



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 10:53 PM UTC

PDB ID : 1P9X / pdb_00001p9x
Title : THE CRYSTAL STRUCTURE OF THE 50S LARGE RIBOSOMAL SUB-UNIT FROM DEINOCOCCUS RADIODURANS COMPLEXED WITH TELITHROMYCIN KETOLIDE ANTIBIOTIC
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Deposited on : 2003-05-13
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

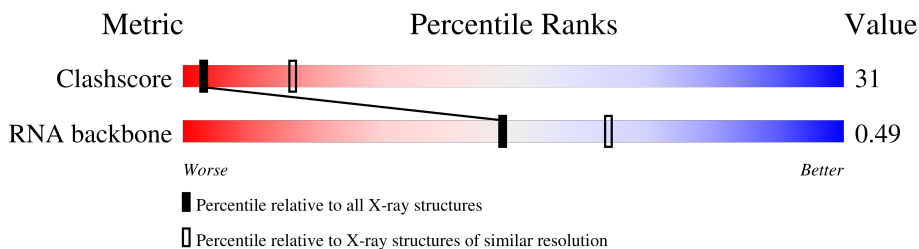
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

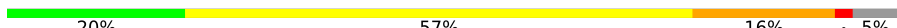
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1022 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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	0	2880	 20% 57% 16% • 5%

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	TEL	0	2881	X	-	-	-

2 Entry composition [i](#)

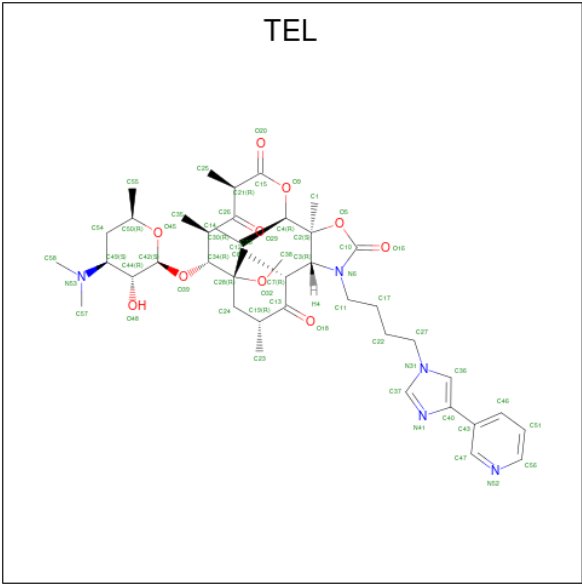
There are 2 unique types of molecules in this entry. The entry contains 58817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2738	58759	26211	10836	18975	2737	0	0	0

- Molecule 2 is TELITHROMYCIN (CCD ID: TEL) (formula: C₄₃H₆₅N₅O₁₀).



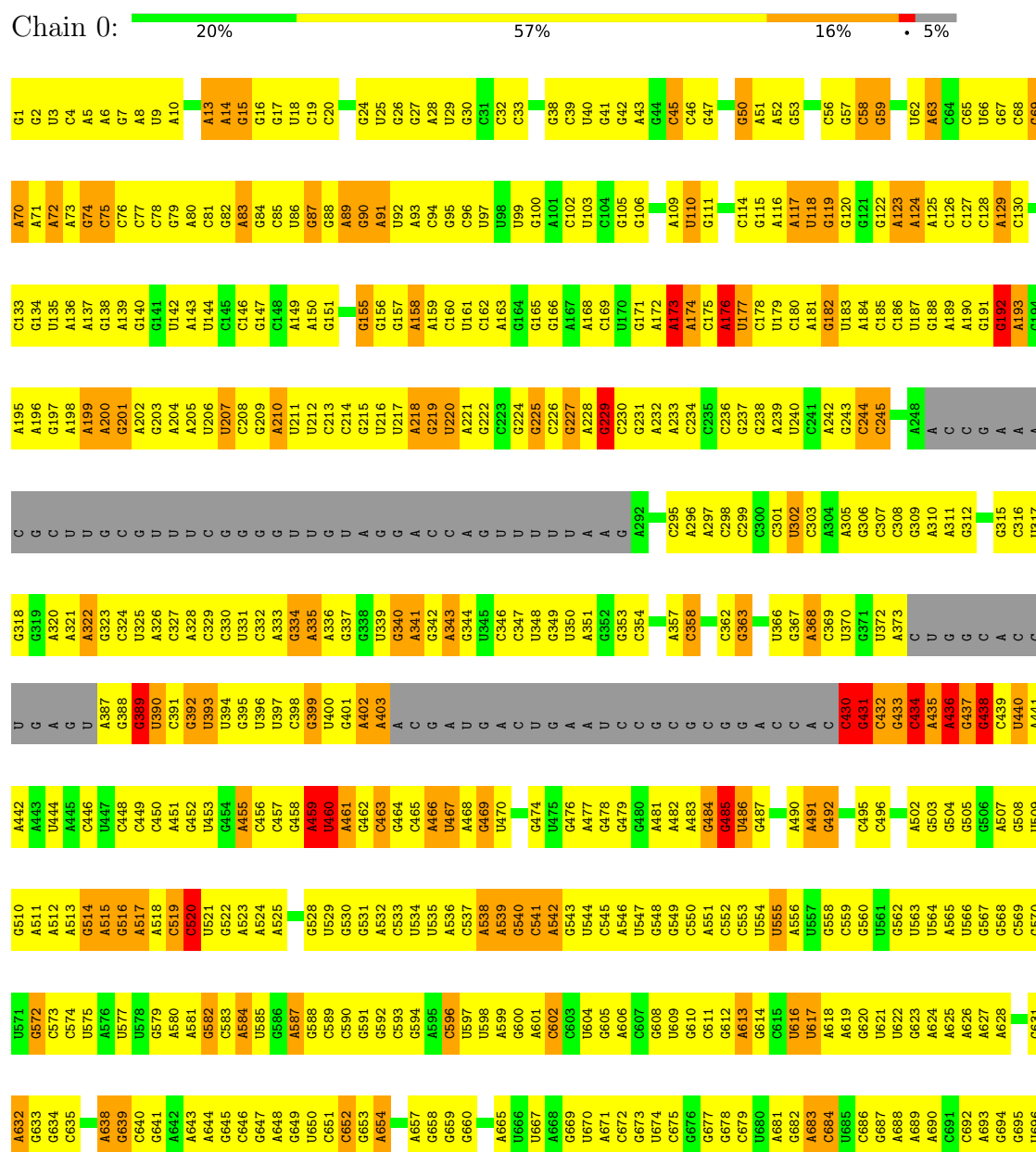
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	0	1	58	43	5	10	0	0

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 RIBOSOMAL RNA



C1615	U1548	U1473	U1410	C1283	G1220	C1152	A1089	C1018	G953	G	C828	C765	C697
C1616	C1549	A1474	C1411	G1284	C1221	A1153	C1089	U1019	U954	G	C829	A766	A698
C1617	C1550	U1475	C1412	A1285	G1222	A1154	C1090	A1020	G767	G	C830	A767	G699
C1618	U1551	G1476	U1413	U1286	C1223	G1155	C1091	A1021	A956	G	G831	U768	C700
C1619	C1552	C1477	G1414	A1287	A1224	U1159	U1092	U1022	G957	C	A832	C769	U701
C1620	G1553	U1478	C1415	A1288	G1225	U1159	C1093	U1023	G958	C	A833	A702	A702
C1621	G1554	G1479	A1416	A1289	A1226	C1160	C1094	G1024	C959	U	A834	G703	G704
C1622	A1555	G1480	C1417	A1293	A1227	U1161	A1095	A1025	U960	C	U837	G773	C705
C1623	A1556	U1481	C1418	A1294	G1228	A1162	A1096	U1026	G961	A	A838	A774	A706
A1624	G1557	U1482	G1419	C1294	C1229	C1163		C1027	C962	C	U839	G776	U707
C1625	C1558	G1483	A1420	U1295	C1230	C1164	A1099	G1028	G963	C	U840	A777	G708
C1626	G1559	U1484		G1296	A1231	G1165		C1029	A964	C	U841	A778	
A1627	A1560	U1485	U1424	A1297	U1232	A1166	G1102	U1030	G965	G	G842	G779	
C1628	A1561	A1486	G1425	C1298	A1233	A1167	C1103	C1031	A966	C	A842	U779	A712
G1629	G1562	C1487	C1364	A1299	C1234	G1168	G1104	A1032	G967	U	G843	U780	G713
A1630		G1488	A1428	A1300	C1235	U1172	U1105	G1033	C968	U	G844	G714	G714
C1631	U1566	C1489	G1429	U1301		A1172	A1106	U1034	U969	A	U845	U782	U715
A1632	A1567	U1490	G1430	C1302	A1238	G1173	A1107	G1035	A970	C	A846	U783	U716
C1633	C1568		U1431	U1303		C1174	U1108	G1036	A971	C	C847		
C1634	A1569	G1494	G1432	G1304	A1242	A1175	A1109	U1038	C972	A911		A787	A718
G1635	C1570	U1495	A1433	C1305	G1243	U1176	G1110	U1038	U973	G	C851	G788	G723
	U1571	G1496	U1434	G1306	U1244	U1177	C1111	A1039	U974		U852	G789	C724
C1641	C1572	C1497	G1435	C1308	G1245	C1178	U1112	U1040	C975		C853	A790	
C1642	G1573	G1498	G1436	G1309	U1246	A1179	C1113	G1041	U978		G854	G791	
A1643	A1574	A1499	A1437	C1310	U1247	A1180	A1114	U1042	A979		G855	U792	U727
G1644	C1575	U1500	G1438	C1311	G1248	C1181	C1115	A1043	A978		A856	G793	G728
C1645	G1576	C1501	U1439	G1312	C1249	U1182	G1118	U1044	C980		U857	A794	A729
G1646	U1577	G1502	G1440	U1313	A1250	C1183	G1119	G1045	C981		G858	G795	
	A1578		A1441	A1314	G1251	G1184	U1119	U1046	C982		U859	A796	G733
U1647	U1579	U1505	C1442	A1315	C1252	C1185	C1120		C983		U860	A797	G734
C1648			G1443	G1316	C1253		G1121	C1052	A984		G861	G798	G735
	A1582	G1508	C1444	G1317	G1254	G1191	A1122	G1053	G985		A862	C799	G736
C1651	A1583	A1584	A1445	A1318	A1255	A1192	G1123	C1054	A986		C863	U800	G737
C1653	G1584	U1513	U1446	C1319	C1256	G1193	U1124	A1055	G987		C864	A801	G738
A1654	A1585	C1514	U1447	A1320	U1257	U1194	G1125	U1056	G988		A865	A802	G739
C1655	A1586	U1515	A1448	A1321	G1258	U1195	A1126	A1057	C989		U866	C803	A740
	A1587		C1449	A1322	A1259	G1196	C1127	U1058	A990		G867	C804	
C1656	A1588	C1522	G1450	G1323	A1260	C1197	G1128	G1058	A991		U868	A805	G742
A1657	G1589	A1523	C1451	G1324	G1261	C1198	A1129	A1059	A992		C869	A806	A743
		C1524	U1452	C1325	U1262	G1199	U1130		C993		C870	A807	C744
C1661	U1592		A1453	U1326	G1263	G1200		G1066	A994		U871	C808	C745
C1663	C1593	G1527	U1454	C1327	C1264	G1201	G1133	A1068	A995		C872	C809	G746
C1664	A1594	C1528	C1455	C1328	G1265	U1202	C1134	G1069	C996		U873	U810	
C1665	A1595	C1529	C1456	U1329	G1266	A1203	G1135	C997	C997		A874	G811	A748
	A1596	U1530	A1457	G1330	A1267	G1204	G1136	U1071	C998		G875	G812	C749
A1669	A1597	C1531	A1458		U1268	G1205	A1137	U1072	A999		A876	A813	C750
C1670	C1598	A1532	U1459	G1333	G1269	G1206	A1138	G1073	G1000		G877	G814	G751
A1671		G1533	C1460	G1334	C1270	G1207	A1139	C1074	A1001		C878	A815	G752
	A1603		C1461	A1335	C1271	A1208	A1140	G1075	C1002		A879	A816	U753
A1672	A1604	U1537	C1462	G1336	G1272	G1209	U1141	U1076			C880	A817	G754
C1673	A1605	A1538	A1463	U1337	G1273	C1210	G1142	U1077	A1007		U881	G818	C755
C1674	C1606	U1539	A1464	G1338	C1274	G1211	A1143	A1078	G1008		C882	C819	G756
C1675	G1607	C1540	G1465	U1339	A	U1212	U1144	G1079			A883	U820	U757
U1676			C1466	C1340	U1276	U1213	C1145		A1011			A821	G758
C1677	U1608	G1541	C1466	C1340	U1276	U1213	C1145	A1080	A1011			A821	G758
	G1609	U1542	U1467	G1341	G1277	C1214	G1146	A1081	A1012		A886	G822	C759
U1678	A1610	G1543	A1468	U1342	A1278	A1215	G1147	G1082	G1013		C887	U823	U760
C1679	C1611	U1544	U1469	C1343	G1279	G1216	G1148	C1083	G1014		G888	U824	G761
A1680	U1611	G1545	G1470	C1344	U1280	U1217	G1149		U1015		C889	C825	A762
A1681	U1612	U1546	G1471	C1344	U1280	U1217	G1149		G1016		C890	G763	A763
C1682	G1613	C1546	C1471	G1345	A1281	C1218	C1150	C1086	C1016		U890	U826	A764
A1683	U1614	U1547	C1472	C1346	A1282	C1219	U1151	C1087	C1017		C891	C827	A765

G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G3009	G3010	G3011	G3012	G3013	G3014	G3015	G3016	G3017	G3018	G3019	G3020	G3021	G3022	G3023	G3024	G3025	G3026	G3027	G3028	G3029	G3030	G3031	G3032	G3033	G3034	G3035	G3036	G3037	G3038	G3039	G3040	G3041	G3042	G3043	G3044	G3045	G3046	G3047	G3048	G3049	G3050	G3051	G3052	G3053	G3054	G3055	G3056	G3057	G3058	G3059	G3060	G3061	G3062	G3063	G3064	G3065	G3066	G3067	G3068	G3069	G3070	G3071	G3072	G3073	G3074	G3075	G3076	G3077	G3078	G3079	G3080	G3081	G3082	G3083	G3084	G3085	G3086	G3087	G3088	G3089	G3090	G3091	G3092	G3093	G3094	G3095	G3096	G3097	G3098	G3099	G3100	G3101	G3102	G3103	G3104	G3105	G3106	G3107	G3108	G3109	G3110	G3111	G3112	G3113	G3114	G3115	G3116	G3117	G3118	G3119	G3120	G3121	G3122	G3123	G3124	G3125	G3126	G3127	G3128	G3129	G3130	G3131	G3132	G3133	G3134	G3135	G3136	G3137	G3138	G3139	G3140	G3141	G3142	G3143	G3144	G3145	G3146	G3147	G3148	G3149	G3150	G3151	G3152	G3153	G3154	G3155	G3156	G3157	G3158	G3159	G3160	G3161	G3162	G3163	G3164	G3165	G3166	G3167	G3168	G3169	G3170	G3171	G3172	G3173	G3174	G3175	G3176	G3177	G3178	G3179	G3180	G3181	G3182	G3183	G3184	G3185	G3186	G3187	G3188	G3189	G3190	G3191	G3192	G3193	G3194	G3195	G3196	G3197	G3198	G3199	G3200	G3201	G3202	G3203	G3204	G3205	G3206	G3207	G3208	G3209	G3210	G3211	G3212	G3213	G3214	G3215	G3216	G3217	G3218	G3219	G3220	G3221	G3222	G3223	G3224	G3225	G3226	G3227	G3228	G3229	G3230	G3231	G3232	G3233	G3234	G3235	G3236	G3237	G3238	G3239	G3240	G3241	G3242	G3243	G3244	G3245	G3246	G3247	G3248	G3249	G3250	G3251	G3252	G3253	G3254	G3255	G3256	G3257	G3258	G3259	G3260	G3261	G3262	G3263	G3264	G3265	G3266	G3267	G3268	G3269	G3270	G3271	G3272	G3273	G3274	G3275	G3276	G3277	G3278	G3279	G3280	G3281	G3282	G3283	G3284	G3285	G3286	G3287	G3288	G3289	G3290	G3291	G3292	G3293	G3294	G3295	G3296	G3297	G3298	G3299	G3300	G3301	G3302	G3303	G3304	G3305	G3306	G3307	G3308	G3309	G3310	G3311	G3312	G3313	G3314	G3315	G3316	G3317	G3318	G3319	G3320	G3321	G3322	G3323	G3324	G3325	G3326	G3327	G3328	G3329	G3330	G3331	G3332	G3333	G3334	G3335	G3336	G3337	G3338	G3339	G3340	G3341	G3342	G3343	G3344	G3345	G3346	G3347	G3348	G3349	G3350	G3351	G3352	G3353	G3354	G3355	G3356	G3357	G3358	G3359	G3360	G3361	G3362	G3363	G3364	G3365	G3366	G3367	G3368	G3369	G3370	G3371	G3372	G3373	G3374	G3375	G3376	G3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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	170.00Å 414.50Å 693.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.40)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.340	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	58817	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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: TEL

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	0.54	2/65792 (0.0%)	0.73	48/102613 (0.0%)

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	28

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	762	A	O3'-P	-6.44	1.51	1.61
1	0	764	A	O5'-C5'	5.38	1.50	1.42

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	765	C	N1-C1'-C2'	9.61	128.42	114.00
1	0	2044	G	P-O3'-C3'	8.87	133.50	120.20
1	0	765	C	O4'-C4'-C3'	-7.29	98.81	106.10
1	0	1182	U	O4'-C1'-N1	7.20	119.30	108.50
1	0	2001	G	N9-C1'-C2'	-7.19	101.22	112.00

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	229	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	389	G	Sidechain
1	0	431	G	Sidechain
1	0	438	G	Sidechain
1	0	459	A	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	58759	0	29615	2736	0
2	0	58	0	65	11	0
All	All	58817	0	29680	2737	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 31.

The worst 5 of 2737 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	1.18
1:0:752:G:H5'	1:0:1775:A:H61	1.07	1.13
1:0:1572:C:H2'	1:0:1573:G:H5''	1.21	1.10
1:0:2451:G:H1'	1:0:2457:A:H61	1.16	1.09
1:0:387:A:H5'	1:0:436:A:H62	1.07	1.08

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	2727/2880 (94%)	580 (21%)	62 (2%)

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	14	A
1	0	15	G
1	0	45	C
1	0	50	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1299	A
1	0	2404	A
1	0	1626	A
1	0	2377	U
1	0	2758	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 oligosaccharides 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	TEL	0	2881	-	60,62,62	3.60	32 (53%)	78,92,92	3.48	36 (46%)

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	TEL	0	2881	-	1/1/19/19	21/73/108/108	0/4/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	2881	TEL	C30-C34	12.76	1.72	1.54
2	0	2881	TEL	C24-C28	7.88	1.64	1.52
2	0	2881	TEL	C47-C43	7.77	1.51	1.39
2	0	2881	TEL	O9-C15	7.45	1.51	1.34
2	0	2881	TEL	C51-C46	6.56	1.50	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	2881	TEL	O9-C15-C21	13.62	124.38	110.93
2	0	2881	TEL	C3-N6-C10	-11.34	96.35	111.64
2	0	2881	TEL	C42-O39-C34	7.35	128.76	116.26
2	0	2881	TEL	O20-C15-C21	-6.88	115.73	124.65
2	0	2881	TEL	O39-C34-C28	-6.48	91.39	106.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	0	2881	TEL	C21

5 of 21 torsion outliers are listed below:

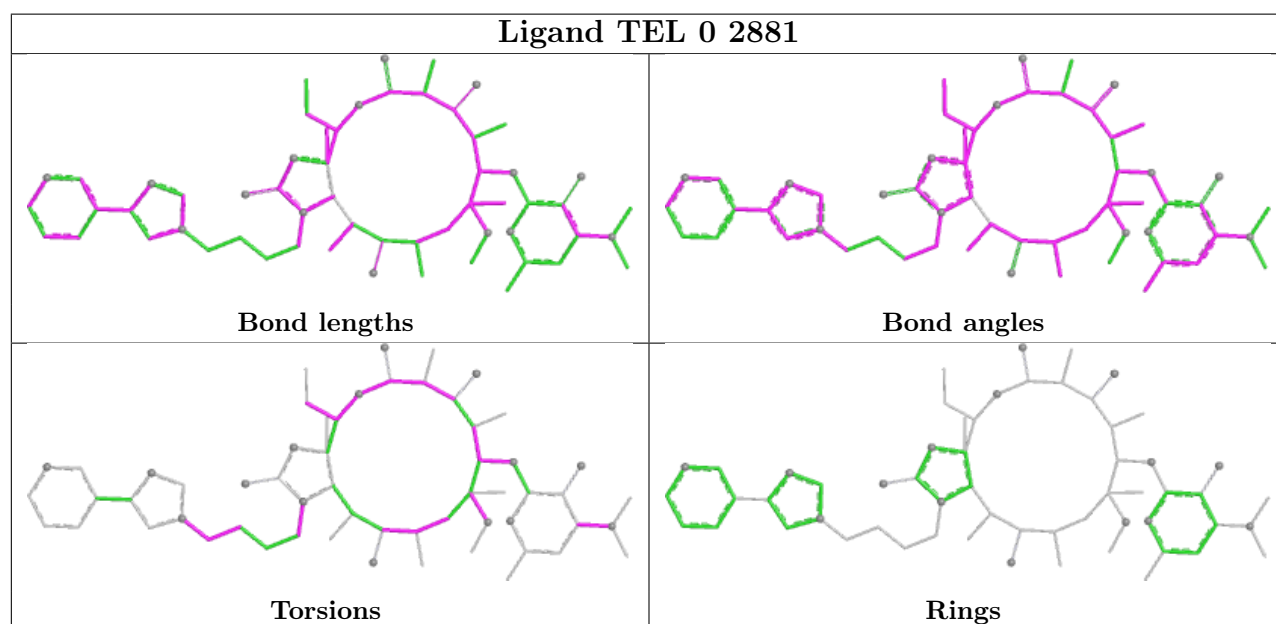
Mol	Chain	Res	Type	Atoms
2	0	2881	TEL	C7-C13-C19-C24
2	0	2881	TEL	C25-C21-C26-O29
2	0	2881	TEL	C25-C21-C26-C30
2	0	2881	TEL	C26-C30-C34-C28
2	0	2881	TEL	C28-C34-O39-C42

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	0	2881	TEL	11	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 [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 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.