



# wwPDB X-ray Structure Validation Summary Report ⓘ

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.; Schlutzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.  
Deposited on : 2003-01-02  
Resolution : 3.70 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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) : **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

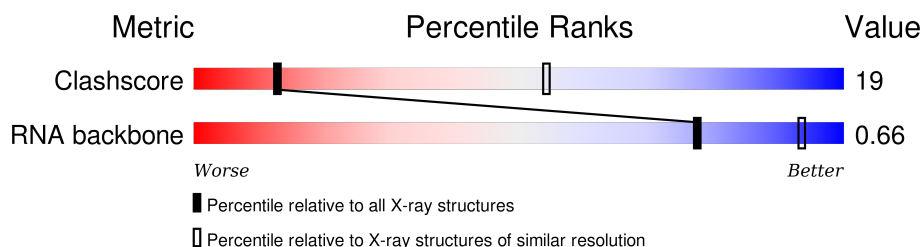
# 1 Overall quality at a glance

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	

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 [i](#)

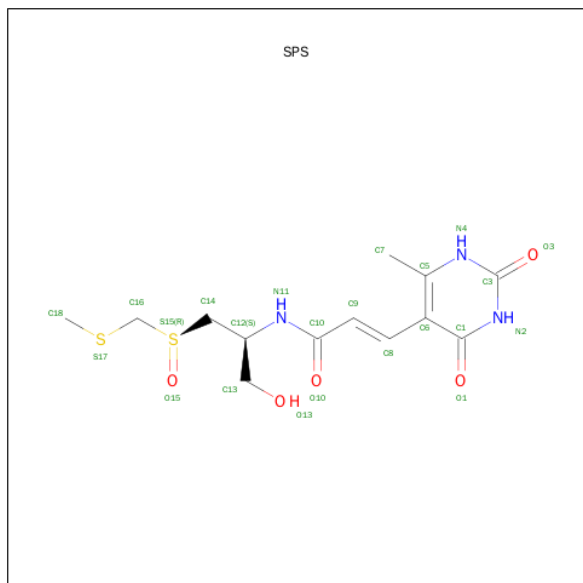
There are 2 unique types of molecules in this entry. The entry contains 59381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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<sub>13</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>S<sub>2</sub>).



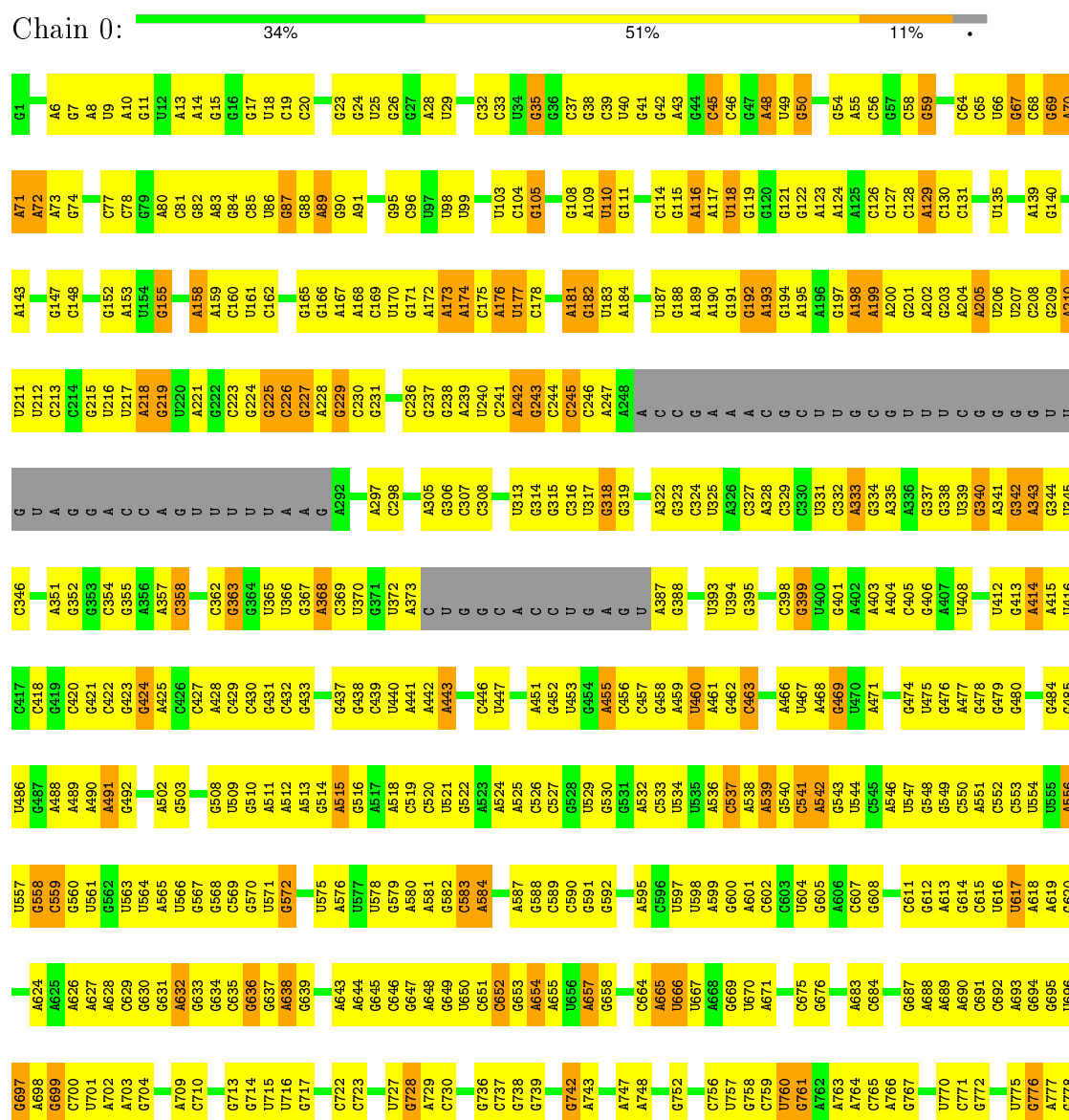
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	0	1	22	13	3	4	2	0	0

### 3 Residue-property plots

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



U1900	U1810	G1730	G1503	A1363	U1286	C1214	U1046	A979	C	A842	U779
A1901	A1811	C1731	G1504	A1364	A1287	A1215	G1047	G980		G843	U780
U1906	U1812	C1732	U1505	A1365	A1288	G1356		C981		G844	G781
C1907	A1813	U1733	G1508	G1436	A1289	U1217	C1052			U845	U782
C1908	G1814	A1658	G1509	U1437	G1290	G1357	G1053	A984		A846	G783
U1909	G1818	A1659	A1509	A1441	G1291	G1218	G1054	G985		C847	U784
A1910	U1819	G1659	A1510	C1442	A1290	C1219	A1055	A986		C848	U785
A1911	G1820	C1661	A1511	C1443	A1292	G1220	A1056	A987		A848	U786
G1912	C1821	G1742	A1512	G1444	A1293	C1221	U1057	G988		G849	
G1913	C1822	C1743	U1513	A1445	G1298	G1223	G1058	A991		U852	G788
A1914	C1825	G1745	U1514	A1446	U1301	A1224	A1065			C853	G789
A1915	U1826	A1665	A1515	U1447	C1302	G1225	G1066	A994		G854	A790
G1916		G1666	U1516	U1447	U1303	A1226	G1067	A995		G855	A791
C1917		A1667	C1517	U1447	U1307	A1227	A1068	C996		A856	U792
G1918	C1829	U1748	U1518	C1451	U1308	C1231	G1069	C997		U857	G793
A1919	U1830	A1668	G1519	A1452	U1309	A1232	A1070	C998		G858	A794
C1920	G1831	A1750	G1520	G1373	G1308	U1232	G1071	C999		U859	A795
A1921		G1670	U1521	G1373	A1309	A1233	G1072	A999		U860	A796
U1922	C1835	G1754	C1524	G1377	G1310	C1234	G1073	G1000		G861	A797
U1923	C1836	A1671	U1527	A1457	G1311	G1235	G1074	A1001		C864	G798
U1926	G1837	A1672	G1528	A1458	G1312	A1242	G1075	C1002		A865	U800
	G1838	U1677	C1529	U1459	U1313	A1243	U1076	C1003			
C1930	A1839	G1678	U1530	A1463	A1314	U1244	A1081	C1004		U868	C804
G1931	A1840	U1679	G1531	A1464	G1315	G1245	A1084	C1006		C869	G805
	G1841	U1680	A1532	G1465	G1316		G1085	A1007		C870	A806
G1937		C1765	G1533	G1466	G1317	G1248	G1086	C1008		U871	A807
U1938	G1850	A1681	U1539	A1467	A1318	G1249	G1087	C1009		G872	C808
U1939	A1851	U1682	C1540	A1468	A1320	A1250	C1088			U873	C809
	G1855	G1684	G1541	U1469	A1323	G1251	A1088	G1014		A874	U810
C1944	U1856	U1771	G1542	G1471	G1324	C1252	C1089	U1015		G875	G811
G1945	G1857	A1685	G1543	C1472	G1325	G1253	C1090	C1016		A876	G812
U1946	C1858	A1686	A1544	A1473	U1326	G1254	C1091	C1017		A877	A813
G1947	A1859	G1691	U1545	U1474	U1327	U1257	C1092	C1018		C878	G814
C1948	A1860	C1692	G1546	U1475	G1328	G1258	U1093	U1019		A879	A815
A1949	G1861	U1696	U1547	U1478	U1329	A1259	A1099	A1020		C880	U816
C1950	C1862	C1696	U1548	U1478	G1330	A1260	G1100	A1021			A817
G1951		U1703	C1552	G1479	G1331	G1261		A1022		G887	G818
A1953	G1866	G1704	G1557	G1480	G1332	U1262	A1114	U1023		G888	C819
A1954	G1871	C1708	C1558	U1481	G1333	G1263		G1024		C889	U820
G1955		A1624	G1561	U1482	G1334	C1264		A1025		U890	A821
G1956	G1880	U1709	A1562	A1486	A1335	G1265		U1026		A891	G822
C1957	U1881	C1711	G1566	C1487	G1336	G1266		C1027		G	U823
	G1882	G1712	A1567	C1488	U1337			U1028		G	U824
A1961	A1883	C1713	G1568	C1489	G1338	G1269		C1029		G	C825
C1962	G1884	A1714	A1569	C1490	U1339	C1270		U1030		G	U826
G1963	C1885	U1715	A1570	C1491	G1340	C1271		C1031		G	C827
A1964	G1886	A1716	A1571	C1492	G1341	C1272		A1032		C	C828
U1965	G1887	A1717	A1572	A1493	U1342	G1273		U1034		C	C829
C1966	G1888	A1718	C1573	G1494	C1343	C1274		G1035		U	C830
G1969	G1890	C1722	G1574	G1495	G1344			U1036		C	G831
	A1895	U1723	A1575	G1496	C1345	A1278		U1037		C	A832
C1970	A1896	G1724	C1576	C1497	G1346	G1279		A1038		C	A833
G1971		A1802	G1577	C1498	C1347	U1280		A1039		A	A834
C1972		C1648	U1578	A1499	G1348	A1281		C972		C	
		A1807	C1579	U1500	A1349	A1282		U973		G	U837
		U1728	U1579	C1501	A1350	G1283		U974		U	A838
		C1729	G1579	U1502	G1352	G1284		C975		A	U839
					G1352	A1285		U1044		C	U840
								G1045			G841

C2855	U2772	G2694	U2616	G2548	G2481	G2617	G2549	G2695	G2618	G2694	G2482	G2619	G2550	G2483	A2418	A2348	A2266	C2195	C2047	U1974
A2858	G2773	C2695	G2549	G2549	A2482	G2617	G2549	C2695	A2618	A2483	A2482	G2618	C2550	U2483	C2419	A2349	A2267	C2125	C2048	G1975
C2860	U2774	G2698	C2550	C2550	U2483	G2618	C2550	G2698	C2420	U2484	U2483	G2619	A2551	G2484	C2420	G2349	G2268	U	C2049	U1976
A2861	U	G2699	A2551	A2551	G2484	G2620	A2551	G2699	C2421	U2485	U2484	G2621	C2552	U2485	C2421	G2353	G2269	U	G2050	C1977
G2862	A	U2700	G2552	G2552	U2486	G2621	G2552	U2700	C2422	U2486	U2485	G2622	C2553	U2486	C2422	G2356	C2271	U	U2051	U1978
U2863	U2778	G2703	G2554	G2554	G2487	G2622	G2554	G2703	G2423	U2487	U2486	G2623	C2555	G2487	G2423	A2356	A2272	G	G2052	C1979
		C2704	G2555	G2555		A2623	G2555	C2704	G2424			G2624	G2556		G2424	A2357	C2273	C	A2054	A1980
		U2704			C2491	G2624		U2704	G2425	C2491		G2625	G2558	C2492	G2425	C2358	C2274	A	A2054	A1981
		A2705			U2492	U2625		A2705	G2426	U2492		U2626	C2558	U2493	G2426	C2359	U2275	G	G2055	
		G2706			U2493	U2626		G2706	A2427	U2493		U2627	C2559	U2494	A2427	G2361	U2276	G	C2056	G1993
		U2707			C2494	U2627		U2707	U2428	C2494		U2628	C2560	U2495	A2428	G2362	A2277	U	U2057	U1994
		C2708			U2495	U2628		C2708	A2429	U2495		U2629	G2561	U2496	A2429	G2363	A2278	U	U2058	G1995
		U2709			U2496	U2629		U2709	A2430	U2496		U2630		C2496	A2430	C2364	U2212	A	A2060	A1996
		C2710						C2710	G2431			U2631	C2565	U2497	A2431	C2365	U2213	U	C2061	A1997
		G2711			U2497			G2711	G2432	U2497		U2632	C2566	U2498	A2432	C2366	G2214	U	U2062	A1998
		A2712			C2499			A2712	G2433	C2499		U2633	G2567	U2499	G2433	A2367	U2215	G	U2069	U2000
		G2713			C2500			G2713	G2434	C2500		U2634	C2568	C2500	G2434	G2368	U2216	A	G2070	G2001
		A2714			U2501			A2714	C2435	U2501		U2635	C2569	U2501	C2435	U2369	U2217	C	A2002	A2002
		U2715			C2502			U2715	U2436	C2502		U2636	C2570	U2502	U2436	G2370	U2218	G	A2003	A2003
		G2716			G2503			G2716	A2437	G2503		U2637	C2571	G2503	A2437	A2371	U2219	C	G2075	A2004
		C2717			U2504			C2717	U2438	U2504		U2638	C2572	G2504	A2438	A2372	U2220	A	U2076	G2005
		A2718			G2505			A2718	U2439	G2505		U2639	C2573	G2505	U2439	C2373	U2221	A	G2077	U2005
		U2719			C2506			U2719	C2440	C2506		U2640	C2574	G2506	C2440		U2222	C	G2078	G2006
		C2800			U2507			C2800		U2507		U2641	C2575	C2507		G2376	U2223	G	U2079	G2007
		A2801			G2508			A2801		G2508		U2642	C2576	U2508		U2377	U2224	U	U2080	C2008
		G2806			C2509			G2806		C2509		U2643	C2577	G2509		U2378	U2225	G	U2081	U2009
		U2807			U2510			U2807		U2510		U2644	C2578	A2510		U2379	U2226	U	U2082	U2010
		C2808			G2511			C2808		G2511		U2645	C2579	G2511		U2380	U2227	G	G2083	U2011
		A2809			U2512			A2809		U2512		U2646	C2580	G2512		U2381	U2228	A	G2084	A2012
		U2810			C2513			U2810		C2513		U2647	C2581	U2513		U2382	U2229	A	G2085	A2013
		G2811			U2514			G2811		U2514		U2648	C2582	G2514		U2383	U2230	A	A2014	A2014
		A2812			G2515			A2812		G2515		U2649	C2583	U2515		U2384	U2231	U	U2086	G2015
		C2815			U2516			C2815		U2516		U2650	C2584	G2516		U2385	U2232	A	G2093	G2016
		G2816			C2517			G2816		C2517		U2651	C2585	U2517		U2386	U2233	C	C2094	U2017
		U2821			U2518			U2821		U2518		U2652	C2586	G2518		U2387	U2234	C	G2095	U2018
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		A2824			C2521			A2824		C2521		U2655	C2589	G2521		U2390	U2237	G	G	G2021
		C2825			U2522			C2825		U2522		U2656	C2590	G2522		U2391	U2238	U	A	C2022
		G2826			G2523			G2826		G2523		U2657	C2591	G2523		U2392	U2239	A	U	C2023
		U2830			U2524			U2830		U2524		U2658	C2592	G2524		U2393	U2240	A	A	U2024
		A2831			C2525			A2831		C2525		U2659	C2593	G2525		U2394	U2241	A	A	A2025
		C2832			U2526			C2832		U2526		U2660	C2594	G2526		C2395	U2242	A	A	C2026
		U2833			U2527			U2833		U2527		U2661	C2595	G2527		C2396	U2243	A	A	C2027
		G2834			C2528			G2834		C2528		U2662	C2596	G2528		C2397	U2244	A	A	C2028
		A2835			U2529			A2835		U2529		U2663	C2597	G2529		U2398	U2245	U	G2103	G2029
		C2836			G2530			C2836		G2530		U2664	C2598	G2530		U2399	U2246	U	G2106	
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		A2839			U2533			A2839		U2533		U2667	C2601	G2533		U2403	U2249	C	C	A2034
		U2840			G2534			U2840		G2534		U2668	C2602	G2534		U2404	U2250	U	C	G2035
		C2841			U2535			C2841		U2535		U2669	C2603	G2535		U2405	U2251	C	C	G2036
		G2842			C2536			G2842		C2536		U2670	C2604	G2536		U2406	U2252	U	C	A2037
		A2843			U2537			A2843		U2537		U2671	C2605	G2537		U2407	U2253	C	C	C2038
		C2844			G2538			C2844		G2538		U2672	C2606	G2538		U2408	U2254	U	C	G2039
		U2845			U2539			U2845		U2539		U2673	C2607	G2539		U2409	U2255	C	A	
		G2846			C2540			G2846		C2540		U2674	C2608	G2540		U2410	U2256	A	A	
		A2847			U2541			A2847		U2541		U2675	C2609	G2541		U2411	U2257	U	A	
		C2848			C2542			C2848		C2542		U2676	C2610	G2542		U2412	U2258	U	A	
		U2849			U2543			U2849		U2543		U2677	C2611	G2543		U2413	U2259	U	A	
		G2850			G2544			G2850		G2544		U2678	C2612	G2544		U2414	U2260	U	A	
		C2851			U2545			C2851		U2545		U2679	C2613	G2545		U2415	U2261	U	A	
		U2852			C2546			U2852		C2546		U2680	C2614	G2546		U2416	U2262	U	A	
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		U2855			U2549			U2855		U2549		U2683	C2617	G2549		U2419	U2265	U	A	
		G2856			C2550			G2856		C2550		U2684	C2618	G2550		U2420	U2266	U	A	
		U2857			U2551			U2857		U2551		U2685	C2619	G2551		U2421	U2267	U	A	
		C2858			C2552			C2858		C2552		U2686	C2620	G2552		U2422	U2268	U	A	
		U2859			U2553			U2859		U2553		U2687	C2621	G2553		U2423	U2269	U	A	
		G2860			C2554			G2860		C2554		U2688	C2622	G2554		U2424	U2270	U	A	
		A2861			U2555			A2861		U2555		U2689	C2623	G2555		U2425	U2271	U	A	
		G2862			C2556			G2862		C2556		U2690	C2624	G2556		U2426	U2272	U	A	
		U2863			U2557			U2863		U2557		U2691	C2625	G2557		U2427	U2273	U	A	
		G2864			C2558			G2864		C2558		U2692	C2626	G2558		U2428	U2274	U	A	
		A2865			U2559			A2865		U2559		U2693	C2627	G2559		U2429	U2275	U	A	
		G2866			C2560			G2866		C2560		U2694	C2628	G2560		U2430	U2276	U	A	
		U2867			U2561			U2867		U2561		U2695	C2629	G2561		U2431	U2277	U	A	
		G2868			C2562			G2868		C2562		U2696	C2630	G2562		U2432	U2278	U	A	
		A2869			U2563			A2869		U2563		U2697	C2631	G2563		U2433	U2279	U	A	
		G2870			C2564			G2870		C2564		U2698	C2632	G2564		U2434	U2280	U	A	
		U2871																		

## 4 Data and refinement statistics

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 a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.10 Å   409.90 Å   696.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	15.00 – 3.70	Depositor
% Data completeness (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 <sup>2</sup> )	82.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 [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	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(°)	Ideal(°)
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.