



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NJM
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a tRNA acceptor stem mimic (ASM) and 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 : 3.60 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) : **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

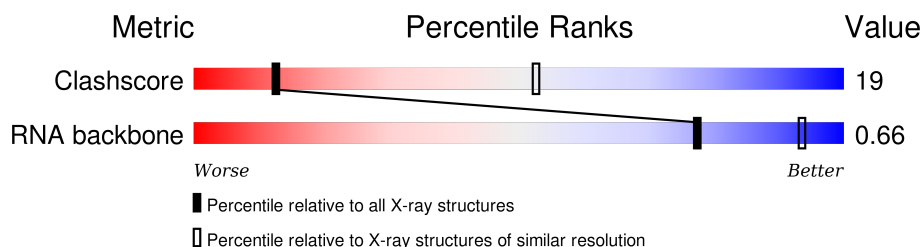
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1010 (3.74-3.46)
RNA backbone	2183	1058 (4.40-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	 33% 51% 11% .
2	5	35	 26% 40% 6% 29%
3	K	141	 88% 12%
4	T	237	 94% 6%

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
5	SPS	0	2881	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60271 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			

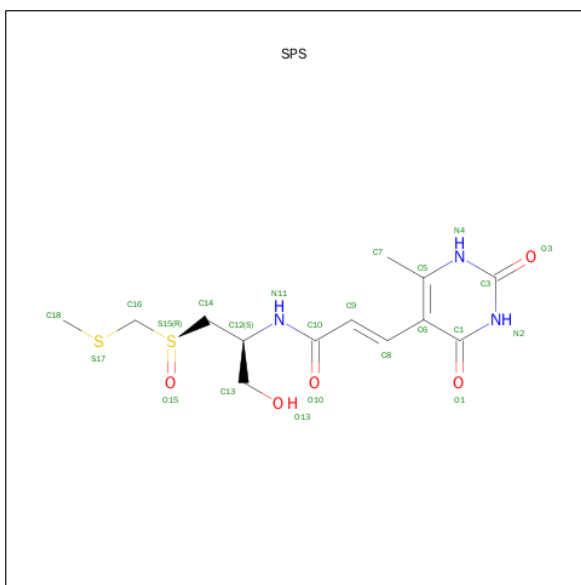
- Molecule 3 is a protein called 50S ribosomal protein L16.

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			

- Molecule 5 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	0	1	Total	C	N	O	S	0	0
			22	13	3	4	2		

A1910	G1818	G1737	A1658	A1586	G1508	A1441	G1369	A1289	G1217	G1142	G1045	U978	C	U840	G778
A1911	U1819	G1742	G1659	A1587	A1509	C1442	U1365	A1290	U1218	A1143	U1046	A979	A911	G841	U779
G1912	G1820	G1743	G1660	U1591	A1510	G1443	U1366	G1291	C1219	U1144	G1047	G980	U916	G842	U780
G1913	A1821	C1743	C1661	U1592	A1511	C1444	A1366	A1292	C1218	G1145	C1052	C981	U917	G843	G781
U1914	C1822	G1745	G1662	U1593	A1512	U1445	A1367	A1293	C1219	G1146	G1053	A984	U918	G844	U782
A1915	C1825	G1746	C1663	U1594	U1513	U1446	G1368	G1298	C1221	G1147	G1054	G985	U919	U845	G783
G1916	U1826	G1747	G1664	A1595	C1514	U1447	G1369	U1298	G1222	G1148	G1055	A986	U920	A846	U784
C1917	G1665	G1748	G1665	A1596	U1515	U1448	U1370	U1301	A1223	G1149	U1056	G987	A921	C847	U785
A1919	C1830	G1749	G1667	A1597	A1516	C1449	G1371	U1307	G1225	G1150	A1057	G988	A922	U852	U786
A1920	G1830	A1750	G1668	C1598	C1518	C1451	G1372	U1308	A1226	U1151	G1058	U991	U925	C853	G788
G1921	G1831	U1750	A1669	G1599	G1519	U1452	G1373	C1309	A1227	A1154	U1059	A994	U926	G854	G789
U1922	G1831	G1754	G1670	U1600	G1520	U1453	G1377	G1310	A1231	A1155	A1065	A994	G927	G855	A790
U1923	C1835	G1755	A1671	U1601	U1521	C1455	U1377	C1311	U1232	U1156	G1066	A995	G928	A856	G791
C1924	G1836	A1756	A1672	G1602	C1522	C1456	C1380	G1312	A1233	A1162	G1067	A996	G929	U857	U792
G1925	G1837	G1760	A1673	A1603	A1523	A1457	G1381	G1313	C1234	C1163	A1068	G997	A930	G858	G793
U1926	G1838	G1761	C1677	A1604	C1524	U1458	A1366	U1313	C1235	C1164	G1069	G998	A931	U859	A794
U1927	A1839	C1762	G1678	A1605	U1527	U1459	G1387	A1314	C1235	G1165	G1070	A999	G932	U860	A795
G1928	A1840	G1763	U1679	C1606	G1527	U1460	G1388	G1315	A1242	A1166	G1073	A1000	G933	G861	A796
U1929	G1841	A1764	U1680	A1607	C1528	A1463	C1389	G1316	G1243	A1167	G1074	A1001	G934	C864	A797
U1930	G1842	C1765	A1681	U1608	C1529	A1464	U1390	A1318	C1243	G1168	G1075	C1002	G935	A865	C799
G1931	G1843	U1766	G1682	G1609	U1530	C1465	G1391	C1319	G1248	C1169	U1076	C1003	A936	U868	U800
U1932	G1844	G1767	G1683	A1610	C1531	C1466	U1392	A1320	G1249	U1172	A1081	U1004	C939	C869	C803
U1933	G1845	U1770	G1684	U1612	G1532	U1467	U1393	G1323	G1251	G1173	C1086	A1005	G940	C870	C804
G1934	A1855	A1771	A1685	G1613	G1533	U1468	G1393	U1324	C1252	U1177	A1084	A1007	U941	U871	G805
U1935	U1856	A1772	C1687	C1614	U1539	U1470	A1397	G1325	C1253	U1178	G1085	A1008	U942	G872	A806
G1936	G1857	A1773	G1688	C1615	C1540	G1471	G1398	U1326	G1254	C1178	C1086	C1009	U943	U873	A807
U1937	C1858	A1774	G1689	G1616	G1543	C1472	C1399	C1327	U1257	A1179	C1087	A944	U944	A874	C808
G1938	G1859	G1775	U1691	U1617	U1544	A1473	G1402	G1328	U1258	A1180	C1088	A945	G945	G875	C809
A1939	A1860	A1776	C1692	A1618	G1545	U1474	U1403	U1329	C1259	C1181	C1089	U1015	C948	A876	U810
U1940	G1861	U1777	G1693	U1619	G1546	U1475	G1407	G1330	A1259	U1182	C1090	C1016	G949	G877	U811
C1941	C1862	C1779	U1696	C1620	C1552	U1478	U1410	G1331	A1260	G1183	C1091	C1017	G950	C878	G812
G1942	G1863	G1780	G1703	G1621	G1557	G1479	C1411	G1332	U1262	C1184	U1093	U1019	G951	A879	A813
U1943	A1864	A1785	C1704	C1622	C1558	U1480	C1411	A1334	G1264	G1185	G1098	A1020	A952	C880	G814
A1944	G1865	C1786	U1708	C1623	G1561	U1481	G1414	G1337	G1265	A1187	A1099	A1021	G953	G887	A815
G1945	U1866	U1787	G1709	A1624	G1562	A1486	C1415	G1338	U1266	A1188	U1022	A1022	U954	G888	A817
U1946	G1867	C1788	U1710	A1625	U1561	C1487	A1416	U1339	G1267	G1189	G1100	U1023	G955	C889	G818
G1947	A1868	U1789	C1711	C1626	G1562	C1488	C1417	U1340	A1268	G1191	A1114	A1024	A956	U890	C819
C1948	G1869	C1791	G1712	C1628	G1566	U1489	G1418	G1341	U1269	U1192	C1120	A1025	G957	A891	U820
U1949	A1870	C1792	G1713	G1629	A1567	C1490	C1419	U1342	C1270	A1193	G1121	U1026	G958	G	A821
C1950	G1871	A1794	A1715	A1632	A1568	U1491	G1419	C1343	G1271	U1194	A1122	C1027	C959	G	G822
G1951	G1872	U1785	G1716	C1633	G1571	A1492	U1424	U1344	C1272	U1195	G1122	G1028	U960	G	U824
A1952	A1873	G1786	A1717	A1634	C1572	A1493	G1425	G1345	G1273	U1196	A1123	C1029	G961	G	U825
U1953	C1874	C1787	C1708	G1635	G1573	G1494	U1426	G1346	C1274	G1197	C1127	U1030	A964	G	C826
G1954	U1875	U1788	U1709	A1636	A1574	G1495	G1427	C1347	A1275	U1198	G1128	A1032	A965	C	U827
U1955	G1876	C1789	G1710	C1637	C1575	G1496	G1428	U1348	A1276	U1199	A1129	G1033	A966	C	C828
G1956	A1877	A1802	C1724	G1644	G1576	C1497	A1429	C1349	A1278	G1200	U1130	U1034	G967	A	G829
U1957	C1878	G1806	C1727	U1648	G1577	C1498	G1430	G1350	G1279	A1203	G1131	G1035	G968	C	C830
C1958	G1879	A1807	A1728	U1649	U1578	A1499	U1431	G1351	U1280	A1204	C1132	G1036	U969	C	G831
A1959	A1880	G1808	C1729	U1651	G1579	U1500	G1432	G1352	A1281	G1204	G1133	U1037	A970	A	A832
U1960	U1900	A1810	G1652	C1580	C1580	C1501	A1433	A1353	U1282	G1205	G1134	A1038	A971	C	G833
C1961	G1881	A1811	C1731	C1653	C1581	G1502	U1434	A1354	G1284	A1137	A1138	U1039	G972	C	A834
U1962	A1882	U1812	U1732	A1654	A1582	G1503	G1435	A1355	A1285	C1210	A1139	A1040	U973	U	U837
G1963	G1883	U1813	U1733	C1655	A1583	G1504	G1436	A1356	U1286	G1211	A1140	G1041	U974	A	A838
A1964	U1965	A1814	C1734	U1656	A1584	U1505	A1437	U1357	A1287	G1214	U1141	U1044	C975	C	U839
U1965	C1884	G1807	C1725	C1657	A1585	U1506	A1438	C1358	A1288						
G1966	G1885	A1808	C1726	C1658	A1586	U1507	A1439	C1359	A1289						
U1967	A1886	A1809	C1727	C1659	A1587	U1508	A1440	C1360	A1290						
C1968	G1887	A1810	C1728	C1660	A1588	U1509	A1441	G1361	U1291						
A1969	C1888	A1811	C1729	C1661	A1589	U1510	A1442	A1362	C1292						
U1970	G1889	A1812	C1730	C1662	C1580	C1501	A1433	A1353	U1282						
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G1972	U1895	G1806	C1727	C1664	G1576	C1497	A1429	G1349	A1278						
U1973	A1896	A1807	A1728	U1648	G1577	C1498	G1430	G1350	A1279						
G1974	C1897	C1808	C1729	U1651	U1578	A1499	U1431	G1351	U1280						
U1975	A1898	G1809	C1730	C1665	G1579	U1500	G1432	G1352	A1281						
C1976	U1900	A1810	G1652	C1580	C1580	C1501	A1433	A1353	U1282						
U1977	G1901	A1811	C1731	C1653	C1581	G1502	U1434	A1354	G1284						
G1978	U1906	U1812	U1732	A1654	A1582	G1503	G1435	A1355	A1285						
C1979	C1907	A1813	U1733	C1655	A1583	G1504	G1436	A1356	U1286						
U1980	A1908	G1814	C1734	U1656	A1584	U1505	A1437	U1357	A1287						
A1981	U1909		C1736	A1657	A1585	U1506	A1438	C1358	A1288						

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A1984	G2052	G2200	C2271	A2357	C2421	U2485	C2552	G2621	C2703	C2778	U2859
G1986	G2055	G2201	C2272	C2358	C2422	G2486	G2553	G2622	U2704	G2779	U2860
	C2056	A2204	C2273	G2361	G2423	G2487	C2554	U2623	A2705	G2780	A2861
G1993	U2057	C2205	U2274	G2362	G2424	G2488	G2555	U2624	U2706	G2781	G2862
U1994	U2058	G2206	U2275	G2363	G2425			U2625			U2863
G1995	U2059	G2207	C2276	G2364	A2426	C2491	C2556	C2628	G2707	G2782	
A1996	U2060	G2208	U2277	G2365	U2427	G2492	U2558	U2629	U2708	A2783	
A1997	C2061	U2211	U2278	G2366	U2428	U2493	C2559	G2630	C2709	A2784	
A1998	U2062	U2212	G2279	U2367	A2429	C2494	G2560	U2631	C2710	A2785	
U1999		G2213	U2285	U2368	A2430	G2495	U2561	A2633	G2711	A2786	
U2000	U2069	G2214	U2286	A2367	C2431	C2496	U2562	U2634	G2712	A2787	
G2001	G2070		G2287	G2368	A2432	A2497	C2563	U2635	A2713		
A2002			G2288	U2369	G2433	U2498	A2566	A2636		G2794	
A2003	U2075		G2289	U2370	G2434	U2499	C2567		G2717	A2795	
U2004	G2076		C2292	C2371	C2435	C2500	C2570	A2639	A2718	A2796	
U2005	G2077		G2293	A2372	U2436	G2501	G2571	G2640		G2797	
G2006	G2078		U2298	C2373	G2437	G2502	U2572	A2641	A2721	C2799	
C2007	U2079		U2299	G2374	A2438	G2503	C2573	G2643	C2725	C2800	
C2008	U2080		U2299	G2375	C2439	G2504	G2574		U2726	A2801	
U2009	U2081		G2300	U2376	C2440	G2505	U2575	C2646	U2727		
U2010	U2082		A2301	G2377	C2441	G2508	A2577	U2651	A2728	G2805	
U2011	G2083		A2302	U2378	C2442	A2509	G2578	G2652	U2729	U2806	
A2012	G2084		U2228	U2380	C2443	A2510	A2579		A2730	U2808	
A2013	G2085		G2229	A2381	A2444	G2511	C2580	A2658	G2731	A2809	
A2014	U2086		A2307	U2382	A2445	G2512	A2581	C2659	C2732	A2810	
G2015	G2093		A2308	C2383	A2446	G2513	G2582	C2660		G2811	
A2016	C2094		G2309	C2384	A2447	G2514	C2583	G2661	C2735	A2812	
U2017	G2095		U2310	U2385	A2448	G2515	G2584		U2736		
G2018	U2096		A2312	U2386	C2449	G2516	G2585	U2666	A2737	C2815	
C2019	G2097		A2313	G2389	A2450	U2517	C2586	U2667		C2816	
G2020	G		A2314	A2390	A2451	G2518	U2587	C2668	C2740	G2821	
C2021	A		A2315	A2391	A2452	A2521	C2588	C2669	G2741	U2822	
C2022	U		G2316	G2392	A2453	G2522	C2589	C2670	G2742	G2823	
C2023	A		U2241	G2393	U2454	G2523	U2590		G2743	U2824	
U2024	U		C2242	G2394	C2455	G2524	U2591	C2671	A2744	A2825	
A2025	A		C2243	C2395	G2456	U2525	U2592	C2672		C2826	
C2026	G2103		C2244	G2396	G2463	U2526	A2593	U2674	C2745	U2830	
C2027	G2106		A2245	A2397	G2464	G2527	C2594	G2675	A2754	A2831	
C2028	G2107		A2246	U2398	G2465	G2528	C2595	U2676	A2755	G2832	
G2029			A2247	U2399	G2466	G2529	C2596	C2677	A2756	C2833	
			U2248	A2401	G2467	U2530	U2597	G2678	G2757	U2834	
			U2249	U2402	A2468	U2531	U2598	U2679	A2758	A2835	
			G2250	U2403	G2469	U2532	A2600	U2680	G2759	U2836	
			U2251	A2404	G2470	U2533	C2601	C2681	G2760	G2837	
				A2405	U2471	U2534	G2602	C2682	A2761		
				G2255	G2472	G2535	G2603	C2683	G2762	U2841	
				A2181	G2473	C2536	G2604	G2684		C2842	
				A2182	G2474	C2537	C2605	G2685	U2766	A2843	
				U2185	G2475	C2538	G2606	C2686	C2767		
				G2186	G2476	C2539	G2607	C2687	C2768		
					C2261	A2540	A2608	C2688	C2769	G2847	
					C2262	A2541	G2609	U2689	A2770	A2848	
					A2265	A2542			C2771		
					A2266	A2543			U2772	G2851	
					A2267	A2544			G2773	G2852	
					G2268	A2545			U2774	U2853	
						A2418			U	G2854	

- Molecule 2: tRNA acceptor stem mimic

Chain 5:  26% 40% 6% 29%

G1	G2	G3	A7	A8	G9	C10	G	U	U	C	C21	G22	U24	U25	A26	G27	U29	C30	C31	A32	C33	C34	A35
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- Molecule 3: 50S ribosomal protein L16

Chain K:

88%

12%

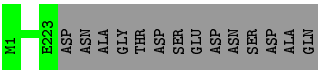


● Molecule 4: GENERAL STRESS PROTEIN CTC

Chain T:

94%

6%



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, α , β , γ	169.60 Å 409.40 Å 695.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	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	60271	wwPDB-VP
Average B, all atoms (Å ²)	74.0	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, 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	0.14	0/66467	0.63	0/103673
2	5	0.16	0/563	0.63	0/873
All	All	0.14	0/67030	0.63	0/104546

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	1742	0
2	5	543	0	290	16	0
3	K	124	0	0	0	0
4	T	223	0	0	0	0
5	0	22	0	19	0	0
All	All	60271	0	30226	1754	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 1754 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	1.05
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.00
1:0:2548:G:H2'	1:0:2549:G:H5''	1.44	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.22	0.98

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%)	416 (15%)	44 (1%)
2	5	22/35 (62%)	2 (9%)	0
All	All	2779/2915 (95%)	418 (15%)	44 (1%)

5 of 418 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	1263	G
1	0	1495	G
1	0	2668	U
1	0	1278	A
1	0	1313	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	1,2	30,40,41	2.78	6 (20%)	37,57,60	1.32	6 (16%)

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	1,2	-	0/21/43/44	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.92	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	CD2-CG	2.59	1.44	1.38
2	5	35	PPU	CE2-CZ	2.68	1.44	1.38
2	5	35	PPU	C6-N1	3.40	1.38	1.34
2	5	35	PPU	CE1-CZ	3.67	1.46	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C4'-C3'-N3'	-3.41	106.49	113.61
2	5	35	PPU	C1'-N9-C4	-2.03	123.88	126.94
2	5	35	PPU	C-CA-N	2.08	117.97	108.73
2	5	35	PPU	C9-N6-C6	2.15	126.26	119.48
2	5	35	PPU	CM-OC-CZ	2.71	123.86	117.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	35	PPU	1	0

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
5	SPS	0	2881	-	17,22,23	4.47	9 (52%)	16,28,30	4.26	8 (50%)

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
5	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)
5	0	2881	SPS	C7-C5	2.47	1.55	1.50
5	0	2881	SPS	C9-C10	3.09	1.54	1.48
5	0	2881	SPS	C6-C8	3.94	1.56	1.47
5	0	2881	SPS	C1-N2	5.02	1.42	1.33
5	0	2881	SPS	C10-N11	5.14	1.50	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	0	2881	SPS	C12-N11-C10	-7.86	112.03	122.58
5	0	2881	SPS	O10-C10-C9	-7.05	109.44	123.01
5	0	2881	SPS	C8-C9-C10	-5.54	109.55	121.63
5	0	2881	SPS	C6-C8-C9	-5.05	110.36	127.09
5	0	2881	SPS	C7-C5-C6	-2.02	121.24	123.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	0	2881	SPS	C12

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	0	2881	SPS	C9-C10-N11-C12
5	0	2881	SPS	O10-C10-N11-C12

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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