



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:00 pm BST

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

<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

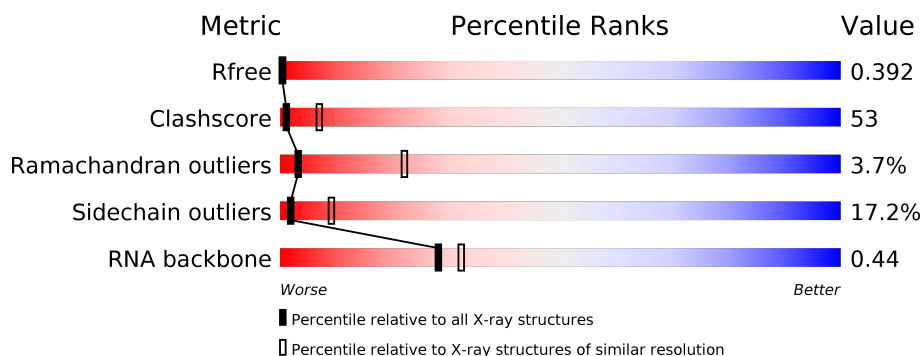
1 Overall quality at a glance

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}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RNA backbone	3102	1129 (3.78-2.90)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	2880	10% 60% 22% . .
2	9	124	13% 69% 14% 5%
3	K	141	33% 43% 19% . .
4	U	91	44% 40% 9% 8%
5	8	113	40% 53% 6% .

2 Entry composition

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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	1526	U	C	conflict	GB 1026245073

- 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			

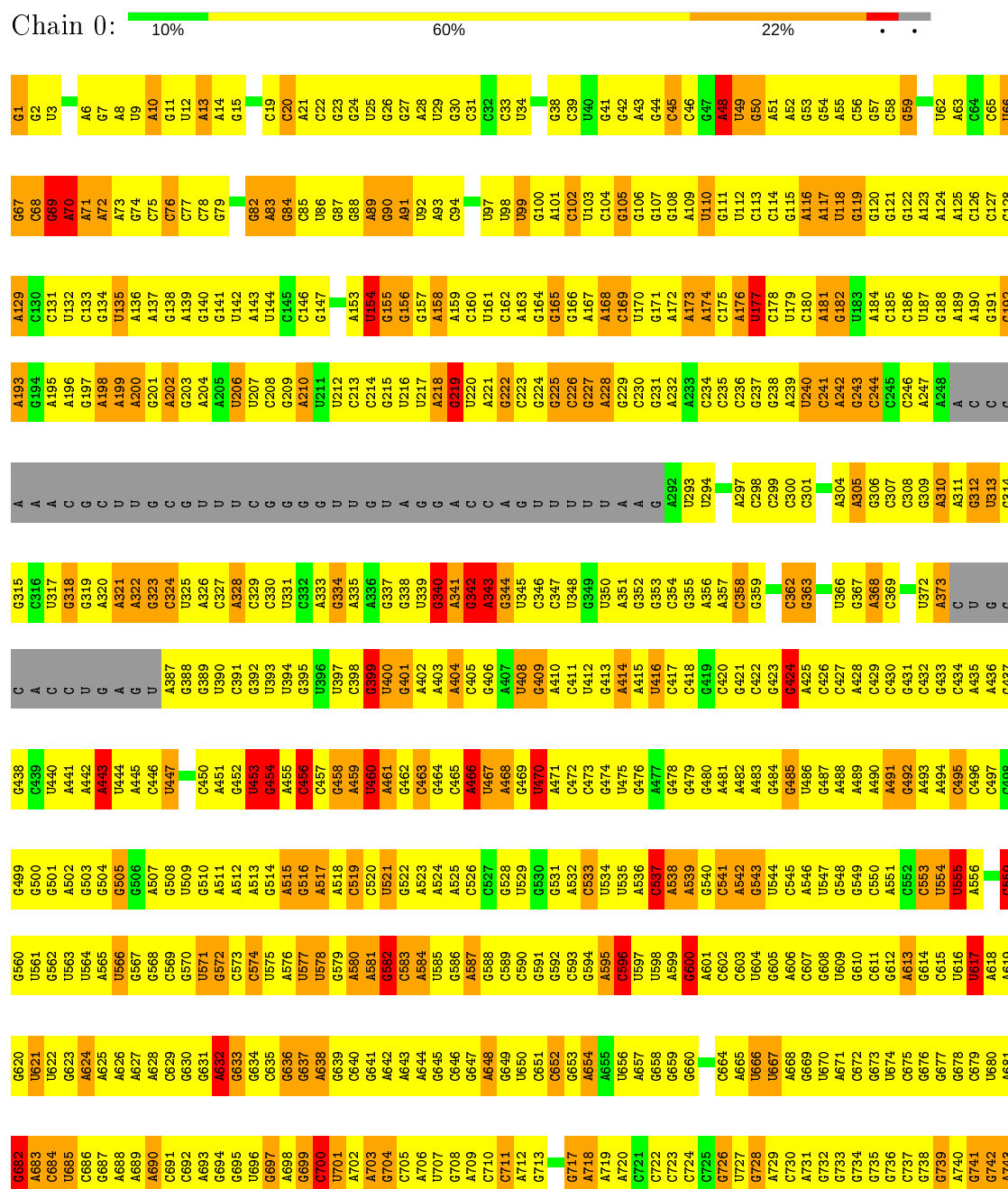
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	31	GLY	-	linker	UNP P0A805
8	32	GLY	-	linker	UNP P0A805
8	33	GLY	-	linker	UNP P0A805

3 Residue-property plots

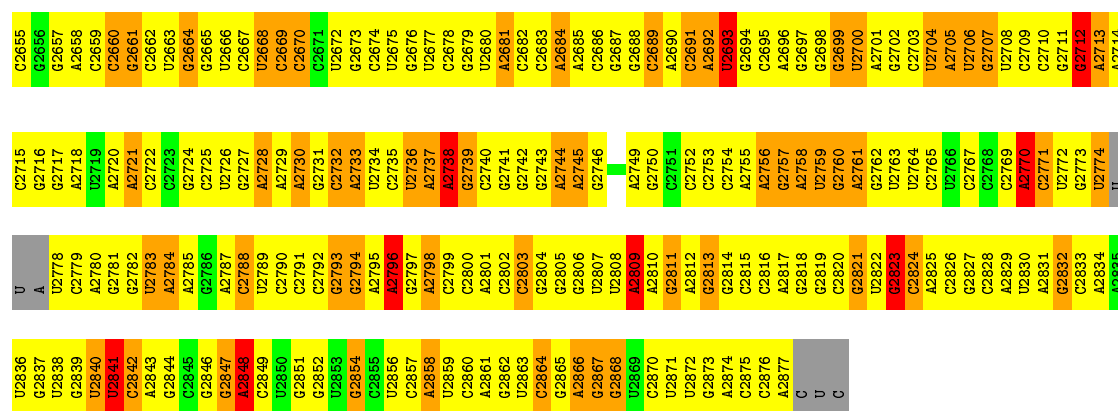
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

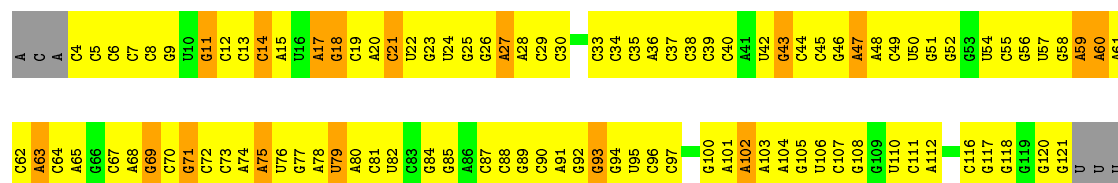


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A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	
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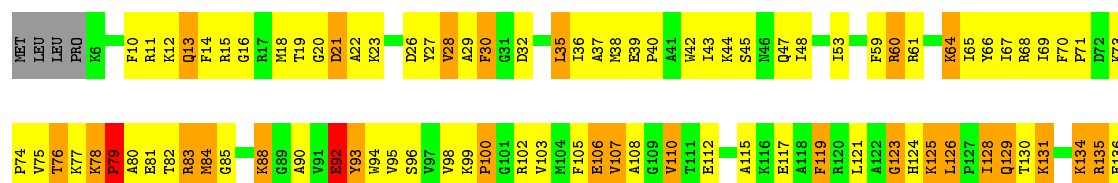
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A2613	G2549	G2489	G2362	A2301	G2238	U2177	C	G2053	U1993	C1930	A1867	A1803	G1739
G2617	C2550	U2490	G2363	G2302	C2239	U2178	A2117	A2054	U1994	G1931	A1868	G1803	G1740
A2618	C2551	U2491	U2364	G2303	C2240	C2179	A2118	G2055	G1995	G1932	A1869	A1804	G1741
G2619	A2552	C2492	U2365	G2304	G2241	U2180	A2119	C2056	A1996	G1933	U1870	G1805	G1742
G2620	C2553	G2493	C2366	C2242	C2242	A2181	C	U2057	A1997	U1934	G1871	G1806	C1743
G2621	G2554	U2493	A2367	A2305	C2243	A2182	G2122	U2058	A1998	A1935	A1872	A1807	G1744
A2622	C2555	G2494	G2368	A2307	C2244	C2183	G2123	U2059	U1999	A1936	A1873	C1808	G1745
A2623	G2556	G2495	U2369	A2308	A2245	C2184	C2124	A2060	G1997	G1937	G1874	G1809	A1746
G2624	G2557	A2497	C2370	G2309	G2246	U2185	C2125	C2061	U1938	U1938	C1875	U1810	G1747
G2625	C2558	G2498	A2371	G2310	A2247	C2186	C2126	A2062	A2003	U1939	C1876	A1811	U1748
U2626	U2559	C2499	C2372	U2311	A2248	A2187	U	G2063	A2002	C1940	C1877	U1812	G1749
G2627	G2560	C2500	C2373	C2312	U2249	A2188	U	U2064	U2004	C1941	C1878	A1813	A1750
U2628	U2561	U2501	G2376	C2313	G2250	U2189	U	A2065	U2005	G1942	G1879	A1751	A1751
G2629	U2562	G2502	U2377	A2314	U2251	A2191	G	G2066	G2006	A1943	G1880	G1815	U1752
C2630	A2563	C2503	U2377	A2315	A2252	C2192	U	U2067	C2007	C1944	U1881	G1816	U1753
G2631	G2564	G2504	U2381	G2316	C2253	C2193	G2132	U2068	C2008	C1945	G1882	A1817	G1754
A2632	A2565	U2505	C2382	C2319	G2254	A2194	U2134	G2070	U2009	U1946	A1883	G1818	G1755
G2633	G2566	C2506	C2383	C2320	G2255	U2196	U2134	G2071	U2011	C1948	C1885	G1820	C1757
A2634	U2567	U2507	G2384	C2321	G2256	U2197	C2135	C2072	A2012	A1949	G1886	A1821	G1758
G2635	A2568	G2508	U2385	U2322	A2257	U2198	U2138	A2073	A2013	C1950	G1887	G1822	A1759
A2636	C2570	A2509	G2386	U2323	G2258	C2199	G2139	U2074	A2014	G1951	G1888	G1823	G1760
G2637	U2571	U2510	U2387	G2324	C2260	G2200	G2139	U2075	A2015	A1952	G1889	G1824	G1761
G2638	C2572	A2511	G2388	A2325	C2261	G2201	G2140	G2076	A2016	A1953	G1890	C1825	G1762
A2639	G2573	A2512	C2389	C2326	G2262	G2202	A	G2077	U2017	A1954	C1891	U1826	G1763
G2640	U2575	G2513	A2390	U2327	C2263	G2203	G	G2078	G2018	G1955	C1892	U1826	A1764
A2641	G2576	G2514	G2391	G2328	C2264	A2204	C	A2079	G2019	G1956	C1893	G1830	C1765
G2642	A2577	G2515	G2392	C2329	A2265	C2205	G	U2080	C2020	C1957	U1894	G1831	U1766
G2643	G2578	A2457	G2393	G2330	A2266	G2206	A	U2081	G2021	G1958	G1895	G1832	G1767
A2644	A2579	U2458	C2394	G2331	A2267	G2207	A	G2082	C2022	U1959	A1896	U1833	U1768
C2645	C2580	C2519	C2395	G2332	G2268	U2208	C	G2083	C2023	U1962	C1897	G1834	U1769
G2646	U2581	A2520	C2396	A2333	G2269	G2209	G	G2084	U2024	C1962	U1898	C1835	U1770
G2647	G2582	G2521	A2397	C2334	U2270	C2210	U	U2088	A2025	G1963	A1899	C1836	A1771
G2648	U2583	C2271	U2398	U2335	U2271	U2211	U	C2089	C2026	A1964	U1899	G1837	C1772
A2649	G2584	A2461	G2399	G2336	A2272	U2212	G	G2090	C2027	U1965	A1902	G1838	C1773
G2650	U2585	C2463	G2400	A2337	C2273	G2213	A	U2091	G2028	C1966	C1903	A1839	A1774
U2651	G2586	G2464	A2401	C2338	C2274	G2214	A	C2091	G2029	U1967	G1904	A1840	A1775
G2652	U2587	U2524	U2402	C2339	U2275	G2215	A	U2092	U2030	G1968	U1908	A1776	A1776
A2653	U2588	G2466	C2403	A2340	A2277	G2216	U	G2093	A2031	G1969	U1909	C1844	U1777
G2654	C2589	G2467	A2404	G2341	C2276	G2217	A	C2094	G2032	G1970	U1909	C1844	U1778
		G2468	A2405	U2342	A2278	G2218	C2157	G2095	C2033	C1971	A1910	A1845	C1779



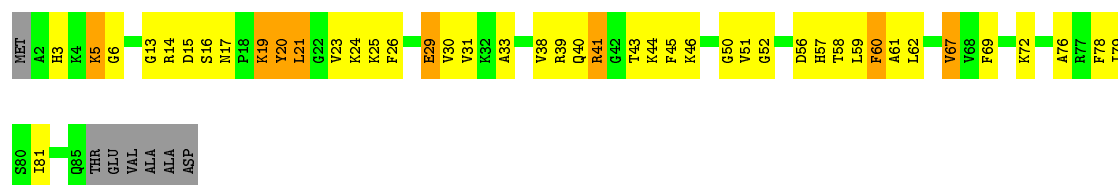
- Molecule 2: 5S ribosomal RNA



- Molecule 3: 50S ribosomal protein L16

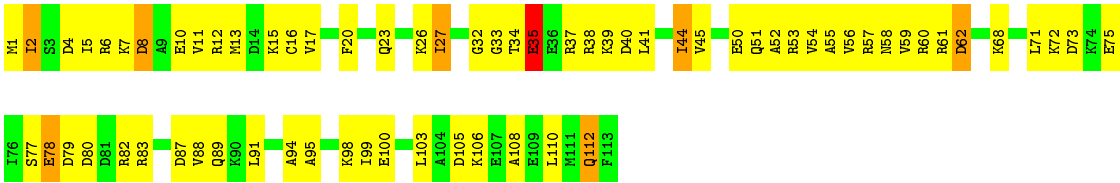


- Molecule 4: 50S ribosomal protein L27



- 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	168.70 Å 405.00 Å 693.00 Å 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 3.31 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.338 0.364 , 0.392	Depositor DCC
R_{free} test set	15675 reflections (5.01%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	4726	0
2	9	2516	0	1286	165	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

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	K	134/141 (95%)	109 (81%)	19 (14%)	6 (4%)	2	17
4	U	82/91 (90%)	63 (77%)	16 (20%)	3 (4%)	3	22
5	8	111/113 (98%)	95 (86%)	13 (12%)	3 (3%)	5	28
All	All	327/345 (95%)	267 (82%)	48 (15%)	12 (4%)	3	22

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

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%)	0	2
4	U	62/67 (92%)	54 (87%)	8 (13%)	4	18
5	8	95/95 (100%)	84 (88%)	11 (12%)	5	22
All	All	267/277 (96%)	221 (83%)	46 (17%)	2	9

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.