



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:56 am GMT

PDB ID : 2F4V
Title : 30S ribosome + designer antibiotic
Authors : Murray, J.B.; Meroueh, S.O.; Russell, R.J.; Lentzen, G.; Haddad, J.; Mobashery, S.
Deposited on : 2005-11-24
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

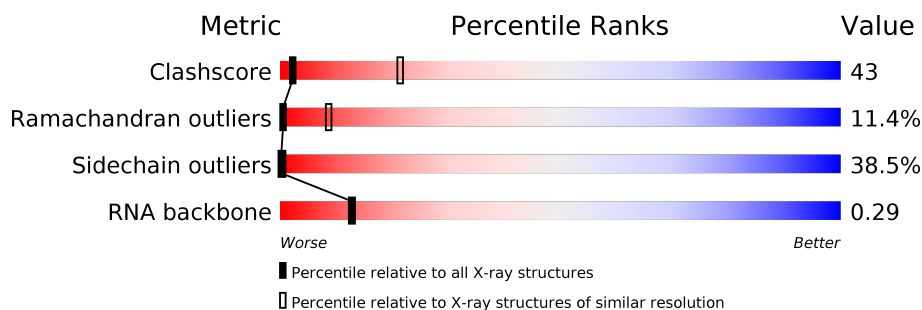
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RNA backbone	2435	1016 (4.70-2.90)

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1511	
2	Z	4	
3	B	256	
4	C	239	
5	D	209	
6	E	162	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	
12	K	129	
13	L	132	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 51728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	22	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	4	Total	C	N	O	P	0	0	0
			80	36	9	31	4			

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	237	Total	C	N	O	S	0	0	0
			1923	1226	344	348	5			

- Molecule 4 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	199	GLN	ASN	CONFLICT	UNP P80373
D	201	ASN	GLN	CONFLICT	UNP P80373

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 7 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 12 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 15 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 16 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 18 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 21 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	D	1	Total	Zn	0	0
			1	1		
22	N	1	Total	Zn	0	0
			1	1		

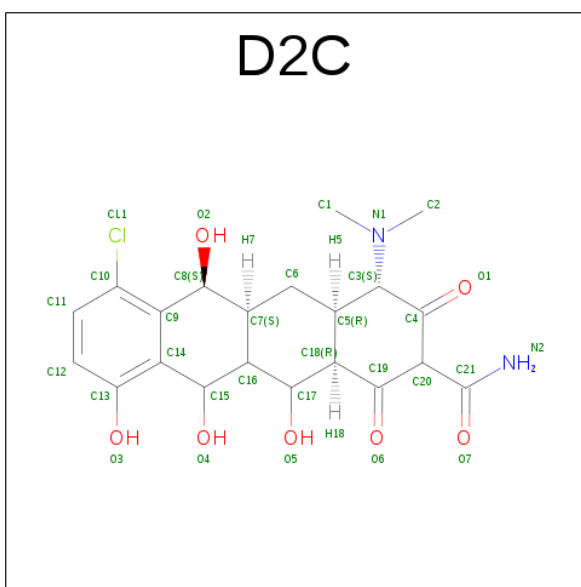
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	Z	1	Total	Mg	0	0
			1	1		
23	A	98	Total	Mg	0	0
			98	98		
23	D	1	Total	Mg	0	0
			1	1		
23	M	1	Total	Mg	0	0
			1	1		

- Molecule 24 is POTASSIUM ION (three-letter code: K) (formula: K).

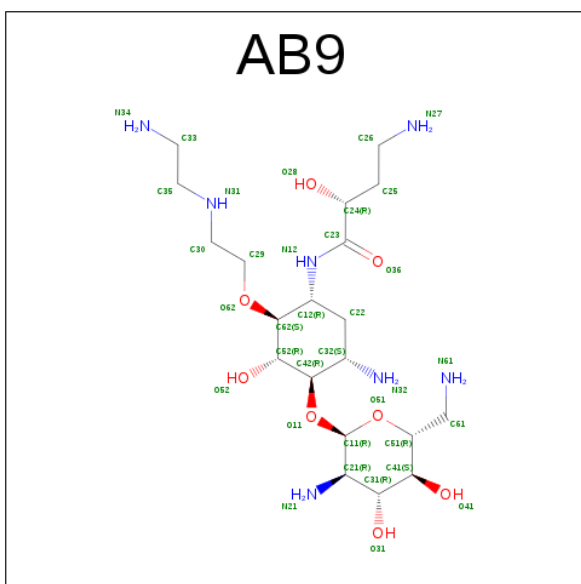
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	12	Total	K	0	0
			12	12		

- Molecule 25 is (2S,4S,4AR,5AS,6S,11R,11AS,12R,12AR)-7-CHLORO-4-(DIMETHYLAMINO)-6,10,11,12-TETRAHYDROXY-1,3-DIOXO-1,2,3,4,4A,5,5A,6,11,11A,12,12A-DODECAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: D2C) (formula: C₂₁H₂₅ClN₂O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	Cl	N	O	
			31	21	1	2	7	
								0
								0

- Molecule 26 is (2R)-4-AMINO-N-[(1R,2S,3R,4R,5S)-5-AMINO-2-[(2-AMINOETHYL)AMINO]ETHOXY]-4-[(2,6-DIAMINO-2,6-DIDEOXY-ALPHA-D-GLUCOPYRANOSYL)OXY]-3-HYDROXYCYCLOHEXYL}-2-HYDROXYBUTANAMIDE (three-letter code: AB9) (formula: C₂₀H₄₃N₇O₈).



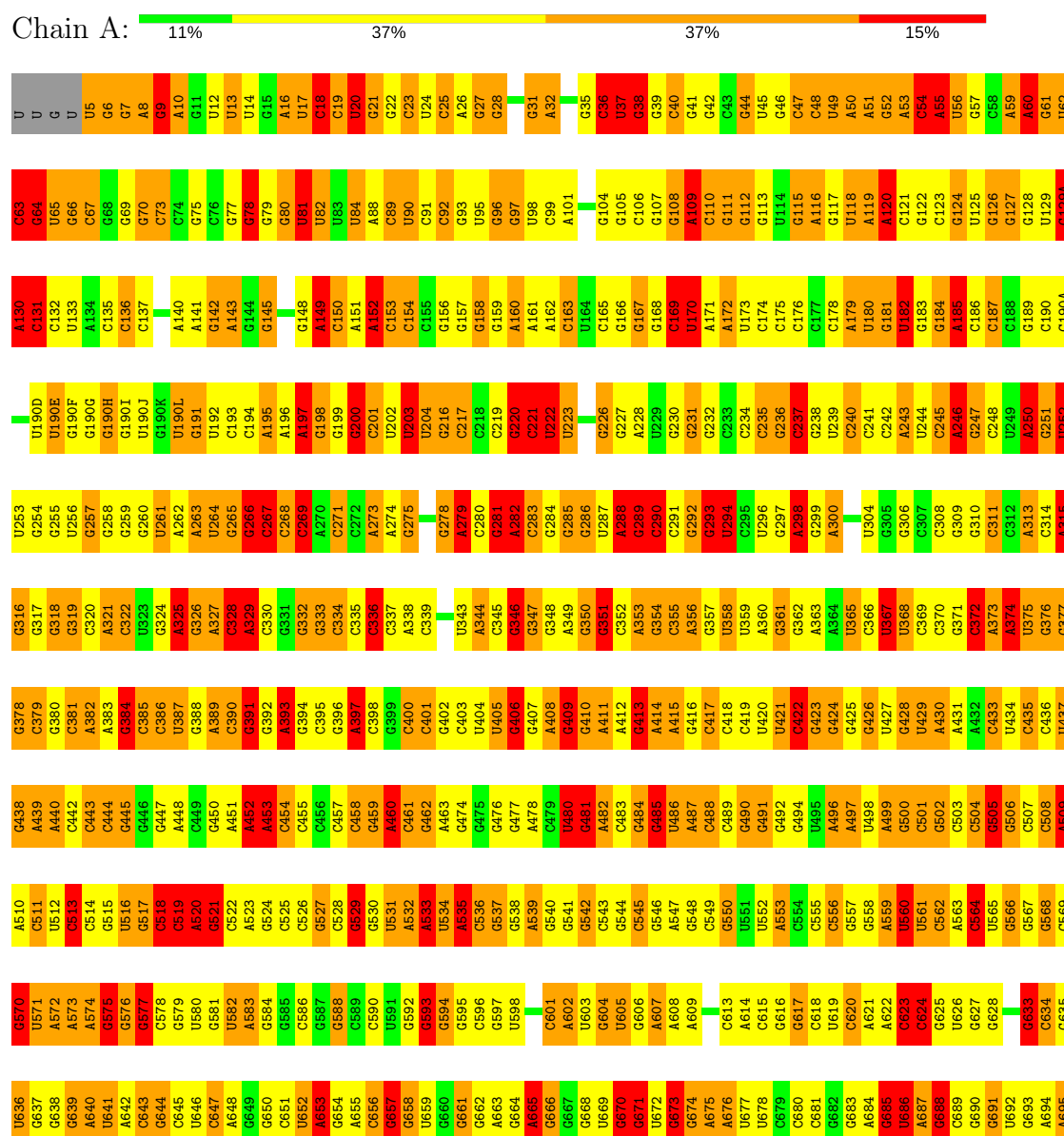
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O		
			35	20	7	8		
							0	
								0

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 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.

Note EDS was not executed.

• Molecule 1: 16S ribosomal RNA



G1497	U1498	A1499	A1500	C1501	A1502	A1503	G1504	A1506	A1507	G1508	C1509	U1510	G1511	U1512	A1513	G1514	C1515	G1516	G1517	A1518	A1519	G1520	G1521	U1522	G1523	G1524	G1525	G1526	U1527	C1528	G1529	G1530	A1531	U1532	C1533	A1534																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
A1428	C1429	C1430	C1431	C1432	A1433	A1434	G1435	U1436	G1437	G1438	C1439	C1440	G1441	G1442	G1443	A1446	G1447	C1448	C1449	U1450	A1451	C1452	G1453	G1454	G1455	C1459	A1460	G1461	G1464	C1465	C1466	G1467	A1468	U1471	U1472	A1473	G1474	G1475																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C1367	G1368	C1369	G1370	G1371	U1372	G1373	A1374	U1376	G1377	C1378	G1379	A1319	C1320	U1381	C1321	C1322	C1383	C1384	G1385	G1386	C1387	C1388	C1389	U1390	U1391	A1332	G1392	U1393	A1394	C1395	C1396	G1397	A1398	C1399	U1340	U1341	C1342	C1343	C1402	C1403	C1404	G1405	U1406	C1407	A1408	C1409	G1410	C1411	C1412	A1413	U1414	U1415	U1485	G1486	G1487	G1488	G1489	C1490	G1491	A1492	A1493	G1494	U1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	C2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	C2130	C2131	C2132	C2133	C2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	C2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	C2366	C2367	C2368	C2369	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389	C2390	C2391	C2392	C2393	C2394	C2395	C2396	C2397	C2398	C2399	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	C2446	C2447	C2448	C2449	C2450	C2451	C2452	C2453	C2454	C2455	C2456	C2457	C2458	C2459	C2460	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	C2479	C2480	C2481	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550	C2551	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625	C2626	C2627	C2628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	C2712	C2713	C2714	C2715	C2716	C2717	C2718	C2719	C2720	C2721	C2722	C2723	C2724	C2725	C2726	C2727

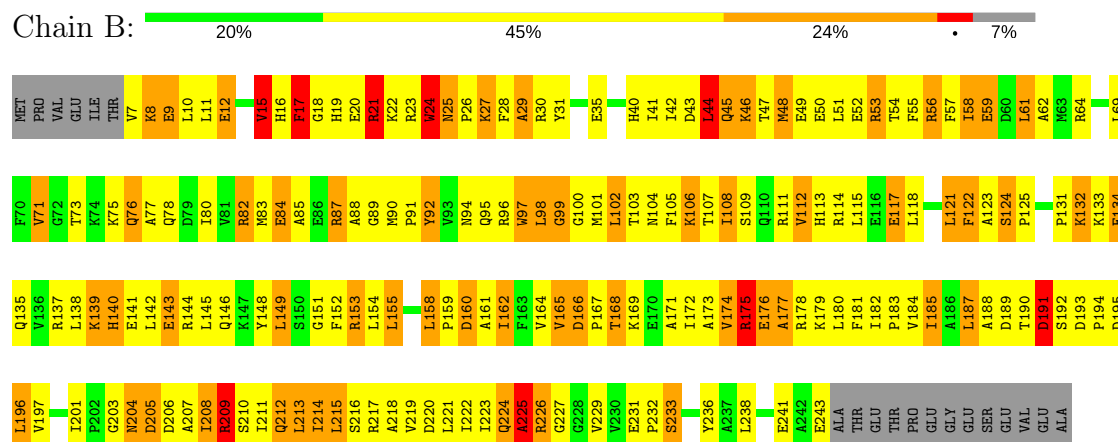
● Molecule 2: 5'-R(P*UP*UP*CP*U)-3'

Chain Z:

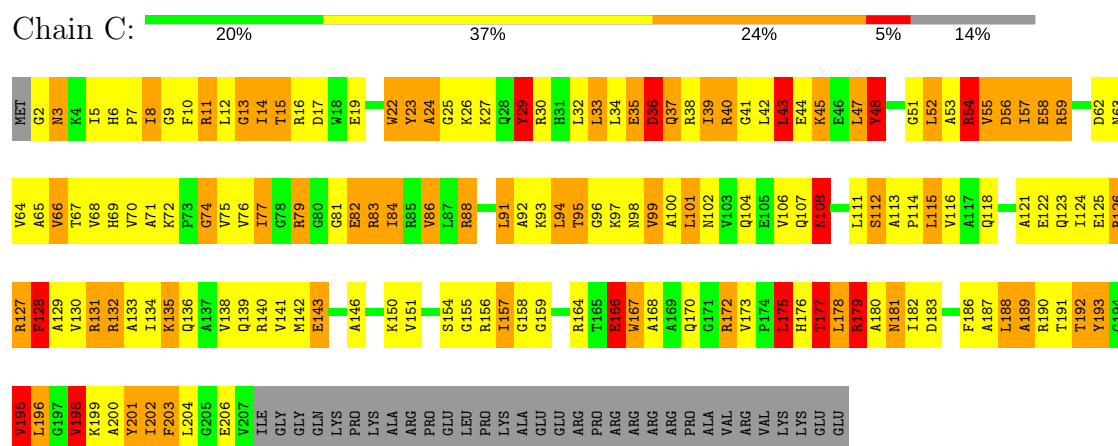
100%

U3
U4
C5
U6

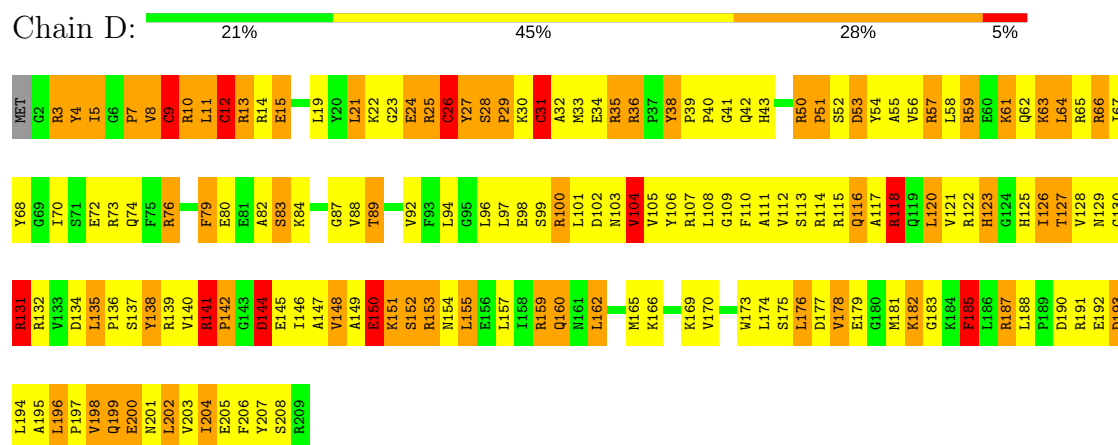
- Molecule 3: 30S ribosomal protein S2



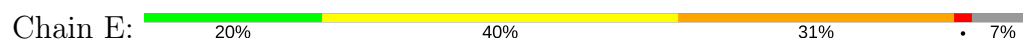
- Molecule 4: 30S ribosomal protein S3

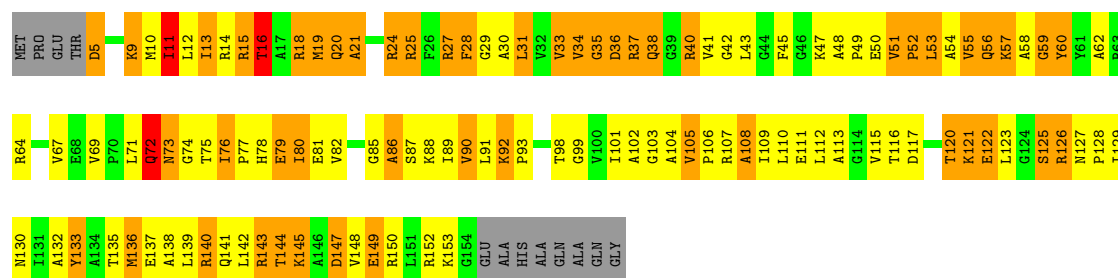


- Molecule 5: 30S ribosomal protein S4



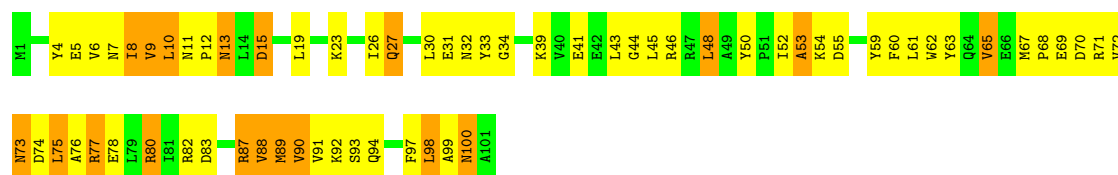
- Molecule 6: 30S ribosomal protein S5





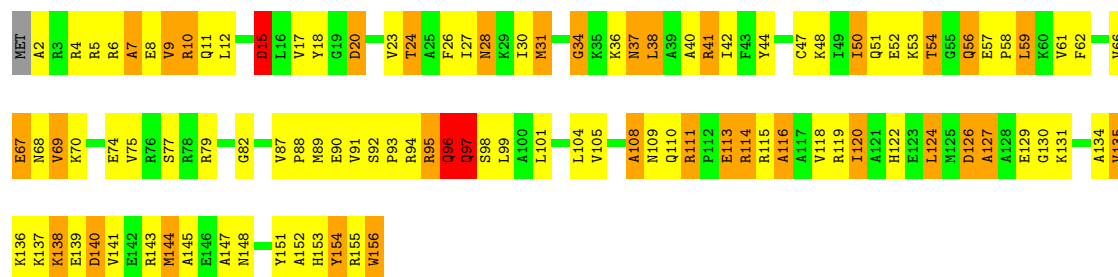
• Molecule 7: 30S ribosomal protein S6

Chain F: 36% 46% 19%



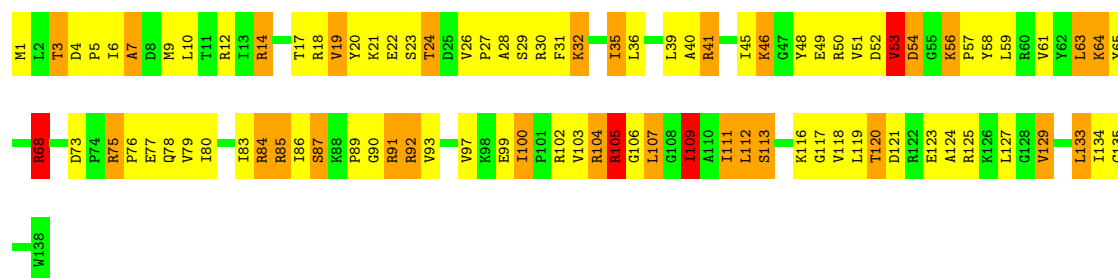
• Molecule 8: 30S ribosomal protein S7

Chain G: 32% 44% 21% ..



• Molecule 9: 30S ribosomal protein S8

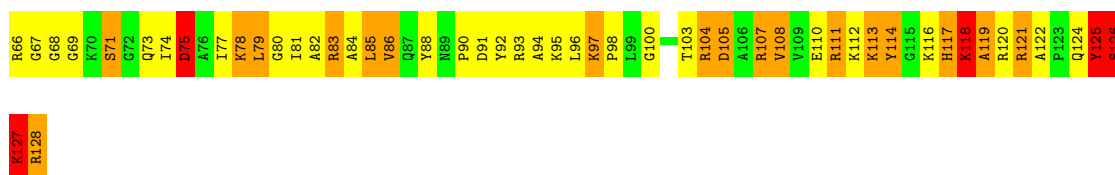
Chain H: 33% 43% 20% .



• Molecule 10: 30S ribosomal protein S9

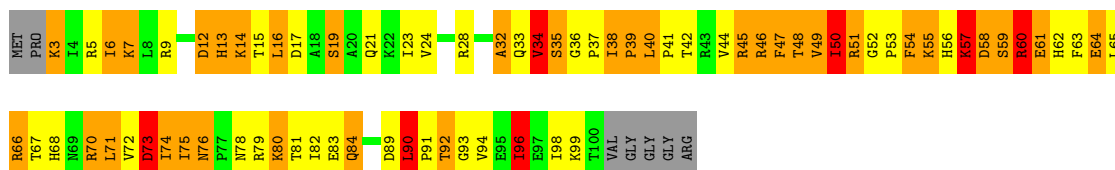
Chain I: 19% 48% 27% 5% .





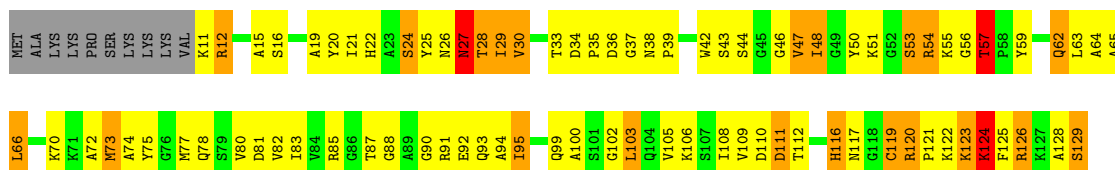
• Molecule 11: 30S ribosomal protein S10

Chain J: 22% 32% 32% 7% 7%



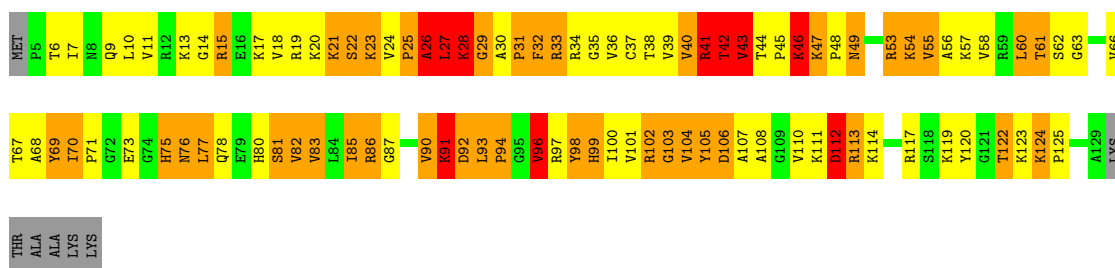
• Molecule 12: 30S ribosomal protein S11

Chain K: 27% 47% 16% 8%



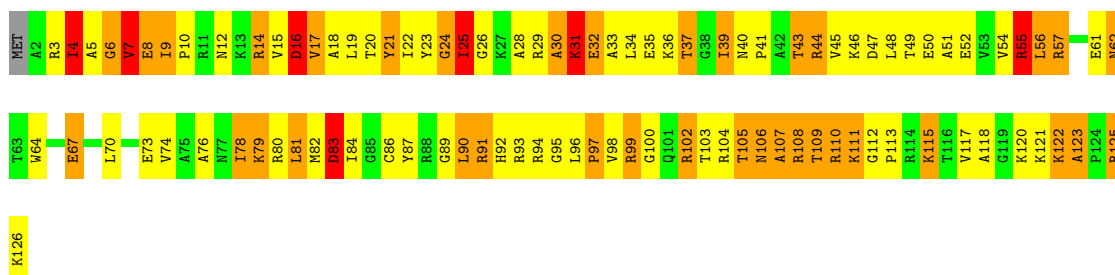
• Molecule 13: 30S ribosomal protein S12

Chain L: 20% 36% 31% 8% 5%

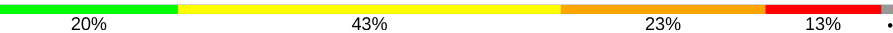


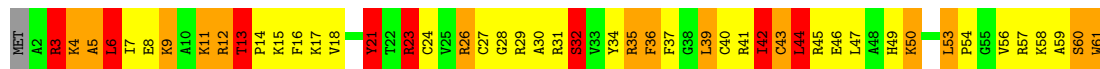
• Molecule 14: 30S ribosomal protein S13

Chain M: 21% 44% 29% 6%



- Molecule 15: 30S ribosomal protein S14

Chain N:  20% 43% 23% 13%

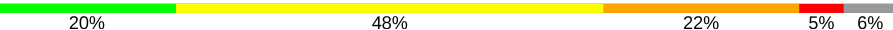


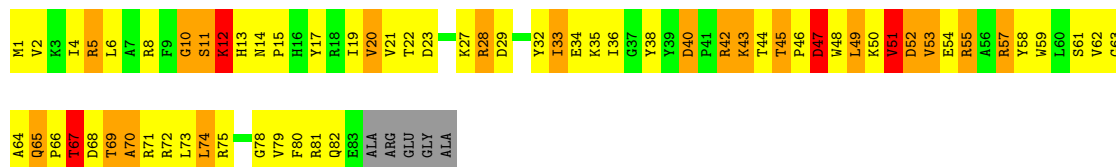
- Molecule 16: 30S ribosomal protein S15

Chain O:  22% 49% 22%



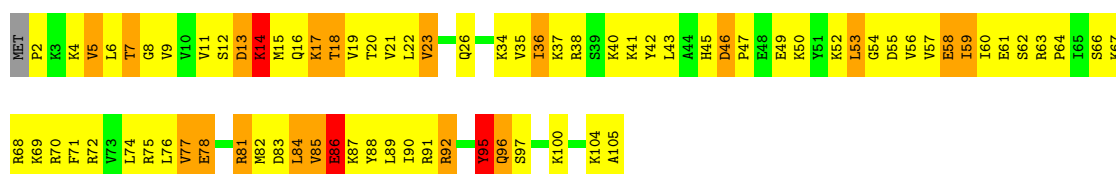
- Molecule 17: 30S ribosomal protein S16

Chain P:  20% 48% 22% 5% 6%



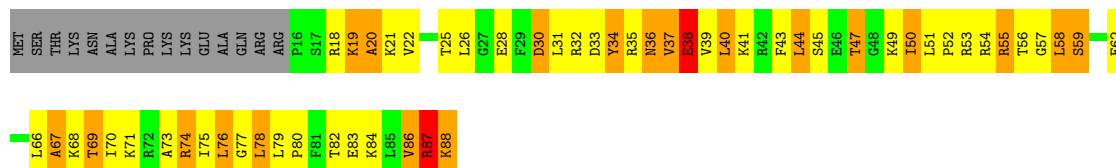
- Molecule 18: 30S ribosomal protein S17

Chain Q:  25% 54% 17%



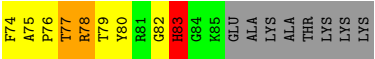
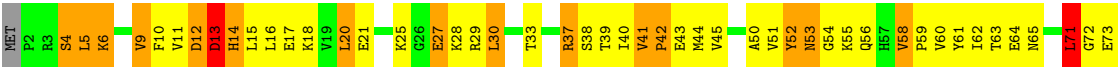
- Molecule 19: 30S ribosomal protein S18

Chain R:  19% 39% 23% 17%

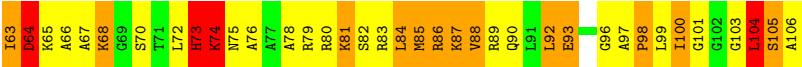
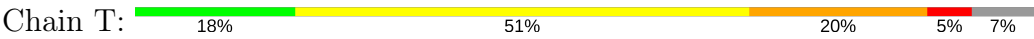


- Molecule 20: 30S ribosomal protein S19

Chain S:  29% 40% 18% 10%



• Molecule 21: 30S ribosomal protein S20



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.32Å 403.32Å 176.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80	Depositor
% Data completeness (in resolution range)	97.2 (30.00-3.80)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.259 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51728	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, AB9, MG, D2C, ZN

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	1.70	440/36247 (1.2%)	1.64	607/56545 (1.1%)
2	Z	2.01	1/87 (1.1%)	1.60	0/132
3	B	0.84	1/1958 (0.1%)	0.69	5/2640 (0.2%)
4	C	0.91	1/1636 (0.1%)	0.66	3/2205 (0.1%)
5	D	0.81	1/1733 (0.1%)	0.66	5/2318 (0.2%)
6	E	1.14	1/1162 (0.1%)	0.75	3/1564 (0.2%)
7	F	0.73	0/856	0.65	2/1154 (0.2%)
8	G	0.89	1/1276 (0.1%)	0.64	4/1709 (0.2%)
9	H	1.18	1/1136 (0.1%)	0.80	2/1527 (0.1%)
10	I	0.79	0/1029	0.67	5/1378 (0.4%)
11	J	0.81	1/805 (0.1%)	0.75	3/1082 (0.3%)
12	K	0.99	0/900	0.73	2/1213 (0.2%)
13	L	0.87	0/991	0.67	3/1327 (0.2%)
14	M	0.87	1/1008 (0.1%)	0.69	3/1347 (0.2%)
15	N	0.86	0/501	0.63	0/664
16	O	0.88	0/745	0.67	3/992 (0.3%)
17	P	1.16	1/716 (0.1%)	0.82	2/963 (0.2%)
18	Q	1.01	0/870	0.71	3/1159 (0.3%)
19	R	0.92	0/603	0.72	1/799 (0.1%)
20	S	0.70	0/689	0.66	2/926 (0.2%)
21	T	1.07	0/764	0.68	0/1006
All	All	1.47	450/55712 (0.8%)	1.41	658/82650 (0.8%)

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
3	B	0	2
4	C	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	0	6
6	E	0	5
7	F	0	1
9	H	0	5
10	I	0	4
11	J	0	6
12	K	0	5
13	L	0	8
14	M	0	4
15	N	0	8
17	P	0	4
18	Q	0	1
20	S	0	5
21	T	0	4
All	All	0	74

The worst 5 of 450 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1169	A	O3'-P	35.46	2.03	1.61
1	A	1227	A	N9-C4	-13.10	1.29	1.37
1	A	1346	A	C3'-O3'	11.14	1.57	1.42
1	A	1224	G	C3'-O3'	10.61	1.57	1.42
1	A	1129	C	C1'-N1	10.46	1.64	1.48

The worst 5 of 658 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1169	A	P-O3'-C3'	29.86	155.53	119.70
1	A	1525	G	C4'-C3'-C2'	-12.91	89.69	102.60
1	A	1346	A	P-O3'-C3'	11.99	134.09	119.70
1	A	1345	U	C1'-O4'-C4'	-11.81	100.45	109.90
1	A	1025	U	C1'-O4'-C4'	-11.60	100.62	109.90

There are no chirality outliers.

5 of 74 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	133	LYS	Peptide
3	B	225	ALA	Peptide
4	C	13	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	C	166	GLU	Peptide
4	C	48	TYR	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	A	32391	0	16359	1894	0
2	Z	80	0	42	4	0
3	B	1923	0	1968	218	0
4	C	1612	0	1677	175	0
5	D	1703	0	1763	198	0
6	E	1146	0	1207	161	0
7	F	843	0	857	58	0
8	G	1257	0	1296	105	0
9	H	1116	0	1177	93	0
10	I	1011	0	1043	122	0
11	J	792	0	835	125	0
12	K	885	0	904	80	0
13	L	975	0	1062	129	0
14	M	997	0	1072	111	0
15	N	492	0	530	84	0
16	O	734	0	771	70	0
17	P	700	0	720	72	0
18	Q	857	0	930	70	0
19	R	597	0	668	68	0
20	S	674	0	699	56	0
21	T	762	0	859	97	0
22	D	1	0	0	0	0
22	N	1	0	0	0	0
23	A	98	0	0	0	0
23	D	1	0	0	0	0
23	M	1	0	0	0	0
23	Z	1	0	0	0	0
24	A	12	0	0	0	0
25	A	31	0	19	4	0
26	A	35	0	43	1	0
All	All	51728	0	36501	3715	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 43.

The worst 5 of 3715 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)
8:G:89:MET:SD	8:G:89:MET:CE	2.02	1.45
1:A:492:G:H3'	1:A:494:G:OP2	1.29	1.32
6:E:80:ILE:CD1	6:E:91:LEU:HB2	1.62	1.29
1:A:70:G:H3'	1:A:73:C:P	1.72	1.27
15:N:40:CYS:O	15:N:43:CYS:HB2	1.23	1.27

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 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	B	235/256 (92%)	153 (65%)	48 (20%)	34 (14%)	0	5
4	C	204/239 (85%)	120 (59%)	51 (25%)	33 (16%)	0	4
5	D	206/209 (99%)	145 (70%)	37 (18%)	24 (12%)	0	8
6	E	148/162 (91%)	110 (74%)	24 (16%)	14 (10%)	1	14
7	F	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	2	25
8	G	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	15
9	H	136/138 (99%)	103 (76%)	26 (19%)	7 (5%)	2	29
10	I	125/128 (98%)	79 (63%)	33 (26%)	13 (10%)	0	11
11	J	96/105 (91%)	63 (66%)	20 (21%)	13 (14%)	0	5
12	K	117/129 (91%)	79 (68%)	25 (21%)	13 (11%)	0	9
13	L	123/132 (93%)	76 (62%)	29 (24%)	18 (15%)	0	5
14	M	123/126 (98%)	75 (61%)	31 (25%)	17 (14%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	58/61 (95%)	43 (74%)	8 (14%)	7 (12%)	0	7
16	O	86/89 (97%)	56 (65%)	22 (26%)	8 (9%)	1	14
17	P	81/88 (92%)	55 (68%)	17 (21%)	9 (11%)	0	9
18	Q	102/105 (97%)	73 (72%)	21 (21%)	8 (8%)	1	19
19	R	71/88 (81%)	50 (70%)	14 (20%)	7 (10%)	1	12
20	S	82/93 (88%)	58 (71%)	17 (21%)	7 (8%)	1	16
21	T	97/106 (92%)	60 (62%)	21 (22%)	16 (16%)	0	4
All	All	2342/2511 (93%)	1577 (67%)	497 (21%)	268 (11%)	0	9

5 of 268 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	17	PHE
3	B	29	ALA
3	B	99	GLY
3	B	106	LYS
3	B	131	PRO

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	B	204/220 (93%)	125 (61%)	79 (39%)	0	0
4	C	160/188 (85%)	90 (56%)	70 (44%)	0	0
5	D	180/181 (99%)	105 (58%)	75 (42%)	0	0
6	E	115/123 (94%)	70 (61%)	45 (39%)	0	0
7	F	90/90 (100%)	63 (70%)	27 (30%)	0	3
8	G	126/127 (99%)	80 (64%)	46 (36%)	0	1
9	H	119/119 (100%)	78 (66%)	41 (34%)	0	1
10	I	98/99 (99%)	61 (62%)	37 (38%)	0	0
11	J	87/92 (95%)	51 (59%)	36 (41%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	90/99 (91%)	62 (69%)	28 (31%)	0	3
13	L	104/109 (95%)	53 (51%)	51 (49%)	0	0
14	M	100/101 (99%)	59 (59%)	41 (41%)	0	0
15	N	49/50 (98%)	26 (53%)	23 (47%)	0	0
16	O	79/80 (99%)	48 (61%)	31 (39%)	0	0
17	P	72/74 (97%)	45 (62%)	27 (38%)	0	0
18	Q	96/97 (99%)	69 (72%)	27 (28%)	0	3
19	R	64/77 (83%)	37 (58%)	27 (42%)	0	0
20	S	73/80 (91%)	47 (64%)	26 (36%)	0	1
21	T	76/82 (93%)	50 (66%)	26 (34%)	0	1
All	All	1982/2088 (95%)	1219 (62%)	763 (38%)	0	0

5 of 763 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	H	18	ARG
11	J	28	ARG
19	R	78	LEU
9	H	49	GLU
10	I	29	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
8	G	148	ASN
11	J	68	HIS
20	S	65	ASN
10	I	34	ASN
11	J	76	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1494/1511 (98%)	656 (43%)	0
2	Z	3/4 (75%)	0	0
All	All	1497/1515 (98%)	656 (43%)	0

5 of 656 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	16	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 117 ligands modelled in this entry, 115 are monoatomic - leaving 2 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	$\# Z > 2$
25	D2C	A	1636	23	33,34,34	2.93	9 (27%)	26,54,54	2.29	10 (38%)
26	AB9	A	1637	-	35,36,36	2.11	2 (5%)	39,49,49	1.37	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	D2C	A	1636	23	-	0/6/64/64	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AB9	A	1637	-	-	0/24/64/64	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1636	D2C	C16-C17	-10.71	1.37	1.53
25	A	1636	D2C	C18-C5	-6.98	1.44	1.54
25	A	1636	D2C	C14-C15	-5.76	1.43	1.52
25	A	1636	D2C	C6-C5	-2.70	1.49	1.53
25	A	1636	D2C	O5-C17	-2.67	1.36	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1637	AB9	O36-C23-N12	-6.89	109.94	122.90
25	A	1636	D2C	O6-C19-C18	-3.63	115.72	122.58
25	A	1636	D2C	C7-C6-C5	-2.64	105.77	110.25
25	A	1636	D2C	C2-N1-C3	-2.60	108.04	114.09
25	A	1636	D2C	C11-C10-C9	-2.53	119.17	122.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1636	D2C	4	0
26	A	1637	AB9	1	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.