U1943	G1875	A1810	U1742	G1587
C2540	A2468	C2339	U2339	U2272	G2210	U2148	A2088	C2022	U1944	A1876	G1811	G1743	U1588
U2541	G2405	U2404	A2340	A2273	A2211	U2149	C2089	C2023	U1944	A1877	G1812	A1744	U1589
C2542	A2406	G2407	G2341	A2274	U2212	C2150	A2090	G2024	G1945	G1878	G1813	A1745	A1590
G2543	A2407	U2342	C2342	C2275	U2213	U2151	C2091	C2025	U1946	G1879	G1814	A1746	A1591
U2544	U2408	U2343	U2343	C2276	C2214	C2152	U2092	U2026	C1947	U1880	A1815	U1747	C1592
C2545	G2409	G2344	G2345	G2279	G2215	C2153	G2093	G2027	G1948	C1881	C1816	C1748	A1593
G2546	A2411	A2346	A2346	C2281	G2216	A2154	A2094	U2028	U1951	U1882	G1817	A1749	U1594
A2547	A2412	G2347	U2348	G2282	G2217	G2156	C2095	G2029	U1951	U1883	U1818	G1750	A1595
U2548	G2481	U2349	U2349	C2283	U2219	C2157	A2097	A2031	A1952	G1884	A1819	G1751	A1596
G2553	A2482	G2415	G2415	U2286	U2220	A	A2098	G2032	A1953	G1888	U1820	C1752	A1597
U2554	C2416	C2416	A2352	C2287	G2221	G	U2099	G2032	G1954	A1821	A1822	G1753	A1598
C2555	U2483	C2417	G2353	A2287	C2222	C	A2101	U2034	U1955	A1889	G1823	U1756	C1600
U2556	G2485	A2418	C2354	A2288	G2223	C	G2100	G2035	C1957	A1890	G1824	A1757	A1603
C2557	U2486	U2419	U2355	U2291	G2224	A	G2102	C2036	C1958	C1893	U1825	U1758	A1607
U2558	G2487	G2420	G2356	U2292	U2225	C	C2103	A2037	C1962	C1894	G1826	A1759	A1608
G2559	U2488	U2421	U2357	U2293	C2226	C	U2104	G2038	U1895	C1896	U1827	C1760	A1609
U2560	C2490	U2422	G2357	G2294	G2227	C	U2105	U2039	U1963	G1828	G1829	A1762	A1610
C2561	G2491	C2423	G2358	C2295	U2229	U	G2107	U2041	C1965	G1829	C1830	G1763	C1611
U2562	U2492	U2424	G2359	U2296	G2230	G	A2108	A2042	A1966	G1831	G1831	U1765	A1616
G2563	A2493	A2426	G2361	A2297	U2231	A	U2109	C2043	C1967	C1902	C1832	U1766	G1623
U2564	C2496	C2427	C2362	A2298	C2232	A	G2110	G2048	G1968	G1903	C1833	G1767	U1624
C2565	A2497	G2428	G2363	U2299	U2233	A	U	G2049	A1969	A1904	C1838	C1771	A1617
U2566	U2498	C2429	G2364	C2300	G2234	U	G	C2050	A1970	C1905	U1841	U1772	A1633
G2567	C2499	A2431	G2365	C2301	U2234	U	A	A2051	U1971	G1906	U1842	A1773	A1634
U2568	U2500	A2432	A2366	U2302	G2238	C	G	A2052	G1972	C1908	C1843	C1774	U1635
C2569	C2501	A2433	C2367	U2306	U2240	C	A	G2053	A1981	C1909	G1844	U1775	U1636
U2570	G2502	A2434	G2370	C2307	A2241	A	G	A2054	U1982	G1910	G1845	U1778	A1637
G2571	A2503	C2435	G2371	G2308	G2242	C	A	C2055	G1983	U1911	G1846	U1779	C1638
C2572	U2504	G2436	U2372	G2309	U2243	C2179	G	G2056	G1984	A1912	A1847	U1784	G1639
U2573	U2506	U2437	G2373	C2310	U2244	U2180	A	A2060	C1985	A1913	G1848	A1784	A1640
G2574	G2507	C2438	C2374	C2311	U2245	U2181	U	G2061	C1986	C1914	G1849	A1785	A1641
U2575	U2508	U2439	G2375	A2312	G2246	U2182	G	A2062	A1987	U1915	U1850	A1786	G1642
C2576	C2440	A2376	C2376	U2247	C2247	A2183	G	C2063	G1988	A1916	U1851	A1787	G1643
U2577	U2441	G2376	A2376	G2248	C2248	A2184	G	C2064	U1991	U1917	U1852	C1788	A1644
G2578	C2512	C2442	G2442	U2249	U2249	U2185	G	C2065	G1992	A1918	U1853	A1789	G1645
U2579	A2513	C2443	G2443	G2250	G2250	G2186	A	C2066	U1993	G1921	A1854	C1790	U1647
C2580	U2514	U2444	G2444	G2251	G2251	U2187	G	G2067	U1994	G1922	U1855	G1723	U1649
U2581	C2515	A2381	C2381	U2252	G2252	U2188	U	C2068	C1997	U1923	U1856	U1724	U1651
G2582	U2516	G2382	U2382	G2253	G2253	U2189	C	U2069	A1998	C1924	G1857	U1725	U1652
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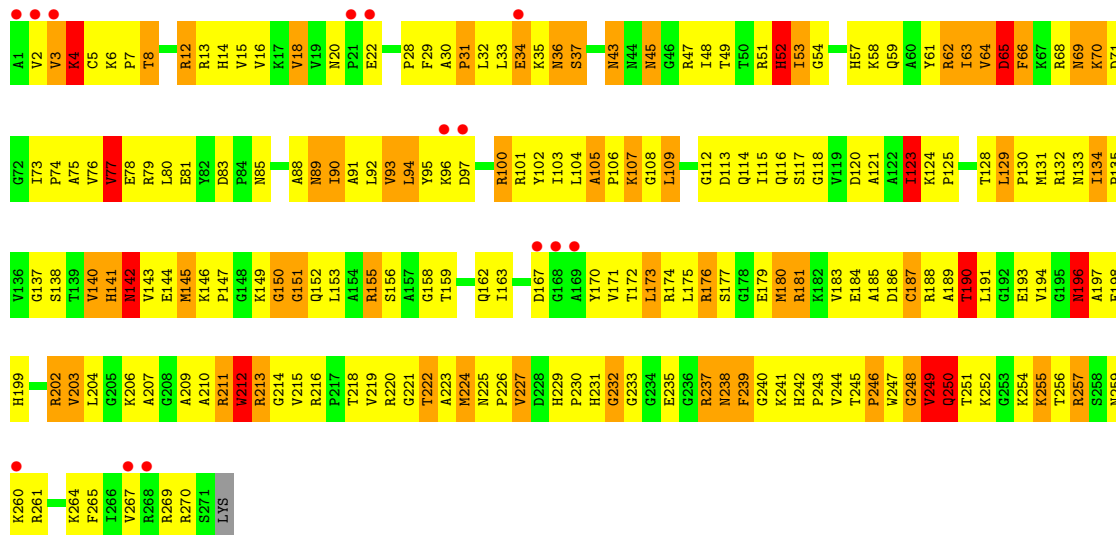
### • Molecule 3: 50S ribosomal protein L11

Chain I:



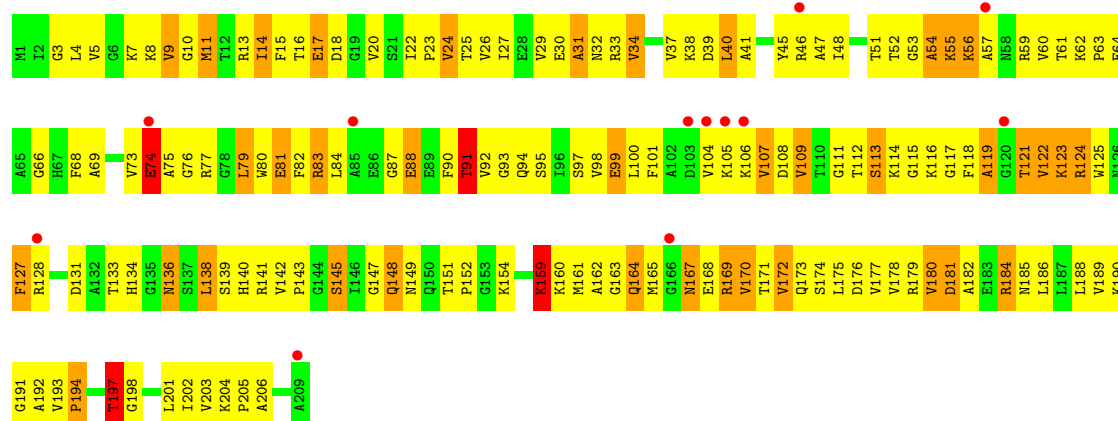
### • Molecule 4: 50S ribosomal protein L2

Chain C:



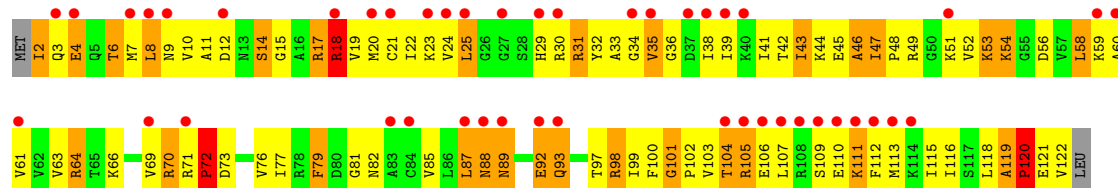
### • Molecule 5: 50S ribosomal protein L3

Chain D: 



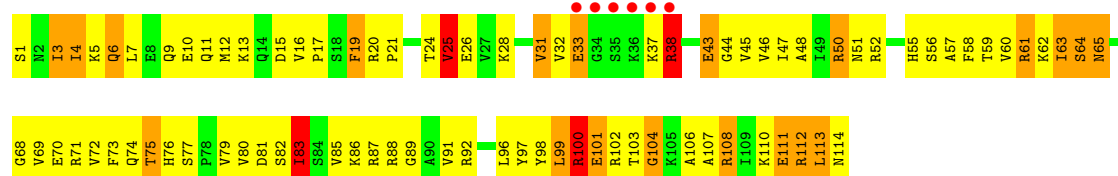
- Molecule 6: 50S ribosomal protein L14

Chain K: 



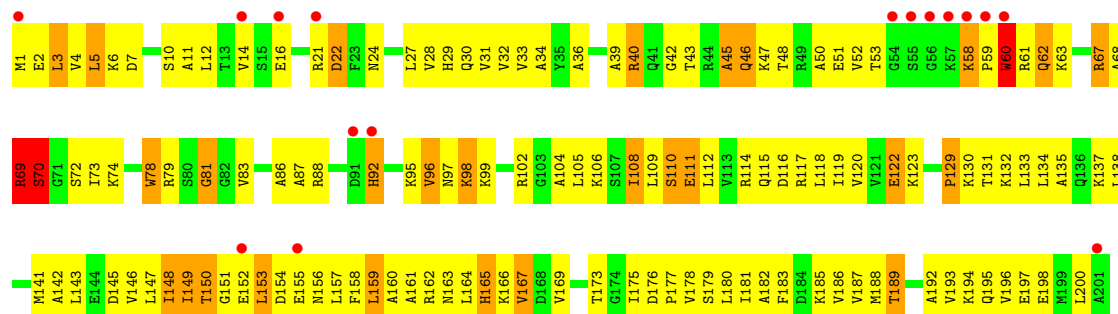
- Molecule 7: 50S ribosomal protein L19

Chain P: 



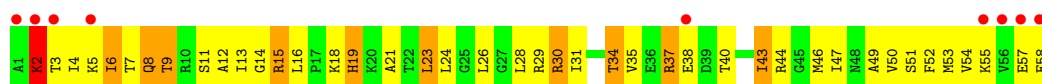
- Molecule 8: 50S ribosomal protein L4

Chain E: 



- Molecule 9: 50S ribosomal protein L30

Chain Y: 



- Molecule 10: 50S ribosomal protein L32

Chain 0:



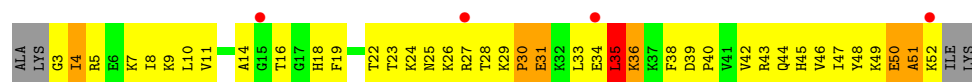
- Molecule 11: 50S ribosomal protein L36

Chain 4:



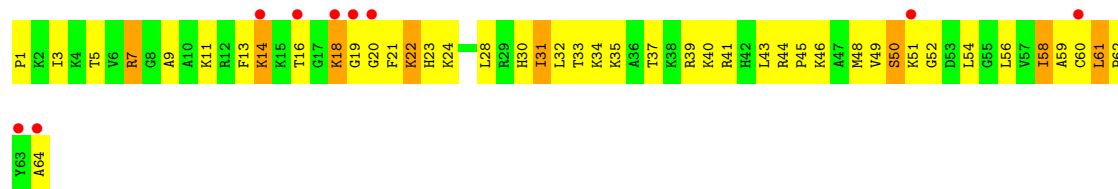
- Molecule 12: 50S ribosomal protein L33

Chain 1:



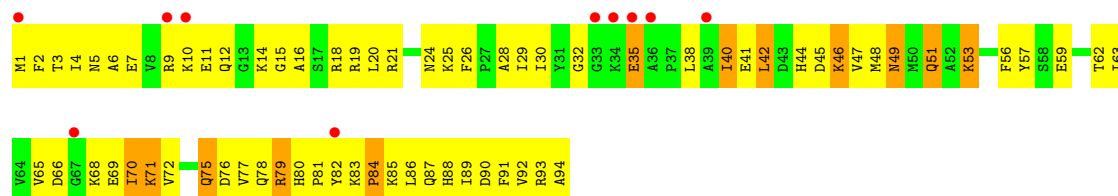
- Molecule 13: 50S ribosomal protein L35

Chain 3:



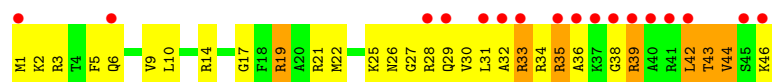
- Molecule 14: 50S ribosomal protein L25

Chain V:



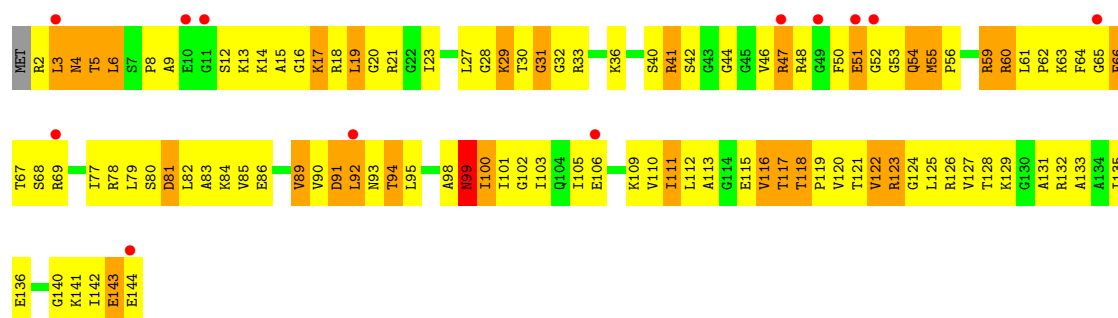
- Molecule 15: 50S ribosomal protein L34

Chain 2:



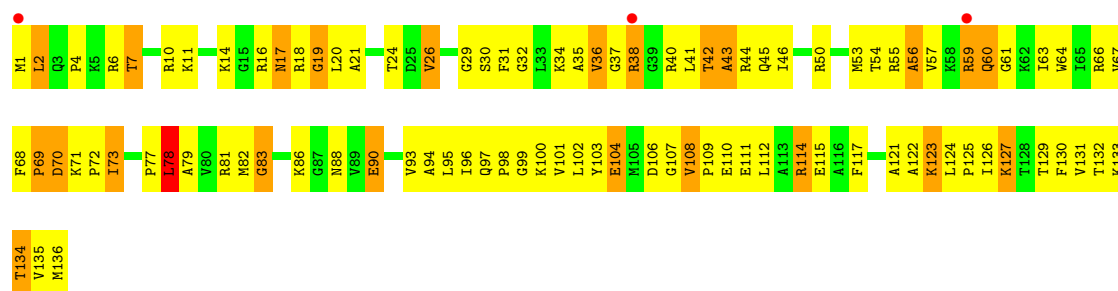
- Molecule 16: 50S ribosomal protein L15

Chain L:



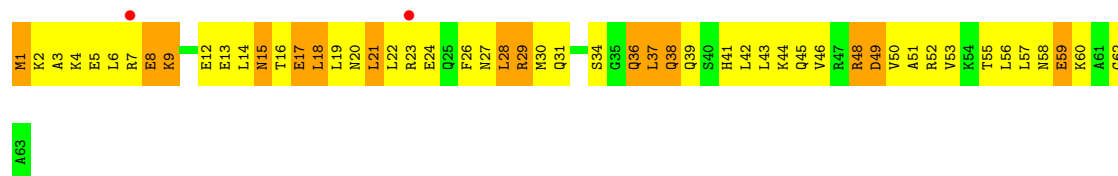
• Molecule 17: 50S ribosomal protein L16

Chain M:



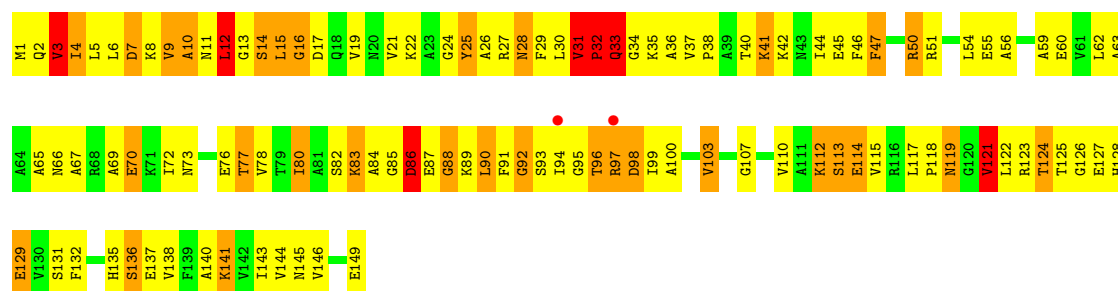
• Molecule 18: 50S ribosomal protein L29

Chain X:



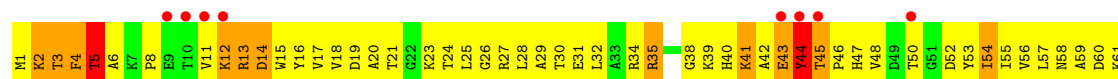
• Molecule 19: 50S ribosomal protein L9

Chain H:



• Molecule 20: 50S ribosomal protein L13

Chain J:

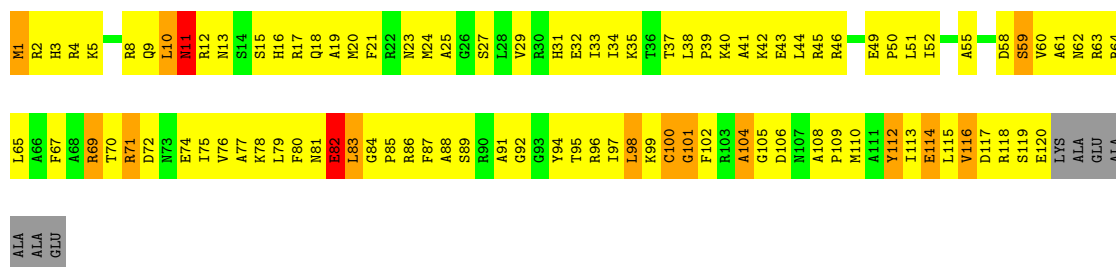






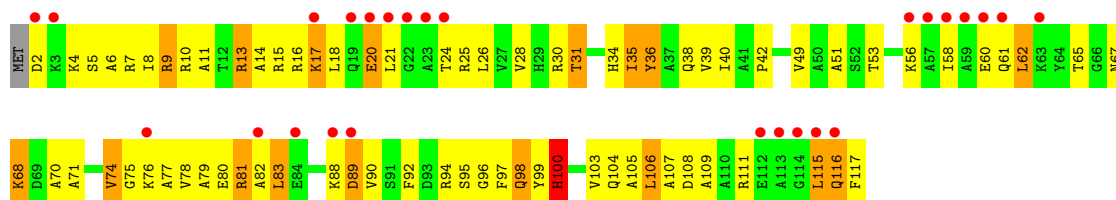
- Molecule 21: 50S ribosomal protein L17

Chain N:



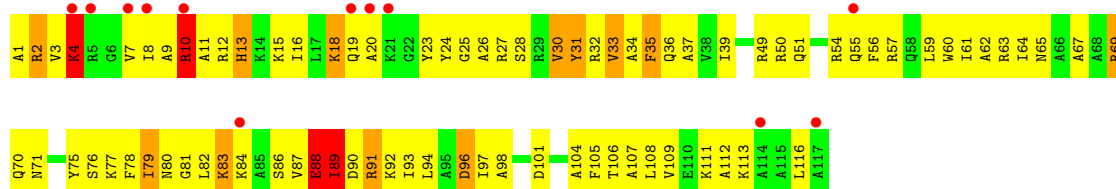
- Molecule 22: 50S ribosomal protein L18

Chain O:



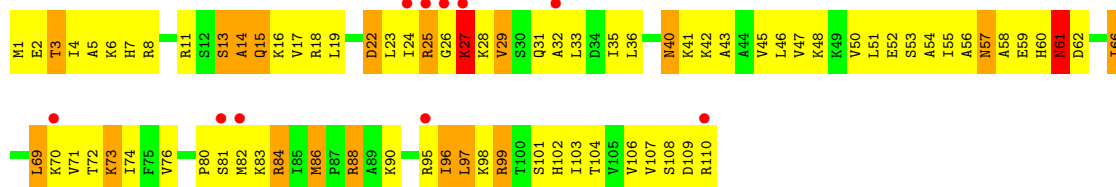
- Molecule 23: 50S ribosomal protein L20

Chain Q:



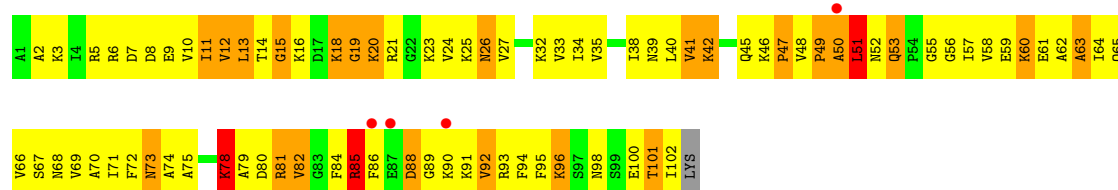
- Molecule 24: 50S ribosomal protein L22

Chain S:



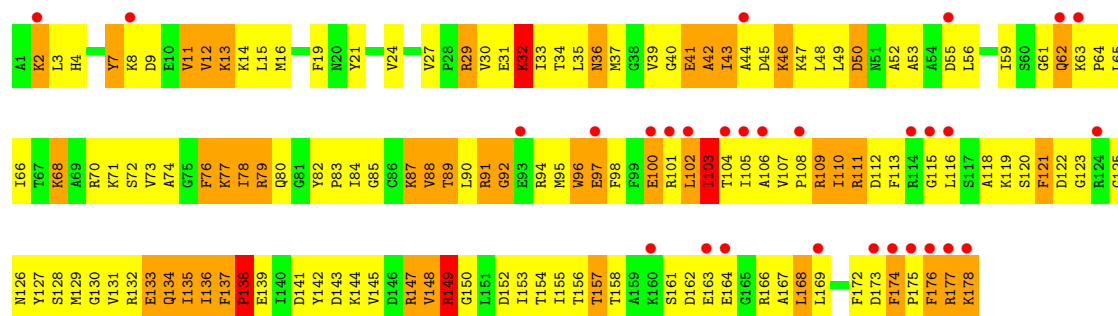
- Molecule 25: 50S ribosomal protein L24

Chain U:



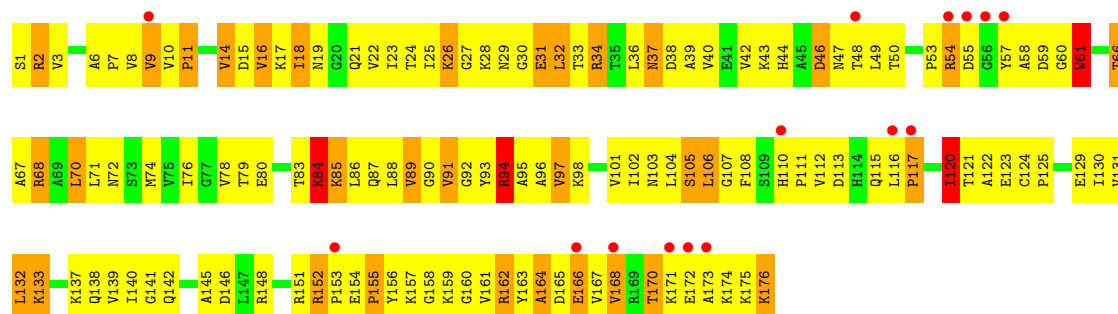
• Molecule 26: 50S ribosomal protein L5

Chain F:



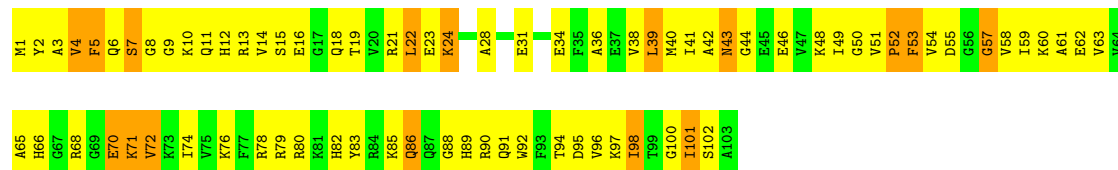
• Molecule 27: 50S ribosomal protein L6

Chain G:



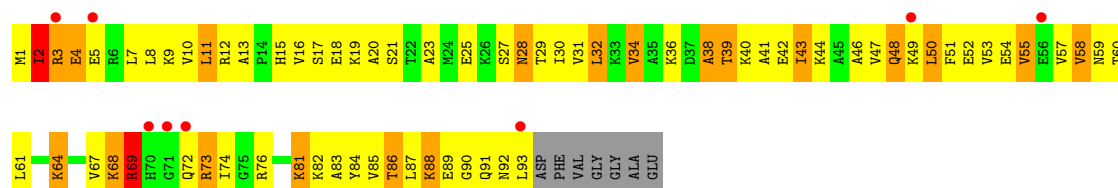
• Molecule 28: 50S ribosomal protein L21

Chain R:



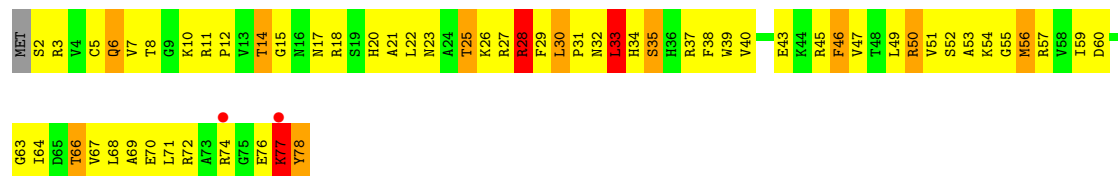
• Molecule 29: 50S ribosomal protein L23

Chain T:



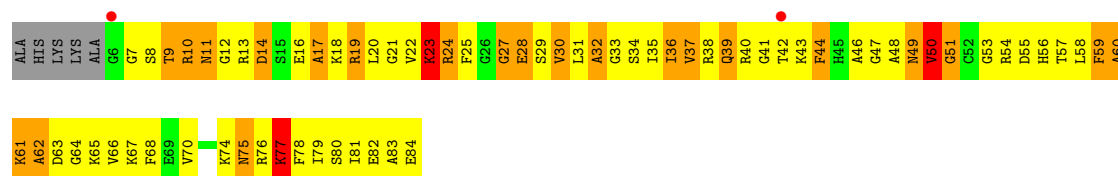
- Molecule 30: 50S ribosomal protein L28

Chain Z: 



- Molecule 31: 50S ribosomal protein L27

Chain W: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.21 138.41 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.21) 66.6 (138.41-3.22)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.274 , 0.309 0.474 , 0.482	Depositor DCC
$R_{free}$ test set	30059 reflections (4.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 9.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 626512 reflections	Xtriage
$F_o, F_c$ correlation	0.62	EDS
Total number of atoms	90305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/2803	0.75	1/4371 (0.0%)
2	B	0.28	9/68314 (0.0%)	0.77	48/106569 (0.0%)
3	I	0.25	0/1046	0.49	0/1410
4	C	0.22	0/2121	0.48	0/2852
5	D	0.24	0/1586	0.49	0/2134
6	K	0.24	0/939	0.56	0/1258
7	P	0.24	0/929	0.51	0/1242
8	E	0.24	0/1571	0.51	0/2113
9	Y	0.23	0/453	0.50	0/605
10	O	0.22	0/450	0.56	0/599
11	4	0.23	0/303	0.47	0/397
12	1	0.27	0/416	0.49	0/554
13	3	0.24	0/513	0.48	0/676
14	V	0.25	0/766	0.42	0/1025
15	2	0.26	0/380	0.47	0/498
16	L	0.24	0/1054	0.49	0/1403
17	M	0.25	0/1093	0.48	0/1460
18	X	0.24	0/510	0.53	0/677
19	H	0.25	0/1122	0.49	0/1515
20	J	0.23	0/1152	0.48	0/1551
21	N	0.24	0/973	0.52	0/1301
22	O	0.23	0/902	0.49	0/1209
23	Q	0.26	0/960	0.50	0/1278
24	S	0.22	0/864	0.52	0/1156
25	U	0.25	0/787	0.48	0/1051
26	F	0.26	0/1444	0.52	0/1937
27	G	0.23	0/1343	0.47	0/1816
28	R	0.25	0/829	0.49	0/1107
29	T	0.23	0/744	0.57	0/994
30	Z	0.25	0/635	0.52	0/848
31	W	0.28	0/603	0.53	0/797
All	All	0.27	9/97605 (0.0%)	0.72	49/146403 (0.0%)

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
2	B	0	42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1086	A	C5-C6	-16.27	1.26	1.41
2	B	1088	A	C6-N1	-10.47	1.28	1.35
2	B	2323	G	O3'-P	9.74	1.72	1.61
2	B	1060	U	C2-N3	7.84	1.43	1.37
2	B	2318	G	O3'-P	-7.29	1.52	1.61

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP1	-29.64	75.14	110.70
2	B	2791	G	O5'-P-OP2	-26.90	78.42	110.70
2	B	2791	G	O5'-P-OP1	18.57	132.98	110.70
2	B	2204	G	O5'-P-OP2	17.72	131.96	110.70
2	B	2790	U	OP2-P-O3'	14.73	137.61	105.20

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	232	G	Sidechain
2	B	299	A	Sidechain
2	B	51	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2507	0	1270	89	0
2	B	60995	0	30677	2244	0
3	I	1032	0	1088	196	0
4	C	2082	0	2157	244	0
5	D	1565	0	1616	214	0
6	K	930	0	1000	121	0
7	P	917	0	965	115	0
8	E	1552	0	1619	165	0
9	Y	449	0	491	47	0
10	0	444	0	461	46	0
11	4	302	0	341	28	0
12	1	409	0	440	42	0
13	3	504	0	574	51	0
14	V	753	0	780	83	0
15	2	377	0	418	47	0
16	L	1045	0	1117	152	0
17	M	1074	0	1157	114	0
18	X	509	0	543	58	0
19	H	1111	0	1148	153	0
20	J	1129	0	1162	148	0
21	N	960	0	1000	116	0
22	O	892	0	923	91	0
23	Q	947	0	1022	147	0
24	S	857	0	922	100	0
25	U	779	0	834	118	0
26	F	1420	0	1460	232	0
27	G	1323	0	1374	189	0
28	R	816	0	839	102	0
29	T	738	0	807	122	0
30	Z	625	0	652	83	0
31	W	596	0	610	143	0
32	B	42	0	46	1	0
33	B	111	0	0	0	0
34	4	1	0	0	0	0
35	B	503	0	0	10	0
35	C	6	0	0	0	0
35	L	2	0	0	0	0
35	R	1	0	0	0	0
All	All	90305	0	59513	5315	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

The worst 5 of 5315 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1099:G:H8	3:I:3:LYS:N	1.38	1.21
19:H:31:VAL:HB	19:H:32:PRO:HD2	1.30	1.11
2:B:1099:G:O5'	3:I:4:VAL:N	1.86	1.06
25:U:85:ARG:HD3	25:U:86:PHE:H	1.19	1.05
2:B:1098:A:H3'	3:I:3:LYS:CA	1.87	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	
3	I	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	5	36
4	C	269/272 (99%)	174 (65%)	47 (18%)	48 (18%)	0	1
5	D	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	1
6	K	119/123 (97%)	75 (63%)	27 (23%)	17 (14%)	0	2
7	P	112/114 (98%)	63 (56%)	34 (30%)	15 (13%)	0	2
8	E	199/201 (99%)	130 (65%)	53 (27%)	16 (8%)	1	11
9	Y	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	1	5
10	0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	1	8
11	4	36/38 (95%)	20 (56%)	7 (19%)	9 (25%)	0	0
12	1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	1	3
13	3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	10
14	V	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	4	31
15	2	44/46 (96%)	28 (64%)	15 (34%)	1 (2%)	10	52
16	L	141/144 (98%)	88 (62%)	29 (21%)	24 (17%)	0	1
17	M	134/136 (98%)	86 (64%)	32 (24%)	16 (12%)	1	4
18	X	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	10
19	H	147/149 (99%)	85 (58%)	39 (26%)	23 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	J	140/142 (99%)	89 (64%)	33 (24%)	18 (13%)	0	3
21	N	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	1	6
22	O	114/117 (97%)	83 (73%)	25 (22%)	6 (5%)	3	24
23	Q	115/117 (98%)	70 (61%)	38 (33%)	7 (6%)	2	19
24	S	108/110 (98%)	69 (64%)	29 (27%)	10 (9%)	1	8
25	U	100/103 (97%)	54 (54%)	23 (23%)	23 (23%)	0	0
26	F	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	2
27	G	174/176 (99%)	101 (58%)	48 (28%)	25 (14%)	0	2
28	R	101/103 (98%)	64 (63%)	28 (28%)	9 (9%)	1	9
29	T	91/100 (91%)	51 (56%)	30 (33%)	10 (11%)	1	5
30	Z	75/78 (96%)	50 (67%)	21 (28%)	4 (5%)	3	24
31	W	77/84 (92%)	29 (38%)	26 (34%)	22 (29%)	0	0
All	All	3309/3397 (97%)	2075 (63%)	823 (25%)	411 (12%)	1	3

5 of 411 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	5	GLN
3	I	18	ASN
4	C	77	VAL
4	C	107	LYS
5	D	9	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 X-ray entries followed by that with respect to entries of similar resolution. 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	
3	I	109/109 (100%)	104 (95%)	5 (5%)	37	80
4	C	216/217 (100%)	176 (82%)	40 (18%)	2	11
5	D	164/164 (100%)	141 (86%)	23 (14%)	5	24
6	K	102/104 (98%)	79 (78%)	23 (22%)	1	6
7	P	99/99 (100%)	81 (82%)	18 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	165/165 (100%)	137 (83%)	28 (17%)	3	14
9	Y	48/48 (100%)	38 (79%)	10 (21%)	2	8
10	0	47/47 (100%)	35 (74%)	12 (26%)	1	2
11	4	34/34 (100%)	28 (82%)	6 (18%)	3	13
12	1	45/48 (94%)	41 (91%)	4 (9%)	14	49
13	3	51/51 (100%)	47 (92%)	4 (8%)	18	58
14	V	78/78 (100%)	62 (80%)	16 (20%)	2	8
15	2	38/38 (100%)	32 (84%)	6 (16%)	4	16
16	L	102/103 (99%)	88 (86%)	14 (14%)	5	25
17	M	109/109 (100%)	91 (84%)	18 (16%)	3	14
18	X	55/55 (100%)	40 (73%)	15 (27%)	0	2
19	H	114/114 (100%)	86 (75%)	28 (25%)	1	3
20	J	116/116 (100%)	100 (86%)	16 (14%)	5	24
21	N	100/103 (97%)	87 (87%)	13 (13%)	6	28
22	O	86/87 (99%)	70 (81%)	16 (19%)	2	11
23	Q	89/89 (100%)	74 (83%)	15 (17%)	3	14
24	S	93/93 (100%)	79 (85%)	14 (15%)	4	19
25	U	83/84 (99%)	68 (82%)	15 (18%)	2	12
26	F	149/149 (100%)	115 (77%)	34 (23%)	1	5
27	G	137/137 (100%)	113 (82%)	24 (18%)	3	13
28	R	84/84 (100%)	73 (87%)	11 (13%)	6	28
29	T	80/84 (95%)	65 (81%)	15 (19%)	2	11
30	Z	67/68 (98%)	52 (78%)	15 (22%)	1	6
31	W	59/62 (95%)	45 (76%)	14 (24%)	1	4
All	All	2719/2739 (99%)	2247 (83%)	472 (17%)	3	13

5 of 472 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	M	38	ARG
19	H	114	GLU
29	T	48	GLN
17	M	104	GLU
18	X	48	ARG

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

Mol	Chain	Res	Type
15	2	16	HIS
19	H	135	HIS
30	Z	6	GLN
16	L	54	GLN
18	X	20	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	17 (14%)	1 (0%)
2	B	2837/2904 (97%)	433 (15%)	20 (0%)
All	All	2953/3024 (97%)	450 (15%)	21 (0%)

5 of 450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	G
1	A	25	U
1	A	26	C
1	A	30	C
1	A	35	C

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1210	G
2	B	1419	A
2	B	2434	A
2	B	1126	A
2	B	2756	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 113 ligands modelled in this entry, 112 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	NMY	B	2905	-	45,45,45	2.26	15 (33%)	67,67,67	1.36	7 (10%)

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
32	NMY	B	2905	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	2905	NMY	C8-C9	6.33	1.57	1.52
32	B	2905	NMY	C8-C7	6.18	1.57	1.52
32	B	2905	NMY	O22-C18	4.50	1.53	1.41
32	B	2905	NMY	C3-C2	4.36	1.59	1.53
32	B	2905	NMY	O16-C13	3.62	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	2905	NMY	O11-C13-O16	5.13	116.41	111.51
32	B	2905	NMY	O22-C22-C23	4.17	112.09	106.97
32	B	2905	NMY	O18-C18-C19	3.55	115.12	108.09
32	B	2905	NMY	O11-C13-C14	2.99	112.83	107.50
32	B	2905	NMY	O5-C5-C6	2.95	110.59	106.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	117/120 (97%)	0.08	7 (5%) 21 5	36, 75, 124, 180	0
2	B	2841/2904 (97%)	-0.03	146 (5%) 27 5	6, 47, 151, 180	0
3	I	141/141 (100%)	-0.35	0 100 100	101, 177, 180, 180	0
4	C	271/272 (99%)	0.13	14 (5%) 26 5	5, 35, 87, 135	0
5	D	209/209 (100%)	0.18	12 (5%) 23 5	5, 50, 126, 180	0
6	K	121/123 (98%)	1.84	45 (37%) 1 0	6, 43, 104, 164	0
7	P	114/114 (100%)	0.19	6 (5%) 25 5	6, 49, 113, 160	0
8	E	201/201 (100%)	0.30	16 (7%) 12 3	5, 72, 137, 180	0
9	Y	58/58 (100%)	0.58	9 (15%) 3 1	21, 60, 141, 177	0
10	0	56/56 (100%)	-0.12	0 100 100	9, 49, 124, 180	0
11	4	38/38 (100%)	-0.17	0 100 100	18, 68, 129, 150	0
12	1	50/54 (92%)	0.26	4 (8%) 12 3	14, 76, 127, 175	0
13	3	64/64 (100%)	0.65	9 (14%) 3 1	9, 49, 112, 156	0
14	V	94/94 (100%)	0.38	10 (10%) 7 2	21, 89, 153, 167	0
15	2	46/46 (100%)	1.38	17 (36%) 1 0	5, 38, 76, 180	0
16	L	143/144 (99%)	0.42	12 (8%) 11 3	9, 59, 117, 147	0
17	M	136/136 (100%)	-0.01	3 (2%) 59 15	13, 54, 118, 167	0
18	X	63/63 (100%)	-0.05	2 (3%) 45 10	38, 97, 156, 180	0
19	H	149/149 (100%)	-0.19	2 (1%) 74 26	32, 110, 160, 180	0
20	J	142/142 (100%)	0.30	8 (5%) 24 5	17, 61, 126, 180	0
21	N	120/127 (94%)	-0.29	0 100 100	7, 43, 91, 172	0
22	O	116/117 (99%)	0.90	26 (22%) 1 1	19, 73, 135, 172	0
23	Q	117/117 (100%)	0.35	12 (10%) 7 2	8, 50, 104, 180	0
24	S	110/110 (100%)	0.53	10 (9%) 9 2	12, 48, 129, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	U	102/103 (99%)	-0.03	4 (3%) 37 8	22, 94, 154, 180	0
26	F	178/178 (100%)	0.75	29 (16%) 2 1	30, 107, 168, 180	0
27	G	176/176 (100%)	0.40	15 (8%) 11 3	35, 97, 161, 180	0
28	R	103/103 (100%)	-0.27	0 100 100	23, 76, 139, 161	0
29	T	93/100 (93%)	0.31	8 (8%) 11 3	24, 64, 156, 179	0
30	Z	77/78 (98%)	-0.03	2 (2%) 53 12	9, 48, 94, 128	0
31	W	79/84 (94%)	0.14	2 (2%) 54 13	20, 71, 134, 180	0
All	All	6325/6421 (98%)	0.14	430 (6%) 17 4	5, 56, 156, 180	0

The worst 5 of 430 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	K	111	LYS	10.4
2	B	645	C	10.3
26	F	178	LYS	9.5
6	K	110	GLU	9.1
25	U	87	GLU	9.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	MG	B	3389	1/1	0.16	28.44	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	NMY	B	2905	42/42	0.45	18.80	88,88,88,88	42
33	MG	B	3337	1/1	0.22	7.21	180,180,180,180	0
33	MG	B	3201	1/1	0.32	6.62	81,81,81,81	0
33	MG	B	3172	1/1	0.39	6.11	74,74,74,74	0
33	MG	B	3452	1/1	0.23	5.55	46,46,46,46	0
33	MG	B	3165	1/1	0.52	5.38	33,33,33,33	0
33	MG	B	3351	1/1	0.24	4.02	115,115,115,115	0
33	MG	B	3592	1/1	0.18	2.26	27,27,27,27	0
33	MG	B	3021	1/1	0.32	1.76	30,30,30,30	0
33	MG	B	3279	1/1	0.22	1.76	46,46,46,46	0
33	MG	B	3207	1/1	0.53	1.51	40,40,40,40	0
33	MG	B	3274	1/1	0.26	1.46	23,23,23,23	0
33	MG	B	3409	1/1	0.27	1.39	23,23,23,23	0
33	MG	B	3308	1/1	0.24	1.07	65,65,65,65	0
33	MG	B	3544	1/1	0.15	0.80	33,33,33,33	0
33	MG	B	3413	1/1	0.27	0.61	61,61,61,61	0
33	MG	B	3515	1/1	0.51	0.48	47,47,47,47	0
33	MG	B	3446	1/1	0.14	0.13	47,47,47,47	0
33	MG	B	3618	1/1	0.19	-0.03	37,37,37,37	0
33	MG	B	3344	1/1	0.16	-0.06	124,124,124,124	0
33	MG	B	3104	1/1	0.18	-0.07	48,48,48,48	0
33	MG	B	3457	1/1	0.17	-0.20	43,43,43,43	0
33	MG	B	3146	1/1	0.20	-0.31	15,15,15,15	0
33	MG	B	3485	1/1	0.17	-0.32	92,92,92,92	0
33	MG	B	3598	1/1	0.26	-0.38	21,21,21,21	0
33	MG	B	3419	1/1	0.22	-0.40	30,30,30,30	0
33	MG	B	3320	1/1	0.25	-0.44	12,12,12,12	0
33	MG	B	3189	1/1	0.18	-0.50	62,62,62,62	0
33	MG	B	3074	1/1	0.16	-0.59	48,48,48,48	0
34	ZN	4	624	1/1	0.13	-0.62	57,57,57,57	0
33	MG	B	3152	1/1	0.14	-0.65	36,36,36,36	0
33	MG	B	3525	1/1	0.12	-0.80	67,67,67,67	0
33	MG	B	3058	1/1	0.24	-0.82	7,7,7,7	0
33	MG	B	3069	1/1	0.15	-0.84	21,21,21,21	0
33	MG	B	3537	1/1	0.12	-0.85	127,127,127,127	0
33	MG	B	3184	1/1	0.13	-0.91	18,18,18,18	0
33	MG	B	3257	1/1	0.25	-1.07	22,22,22,22	0
33	MG	B	3052	1/1	0.13	-1.09	5,5,5,5	0
33	MG	B	3214	1/1	0.14	-1.17	15,15,15,15	0
33	MG	B	3239	1/1	0.18	-1.32	7,7,7,7	0
33	MG	B	3127	1/1	0.13	-1.34	29,29,29,29	0
33	MG	B	3315	1/1	0.12	-1.35	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	3370	1/1	0.12	-1.35	33,33,33,33	0
33	MG	B	3332	1/1	0.09	-1.37	43,43,43,43	0
33	MG	B	3220	1/1	0.13	-1.39	17,17,17,17	0
33	MG	B	3357	1/1	0.11	-1.41	47,47,47,47	0
33	MG	B	3492	1/1	0.13	-1.42	25,25,25,25	0
33	MG	B	3564	1/1	0.09	-1.44	5,5,5,5	0
33	MG	B	3463	1/1	0.19	-1.54	39,39,39,39	0
33	MG	B	3225	1/1	0.12	-1.57	19,19,19,19	0
33	MG	B	3609	1/1	0.13	-1.58	19,19,19,19	0
33	MG	B	3301	1/1	0.37	-1.59	102,102,102,102	0
33	MG	B	3081	1/1	0.06	-1.85	22,22,22,22	0
33	MG	B	3425	1/1	0.14	-1.89	33,33,33,33	0
33	MG	B	3262	1/1	0.14	-1.93	55,55,55,55	0
33	MG	B	3382	1/1	0.05	-1.94	29,29,29,29	0
33	MG	B	3570	1/1	0.14	-2.01	14,14,14,14	0
33	MG	B	3579	1/1	0.12	-2.16	21,21,21,21	0
33	MG	B	3040	1/1	0.08	-2.18	16,16,16,16	0
33	MG	B	3014	1/1	0.07	-2.19	14,14,14,14	0
33	MG	B	3140	1/1	0.09	-2.19	44,44,44,44	0
33	MG	B	3468	1/1	0.10	-2.26	18,18,18,18	0
33	MG	B	3553	1/1	0.07	-2.29	29,29,29,29	0
33	MG	B	3512	1/1	0.07	-2.30	34,34,34,34	0
33	MG	B	3268	1/1	0.07	-2.39	24,24,24,24	0
33	MG	B	3159	1/1	0.03	-2.46	8,8,8,8	0
33	MG	B	3614	1/1	0.07	-2.48	28,28,28,28	0
33	MG	B	3245	1/1	0.08	-2.48	15,15,15,15	0
33	MG	B	3292	1/1	0.05	-2.51	87,87,87,87	0
33	MG	B	3504	1/1	0.10	-2.53	48,48,48,48	0
33	MG	B	3584	1/1	0.06	-2.63	40,40,40,40	0
33	MG	B	3496	1/1	0.07	-2.69	18,18,18,18	0
33	MG	B	3235	1/1	0.07	-2.70	15,15,15,15	0
33	MG	B	3001	1/1	0.04	-2.72	5,5,5,5	0
33	MG	B	3532	1/1	0.04	-2.73	39,39,39,39	0
33	MG	B	3133	1/1	0.13	-2.74	55,55,55,55	0
33	MG	B	3474	1/1	0.14	-2.82	6,6,6,6	0
33	MG	B	3500	1/1	0.07	-2.91	25,25,25,25	0
33	MG	B	3064	1/1	0.08	-2.91	37,37,37,37	0
33	MG	B	3528	1/1	0.08	-2.91	21,21,21,21	0
33	MG	B	3588	1/1	0.11	-2.95	39,39,39,39	0
33	MG	B	3026	1/1	0.05	-3.01	20,20,20,20	0
33	MG	B	3327	1/1	0.04	-3.04	5,5,5,5	0
33	MG	B	3033	1/1	0.06	-3.06	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	3559	1/1	0.05	-3.12	9,9,9,9	0
33	MG	B	3575	1/1	0.04	-3.13	16,16,16,16	0
33	MG	B	3431	1/1	0.08	-3.19	28,28,28,28	0
33	MG	B	3440	1/1	0.06	-3.37	26,26,26,26	0
33	MG	B	3179	1/1	0.08	-3.68	32,32,32,32	0
33	MG	B	3196	1/1	0.10	-3.72	43,43,43,43	0
33	MG	B	3602	1/1	0.04	-3.81	10,10,10,10	0
33	MG	B	3110	1/1	0.07	-3.97	5,5,5,5	0
33	MG	B	3286	1/1	0.05	-4.26	32,32,32,32	0
33	MG	B	3403	1/1	0.11	-4.27	6,6,6,6	0
33	MG	B	3375	1/1	0.04	-4.54	16,16,16,16	0
33	MG	B	3229	1/1	0.08	-4.57	58,58,58,58	0
33	MG	B	3436	1/1	0.05	-4.59	7,7,7,7	0
33	MG	B	3547	1/1	0.06	-4.67	36,36,36,36	0
33	MG	B	3117	1/1	0.04	-4.81	9,9,9,9	0
33	MG	B	3008	1/1	0.07	-4.83	9,9,9,9	0
33	MG	B	3298	1/1	0.06	-5.24	32,32,32,32	0
33	MG	B	3364	1/1	0.04	-6.49	71,71,71,71	0
33	MG	B	3480	1/1	0.04	-6.57	24,24,24,24	0
33	MG	B	3508	1/1	0.05	-6.65	10,10,10,10	0
33	MG	B	3099	1/1	0.07	-6.91	8,8,8,8	0
33	MG	B	3046	1/1	0.09	-8.22	19,19,19,19	0
33	MG	B	3521	1/1	0.04	-9.20	46,46,46,46	0
33	MG	B	3092	1/1	0.06	-9.46	6,6,6,6	0
33	MG	B	3251	1/1	0.06	-9.88	12,12,12,12	0
33	MG	B	3396	1/1	0.08	-10.17	19,19,19,19	0
33	MG	B	3087	1/1	0.08	-12.55	49,49,49,49	0
33	MG	B	3122	1/1	0.05	-12.80	5,5,5,5	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.