



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:18 am BST

PDB ID : 2ZJR  
Title : Refined native structure of the large ribosomal subunit (50S) from *Deinococcus radiodurans*  
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 : 2.91 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

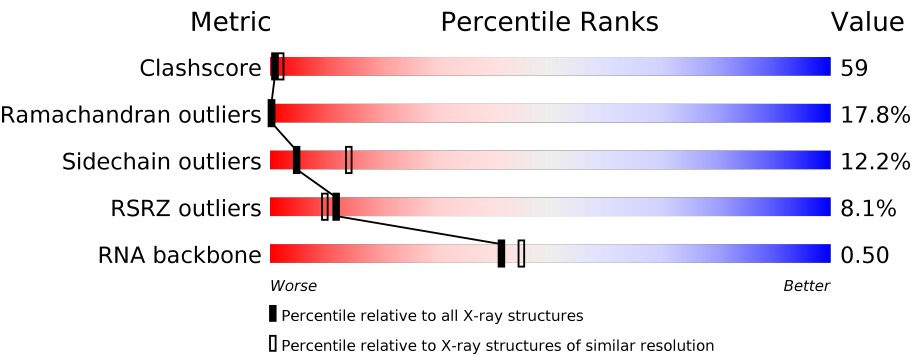
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)
RNA backbone	3102	1001 (3.18-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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>4%</div><div>16%46%20%10%7%</div></div>
2	Y	123	<div><div>2%</div><div>23%59%15%</div></div>
3	A	274	<div><div>7%</div><div>16%54%16%12%</div></div>
4	B	211	<div><div></div><div>29%52%12%</div></div>
5	C	205	<div><div>5%</div><div>11%56%25%</div></div>
6	D	180	<div><div>7%</div><div>11%69%16%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	2884	-	-	-	X
31	MG	X	2908	-	-	-	X
31	MG	Y	124	-	-	-	X

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 83819 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	71	Total	C	N	O	S	0	0	0
			503	310	91	99	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		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	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

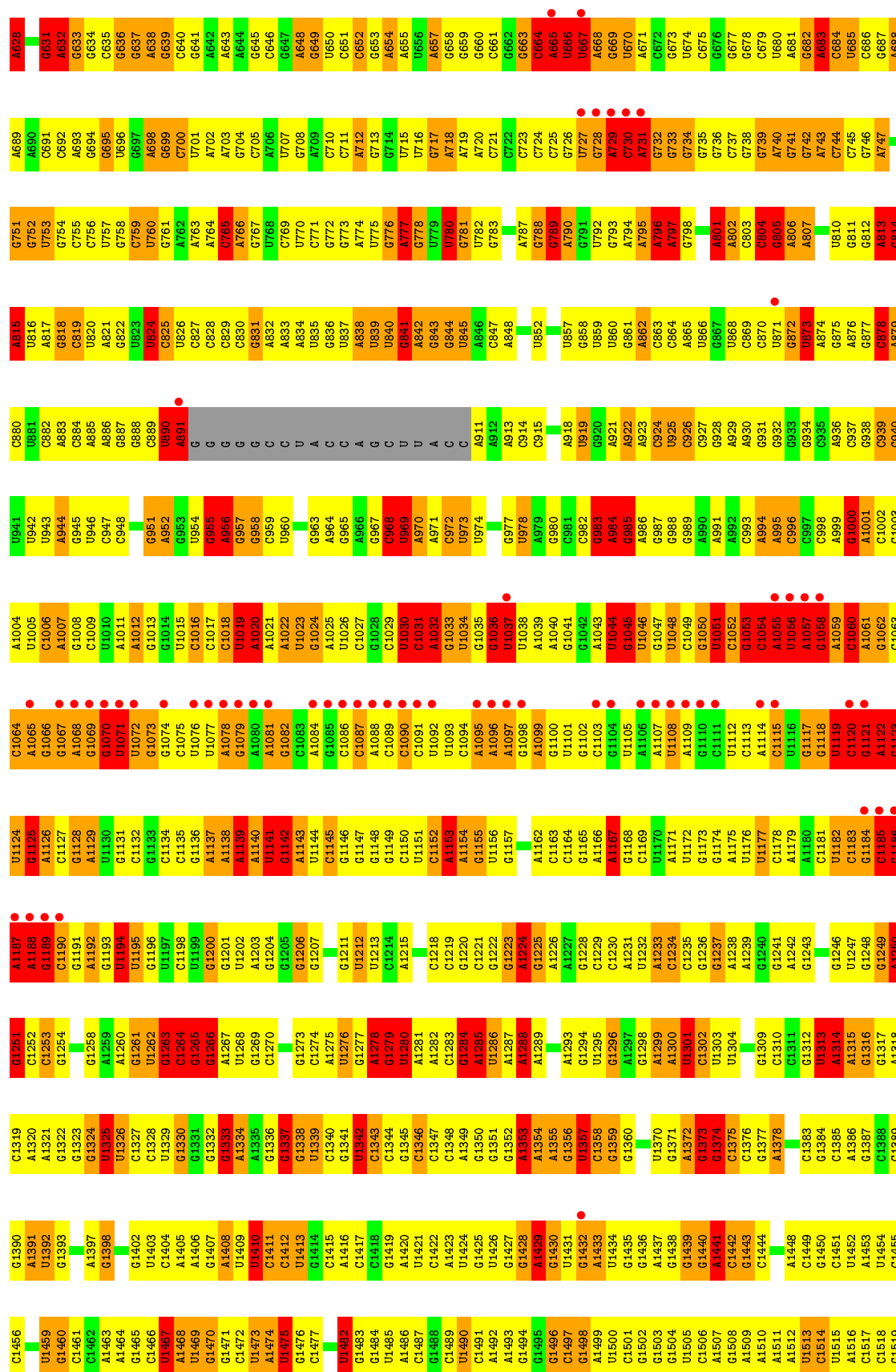
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

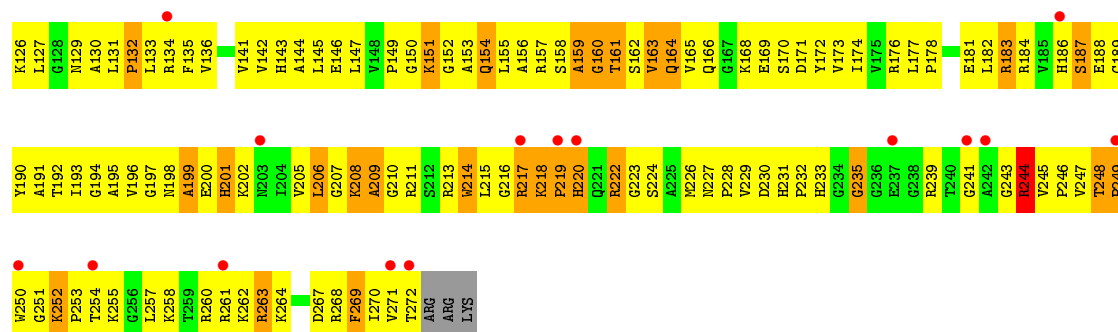
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0





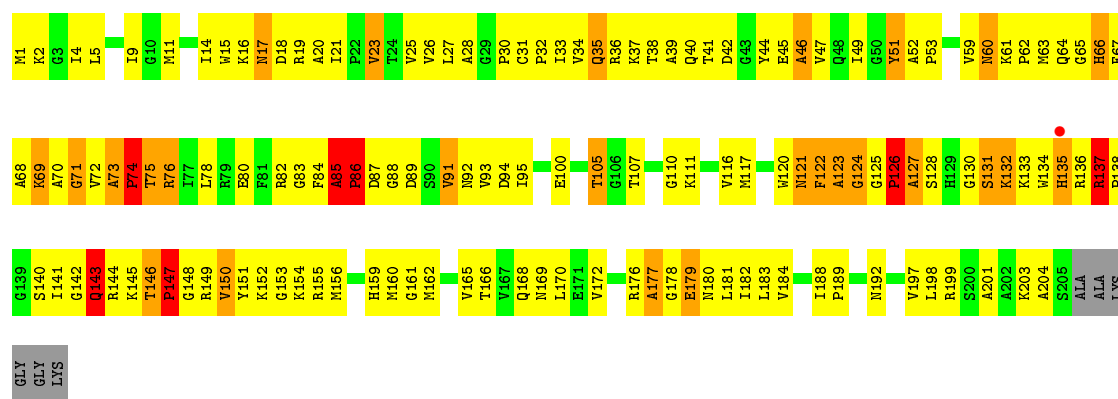
U2342	A2278	G2217	C	G2035	G1975	A1910	G1849	A1785	A1718	C1655	A1585	G1520
C2343	G2279	G2218	C	G2036	U1976	A1911	G1850	C1786	G1719	U1656	A1586	U1521
G2344	U2219	U2219	C	A2037	C1977	G1912	A1851	U1787	G1722	A1657	A1587	A1522
A2345	C2281	C2220	C	C2038	U1978	G1913	G1852	C1788	U1723	G1658	A1588	A1523
G2350	G2282	G2221	C	G2039	A1980	U1914	G1853	G1790	U1724	G1659	A1589	A1524
G2351	U2223	U2222	C	A2040	C1979	A1915	G1854	G1791	C1725	G1660	A1590	A1525
A2352	U2284	U2224	U	A2041	A1981	G1916	G1855	C1792	C1726	C1661	U1594	U1526
G2353	G2285	G2225	G	A2042	C1982	C1917	U1856	A1793	G1727	G1662	A1595	G1527
G2354	G2286	G2226	U	A2043	G1983	G1918	G1857	C1795	A1728	G1663	A1596	U1528
G2355	G2287	A2227	G	G2044	A1984	A1919	A1858	A1794	C1729	G1664	A1597	U1529
G2356	A2288	C2227	G	A2045	G1985	A1920	A1859	A1795	C1730	G1665	C1598	U1530
A2357	G2289	U2228	A	C2046	G1986	A1921	A1860	A1796	G1731	G1666	C1599	G1531
A2358	A2290	G2229	G	C2047	G1987	U1922	G1861	A1800	A1667	A1667	A1600	A1532
C2359	U2291	G2230	G	C2048	A1988	U1923	C1862	C1801	U1732	G1668	U1601	G1533
C2360	G2292	G2231	C	C2049	C1989	C1924	U1863	A1802	C1733	A1669	A1602	G1536
G2361	G2293	G2232	C	G2050	U1990	C1925	G1864	G1803	C1734	G1670	A1603	U1537
G2362	U2294	G2233	U	U2051	C1991	U1926	C1865	U1804	G1735	A1671	A1538	U1538
G2363	G2297	G2234	G	G2052	G1992	U1927	G1866	G1805	C1736	A1672	U1539	U1539
G2364	U2298	G2235	C	G2053	G1993	G1928	A1867	A1806	G1737	C1673	C1606	A1540
G2365	U2299	U2236	C	A2054	U1994	U1929	A1868	A1807	U1738	C1674	A1607	U1541
U2366	G2300	G2237	A	G2055	G1995	U1930	A1869	C1808	G1741	C1675	U1608	U1542
A2367	G2301	U2178	A	C2056	A1996	G1933	G1871	G1810	G1742	U1676	G1609	G1543
G2368	A2301	C2179	A	U2057	A1997	A1872	A1873	A1811	C1743	G1677	A1610	U1611
G2369	G2302	U2180	C	U2058	A1998	U1935	G1874	A1812	G1744	U1678	U1612	A1544
G2370	G2303	A2181	U	G2060	U1999	A1936	G1875	A1813	C1745	U1680	G1613	U1547
A2371	G2304	A2182	G	C2061	G2001	G1937	C1876	G1814	A1746	A1681	G1614	U1548
A2372	G2305	C2183	G	U2062	A2002	U1938	C1877	G1815	C1747	A1682	C1615	U1549
C2373	A2306	C2184	C	G2063	U2003	A1940	C1878	G1816	U1748	G1683	U1618	U1550
A2374	A2307	U2185	U	U2064	U2004	C1940	G1885	A1817	G1749	A1684	A1619	U1551
G2375	A2308	G2186	C	A2065	U2005	U1949	G1886	G1824	C1757	A1685	C1620	C1552
G2376	A2309	A2187	U	U2066	U2006	C1950	G1887	U1825	G1762	A1686	G1621	G1553
G2377	G2310	A2188	U	U2067	G2007	G1951	C1888	U1826	C1763	C1687	C1622	U1554
G2378	U2311	A2189	U	C2068	G2008	U1952	G	U1827	A1763	U1693	C1627	A1560
G2379	G2312	A2190	G	U2069	C2009	A1953	G	C1830	C1764	U1697	C1628	A1561
U2380	G2313	A2191	G	G2070	U2010	A1954	C	G1831	C1765	C1698	G1629	U1562
A2381	A2314	U2192	G	G2071	U2011	G1955	C	G1832	U1766	A1699	A1630	U1563
A2382	G2253	U2193	G	C2072	U2012	G1956	U	U1833	G1767	C1700	A1631	U1564
A2383	G2254	A2194	U	A2073	A2013	C1957	G	U1834	G1770	C1701	C1632	A1569
G2384	G2255	C2195	C	U2074	A2014	A1958	A	G1835	A1771	G1704	C1633	C1570
U2385	G2256	U2196	C	U2075	G2015	A1959	C	C1836	C1772	U1705	G1635	G1571
G2386	A2257	U2197	U	G2076	A2016	G1956	U	C1837	C1773	A1706	G1636	G1572
G2387	G2258	U2198	U	U2077	U2017	G1957	A	G1838	A1774	A1707	U1637	A1574
G2388	G2259	C2199	G	A2079	G2018	C1958	U	A1839	A1775	C1708	G1642	C1575
G2389	C2260	G2200	G	U2080	C2019	G1959	U	A1840	A1776	U1709	A1643	C1576
G2390	G2261	G2201	A	U2081	G2020	U1960	A	G1841	A1777	U1710	G1644	U1577
G2391	C2262	G2202	G	C2082	G2021	U1961	C	C1842	U1778	C1711	U1645	G1578
G2392	C2263	G2203	C	G2083	C2022	G1962	C	G1843	C1779	G1712	G1579	U1579
G2393	A2264	A2204	C	G2084	C2023	G1963	U	U1844	A1774	G1713	C1580	C1581
C2394	A2265	C2205	A	A2085	C2024	U1964	U	C1845	A1775	A1714	G1648	A1582
C2395	A2266	C2206	C	U2086	A2025	U1965	A	A1846	A1776	A1715	U1651	A1583
C2396	A2267	G2207	C	U2087	C2026	G1966	U	G1847	A1777	G1716	G1652	U1584
A2397	G2268	U2208	G	C2088	C2027	U1967	A	U1848	U1778	C1717	A1653	
U2398	G2269	C2209	G	C2089	C2028	U1968	C	G1849	U1779	A1718	A1654	
G2399	U2270	G2210	U	U2090	G2029	G1969	G	C1850	A1780	G1719	C1585	
G2400	C2271	U2211	G	U2091	U2030	C1971	U	A1845	A1781	A1714	A1655	
U2401	A2272	U2212	A	C	A2031	G1972	C	A1846	A1782	A1715	A1656	
U2402	C2273	G2213	A	U	G2032	C1973	C	G1847	C1783	G1716	A1583	
U2403	C2274	G2214	U	C	C2033	U1974	C	U1848	C1784	A1717	G1584	
U2404	U2275	G2215	A	U	A2034							
C2405	G2276	G2216	A	U								
G2407	A2277											





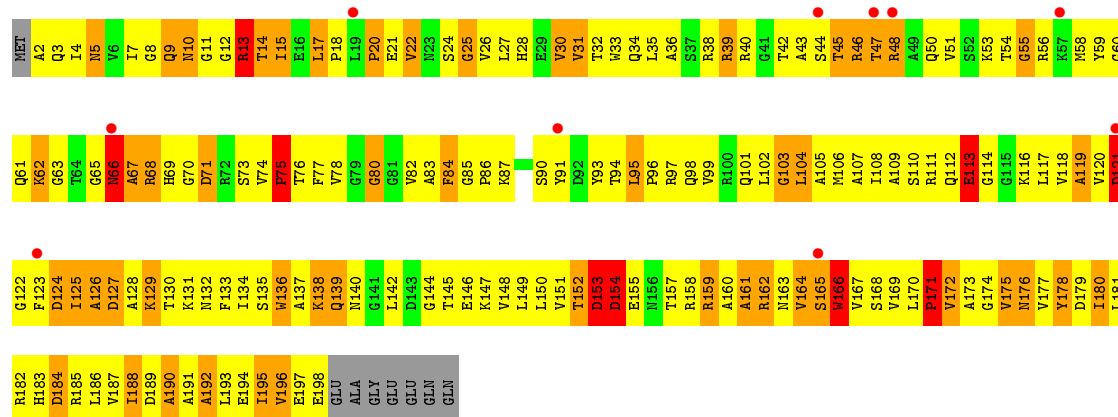
• Molecule 4: 50S ribosomal protein L3

Chain B: 29% 52% 12% . .



• Molecule 5: 50S ribosomal protein L4

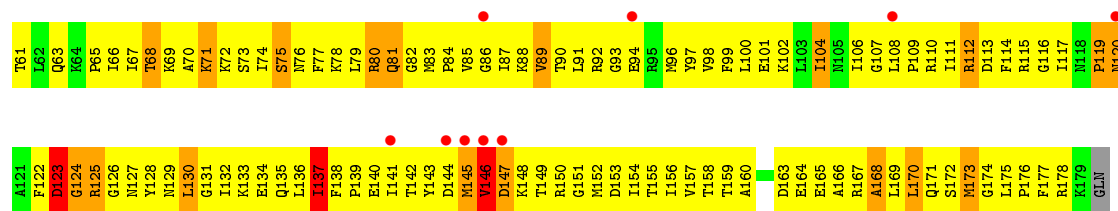
Chain C: 5% 11% 56% 25% . .



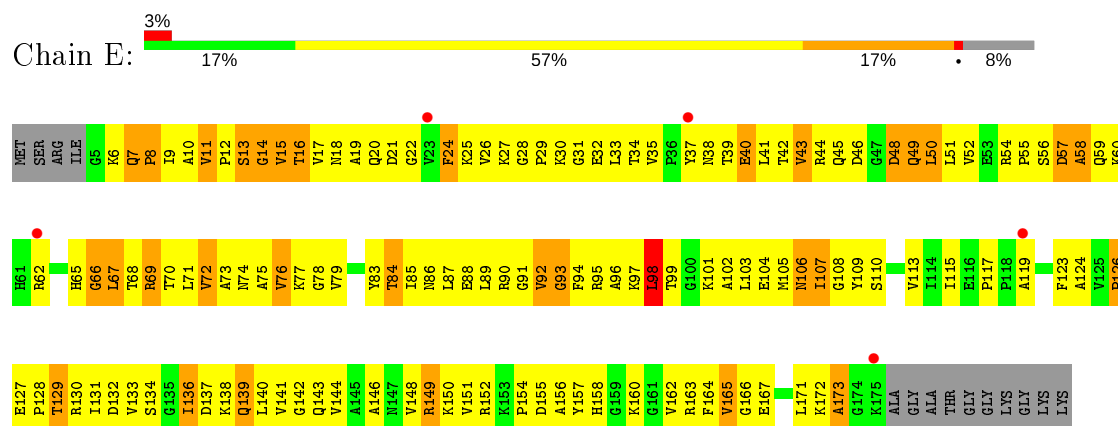
• Molecule 6: 50S ribosomal protein L5

Chain D: 7% 11% 69% 16% . .

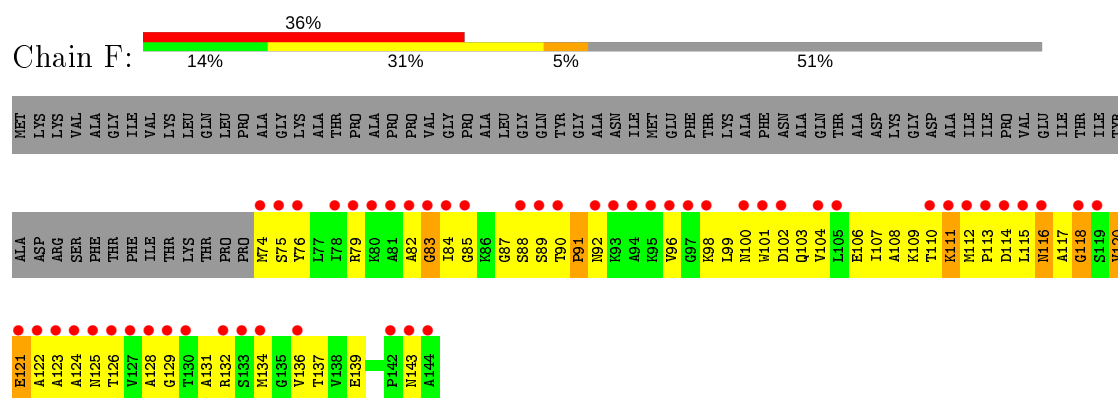




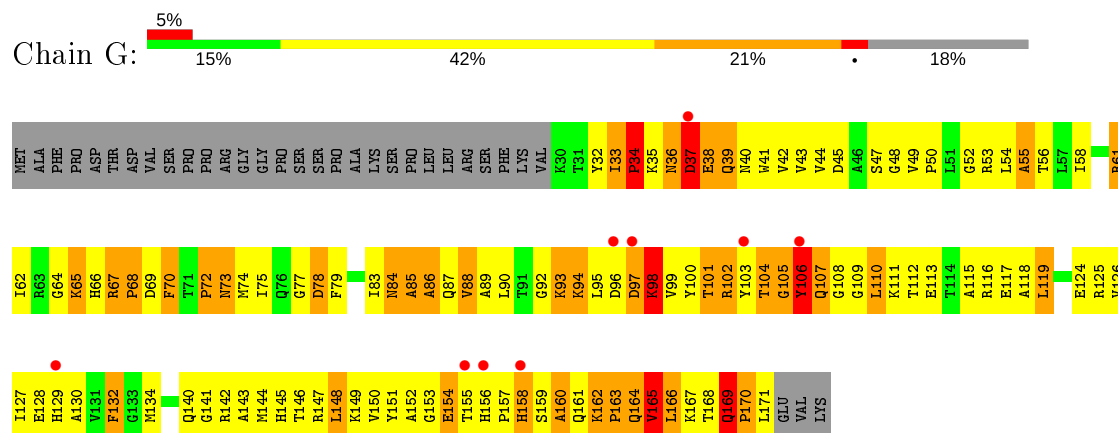
• Molecule 7: 50S ribosomal protein L6



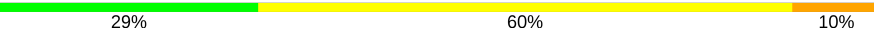
• Molecule 8: 50S ribosomal protein L11

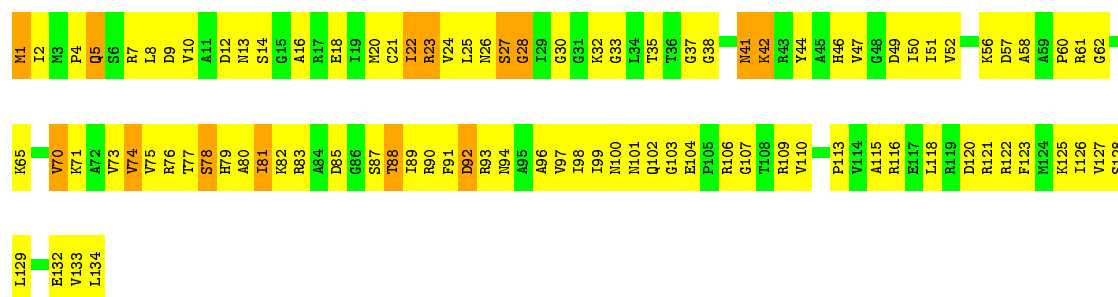


• Molecule 9: 50S ribosomal protein L13




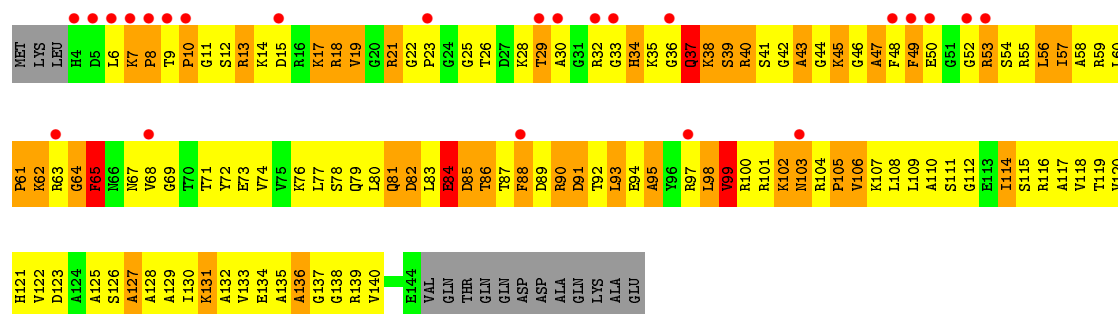
• Molecule 10: 50S ribosomal protein L14

Chain H: 



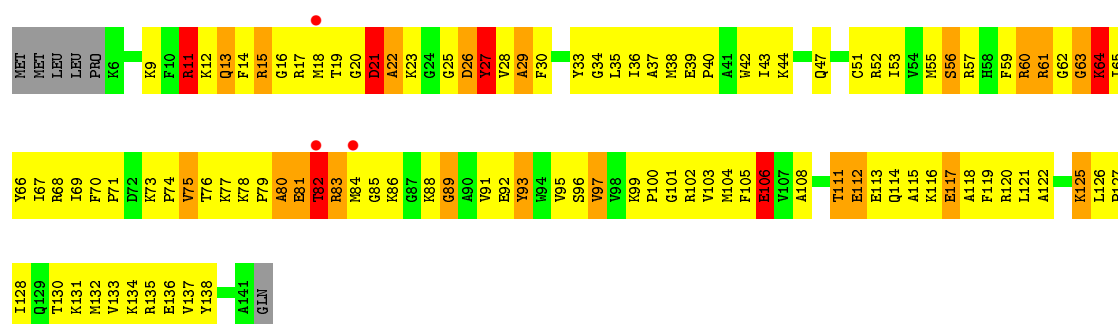
• Molecule 11: 50S ribosomal protein L15

Chain I: 



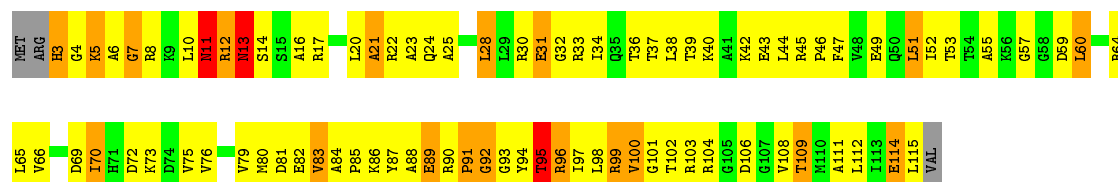
• Molecule 12: 50S ribosomal protein L16

Chain J: 



• Molecule 13: 50S ribosomal protein L17

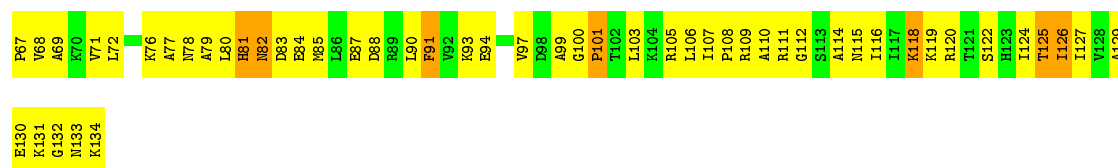
Chain K: 



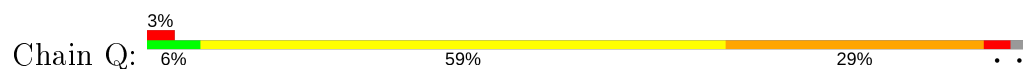
• Molecule 14: 50S ribosomal protein L18



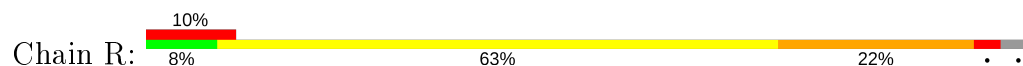




• Molecule 19: 50S ribosomal protein L23



• Molecule 20: 50S ribosomal protein L24

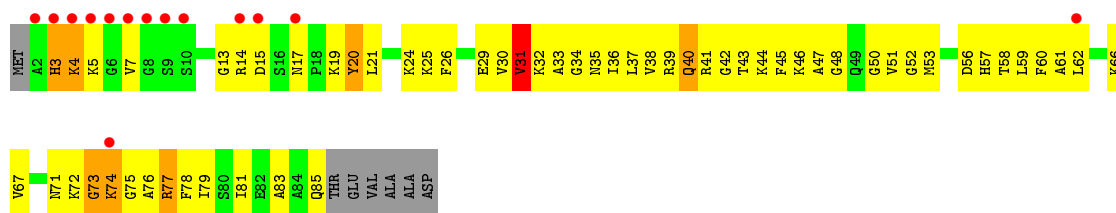


• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27

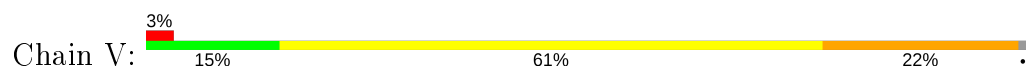




• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



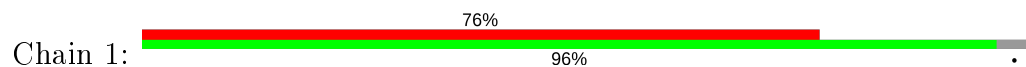
• Molecule 25: 50S ribosomal protein L30



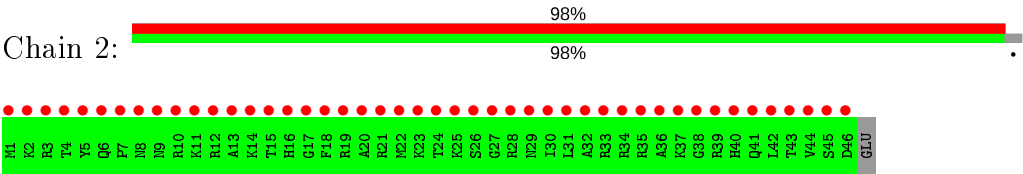
• Molecule 26: 50S ribosomal protein L32



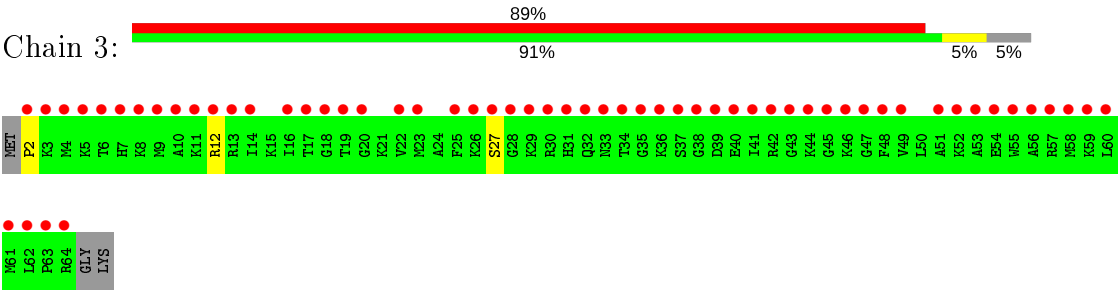
• Molecule 27: 50S ribosomal protein L33



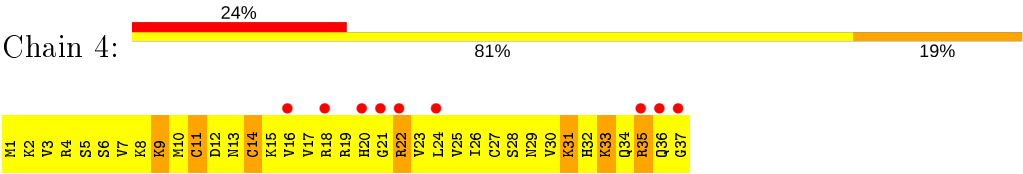
• Molecule 28: 50S ribosomal protein L34



• Molecule 29: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90 Å   408.90 Å   694.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.90 – 2.91 29.92 – 2.91	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.90-2.91) 94.1 (29.92-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.90 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.277   ,   0.311 0.265   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	83819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.90	156/64561 (0.2%)	1.15	809/100708 (0.8%)
2	Y	0.50	0/2904	0.73	0/4525
3	A	0.50	0/1862	0.82	0/2510
4	B	0.70	0/1567	0.99	6/2105 (0.3%)
5	C	0.60	0/1529	0.87	0/2070
6	D	0.47	0/1419	0.70	0/1903
7	E	0.46	0/1308	0.76	0/1771
8	F	0.65	0/508	1.11	2/683 (0.3%)
9	G	0.59	0/1138	0.92	2/1539 (0.1%)
10	H	0.72	0/1007	0.93	1/1352 (0.1%)
11	I	0.60	0/1081	0.89	0/1448
12	J	0.59	0/1113	0.86	1/1486 (0.1%)
13	K	0.83	0/886	1.04	1/1188 (0.1%)
14	L	0.48	0/785	0.82	1/1048 (0.1%)
15	M	0.72	0/884	1.15	6/1186 (0.5%)
16	N	0.54	0/994	0.80	0/1323
17	O	0.54	0/750	0.83	0/1000
18	P	0.73	0/1027	0.90	0/1373
19	Q	0.58	0/737	0.88	3/988 (0.3%)
20	R	0.48	0/835	0.84	0/1121
21	S	0.48	0/1370	0.71	0/1862
22	T	0.52	0/633	0.77	0/838
23	U	0.51	0/556	0.87	0/741
24	V	0.44	0/537	0.67	0/714
25	W	0.51	0/426	0.83	0/568
26	Z	0.68	0/469	0.95	1/629 (0.2%)
30	4	0.45	0/298	0.65	0/390
All	All	0.82	156/91184 (0.2%)	1.08	833/137069 (0.6%)

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	225
2	Y	0	4
9	G	0	1
16	N	0	1
19	Q	0	1
All	All	0	232

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1123	G	C3'-O3'	14.43	1.62	1.42
1	X	1123	G	C4'-C3'	13.55	1.68	1.53
1	X	2322	U	C3'-O3'	12.22	1.59	1.42
1	X	1187	A	C2'-C1'	11.44	1.66	1.53
1	X	100	G	C3'-O3'	10.61	1.57	1.42

The worst 5 of 833 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1055	A	N9-C1'-C2'	-29.46	75.70	114.00
1	X	513	A	N9-C1'-C2'	24.54	145.90	114.00
1	X	2297	G	N9-C1'-C2'	21.75	142.27	114.00
1	X	557	U	N1-C1'-C2'	19.63	139.52	114.00
1	X	2298	U	N1-C1'-C2'	19.50	139.35	114.00

There are no chirality outliers.

5 of 232 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	13	A	Sidechain
1	X	15	G	Sidechain
1	X	32	C	Sidechain
1	X	34	U	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	29047	3656	0
2	Y	2598	0	1328	160	0
3	A	1826	0	1885	387	0
4	B	1539	0	1600	265	0
5	C	1506	0	1525	369	0
6	D	1400	0	1481	377	0
7	E	1286	0	1336	242	0
8	F	503	0	520	94	0
9	G	1114	0	1144	264	0
10	H	997	0	1046	152	0
11	I	1067	0	1103	273	0
12	J	1090	0	1125	254	0
13	K	878	0	930	120	0
14	L	779	0	820	236	0
15	M	871	0	894	198	0
16	N	978	0	1020	216	0
17	O	741	0	756	192	0
18	P	1014	0	1096	152	0
19	Q	726	0	753	183	0
20	R	825	0	881	263	0
21	S	1345	0	1372	294	0
22	T	625	0	655	97	0
23	U	552	0	604	201	0
24	V	533	0	558	107	0
25	W	424	0	470	67	0
26	Z	457	0	464	67	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	3	0
30	4	297	0	330	68	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
All	All	83819	0	54743	8176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

The worst 5 of 8176 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:135:U:H2'	1:X:136:A:C8	1.59	1.37
1:X:2195:C:C5	1:X:2196:U:C5	2.22	1.28
1:X:623:G:N2	1:X:626:A:C2	2.01	1.26
1:X:1053:G:H2'	1:X:1054:C:C6	1.71	1.25
1:X:333:A:H3'	5:C:162:ARG:NH2	1.49	1.24

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	A	238/274 (87%)	147 (62%)	53 (22%)	38 (16%)	0	0
4	B	203/211 (96%)	147 (72%)	31 (15%)	25 (12%)	0	1
5	C	195/205 (95%)	99 (51%)	48 (25%)	48 (25%)	0	0
6	D	175/180 (97%)	91 (52%)	59 (34%)	25 (14%)	0	0
7	E	169/185 (91%)	100 (59%)	39 (23%)	30 (18%)	0	0
8	F	69/144 (48%)	45 (65%)	19 (28%)	5 (7%)	1	2
9	G	140/174 (80%)	80 (57%)	28 (20%)	32 (23%)	0	0
10	H	132/134 (98%)	114 (86%)	11 (8%)	7 (5%)	2	5
11	I	139/156 (89%)	62 (45%)	33 (24%)	44 (32%)	0	0
12	J	134/142 (94%)	74 (55%)	36 (27%)	24 (18%)	0	0
13	K	111/116 (96%)	85 (77%)	12 (11%)	14 (13%)	0	0
14	L	102/114 (90%)	55 (54%)	22 (22%)	25 (24%)	0	0
15	M	106/166 (64%)	71 (67%)	21 (20%)	14 (13%)	0	0
16	N	115/118 (98%)	72 (63%)	25 (22%)	18 (16%)	0	0
17	O	92/100 (92%)	57 (62%)	16 (17%)	19 (21%)	0	0
18	P	125/134 (93%)	94 (75%)	20 (16%)	11 (9%)	1	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	44 (48%)	23 (25%)	24 (26%)	0	0
20	R	108/115 (94%)	60 (56%)	24 (22%)	24 (22%)	0	0
21	S	173/237 (73%)	94 (54%)	40 (23%)	39 (22%)	0	0
22	T	82/91 (90%)	48 (58%)	20 (24%)	14 (17%)	0	0
23	U	70/81 (86%)	35 (50%)	18 (26%)	17 (24%)	0	0
24	V	64/67 (96%)	32 (50%)	20 (31%)	12 (19%)	0	0
25	W	53/55 (96%)	42 (79%)	6 (11%)	5 (9%)	0	1
26	Z	56/60 (93%)	41 (73%)	7 (12%)	8 (14%)	0	0
30	4	35/37 (95%)	17 (49%)	9 (26%)	9 (26%)	0	0
All	All	2977/3391 (88%)	1806 (61%)	640 (22%)	531 (18%)	0	0

5 of 531 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	187	SER
3	A	209	ALA
3	A	217	ARG
3	A	220	HIS

### 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%)	167 (90%)	18 (10%)	8	24
4	B	155/157 (99%)	139 (90%)	16 (10%)	7	21
5	C	157/163 (96%)	132 (84%)	25 (16%)	2	7
6	D	153/156 (98%)	136 (89%)	17 (11%)	6	18
7	E	136/144 (94%)	124 (91%)	12 (9%)	10	28
8	F	51/107 (48%)	49 (96%)	2 (4%)	32	64
9	G	118/146 (81%)	101 (86%)	17 (14%)	3	9

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	103/103 (100%)	93 (90%)	10 (10%)	8	24
11	I	108/121 (89%)	91 (84%)	17 (16%)	2	7
12	J	110/116 (95%)	97 (88%)	13 (12%)	5	15
13	K	90/93 (97%)	73 (81%)	17 (19%)	1	4
14	L	74/82 (90%)	57 (77%)	17 (23%)	1	2
15	M	94/134 (70%)	81 (86%)	13 (14%)	3	10
16	N	96/97 (99%)	85 (88%)	11 (12%)	5	16
17	O	75/79 (95%)	66 (88%)	9 (12%)	5	14
18	P	109/115 (95%)	100 (92%)	9 (8%)	11	30
19	Q	75/76 (99%)	67 (89%)	8 (11%)	6	19
20	R	91/96 (95%)	79 (87%)	12 (13%)	4	11
21	S	149/192 (78%)	133 (89%)	16 (11%)	6	19
22	T	62/67 (92%)	58 (94%)	4 (6%)	17	43
23	U	57/66 (86%)	44 (77%)	13 (23%)	1	2
24	V	54/55 (98%)	48 (89%)	6 (11%)	6	18
25	W	48/48 (100%)	43 (90%)	5 (10%)	7	20
26	Z	51/53 (96%)	43 (84%)	8 (16%)	2	7
30	4	35/35 (100%)	33 (94%)	2 (6%)	20	49
All	All	2436/2716 (90%)	2139 (88%)	297 (12%)	5	14

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	11	ARG
14	L	37	HIS
23	U	70	LEU
12	J	64	LYS
13	K	13	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
13	K	13	ASN
16	N	34	ASN
25	W	49	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	L	37	HIS
14	L	97	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	695 (25%)	324 (12%)
2	Y	121/123 (98%)	25 (20%)	1 (0%)
All	All	2801/3003 (93%)	720 (25%)	325 (11%)

5 of 720 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	13	A
1	X	14	A
1	X	25	U

5 of 325 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1194	U
1	X	1439	G
1	X	2608	A
1	X	1249	G
1	X	1315	A

## 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 35 ligands modelled in this entry, 35 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	X	2686/2880 (93%)	-0.22	110 (4%) 37 34	3, 38, 98, 118	0
2	Y	122/123 (99%)	-0.03	3 (2%) 57 56	24, 67, 89, 101	0
3	A	240/274 (87%)	0.27	20 (8%) 11 9	17, 53, 65, 71	0
4	B	205/211 (97%)	-0.45	1 (0%) 91 91	2, 21, 43, 56	0
5	C	197/205 (96%)	0.02	10 (5%) 28 24	14, 43, 58, 66	0
6	D	177/180 (98%)	0.45	13 (7%) 15 12	50, 60, 67, 69	0
7	E	171/185 (92%)	-0.09	5 (2%) 51 48	38, 53, 64, 68	0
8	F	71/144 (49%)	2.85	52 (73%) 0 0	0, 77, 83, 85	0
9	G	142/174 (81%)	0.10	9 (6%) 20 17	24, 39, 53, 63	0
10	H	134/134 (100%)	-0.53	0 100 100	3, 17, 33, 42	0
11	I	141/156 (90%)	0.77	24 (17%) 1 1	21, 53, 62, 71	0
12	J	136/142 (95%)	-0.03	3 (2%) 62 60	28, 43, 60, 65	0
13	K	113/116 (97%)	-0.47	0 100 100	2, 10, 24, 34	0
14	L	104/114 (91%)	0.28	10 (9%) 8 6	38, 51, 58, 63	0
15	M	108/166 (65%)	-0.54	1 (0%) 84 84	3, 18, 43, 55	0
16	N	117/118 (99%)	-0.19	2 (1%) 70 70	5, 37, 54, 61	0
17	O	94/100 (94%)	-0.17	3 (3%) 47 44	22, 47, 59, 64	0
18	P	127/134 (94%)	-0.50	0 100 100	4, 18, 47, 59	0
19	Q	93/95 (97%)	-0.00	3 (3%) 47 44	29, 42, 57, 68	0
20	R	110/115 (95%)	0.35	12 (10%) 5 4	35, 46, 61, 65	0
21	S	175/237 (73%)	0.64	18 (10%) 6 5	49, 58, 64, 68	0
22	T	84/91 (92%)	0.62	14 (16%) 1 1	26, 44, 59, 70	0
23	U	72/81 (88%)	0.74	11 (15%) 2 1	41, 53, 63, 67	0
24	V	66/67 (98%)	-0.12	2 (3%) 50 46	38, 52, 65, 67	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	-0.40	0 100 100	21, 37, 49, 64	0
26	Z	58/60 (96%)	-0.42	1 (1%) 70 70	4, 16, 38, 44	0
27	1	53/55 (96%)	3.46	42 (79%) 0 0	37, 47, 56, 60	0
28	2	46/47 (97%)	6.25	46 (100%) 0 0	11, 27, 34, 37	0
29	3	63/66 (95%)	5.67	59 (93%) 0 0	21, 36, 46, 48	0
30	4	37/37 (100%)	1.02	9 (24%) 0 0	44, 52, 58, 59	0
All	All	5997/6562 (91%)	0.10	483 (8%) 12 10	0, 43, 85, 118	0

The worst 5 of 483 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	37	SER	16.5
29	3	38	GLY	16.4
29	3	39	ASP	11.4
29	3	33	ASN	11.4
29	3	43	GLY	11.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	2886	1/1	0.52	0.33	41,41,41,41	0
31	MG	X	2884	1/1	0.53	0.42	55,55,55,55	0
31	MG	X	2910	1/1	0.63	0.37	19,19,19,19	0
31	MG	X	2882	1/1	0.66	0.29	12,12,12,12	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2908	1/1	0.72	0.49	17,17,17,17	0
31	MG	Y	126	1/1	0.73	0.29	25,25,25,25	0
31	MG	X	2883	1/1	0.76	0.19	49,49,49,49	0
31	MG	Y	124	1/1	0.80	0.42	26,26,26,26	0
31	MG	Y	128	1/1	0.82	0.16	41,41,41,41	0
31	MG	X	2881	1/1	0.82	0.26	59,59,59,59	0
31	MG	X	2888	1/1	0.83	0.23	3,3,3,3	0
31	MG	X	2890	1/1	0.83	0.20	49,49,49,49	0
31	MG	X	2900	1/1	0.83	0.40	3,3,3,3	0
31	MG	X	2893	1/1	0.83	0.21	13,13,13,13	0
31	MG	X	2885	1/1	0.84	0.52	56,56,56,56	0
31	MG	X	2909	1/1	0.86	0.12	3,3,3,3	0
31	MG	X	2892	1/1	0.87	0.19	22,22,22,22	0
31	MG	X	2899	1/1	0.88	0.22	19,19,19,19	0
31	MG	Y	127	1/1	0.90	0.18	12,12,12,12	0
31	MG	X	2906	1/1	0.91	0.44	13,13,13,13	0
31	MG	X	2896	1/1	0.92	0.25	3,3,3,3	0
31	MG	X	2898	1/1	0.92	0.42	3,3,3,3	0
31	MG	X	2905	1/1	0.92	0.28	6,6,6,6	0
31	MG	X	2903	1/1	0.93	0.24	24,24,24,24	0
31	MG	X	2897	1/1	0.93	0.51	3,3,3,3	0
31	MG	X	2901	1/1	0.93	0.28	3,3,3,3	0
31	MG	X	2887	1/1	0.94	0.15	3,3,3,3	0
31	MG	X	2894	1/1	0.95	0.39	15,15,15,15	0
31	MG	X	2907	1/1	0.96	0.17	58,58,58,58	0
31	MG	X	2904	1/1	0.96	0.13	3,3,3,3	0
31	MG	X	2902	1/1	0.97	0.11	60,60,60,60	0
31	MG	Y	125	1/1	0.97	0.20	9,9,9,9	0
31	MG	X	2895	1/1	0.97	0.35	3,3,3,3	0
31	MG	X	2889	1/1	0.98	0.36	3,3,3,3	0
31	MG	X	2891	1/1	0.99	0.51	12,12,12,12	0

## 6.5 Other polymers

There are no such residues in this entry.