



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:41 PM GMT

PDB ID : 1Y69
Title : RRF domain I in complex with the 50S ribosomal subunit from *Deinococcus radiodurans*
Authors : Wilson, D.N.; Schlutzen, F.; Harms, J.M.; Yoshida, T.; Ohkubo, T.; Albrecht, R.; Buerger, J.; Kobayashi, Y.; Fucini, P.
Deposited on : 2004-12-04
Resolution : 3.33 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

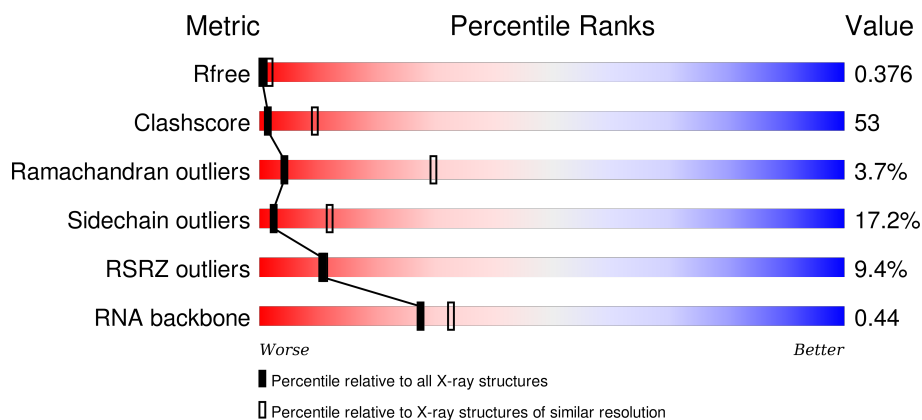
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)
RNA backbone	2183	1007 (3.88-2.80)

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	0	2880	<div> <div>8%</div> <div>10%</div> <div>60%</div> <div>22%</div> <div>• •</div> </div>
2	9	124	<div> <div>6%</div> <div>13%</div> <div>69%</div> <div>14%</div> <div>5%</div> </div>
3	K	141	<div> <div>16%</div> <div>33%</div> <div>43%</div> <div>19%</div> <div>• •</div> </div>
4	U	91	<div> <div>19%</div> <div>44%</div> <div>40%</div> <div>9%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
5	8	113	<p>16% 40% 53% 6%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 64484 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	118	Total	C	N	O	P	0	0	0
			2516	1124	464	811	117			

- Molecule 3 is a protein called 50S ribosomal protein L16.

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

- Molecule 4 is a protein called 50S ribosomal protein L27.

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

- Molecule 5 is a protein called Ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	8	113	Total	C	N	O	S	0	0	0
			894	541	170	179	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	31	GLY	-	see remark 999	UNP P16174
8	32	GLY	-	see remark 999	UNP P16174

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Chain	Residue	Modelled	Actual	Comment	Reference
8	33	GLY	-	see remark 999	UNP P16174

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.

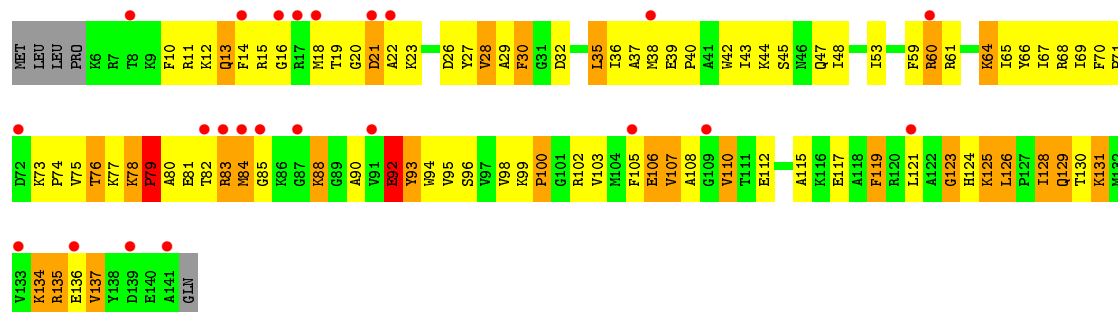
Chain 0:

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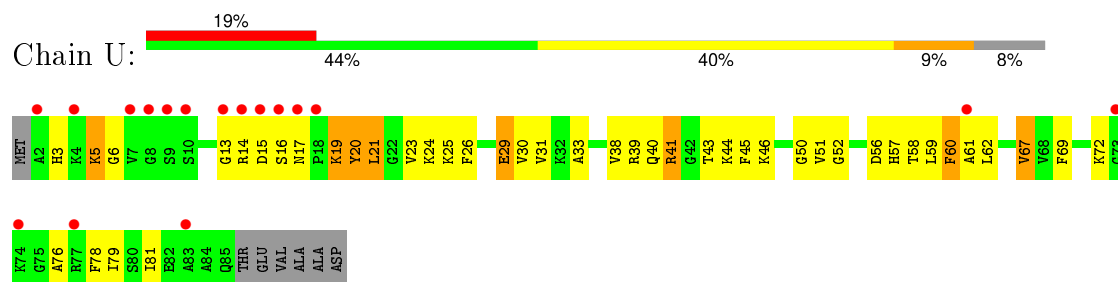
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A1468	A1408	A1287	A1106	G1041	G981	A921	G861	A801	G741	C679	U617
U1469	U1409	A1288	A1107	G1042	G982	A922	A862	A802	A742	U680	A618
U1470	U1410	A1289	U1108	A1043	G983	A923	C863	C803	A743	A619	A619
G1471	G1350	A1290	U1109	U1044	G984	C924	C864	C804	C744	C682	G620
C1472	C1411	G1291	G1110	G1045	G985	U925	A865	G805	C745	A683	U621
U1473	U1412	A1292	C1111	U1046	A986	C926	U866	A806	G746	C684	U622
A1474	U1413	U1232	C1112	U1047	G987	C927	U867	A807	A747	U685	G623
U1475	G1414	A1233	C1113		G988	C928	U868	C808	A748	C686	A624
G1476	G1415	C1234	C1114	C1054	G989	A929	C869	C809	C749	A625	A625
C1477	C1416	G1235	C1115	A1055	G990	A930	C870	U810	C750	A688	A626
G1478	C1417	G1236	U1116	U1056	A991	G931	U871	G811	C751	A690	A627
C1479	G1418	G1237	U1117	U1057	A992	G932	U872	G812	G752	A691	A628
G1480	A1420	A1238	U1118	G1058	C993	G933	U873	A813	U753	C691	C629
U1481	U1421	A1239	U1119	A1059	A994	G934	A874	G814	G754	C692	G630
U1482	C1422	G1240	U1120	C1060	A995	G935	C875	C815	C755	A693	G631
G1483	A1423	A1241	C1121	A1061	C996	A936	A876	U816	C756	C694	A632
G1484	U1424	G1242	G1122	G1062	C997	C937	C877	A817	C757	G695	G633
U1485	U1304	C1243	G1123	C1063	C998	G938	C878	G818	C758	U696	G634
C1486	G1305	G1245	U1124	C1064	A999	C939	A879	C819	C759	G697	C635
U1487	U1306	G1246	G1125	A1065	G1000	G940	C880	U820	U760	A698	
G1488	A1367	U1247	A1126	G1066	A1001	C941	U881	A821	G761	G699	G637
G1489	G1368	G1248	C1127	G1067	C1002	U942	C882	G822	A762	C700	A638
U1490	G1369	G1249	G1128	A1068	C1003	U943	A883	U823	A763	U701	G639
U1491	U1370	A1250	A1129	G1069	A1004	A944	C884	U824	A764	A702	C640
A1492	G1371	G1251	U1130	G1070	U1005	G945	A885	C825	C765	A703	G641
A1493	A1372	C1252	G1131	U1071	C1006	U946	A886	U826	A766	G704	A642
G1494	G1373	G1253	C1132	U1072	A1007	C947	C887	C827	A767	C643	
G1495	G1374	A1314	G1133	G1073	G1008	C948	C888	C828	U768	A706	A644
G1496	G1375	A1255	G1134	G1074	C1009	G949	C889	C829	C769	U707	G645
A1497	C1376	C1256	G1135	C1075	U1010	G950	U890	C830	U770	G708	C646
G1498	G1377	U1257	G1136	U1076	A1011	G951	A891	G831	C771	A709	G647
A1499	A1378	C1258	A1137	U1077	A1012	C952	G	A832	G772	C710	A648
G1500	G1379	A1259	A1138	A1078	G1013	G953	G	A833	G773	C711	G649
G1501	A1320	A1260	A1139	G1079	G1014	U954	G	A834	A774	A712	U650
G1502	A1321	G1261	A1140	A1080	U1015	G955	G	U835	U775	C651	
G1503	G1322	U1262	U1141	A1081	G1016	A956	G	G836	G776	C652	
G1504	C1323	G1263	G1142	G1082	C1017	C957	C	U837	A777	G653	
U1505	G1324	A1264	A1143	C1083	C1018	G958	C	A838	G778	A654	
G1506	U1325	G1265	U1144	A1084	U1019	C959	U	U839	U779	A719	
G1507	U1326	G1266	C1145	G1085	A1020	U960	C	U840	U780	A720	U656
U1508	U1327	A1267	G1146	C1086	A1021	G961	C	G841	G781	G721	A657
A1509	C1328	U1268	G1147	C1087	A1022	C962	C	A842	U782	G722	G658
A1510	U1329	G1269	G1148	A1088	U1023	G963	C	G843	C783	C723	G659
A1511	G1330	C1270	G1149	C1089	G1024	A964	G	U844	U784	C724	G660
A1512	G1331	G1271	C1150	C1090	A1025	G965	C	U845	U785	G725	
U1513	A1391	G1272	U1151	C1091	U1026	A966	U	A846	U786	G726	C664
C1514	G1332	G1273	C1152	U1092	C1027	G967	U	C847	A787	U727	A665
U1515	A1333	C1274	A1153	U1093	G1028	C968	A	A848	G788	G728	U666
U1516	A1334	A1275	G1154	C1094	C1029	U969	C	G849	U789	A729	U667
G1517	A1335	U1276	G1155	A1095	U1030	A970	C	C850	A790	C730	A668
A1518	A1397	U1277	U1156	A1096	C1031	A971	A911	C851	G791	A731	
G1519	G1398	C1278	G1157	A1097	A1032	C972	A912	U852	U792	G732	
U1520	C1399	A1279	C1218	G1098	G1033	U973	A913	C853	U793	G733	U670
U1521	A1400	U1339	C1219	G1099	U1034	U974	C914	G854	A794	G734	A671
G1522	G1401	U1280	G1160	A1099	U1035	C975	C915	G855	A795	G735	C672
C1523	G1402	A1281	U1161	G1100	G1036	C976	U916	A856	A796	G736	G673
A1524	A1463	A1282	A1162	U1101	G1037	C977	U917	U857	A797	G737	U674
G1525	A1464	C1283	C1163	G1102	U1038	G978	A918	G858	G798	C738	G675
U1526	A1465	G1284	C1164	C1103	U1039	U979	U919		C799	G739	
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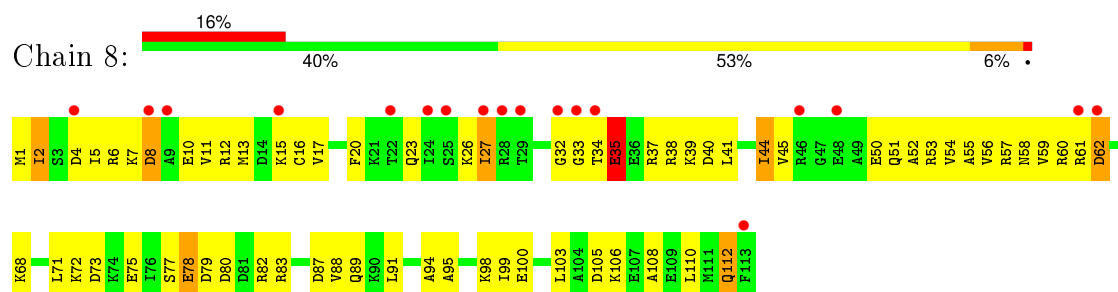
G2328	A2266	C2206	A	G2084	U2024	C1962	A1901	G1838	C1773	G1713	A1950	G1589	C1528
C2329	A2267	G2208	C	G	A2025	A1964	A1902	A1839	A1774	A1714	G1651	C1590	C1529
G2330	G2268	G2208	C	U2088	C2026	G1964	C1903	A1840	A1775	A1715	G1652	U1591	U1530
G2331	G2269	G	G	C2089	C2027	U1965	G1904	G1766	A1776	G1716	C1653	U1592	C1531
G2332	U2270	U	U	U2090	C2028	C1966	G1905	G1841	A1777	A1717	A1554	U1593	A1532
A2333	C2271	G	G	C2091	G2029	U1967	U1906	C1844	U1778	A1718	C1655	U1594	G1533
C2334	A2272	A	A	U2092	U2030	G1968	C1907	A1845	C1779	G1719	U1656	A1596	A1534
U2335	C2273	G	A	G2093	A2031	G1969	C1908	A1846	A1780	G1720	U1657	A1595	C1535
C2336	C2274	A	A	C2094	G2032	G1970	U1909	G1847	C1781	G1721	A1658	A1597	G1536
U2275	G2215	U	U	G2095	C2033	C1971	A1910	U1848	A1782	G1722	G1659	C1598	U1537
C2276	U2275	A	A	U2096	A2034	G1972	A1911	G1849	G1783	U1723	G1660	G1599	A1538
A2277	G2216	C2157	C2157	A2097	G2035	G1973	G1912	G1850	C1784	C1724	G1661	U1600	U1539
A2278	G2217	C2158	C2158	G	G2036	U1974	G1913	A1851	A1785	C1725	G1662	U1601	C1540
G2279	U2219	A2159	A2159	G	A2037	G1975	U1914	G1852	C1786	C1726	G1663	A1602	G1541
A2280	U2220	C2160	C2160	A	C2038	U1976	A1915		U1787	C1727	G1664	A1603	G1542
C2281	G2221	C2161	C2161	U	G2039	C1977	G1916	U1856	C1788	A1728	C1665	A1604	G1543
G2282	U2222	G2282	C2162	A	A2040	U1978	C1917	G1857	U1789	G1729	G1666	A1605	A1544
U2223	U2223	U2223	U2163	G2103	A2041	C1979	G1918	C1858	G1790	G1730	A1667	C1606	G1545
G2284	U2224	G2284	G2164	G2104	A2042	A1980	A1919	A1859	C1791	C1731	G1668	A1607	C1546
U2285	G2225	U2285	A2165	U2105	A2043	A1981	A1920	A1860	C1792	U1732	C1669	U1608	U1547
G2286	A2226	G2286	C2166	G2106	G2044	A1982	A1921	G1861	A1793	U1733	G1670	G1609	U1548
C2227	G2227	A2167	G2107	G2107	A2045	G1983	U1922	C1862	A1794	C1734	A1671	A1610	C1549
U2228	A2288	A2168	G2108	G2108	C2046	A1984	U1923	U1863	C1795	G1735	A1672	U1611	C1550
A2289	G2229	A2169	A2109	A2109	C2047	G1985	C1924	G1864		G1736	A1673		U1551
C2230	G2230	C2170	G2110	G2110	C2048	G1986	C1925	C1865	A1800	G1737	C1674	C1614	C1552
G2231	U2231	U2171	C	C	C2049		U1926	C1866	C1801	C1738	C1675	G1615	G1553
C2232	G2232	U2172	G	G	G2050	U1990	C1927	A1867	A1802	G1739	U1676	C1616	G1554
G2293	C2293	G2173	U	U	U2051	A1991	G1928	A1868	G1803	G1803	C1677	C1617	A1555
C2294	G2294	G2174	G	G	G2052	G1992	U1929	A1869	U1804	G1741	G1618	U1618	A1556
G2235	G2235	A2175	C	C	G2053	G1993	C1930	U1870	G1805	G1742	A1619	G157	
U2236	U2236	U2176	G	G	A2054	A1994	G1931	A1871	G1806	C1743	C1520	C1520	
C2237	C2237	U2177	A	A	G2055	G1995	G1932	A1872	A1807	G1744	A1681	C1621	G1559
A2299	G2238	U2178	C	C	C2056	G1996	G1933	A1873	C1808	C1745	U1688	G1622	A1560
G2300	C2239	C2179	A2119	A2119	U2057	A1997	U1934	G1874	G1809	C1746	G1684	C1623	A1561
A2301	C2240	U2180	U2120	U2120	U2058	A1998	A1935	C1875	U1810	G1747	A1685	A1624	G1562
C2302	U2241	A2181	U2121	U2121	U2059	U1999	A1936	C1876	A1811	U1748	A1886	U1625	U1583
G2303	C2242	A2182	G2122	G2122	A2060	U2000	G1937	C1877	U1812	G1749	C1687	A1826	U1584
C2304	C2243	C2183	C2123	C2123	G2061	G2001	U1938	A1878	A1813	C1750	U1688	C1627	
G2305	C2244	C2184	C2124	C2124	U2062	A2002	U1939	G1879	G1814	A1751	U1689	C1628	A1567
A2306	A2245	U2185	C2125	C2125	A2063	A2003	C1940	G1880	G1815	U1752	G1629	C1629	
C2307	A2246	C2186	U	U	U2064	U2004	C1941	U1881	G1816	A1753	G1691	A1630	A1569
A2308	A2247	A2187	U	U	A2065	U2005	G1942	G1882	U1817	G1754	C1692	C1631	C1570
G2309	A2248	C2188	U	U	G2066	G2006	C1943	A1883	G1818	G1755	A1993	G1571	G1571
C2310	U2249	A2189	G	G	U2067	G2007	C1944	A1884	U1819	C1756	C1696	C1633	C1572
U2311	G2250	A2190			C2068	C2008	C1945	C1885	G1820	C1757	G1697	A1634	A1574
A2312	U2251	A2191	G	U	U2069	U2009	U1946	G1886	A1821	C1758	A1697	G1635	C1575
G2313	A2252	U2192	G2132	G2132	G2070	G2010	G1947	G1887	C1822	A1759	C1698	C1636	C1576
A2314	A2253	G2193	G2133	G2133	G2071	U2011	G1948	C1888	G1823	G1760	A1699	U1637	G1576
G2315	C2254	A2194	U2134	U2134	C2072	A2012	A1949	G1889	C1824	C1761	C1700	G1538	
G2316	G2255	C2195	C2135	C2135	A2073	A2013	C1950	G1890	U1826	G1762	C1701	C1639	U1578
	U2256	U2196	G2136	G2136	U2074	A2014	G1951	C1891	C1825	G1763	C1702	C1640	G1579
G2319	A2257	U2197	G2137	G2137	G2075	G2015	A1952	G1892	A1764	C1703	G1580	C1641	C1580
C2320	G2258	U2198	U2138	U2138	G2076	A2016	A1953	G1893		G1765	C1704	G1642	C1581
C2321	G2259	C2199	G2139	G2139	G2077	U2017	A1954	U1894	G1830	U1766	A1643	A1582	
U2322	C2260	G2200	G2140	G2140	G2078	G2018	G1955	A1895	G1831	G1767	C1708	G1644	A1583
G2323	G2261	G2201	A	A	A2079	C2019	G1956	A1896	U1833	C1768	C1709	U1645	G1584
A2324	C2262	G2202	G	G	U2081	G2021	C1957	C1894	C1835	U1769	U1740	G1646	A1585
G2325	G2263	G2203	G	G	U2081	G2021	G1958	C1897	C1835	U1770	U1647	A1586	
C2326	C2264	A2204	C	C	C2082	C2022	U1959	A1899	C1836	A1771	C1648	A1587	A1588
U2327	U2265	C2205	A	A	C2083	C2023	C2023	U1900	C1837	G1772	C1649	A1589	



- Molecule 4: 50S ribosomal protein L27



- Molecule 5: Ribosome recycling factor



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.70Å 405.00Å 693.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.13 – 3.33 29.66 – 3.30	Depositor EDS
% Data completeness (in resolution range)	74.5 (8.13-3.33) 89.1 (29.66-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.338 0.340 , 0.376	Depositor DCC
R_{free} test set	8852 reflections (2.83%)	DCC
Wilson B-factor (Å ²)	74.3	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 6.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	5 of 313046 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	64484	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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	0	0.71	2/66467 (0.0%)	0.85	112/103673 (0.1%)
2	9	0.53	0/2813	0.78	0/4384
3	K	0.59	0/1113	0.80	2/1486 (0.1%)
4	U	0.55	0/633	0.69	0/838
5	8	0.57	0/895	0.71	0/1189
All	All	0.70	2/71921 (0.0%)	0.85	114/111570 (0.1%)

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	0	0	217
2	9	0	2
All	All	0	219

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	841	G	C5-C6	-5.21	1.37	1.42
1	0	1285	A	N9-C4	5.07	1.40	1.37

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	582	G	N9-C1'-C2'	10.45	127.58	114.00
1	0	1154	A	OP1-P-O3'	8.68	124.30	105.20
1	0	466	A	N9-C1'-C2'	8.54	125.10	114.00
1	0	788	G	N9-C1'-C2'	8.41	124.94	114.00
1	0	1979	C	N1-C1'-C2'	8.27	124.75	114.00

There are no chirality outliers.

5 of 219 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1	G	Sidechain
1	0	10	A	Sidechain
1	0	20	C	Sidechain
1	0	48	A	Sidechain
1	0	66	U	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	0	59359	0	29917	4727	0
2	9	2516	0	1286	164	0
3	K	1090	0	1125	185	0
4	U	625	0	655	83	0
5	8	894	0	925	101	0
All	All	64484	0	33908	5144	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 53.

The worst 5 of 5144 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)
1:0:1333:G:N2	1:0:1344:C:H41	1.39	1.21
1:0:2548:G:C2'	1:0:2549:G:H5''	1.73	1.17
1:0:1073:G:H2'	1:0:1074:G:H5''	1.18	1.17
1:0:1978:U:H3'	1:0:1979:C:H5''	1.28	1.15
3:K:76:THR:HG21	3:K:88:LYS:HB2	1.22	1.15

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	134/141 (95%)	109 (81%)	19 (14%)	6 (4%)	3	24
4	U	82/91 (90%)	63 (77%)	16 (20%)	3 (4%)	4	30
5	8	111/113 (98%)	95 (86%)	13 (12%)	3 (3%)	6	37
All	All	327/345 (95%)	267 (82%)	48 (15%)	12 (4%)	4	30

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	79	PRO
5	8	112	GLN
3	K	80	ALA
3	K	135	ARG
4	U	13	GLY

5.3.2 Protein sidechains [i](#)

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	K	110/115 (96%)	83 (76%)	27 (24%)	1	3
4	U	62/67 (92%)	54 (87%)	8 (13%)	5	23
5	8	95/95 (100%)	84 (88%)	11 (12%)	7	28
All	All	267/277 (96%)	221 (83%)	46 (17%)	2	12

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	119	PHE
3	K	134	LYS
5	8	62	ASP
3	K	125	LYS
3	K	129	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	U	57	HIS
5	8	89	GLN
5	8	51	GLN
4	U	40	GLN
5	8	23	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	636 (23%)	121 (4%)
2	9	117/124 (94%)	16 (13%)	0
All	All	2874/3004 (95%)	652 (22%)	121 (4%)

5 of 652 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	45	C
1	0	48	A
1	0	49	U
1	0	50	G
1	0	51	A

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1626	A
1	0	1775	A
1	0	2633	A
1	0	1633	C
1	0	1691	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0	2766/2880 (96%)	0.48	239 (8%) 13 12	20, 43, 100, 131	0
2	9	118/124 (95%)	0.48	7 (5%) 26 25	33, 70, 94, 106	0
3	K	136/141 (96%)	1.14	23 (16%) 2 2	20, 50, 68, 80	0
4	U	84/91 (92%)	1.19	17 (20%) 1 1	21, 49, 63, 66	0
5	8	113/113 (100%)	0.75	18 (15%) 3 2	28, 52, 66, 82	0
All	All	3217/3349 (96%)	0.53	304 (9%) 11 11	20, 45, 98, 131	0

The worst 5 of 304 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	0	558	G	9.5
1	0	1086	C	8.1
1	0	248	A	7.9
1	0	1902	A	7.5
4	U	15	ASP	7.2

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.