



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:13 AM GMT

PDB ID : 2ZJQ
Title : Interaction of L7 with L11 induced by Micrococin binding to the Deinococcus radiodurans 50S subunit
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on : 2008-03-08
Resolution : 3.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

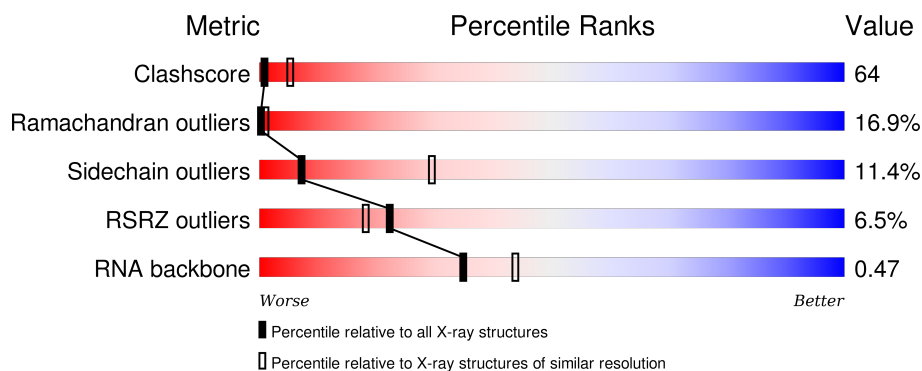
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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.

Mol	Chain	Length	Quality of chain
1	X	2880	<div> <div></div> <div>11% 50% 23% 10% 7%</div> </div>
2	Y	122	<div> <div>2%</div> <div>16% 69% 14%</div> </div>
3	A	274	<div> <div>2%</div> <div>19% 55% 14% 12%</div> </div>
4	B	211	<div> <div></div> <div>25% 56% 13%</div> </div>
5	C	205	<div> <div></div> <div>14% 54% 24% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	142	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	

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Mol	Chain	Length	Quality of chain
31	5	122	<div> <div>49%</div> <div>58%</div> <div>42%</div> </div>

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 84395 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 ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 2 is a RNA chain called ribosomal 5S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	144	Total	C	N	O	S	0	0	0
			1043	663	179	196	5			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	S	0	0	0
			1067	655	216	196				

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	INITIATING METHIONINE	UNP Q9RXJ5

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O		0	0	0
			779	476	161	142				

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O		0	0	0
			871	543	172	156				

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O		0	0	0
			741	465	139	137				

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O	0	0	0
			552	341	116	95			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

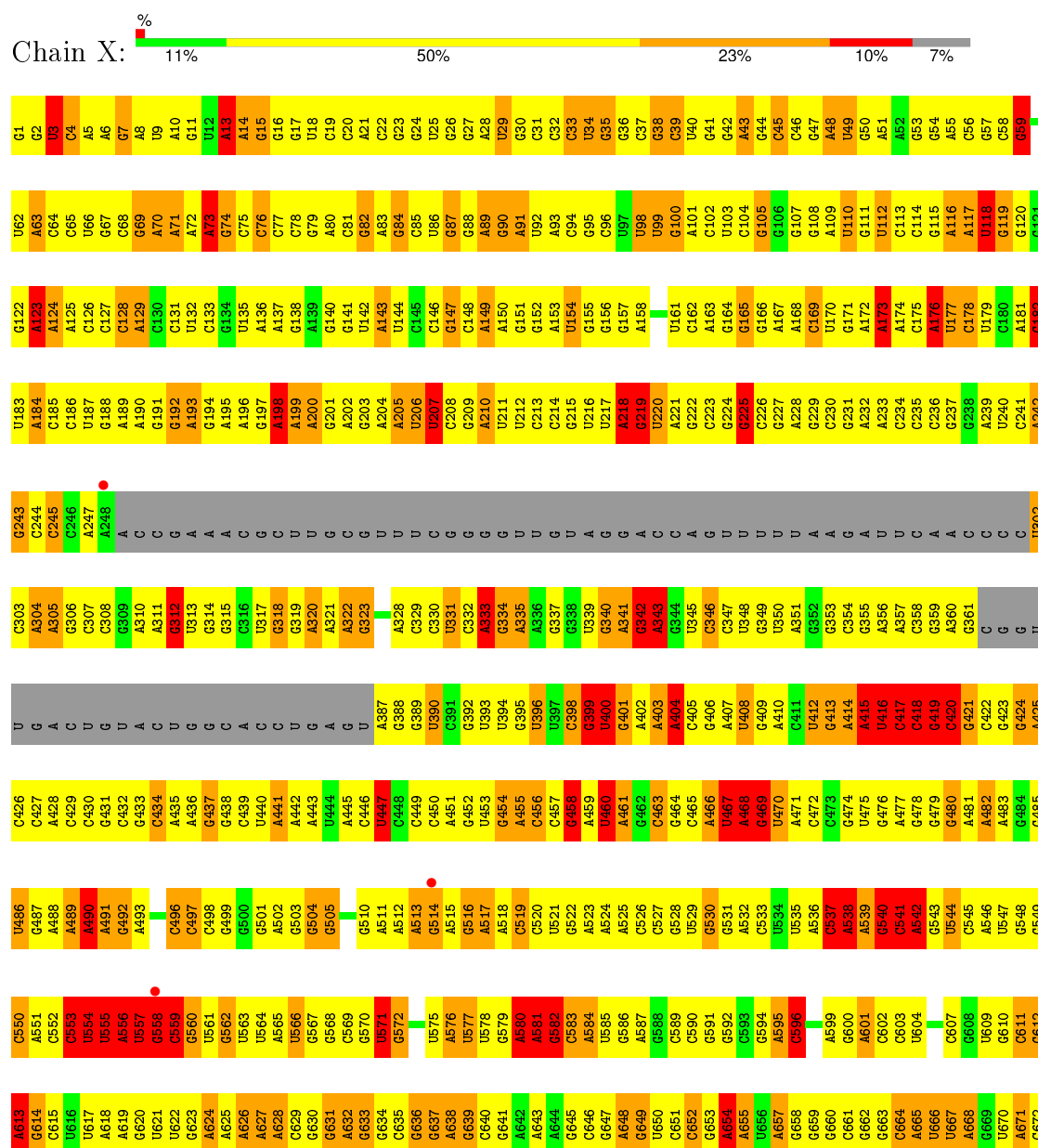
- Molecule 31 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	5	71	Total C 71 71	0	0	71

3 Residue-property plots

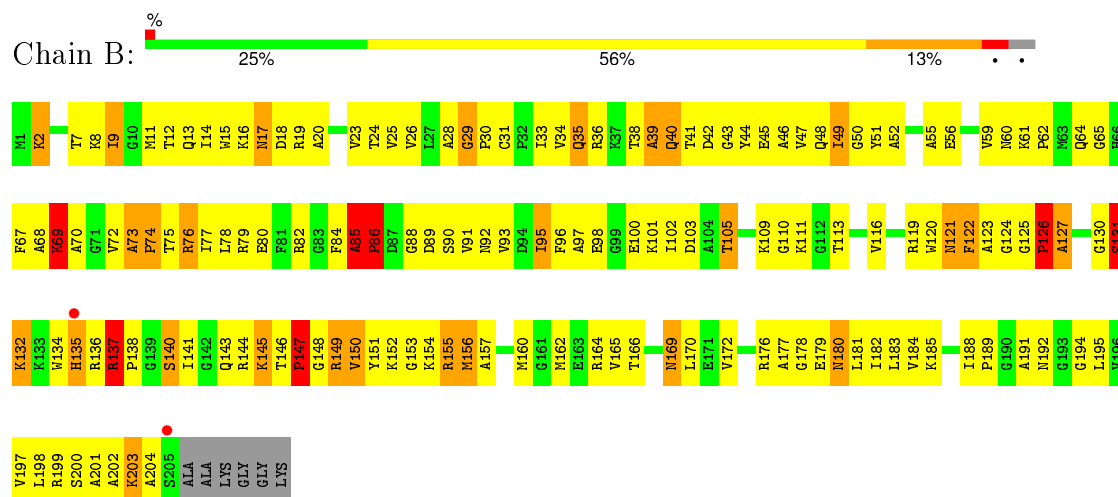
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ribosomal 23S RNA

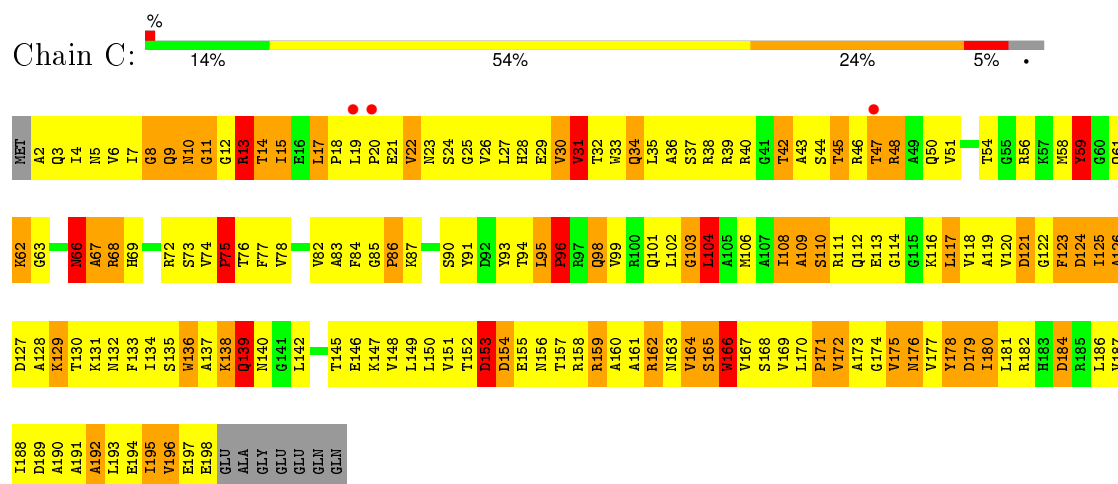




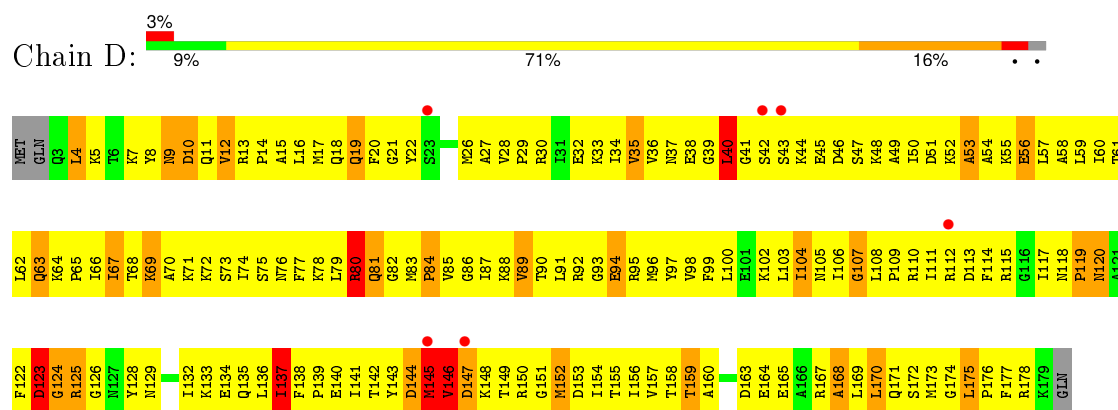
G2485	C2403	U2342	C2281	G2218	C	A	G2036	U1974	U1914	C1853	U1789	C1725	A1658	U1594
G2486	A2404	C2343	G2282	U2219	C	G	A2037	G1976	A1915	G1854	G1790	C1726	G1659	A1595
A2487	A2405	G2344	G2283	A2220	A	G	C2038	U1977	G1916	G1855	C1791	C1727	G1660	A1596
G2488	A2406	A2345	U2284	G2221	C	A	G2039	C1977	C1917	U1856	C1792	A1728	C1661	A1597
U2489	G2407	G2346	U2285	U2222	C	U	A2040	U1978	G1918	G1857	A1793	C1729	G1662	C1598
G2490	G2408	C2347	G2286	A2041	C	A	A2041	C1979	A1919	C1858	A1794	G1730	C1663	G1599
U2491	A2409	A2348	G2287	G2224	U	G	A2042	A1980	A1920	A1859	C1795	C1731	G1664	U1600
U2492	U2410	G2349	A2288	G2225	G	G	G2043	A1981	A1921	A1860	U1732	U1732	G1665	U1601
A2493	A2411	G2350	A2289	G2226	A2165	U	G2044	C1982	U1922	G1861	U1733	U1733	G1666	G1602
G2494	A2412	G2351	G2290	C2227	A2166	G	A2045	A1983	U1923	A1800	G1734	A1667	A1667	A1603
A2495	A2413	A2352	U2291	U2228	A2167	G	G2046	A1984	C1924	C1863	C1801	G1735	G1668	A1604
G2496	G2414	G2353	C2292	G2229	A2168	G	C2047	G1985	C1925	G1864	A1802	G1736	A1669	A1605
U2497	G2415	G2354	G2293	G2230	A2169	A	G2048	G1986	U1926	C1865	G1803	G1737	G1670	C1606
C2498	U2416	A2355	U2294	G2230	C2170	G	C2049	G1987	U1927	G1866	U1804	U1738	A1671	A1607
G2499	U2417	A2356	C2295	G2234	U2171	C	G2050	U1988	G1928	A1867	G1739	U1739	A1672	U1608
C2500	A2418	A2357	G2296	G2235	U2172	C	U2051	C1991	G1928	G1868	G1673	G1740	C1673	G1609
A2501	C2419	C2358	U2297	U2236	G2173	G	G2052	G1992	C1930	A1869	A1807	G1741	C1674	A1610
G2502	C2420	G2359	G2298	U2237	G2174	G	G2053	G1993	G1931	C1870	A1808	G1742	C1675	U1611
U2503	C2421	C2360	A2299	G2238	A2175	C	A2054	U1994	G1932	G1871	G1809	C1743	U1676	U1612
G2504	C2422	G2361	G2300	C2239	U2176	G	G2055	G1995	G1933	A1872	U1810	G1744	C1677	G1613
U2505	G2423	G2362	A2301	C2240	U2177	A	C2056	A1996	U1934	C1873	A1811	C1745	G1678	C1614
C2506	G2424	C2363	G2302	U2241	U2178	A	U2057	A1997	A1935	G1874	U1812	A1746	U1679	C1615
G2507	G2425	C2364	C2303	G2242	C2179	A	U2058	A1998	A1936	C1875	A1813	G1747	U1680	C1616
U2508	G2426	U2365	G2304	C2243	U2180	C	U2059	U1999	G1937	U1875	G1814	U1748	A1681	G1617
C2509	A2427	U2366	C2305	C2244	A2181	U	A2060	U2000	U1938	C1878	G1815	G1749	A1682	U1618
G2510	U2428	A2367	A2306	A2245	G2182	G	C2061	G2001	U1939	G1879	G1816	A1750	G1683	A1619
U2511	A2429	G2368	A2307	A2246	G2184	C	U2062	A2002	C1940	G1880	U1817	A1751	G1684	C1620
C2512	C2430	U2369	A2308	A2247	U2185	G	A2063	A2003	C1941	U1881	U1818	U1752	A1685	C1621
G2513	G2431	G2370	G2309	G2248	G2186	C	U2064	U2004	G1942	G1882	U1819	A1753	A1686	G1622
U2514	A2432	A2371	G2310	U2249	A2187	C	A2065	U2005	A1943	A1883	G1820	G1754	C1687	C1623
G2515	G2433	A2372	U2311	G2250	A2188	U	G2066	G2006	C1944	A1884	A1821	G1755	U1688	A1624
C2516	C2434	C2373	A2312	U2251	A2189	U	U2067	G2007	C1945	C1885	C1822	G1756	U1689	A1625
U2517	U2435	G2374	G2313	A2252	A2190	C	C2068	C2008	U1946	G1886	G1823	C1757	U1690	A1626
G2518	A2436	G2375	A2314	G2253	A2191	G	U2069	U2009	G1947	G1887	C1824	C1758	C1692	C1627
C2519	G2437	G2376	A2315	C2254	U2192	G	G2070	U2010	C1948	C1888	C1825	U1759	A1693	G1628
U2520	A2438	U2377	G2316	G2255	C2193	G	G2071	U2011	A1949	C1889	U1826	U1760	A1694	G1629
G2521	U2439	G2378	G2317	G2256	A2194	C	C2072	A2012	C1950	A1890	A1827	A1771	U1695	A1630
C2522	C2440	G2379	G2318	A2257	G2195	U	U2073	A2013	G1951	C1891	C1828	C1772	U1705	G1636
U2523	U2441	U2380	G2319	G2258	U2196	C	U2074	A2014	A1952	C1892	U1830	C1773	A1706	G1638
G2524	C2442	A2381	C2321	G2259	U2197	G	U2075	G2015	A1953	C1893	G1831	U1774	A1707	G1642
C2525	G2443	C2382	U2322	G2260	U2198	C	G2076	A2016	A1954	U1893	U1832	A1775	C1708	A1643
U2526	C2444	C2383	G2323	G2261	C2199	G	G2081	U2017	G1955	A1894	U1833	A1776	U1709	A1644
G2527	G2445	G2384	G2324	G2262	G2200	G	G2082	G2018	G1956	A1895	G1834	A1777	U1710	G1645
U2528	C2446	C2385	A2325	C2263	G2201	C	U2083	G2019	C1957	C1896	C1835	C1778	C1711	U1646
C2529	G2447	U2386	C2326	C2264	G2202	A	U2084	G2020	G1958	U1897	U1836	U1779	G1712	G1647
U2530	A2448	G2387	U2327	A2265	G2203	G	G2085	G2021	A1960	A1898	G1837	A1774	A1708	C1648
G2531	G2449	G2388	G2328	A2266	A2204	G	G2086	C2022	A1961	U1899	A1839	A1775	C1709	A1649
C2532	A2450	C2389	C2329	A2267	G2205	C	G2087	C2023	C1962	A1896	U1841	A1776	U1711	A1650
U2533	G2451	A2391	G2330	G2268	C2206	G	U2088	U2024	G1963	A1897	G1842	U1778	C1712	U1645
G2534	U2452	G2392	A2331	G2269	G2207	A	U2089	A2025	G1964	C1898	U1843	C1779	G1713	C1648
C2535	C2453	G2393	G2332	U2270	U2208	C	U2090	C2026	U1965	U1899	A1844	A1780	G1714	C1649
U2536	G2454	G2394	A2333	C2271	G2209	G	U2091	G2027	C1966	U1967	U1845	C1781	A1715	A1650
C2537	A2455	C2395	C2334	A2272	C2210	G	C2092	C2028	C1967	C1899	A1846	A1782	A1716	A1651
U2538	U2456	C2396	U2335	C2273	U2211	G	U2093	G2029	U1968	C1900	C1847	G1783	G1717	G1652
G2539	G2457	A2397	G2336	C2274	U2212	C	C	U2030	G1969	U1909	U1848	C1784	A1718	G1653
C2540	U2458	U2398	A2337	U2275	G2213	A	U	A2031	C1970	A1910	G1849	A1785	U1719	G1654
U2541	G2460	G2399	C2338	G2276	G2214	A	U	G2032	G1971	A1911	C1890	A1786	U1723	C1655
C2542	G2461	A2400	A2339	G2277	C2215	A	C	C2033	G1972	G1912	A1850	U1787	U1724	U1656
G2543	C2462	G2401	C2340	U2279	G2216	U	G	A2034	C1973	G1913	G1852	C1788	C1724	A1657
U2544	G2463	U2402	G2341	A2280	G2217	A	U	G2035	C1973					

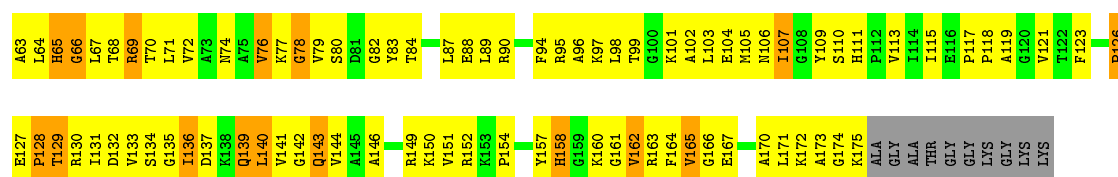


• Molecule 5: 50S ribosomal protein L4

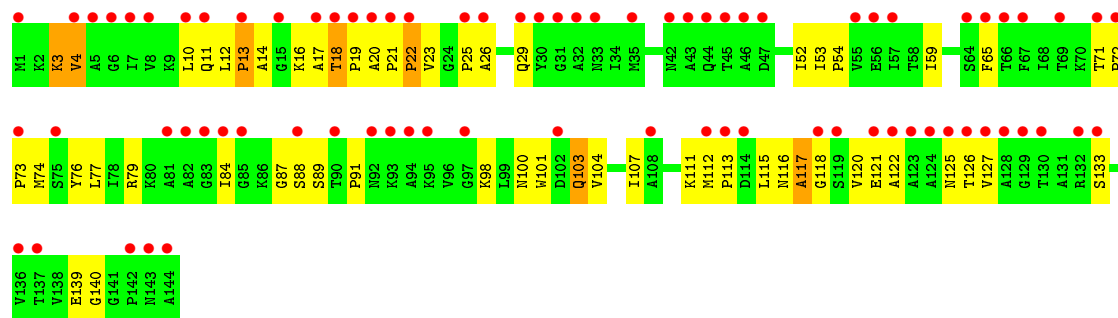


• Molecule 6: 50S ribosomal protein L5

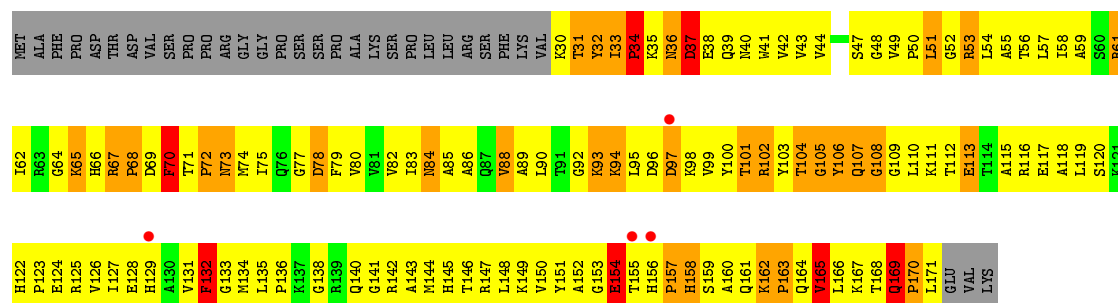




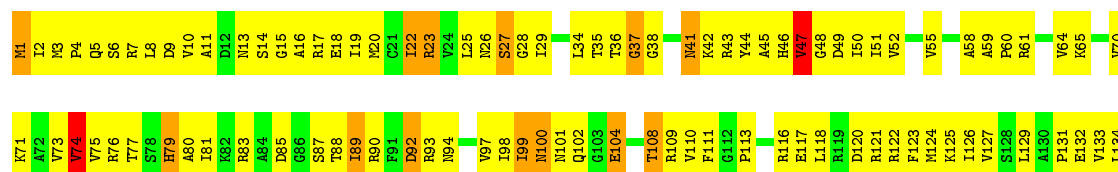
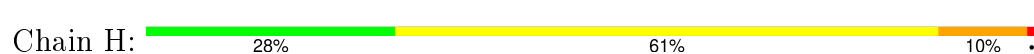
• Molecule 8: 50S ribosomal protein L11



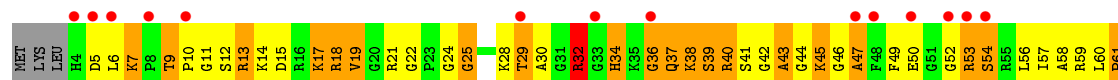
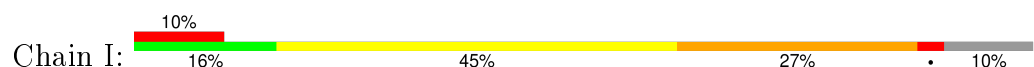
• Molecule 9: 50S ribosomal protein L13

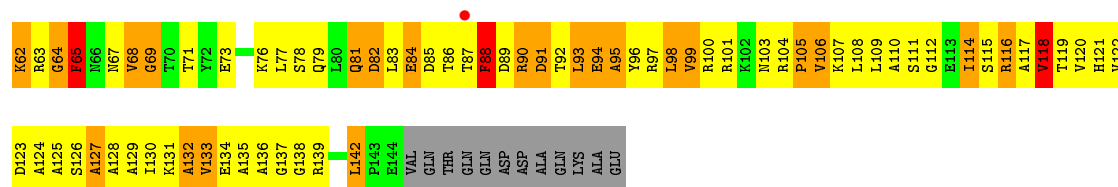


• Molecule 10: 50S ribosomal protein L14

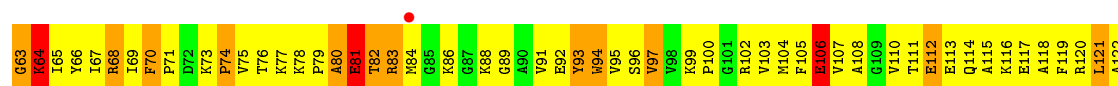
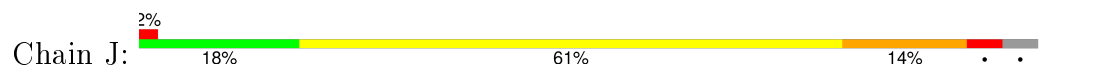


• Molecule 11: 50S ribosomal protein L15

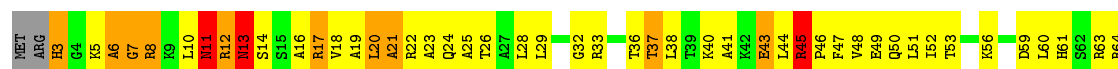




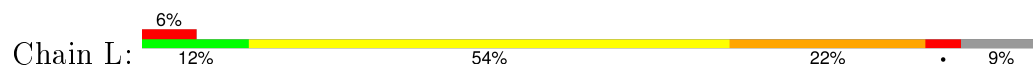
• Molecule 12: 50S ribosomal protein L16



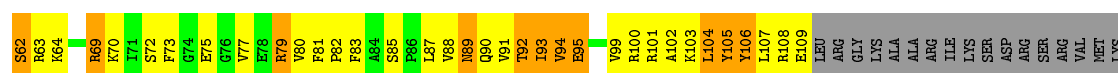
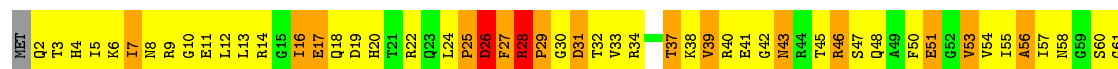
• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18

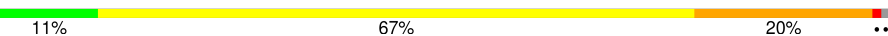


• Molecule 15: 50S ribosomal protein L19



ASP
ALA
ALA
ARG
ALA
ALA
GLN
GLN
ASP
LYS
ALA
ALA
ASU
ALA
SER
ALA
ALA
GLN
ALA
ASP
VAL
THR
VAL
ILE
SER
ALA
ALA
ALA
PRO
GLU
VAL
ALA
PRO
GLU
THR
GLN
GLY
GLU

• Molecule 16: 50S ribosomal protein L20

Chain N: 

MET	F2	R3	A4	R5	T6	G7	I8	V9	R10	R11	R12	R13	H14	K15	V17	L18	F19	R20	A21	G22	G23	F24	I25	G26	S27	R28	S29	K30	O31	R32	R33	N34	A35	F36	D37	T38	L39	L40	N41	A42	A43	T44	Y45	E46	Y47	R48	D49	L109	R50	R51	R52	K53	R54	R55	D56	F57	R58	R59	L60
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• Molecule 17: 50S ribosomal protein L21

Chain O: 

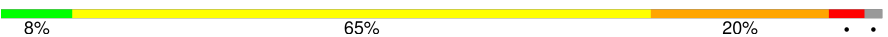
MET	PHE	ALA	ILE	I6	Q6	T7	G8	G9	K10	Q11	Y12	R13	R14	S15	E16	G17	D18	V19	I20	R21	V22	E23	S24	L25	Q26	G27	E28	A29	G30	D31	K32	V33	E34	L35	K36	L37	L38	F39	V40	G41	G42	E43	Q44	T45	V46	F47	R48	E49	D50	A51	G52	K53	Y54	T55	V56	Q57	A58	E59	V60
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• Molecule 18: 50S ribosomal protein L22

Chain P: 

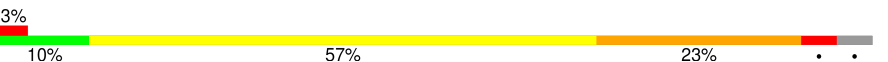
MET	THR	ALA	PRO	GLN	THR	F8	R9	L10	M11	K12	Q13	Q14	R15	Q16	Q17	V18	K19	L20	G24	F25	A26	V27	A28	E29	V30	V31	R32	K33	S34	F35	R36	K37	V38	R39	L40	V41	V42	D43	V44	I45	R46	G47	R48	S49	V50	Q51	D52	A53	E54	L57	R58	F59	I60	P61	R62	S63
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• Molecule 19: 50S ribosomal protein L23

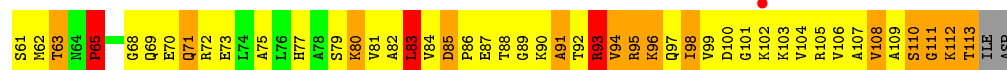
Chain Q: 

MET	S2	H3	Y4	D5	I6	L7	Q8	A9	P10	V11	I12	E13	E14	K15	Y16	S17	I18	A19	M20	E21	G22	G23	V24	Y25	S26	F27	W28	K29	S30	P31	K32	A33	T34	K35	T36	E37	I38	K39	D40	A41	I42	Q43	Q44	A45	F46	G47	V48	R49	V50	I51	G52	I53	S54	T55	M56	P59	G60	K61
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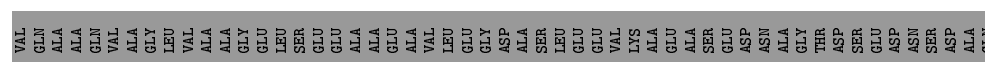
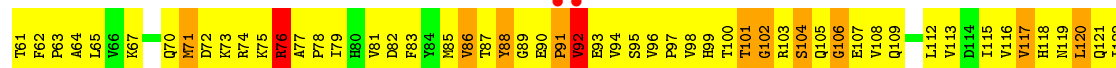
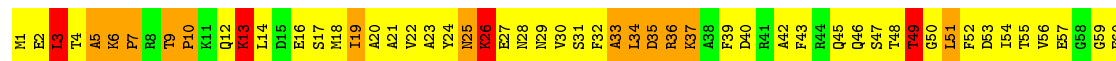
• Molecule 20: 50S ribosomal protein L24

Chain R: 

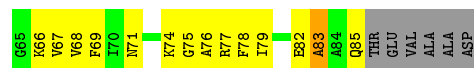
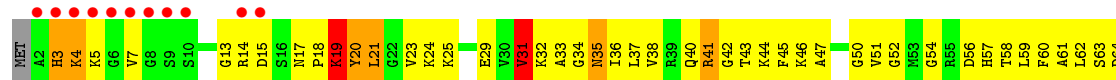
MET	PRO	ARG	P4	S5	A6	G7	S8	H9	R10	R11	D12	K13	L14	R15	F16	K17	I18	G19	D20	T21	V22	I23	V24	L25	S26	G27	K28	R29	K30	A31	Q32	I33	G34	K35	V36	L37	L38	A39	P41	R42	D43	Q44	K45	V46	V47	V48	R49	G50	V51	N52	V53	L54	T55	K56	R57	V58	K59	P60
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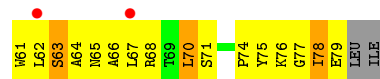
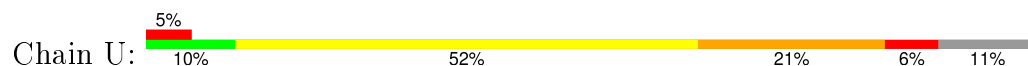
• Molecule 21: 50S ribosomal protein L25



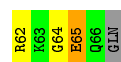
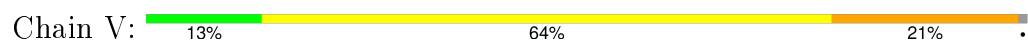
• Molecule 22: 50S ribosomal protein L27



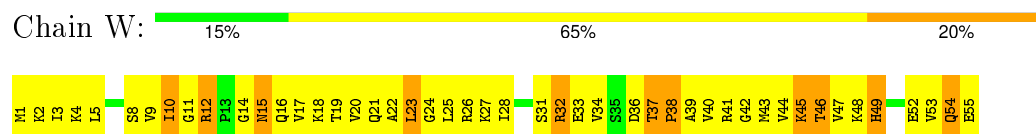
• Molecule 23: 50S ribosomal protein L28



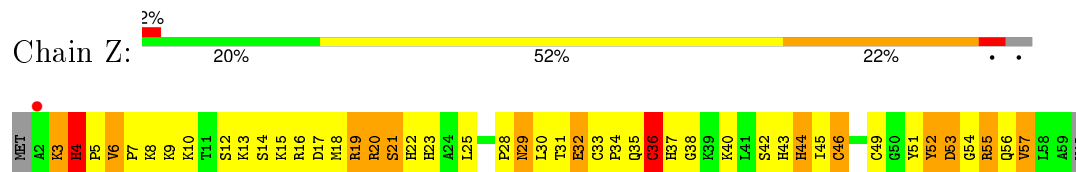
• Molecule 24: 50S ribosomal protein L29



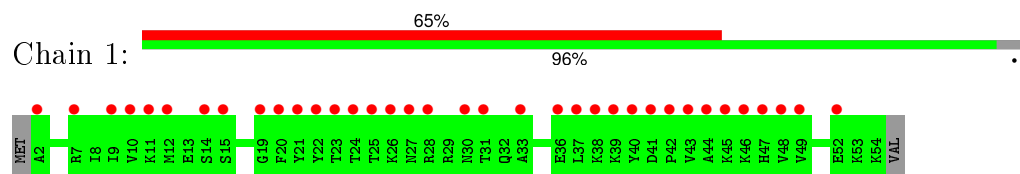
• Molecule 25: 50S ribosomal protein L30



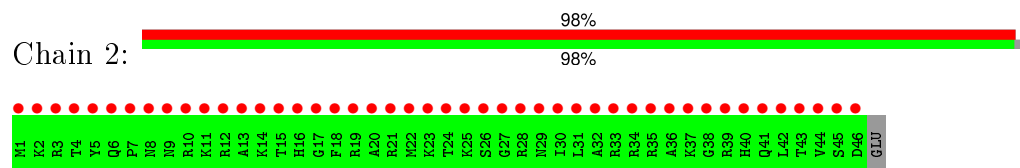
- Molecule 26: 50S ribosomal protein L32



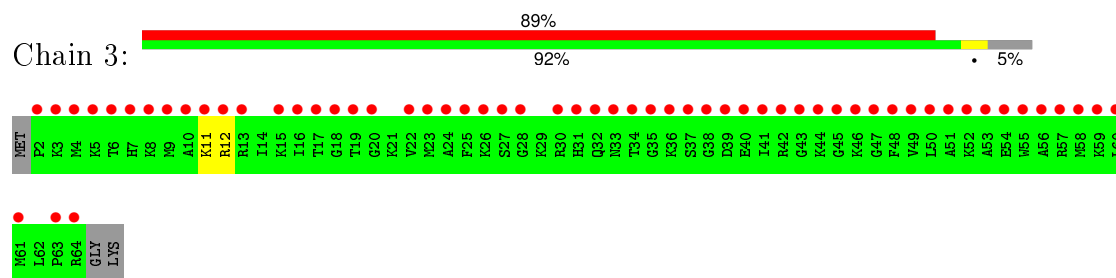
- Molecule 27: 50S ribosomal protein L33



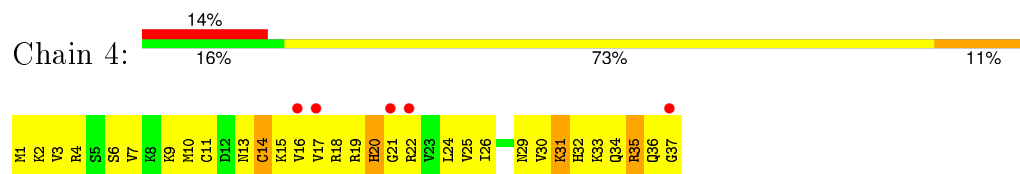
- Molecule 28: 50S ribosomal protein L34



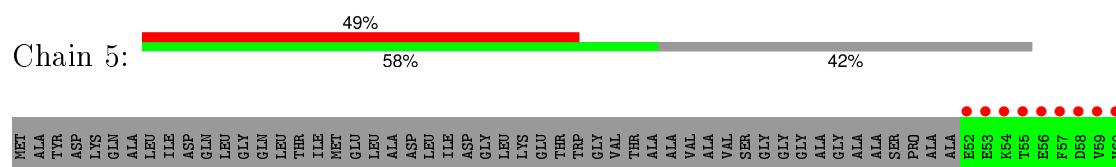
- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L7/L12



L61	L62	D63	A64	G65	A66	S67	R68	I69	N70	V71	I72	K73	E74	I75	R76	G77	I78	T79	G80	L81	G82	L83	K84	E85	A86	K87	D88	M89	S90	E91	K92	G93	G94	V95	L96	K97	E98	G99	V100	A101	K102	D103	E104	A105	E106	K109	L112	E113	A114	A115	G116	A117	R118	V119	E120	L121	K122
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.92 – 3.31	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-3.30) 97.2 (29.92-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.302 , 0.339 0.277 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 346473 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	84395	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	X	0.90	77/64561 (0.1%)	1.04	462/100708 (0.5%)
2	Y	0.60	0/2904	0.77	0/4525
3	A	0.60	0/1862	0.83	0/2510
4	B	0.72	0/1567	0.95	2/2105 (0.1%)
5	C	0.63	0/1529	0.86	0/2070
6	D	0.60	0/1419	0.77	0/1903
7	E	0.55	0/1308	0.82	0/1771
8	F	0.23	0/1062	0.41	0/1440
9	G	0.65	0/1138	0.93	2/1539 (0.1%)
10	H	0.77	0/1007	0.85	0/1352
11	I	0.65	0/1081	0.93	1/1448 (0.1%)
12	J	0.68	0/1113	0.87	0/1486
13	K	0.80	0/886	0.95	0/1188
14	L	0.56	0/785	0.83	0/1048
15	M	0.73	0/884	0.97	2/1186 (0.2%)
16	N	0.60	0/994	0.81	0/1323
17	O	0.62	0/750	0.85	1/1000 (0.1%)
18	P	0.78	0/1027	0.89	0/1373
19	Q	0.67	0/737	0.94	1/988 (0.1%)
20	R	0.57	0/835	0.90	1/1121 (0.1%)
21	S	0.56	0/1370	0.79	0/1862
22	T	0.62	0/633	0.81	1/838 (0.1%)
23	U	0.58	0/556	0.94	0/741
24	V	0.54	0/537	0.75	0/714
25	W	0.55	0/426	0.82	0/568
26	Z	0.62	0/469	0.87	0/629
30	4	0.54	0/298	0.75	0/390
All	All	0.83	77/91738 (0.1%)	0.99	473/137826 (0.3%)

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
1	X	2	281
2	Y	0	2
5	C	0	1
9	G	0	1
16	N	0	1
17	O	0	1
22	T	0	1
All	All	2	288

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1056	U	P-O5'	8.88	1.68	1.59
1	X	1750	A	C5-C6	-7.65	1.34	1.41
1	X	1688	U	C4-O4	7.39	1.29	1.23
1	X	2189	A	N9-C4	7.30	1.42	1.37
1	X	1981	A	C5-C6	-7.18	1.34	1.41

The worst 5 of 473 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1055	A	N9-C1'-C2'	-32.03	72.36	114.00
1	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
1	X	417	C	N1-C1'-C2'	17.87	137.24	114.00
1	X	2323	U	O4'-C1'-N1	13.98	119.39	108.20
1	X	558	G	C3'-C2'-C1'	-13.92	90.37	101.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1278	A	C1'
1	X	2592	U	C1'

5 of 288 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	13	A	Sidechain
1	X	15	G	Sidechain
1	X	29	U	Sidechain
1	X	43	A	Sidechain
1	X	59	G	Sidechain

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	X	57651	0	29046	4354	0
2	Y	2598	0	1328	184	0
3	A	1826	0	1885	379	0
4	B	1539	0	1600	236	0
5	C	1506	0	1525	356	0
6	D	1400	0	1481	400	0
7	E	1286	0	1336	249	0
8	F	1043	0	1088	71	0
9	G	1114	0	1144	282	0
10	H	997	0	1046	167	1
11	I	1067	0	1103	286	0
12	J	1090	0	1125	268	0
13	K	878	0	930	131	1
14	L	779	0	820	227	0
15	M	871	0	894	183	0
16	N	978	0	1020	234	0
17	O	741	0	756	200	0
18	P	1014	0	1096	184	0
19	Q	726	0	753	159	0
20	R	825	0	881	266	0
21	S	1345	0	1372	276	0
22	T	625	0	655	99	0
23	U	552	0	604	209	0
24	V	533	0	558	86	0
25	W	424	0	470	84	0
26	Z	457	0	464	81	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	2	0
30	4	297	0	330	69	0
31	5	71	0	0	0	0
All	All	84395	0	55310	8913	1

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 64.

The worst 5 of 8913 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)
1:X:1854:G:O2'	1:X:1855:G:H5'	1.31	1.28
1:X:2195:C:C5	1:X:2196:U:C5	2.22	1.28
1:X:729:A:H2'	1:X:730:C:O4'	1.19	1.25
1:X:2196:U:H2'	1:X:2197:U:C6	1.74	1.21
1:X:731:A:H2'	1:X:732:G:O4'	1.34	1.21

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:125:LYS:NZ	13:K:82:GLU:OE2[8_555]	2.08	0.12

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	A	238/274 (87%)	150 (63%)	62 (26%)	26 (11%)	0	4
4	B	203/211 (96%)	143 (70%)	29 (14%)	31 (15%)	0	1
5	C	195/205 (95%)	89 (46%)	60 (31%)	46 (24%)	0	0
6	D	175/180 (97%)	101 (58%)	44 (25%)	30 (17%)	0	1
7	E	169/185 (91%)	98 (58%)	43 (25%)	28 (17%)	0	1
8	F	142/144 (99%)	113 (80%)	22 (16%)	7 (5%)	3	19
9	G	140/174 (80%)	76 (54%)	35 (25%)	29 (21%)	0	1
10	H	132/134 (98%)	108 (82%)	16 (12%)	8 (6%)	2	14
11	I	139/156 (89%)	63 (45%)	36 (26%)	40 (29%)	0	0
12	J	134/142 (94%)	74 (55%)	39 (29%)	21 (16%)	0	1
13	K	111/116 (96%)	75 (68%)	20 (18%)	16 (14%)	0	1
14	L	102/114 (90%)	52 (51%)	31 (30%)	19 (19%)	0	1
15	M	106/166 (64%)	57 (54%)	32 (30%)	17 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	68 (59%)	30 (26%)	17 (15%)	0	1
17	O	92/100 (92%)	53 (58%)	14 (15%)	25 (27%)	0	0
18	P	125/134 (93%)	87 (70%)	20 (16%)	18 (14%)	0	1
19	Q	91/95 (96%)	46 (50%)	23 (25%)	22 (24%)	0	0
20	R	108/115 (94%)	57 (53%)	28 (26%)	23 (21%)	0	0
21	S	173/237 (73%)	99 (57%)	43 (25%)	31 (18%)	0	1
22	T	82/91 (90%)	48 (58%)	24 (29%)	10 (12%)	0	2
23	U	70/81 (86%)	35 (50%)	18 (26%)	17 (24%)	0	0
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0	1
25	W	53/55 (96%)	36 (68%)	11 (21%)	6 (11%)	0	3
26	Z	56/60 (93%)	35 (62%)	13 (23%)	8 (14%)	0	1
30	4	35/37 (95%)	23 (66%)	6 (17%)	6 (17%)	0	1
All	All	3050/3391 (90%)	1818 (60%)	718 (24%)	514 (17%)	0	1

5 of 514 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	54	ILE
3	A	59	LYS
3	A	60	ARG
3	A	153	ALA
3	A	154	GLN

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	A	185/215 (86%)	165 (89%)	20 (11%)	8	32
4	B	155/157 (99%)	140 (90%)	15 (10%)	10	38
5	C	157/163 (96%)	133 (85%)	24 (15%)	3	16
6	D	153/156 (98%)	137 (90%)	16 (10%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	136/144 (94%)	126 (93%)	10 (7%)	17	52
8	F	107/107 (100%)	105 (98%)	2 (2%)	65	85
9	G	118/146 (81%)	102 (86%)	16 (14%)	5	21
10	H	103/103 (100%)	90 (87%)	13 (13%)	5	24
11	I	108/121 (89%)	95 (88%)	13 (12%)	6	27
12	J	110/116 (95%)	99 (90%)	11 (10%)	9	36
13	K	90/93 (97%)	79 (88%)	11 (12%)	6	26
14	L	74/82 (90%)	57 (77%)	17 (23%)	1	4
15	M	94/134 (70%)	82 (87%)	12 (13%)	5	23
16	N	96/97 (99%)	87 (91%)	9 (9%)	11	39
17	O	75/79 (95%)	65 (87%)	10 (13%)	5	21
18	P	109/115 (95%)	103 (94%)	6 (6%)	27	66
19	Q	75/76 (99%)	66 (88%)	9 (12%)	6	27
20	R	91/96 (95%)	76 (84%)	15 (16%)	3	14
21	S	149/192 (78%)	131 (88%)	18 (12%)	6	26
22	T	62/67 (92%)	57 (92%)	5 (8%)	15	48
23	U	57/66 (86%)	46 (81%)	11 (19%)	2	7
24	V	54/55 (98%)	50 (93%)	4 (7%)	17	52
25	W	48/48 (100%)	42 (88%)	6 (12%)	6	24
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1	7
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2492/2716 (92%)	2209 (89%)	283 (11%)	7	29

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	142	LEU
14	L	44	ASP
23	U	70	LEU
12	J	60	ARG
13	K	12	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
11	I	34	HIS
14	L	63	ASN
24	V	52	GLN
11	I	37	GLN
11	I	121	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	695 (25%)	301 (11%)
2	Y	121/122 (99%)	23 (19%)	0
All	All	2801/3002 (93%)	718 (25%)	301 (10%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	13	A
1	X	14	A
1	X	34	U
1	X	35	G

5 of 301 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1278	A
1	X	1581	C
1	X	2633	A
1	X	1313	U
1	X	1357	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	2686/2880 (93%)	-0.27	40 (1%) 76 71	11, 57, 103, 131	0
2	Y	122/122 (100%)	-0.00	2 (1%) 74 69	29, 81, 102, 108	0
3	A	240/274 (87%)	-0.01	6 (2%) 61 54	35, 65, 77, 90	0
4	B	205/211 (97%)	-0.24	2 (0%) 84 80	30, 53, 64, 77	0
5	C	197/205 (96%)	-0.22	3 (1%) 76 71	38, 60, 71, 83	0
6	D	177/180 (98%)	0.10	6 (3%) 49 42	54, 67, 76, 84	0
7	E	171/185 (92%)	-0.38	1 (0%) 90 88	50, 64, 75, 80	0
8	F	144/144 (100%)	2.21	78 (54%) 0 0	0, 0, 83, 88	0
9	G	142/174 (81%)	-0.12	4 (2%) 56 50	47, 59, 69, 77	0
10	H	134/134 (100%)	-0.27	0 100 100	27, 52, 62, 69	0
11	I	141/156 (90%)	0.38	15 (10%) 8 6	40, 63, 75, 83	0
12	J	136/142 (95%)	-0.20	3 (2%) 65 59	45, 61, 72, 78	0
13	K	113/116 (97%)	-0.22	0 100 100	37, 50, 60, 63	0
14	L	104/114 (91%)	0.08	7 (6%) 21 17	52, 63, 73, 78	0
15	M	108/166 (65%)	-0.31	0 100 100	23, 53, 65, 73	0
16	N	117/118 (99%)	-0.34	0 100 100	39, 57, 69, 75	0
17	O	94/100 (94%)	-0.38	0 100 100	42, 61, 72, 79	0
18	P	127/134 (94%)	-0.36	0 100 100	34, 52, 66, 76	0
19	Q	93/95 (97%)	-0.31	0 100 100	47, 58, 73, 78	0
20	R	110/115 (95%)	-0.03	4 (3%) 46 39	49, 62, 73, 85	0
21	S	175/237 (73%)	0.06	7 (4%) 42 34	55, 65, 76, 87	0
22	T	84/91 (92%)	0.30	11 (13%) 5 3	50, 61, 74, 80	0
23	U	72/81 (88%)	0.14	4 (5%) 28 22	52, 64, 73, 78	0
24	V	66/67 (98%)	-0.28	0 100 100	54, 63, 75, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.49	0	100 100	48, 58, 70, 79	0
26	Z	58/60 (96%)	-0.24	1 (1%)	73 67	35, 53, 66, 69	0
27	1	53/55 (96%)	3.30	36 (67%)	0 0	53, 61, 68, 71	0
28	2	46/47 (97%)	6.76	46 (100%)	0 0	43, 56, 62, 63	0
29	3	63/66 (95%)	5.35	59 (93%)	0 0	50, 58, 65, 67	0
30	4	37/37 (100%)	0.38	5 (13%)	4 3	52, 63, 71, 76	0
31	5	71/122 (58%)	5.13	60 (84%)	0 0	0, 0, 0, 0	0
All	All	6141/6683 (91%)	0.07	400 (6%)	22 18	0, 60, 91, 131	0

The worst 5 of 400 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	5	101	ALA	22.5
29	3	37	SER	16.6
28	2	4	THR	13.7
31	5	70	ASN	13.0
31	5	104	GLU	13.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.