



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:55 PM GMT

PDB ID : 2QBC
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin. This file contains the 50S subunit of the second 70S ribosome, with gentamicin 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 : 2007-06-16
Resolution : 3.54 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

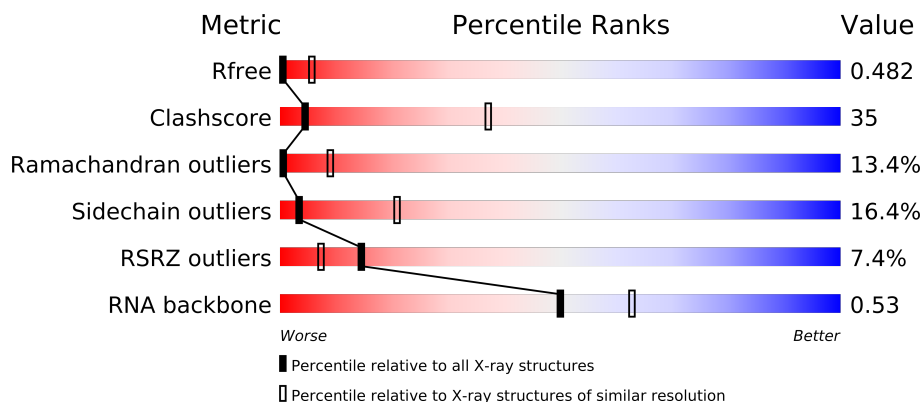
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.54 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	1270 (3.78-3.30)
Clashscore	79885	1033 (3.70-3.38)
Ramachandran outliers	78287	1067 (3.72-3.36)
Sidechain outliers	78261	1067 (3.72-3.36)
RSRZ outliers	66119	1270 (3.78-3.30)
RNA backbone	1838	1011 (4.30-2.76)

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. 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	MG	B	3165	-	X
32	MG	B	3201	-	X
32	MG	B	3207	-	X
32	MG	B	3262	-	X
32	MG	B	3279	-	X
32	MG	B	3337	-	X
32	MG	B	3452	-	X
32	MG	B	3515	-	X
34	LLL	B	3619	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 90294 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			

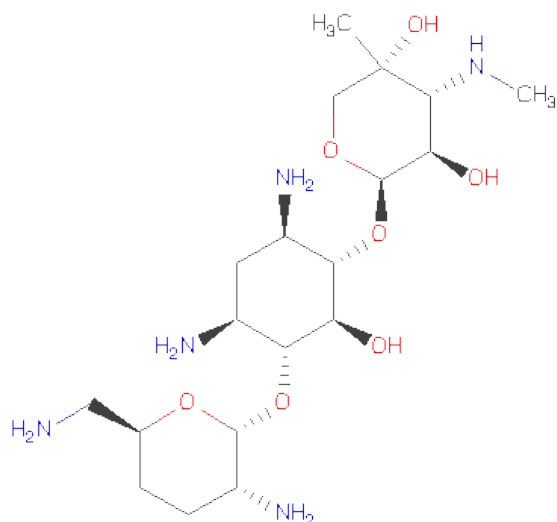
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	4	1	Total	Zn	0	0
			1	1		

- Molecule 34 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 35 is water.

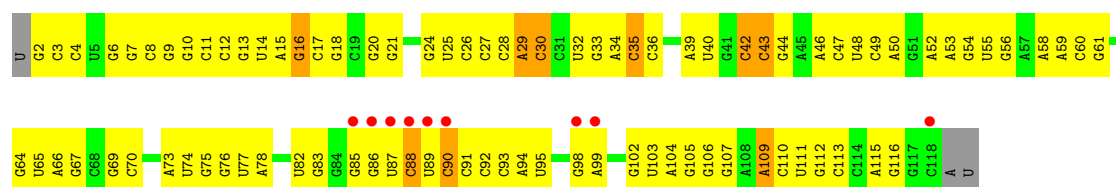
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	502	Total	O	0	0
			502	502		
35	C	4	Total	O	0	0
			4	4		
35	E	2	Total	O	0	0
			2	2		
35	L	4	Total	O	0	0
			4	4		

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.

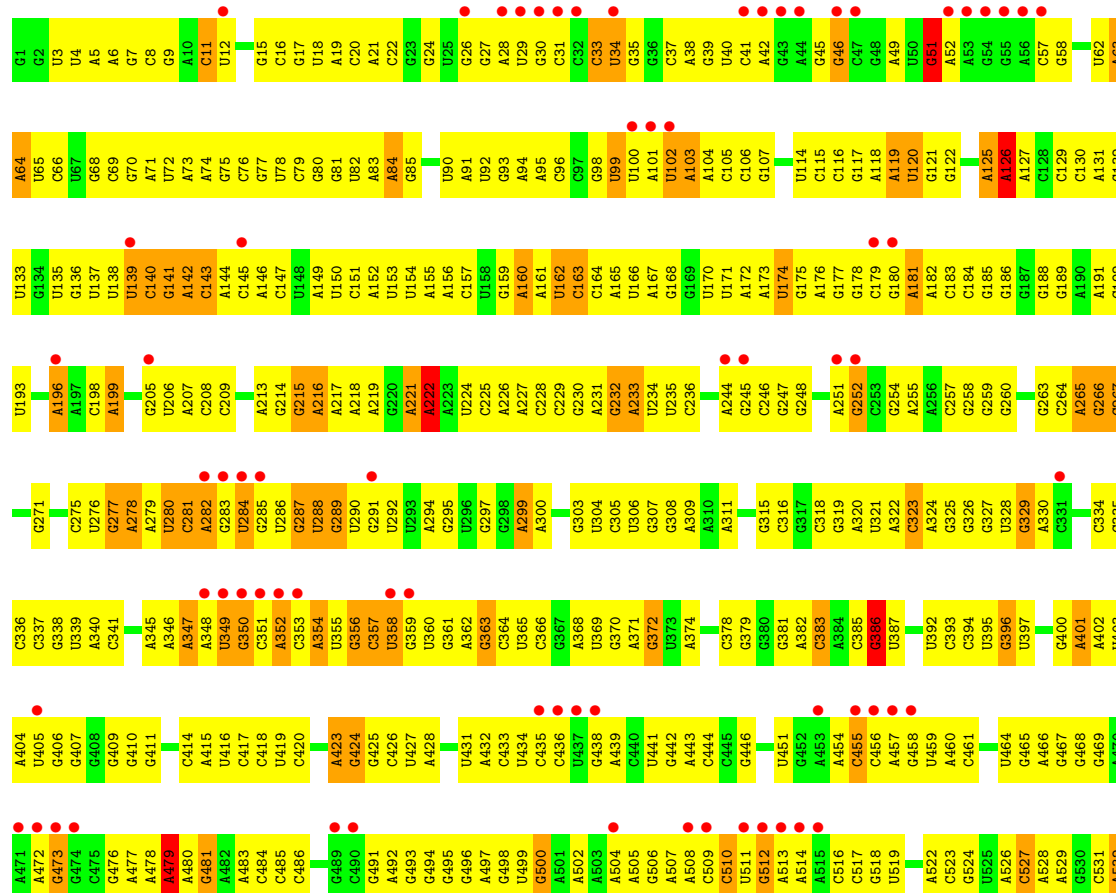
• Molecule 1: 5S rRNA

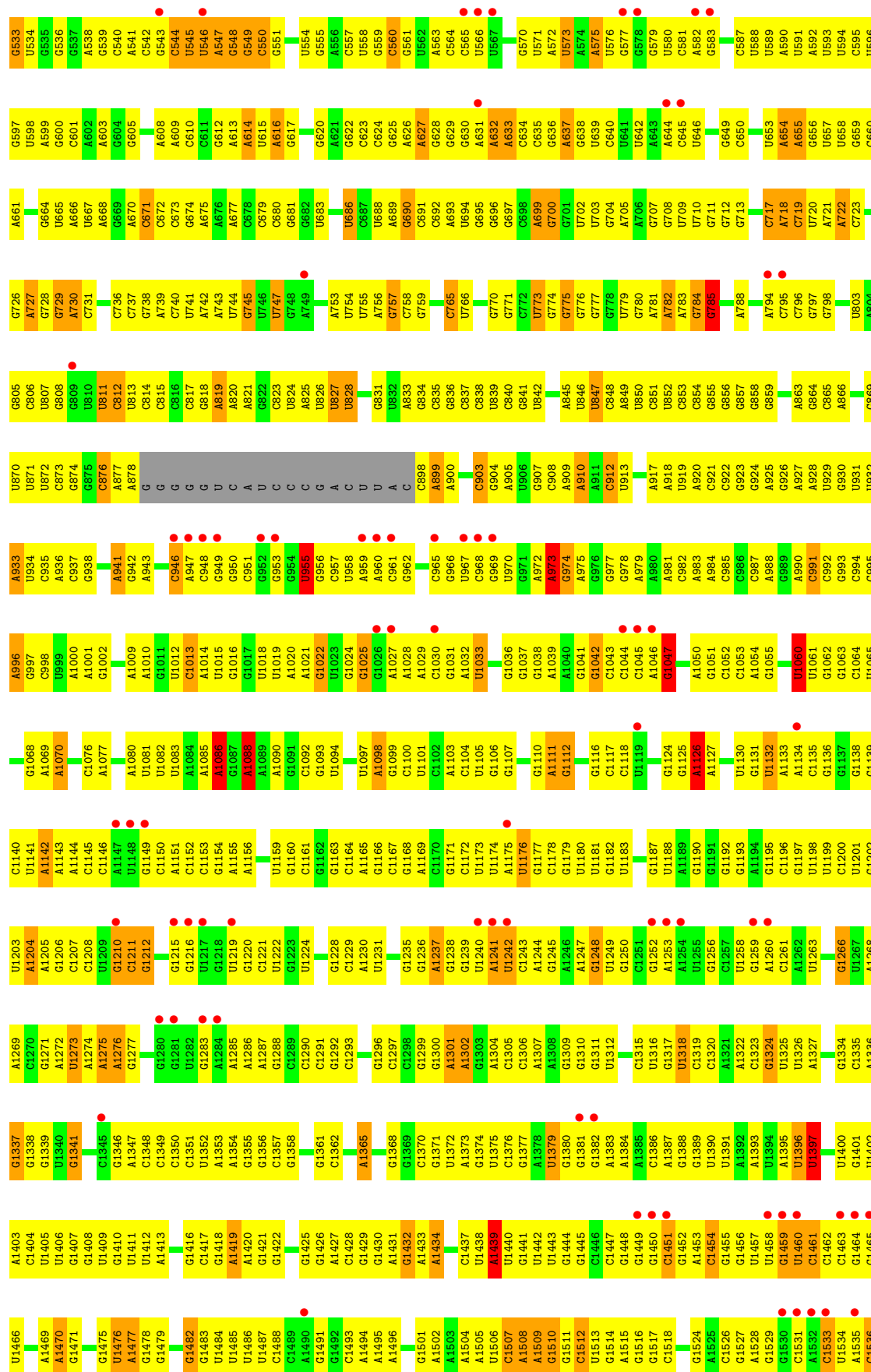
Chain A: 



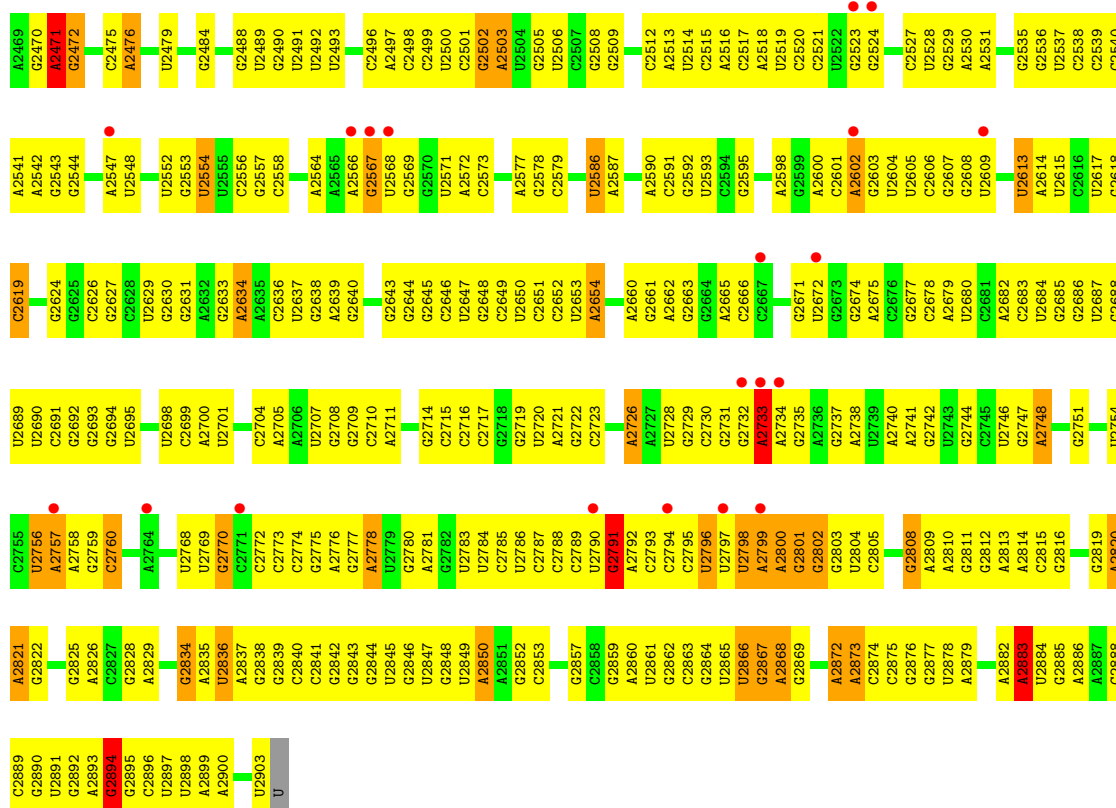
• Molecule 2: 23S rRNA

Chain B: 



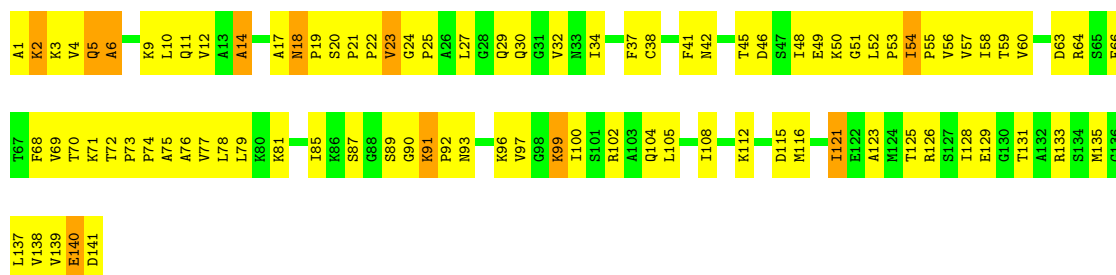


G2405	A2406	A2407	U2408	G2409	U2343	U2344	G2345	G2346	A2347	U2348	G2349	A2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	A2298	G2299	G2363	G2364	G2365	A2366	G2367	G2368	A2369	G2370	G2371	A2434	A2435	U2438	A2439	U2440	U2441	G2375	G2376	G2443	G2444	G2445	G2446	G2447	A2448	U2449	A2450	A2451	G2454	G2455	G2456	U2457	G2458	A2459	U2460	A2461	G2462	G2463	G2464	G2465	G2466	G2467	A2468
C2339	A2340	G2341	G2342	U2343	U2344	G2345	G2346	A2347	U2348	G2349	A2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	A2298	G2299	G2363	G2364	G2365	A2366	G2367	G2368	A2369	G2370	G2371	A2434	A2435	U2438	A2439	U2440	U2441	G2375	G2376	G2443	G2444	G2445	G2446	G2447	A2448	U2449	A2450	A2451	G2454	G2455	G2456	U2457	G2458	A2459	U2460	A2461	G2462	G2463	G2464	G2465	G2466	G2467	A2468	
A2274	C2275	G2276	G2279	G2280	A2281	G2282	G2283	U2284	A2285	G2286	G2287	A2288	U2291	U2292	G2293	G2294	G2295	G2296	A2297	A2298	G2299	G2300	C2301	U2302	G2303	G2304	U2305	G2306	G2307	G2308	A2309	G2310	A2311	U2312	A2313	A2314	G2315	G2316	U2320	U2321	A2322	G2323	U2324	G2325	U2328	U2329	G2330	G2331	G2332	A2333	G2334	A2335	A2336	G2337	U2402									
A2212	U2213	C2214	G2215	G2216	G2217	G2218	U2219	U2220	G2221	G2222	G2223	G2224	A2225	G2226	A2227	G2228	U2229	G2230	U2231	U2232	U2233	G2234	U2235	G2236	G2237	G2238	G2239	U2240	A2241	G2242	U2243	U2244	U2245	G2246	A2247	G2248	U2249	G2250	G2251	G2256	G2257	G2258	U2259	G2260	G2261	U2262	G2263	G2264	U2265	A2266	A2267	A2268	G2269	G2270	U2271	U2272	A2273							
C2025	U2026	G2027	U2028	G2029	U2030	A2031	G2032	A2033	A2037	G2038	U2039	G2040	U2041	A2042	C2043	G2046	G2047	G2048	G2049	C2050	A2051	G2052	G2053	A2054	G2055	G2056	A2060	G2061	A2062	G2063	C2064	G2065	C2066	G2067	U2068	G2069	A2070	A2071	A2072	C2073	U2074	U2075	U2076	A2077	C2078	U2079	A2080	U2081	G2082	G2083	G2084	A2085	U2086	G2087	A2088	C2089								
U1946	C1947	G1948	U1955	U1956	C1957	G1958	G1959	G1964	C1967	G1968	A1969	U1970	U1971	G1972	G1973	C1974	U1979	G1980	A1981	U1982	G1983	G1984	U1985	G1986	U1987	U1988	U1991	U1992	G1993	G1994	U1995	C1996	C1997	A1998	U1999	G2000	C2001	U2007	C2008	A2009	U2010	G2012	A2015	U2016	U2017	G2018	A2019	U2020	C2021	U2022	G2023	G2024												
C1874	G1875	A1876	A1877	G1878	C1879	U1880	C1881	U1882	G1883	G1884	G1888	A1889	A1890	C1891	C1892	C1893	U1898	U1899	C1902	G1906	C1909	G1910	U1911	A1912	C1913	C1914	U1915	A1916	U1917	A1918	G1921	G1922	U1923	C1924	C1925	U1926	A1927	U1928	G1929	U1930	U1931	A1932	G1933	G1934	G1935	U1936	A1937	U1938	A1939	U1940	U1943													
A1805	A1808	U1812	G1813	A1814	A1815	C1816	G1817	U1818	A1819	U1820	A1821	G1824	U1825	G1826	U1827	G1828	A1829	G1830	G1831	C1832	G1838	U1841	C1842	C1843	C1844	G1845	G1846	A1847	U1848	G1849	G1850	U1851	U1852	A1853	U1854	U1855	A1856	G1857	A1858	U1859	G1860	G1861	G1862	G1863	U1864	U1865	G1866	U1867	C1868	G1869	A1870	A1871	A1872	U1873										
U1736	G1737	A1738	G1739	C1740	U1741	U1742	G1743	A1744	U1745	A1746	A1754	U1755	G1756	U1757	U1758	A1759	C1760	C1761	A1762	G1763	C1764	U1765	G1766	G1767	C1768	A1771	A1772	A1773	C1774	U1775	G1776	U1777	U1778	U1779	A1783	A1784	U1785	A1786	A1787	G1788	A1789	C1790	A1791	G1792	C1793	A1794	C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	G1803	C1804								
G1537	G1538	U1539	G1540	C1541	U1542	G1543	A1544	A1545	G1546	C1547	A1548	A1549	C1550	A1551	A1552	U1554	C1555	C1556	C1557	C1558	U1559	G1560	C1561	U1562	C1563	C1564	C1565	A1566	G1567	C1568	A1569	A1570	U1571	A1572	G1573	C1574	G1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	U1583	U1584	C1585	A1586	G1587	A1590	A1591	C1592	G1593	U1594	C1595	A1597								
A1598	U1599	G1600	A1603	C1607	A1608	A1609	A1610	G1613	A1616	C1617	G1622	U1623	U1624	G1628	U1629	A1633	A1634	A1635	U1636	A1637	C1638	C1639	A1640	A1641	G1642	G1643	U1647	U1648	G1649	A1650	G1651	A1652	G1653	A1654	A1655	C1656	U1657	C1658	G1661	U1662	G1663	A1664	G1665	G1666	G1667	G1668	A1669	C1670	G1674															
G1675	A1676	A1677	U1679	U1680	G1681	G1682	U1683	C1685	A1686	G1687	U1688	A1689	C1691	U1692	U1693	G1694	G1695	G1696	G1697	A1698	G1699	A1700	G1702	C1703	C1704	A1705	C1706	G1707	C1708	U1709	G1710	A1711	U1712	A1713	U1714	G1715	U1716	A1717	G1718	G1719	U1720	A1721	A1722	G1723	G1726	C1727	C1728	U1729	G1730	G1731	G1732	G1733	A1735											



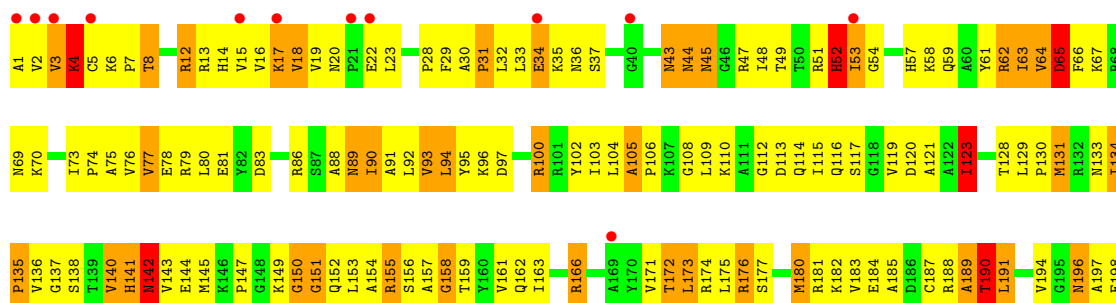
• Molecule 3: 50S ribosomal protein L11

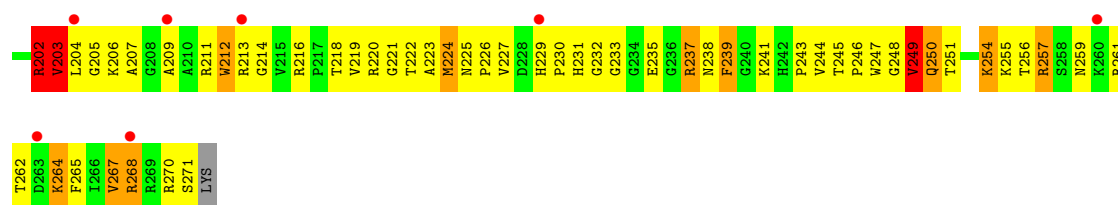
Chain I:



• Molecule 4: 50S ribosomal protein L2

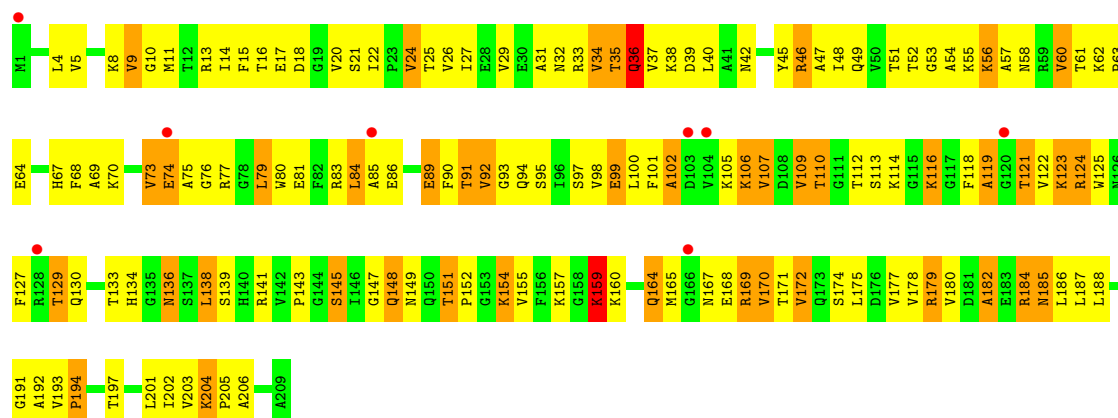
Chain C:





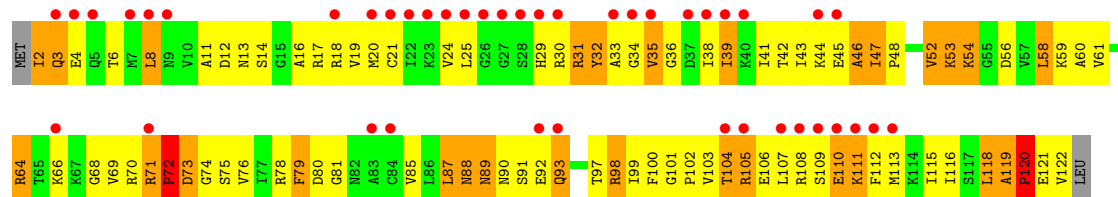
• Molecule 5: 50S ribosomal protein L3

Chain D:



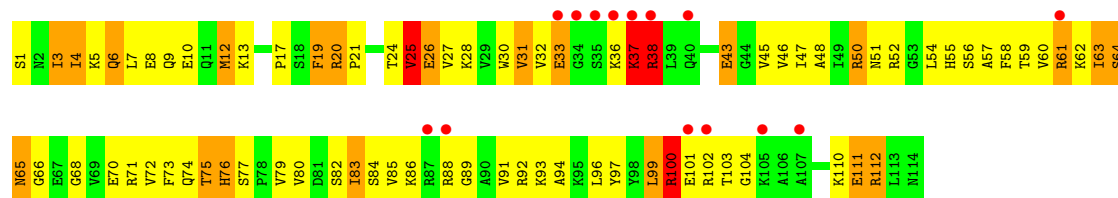
• Molecule 6: 50S ribosomal protein L14

Chain K:



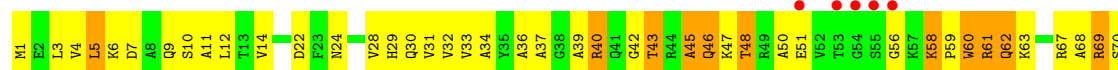
• Molecule 7: 50S ribosomal protein L19

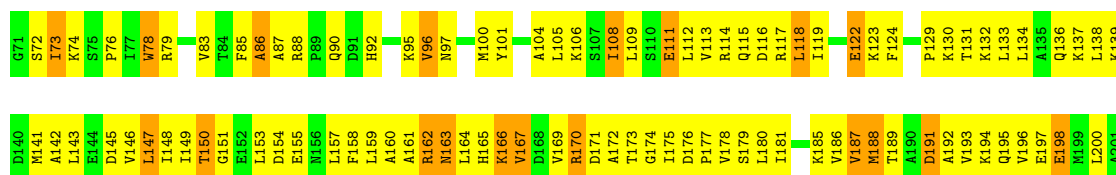
Chain P:



• Molecule 8: 50S ribosomal protein L4

Chain E:





- Molecule 9: 50S ribosomal protein L30

Chain Y:



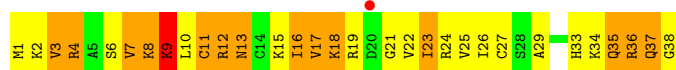
- Molecule 10: 50S ribosomal protein L32

Chain 0:



- Molecule 11: 50S ribosomal protein L36

Chain 4:



- Molecule 12: 50S ribosomal protein L33

Chain 1:



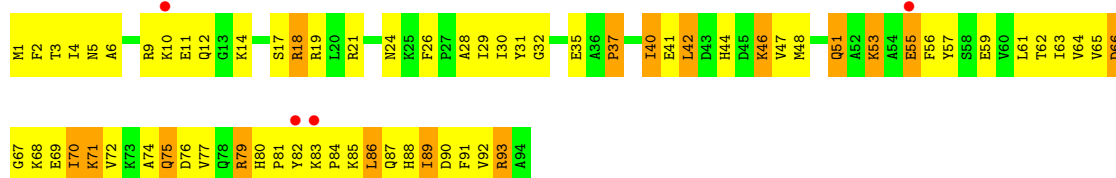
- Molecule 13: 50S ribosomal protein L35

Chain 3:



- Molecule 14: 50S ribosomal protein L25

Chain V:



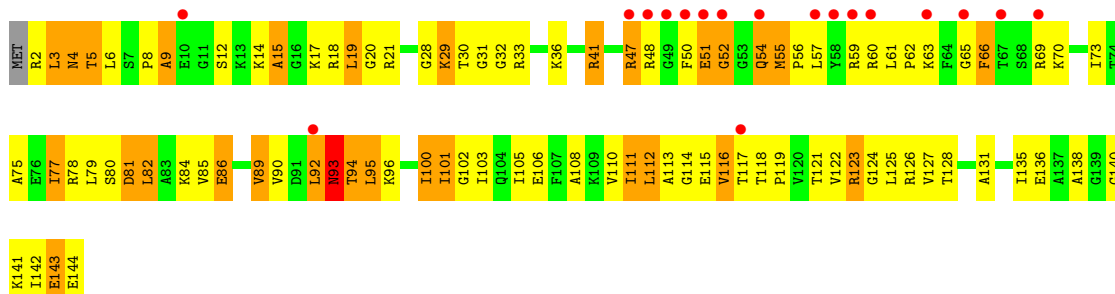
- Molecule 15: 50S ribosomal protein L34

Chain 2:



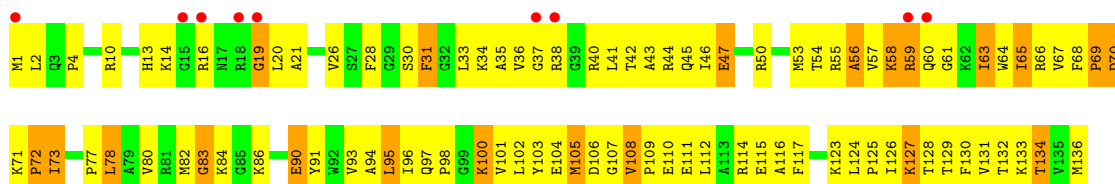
• Molecule 16: 50S ribosomal protein L15

Chain L:



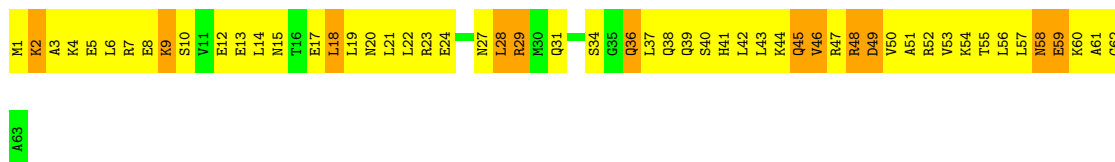
• Molecule 17: 50S ribosomal protein L16

Chain M:



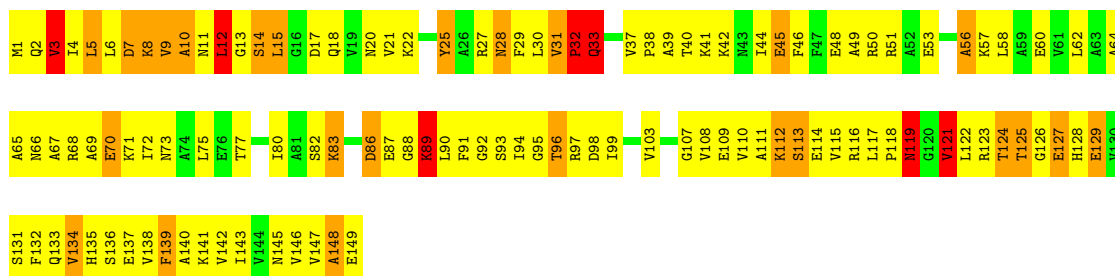
• Molecule 18: 50S ribosomal protein L29

Chain X:



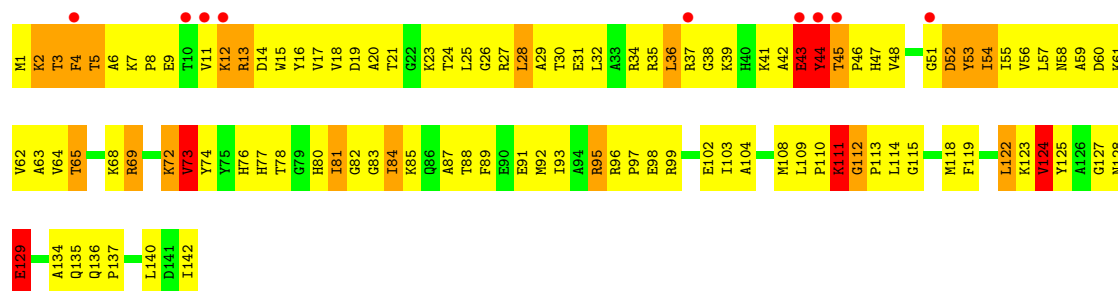
• Molecule 19: 50S ribosomal protein L9

Chain H:



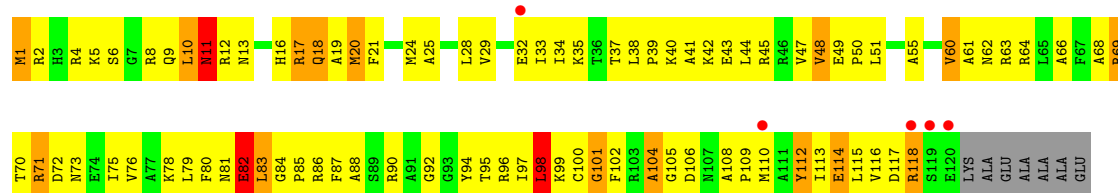
• Molecule 20: 50S ribosomal protein L13

Chain J:



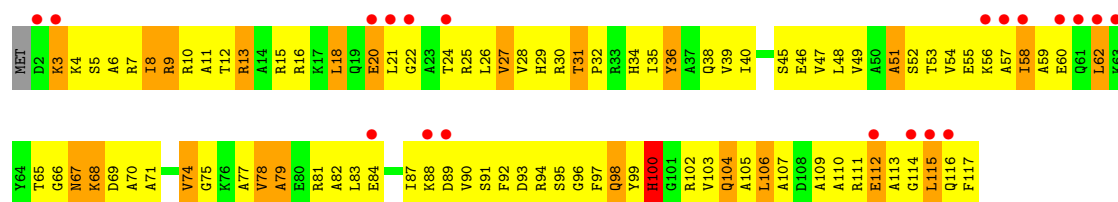
- Molecule 21: 50S ribosomal protein L17

Chain N:



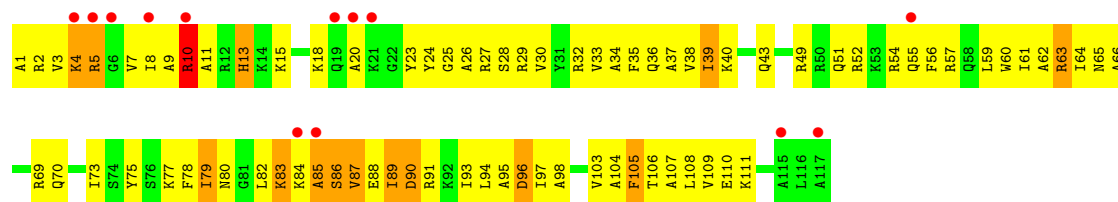
- Molecule 22: 50S ribosomal protein L18

Chain O:



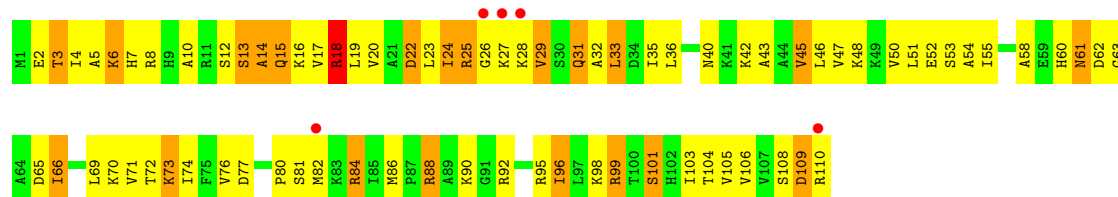
- Molecule 23: 50S ribosomal protein L20

Chain Q:



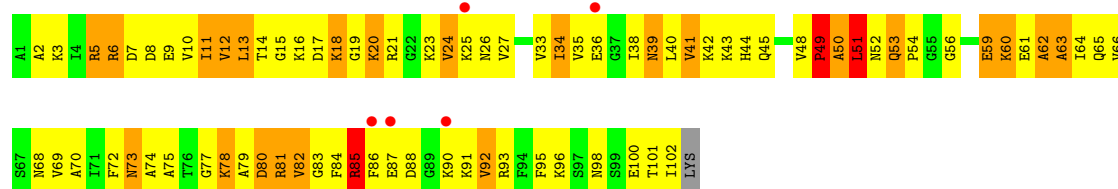
- Molecule 24: 50S ribosomal protein L22

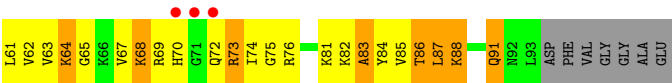
Chain S:



- Molecule 25: 50S ribosomal protein L24

Chain U: 

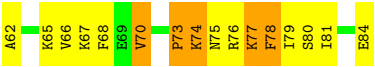
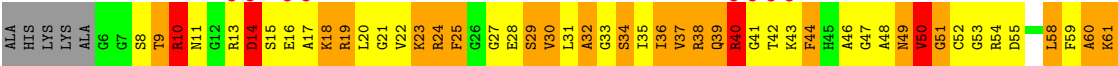
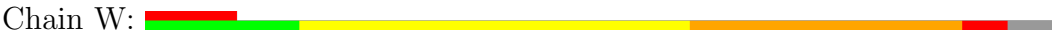




● Molecule 30: 50S ribosomal protein L28



● Molecule 31: 50S ribosomal protein L27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.54 138.41 – 3.55	Depositor EDS
% Data completeness (in resolution range)	88.8 (70.00-3.54) 89.9 (138.41-3.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.320 0.474 , 0.482	Depositor DCC
R_{free} test set	30187 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 4.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 627888 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	90294	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, LLL

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	0.23	0/2803	0.74	0/4371
2	B	0.28	9/68314 (0.0%)	0.78	58/106569 (0.1%)
3	I	0.25	0/1046	0.48	0/1410
4	C	0.22	0/2121	0.48	0/2852
5	D	0.24	0/1586	0.48	0/2134
6	K	0.24	0/939	0.53	0/1258
7	P	0.24	0/929	0.50	0/1242
8	E	0.24	0/1571	0.50	0/2113
9	Y	0.23	0/453	0.48	0/605
10	O	0.22	0/450	0.53	0/599
11	4	0.23	0/303	0.46	0/397
12	1	0.27	0/416	0.48	0/554
13	3	0.24	0/513	0.47	0/676
14	V	0.25	0/766	0.42	0/1025
15	2	0.25	0/380	0.45	0/498
16	L	0.24	0/1054	0.47	0/1403
17	M	0.25	0/1093	0.47	0/1460
18	X	0.24	0/510	0.52	0/677
19	H	0.25	0/1122	0.47	0/1515
20	J	0.23	0/1152	0.48	0/1551
21	N	0.24	0/973	0.51	0/1301
22	O	0.23	0/902	0.48	0/1209
23	Q	0.25	0/960	0.47	0/1278
24	S	0.22	0/864	0.51	0/1156
25	U	0.26	0/787	0.46	0/1051
26	F	0.26	0/1444	0.50	0/1937
27	G	0.23	0/1343	0.47	0/1816
28	R	0.25	0/829	0.48	0/1107
29	T	0.22	0/744	0.54	0/994
30	Z	0.25	0/635	0.50	0/848
31	W	0.28	0/603	0.48	0/797
All	All	0.27	9/97605 (0.0%)	0.72	58/146403 (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	40

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	-16.38	1.26	1.41
2	B	1088	A	C6-N1	-10.61	1.28	1.35
2	B	1060	U	C2-N3	8.04	1.43	1.37
2	B	2276	G	O3'-P	-8.01	1.51	1.61
2	B	2280	G	O3'-P	7.60	1.70	1.61

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP1	-29.68	75.08	110.70
2	B	2791	G	O5'-P-OP2	-27.65	77.52	110.70
2	B	2791	G	O5'-P-OP1	17.94	132.23	110.70
2	B	2204	G	O5'-P-OP2	17.92	132.20	110.70
2	B	2790	U	OP2-P-O3'	14.55	137.22	105.20

There are no chirality outliers.

5 of 40 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	96	0
2	B	60995	0	30677	2298	0
3	I	1032	0	1088	176	0
4	C	2082	0	2157	245	0
5	D	1565	0	1616	186	0
6	K	930	0	1000	108	0
7	P	917	0	965	107	0
8	E	1552	0	1619	153	0
9	Y	449	0	491	59	0
10	0	444	0	461	45	0
11	4	302	0	340	42	0
12	1	409	0	440	47	0
13	3	504	0	574	45	0
14	V	753	0	780	97	0
15	2	377	0	418	34	0
16	L	1045	0	1117	153	0
17	M	1074	0	1157	119	0
18	X	509	0	543	72	0
19	H	1111	0	1148	150	0
20	J	1129	0	1162	144	0
21	N	960	0	1000	118	0
22	O	892	0	923	103	0
23	Q	947	0	1022	141	0
24	S	857	0	922	87	0
25	U	779	0	834	114	0
26	F	1420	0	1460	224	0
27	G	1323	0	1374	191	0
28	R	816	0	839	112	0
29	T	738	0	807	128	0
30	Z	625	0	652	77	0
31	W	596	0	610	131	0
32	B	111	0	0	0	0
33	4	1	0	0	0	0
34	B	31	0	39	0	0
35	B	502	0	0	8	0
35	C	4	0	0	0	0
35	E	2	0	0	0	0
35	L	4	0	0	0	0
All	All	90294	0	59505	5289	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 35.

The worst 5 of 5289 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	1.42	1.17
2:B:855:G:H21	31:W:23:LYS:HG2	1.12	1.14
5:D:106:LYS:HB3	5:D:206:ALA:H	1.13	1.09
2:B:1098:A:H3'	3:I:3:LYS:CA	1.84	1.07
16:L:143:GLU:HG2	16:L:144:GLU:H	1.17	1.07

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%)	115 (83%)	19 (14%)	5 (4%)	5	50
4	C	269/272 (99%)	167 (62%)	59 (22%)	43 (16%)	0	5
5	D	207/209 (99%)	119 (58%)	59 (28%)	29 (14%)	0	8
6	K	119/123 (97%)	78 (66%)	23 (19%)	18 (15%)	0	6
7	P	112/114 (98%)	60 (54%)	37 (33%)	15 (13%)	0	9
8	E	199/201 (99%)	127 (64%)	46 (23%)	26 (13%)	0	10
9	Y	56/58 (97%)	40 (71%)	13 (23%)	3 (5%)	3	36
10	0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	1	18
11	4	36/38 (95%)	18 (50%)	7 (19%)	11 (31%)	0	0
12	1	48/54 (89%)	33 (69%)	10 (21%)	5 (10%)	1	15
13	3	62/64 (97%)	41 (66%)	16 (26%)	5 (8%)	1	22
14	V	92/94 (98%)	67 (73%)	21 (23%)	4 (4%)	4	43
15	2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	2	28
16	L	141/144 (98%)	90 (64%)	27 (19%)	24 (17%)	0	4
17	M	134/136 (98%)	81 (60%)	39 (29%)	14 (10%)	1	15
18	X	61/63 (97%)	37 (61%)	17 (28%)	7 (12%)	1	13
19	H	147/149 (99%)	89 (60%)	30 (20%)	28 (19%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	J	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	8
21	N	118/127 (93%)	76 (64%)	30 (25%)	12 (10%)	1	15
22	O	114/117 (97%)	80 (70%)	23 (20%)	11 (10%)	1	17
23	Q	115/117 (98%)	77 (67%)	30 (26%)	8 (7%)	2	27
24	S	108/110 (98%)	66 (61%)	29 (27%)	13 (12%)	1	12
25	U	100/103 (97%)	59 (59%)	23 (23%)	18 (18%)	0	4
26	F	176/178 (99%)	102 (58%)	49 (28%)	25 (14%)	0	8
27	G	174/176 (99%)	94 (54%)	50 (29%)	30 (17%)	0	4
28	R	101/103 (98%)	62 (61%)	26 (26%)	13 (13%)	0	10
29	T	91/100 (91%)	51 (56%)	23 (25%)	17 (19%)	0	3
30	Z	75/78 (96%)	50 (67%)	15 (20%)	10 (13%)	0	9
31	W	77/84 (92%)	30 (39%)	24 (31%)	23 (30%)	0	0
All	All	3309/3397 (97%)	2073 (63%)	792 (24%)	444 (13%)	0	9

5 of 444 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	5	GLN
3	I	18	ASN
4	C	4	LYS
4	C	53	ILE
4	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 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%)	103 (94%)	6 (6%)	30	78
4	C	216/217 (100%)	183 (85%)	33 (15%)	4	25
5	D	164/164 (100%)	138 (84%)	26 (16%)	4	22
6	K	102/104 (98%)	77 (76%)	25 (24%)	1	6
7	P	99/99 (100%)	81 (82%)	18 (18%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	165/165 (100%)	144 (87%)	21 (13%)	6	34
9	Y	48/48 (100%)	37 (77%)	11 (23%)	1	7
10	0	47/47 (100%)	38 (81%)	9 (19%)	2	13
11	4	34/34 (100%)	28 (82%)	6 (18%)	3	16
12	1	45/48 (94%)	37 (82%)	8 (18%)	2	16
13	3	51/51 (100%)	46 (90%)	5 (10%)	12	50
14	V	78/78 (100%)	63 (81%)	15 (19%)	2	12
15	2	38/38 (100%)	31 (82%)	7 (18%)	2	14
16	L	102/103 (99%)	91 (89%)	11 (11%)	9	44
17	M	109/109 (100%)	93 (85%)	16 (15%)	4	27
18	X	55/55 (100%)	49 (89%)	6 (11%)	9	44
19	H	114/114 (100%)	91 (80%)	23 (20%)	2	11
20	J	116/116 (100%)	98 (84%)	18 (16%)	4	24
21	N	100/103 (97%)	86 (86%)	14 (14%)	5	29
22	O	86/87 (99%)	68 (79%)	18 (21%)	1	10
23	Q	89/89 (100%)	80 (90%)	9 (10%)	11	49
24	S	93/93 (100%)	76 (82%)	17 (18%)	2	14
25	U	83/84 (99%)	68 (82%)	15 (18%)	2	15
26	F	149/149 (100%)	116 (78%)	33 (22%)	1	8
27	G	137/137 (100%)	113 (82%)	24 (18%)	3	17
28	R	84/84 (100%)	71 (84%)	13 (16%)	4	24
29	T	80/84 (95%)	68 (85%)	12 (15%)	4	26
30	Z	67/68 (98%)	54 (81%)	13 (19%)	2	12
31	W	59/62 (95%)	44 (75%)	15 (25%)	1	6
All	All	2719/2739 (99%)	2272 (84%)	447 (16%)	3	21

5 of 447 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	M	30	SER
20	J	35	ARG
29	T	24	MET
17	M	70	ASP
19	H	28	ASN

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

Mol	Chain	Res	Type
14	V	80	HIS
18	X	25	GLN
29	T	48	GLN
16	L	4	ASN
17	M	3	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	14 (12%)	0
2	B	2837/2904 (97%)	424 (14%)	21 (0%)
All	All	2953/3024 (97%)	438 (14%)	21 (0%)

5 of 438 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	15	A
1	A	16	G
1	A	26	C
1	A	29	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1301	A
2	B	1911	U
2	B	2756	U
2	B	1210	G
2	B	2798	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$
34	LLL	B	3619	-	33,33,33	3.19	14 (42%)	49,49,49	1.48	6 (12%)

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
34	LLL	B	3619	-	-	0/12/65/65	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	3619	LLL	C22-C32	8.92	1.59	1.52
34	B	3619	LLL	C22-C12	7.45	1.58	1.52
34	B	3619	LLL	O53-C53	6.07	1.52	1.43
34	B	3619	LLL	C43-C33	4.96	1.63	1.54
34	B	3619	LLL	C42-C32	4.78	1.59	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	3619	LLL	C93-N33-C33	5.90	117.21	113.85
34	B	3619	LLL	C53-O53-C13	4.50	117.63	111.22
34	B	3619	LLL	C83-C43-C33	2.73	116.68	112.15
34	B	3619	LLL	O43-C43-C83	-2.52	102.51	108.08
34	B	3619	LLL	C11-O51-C51	2.02	115.23	113.19

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, 95th 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 ²)	Q<0.9
1	A	117/120 (97%)	0.13	9 (7%) 13 7	30, 80, 115, 155	0
2	B	2841/2904 (97%)	0.17	213 (7%) 14 7	5, 45, 124, 163	0
3	I	141/141 (100%)	-0.50	0 100 100	70, 117, 148, 160	0
4	C	271/272 (99%)	0.16	19 (7%) 16 8	5, 32, 80, 112	0
5	D	209/209 (100%)	0.14	8 (3%) 38 18	5, 49, 98, 135	0
6	K	121/123 (98%)	1.55	42 (34%) 1 1	5, 37, 90, 130	0
7	P	114/114 (100%)	0.45	14 (12%) 5 4	7, 49, 94, 112	0
8	E	201/201 (100%)	-0.18	5 (2%) 54 26	5, 62, 107, 138	0
9	Y	58/58 (100%)	0.52	9 (15%) 3 3	6, 64, 110, 117	0
10	0	56/56 (100%)	0.07	3 (5%) 25 11	10, 43, 99, 104	0
11	4	38/38 (100%)	0.18	1 (2%) 53 25	15, 65, 94, 105	0
12	1	50/54 (92%)	-0.19	0 100 100	27, 74, 105, 118	0
13	3	64/64 (100%)	1.09	14 (21%) 1 2	5, 39, 84, 101	0
14	V	94/94 (100%)	-0.06	4 (4%) 34 15	8, 79, 108, 125	0
15	2	46/46 (100%)	1.32	14 (30%) 1 1	5, 28, 69, 113	0
16	L	143/144 (99%)	0.44	18 (12%) 4 3	5, 55, 95, 123	0
17	M	136/136 (100%)	0.22	9 (6%) 18 9	5, 55, 94, 134	0
18	X	63/63 (100%)	-0.36	0 100 100	36, 82, 107, 142	0
19	H	149/149 (100%)	-0.47	0 100 100	18, 88, 112, 141	0
20	J	142/142 (100%)	0.17	9 (6%) 19 9	5, 60, 101, 131	0
21	N	120/127 (94%)	-0.05	5 (4%) 35 15	5, 42, 75, 118	0
22	O	116/117 (99%)	0.59	20 (17%) 2 2	5, 73, 106, 157	0
23	Q	117/117 (100%)	0.42	13 (11%) 6 4	5, 50, 92, 120	0
24	S	110/110 (100%)	0.22	5 (4%) 32 14	5, 48, 95, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	U	102/103 (99%)	-0.04	5 (4%) 28 13	34, 80, 112, 130	0
26	F	178/178 (100%)	0.06	9 (5%) 27 12	38, 85, 125, 138	0
27	G	176/176 (100%)	0.02	9 (5%) 27 12	17, 82, 110, 133	0
28	R	103/103 (100%)	-0.21	0 100 100	15, 72, 111, 128	0
29	T	93/100 (93%)	0.33	5 (5%) 25 11	8, 66, 108, 120	0
30	Z	77/78 (98%)	0.03	3 (3%) 37 17	5, 43, 87, 114	0
31	W	79/84 (94%)	0.59	8 (10%) 7 5	12, 65, 103, 122	0
All	All	6325/6421 (98%)	0.17	473 (7%) 14 7	5, 55, 118, 163	0

The worst 5 of 473 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	645	C	12.3
1	A	88	C	10.6
6	K	110	GLU	8.3
22	O	3	LYS	8.0
2	B	350	G	7.7

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, 95th 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 ²)	Q<0.9
32	MG	B	3452	1/1	0.33	14.67	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	3337	1/1	0.37	13.41	96,96,96,96	0
32	MG	B	3279	1/1	0.63	10.55	36,36,36,36	0
34	LLL	B	3619	31/31	0.25	9.38	54,54,54,54	0
32	MG	B	3165	1/1	1.10	5.74	37,37,37,37	0
32	MG	B	3515	1/1	1.45	5.47	57,57,57,57	0
32	MG	B	3262	1/1	0.25	5.17	66,66,66,66	0
32	MG	B	3207	1/1	0.98	3.34	54,54,54,54	0
32	MG	B	3201	1/1	0.41	2.61	74,74,74,74	0
32	MG	B	3351	1/1	0.23	1.53	79,79,79,79	0
32	MG	B	3274	1/1	0.30	1.43	5,5,5,5	0
32	MG	B	3570	1/1	0.23	1.23	26,26,26,26	0
32	MG	B	3184	1/1	0.24	0.86	8,8,8,8	0
32	MG	B	3087	1/1	0.15	0.79	50,50,50,50	0
32	MG	B	3409	1/1	0.28	0.74	21,21,21,21	0
32	MG	B	3457	1/1	0.28	0.51	48,48,48,48	0
32	MG	B	3618	1/1	0.31	0.51	43,43,43,43	0
32	MG	B	3592	1/1	0.17	0.51	37,37,37,37	0
32	MG	B	3419	1/1	0.28	0.17	34,34,34,34	0
32	MG	B	3239	1/1	0.30	0.03	41,41,41,41	0
32	MG	B	3021	1/1	0.24	-0.27	21,21,21,21	0
32	MG	B	3301	1/1	0.48	-0.32	62,62,62,62	0
32	MG	B	3257	1/1	0.37	-0.35	18,18,18,18	0
32	MG	B	3598	1/1	0.36	-0.47	15,15,15,15	0
32	MG	B	3220	1/1	0.17	-0.48	5,5,5,5	0
32	MG	B	3033	1/1	0.15	-0.52	5,5,5,5	0
32	MG	B	3127	1/1	0.15	-0.58	23,23,23,23	0
32	MG	B	3001	1/1	0.14	-0.73	5,5,5,5	0
32	MG	B	3069	1/1	0.19	-0.74	14,14,14,14	0
32	MG	B	3320	1/1	0.27	-0.83	11,11,11,11	0
32	MG	B	3357	1/1	0.15	-0.84	58,58,58,58	0
32	MG	B	3525	1/1	0.11	-0.86	76,76,76,76	0
32	MG	B	3104	1/1	0.16	-0.89	48,48,48,48	0
32	MG	B	3172	1/1	0.15	-0.91	66,66,66,66	0
32	MG	B	3547	1/1	0.17	-0.95	42,42,42,42	0
32	MG	B	3544	1/1	0.12	-0.97	5,5,5,5	0
32	MG	B	3485	1/1	0.17	-0.98	56,56,56,56	0
32	MG	B	3537	1/1	0.13	-0.99	96,96,96,96	0
32	MG	B	3308	1/1	0.18	-1.04	66,66,66,66	0
32	MG	B	3492	1/1	0.16	-1.05	25,25,25,25	0
32	MG	B	3564	1/1	0.11	-1.06	5,5,5,5	0
32	MG	B	3026	1/1	0.13	-1.17	6,6,6,6	0
32	MG	B	3140	1/1	0.14	-1.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	3081	1/1	0.10	-1.21	13,13,13,13	0
32	MG	B	3189	1/1	0.16	-1.23	45,45,45,45	0
32	MG	B	3327	1/1	0.16	-1.26	5,5,5,5	0
33	ZN	4	624	1/1	0.06	-1.30	45,45,45,45	0
32	MG	B	3008	1/1	0.13	-1.32	12,12,12,12	0
32	MG	B	3225	1/1	0.16	-1.39	17,17,17,17	0
32	MG	B	3614	1/1	0.08	-1.39	29,29,29,29	0
32	MG	B	3052	1/1	0.11	-1.43	5,5,5,5	0
32	MG	B	3474	1/1	0.23	-1.45	5,5,5,5	0
32	MG	B	3040	1/1	0.09	-1.49	18,18,18,18	0
32	MG	B	3196	1/1	0.08	-1.51	18,18,18,18	0
32	MG	B	3064	1/1	0.09	-1.63	35,35,35,35	0
32	MG	B	3584	1/1	0.10	-1.74	55,55,55,55	0
32	MG	B	3152	1/1	0.13	-1.76	33,33,33,33	0
32	MG	B	3332	1/1	0.07	-1.79	53,53,53,53	0
32	MG	B	3292	1/1	0.03	-1.80	73,73,73,73	0
32	MG	B	3446	1/1	0.11	-1.81	43,43,43,43	0
32	MG	B	3440	1/1	0.08	-1.82	41,41,41,41	0
32	MG	B	3370	1/1	0.09	-1.84	21,21,21,21	0
32	MG	B	3074	1/1	0.14	-1.89	37,37,37,37	0
32	MG	B	3214	1/1	0.09	-1.89	26,26,26,26	0
32	MG	B	3413	1/1	0.14	-1.94	43,43,43,43	0
32	MG	B	3298	1/1	0.07	-1.96	57,57,57,57	0
32	MG	B	3268	1/1	0.10	-2.04	5,5,5,5	0
32	MG	B	3463	1/1	0.09	-2.05	43,43,43,43	0
32	MG	B	3559	1/1	0.07	-2.07	5,5,5,5	0
32	MG	B	3058	1/1	0.29	-2.09	14,14,14,14	0
32	MG	B	3480	1/1	0.09	-2.10	42,42,42,42	0
32	MG	B	3382	1/1	0.07	-2.15	16,16,16,16	0
32	MG	B	3512	1/1	0.07	-2.19	52,52,52,52	0
32	MG	B	3014	1/1	0.12	-2.22	17,17,17,17	0
32	MG	B	3425	1/1	0.15	-2.24	25,25,25,25	0
32	MG	B	3532	1/1	0.12	-2.24	14,14,14,14	0
32	MG	B	3528	1/1	0.10	-2.26	7,7,7,7	0
32	MG	B	3179	1/1	0.11	-2.45	26,26,26,26	0
32	MG	B	3504	1/1	0.08	-2.52	63,63,63,63	0
32	MG	B	3496	1/1	0.09	-2.54	5,5,5,5	0
32	MG	B	3235	1/1	0.05	-2.63	5,5,5,5	0
32	MG	B	3117	1/1	0.09	-2.64	5,5,5,5	0
32	MG	B	3245	1/1	0.08	-2.65	22,22,22,22	0
32	MG	B	3375	1/1	0.07	-2.82	11,11,11,11	0
32	MG	B	3468	1/1	0.10	-2.86	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	3575	1/1	0.05	-3.08	16,16,16,16	0
32	MG	B	3092	1/1	0.13	-3.16	17,17,17,17	0
32	MG	B	3099	1/1	0.08	-3.23	5,5,5,5	0
32	MG	B	3344	1/1	0.10	-3.29	100,100,100,100	0
32	MG	B	3315	1/1	0.06	-3.32	13,13,13,13	0
32	MG	B	3553	1/1	0.07	-3.34	23,23,23,23	0
32	MG	B	3436	1/1	0.07	-3.34	5,5,5,5	0
32	MG	B	3251	1/1	0.08	-3.43	5,5,5,5	0
32	MG	B	3521	1/1	0.07	-3.51	45,45,45,45	0
32	MG	B	3579	1/1	0.09	-3.54	7,7,7,7	0
32	MG	B	3396	1/1	0.12	-3.57	5,5,5,5	0
32	MG	B	3403	1/1	0.09	-3.73	5,5,5,5	0
32	MG	B	3431	1/1	0.09	-3.74	33,33,33,33	0
32	MG	B	3286	1/1	0.06	-3.79	5,5,5,5	0
32	MG	B	3133	1/1	0.15	-3.83	13,13,13,13	0
32	MG	B	3602	1/1	0.06	-3.84	5,5,5,5	0
32	MG	B	3146	1/1	0.07	-4.16	5,5,5,5	0
32	MG	B	3500	1/1	0.07	-4.17	24,24,24,24	0
32	MG	B	3229	1/1	0.05	-4.24	36,36,36,36	0
32	MG	B	3110	1/1	0.08	-4.40	6,6,6,6	0
32	MG	B	3364	1/1	0.04	-4.64	43,43,43,43	0
32	MG	B	3609	1/1	0.15	-4.68	28,28,28,28	0
32	MG	B	3508	1/1	0.06	-5.69	18,18,18,18	0
32	MG	B	3122	1/1	0.07	-5.78	5,5,5,5	0
32	MG	B	3159	1/1	0.06	-6.15	12,12,12,12	0
32	MG	B	3588	1/1	0.11	-7.38	30,30,30,30	0
32	MG	B	3046	1/1	0.09	-10.43	8,8,8,8	0
32	MG	B	3389	1/1	0.42	-	100,100,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.