



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:19 PM UTC

PDB ID : 1NJP / pdb_00001njp
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a tRNA acceptor stem mimic (ASM)
Authors : Bashan, A.; Agmon, I.; Zarivatch, R.; Schlutzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on : 2003-01-02
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

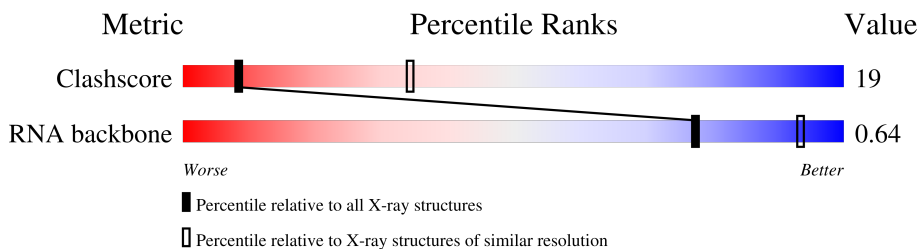
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

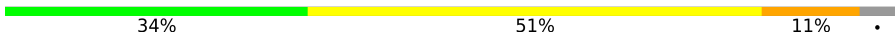
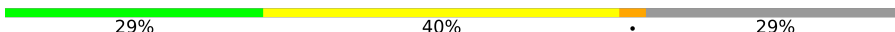
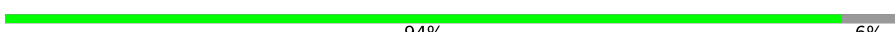
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	 34% 51% 11% .
2	5	35	 29% 40% . 29%
3	K	141	 88% 12%
4	T	237	 94% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60249 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 tRNA acceptor stem mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	5	25	Total	C	N	O	P	0	0	0
			543	249	97	173	24			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	K	124	Total	C	0	0	124
			124	124			

- Molecule 4 is a protein called GENERAL STRESS PROTEIN CTC.

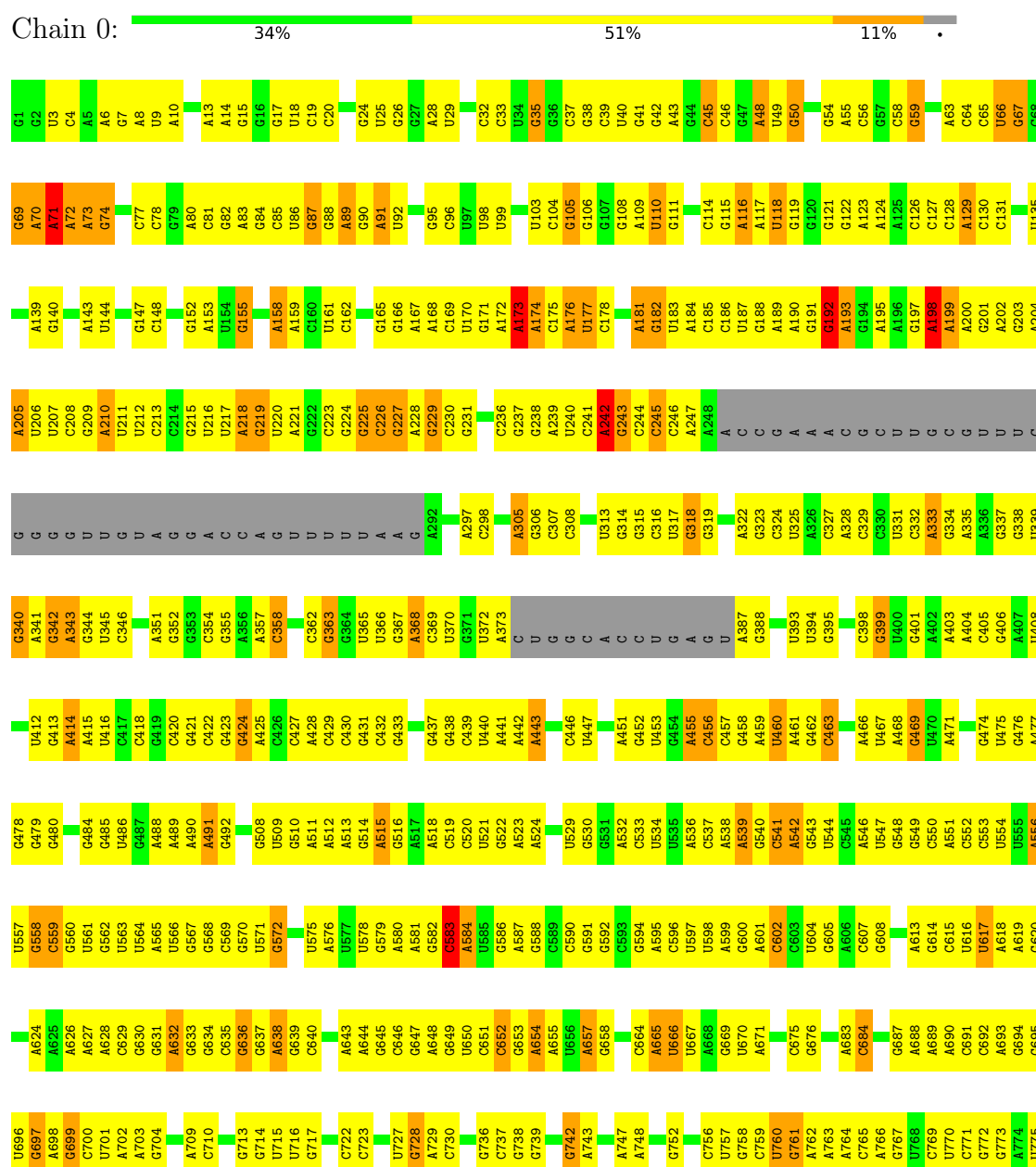
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	T	223	Total	C	0	0	223
			223	223			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA



U1819	G1820	A1821	C1822	C1825	U1826	C1829	A1830	G1831	C1835	C1836	G1837	A1838	C1839	A1840	G1841	C1845	G1846	C1847	A1848	C1849	G1850	A1851	C1855	U1856	C1857	A1858	C1859	G1860	A1861	C1862	C1865	G1866	C1871	A1875	C1876	G1877	A1878	C1879	G1880	U1881	A1882	C1883	A1884	C1885	G1886	C1887	C1888	G1889	C1890	G1893	U1894	A1895	C1896	A1899	U1900	U1906	C1907	C1908					
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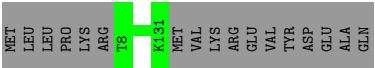
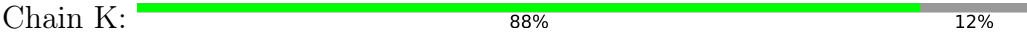
A2861	G2862	U2863	G2867	U2871	U2872	A2873	G2875	C2876	A2877	C	U	C	U1909	A1910	A1911	G1912	G1913	U1914	A1915	G1916	C1917	G1918	A1919	G1920	A1921	U1922	U1923	A1924	C1925	U1926	U1927	G1928	U1929	G1930	G1931	G1937	U1938	U1939	U1946	G1947	C1948	A1949	C1950	G1951	A1952	A1953	A1954	G1955	G1956	C1957	G1958	A1961	C1962	G1963	A1964	U1965	C1966	U1967	G1968	G1969	G1970	C1971	A2002	A2003	U2004	U2005	G2006	G2007	C2008	C1930	U2009	G2010	U2011	A2012	A2013	A2014	U2015	U2016	G2017	G2018	C2019	G2020	C2021	G2022	C2023	U2024	A2025	C2026	C2027	C2028	G2029	G2032	C2033	A2034	G2035	G2036	A2037	G2038	G2039	A2043	G2044	A2045	G2046	C2047	C2048	U2049	U2050	U2051	G2052	G2055	C2056	U2057	U2058	U2059	A2060	C2061	U2062	U2069	G2070	A2071	U2075	G2076	G2077	G2078	A2079	U2080	U2081	C2082	G2083	G2084	G2085	U2086	G2093	C2094	G2095	U2096	A2097	G	A	U	A	G2103	G2106	G2107	G2110	C	C	U	G	C	A2117	A2118	A2119	A2120	U2121	C2125	U	U	U	G	G	G2132	G2133	U2134	C2135	U2136	U2137	U2138	G2139	G2140	A	G	G	C	A	A	U	A	C2157	C2158	A2159	C2160	C2161	C2162	U2163	A2168	A2169	U2172	U2177	U2178	C2179	U2180	A2181	A2182	U2185	G2186	A2191	U2192	C2193	A2194	C2195	U2196	U2197	U2198	C2199	G2200	G2201	A2204	C2205	C2206	U2211	U2212	G2213	G2214	G2217	G2218	U2219	G2220	G2221	U2222	U2223	U2224	G2225	A2226	C2227	U2228	G2229	G2234	U2235	U2236	C2237	C2238	C2239	C2240	U2241	C2242	C2243	C2244	A2245	A2246	A2247	U2248	U2249	U2250	U2251	G2255	G2256	A2257	G2258	C2259	C2260	C2261	C2262	A2265	A2266	A2267	C2268	C2269	C2271	C2272	C2273	C2274	C2275	C2276	A2277	U2278	G2279	U2285	U2286	C2287	A2288	U2298	A2299	G2300	A2301	G2302	A2307	A2308	G2309	G2310	U2311	U2312	A2313	C2314	A2315	G2316	G2317	U2318	G2319	G2320	C2321	U2322	U2323	G2324	C2325	C2326	U2327	G2328	C2329	G2330	A2331	G2332	A2333	C2334	C2343	G2344	A2348	G2349	C2353	C2354	G2355	A2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	A2364	U2365	U2366	A2367	G2368	C2369	U2370	G2371	A2372	C2373	U2376	U2377	G2378	G2379	U2380	A2381	C2382	C2383	G2384	U2385	G2389	A2390	G2391	G2392	G2393	G2394	C2395	C2396	A2397	U2398	A2401	U2402	C2403	A2404	A2405	C2406	G2407	G2408	A2409	U2410	A2411	A2412	A2413	A2414	U2417	A2418	U2419	C2420	C2421	A2422	G2423	G2424	G2425	G2426	A2427	U2428	C2429	A2430	U2431	C2432	G2433	C2434	G2435	U2436	G2437	A2438	U2439	C2440	C2444	C2445	C2446	G2447	A2448	C2449	A2450	G2451	C2454	A2455	U2456	A2457	U2458	C2459	G2460	G2463	G2464	G2465	A2466	A2467	G2468	G2469	U2470	U2471	U2472	G2473	G2474	C2475	A2476	C2477	U2478	G2479	C2480	G2481	A2482	U2483	G2484	G2485	G2486	G2487	G2488	G2489	A2490	U2491	U2492	U2493	C2494	C2495	U2496	U2497	U2498	U2499	U2500	U2501	G2502	G2503	G2504	G2505	G2508	A2509	A2510	G2511	A2512	A2513	G2514	U2515	U2516	C2517	A2521	G2522	G2523	G2524	U2525	U2526	G2527	G2528	G2529	C2530	U2533	U2534	C2535	G2536	C2537	C2538	C2539	A2540	A2544	A2545	G2546	C2547	G2548	G2549	C2550	A2551	C2552	G2553	C2554	G2555	U2559	U2560	G2561	G2562	U2563	U2564	C2565	A2566	C2570	G2571	U2572	C2573	G2574	U2575	G2576	A2577	U2578	A2579	C2580	A2581	U2582	C2585	U2586	U2587	U2588	C2589	U2590	C2591	U2592	A2593	U2594	C2595	G2596	C2597	C2598	U2599	A2600	C2601	G2602	G2603	G2604	C2605	G2606	A2607	A2608	G2609	U2615	U2616	G2617	A2618	U2619	G2620	G2621	G2622	A2623	G2624	U2625	C2628	U2629	A2633	G2634	U2635	A2636	A2639	G2640	A2641	G2642	G2643	C2646	U2651	A2652	G2658	C2659	G2660	G2661	U2666	G2667	U2668	C2669	C2670	U2674	U2675	U2676	U2677	G2678	G2679	U2680	A2681	C2682	C2686	G2687	G2688	C2689	A2690	C2691	U2692	A2693	G2694	C2695	G2698	G2699	U2700	C2703	U2704	A2705	U2706	U2707	U2708	C2709	C2710	U2711	G2712	G2713	A2714	U2715	G2717	A2718	C2719	C2720	A2721	U2725	U2726	G2727	A2728	U2729	A2730	G2731	C2732	C2735	U2736	A2737	G2740	G2741	G2742	A2743	G2744	A2745	C2754	A2755	A2756	G2757	U2758	U2759	G2760	A2761	G2762	U2766	C2767	C2768	C2769	A2770	C2771	U2772	G2773	U2774	U	U	A
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• Molecule 2: tRNA acceptor stem mimic

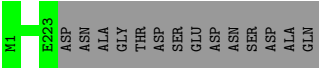
Chain 5:  29%  40%  29%



- Molecule 3: 50S ribosomal protein L16



- Molecule 4: GENERAL STRESS PROTEIN CTC



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 409.90Å 695.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	60249	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPU

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	0.25	0/66467	0.50	7/103673 (0.0%)
2	5	0.25	0/563	0.50	0/873
All	All	0.25	0/67030	0.50	7/104546 (0.0%)

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	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	0	2426	G	C2'-C3'-O3'	6.11	118.67	109.50
1	0	192	G	C2'-C3'-O3'	5.89	118.34	109.50
1	0	71	A	C2'-C3'-O3'	5.78	118.17	109.50
1	0	242	A	C2'-C3'-O3'	5.74	118.11	109.50
1	0	583	C	C2'-C3'-O3'	5.58	117.87	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	873	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	0	59359	0	29917	1715	0
2	5	543	0	290	11	0
3	K	124	0	0	0	0
4	T	223	0	0	0	0
All	All	60249	0	30207	1722	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 19.

The worst 5 of 1722 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)
1:0:940:G:H3'	1:0:941:U:H5''	1.22	1.14
1:0:1141:U:H3	1:0:2008:C:H5''	1.20	1.04
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.01
1:0:2548:G:H2'	1:0:2549:G:H5''	1.44	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.21	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	413 (14%)	44 (1%)
2	5	22/35 (62%)	2 (9%)	0
All	All	2779/2915 (95%)	415 (14%)	44 (1%)

5 of 415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1807	A
1	0	2245	A
1	0	1820	G
1	0	2093	G
1	0	2377	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	PPU	5	35	2	37,40,41	2.63	7 (18%)	47,57,60	0.99	4 (8%)

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
2	PPU	5	35	2	-	1/25/43/44	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	C-N3'	12.76	1.61	1.34
2	5	35	PPU	OC-CM	-5.27	1.28	1.42
2	5	35	PPU	CE1-CZ	3.90	1.46	1.38
2	5	35	PPU	CE2-CZ	2.86	1.44	1.38
2	5	35	PPU	CD2-CG	2.75	1.44	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C2-N1-C6	3.30	119.89	111.83
2	5	35	PPU	CM-OC-CZ	2.91	123.75	117.50
2	5	35	PPU	C9-N6-C6	2.35	126.49	120.52
2	5	35	PPU	C-CA-N	2.27	117.94	109.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	35	PPU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.