



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2023 – 04:37 AM EDT

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.; Schluenzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on : 2003-01-02
Resolution : 3.60 Å(reported)

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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

2 Entry composition [i](#)

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

- Molecule 2 is a RNA chain called tRNA acceptor stem mimic.

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

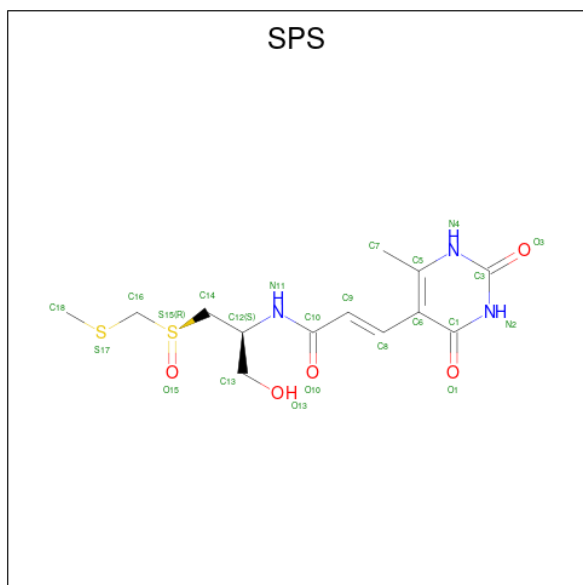
- Molecule 3 is a protein called 50S ribosomal protein L16.

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

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

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

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



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

G1818	G1737	A1858	A1586	G1508	A1441	G1359	A1289	G1045	U978	C	U840	G778
U1819	G1742	G1659	A1587	A1509	C1442	U1365	A1290	U1046	A979	A911	G841	U719
A1820	C1743	G1660	U1510	A1511	C1443	U1366	G1291	G1047	G980	U916	A842	U780
C1822	G1744	C1661	U1591	A1512	C1444	A1365	A1292	C1219	C981	U917	G843	G781
C1825	C1745	G1662	C1592	U1513	U1445	A1366	A1293	C1220	G1146	U918	G844	U782
U1826	A1746	C1663	U1593	U1514	U1446	G1366	G1288	C1053	A984	U919	U845	G783
C1829	G1747	G1664	U1594	C1514	U1447	G1367	U1298	G1052	G985	G920	A846	U784
U1830	U1748	C1665	A1595	U1515	A1448	U1370	G1288	A1055	A886	A921	C847	U785
G1831	G1749	A1666	A1596	A1516	C1449	G1371	U1301	A1056	G987	A922	U852	U786
C1835	A1750	C1667	C1597	C1450	G1450	A1372	U1307	A1057	C853	A923	C854	A787
G1836	U1751	G1668	C1598	C1451	G1451	G1373	U1307	U1057	G854	U924	G855	G788
U1837	G1752	A1669	U1599	G1452	U1452	G1374	U1307	G1058	G855	U925	G856	G789
C1838	G1753	G1670	U1600	U1453	C1453	G1375	G1308	A1065	U926	U926	U857	G790
G1839	G1754	U1601	U1601	C1454	C1454	G1376	G1310	A1066	C927	U927	U858	G791
U1840	G1755	C1602	A1602	C1455	C1455	C1380	C1310	G1066	A994	C927	U859	G792
C1841	C1756	G1603	A1603	C1456	C1456	G1381	G1311	G1067	A995	G928	U860	U793
G1850	G1760	C1604	A1604	A1457	A1457	G1382	A1162	A1068	C996	A929	G858	G794
U1851	C1761	U1605	U1605	C1458	C1458	G1383	C1163	C1069	C997	A930	U859	A794
G1855	G1762	A1606	A1606	A1459	A1459	A1384	A1314	G1070	C998	G931	U860	A795
U1856	C1763	C1606	C1606	U1460	U1460	G1385	G1315	G1073	A999	G932	G861	A796
C1857	A1764	U1607	U1607	A1463	A1463	G1386	G1316	G1074	G1000	G933	C864	A797
G1858	U1765	C1608	A1608	A1464	A1464	C1387	G1317	G1075	A1001	G934	C865	A798
U1859	C1766	U1609	U1609	C1465	C1465	C1388	G1317	C1076	A1002	G935	A865	U800
C1861	G1767	C1610	A1610	C1466	C1466	A1390	A1318	U1076	C1003	A936	G866	C803
U1862	U1768	A1611	U1611	C1467	C1467	A1391	C1319	C1077	U1004	C939	U867	C804
G1865	A1769	U1612	U1612	U1468	U1468	U1392	A1320	C1078	U1005	G940	C870	G805
U1866	C1770	G1613	G1613	U1469	U1469	G1393	G1323	A1081	U1006	G941	C871	G806
C1867	G1771	C1614	C1614	G1470	G1470	U1397	G1324	A1082	A1007	U942	U872	A807
U1868	U1772	U1615	U1615	C1471	C1471	G1398	U1325	A1083	A806	U943	G873	C808
G1869	C1773	C1616	A1616	C1472	C1472	C1399	U1326	C1086	U944	U944	U874	C809
U1870	A1774	G1617	U1617	C1473	C1473	G1400	C1327	C1087	A874	G945	G875	U810
C1871	U1775	U1618	U1618	A1474	A1474	G1401	U1329	C1088	U1015	C948	G876	G811
U1872	G1776	A1619	A1619	U1475	U1475	U1402	U1329	C1089	U1016	G949	C877	G812
G1873	C1777	C1620	C1620	U1476	U1476	U1403	U1330	C1090	G950	G949	C878	G813
U1874	A1778	U1621	U1621	U1477	U1477	U1404	G1331	C1091	U1017	G950	C879	G814
C1875	U1779	G1622	A1622	C1478	C1478	C1411	U1332	U1093	G815	G951	C880	A815
U1876	G1780	C1623	A1623	U1479	U1479	C1412	G1333	G1098	U1020	G952	G887	U816
G1877	U1781	U1624	U1624	U1480	U1480	G1413	U1334	A1099	A1021	G953	G888	A817
U1878	A1695	C1625	C1625	U1481	U1481	G1414	G1337	A1099	A1022	U954	G889	G818
C1879	U1626	U1626	U1626	U1482	U1482	C1415	U1338	G1100	U1023	U955	U890	C819
U1880	A1627	C1627	A1627	A1486	A1486	C1416	U1339	G1101	G1024	A956	U891	U820
G1881	C1628	C1628	C1628	C1487	C1487	C1417	C1340	A1114	A1025	G957	G	A821
U1882	G1629	U1629	U1629	C1488	C1488	C1418	G1341	G1120	U1026	G958	G	U822
C1883	A1632	A1632	A1632	C1489	C1489	G1419	U1342	G1121	C1027	C859	G	U823
U1884	C1633	C1633	C1633	U1490	U1490	U1420	U1343	G1122	G1028	U960	G	U824
G1885	U1634	U1634	U1634	A1492	A1492	U1421	C1344	A1122	C1029	G961	G	C825
U1886	A1635	C1635	C1635	C1493	C1493	U1422	G1345	G1127	U1030	A964	G	C826
C1887	G1643	U1636	U1636	C1494	C1494	U1423	U1346	C1128	A1032	A965	G	U827
U1888	C1644	C1644	C1644	G1496	G1496	G1424	C1347	G1129	A1033	A966	U	C828
G1889	U1644	U1644	U1644	C1497	C1497	U1425	U1348	U1130	G967	G967	A	C829
U1890	G1644	C1644	C1644	U1498	U1498	U1426	A1349	G1131	U1034	U968	C	C830
C1891	C1644	C1644	C1644	C1499	C1499	U1427	G1350	G1132	G1035	C968	C	C831
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G1893	U1644	C1644	C1644	U1500	U1500	U1429	G1352	G1134	U1037	A970	A	A833
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C1895	U1644	C1644	C1644	U1502	U1502	U1431	U1354	A1137	A1039	C972	C	U835
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U1898	C1644	C1644	C1644	U1505	U1505	U1434	U1357	A1140	U1044	C975	C	U838
C1899	U1644	C1644	C1644	U1506	U1506	U1435	U1358	U1141				U839

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A2858	A1911	G1983	U2051	C2199	U2270	G2363	G2484	A2551	G2620	U2700	U2778	A2858
U2859	G1912	G1984	G2052	C2199	C2271	G2364	U2485	C2552	G2621	U2701	C2779	U2859
C2860	G1913	G1985	G2055	G2201	A2272	A2356	U2486	G2553	C2422	C2703	C2779	C2860
A2861	U1914	G1986	C2056	C2202	C2273	C2357	C2487	G2554	C2423	U2704	A2780	A2861
G2862	G1915	G1987	U2057	A2204	C2274	A2358	G2488	G2555	G2424	A2705	A2781	G2862
U2863	G1916	G1988	U2058	C2205	U2275	G2361	C2489	C2556	G2425	U2706	G2782	U2863
G2867	G1917	G1989	U2059	C2206	C2276	G2362	A2490	C2557	A2426	G2707	U2783	G2867
U2872	G1918	G1990	U2060	C2207	A2277	G2363	U2491	C2558	U2427	U2708	A2784	U2872
G2873	A1919	A1996	U2061	U2211	C2278	G2364	U2492	C2559	A2428	U2709	A2785	G2873
A2874	A1920	A1997	C2061	U2212	G2279	C2365	U2493	C2560	U2429	C2710	G2786	A2874
C2875	A1921	A1998	U2062	G2213	G2279	U2366	A2494	C2561	A2430	G2711	A2787	C2875
A2877	U1922	A1999	U2063	G2214	U2285	A2367	C2431	C2562	A2432	G2712	G2792	A2877
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U	C1948	A2014	U2087	U	A2311	G2382	A2447	C2577	U2447	C2734	A2811	U
U	A1949	A2015	G2093	A	G2312	C2383	A2448	C2578	U2448	U2735	A2812	U
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U	C1957	A2025	A	A	G2320	C2391	C2456	C2586	U2456	C2745	C2826	U
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U	G2044	G2044	A2119	A	U2333	A2413	U2476	U2539	A2477	C2758	G2846	U
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U	G2046	G2046	U2121	U	C2335	A2414	C2477	U2541	U2479	C2760	G2848	U
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U	U	U	U	U	G2354	U2426	U2491	U2553	U2491	C2772	G2860	U
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U	U	U	U	U	G2357	U2429	U2494	U2556	U2494	C2775	G2863	U
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U	U	U	U	U	G2367	U2439	U2504	U2566	U2504	C2785	G2873	U
U	U	U	U	U	G2368	C2440	U2505	U2567	U2505	C2786	G2874	U
U	U	U	U	U	G2369	C2441	U2506	U2568	U2506	C2787	G2875	U
U	U	U	U	U	G2370	C2442	U2507	U2569	U2507	C2788	G2876	U
U	U	U	U	U	G2371	C2443	U2508	U2570	U2508	C2789	G2877	U
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U	U	U	U	U	G2373	C2445	U2510	U2572	U2510	C2791	G2879	U
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U	U	U	U	U	G2376	C2448	U2513	U2575	U2513	C2794	G2882	U
U	U	U	U	U	G2377	C2449	U2514	U2576	U2514	C2795	G2883	U
U	U	U	U	U	G2378	C2450	U2515	U2577	U2515	C2796	G2884	U
U	U	U	U	U	G2379	U2385	U2516	U2578	U2516	C2797	G2885	U
U	U	U	U	U	U2380	U2386	U2517	U2579	U2517	C2798	G2886	U
U	U	U	U	U	A2381	G2387	C2517	U2580	U2518	C2799	G2887	U
U	U	U	U	U	A2382	U2388	C2518	U2581	U2519	C2800	G2888	U
U	U	U	U	U	A2383	U2389	C2519	U2582	U2520	C2801	G2889	U
U	U	U	U	U	A2384	U2390	C2520	U2583	U2521	C2802	G2890	U
U	U	U	U	U	A2385	U2391	C2521	U2584	U2522	C2803	G2891	U
U	U	U	U	U	A2386	U2392	C2522	U2585	U2523	C2804	G2892	U
U	U	U	U	U	A2387	U2393	C2523	U2586	U2524	C2805	G2893	U
U	U	U	U	U	A2388	U2394	C2524	U2587	U2525	C2806	G2894	U
U	U	U	U	U	U2389	C2395	C2525	U2588	U2526	C2807	G2895	U
U	U	U	U	U	G2390	C2396	U2526	U2589	U2527	C2808	G2896	U
U	U	U	U	U	A2391	A2397	U2527	U2590	C2528	C2809	G2897	U
U	U	U	U	U	A2392	U2398	U2528	C2590	U2529	C2810	G2898	U
U	U	U	U	U	G2393	U2398	U2529	U2591	U2530	C2811	G2899	U
U	U	U	U	U	U2394	C2396	U2530	U2592	U2531	C2812	G2900	U
U	U	U	U	U	U2395	C2396	U2531	U2593	U2532	C2813	G2901	U
U	U	U	U	U	G2396	C2396	U2532	U2594	U2533	C2814	G2902	U
U	U	U	U	U	A2401	A2401	U2533	U2595	U2534	C2815	G2903	U
U	U	U	U	U	U2402	U2402	U2534	U2596	U2535	C2816	G2904	U
U	U	U	U	U	C2403	C2403	U2535	U2597	U2536	C2817	G2905	U
U	U</											

4 Data and refinement statistics

Xtrriage (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	169.60Å 409.40Å 695.10Å 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.	Xtrriage
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	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 [i](#)

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	2,1	32,40,41	2.81	6 (18%)	33,57,60	0.98	3 (9%)

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	-	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	C-N3'	12.63	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.96	1.27	1.42
2	5	35	PPU	C6-N1	3.86	1.38	1.33
2	5	35	PPU	CE1-CZ	3.70	1.46	1.38
2	5	35	PPU	CE2-CZ	2.70	1.44	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	CM-OC-CZ	2.93	123.86	117.51
2	5	35	PPU	C9-N6-C6	2.23	126.26	119.51
2	5	35	PPU	C-CA-N	2.22	117.97	109.40

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 monosaccharides 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	-	19,22,23	4.43	9 (47%)	17,28,30	4.15	8 (47%)

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	9/15/16/18	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	O10-C10	9.82	1.43	1.24
5	0	2881	SPS	C9-C8	8.40	1.54	1.33
5	0	2881	SPS	O1-C1	7.67	1.43	1.24
5	0	2881	SPS	C10-N11	6.56	1.50	1.34
5	0	2881	SPS	C5-N4	5.43	1.42	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	-7.47	112.03	122.57
5	0	2881	SPS	C3-N2-C1	6.40	120.55	115.14
5	0	2881	SPS	C8-C9-C10	-6.14	109.55	121.56
5	0	2881	SPS	C14-S15-C16	6.14	109.42	101.04
5	0	2881	SPS	O10-C10-C9	-5.96	109.44	123.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	0	2881	SPS	C12

5 of 9 torsion outliers are listed below:

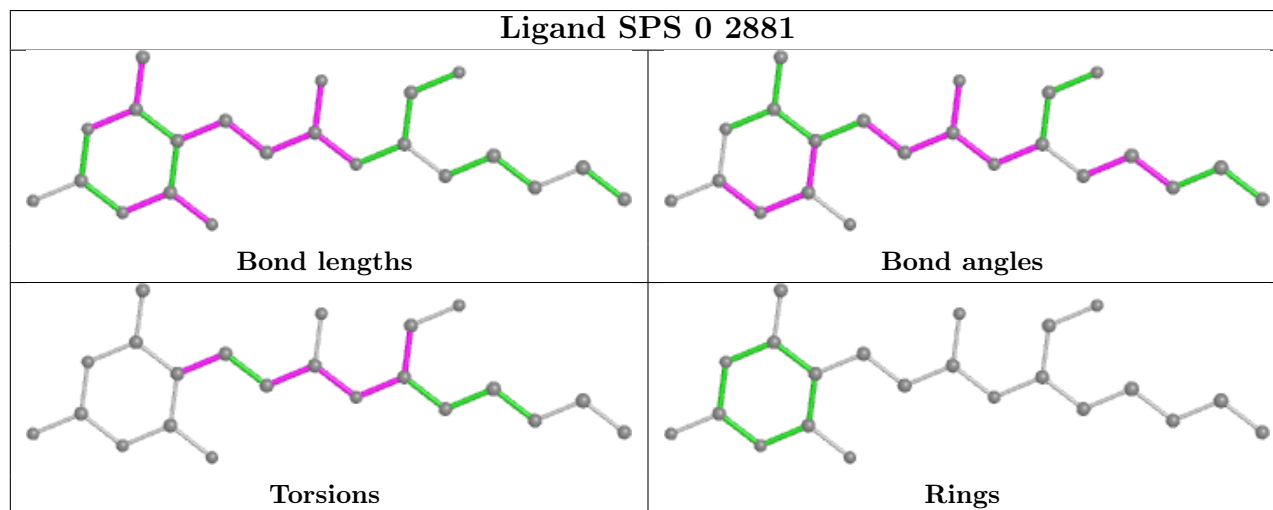
Mol	Chain	Res	Type	Atoms
5	0	2881	SPS	C1-C6-C8-C9
5	0	2881	SPS	C9-C10-N11-C12
5	0	2881	SPS	O10-C10-N11-C12
5	0	2881	SPS	C14-C12-C13-O13
5	0	2881	SPS	N11-C12-C13-O13

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.