# wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:07 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1NJN |
| Title | : | The crystal structure of the 50S Large ribosomal subunit from Deinococcus radiodurans complexed with the antibiotic sparsomycin |
| Authors | : | Bashan, A.; Agmon, I.; Zarivatch, R.; Schluenzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A. |
| Deposited on | : | 2003-01-02 |
| Resolution | : | 3.70 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 (i) symbol.

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

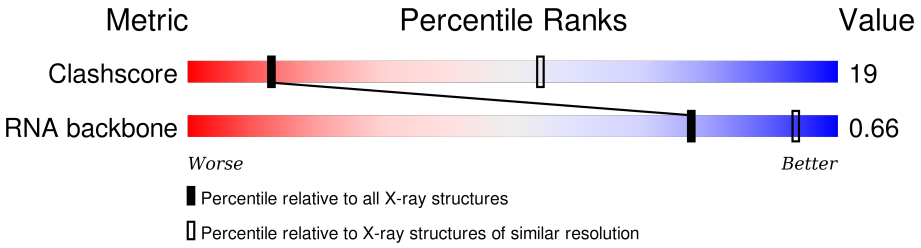
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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 | 102246 | 1224 (3.90-3.50) |
| RNA backbone | 2183 | 1067 (4.60-2.80) |

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 <=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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0 | 2880 | 34% 51% 11% • |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 2 | SPS | 0 | 2881 | X | - | - | - |

## 2 Entry composition

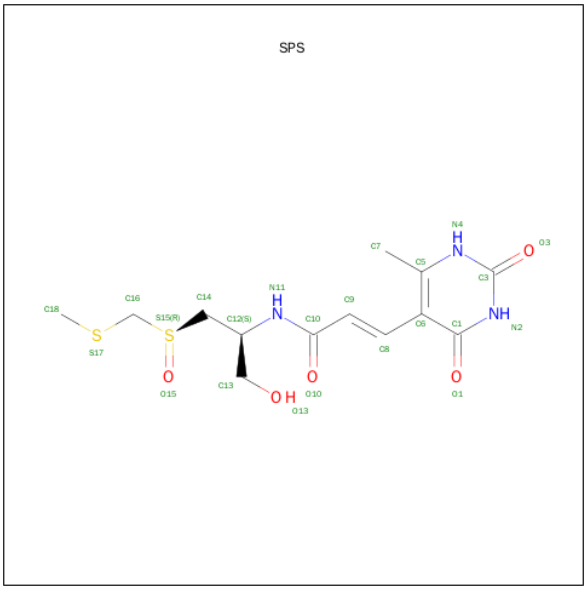
There are 2 unique types of molecules in this entry. The entry contains 59381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | 0 | 2766 | 59359 | 26479 | 10949 | 19166 | 2765 | 0 | 0 | 0 |

- Molecule 2 is SPARSOMYCIN (three-letter code: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 0 | 1 | 22 | 13 | 3 | 4 | 2 | 0 | 0 |

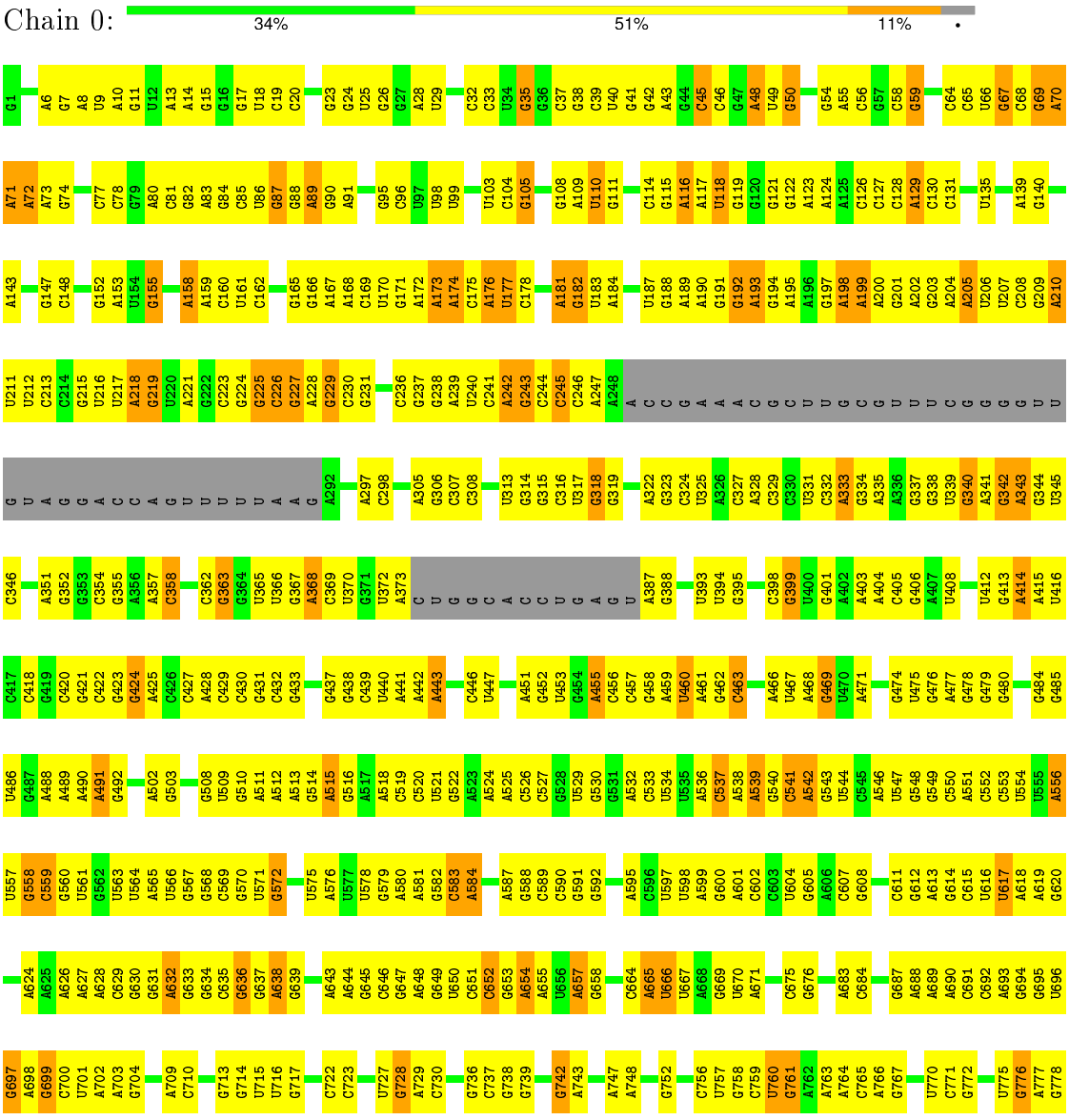
# 3 Residue-property plots (i)

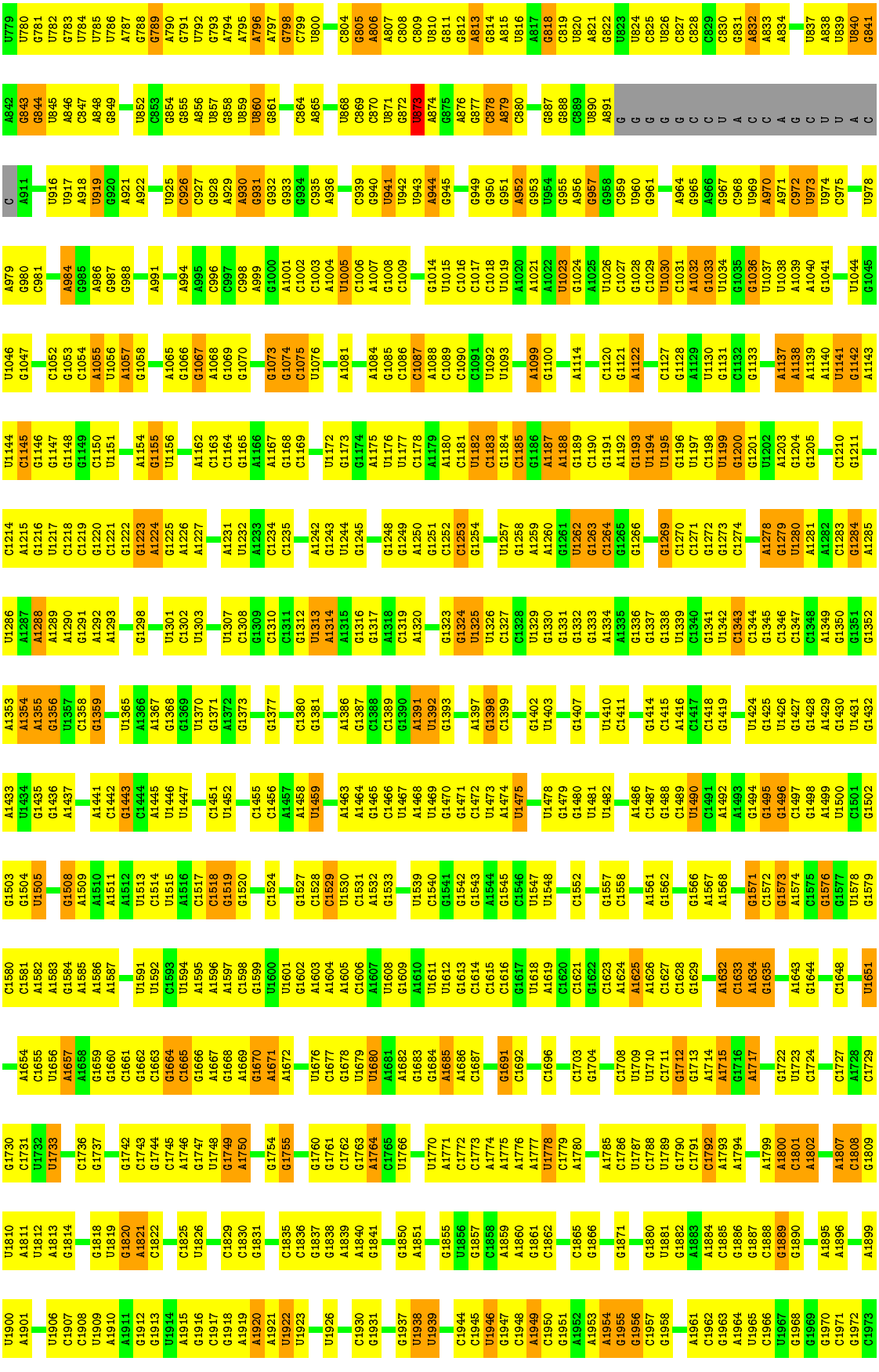
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 (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.

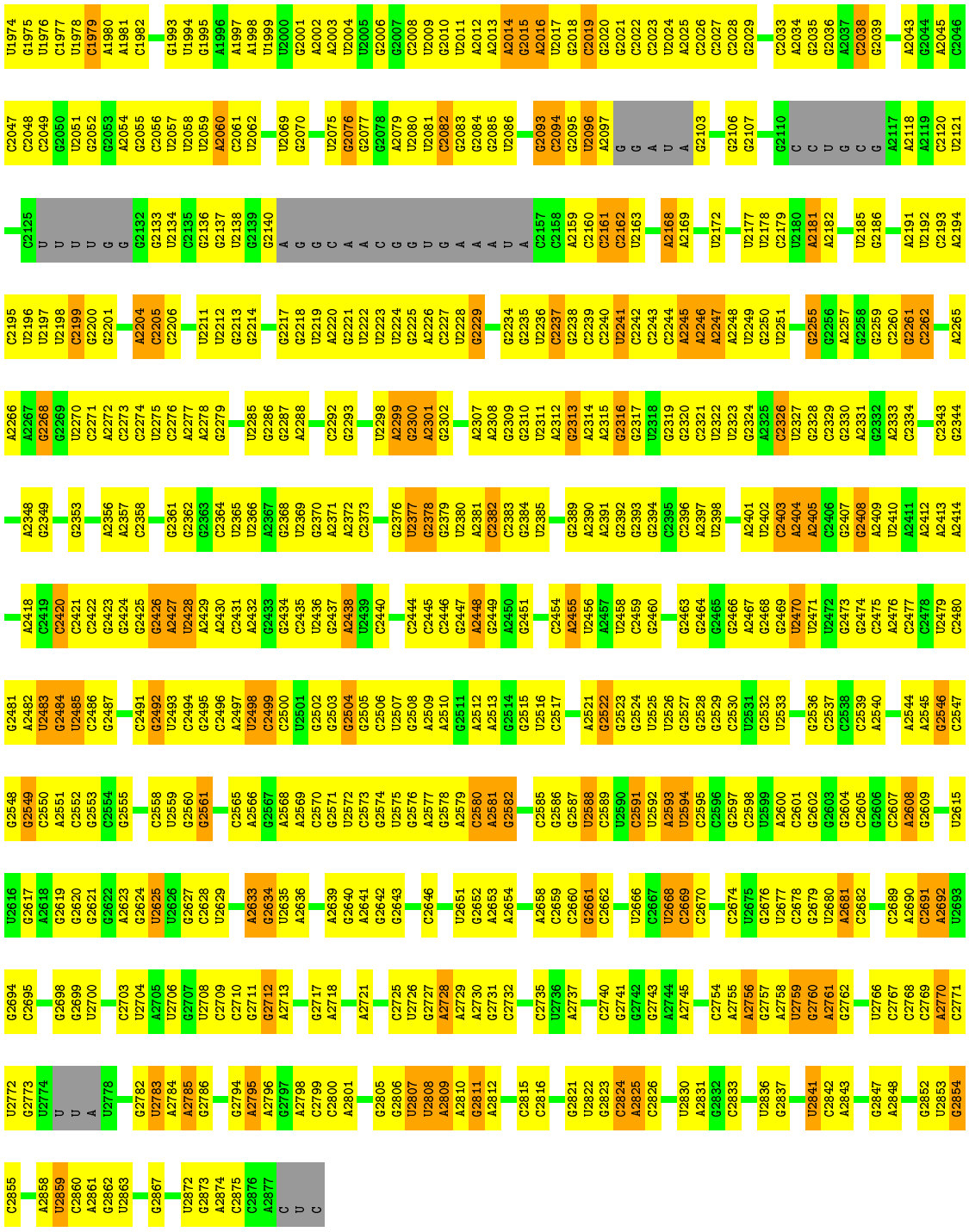
Note EDS was not executed.

- Molecule 1: 23S ribosomal RNA

Chain 0:






U1974 G1975 U1976 C1977 U1978 C1979 A1980 A1981 C1982 G1993 U1994 G1995 A1996 A1997 A1998 U1999 U2000 G2001 A2002 A2003 U2004 U2005 G2006 G2007 C2008 U2009 G2010 U2011 A2012 A2013 A2014 G2015 A2016 U2017 G2018 C2019 G2020 G2021 C2022 C2023 U2024 A2025 C2026 C2027 C2028 G2029 C2033 A2034 G2035 G2036 A2037 C2038 G2039 A2043 G2044 A2045 C2046
C2047 C2048 C2049 G2050 U2051 G2052 G2053 A2054 G2055 C2056 U2057 U2058 U2059 A2060 C2061 U2062 U2069 G2070 U2075 G2076 G2077 G2078 A2079 U2080 U2081 C2082 G2083 G2084 G2085 U2086 G2093 C2094 G2095 U2096 A2097 G C G A U A G2103 G2106 G2107 G2110 C C C U G C G A2117 A2118 A2119 C2120 U2121
C2125 U U U U U G G G2132 G2133 U2134 C2135 G2136 G2137 U2138 G2139 G2140 A G G G C A A C G G U G A A 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 A2220 G2221 U2222 U2223 U2224 G2225 A2226 C2227 U2228 G2229 G2234 G2235 U2236 C2237 G2238 C2239 C2240 U2241 C2242 C2243 C2244 A2245 A2246 A2247 A2248 U2249 G2250 U2251 G2255 G2256 A2257 G2258 G2259 C2260 G2261 C2262 A2265
A2266 A2267 G2268 G2269 U2270 C2271 A2272 C2273 C2274 U2275 C2276 A2277 A2278 G2279 U2285 G2286 G2287 A2288 C2292 G2293 U2298 A2299 G2300 A2301 G2302 A2307 A2308 G2309 G2310 U2311 A2312 G2313 A2314 A2315 G2316 G2317 U2318 G2319 G2320 C2321 U2322 U2323 G2324 A2325 C2326 U2327 G2328 C2329 G2330 A2331 G2332 A2333 C2334 C2343 G2344
A2348 G2349 G2353 A2356 A2357 C2358 G2361 G2362 G2363 C2364 U2365 U2366 A2367 G2368 U2369 G2370 A2371 A2372 C2373 G2376 U2377 G2378 G2379 U2380 A2381 C2382 C2383 G2384 U2385 G2389 A2390 A2391 G2392 G2393 G2394 C2395 C2396 A2397 U2398 A2401 U2402 C2403 A2404 A2405 C2406 G2407 G2408 A2409 U2410 A2411 A2412 A2413 A2414
A2418 C2419 C2420 C2421 C2422 G2423 G2424 G2425 G2426 A2427 U2428 A2429 A2430 C2431 A2432 G2433 G2434 C2435 U2436 G2437 A2438 U2439 C2440 C2444 C2445 C2446 G2447 A2448 G2449 A2450 G2451 C2454 A2455 U2456 A2457 U2458 C2459 G2460 G2463 G2464 G2465 G2466 A2467 G2468 G2469 U2470 U2471 U2472 G2473 G2474 C2475 A2476 C2477 C2478 U2479 C2480
G2481 A2482 U2483 G2484 U2485 C2486 G2487 C2491 G2492 U2493 C2494 G2495 C2496 A2497 U2498 C2499 C2500 U2501 G2502 G2503 G2504 G2505 C2506 U2507 G2508 A2509 A2510 G2511 A2512 A2513 G2514 G2515 C2516 C2517 A2521 G2522 G2523 G2524 U2525 U2526 G2527 G2528 G2529 C2530 U2531 G2532 U2533 G2536 C2537 C2538 G2539 A2540 A2544 A2545 G2546 C2547
G2548 G2549 C2550 A2551 C2552 G2553 C2554 G2555 C2558 U2559 G2560 G2561 C2565 A2566 G2567 A2568 A2569 C2570 G2571 U2572 C2573 G2574 U2575 G2576 A2577 G2578 A2579 C2580 A2581 G2582 C2585 G2586 G2587 U2588 C2589 U2590 C2591 U2592 A2593 U2594 C2595 C2596 G2597 C2598 U2599 A2600 C2601 G2602 G2603 G2604 C2605 G2606 C2607 A2608 G2609 U2615
U2616 G2617 A2618 G2619 G2620 G2621 G2622 A2623 G2624 G2625 U2626 G2627 C2628 U2629 A2633 G2634 U2635 A2636 A2639 G2640 A2641 G2642 G2643 C2646 U2651 G2652 A2653 A2654 A2658 C2659 C2660 G2661 C2662 U2666 C2667 U2668 C2669 C2670 C2674 U2675 G2676 U2677 C2678 G2679 U2680 A2681 C2682 C2689 A2690 C2691 A2692 U2693
G2694 C2695 G2698 G2699 U2700 C2703 U2704 A2705 U2706 G2707 U2708 C2709 C2710 G2711 G2712 A2713 G2717 A2718 A2721 C2725 U2726 G2727 A2728 A2729 A2730 G2731 C2732 C2735 U2736 A2737 C2740 G2741 G2742 G2743 A2744 A2745 C2754 A2755 A2756 G2757 A2758 U2759 G2760 A2761 G2762 C2766 C2767 C2768 C2769 A2770 C2771
U2772 G2773 U2774 U U U A U2778 G2782 U2783 A2784 A2785 G2786 G2794 A2795 A2796 G2797 A2798 C2799 C2800 A2801 G2805 G2806 U2807 U2808 A2809 A2810 G2811 A2812 C2815 C2816 G2821 U2822 G2823 C2824 A2825 C2826 U2830 A2831 G2832 C2833 U2836 G2837 U2841 C2842 A2843 G2847 A2848 G2852 U2853 G2854
C2855 A2858 U2859 C2860 A2861 G2862 U2863 G2867 U2872 G2873 A2874 C2875 C2876 A2877 C U C

# 4 Data and refinement statistics (i)

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

| Property | Value | Source |
|---|---|---|
| Space group | I 2 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 169.10Å 409.90Å 696.30Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 3.70 | Depositor |
| % Data completeness<br>(in resolution range) | (Not available) (15.00-3.70) | Depositor |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.13 | Depositor |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.284 , 0.308 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 59381 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 82.0 | 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: SPS

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 | 0.14 | 0/66467 | 0.63 | 0/103673 |

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.

There are no bond angle outliers.

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

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 | 1711 | 0 |
| 2 | 0 | 22 | 0 | 19 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 59381 | 0 | 29936 | 1711 | 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 1711 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" | 1.24 | 1.14 |
| 1:0:1073:G:H2' | 1:0:1074:G:H4' | 1.39 | 1.02 |
| 1:0:2769:C:H2' | 1:0:2867:G:H22 | 1.23 | 1.01 |
| 1:0:1141:U:H3 | 1:0:2008:C:H5" | 1.22 | 1.01 |
| 1:0:2548:G:H2' | 1:0:2549:G:H5" | 1.44 | 0.99 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 0 | 2757/2880 (95%) | 413 (14%) | 39 (1%) |

5 of 413 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 |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 49 | U |

5 of 39 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 1279 | G |
| 1 | 0 | 1518 | C |
| 1 | 0 | 2668 | U |
| 1 | 0 | 1313 | U |
| 1 | 0 | 1354 | A |

## 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)

1 ligand 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 | SPS | 0 | 2881 | - | 17,22,23 | 4.43 | 9 (52%) | 16,28,30 | 4.27 | 9 (56%) |

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 | SPS | 0 | 2881 | - | 1/1/2/6 | 2/15/16/18 | 0/1/1/1 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 0 | 2881 | SPS | C7-C5 | 2.48 | 1.55 | 1.50 |
| 2 | 0 | 2881 | SPS | C9-C10 | 3.01 | 1.54 | 1.48 |
| 2 | 0 | 2881 | SPS | C6-C8 | 3.85 | 1.55 | 1.47 |
| 2 | 0 | 2881 | SPS | C1-N2 | 5.03 | 1.42 | 1.33 |
| 2 | 0 | 2881 | SPS | C10-N11 | 5.11 | 1.50 | 1.34 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 0 | 2881 | SPS | C12-N11-C10 | -7.90 | 111.98 | 122.58 |
| 2 | 0 | 2881 | SPS | O10-C10-C9 | -6.92 | 109.69 | 123.01 |
| 2 | 0 | 2881 | SPS | C8-C9-C10 | -5.49 | 109.64 | 121.63 |
| 2 | 0 | 2881 | SPS | C6-C8-C9 | -5.17 | 109.95 | 127.09 |
| 2 | 0 | 2881 | SPS | C14-C12-C13 | -2.09 | 108.36 | 111.44 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 2 | 0 | 2881 | SPS | C12 |

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | 0 | 2881 | SPS | C9-C10-N11-C12 |
| 2 | 0 | 2881 | SPS | O10-C10-N11-C12 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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

## 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

## 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

## 6.4 Ligands

EDS was not executed - this section will therefore be empty.

## 6.5 Other polymers

EDS was not executed - this section will therefore be empty.