



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:46 PM UTC

PDB ID : 2O44 / pdb_00002o44
Title : Structure of 23S rRNA of the large ribosomal subunit from *Deinococcus radiodurans* in complex with the macrolide josamycin
Authors : Pyetan, E.; Daram, D.; Auerbach-Nevo, T.; Yonath, A.
Deposited on : 2006-12-03
Resolution : 3.30 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

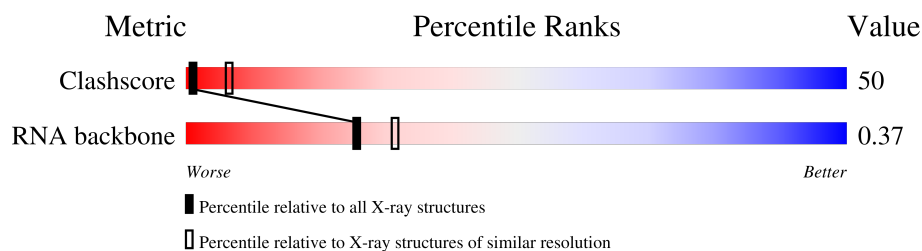
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

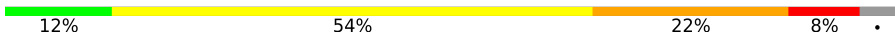
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	A	2880	 12% 54% 22% 8% .

2 Entry composition ⓘ

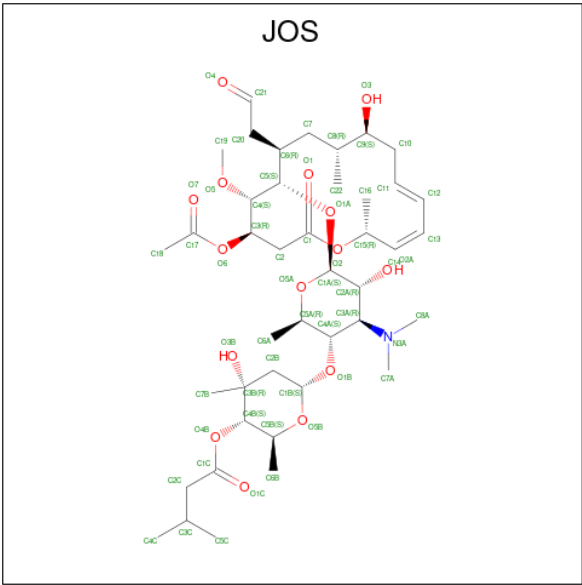
There are 2 unique types of molecules in this entry. The entry contains 59417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is (2S,3S,4R,6S)-6-{[(2R,3S,4R,5R,6S)-6-{[(4R,5S,6S,7R,9R,10S,12E,14Z,16R)-4-(ACETYLOXY)-10-HYDROXY-5-METHOXY-9,16-DIMETHYL-2-OXO-7-(2-OXOETHYL)OXACYCLOHEXADECA-12,14-DIEN-6-YL]OXY}-4-(DIMETHYLAMINO)-5-HYDROXY-2-METHYLTETRAHYDRO-2H-PYRAN-3-YL]OXY}-4-HYDROXY-2,4-DIMETHYLTETRAHYDRO-2H-PYRAN-3-YL 3-METHYLBUTANOATE (CCD ID: JOS) (formula: C₄₂H₆₉NO₁₅).



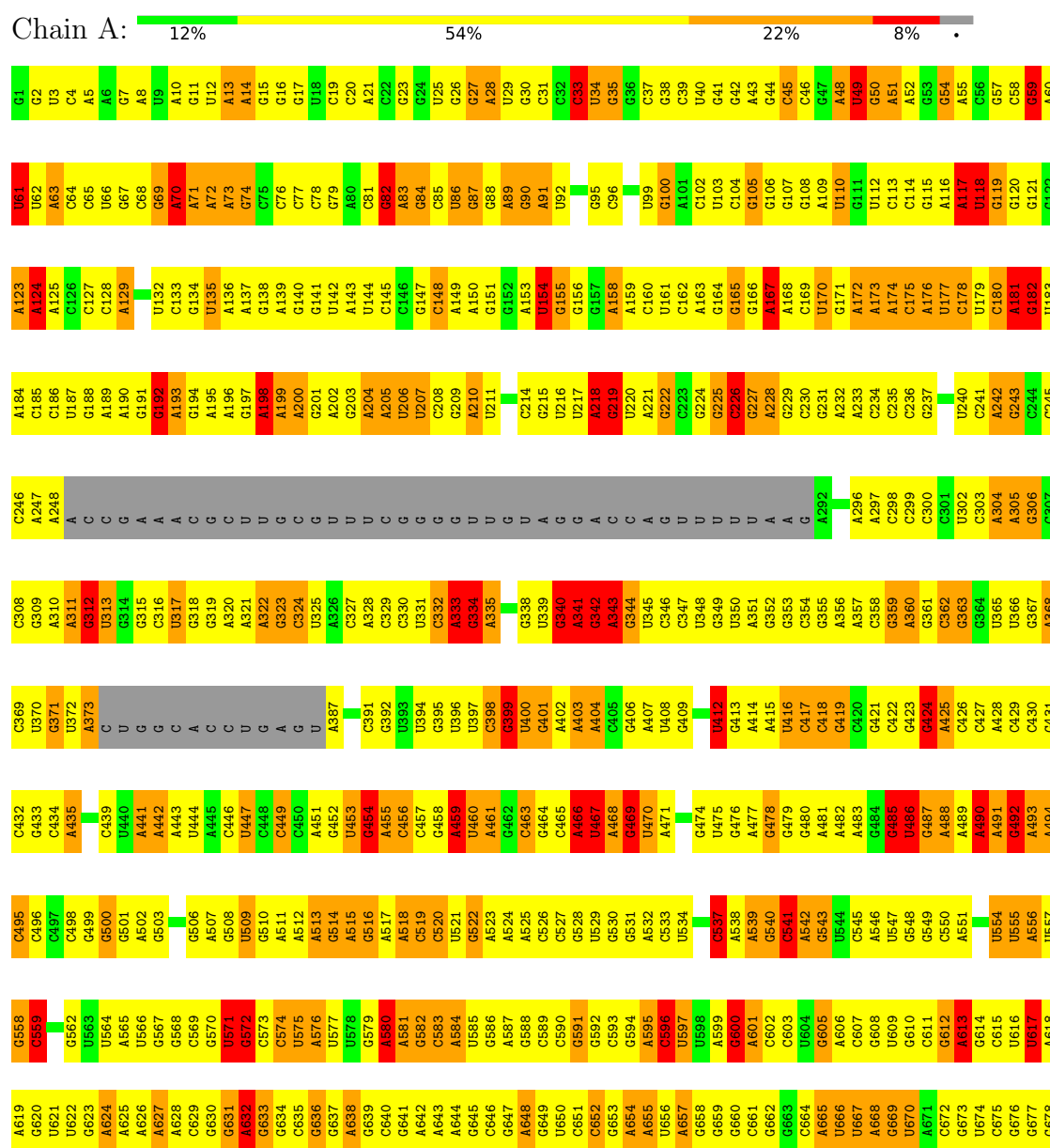
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	58	42	1	15	0	0

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 rRNA



G1540	G1478	G1352	A1292	C1169	U1108	G1047	A984	A923	C863	A802	G741	C679
G1541	G1479	A1353	A1293	U1170	A1109	U1045	G885	C924	C864	C803	G742	U680
G1542	G1480	A1354	G1294	A1171	G1110	C1049	A986	U925	A865	C804	A743	G681
G1543	G1481	A1355	C1235	U1172	C1111	G1050	G987	C926	U866	C805	G744	G682
G1544	U1482	A1356	G1296	G1173	G1112	U1051	G988	C927	A806	A806	G745	G683
G1545	G1483	U1357	G1237	G1174	C1113	C1052	G989	G928	U868	A807	G746	C684
G1546	G1484	C1358	A1238	A1175	A1114	G1053	U992	A929	C869	C806	A747	U685
G1547	U1485	G1361	A1299	U1176	C1115	C1054	A992	A930	G870	C809	A748	C686
G1548	A1486	A1362	G1240	U1177	U1116	A1055	C993	G931	U871	U810	G749	C687
G1549	G1487	U1363	U1301	C1178	G1117	U1056	A994	G932	C872	G811	G750	A688
C1550	G1488	C1363	C1242	A1179	G1118	A1057	A995	G933	U873	G812	G751	A689
U1551	A1489	G1364	U1303	A1180	U1119	G1058	C996	G934	A874	A813	G752	A690
C1552	U1490	U1365	U1304	C1181	C1120	A1059	G995	G935	G875	G814	U753	C691
G1553	G1491	A1366	C1305	U1182	G1121	C1060	G1000	A936	A876	A815	U754	C692
U1554	U1492	U1367	U1306	U1246	A1122	A1061	A1001	A937	C877	U816	G755	A693
A1555	A1493	G1368	U1307	G1184	G1123	G1062	C1002	G938	C878	A817	G756	G694
A1556	G1494	G1369	C1308	C1185	U1124	C1063	A996	C939	A879	G818	U757	U695
G1557	G1495	U1370	G1309	G1186	G1125	A1064	C997	G940	C880	C819	G758	A698
C1558	U1496	G1371	C1310	A1187	A1126	A1065	U1005	U941	U881	U822	G759	G699
G1559	G1497	A1372	G1311	U1188	A1129	G1066	C1006	U942	C882	G823	U760	C700
A1560	A1498	G1373	G1312	C1251	G1189	G1067	A1007	U943	A883	U824	U761	U701
A1561	U1499	G1374	U1313	C1253	U1130	A1068	G1008	A944	C884	U825	A762	A702
G1562	U1500	C1375	A1314	G1191	G1131	G1069	C1009	G945	A885	C826	A763	A703
U1563	C1501	G1376	A1315	A1192	G1132	U1070	U1010	U946	A886	U827	G764	G704
U1564	G1502	G1377	G1316	G1193	G1133	U1071	A1011	C947	G887	C828	G765	C705
G1565	A1441	A1378	G1317	U1194	C1134	U1072	A1012	C948	C888	C829	A766	A706
G1566	G1504	A1379	A1318	U1195	C1135	G1073	G1013	G949	C889	C830	G767	U707
A1567	U1505	C1380	C1319	U1196	G1136	G1074	G1014	G950	U890	G831	U768	G708
A1568	A1506	G1381	A1260	U1197	A1137	C1075	U1015	G951	U891	G832	A769	A709
A1569	U1507	C1382	C1321	C1198	A1138	U1076	G1016	A952	G	A833	G772	C710
C1570	G1508	C1383	G1322	U1199	A1139	U1077	C1017	G953	G	U834	G773	G711
A1509	A1509	G1384	G1323	G1200	A1140	A1078	C1018	U954	G	U835	A774	A712
C1572	U1510	C1385	G1324	C1201	U1141	G1079	U1019	G955	G	A836	U775	G713
G1573	A1511	A1386	A1325	U1202	G1142	A1080	A1020	A956	G	U837	G776	G714
A1574	U1512	G1387	U1326	G1266	A1143	A1081	A1021	G957	C	A838	U777	U715
C1575	U1513	G1388	C1327	A1267	G1144	C1082	A1022	G958	C	U839	G778	U716
A1576	U1514	C1389	G1328	G1206	C1145	C1083	U1023	C959	U	U840	U779	G717
G1577	U1515	G1390	U1329	G1269	G1146	A1084	G1024	U960	A	G841	U780	A718
U1578	U1578	A1391	G1330	C1270	G1147	G1085	A1025	G	C	A842	U781	A719
G1579	G1579	U1392	C1331	C1271	G1148	C1086	U1026	G963	C	G843	U782	A720
C1580	A1581	G1393	G1332	G1272	G1149	C1087	C1027	A964	A	G844	U783	G721
A1582	C1522	U1460	C1333	C1273	C1150	A1088	G1028	G965	G	U845	U784	C722
G1583	U1523	A1397	A1334	G1274	U1151	C1089	C1029	A966	C	A846	U785	C723
G1584	C1524	G1398	G1335	A1275	C1152	C1090	G967	G968	U	C847	U786	C724
A1585	A1525	G1401	G1337	U1276	A1153	C1091	C1031	C969	A	A848	G787	C725
A1586	U1526	U1409	G1338	G1277	A1154	C1092	A1032	U969	C	G849	G788	G726
A1587	G1527	G1402	U1339	A1215	G1155	A1095	G1033	A970	C	C850	G789	U727
A1588	C1528	U1403	C1340	U1217	G1157	A1096	U1034	G971	C	C851	A790	A728
G1589	U1529	G1407	G1341	C1218	U1158	A1097	G1035	G972	A911	U852	G791	A729
C1590	U1530	U1468	U1342	C1219	U1159	G1098	U1036	U973	A912	C853	U792	C730
U1591	G1531	A1408	C1343	G1220	C1160	A1099	U1037	U974	A913	C854	U793	A731
U1592	A1532	U1409	U1344	U1221	U1161	G1100	A1038	U975	C914	G855	G794	G732
C1593	G1533	U1410	G1345	A1285	A1162	U1101	A1039	C976	C915	G856	U795	G733
U1594	A1534	C1411	C1346	U1286	C1163	G1102	U1011	G977	U916	U857	A796	G734
A1595	U1535	C1412	C1347	A1287	C1164	C1103	G1041	U978	U917	U858	A797	G735
A1596	G1536	U1413	G1348	A1288	G1165	G1104	A1042	A979	A918	U859	G798	G736
A1597	U1537	G1414	A1349	A1289	A1166	U1105	U1044	C980	U919	U860	C799	G737
A1598	G1476	C1415	G1350	A1290	A1167	A1106	G1045	C981	U920	U861	U799	G738
G1599	U1539	A1416	G1351	C1291	G1168	A1107	U1046	G983	A922	A862	A801	A740



C2855	C2856	C2857	A2858	C2859	C2860	A2861	C2862	C2863	C2864	C2865	A2866	C2867	C2868		U2872	C2873	C2874	C2875	C2876	A2877	C	U	C																																				
G2793	G2794	A2795	A2796	G2797	A2798	C2799	C2800	A2801	C2802	C2803	C2804	G2805	G2806	U2807	U2808	A2809	A2810	C2811	A2812	G2813	G2814	C2815	C2816	C2817	G2818	G2819	C2820	G2821	U2822	G2823	C2824	A2825	C2826	G2827	C2828	A2829	U2830	A2831	C2832	C2833	A2834	A2835	U2836	G2837	U2838	G2839	U2840	U2841	C2842	A2843	G2844	C2845	C2846	G2847	A2848	C2849		U2853	C2854
A2733	U2734	C2735	U2736	C2737	A2738	G2739	C2740	G2741	G2742	G2743	A2744	A2745	G2746	C2747	C2748	A2749	G2750	C2751	C2752	C2753	C2754	A2755	A2756	G2757	A2758	U2759	G2760	A2761	G2762	U2763	U2764	C2765	U2766	C2767	C2768	C2769	A2770	C2771	U2772	G2773	U2774	U	U	A	U2778	C2779	U2780	G2781	G2782	U2783	A2784	A2785	C2786	G2787	C2788	U2789	C2790	C2791	C2792
C2671	U2672	C2673	C2674	U2675		G2679	U2680	A2681	C2682	C2683	A2684	A2685	C2686	G2687	G2688	C2689	A2690	C2691	A2692	U2693	C2694	C2695	A2696	G2697	G2698	U2699	U2700	A2701	G2702	C2703	U2704	A2705	U2706	G2707	U2708	C2709	C2710	G2711	G2712	A2713	A2714	C2715	G2716	G2717	A2718	U2719	A2720	A2721	C2722	G2723	G2724	C2725	U2726	G2727	A2728	A2729	A2730	G2731	C2732
A2545	G2546	C2547	G2548	G2549	C2550	A2551	C2552	G2553	C2554	G2555	A2556	G2557	C2558	U2559	G2560	G2561	G2562	U2563	U2564	C2565	A2566	G2567	A2568	A2569	C2570	U2571	G2572	C2573	G2574	U2575	G2576	A2577	G2578		A2581	G2582	U2583	U2584	C2585	G2586	G2587	U2588	C2589	U2590	C2591	U2592	A2593	U2594	C2595	C2596	G2597	C2598	U2599	A2600	C2601		G2606	C2607	A2608
C2609	G2610		A2613	U2614	U2615	U2616	G2617	A2618	G2619	G2620	G2621	G2622	A2623	U2624	U2625	U2626	G2627	C2628	U2629	C2630	C2631	U2632	A2633	A2634	G2635	A2636	C2637	G2638	A2639	G2640	A2641	G2642	G2643	A2644	C2645	G2646	G2647	G2648	A2649	G2650	U2651	G2652	A2653	A2654	C2655	U2656	A2657	U2658	C2659	C2660	C2661	C2662		G2665	A2666	C2667	U2668	C2669	C2670

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	172.80Å 411.48Å 697.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59417	wwPDB-VP
Average B, all atoms (Å ²)	83.0	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: JOS

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	A	0.49	0/66467	0.90	230/103673 (0.2%)

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	A	1	200

There are no bond length outliers.

The worst 5 of 230 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2660	C	C2'-C3'-O3'	11.09	126.14	109.50
1	A	2044	G	N9-C1'-C2'	10.06	129.09	114.00
1	A	1975	G	C2'-C3'-O3'	9.25	123.37	109.50
1	A	2841	U	C2'-C3'-O3'	8.59	122.38	109.50
1	A	2237	C	N1-C1'-C2'	8.51	126.77	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	541	C	C1'

5 of 200 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	U	Sidechain
1	A	49	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	54	G	Sidechain
1	A	59	G	Sidechain
1	A	86	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	A	59359	0	29916	4364	0
2	A	58	0	68	7	0
All	All	59417	0	29984	4366	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 50.

The worst 5 of 4366 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:A:1435:G:C2	1:A:1436:G:H1'	1.70	1.25
1:A:2094:C:N4	1:A:2162:C:H42	1.40	1.19
1:A:793:G:H21	1:A:796:A:N6	1.41	1.17
1:A:1463:A:H1'	1:A:1543:G:N2	1.59	1.17
1:A:2498:U:H4'	1:A:2499:C:OP1	1.40	1.14

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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2757/2880 (95%)	722 (26%)	224 (8%)

5 of 722 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	23	G
1	A	28	A
1	A	33	C

5 of 224 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1333	G
1	A	2823	G
1	A	1710	U
1	A	2760	G
1	A	2521	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	JOS	A	2881	-	60,60,60	2.65	18 (30%)	73,85,85	2.16	23 (31%)

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	JOS	A	2881	-	-	18/65/104/104	0/2/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	JOS	C2A-C3A	10.08	1.70	1.53
2	A	2881	JOS	C10-C11	-6.64	1.30	1.50
2	A	2881	JOS	O4B-C4B	6.45	1.56	1.45
2	A	2881	JOS	C8-C9	5.14	1.61	1.53
2	A	2881	JOS	C4A-C5A	5.14	1.61	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	JOS	C15-O2-C1	6.78	125.74	117.48
2	A	2881	JOS	C9-C10-C11	6.62	123.26	112.88
2	A	2881	JOS	O6-C17-C18	4.89	119.80	111.09
2	A	2881	JOS	O1B-C4A-C5A	4.27	117.65	106.77
2	A	2881	JOS	O2-C1-C2	4.09	118.76	111.43

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

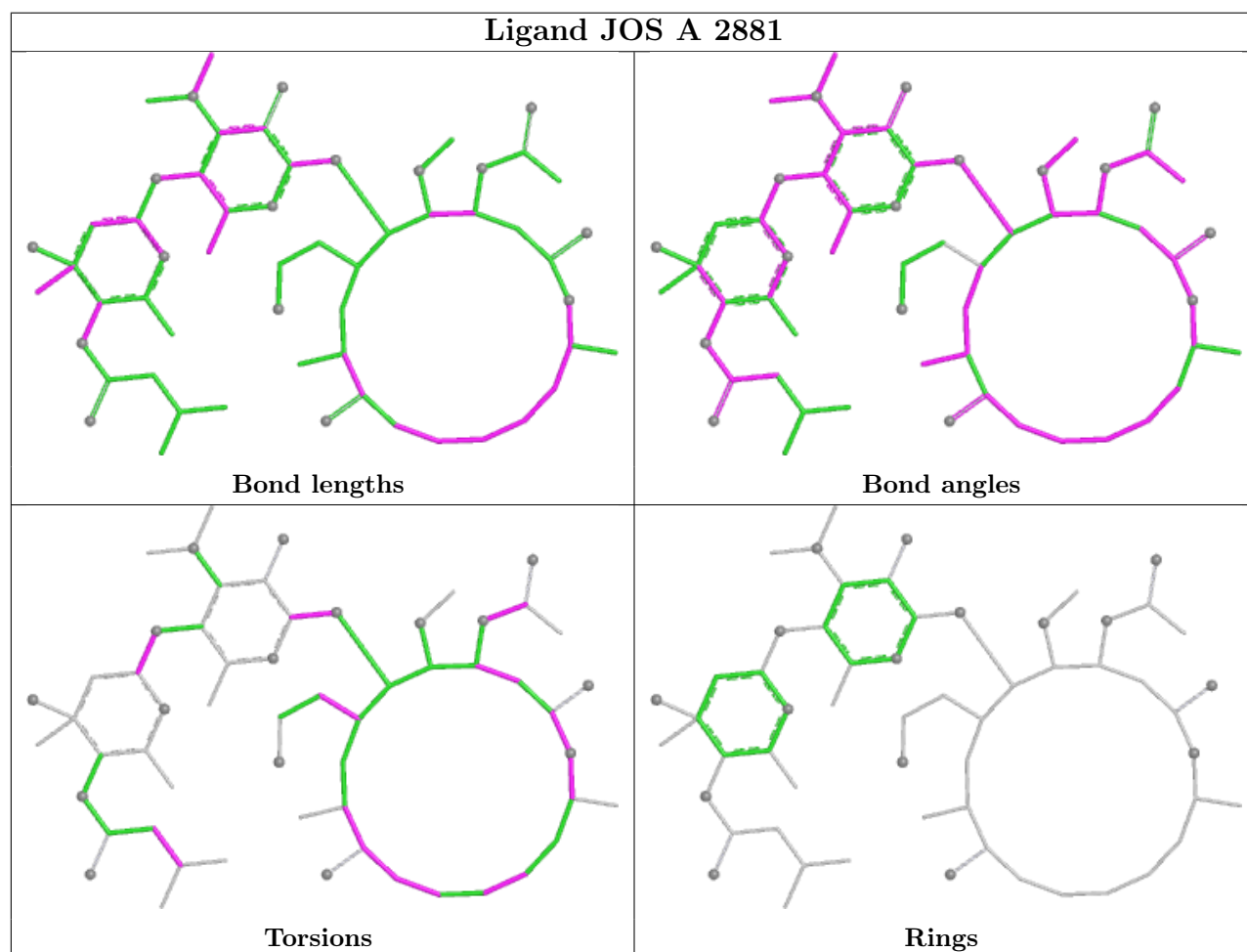
Mol	Chain	Res	Type	Atoms
2	A	2881	JOS	C11-C10-C9-C8
2	A	2881	JOS	C11-C10-C9-O3
2	A	2881	JOS	C22-C8-C9-C10
2	A	2881	JOS	C18-C17-O6-C3
2	A	2881	JOS	O7-C17-O6-C3

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2881	JOS	7	0

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 ⓘ

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.