



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DLL
Title : The oxazolidinone antibiotics perturb the ribosomal peptidyl-transferase center and effect tRNA positioning
Authors : Wilson, D.N.; Schlutzen, F.; Harms, J.M.; Starosta, A.L.; Connell, S.R.; Fucini, P.
Deposited on : 2008-06-27
Resolution : 3.50 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

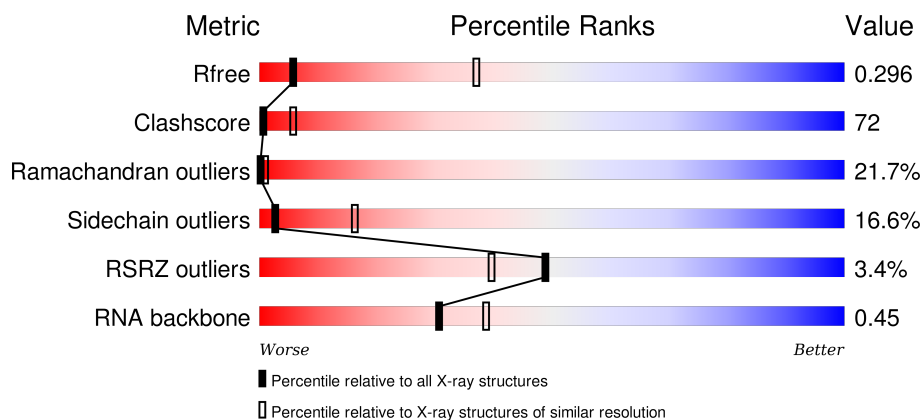
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


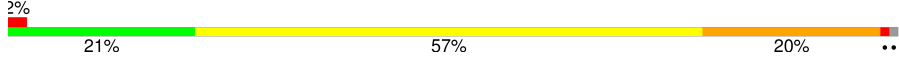

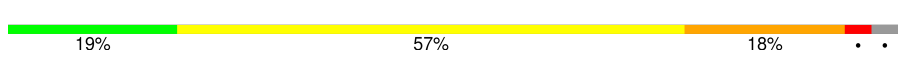
The reported resolution of this entry is 3.50 Å.

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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	
2	Z	123	
3	A	274	
4	B	211	


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	205	
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	Y	60	
27	1	55	
28	2	47	
29	3	66	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	4	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	M	167	-	-	-	X
32	MG	X	2885	-	-	-	X
32	MG	X	2889	-	-	-	X
32	MG	X	2896	-	-	-	X
32	MG	X	2899	-	-	-	X
32	MG	X	2903	-	-	-	X
32	MG	X	2907	-	-	-	X
32	MG	X	2909	-	-	-	X
33	ZLD	X	2911	-	-	X	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 83657 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 rRNA-23S ribosomal 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 rRNA-5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	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	218	Total	C	N	O	S	0	0	0
			1637	1017	326	292	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	70	Total	C	N	O	S	0	0	0
			504	314	90	97	3			

- 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	S	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	Y	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

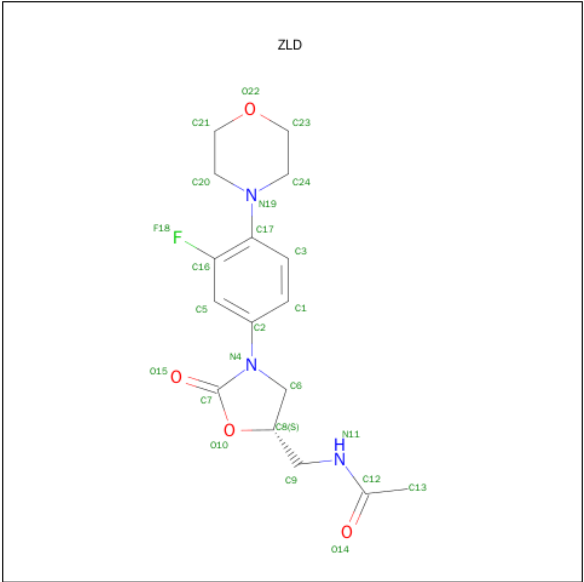
- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	Y	1	Total Zn 1 1	0	0
31	4	1	Total Zn 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	30	Total Mg 30 30	0	0
32	Z	4	Total Mg 4 4	0	0
32	M	1	Total Mg 1 1	0	0

- Molecule 33 is N-{|(5S)-3-(3-FLUORO-4-MORPHOLIN-4-YLPHENYL)-2-OXO-1,3-OXAZOLIDIN-5-YL|METHYL}ACETAMIDE (three-letter code: ZLD) (formula: C₁₆H₂₀FN₃O₄).

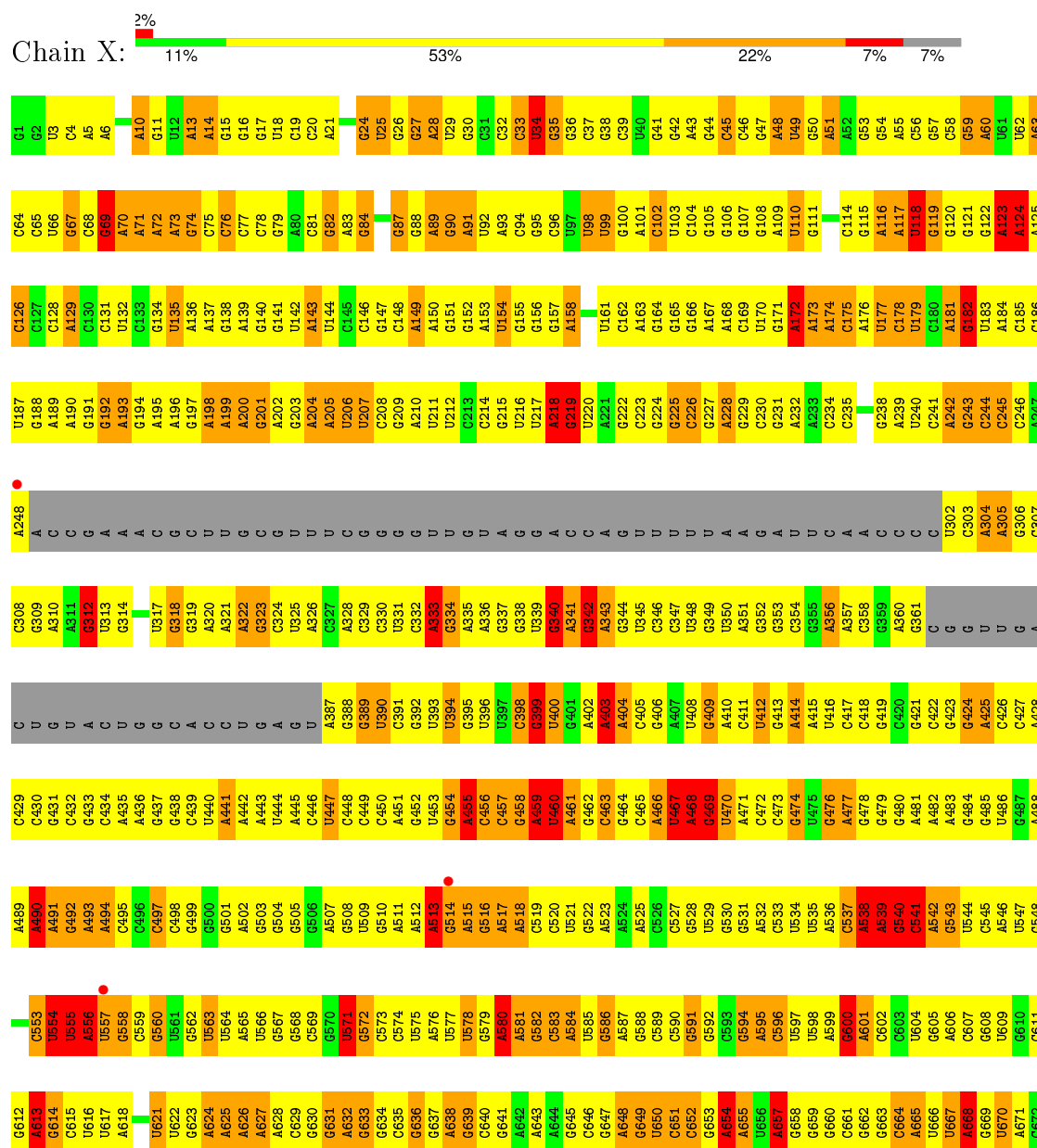


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

3 Residue-property plots

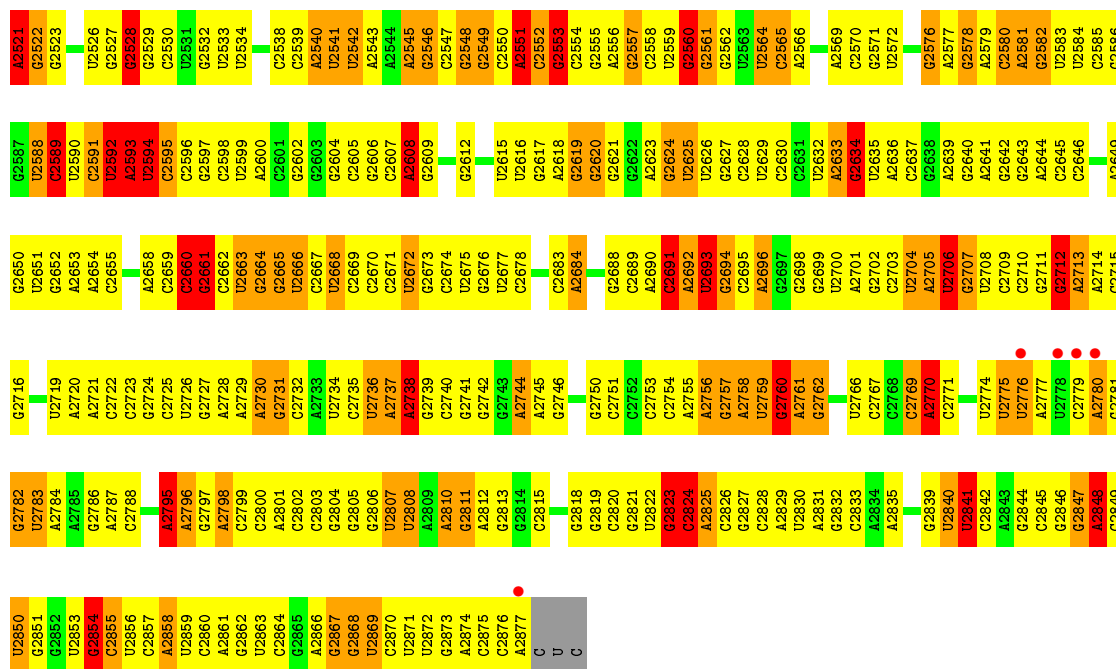
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: rRNA-23S ribosomal RNA

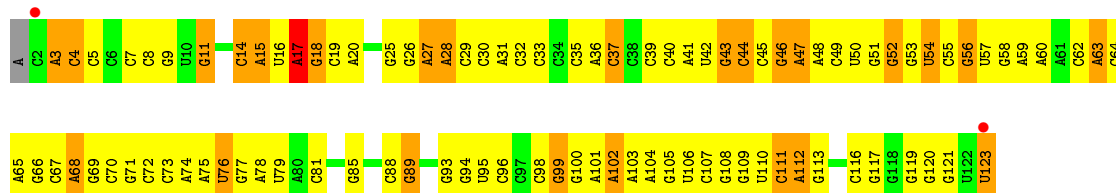




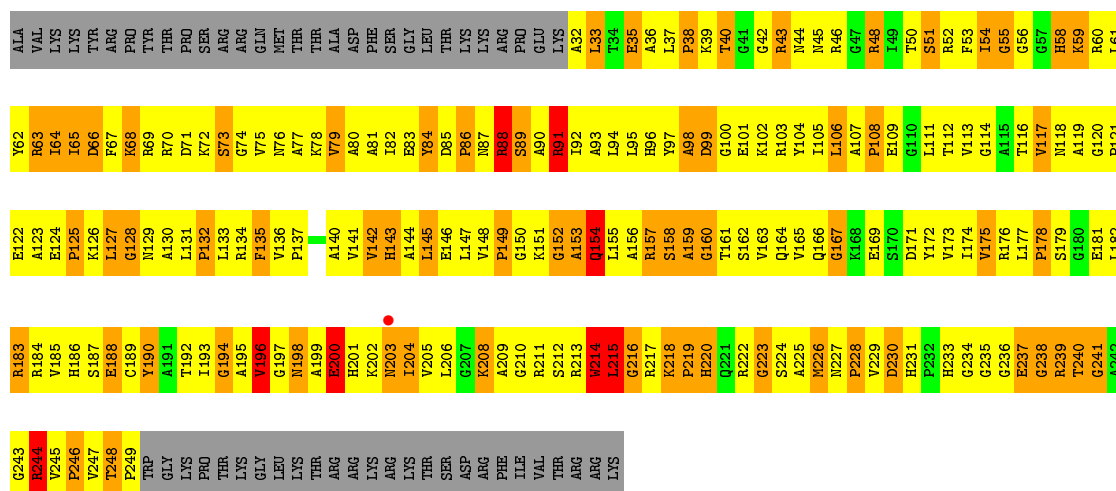
G2461	A2401	A2339	U2275	U2212	G	C	G2029	G1969	C	G1847	A1785	C1725	A1596
G2462	U2402	C2340	C2276	G2213	A	U	U2030	G1970	U1909	U1848	C1786	C1726	A1597
G2463	C2341	G2341	C2281	G2214	A	G	A2031	G1971	A1910	G1849	C1787	C1727	C1598
G2464	A2404	U2342	C2281	G2215	A	C	G2032	G1972	A1911	G1850	C1788	A1728	G1599
G2465	A2405	C2343	G2282	G2216	U	G	C2033	C1973	G1912	A1851	U1789	C1729	G1600
G2466	A2406	G2344	G2283	G2217	A	U	A2034	U1974	G1913	G1852	G1790	G1730	U1601
G2467	G2407	A2345	G2284	G2218	C	A	G2035	G1975	U1914	U1853	C1791	G1731	G1602
G2468	G2408	U2346	U2285	G2219	C	G	G2036	U1976	A1915	G1854	C1792	U1732	A1603
G2469	A2409	G2347	G2286	A2220	A	G	A2037	G1977	G1916	G1855	C1793	U1733	A1604
U2470	U2410	A2348	G2287	G2221	C	A	G2038	U1978	C1917	U1856	A1793	G1734	A1605
U2471	A2411	G2349	U2288	G2222	C	U	G2039	C1979	G1918	G1857	A1794	C1735	A1606
U2472	A2412	G2350	U2289	U2223	C	A	A2040	A1980	A1919	U1858	C1795	G1736	A1607
G2473	A2413	G2351	U2290	U2224	C	A	A2041	A1981	A1920	A1859	A1799	G1737	U1608
G2474	A2414	A2352	U2291	G2225	G	U	A2042	C1982	A1921	A1860	A1799	G1738	G1609
C2475	G2415	G2353	A2292	A2226	U	U	A2043	G1983	U1922	G1861	C1792	U1739	G1613
A2476	U2416	G2354	C2227	U2227	G	G	U2044	U1984	U1923	G1862	C1793	G1740	C1614
C2477	U2417	G2355	U2228	U2228	G	G	A2045	G1985	C1924	U1863	A1802	G1741	C1615
C2478	A2418	A2356	G2229	G2230	A	A	G2046	G1986	G1925	G1864	G1741	G1742	C1616
U2479	C2419	A2357	G2230	G2231	U	G	C2047	G1987	U1926	G1865	G1743	G1744	G1617
C2480	C2420	U2358	U2289	G2231	C	C	G2048	A1988	U1927	A1866	A1806	G1745	U1618
G2481	C2421	G2359	A2299	G2232	U	U	C2049	C1989	U1928	A1867	A1807	C1746	A1682
A2482	C2422	G2360	G2300	G2233	C	C	U2050	U1990	U1929	A1869	C1808	A1746	G1618
U2483	G2423	G2361	A2301	U2236	C	U	G2051	C1991	G1930	U1870	G1809	G1747	A1619
G2484	G2424	G2362	G2302	G2237	A2173	G	U2052	G1992	G1931	A1871	U1810	G1748	C1620
U2485	G2425	C2363	C2303	G2238	A2175	C	G2053	G1993	G1932	A1872	A1811	G1749	C1621
C2486	G2426	C2364	G2304	G2239	U2177	G	A2054	U1994	G1933	A1873	U1812	A1750	G1622
G2487	A2427	U2365	U2305	G2240	U2178	A	G2055	G1995	A1936	G1874	A1813	A1751	C1623
G2488	U2428	G2366	A2306	U2241	C	A	C2056	A1996	A1937	C1875	U1752	A1752	A1624
A2489	A2429	A2367	G2307	G2242	U2180	A	U2057	A1997	G1938	C1876	G1815	A1753	A1625
U2490	A2430	G2368	C2308	C2243	A2181	C	G2058	A1998	U1939	C1877	G1816	G1754	A1626
C2491	C2431	U2369	G2309	U2244	A2182	U	U2059	U1999	U1940	C1878	U1817	G1755	C1627
G2492	A2432	G2370	G2310	A2245	C2183	G	A2060	U2000	C1941	G1879	G1818	C1756	C1628
U2493	C2433	A2371	U2311	A2246	G2184	U	G2061	G2001	C1942	U1880	U1819	C1757	A1630
G2494	G2434	C2372	A2312	A2247	U2185	C	U2064	A2002	G1943	C1881	G1820	C1758	C1631
G2495	U2435	G2373	A2248	G2248	G2186	C	U2067	A2003	C1944	A1882	A1821	G1759	A1632
C2496	U2436	G2374	U2249	U2249	A2187	U	U2068	U2004	C1945	A1883	G1822	G1760	C1633
A2497	G2437	G2375	A2315	G2250	A2188	U	U2069	U2005	G1946	A1884	C1823	G1761	A1634
U2498	A2438	G2376	G2316	U2251	C2189	U	C2068	G2006	U1947	C1885	C1824	C1762	G1635
C2499	U2439	G2377	U2317	A2252	A2190	U	G2069	G2007	C1948	G1886	C1825	G1763	C1703
C2500	C2440	U2318	A2253	G2253	A2191	G	G2070	C2008	A1949	G1887	U1826	A1764	U1639
U2501	U2441	G2319	G2254	G2254	U2192	G	C2071	U2009	G1950	C1888	G1827	C1765	G1704
G2502	C2442	A2381	G2255	G2255	C2193	G	G2072	G2010	G1951	G	C1828	U1766	U1705
G2503	C2443	G2382	G2256	G2256	A2194	G	C2073	U2011	A1952	C	C1829	G1767	A1706
G2504	G2444	C2383	A2257	G2257	C2195	U	U2074	U2012	G1953	C	C1830	U1768	G1642
G2505	C2445	G2384	G2258	G2258	U2196	C	U2075	A2013	A1954	C	G1831	U1769	A1643
C2506	C2446	U2385	G2259	G2259	U2197	G	G2076	A2014	A1954	G	U1832	U1770	G1644
U2507	G2447	G2386	G2260	G2260	U2198	G	G2077	G2015	G1955	U	U1833	A1771	U1645
G2508	A2448	U2387	C2261	G2261	C2199	U	G2078	A2016	G1956	A	G1834	C1772	G1646
A2509	U2449	G2388	C2262	C2262	G2200	G	A2079	U2017	C1957	A	C1835	C1773	U1647
A2510	G2450	G2389	G2263	C2263	G2201	G	U2080	G2018	G1958	C	C1836	A1774	C1648
G2511	U2451	C2390	A2265	G2265	G2202	A	U2081	C2019	U1959	U	G1837	A1775	A1649
A2512	C2452	G2391	A2266	G2266	G2203	G	C2082	G2020	A1960	A	G1838	A1776	U1650
G2513	C2453	A2392	A2267	G2267	A2204	G	G2083	G2021	A1961	U	U1839	A1777	U1651
G2514	G2454	G2393	G2268	G2268	C2205	G	G2084	C2022	G1962	A	A1840	U1778	G1652
G2515	A2455	A2394	G2269	G2269	C2206	A	G2085	C2023	G1963	A	G1841	C1779	C1653
U2516	U2456	G2395	U2270	U2270	G2207	A	U2086	U2024	A1964	C	G1842	A1780	A1654
C2517	A2457	U2396	C2271	C2271	U2208	C	U2087	A2025	U1965	G	U1843	C1781	C1655
C2518	U2458	G2397	A2272	C2272	G2209	G	U2088	C2026	C1966	U	C1844	A1782	U1656
C2519	G2459	U2398	C2273	C2273	G2210	G	C2089	C2027	U1967	U	G1783	G1723	A1657
A2520	G2460	C2398	C2274	U2090	U2211	U	U2090	C2028	G1968	C	A1846	C1784	G1659



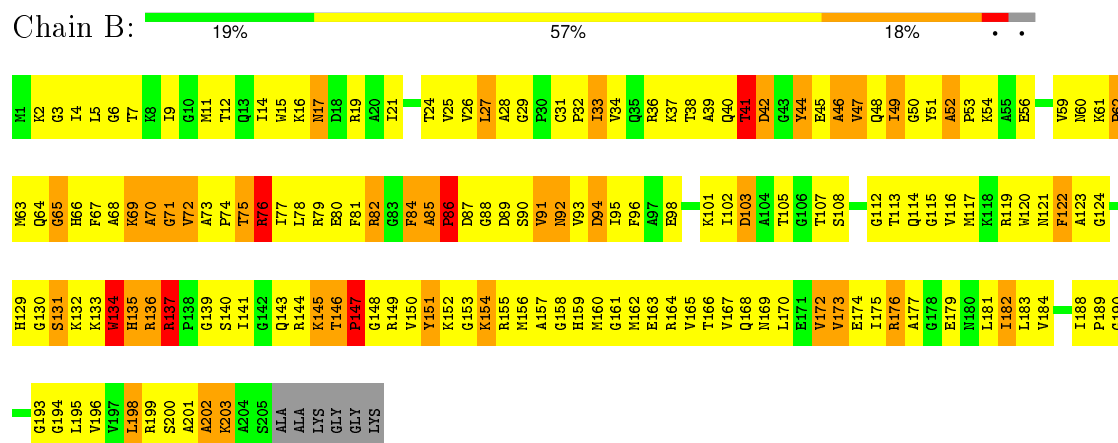
• Molecule 2: rRNA-5S ribosomal RNA



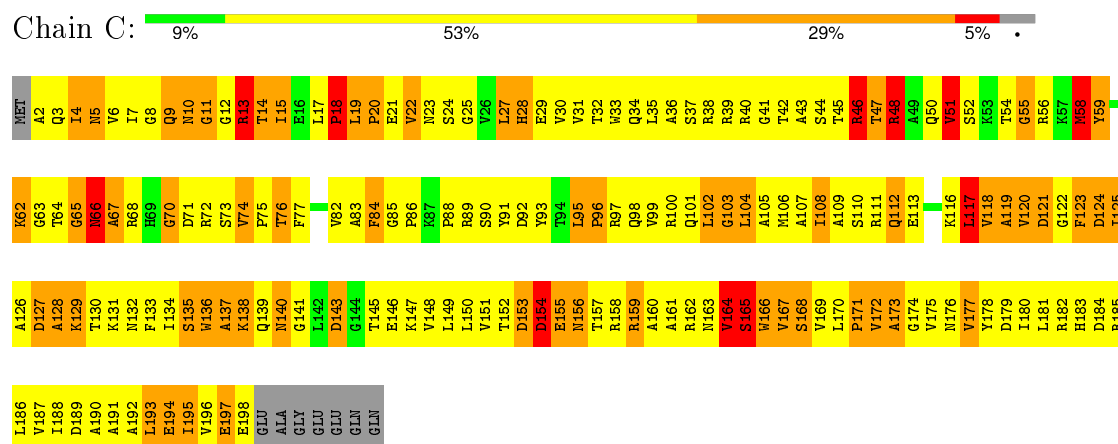
• Molecule 3: 50S ribosomal protein L2



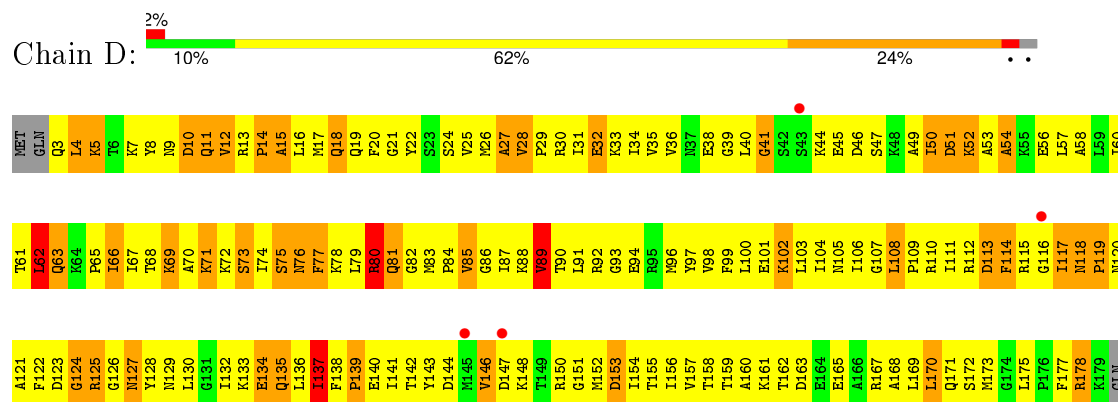
• Molecule 4: 50S ribosomal protein L3



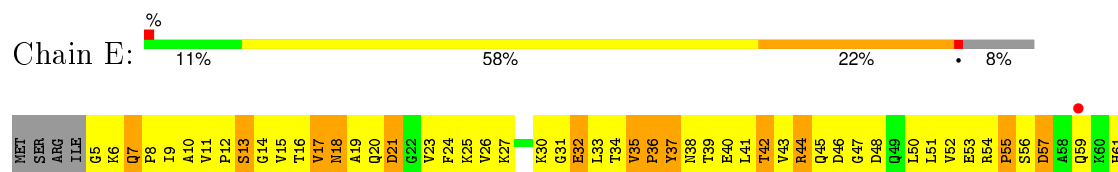
• Molecule 5: 50S ribosomal protein L4

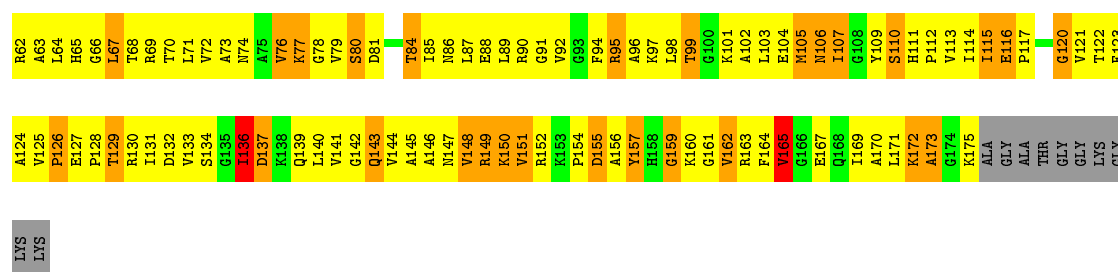


• Molecule 6: 50S ribosomal protein L5

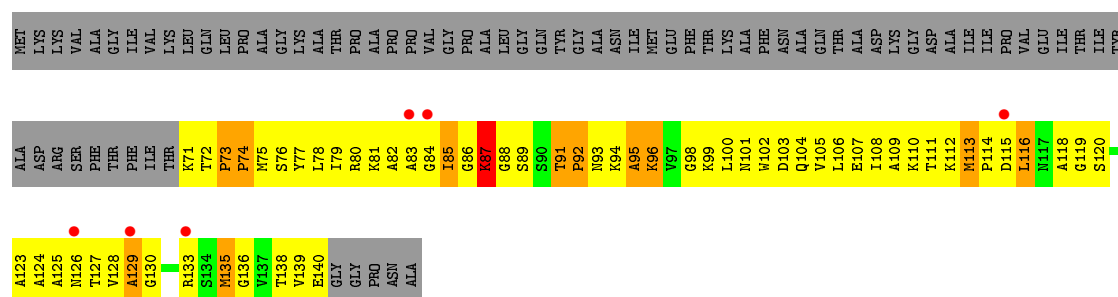
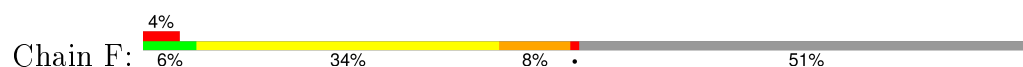


• Molecule 7: 50S ribosomal protein L6

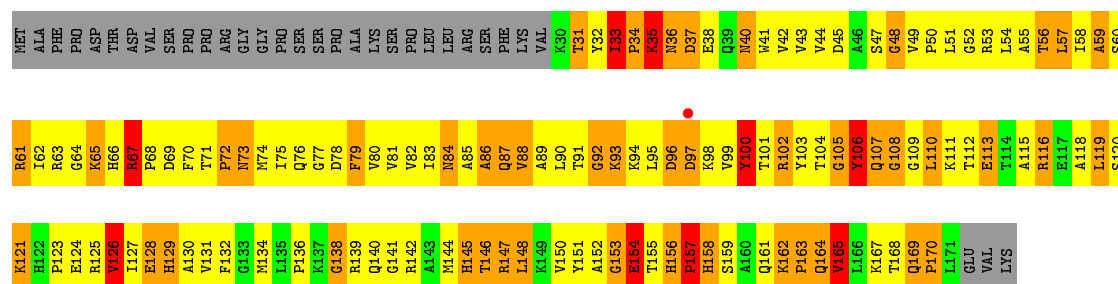




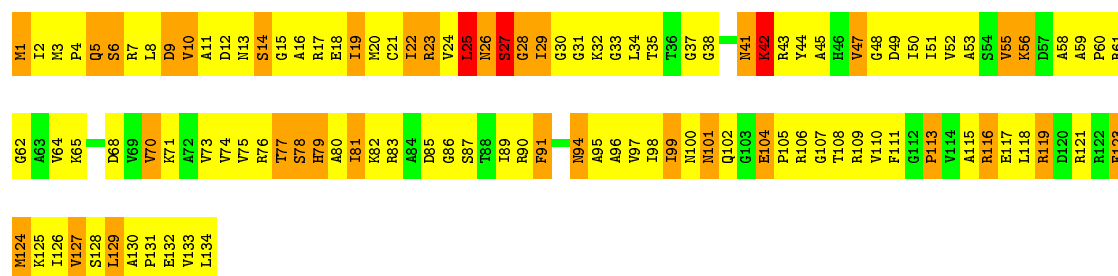
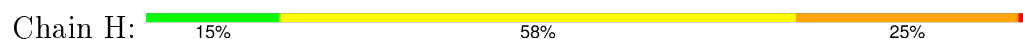
• Molecule 8: 50S ribosomal protein L11



• Molecule 9: 50S ribosomal protein L13

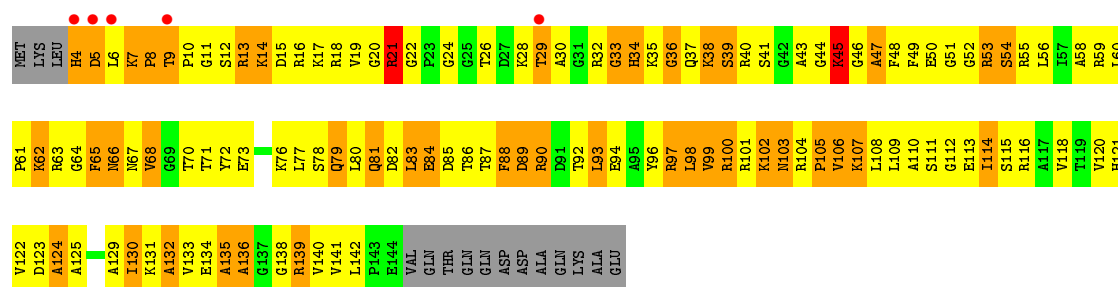


• Molecule 10: 50S ribosomal protein L14

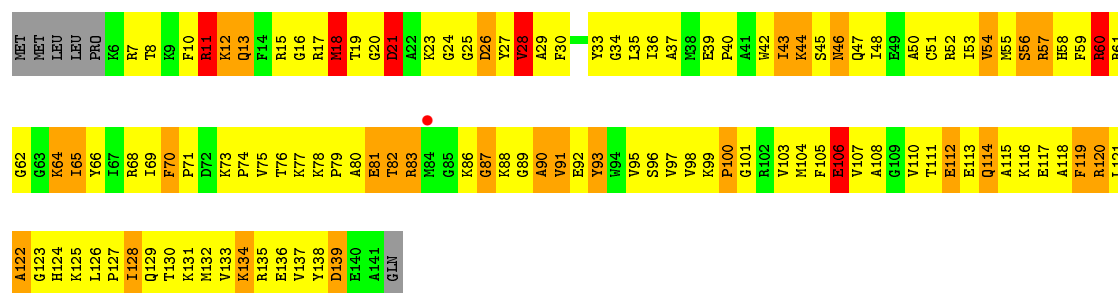
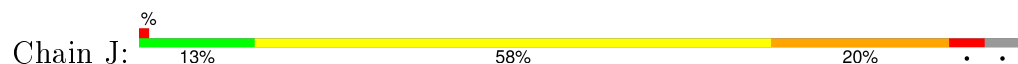


• Molecule 11: 50S ribosomal protein L15

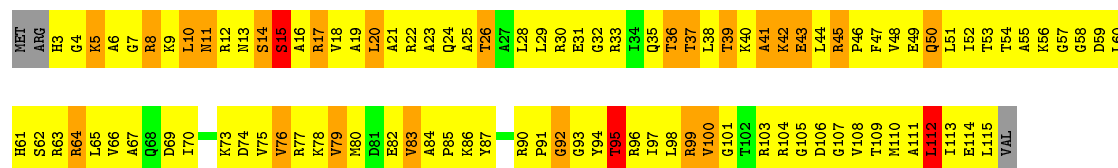
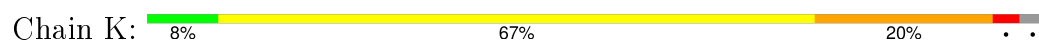




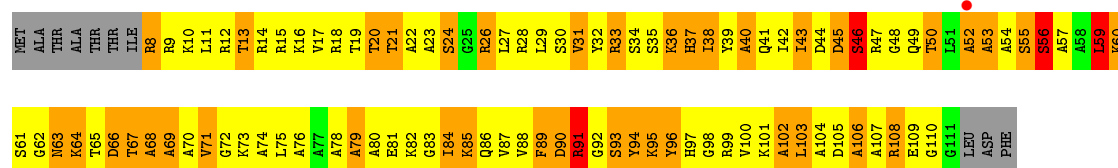
- Molecule 12: 50S ribosomal protein L16



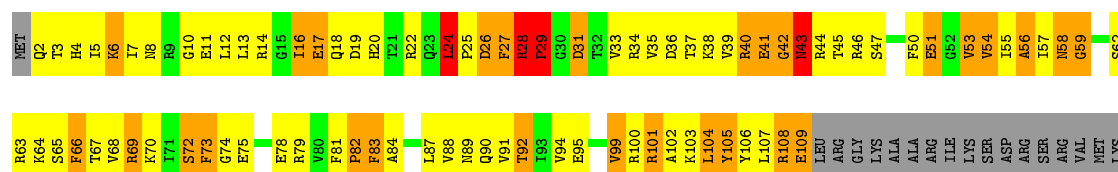
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



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

• Molecule 16: 50S ribosomal protein L20

Chain N: 9% 56% 31% . .

MET F2 R3 A4 ILE K5 T6 G7 I8 V9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

• Molecule 17: 50S ribosomal protein L21

Chain O: 11% 56% 25% . 6%

MET PHE ALA ILE I6 Q6 T7 G8 G9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 K32 K33 K34 K35 K36 K37 K38 K39 K40 K41 K42 K43 K44 K45 K46 K47 K48 K49 K50 K51 K52 K53 K54 K55 K56 K57 K58 K59 K60

• Molecule 18: 50S ribosomal protein L22

Chain P: 16% 63% 13% . 5%

MET THR PRO GLU THR F8 R9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 K32 K33 K34 K35 K36 K37 K38 K39 K40 K41 K42 K43 K44 K45 K46 K47 K48 K49 K50 K51 K52 K53 K54 K55 K56 K57 K58 K59 K60

• Molecule 19: 50S ribosomal protein L23

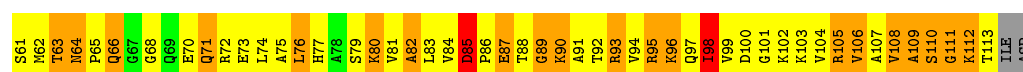
Chain Q: 9% 52% 33% . .

MET S2 R3 Y4 D5 I6 L7 F8 I9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

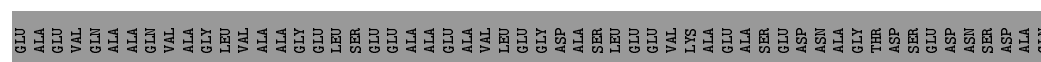
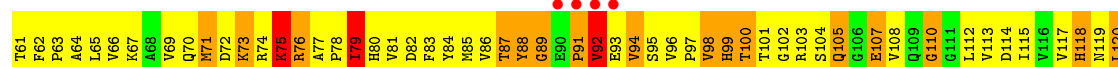
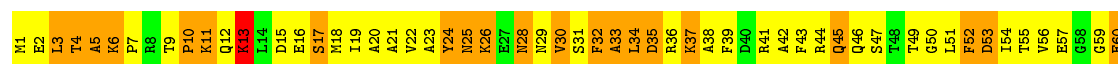
• Molecule 20: 50S ribosomal protein L24

Chain R: 5% 53% 32% 5% .

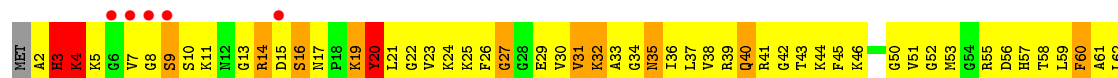
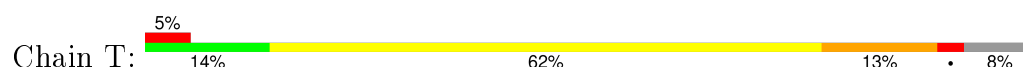
MET PRO ARG P4 S5 A6 G7 S8 H9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60



• Molecule 21: 50S ribosomal protein L25



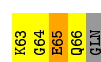
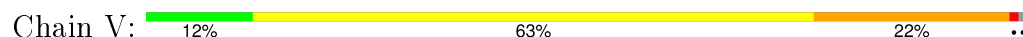
• Molecule 22: 50S ribosomal protein L27



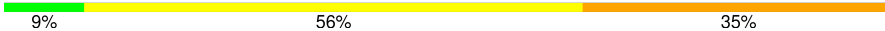
• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



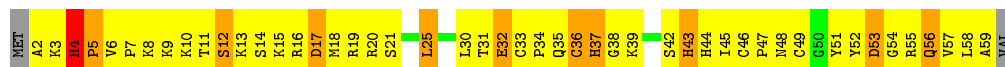
• Molecule 25: 50S ribosomal protein L30

Chain W: 



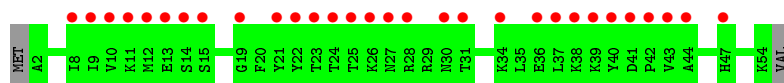
- Molecule 26: 50S ribosomal protein L32

Chain Y: 

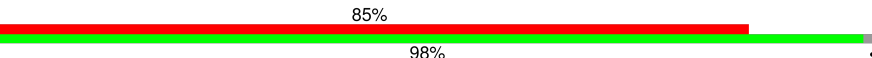


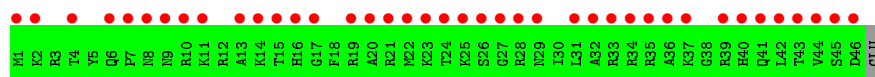
- Molecule 27: 50S ribosomal protein L33

Chain 1: 



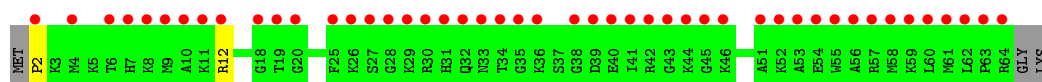
- Molecule 28: 50S ribosomal protein L34

Chain 2: 




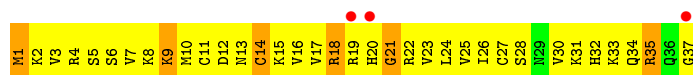
- Molecule 29: 50S ribosomal protein L35

Chain 3: 



- Molecule 30: 50S ribosomal protein L36

Chain 4: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.70Å 410.00Å 695.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 30.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.98-3.50) 85.7 (30.06-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.280 0.250 , 0.296	Depositor DCC
R_{free} test set	13552 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 38.0	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 308916 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	83657	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 ⓘ

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

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	0.83	19/64561 (0.0%)	0.93	192/100708 (0.2%)
2	Z	0.56	0/2904	0.78	0/4525
3	A	0.62	0/1669	0.95	1/2254 (0.0%)
4	B	0.76	0/1567	0.99	1/2105 (0.0%)
5	C	0.62	0/1529	0.92	1/2070 (0.0%)
6	D	0.50	0/1419	0.79	0/1903
7	E	0.49	0/1308	0.80	0/1771
8	F	0.51	0/510	0.82	0/688
9	G	0.62	0/1138	0.95	2/1539 (0.1%)
10	H	0.75	0/1007	0.99	2/1352 (0.1%)
11	I	0.66	1/1081 (0.1%)	0.98	0/1448
12	J	0.68	1/1113 (0.1%)	0.87	0/1486
13	K	0.90	0/886	1.07	1/1188 (0.1%)
14	L	0.53	0/785	0.84	0/1048
15	M	0.76	0/884	1.24	5/1186 (0.4%)
16	N	0.64	0/994	0.84	0/1323
17	O	0.60	0/750	0.92	1/1000 (0.1%)
18	P	0.76	0/1027	0.99	1/1373 (0.1%)
19	Q	0.62	0/737	0.93	2/988 (0.2%)
20	R	0.53	0/835	0.91	3/1121 (0.3%)
21	S	0.51	0/1370	0.82	0/1862
22	T	0.59	0/633	0.89	0/838
23	U	0.57	0/556	0.92	0/741
24	V	0.51	0/537	0.82	0/714
25	W	0.54	0/426	0.86	0/568
26	Y	0.71	0/469	1.01	0/629
30	4	0.48	0/298	0.77	0/390
All	All	0.78	21/90993 (0.0%)	0.92	212/136818 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	228
2	Z	0	4
9	G	0	1
17	O	0	1
All	All	0	234

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2594	U	P-OP2	17.32	1.78	1.49
1	X	2594	U	P-OP1	-13.28	1.26	1.49
1	X	2592	U	P-OP2	-12.20	1.28	1.49
1	X	28	A	C5-C6	-6.98	1.34	1.41
1	X	1333	G	N9-C4	-6.33	1.32	1.38

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	28	ARG	C-N-CD	-19.65	77.37	120.60
1	X	2594	U	O5'-P-OP2	-18.88	88.04	110.70
1	X	2592	U	O5'-P-OP2	-15.03	92.18	105.70
1	X	2592	U	N1-C1'-C2'	14.74	133.17	114.00
1	X	2592	U	C1'-O4'-C4'	-12.24	100.11	109.90

There are no chirality outliers.

5 of 234 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	10	A	Sidechain
1	X	24	G	Sidechain
1	X	25	U	Sidechain
1	X	34	U	Sidechain
1	X	98	U	Sidechain

5.2 Too-close contacts [i](#)

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	29049	4430	0
2	Z	2598	0	1328	213	0
3	A	1637	0	1673	471	0
4	B	1539	0	1600	358	0
5	C	1506	0	1525	400	0
6	D	1400	0	1481	437	0
7	E	1286	0	1336	330	0
8	F	504	0	530	125	0
9	G	1114	0	1144	371	0
10	H	997	0	1046	213	1
11	I	1067	0	1103	324	0
12	J	1090	0	1125	259	0
13	K	878	0	930	165	1
14	L	779	0	820	275	0
15	M	871	0	894	204	0
16	N	978	0	1020	288	0
17	O	741	0	756	242	0
18	P	1014	0	1096	191	0
19	Q	726	0	753	197	0
20	R	825	0	881	271	0
21	S	1345	0	1372	323	0
22	T	625	0	655	144	0
23	U	552	0	604	192	0
24	V	533	0	558	133	0
25	W	424	0	470	103	0
26	Y	457	0	462	86	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	329	83	0
31	4	1	0	0	0	0
31	Y	1	0	0	0	0
32	M	1	0	0	0	0
32	X	30	0	0	0	0
32	Z	4	0	0	0	0
33	X	24	0	19	22	0
All	All	83657	0	54559	9938	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 72.

The worst 5 of 9938 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:1281:A:H1'	1:X:2592:U:C5	1.68	1.26
1:X:2198:U:H3'	1:X:2199:C:C4'	1.66	1.24
1:X:2198:U:C3'	1:X:2199:C:H4'	1.68	1.23
1:X:1781:C:OP1	3:A:219:PRO:HB2	1.41	1.20
1:X:1281:A:C1'	1:X:2592:U:H5	1.55	1.20

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:107:GLY:O	13:K:86:LYS:NZ[8_555]	2.03	0.17

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	A	216/274 (79%)	109 (50%)	52 (24%)	55 (26%)	0	1
4	B	203/211 (96%)	124 (61%)	47 (23%)	32 (16%)	0	3
5	C	195/205 (95%)	92 (47%)	46 (24%)	57 (29%)	0	0
6	D	175/180 (97%)	78 (45%)	54 (31%)	43 (25%)	0	1
7	E	169/185 (91%)	91 (54%)	42 (25%)	36 (21%)	0	1
8	F	68/144 (47%)	37 (54%)	21 (31%)	10 (15%)	0	4
9	G	140/174 (80%)	66 (47%)	32 (23%)	42 (30%)	0	0
10	H	132/134 (98%)	91 (69%)	26 (20%)	15 (11%)	0	7
11	I	139/156 (89%)	51 (37%)	50 (36%)	38 (27%)	0	0
12	J	134/142 (94%)	63 (47%)	46 (34%)	25 (19%)	0	2
13	K	111/116 (96%)	61 (55%)	31 (28%)	19 (17%)	0	3
14	L	102/114 (90%)	48 (47%)	25 (24%)	29 (28%)	0	0
15	M	106/166 (64%)	68 (64%)	17 (16%)	21 (20%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	56 (49%)	30 (26%)	29 (25%)	0	1
17	O	92/100 (92%)	52 (56%)	19 (21%)	21 (23%)	0	1
18	P	125/134 (93%)	75 (60%)	35 (28%)	15 (12%)	0	6
19	Q	91/95 (96%)	44 (48%)	23 (25%)	24 (26%)	0	1
20	R	108/115 (94%)	63 (58%)	17 (16%)	28 (26%)	0	1
21	S	173/237 (73%)	97 (56%)	40 (23%)	36 (21%)	0	1
22	T	82/91 (90%)	51 (62%)	16 (20%)	15 (18%)	0	2
23	U	70/81 (86%)	39 (56%)	15 (21%)	16 (23%)	0	1
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0	1
25	W	53/55 (96%)	22 (42%)	18 (34%)	13 (24%)	0	1
26	Y	56/60 (93%)	31 (55%)	17 (30%)	8 (14%)	0	4
30	4	35/37 (95%)	22 (63%)	11 (31%)	2 (6%)	2	23
All	All	2954/3391 (87%)	1563 (53%)	749 (25%)	642 (22%)	0	1

5 of 642 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	58	HIS
3	A	66	ASP
3	A	91	ARG
3	A	98	ALA

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	164/215 (76%)	130 (79%)	34 (21%)	1	8
4	B	155/157 (99%)	132 (85%)	23 (15%)	4	22
5	C	157/163 (96%)	126 (80%)	31 (20%)	1	9
6	D	153/156 (98%)	139 (91%)	14 (9%)	11	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	136/144 (94%)	119 (88%)	17 (12%)	6	29
8	F	53/107 (50%)	48 (91%)	5 (9%)	11	44
9	G	118/146 (81%)	96 (81%)	22 (19%)	2	11
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	6
11	I	108/121 (89%)	91 (84%)	17 (16%)	3	19
12	J	110/116 (95%)	92 (84%)	18 (16%)	3	17
13	K	90/93 (97%)	71 (79%)	19 (21%)	1	8
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	4
15	M	94/134 (70%)	81 (86%)	13 (14%)	4	25
16	N	96/97 (99%)	80 (83%)	16 (17%)	3	16
17	O	75/79 (95%)	69 (92%)	6 (8%)	15	52
18	P	109/115 (95%)	92 (84%)	17 (16%)	3	20
19	Q	75/76 (99%)	62 (83%)	13 (17%)	2	14
20	R	91/96 (95%)	70 (77%)	21 (23%)	1	5
21	S	149/192 (78%)	123 (83%)	26 (17%)	2	14
22	T	62/67 (92%)	53 (86%)	9 (14%)	4	23
23	U	57/66 (86%)	46 (81%)	11 (19%)	2	10
24	V	54/55 (98%)	45 (83%)	9 (17%)	3	16
25	W	48/48 (100%)	41 (85%)	7 (15%)	4	22
26	Y	51/53 (96%)	45 (88%)	6 (12%)	6	31
30	4	35/35 (100%)	30 (86%)	5 (14%)	4	24
All	All	2417/2716 (89%)	2015 (83%)	402 (17%)	3	16

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	88	PHE
14	L	24	SER
23	U	61	TRP
12	J	10	PHE
13	K	5	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
11	I	121	HIS
15	M	48	GLN
24	V	36	GLN
12	J	13	GLN
14	L	86	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	678 (25%)	283 (10%)
2	Z	121/123 (98%)	24 (19%)	0
All	All	2801/3003 (93%)	702 (25%)	283 (10%)

5 of 702 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	14	A
1	X	27	G
1	X	34	U
1	X	35	G

5 of 283 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1314	A
1	X	1607	A
1	X	2633	A
1	X	1325	U
1	X	1409	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 38 ligands modelled in this entry, 37 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	$\# Z > 2$
33	ZLD	X	2911	-	26,26,26	1.22	2 (7%)	35,36,36	2.14	8 (22%)

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
33	ZLD	X	2911	-	-	2/13/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	2911	ZLD	C5-C16	2.05	1.41	1.37
33	X	2911	ZLD	O10-C7	3.39	1.40	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	X	2911	ZLD	C2-N4-C7	-5.48	119.25	125.80
33	X	2911	ZLD	O10-C7-N4	-5.28	106.55	109.97
33	X	2911	ZLD	C5-C16-C17	-4.20	119.97	123.39
33	X	2911	ZLD	F18-C16-C17	2.28	120.61	118.45
33	X	2911	ZLD	C5-C2-N4	2.36	122.59	119.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	X	2911	ZLD	C13-C12-N11-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	X	2911	ZLD	O14-C12-N11-C9

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	2911	ZLD	22	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 [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%)	-0.41	53 (1%) 68 59	1, 35, 97, 115	0
2	Z	122/123 (99%)	0.05	2 (1%) 74 65	28, 74, 94, 101	0
3	A	218/274 (79%)	-0.50	1 (0%) 91 88	8, 44, 57, 63	0
4	B	205/211 (97%)	-0.85	0 100 100	1, 12, 35, 53	0
5	C	197/205 (96%)	-0.52	0 100 100	2, 45, 62, 78	0
6	D	177/180 (98%)	-0.09	4 (2%) 64 54	54, 65, 73, 76	0
7	E	171/185 (92%)	-0.45	1 (0%) 90 85	38, 59, 72, 76	0
8	F	70/144 (48%)	0.72	6 (8%) 13 12	62, 71, 75, 76	0
9	G	142/174 (81%)	-0.59	1 (0%) 89 82	19, 37, 53, 57	0
10	H	134/134 (100%)	-0.87	0 100 100	1, 8, 30, 42	0
11	I	141/156 (90%)	-0.06	5 (3%) 48 38	10, 54, 69, 84	0
12	J	136/142 (95%)	-0.49	1 (0%) 89 82	25, 44, 59, 66	0
13	K	113/116 (97%)	-0.88	0 100 100	1, 2, 13, 23	0
14	L	104/114 (91%)	-0.24	1 (0%) 84 76	38, 54, 61, 67	0
15	M	108/166 (65%)	-0.92	0 100 100	1, 11, 40, 46	0
16	N	117/118 (99%)	-0.73	0 100 100	2, 33, 55, 64	0
17	O	94/100 (94%)	-0.66	0 100 100	13, 46, 63, 66	0
18	P	127/134 (94%)	-0.85	0 100 100	1, 10, 40, 57	0
19	Q	93/95 (97%)	-0.59	0 100 100	23, 36, 60, 63	0
20	R	110/115 (95%)	-0.52	0 100 100	32, 44, 66, 70	0
21	S	175/237 (73%)	-0.10	5 (2%) 55 45	53, 62, 72, 79	0
22	T	84/91 (92%)	-0.01	5 (5%) 25 19	23, 47, 66, 69	0
23	U	72/81 (88%)	-0.34	0 100 100	39, 52, 63, 64	0
24	V	66/67 (98%)	-0.72	0 100 100	34, 52, 72, 76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.64	0	100	32, 41, 57, 66	0
26	Y	58/60 (96%)	-0.78	0	100	1, 7, 32, 34	0
27	1	53/55 (96%)	2.49	30 (56%)	0	33, 47, 62, 65	0
28	2	46/47 (97%)	3.35	40 (86%)	0	1, 12, 25, 35	0
29	3	63/66 (95%)	3.43	47 (74%)	0	23, 34, 43, 50	0
30	4	37/37 (100%)	0.51	3 (8%)	15	52, 65, 72, 73	0
All	All	5974/6562 (91%)	-0.34	205 (3%)	49	1, 41, 84, 115	0

The worst 5 of 205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	34	THR	8.7
29	3	33	ASN	8.7
27	1	40	TYR	8.4
29	3	39	ASP	7.9
29	3	32	GLN	7.3

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	X	2907	1/1	0.97	0.62	47.58	1,1,1,1	0
32	MG	X	2899	1/1	0.99	0.53	45.13	1,1,1,1	0
32	MG	M	167	1/1	0.98	0.55	19.63	1,1,1,1	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	X	2889	1/1	0.95	0.43	12.66	1,1,1,1	0
32	MG	X	2909	1/1	0.98	0.36	12.09	1,1,1,1	0
32	MG	X	2903	1/1	0.93	0.31	11.39	1,1,1,1	0
33	ZLD	X	2911	24/24	0.90	0.48	8.50	28,31,37,37	0
32	MG	X	2896	1/1	0.99	0.28	5.66	1,1,1,1	0
32	MG	X	2885	1/1	0.88	0.21	2.47	45,45,45,45	0
32	MG	X	2883	1/1	0.97	0.19	1.61	1,1,1,1	0
31	ZN	Y	61	1/1	0.98	0.13	-0.27	89,89,89,89	0
31	ZN	4	38	1/1	0.98	0.03	-1.94	78,78,78,78	0
32	MG	X	2887	1/1	0.96	0.17	-	37,37,37,37	0
32	MG	X	2888	1/1	0.99	0.38	-	1,1,1,1	0
32	MG	Z	125	1/1	0.98	0.17	-	1,1,1,1	0
32	MG	X	2884	1/1	0.97	0.23	-	19,19,19,19	0
32	MG	X	2900	1/1	0.92	0.52	-	1,1,1,1	0
32	MG	X	2901	1/1	0.98	0.35	-	1,1,1,1	0
32	MG	X	2895	1/1	0.98	0.31	-	1,1,1,1	0
32	MG	Z	127	1/1	0.97	0.20	-	3,3,3,3	0
32	MG	X	2893	1/1	0.95	0.20	-	3,3,3,3	0
32	MG	X	2902	1/1	0.97	0.80	-	61,61,61,61	0
32	MG	X	2881	1/1	0.95	0.50	-	10,10,10,10	0
32	MG	X	2886	1/1	0.96	0.25	-	15,15,15,15	0
32	MG	X	2905	1/1	0.96	0.36	-	18,18,18,18	0
32	MG	X	2882	1/1	0.96	0.38	-	49,49,49,49	0
32	MG	Z	126	1/1	0.95	0.13	-	12,12,12,12	0
32	MG	X	2892	1/1	0.98	0.19	-	1,1,1,1	0
32	MG	X	2897	1/1	0.90	0.27	-	1,1,1,1	0
32	MG	X	2908	1/1	0.96	0.46	-	48,48,48,48	0
32	MG	Z	124	1/1	0.90	0.19	-	11,11,11,11	0
32	MG	X	2891	1/1	0.94	0.11	-	23,23,23,23	0
32	MG	X	2904	1/1	0.94	0.40	-	1,1,1,1	0
32	MG	X	2906	1/1	0.99	0.09	-	40,40,40,40	0
32	MG	X	2890	1/1	0.95	0.65	-	1,1,1,1	0
32	MG	X	2910	1/1	0.94	0.26	-	14,14,14,14	0
32	MG	X	2898	1/1	0.97	0.40	-	1,1,1,1	0
32	MG	X	2894	1/1	0.94	0.36	-	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.