



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:58 PM GMT

PDB ID : 2OGN
Title : The crystal structure of the large ribosomal subunit from *Deinococcus radiodurans* complexed with the pleuromutilin derivative SB-280080
Authors : Davidovich, C.; Bashan, A.; Auerbach-Nevo, T.; Yonath, A.
Deposited on : 2007-01-07
Resolution : 3.56 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

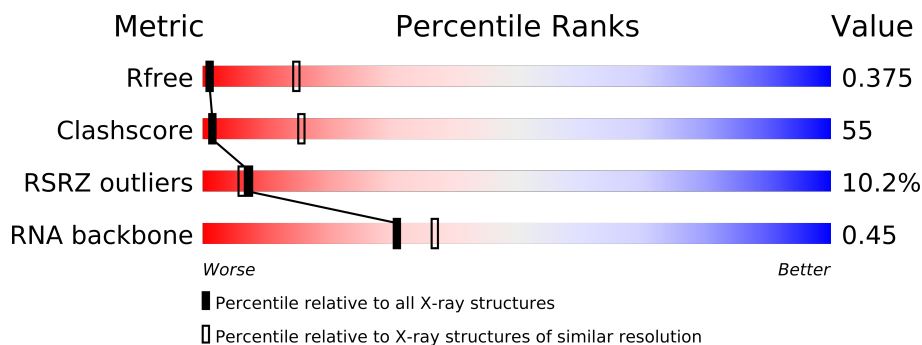
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.56 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))
R_{free}	66092	1024 (3.80-3.32)
Clashscore	79885	1022 (3.72-3.40)
RSRZ outliers	66119	1025 (3.80-3.32)
RNA backbone	1838	1011 (4.30-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	B	211	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 59597 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

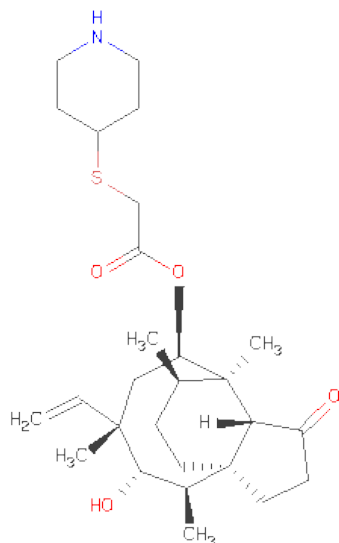
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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 protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	205	Total	C	0	0	205
			205	205			

- Molecule 3 is (3AS,4R,5S,6S,8R,9R,9AR,10R)-5-HYDROXY-4,6,9,10-TETRAMETHYL-1-OXO-6-VINYLDECAHYDRO-3A,9-PROPANOCYCLOPENTA[8]ANNULEN-8-YL(PIPERIDIN-4-YLTHIO)ACETATE (three-letter code: G80) (formula: C₂₇H₄₃NO₄S).



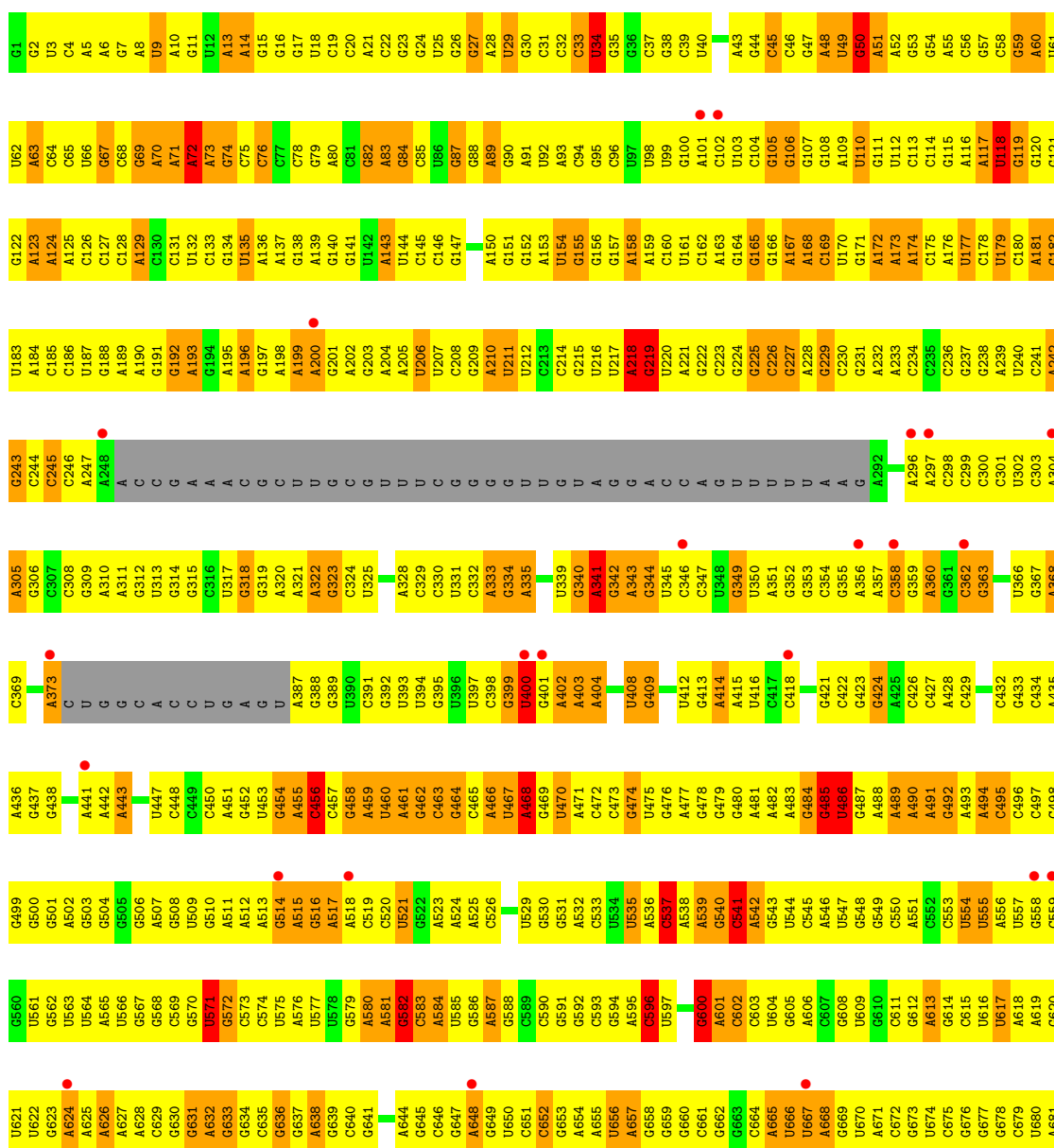
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	0	1	Total	C	N	O	S	0	0
			33	27	1	4	1		

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.

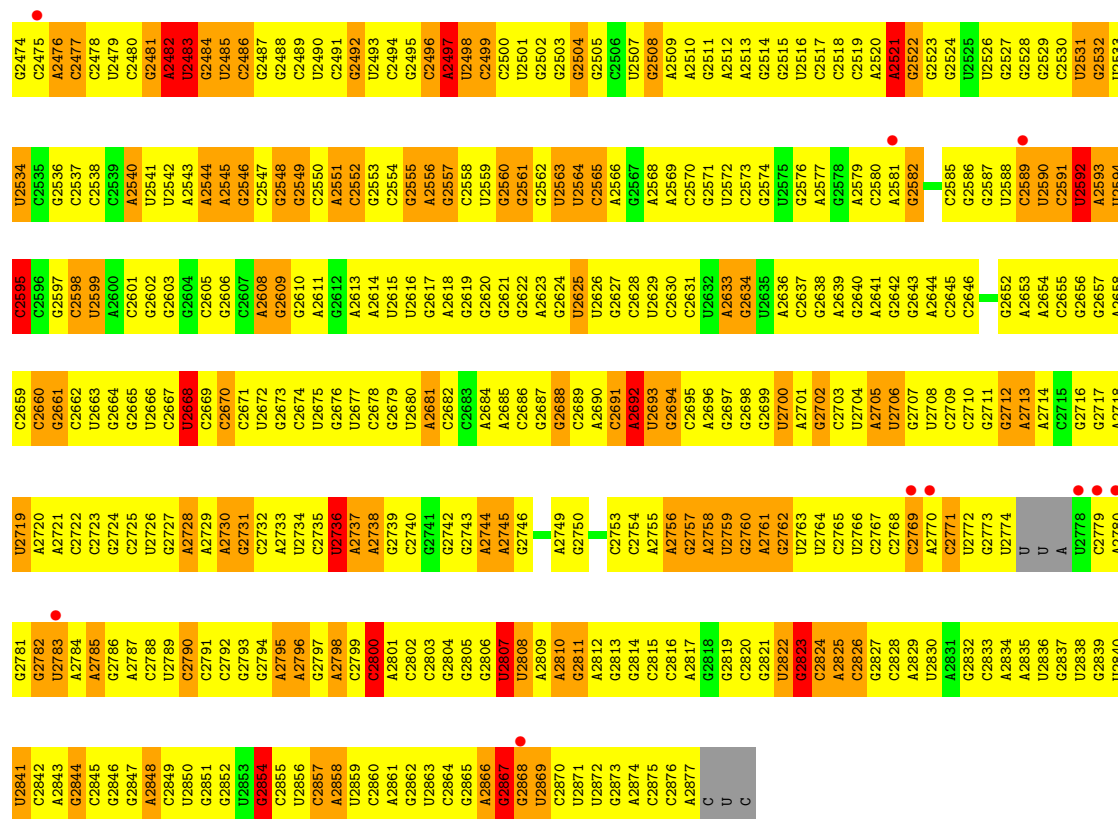
• Molecule 1: 23S ribosomal RNA

Chain 0: 



U1551	C1489	G1428	A1367	G1241	A1180	U1116	G1053	C927	A865	G805	A743	G682
C1552	U1490	A1429	G1368	A1242	C1181	G1117	C1094	G928	U866	A806	G746	A683
G1553	C1369	G1430	G1369	G1243	U1182	G1118	A1055	A929	G867	A807	G747	C684
G1554	U1431	U1370	G1370	G1244	C1185	U1119	U1056	A930	C985	C808	A748	U685
A1555	G1371	G1245	G1371	G1245	C1186	G1121	A1057	G931	U871	C809	A749	G686
C1558	A1494	A1432	U1307	G1246	A1187	G1122	G1058	G932	G872	U810	C749	G687
G1559	G1308	U1307	U1247	U1247	A1187	A1122	A1059	G933	U873	G811	C750	A688
G1495	C1308	G1308	G1373	G1248	A1188	G1123	C1060	G934	A874	G812	G751	A689
C1497	G1309	G1309	G1374	G1249	A1189	G1124	A1061	G935	G875	A813	G752	A690
G1498	C1310	C1310	C1375	G1250	C1190	G1125	A1062	A936	A876	C814	G753	C691
A1499	G1311	G1311	G1376	A1250	C1191	A1126	G1000	G937	A877	A815	G754	C692
U1500	G1312	G1312	G1377	G1251	G1191	A1127	G1001	G938	G878	U816	C755	G693
U1563	U1313	U1313	A1378	C1252	A1192	G1128	A1002	C939	A879	A817	C756	G694
G1501	A1314	C1253	C1253	G1254	U1194	G1129	C1003	G940	C880	G818	U757	G695
G1502	A1441	A1315	A1315	A1255	U1195	U1130	C1004	U941	U881	C819	G758	U696
G1566	G1442	G1316	G1316	C1256	G1196	G1133	U1005	U942	C882	U820	C759	G697
A1568	G1443	C1322	G1322	A1257	U1197	G1134	A1007	U943	A883	G822	U760	A698
U1505	G1444	G1323	G1323	G1258	C1198	G1134	U1072	A944	C884	G823	G761	G699
C1506	C1445	G1324	A1259	A1260	U1199	A1137	G1074	G945	A885	U824	A762	C700
C1570	U1446	G1325	G1260	G1261	G1201	A1138	U1077	U946	A886	C825	A763	U701
G1571	U1447	G1326	G1262	G1262	U1202	A1139	A1078	C947	G887	G826	A764	A702
A1574	G1450	C1327	G1263	G1263	A1203	A1140	A1011	C948	C888	U826	C765	A703
C1577	U1451	G1328	G1264	G1264	G1204	U1141	G1079	G949	C889	C927	A766	G704
U1578	U1452	U1329	G1265	G1265	G1205	G1142	G1013	G950	U890	C928	G767	C705
G1579	U1453	G1330	G1266	G1266	G1206	A1143	A1080	G951	A891	C929	U768	A706
C1580	U1454	G1331	G1267	G1267	G1207	A1144	A1081	A952	G	C930	C769	U707
C1581	U1455	G1332	G1268	G1268	A1208	C1145	G1082	U953	G	G831	G772	G708
A1582	A1457	C1333	G1269	G1269	G1209	G1146	A1083	U954	G	A832	G773	A709
U1583	C1397	A1397	C1270	C1270	C1210	G1147	G1084	G955	G	A833	A774	C710
G1584	G1398	G1398	C1271	C1271	G1211	G1148	C1086	G957	C	U835	U775	A712
A1585	C1399	C1399	G1272	G1272	U1212	G1149	G1087	G958	C	G836	G776	G713
U1586	A1400	A1400	G1273	G1273	U1213	C1150	A1088	U959	U	U837	A777	G714
C1587	C1462	G1401	C1274	C1274	C1214	U1151	C1089	U960	A	A838	G778	U715
A1588	A1463	G1341	A1275	A1275	A1215	G1152	G1090	G	C	U839	U779	U716
U1526	A1464	U1342	C1342	C1342	G1216	A1153	C1091	A964	C	U840	U780	G717
G1527	C1466	C1344	A1405	A1405	U1217	A1154	U1092	G965	A	G841	G781	A718
C1528	U1467	G1406	A1406	A1406	C1218	G1155	U1093	A966	G	A842	U782	A719
A1529	A1468	G1407	G1407	G1407	C1219	U1159	C1094	C967	C	G843	G783	A720
U1530	U1469	C1347	A1281	A1281	C1221	C1160	A1095	U968	U	U844	U784	C721
U1531	C1348	C1348	A1282	A1282	G1222	U1161	U1030	A970	U	U845	U785	C722
A1532	U1409	U1409	C1283	C1283	G1223	A1162	C1031	A971	A	A846	U786	C723
G1533	C1349	G1349	G1284	G1284	A1224	C1163	G1098	G972	C	C847	A787	G726
A1534	G1350	G1350	A1285	A1285	G1225	C1164	A1099	U973	A911	A848	G788	U727
C1535	C1351	G1351	U1286	U1286	A1226	G1165	G1109	U974	A912	G849	G789	G728
U1473	G1412	C1412	A1287	A1287	A1227	G1166	U1101	C975	A913	C850	A790	A729
A1474	U1413	G1413	A1288	A1288	G1228	A1167	G1102	G976	C914	C851	G791	G730
C1475	C1415	C1415	A1289	A1289	C1229	G1168	C1103	G977	C915	U852	U792	C731
U1476	A1416	A1355	A1290	A1290	G1230	U1169	U1038	U978	U916	C853	G793	G732
C1477	C1417	G1356	G1291	G1291	C1231	C1169	A1039	U979	U917	G854	A794	G733
U1478	U1418	A1292	A1292	A1292	A1232	U1170	A1040	A980	A918	G855	A795	G734
G1479	G1419	C1358	A1293	A1293	U1233	A1171	G1041	G981	U919	A956	A796	G735
A1604	A1480	G1359	G1294	G1294	A1233	U1172	A1042	C982	G920	U857	A797	G736
U1481	U1420	G1360	U1295	U1295	C1234	G1173	G1043	G983	A921	G858	G798	G737
A1544	U1482	C1421	G1296	G1296	C1235	G1174	C1110	U984	A922	U859	C799	G738
G1545	G1483	C1422	A1361	A1361	G1236	A1175	U1045	G985	A923	U860	U800	G739
U1608	A1546	A1362	A1297	A1297	G1237	U1176	U1046	A986	C924	C861	A801	A740
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U1548	A1486	C1364	A1299	A1299	A1239	U1178	U1051	C988	U925	C863	C803	G742
U1611	U1487	A1365	A1300	A1300	A1239	C1178	C1052			C864	C804	
U1612	G1488	A1366	U1301	U1301	G1240	A1179	C1115					

A2410	A2411	A2412	A2413	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	G2287	A2288	A2289	A2290	A2291	C2292	C2293	A2294	C2295	C2296	C2297	C2298	C2299	C2300	A2301	C2302	C2303	A2306	A2307	A2308	A2309	G2310	A2311	A2312	C2313	A2314	A2315	C2316	C2317	U2318	C2319	G2320	C2321	C2322	U2323	C2324	A2325	C2326	A2265	A2266	A2267	G2268	G2269	U2270	C2271	A2272	C2273	C2274	U2275	C2276	A2277	A2278	A2279	A2280	U2281	A2282	C2283	U2284	U2285	C2286	G2166	A2167	A2168	A2169	C2170	U2171	U2172	C2173	C2174	C2175	C2237	C2238	U2177	U2178	C2179	U2180	A2182	C2183	C2184	U2185	A2187	A2188	A2189	A2190	U2197	U2198	C2199	G2200	G2201	C2202	C2203	A2204	C2205	C2206	G2207	C2208	C2209	C2210	U2211	U2212	G2213	G2214	C2215	G2216	G2217	U2218	U2219	A2220	G2221	U2222	U2223	U2224	G2225	U2105	G2106	G2107	A2108	A2109	C2110	C	C	U	C	U	G	A2117	A2118	C2119	C2120	C2121	G2123	C2124	C2125	U	U	U	U	G	U	G	U2067	C2068	U2069	U2070	U2071	C2072	A2073	U2074	U2075	U2076	U2077	G2078	A2079	U2080	U2081	C2082	C2083	A2084	C2085	U2086	C2089	U2090	C2091	U2092	A2093	A2094	C2095	U2096	A2097	G	A	U	A	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2446	A2447	A2448	A2449	A2450	A2451	A2452	A2453	A2454	A2455	A2456	A2457	A2458	A2459	A2460	A2461	A2462	A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	A2485	A2486	A2487	A2488	A2489	A2490	A2491	A2492	A2493	A2494	A2495	A2496	A2497	A2498	A2499	A2500	A2501	A2502	A2503	A2504	A2505	A2506	A2507	A2508	A2509	A2510	A2511	A2512	A2513	A2514	A2515	A2516	A2517	A2518	A2519	A2520	A2521	A2522	A2523	A2524	A2525	A2526	A2527	A2528	A2529	A2530	A2531	A2532	A2533	A2534	A2535	A2536	A2537	A2538	A2539	A2540	A2541	A2542	A2543	A2544	A2545	A2546	A2547	A2548	A2549	A2550	A2551	A2552	A2553	A2554	A2555	A2556	A2557	A2558	A2559	A2560	A2561	A2562	A2563	A2564	A2565	A2566	A2567	A2568	A2569	A2570	A2571	A2572	A2573	A2574	A2575	A2576	A2577	A2578	A2579	A2580	A2581	A2582	A2583	A2584	A2585	A2586	A2587	A2588	A2589	A2590	A2591	A2592	A2593	A2594	A2595	A2596	A2597	A2598	A2599	A2600	A2601	A2602	A2603	A2604	A2605	A2606	A2607	A2608	A2609	A2610	A2611	A2612	A2613	A2614	A2615	A2616	A2617	A2618	A2619	A2620	A2621	A2622	A2623	A2624	A2625	A2626	A2627	A2628	A2629	A2630	A2631	A2632	A2633	A2634	A2635	A2636	A2637	A2638	A2639	A2640	A2641	A2642	A2643	A2644	A2645	A2646	A2647	A2648	A2649	A2650	A2651	A2652	A2653	A2654	A2655	A2656	A2657	A2658	A2659	A2660	A2661	A2662	A2663	A2664	A2665	A2666	A2667	A2668	A2669	A2670	A2671	A2672	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2682	A2683	A2684	A2685	A2686	A2687	A2688	A2689	A2690	A2691	A2692	A2693	A2694	A2695	A2696	A2697	A2698	A2699	A2700	A2701	A2702	A2703	A2704	A2705	A2706	A2707	A2708	A2709	A2710	A2711	A2712	A2713	A271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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.47Å 412.74Å 696.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.56 29.95 – 3.56	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.96-3.56) 90.6 (29.95-3.56)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.338 0.358 , 0.375	Depositor DCC
R_{free} test set	13108 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 33.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 263343 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	59597	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G80

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	0.62	9/66467 (0.0%)	0.83	95/103673 (0.1%)

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	158

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	788	G	N9-C4	8.60	1.44	1.38
1	0	700	C	N1-C2	8.52	1.48	1.40
1	0	788	G	C5-C6	6.89	1.49	1.42
1	0	824	U	N1-C2	6.74	1.44	1.38
1	0	788	G	C2-N3	5.96	1.37	1.32

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1342	U	N1-C1'-C2'	10.68	127.89	114.00
1	0	985	G	N9-C1'-C2'	10.52	127.68	114.00
1	0	2497	A	N9-C1'-C2'	10.09	127.12	114.00
1	0	1975	G	N9-C1'-C2'	9.37	126.19	114.00
1	0	2660	C	N1-C1'-C2'	9.30	126.09	114.00

There are no chirality outliers.

5 of 158 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	154	U	Sidechain
1	0	29	U	Sidechain
1	0	50	G	Sidechain
1	0	67	G	Sidechain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	4825	0
2	B	205	0	0	2	0
3	0	33	0	43	7	0
All	All	59597	0	29960	4828	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 55.

The worst 5 of 4828 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2040:A:H2'	1:0:2041:A:C8	1.52	1.42
1:0:2040:A:C2'	1:0:2041:A:H8	1.48	1.27
1:0:2564:U:O2'	1:0:2565:C:H5'	1.34	1.26
1:0:2418:A:H1'	1:0:2565:C:O2'	1.31	1.24
1:0:2810:A:C6	1:0:2854:G:C8	2.27	1.22

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	664 (24%)	167 (6%)

5 of 664 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	9	U
1	0	13	A
1	0	14	A
1	0	27	G
1	0	33	C

5 of 167 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1326	U
1	0	1634	A
1	0	2660	C
1	0	1337	G
1	0	1407	G

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 carbohydrates 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	$\# Z > 2$
3	G80	0	2881	-	36,36,36	2.91	13 (36%)	56,56,56	2.02	14 (25%)

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
3	G80	0	2881	-	-	1/12/81/81	0/1/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	2881	G80	C12-C11	7.73	1.67	1.55
3	0	2881	G80	C5-C6	6.30	1.70	1.56
3	0	2881	G80	C10-C11	5.08	1.63	1.55
3	0	2881	G80	C5-C4	4.92	1.63	1.56
3	0	2881	G80	C8-C7	4.58	1.64	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0	2881	G80	C7-C6-C5	5.69	118.59	111.21
3	0	2881	G80	C4-C5-C6	-5.68	97.21	106.87
3	0	2881	G80	C16-C6-C7	-4.54	103.04	110.43
3	0	2881	G80	C18-C12-C11	4.49	111.80	107.43
3	0	2881	G80	C12-C11-C10	-4.17	107.83	116.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	0	2881	G80	C20-C19-C12-C13

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	0	2766/2880 (96%)	0.22	188 (6%)	17 9	12, 79, 200, 200	0
2	B	205/211 (97%)	2.48	115 (56%)	0 1	3, 58, 141, 202	0
All	All	2971/3091 (96%)	0.37	303 (10%)	7 6	3, 77, 200, 202	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	144	ARG	10.9
2	B	146	THR	10.4
1	0	558	G	10.1
1	0	730	C	8.3
1	0	2096	U	8.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	G80	0	2881	33/33	0.25	0.78	62,62,62,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.