



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 05:40 am BST

PDB ID : 1NWY
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOC-
CUS RADIODURANS WITH AZITHROMYCIN
Authors : Schlutzen, F.; Harms, J.; Franceschi, F.; Hansen, H.A.S.; Bartels, H.; Zari-
vach, R.; Yonath, A.
Deposited on : 2003-02-07
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 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)
Xtriage (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) : 2.11

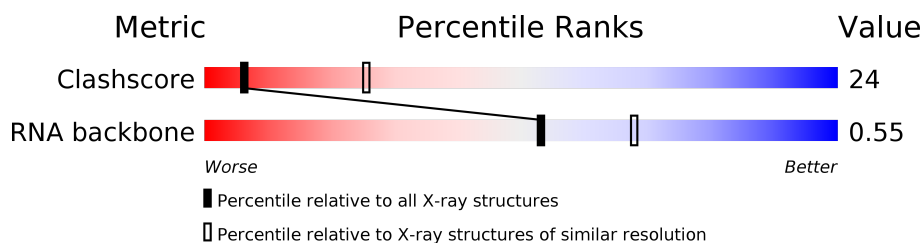
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.


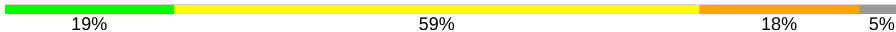

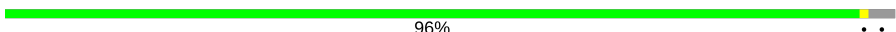
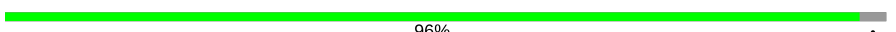
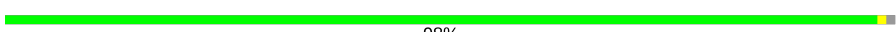
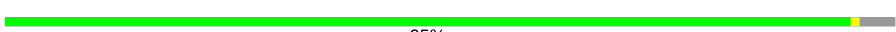


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1205 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)
















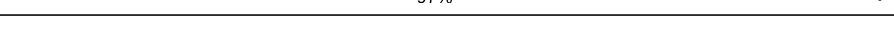
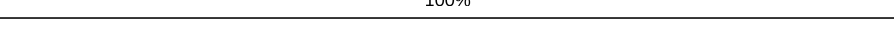
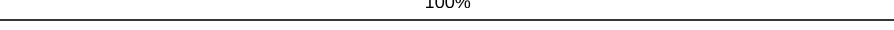
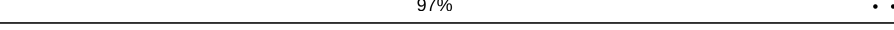
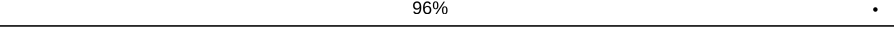
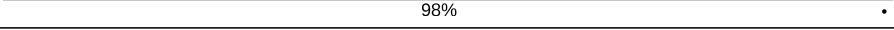
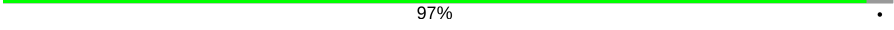
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 26% 57% 13% .
2	9	124	 19% 59% 18% 5%
3	A	274	 99% .
4	B	211	 96% ..
5	C	204	 96% .
6	D	180	 98% ..
7	E	185	 95% . .
8	F	146	 34% . 64%
9	G	144	 99% .

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Mol	Chain	Length	Quality of chain
10	H	174	 82% 18%
11	I	134	 99% .
12	J	156	 90% 10%
13	K	141	 87% . 12%
14	L	116	 97% ..
15	M	113	 97% ..
16	N	166	 75% . 25%
17	O	118	 99% .
18	P	100	 100%
19	Q	134	 97% .
20	R	94	 99% .
21	S	115	 98% .
22	T	237	 94% 6%
23	U	91	 95% 5%
24	W	67	 97% .
25	X	55	 100%
26	Y	73	 100%
27	Z	59	 97% ..
28	1	55	 96% .
29	2	47	 98% .
30	3	65	 97% .
31	4	37	 95% 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
32	ZIT	0	2881	-	-	X	-
32	ZIT	0	2882	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65404 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 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			

- Molecule 3 is a protein called ribosomal protein L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	270	Total	C	0	0	270
			270	270			

- Molecule 4 is a protein called ribosomal protein L3.

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

- Molecule 5 is a protein called ribosomal protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	C	197	Total	C	0	0	197
			197	197			

- Molecule 6 is a protein called ribosomal protein L5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	D	178	Total	C	0	0	178
			178	178			

- Molecule 7 is a protein called ribosomal protein L6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	E	177	Total	C	0	0	177
			177	177			

- Molecule 8 is a protein called ribosomal protein L9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	F	52	Total	C	0	0	52
			52	52			

- Molecule 9 is a protein called ribosomal protein L11.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	G	143	Total	C	0	0	143
			143	143			

- Molecule 10 is a protein called ribosomal protein L13.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	H	143	Total	C	0	0	143
			143	143			

- Molecule 11 is a protein called ribosomal protein L14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	I	132	Total	C	0	0	132
			132	132			

- Molecule 12 is a protein called ribosomal protein L15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	J	141	Total	C	0	0	141
			141	141			

- Molecule 13 is a protein called ribosomal protein L16.

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

- Molecule 14 is a protein called ribosomal protein L17.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	L	114	Total	C	0	0	114
			114	114			

- Molecule 15 is a protein called ribosomal protein L18.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	M	111	Total	C	8	0	111
			111	111			

- Molecule 16 is a protein called ribosomal protein L19.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
16	N	125	Total	C	0	0	125
			125	125			

- Molecule 17 is a protein called ribosomal protein L20.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
17	O	117	Total	C	16	0	117
			117	117			

- Molecule 18 is a protein called ribosomal protein L21.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
18	P	100	Total	C	0	0	100
			100	100			

- Molecule 19 is a protein called ribosomal protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
19	Q	130	Total	C	0	0	130
			130	130			

- Molecule 20 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
20	R	93	Total	C	0	0	93
			93	93			

- Molecule 21 is a protein called ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	113	Total C 113 113	0	0	113

- Molecule 22 is a protein called general stress protein Ctc.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	223	Total C 223 223	43	0	223

- Molecule 23 is a protein called ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	86	Total C 86 86	0	0	86

- Molecule 24 is a protein called ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	W	65	Total C 65 65	0	0	65

- Molecule 25 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	X	55	Total C 55 55	4	0	55

- Molecule 26 is a protein called ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Y	73	Total C 73 73	0	0	73

- Molecule 27 is a protein called ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Z	58	Total C 58 58	0	0	58

- Molecule 28 is a protein called ribosomal protein L33.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
28	1	53	Total	C		0	0	53
			53	53				

- Molecule 29 is a protein called ribosomal protein L34.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
29	2	46	Total	C		0	0	46
			46	46				

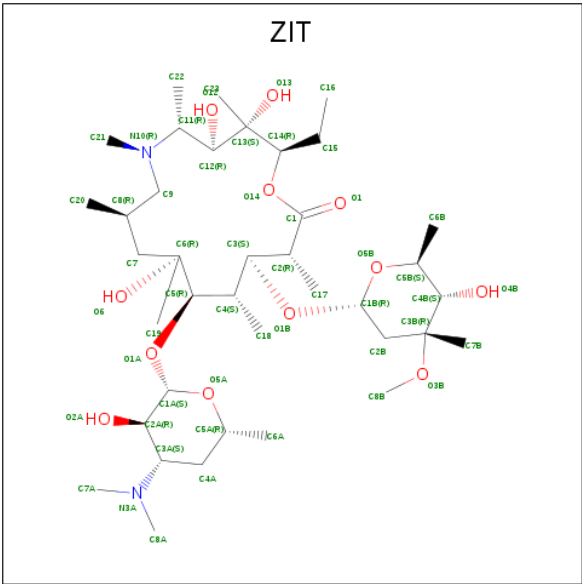
- Molecule 30 is a protein called ribosomal protein L35.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
30	3	63	Total	C		0	0	63
			63	63				

- Molecule 31 is a protein called ribosomal protein L36.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
31	4	35	Total	C		0	0	35
			35	35				

- Molecule 32 is AZITHROMYCIN (three-letter code: ZIT) (formula: C₃₈H₇₂N₂O₁₂).



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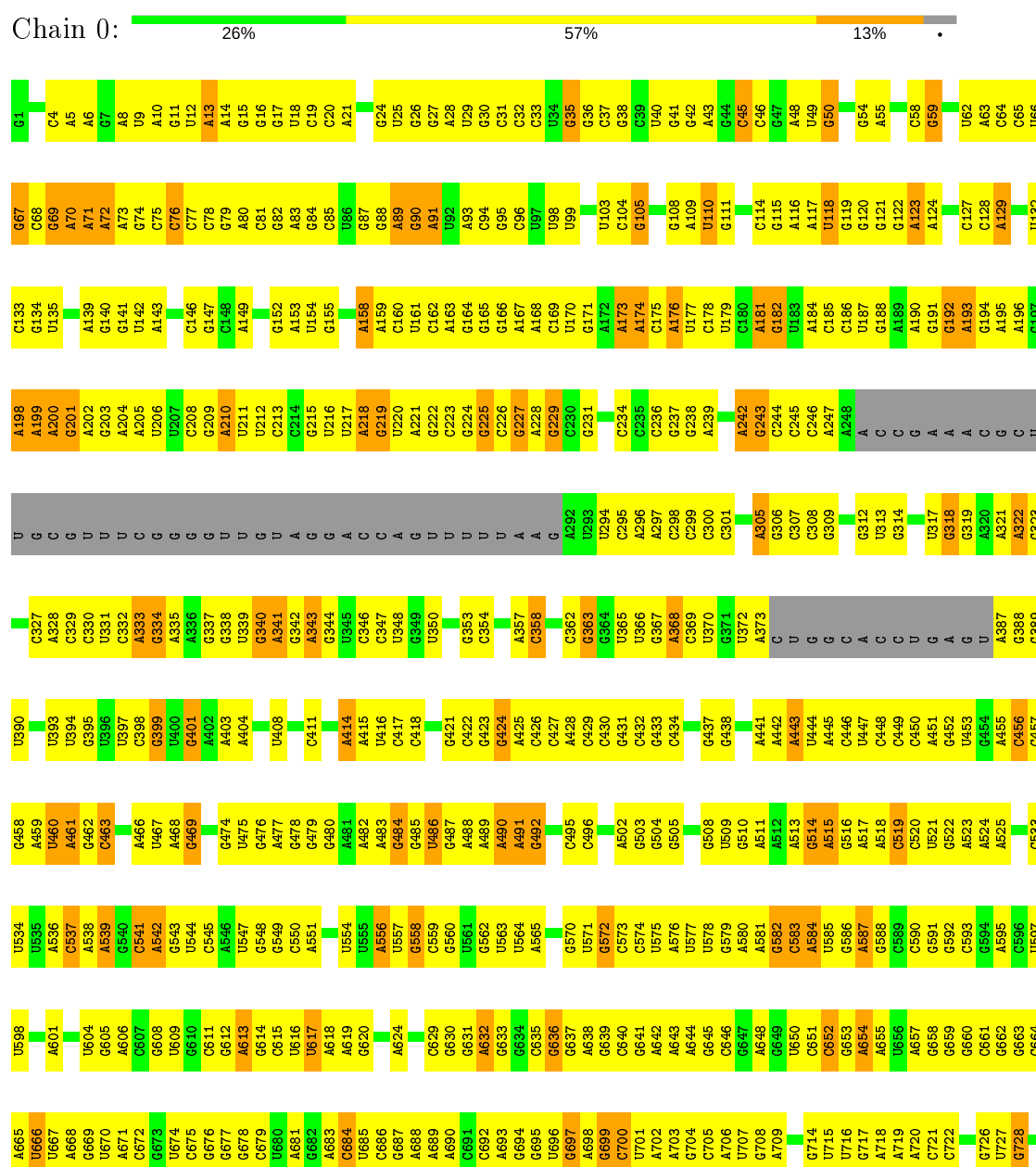
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	0	1	52	38	2	12	0	0

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 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.

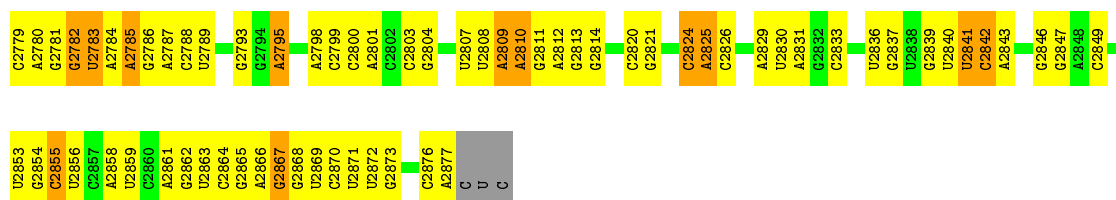
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RRNA



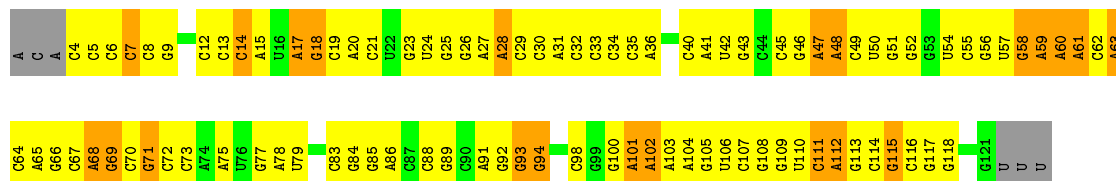
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G1559	A1560	A1561	G1562	G1566	A1567	A1568	A1569	C1570	G1571	A1572	G1573	A1574	C1575	G1576	A1577	G1578	G1579	C1580	C1581	A1582	A1583	G1584	A1585	A1586	A1587	A1588	G1589	C1590	G1591	G1592	C1593	U1594	A1595	A1596	A1597	C1598	G1599	U1600	A1601	G1602	A1603	A1604	A1605	U1608	G1609	A1610	U1611	U1612	G1613	C1614	C1615	C1616	A1685	A1686	U1687	G1688	A1689	C1690	C1691
C1489	U1490	C1491	A1492	A1493	G1494	G1495	G1496	U1500	C1501	G1502	G1503	G1504	U1505	A1509	A1512	U1513	A1514	U1515	A1516	C1517	C1518	G1519	G1520	C1524	G1527	C1528	A1529	U1530	C1531	A1532	G1533	A1534	C1535	G1536	U1537	A1538	U1539	C1540	G1541	G1542	G1543	A1544	G1545	C1546	U1547	U1548	C1552	G1553	U1554	A1555	U1556	C1557	C1558						
G1427	G1428	A1429	G1430	U1431	G1432	A1433	G1436	A1437	G1438	G1439	G1440	A1441	G1442	G1443	A1444	A1445	U1446	U1447	A1448	G1449	G1450	U1451	U1452	C1455	C1456	A1457	A1458	U1459	A1460	C1461	C1462	A1463	A1464	G1465	C1466	A1467	A1468	U1469	G1470	G1471	C1472	U1473	A1474	G1475	G1476	U1477	U1478	G1479	G1480	U1481	U1482	G1483	U1485	A1486	G1487	G1488			
C1358	G1359	C1363	C1364	U1365	G1368	A1371	A1372	G1373	G1374	C1375	G1376	G1377	G1378	A1379	A1380	C1381	G1382	C1383	G1384	C1385	A1386	G1387	C1388	C1389	G1390	A1391	U1392	G1393	A1397	C1398	C1399	A1400	G1401	G1402	U1403	A1404	A1405	A1406	G1407	U1408	U1409	C1411	G1412	A1416	C1417	C1418	G1419	C1422	A1423	U1424	U1426	U1426							
A1297	G1298	A1299	A1300	U1301	C1302	U1303	U1304	C1305	U1306	G1307	G1308	G1309	C1310	C1311	G1312	A1313	A1314	A1315	G1316	G1317	A1318	C1319	A1320	A1321	G1322	G1323	G1324	U1325	U1326	C1327	G1328	U1329	G1332	G1333	A1334	A1335	G1336	G1337	G1338	G1339	G1340	G1341	U1342	C1343	G1344	G1345	G1346	C1347	C1348	A1349	G1350	G1351	G1352	A1353	A1354	G1355	A1356	U1357	
A1283	C1284	C1285	C1286	A1288	A1289	G1241	A1242	G1243	U1244	G1245	G1246	U1247	G1248	G1249	A1250	G1251	C1252	G1253	A1254	A1255	G1256	U1257	A1258	A1259	A1260	G1261	U1262	G1263	C1264	G1265	G1266	A1267	U1268	G1269	C1270	C1271	G1272	G1273	G1277	A1278	G1279	U1280	A1281	G1284	A1285	U1286	A1287	A1288	A1289	A1290	G1291	A1292	A1293	G1294	U1295	G1296			
U1156	A1162	C1163	C1164	G1165	A1166	A1167	G1168	U1169	U1170	A1171	U1172	A1179	A1180	U1181	C1182	C1183	G1184	C1185	C1190	G1191	A1192	G1193	U1194	U1195	G1196	U1197	C1198	U1199	G1200	G1201	U1202	A1203	G1204	G1205	G1206	G1207	U1212	U1213	C1214	A1215	G1216	U1217	C1218	C1219	G1220	C1221	G1222	G1223	A1224	G1225	A1226	A1227	G1228	A1229	C1230				
G1082	C1083	C1086	C1087	A1088	C1089	C1090	U1091	U1092	A1095	A1096	A1099	U1100	U1101	G1102	C1103	G1110	C1111	C1113	A1114	C1115	U1116	G1117	G1121	A1122	G1123	U1124	G1125	A1126	U1130	G1131	C1132	G1133	C1134	C1135	A1136	A1137	A1138	A1139	U1141	U1141	G1142	C1145	G1146	G1147	G1148	U1151	C1152	A1153	A1154	G1155									
C1002	C1003	U1004	C1005	C1006	A1007	G1008	C1009	U1010	A1011	A1012	C1016	C1017	C1018	U1019	A1020	A1021	A1022	U1023	G1024	A1025	U1026	C1027	G1028	C1029	U1030	C1031	A1032	G1033	U1034	G1035	C1036	U1037	U1038	A1039	A1040	G1041	U1044	C1054	A1055	U1056	A1057	G1058	C1064	A1065	G1066	G1067	A1068	G1069	G1073	G1074	C1075	U1076	A1081						
A794	A795	A796	A797	G798	G799	U800	A801	A802	C803	C804	G805	A806	A807	C808	U809	G810	G811	G812	A813	G814	A815	U816	G817	G818	C819	U820	A821	U824	C825	U826	C829	C830	G831	A832	U837	A838	U839	U840	A841	A842	G843	G844	C847	A848	U852	C853	G854	G855	C926	C927	A856	C928	A857	A858	U859	U860	G861		
G732	G733	G734	G735	G736	G737	G738	G739	A740	G741	G742	A743	G744	C745	G746	C749	G750	G751	G752	G753	G754	C755	G756	U757	G758	U760	A761	A762	A763	A764	C765	A766	U768	U769	G771	G772	G773	A774	U775	G776	A777	G778	G781	U782	G783	U784	U785	U786	A787	G788	G789	A790	G791	U792	G793					

G2717	G2718	A2581	G2582	G2449	G2378	A2306	U2228	C2162	G	U2030	C1962	U1900	A1821	G1760
G2652	A2653	G2583	G2584	A2450	G2379	A2307	G2229	U2163	A	A2031	G1963	U1901	C1822	G1761
A2654	G2585	C2454	G2586	G2455	U2380	A2308	G2230	G2164	A	G2032	U1964	A1902	G1823	G1762
G2721	G2587	U2456	G2588	U2457	C2382	G2309	G2232	A2165		G2035	C1903	G1904	G1824	G1763
G2722	G2589	A2457	G2590	A2458	C2383	G2310	G2233	A2166	G2104	G2036	G1905	G1906	U1826	A1764
A2658	G2591	U2459	U2385	G2460	U2384	U2311	G2234	A2168	U2105	A2037	G1907	U1908	G1827	C1765
G2725	U2592	G2461	U2386	G2462	U2387	A2312		C2170	G2107	G2038	G1971	C1909	C1830	U1766
G2726	U2593	G2463	A2391	G2464	U2388	G2313	G2238	C2171	G2110	G2039	G1972	U1909	G1831	U1767
G2727	A2593	G2465	A2392	G2466	U2389	A2314	G2239	U2172	C	A2043	C1973	U1910	U1768	U1769
A2728	G2594	G2467	A2393	G2468	C2390	G2315	G2240	G2173	C	G2044	C1974	A1911	U1770	U1771
G2729	G2595	G2469	G2394	G2470	C2391	G2316	U2241	G2174	U	A2045	C1975	A1912	C1836	C1772
A2730	G2596	U2471	C2395	U2472	C2396	U2318	C2443	A2175	U	C2046	U1976	G1913	G1837	C1773
G2731	G2597	G2473	C2397	G2474	A2397	G2319	C2444	U2176	C	G2047	C1977	G1914	G1838	G1774
G2732	G2598	G2475	A2398	G2476	U2397	G2320	A2445	U2177	G	C2048	U1978	A1915	A1840	A1775
A2733	U2599	A2467	C2399	G2477	U2398	G2321	A2446	C2178	G	U2051	C1979	G1916	G1841	A1776
G2734	A2600	G2468	C2399	G2478	C2399	U2322	A2477	C2179	A2117	G2052	C1980	G1917	A1777	U1777
G2735	G2600	G2469	U2402	U2470	U2402	U2323	U2448	U2180	A2118	U2053	A1981	G1918	G1842	U1778
G2736	G2601	U2470	C2403	U2471	C2403	G2324	U2449	A2181	A2119	G2054	C1982	G1919	U1843	
U2737	G2602	G2472	U2404	G2473	U2404	A2325	U2450	A2182	C2120	A2054		A1920	A1844	
A2738	G2603	G2474	A2404	G2475	A2404	C2326	U2451	C2183	U2121	G2055	U1990	A1921	A1845	C1781
G2739	C2607	G2476	A2405	G2477	A2405	U2327	U2452	C2184	C2181	G2056	C1991	A1922	A1846	A1782
U2740	A2607	A2477	G2406	G2478	G2406	G2328	A2453	U2185	G2122	U2057	G1992	U1923	G1847	G1783
G2741	G2608	A2478	G2407	G2479	G2407	C2329	C2454	C2186	C2124	U2058	G1993	C1924	U1848	G1784
G2742	G2609	C2477	G2408	G2480	G2408	G2330	G2455		C2125	U2059	U1994	G1925	G1849	A1785
G2743	G2610	U2479	U2409	U2481	U2409	A2331	G2456	A2191	U	A2060	G1995	U1926	G1850	C1786
A2744	G2611	G2479	U2410	G2482	U2410	U2332	G2457	U2192	U	U2064	A1996	U1927	A1851	U1787
A2745	A2612	G2480	A2413	G2482	A2413	U2333	C2263	C2193	U	A2065	A1997	G1928	G1854	U1788
G2746	U2615	G2481	A2414	G2483	A2414	A2337	C2264	C2195	U	G2066	U1998		G1855	U1789
G2747	U2616	U2482	A2415	U2483	A2415	A2337	A2265	U2196	G	U2067	G2000	G1933	U1856	G1790
A2748	G2617	U2483	U2417	U2484	U2417	G2341	A2266	U2197	G2132	G2070	G2001	U1934	G1857	C1791
G2749	G2618	G2484	U2418	U2485	U2418	U2342	A2267	U2198	G2136	A2071	A2002	A1935	C1858	C1792
G2750	G2619	U2485	C2419	U2486	C2419	G2343	G2268	G2200	U2137	C2072	A2003	A1936	A1859	A1794
G2751	G2620	G2486	G2419	G2487	G2419	G2344	U2269	G2201	U2138	A2073	U2004	G1937	A1860	G1795
G2752	G2621	G2487	C2420	G2488	C2420	A2345	G2270	G2202	G2139	U2074	U2005	U1938	G1861	G1796
G2753	G2622	G2488	C2421	C2489	C2421	G2346		G2203	G2140	U2075	G2006	U1939	C1862	
G2754	G2623	C2489	G2423	C2490	G2423	G2347	C2273	A2204	A	G2076		C1940	G1863	A1799
A2755	G2624	U2490	G2424	U2491	G2424	A2348	C2274	C2205	G	G2077	G2010	G1942	G1865	A1800
G2756	U2625	G2491	G2425	G2492	G2425	G2349	U2275	C2206	C	A2078	G2011	A1943	C1866	C1801
G2757	G2626	G2492	G2426	G2493	G2426	G2351	C2276	G2207	U	U2080	A2012	C1944	G1867	A1802
U2758	U2627	G2493	G2427	G2494	G2427	G2352	A2277	U2208	C	U2081	A2013	C1945	U1804	G1803
G2759	G2628	C2494	U2428	G2495	U2428	G2353	G2278	G2209	A	C2082	A2014	U1946	G1868	G1804
G2760	G2629	G2495	A2429	G2496	A2429	G2354	A2280	G2210	C	G2083	G2015	G1947	G1869	G1805
A2761	U2630	U2496	A2430	G2497	A2430	G2355	G2279	G2211	G	G2084	G2016	C1948	U1870	A1807
G2762	C2631	A2497	C2431	U2498	C2431	G2361	U2285	U2212	C	G2085	A2017	A1949	A1871	C1808
U2763	U2632	U2498	A2432	U2499	A2432	G2362	U2286	G2213	U	U2086	G2018	C1950	A1872	G1809
C2765	G2633	C2499	G2433	G2500	G2433	G2363	G2287	G2214	G		G2019	G1951	A1873	U1810
U2764	G2634	U2501	C2435	U2502	C2435	G2364	A2288	G2215	A		G2020	A1952	U1881	A1811
G2765	U2635	G2502	U2436	G2503	U2436	U2365	A2289	G2216	A	U2090	G2021	A1953	G1882	U1812
C2768	A2636	G2503	A2437	G2504	A2437	U2369	U2290	G2217	A	C2091	C2022	A1954	A1883	A1813
G2769	G2640	G2504	A2438	G2505	A2438	U2370	U2291	G2218	U	U2092	G2023	G1955	A1884	G1814
A2770	U2507	G2506	C2443	U2508	C2443	A2371	U2298	U2219	A	G2093	U2024	G1956	G1885	G1815
U2771	G2508	C2445	C2445	U2509	C2445	A2372	A2299	U2220		C2094	A2025	C1957	G1886	G1816
G2772	A2510	G2446	G2446	U2511	G2446	G2375	G2300		C2158	G2095	G2026	G1958	G1887	U1817
G2773	G2512	G2447	G2447	U2513	G2447	A2377	A2301	G2225	A2159	U2096	G2027	U1959	G1888	U1818
U2774	G2514	U2377	U2377	U2515	U2377		C2302	A2226	C2160	A2097	G2028	A1960	G1889	U1819
G2775	G2516			U2517			C2303	C2227	C2161	G	G2029	A1961	G1890	G1820



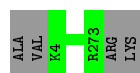
- Molecule 2: 5S RIBOSOMAL RRNA

Chain 9: 19% 59% 18% 5%



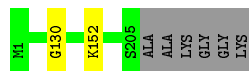
- Molecule 3: ribosomal protein L2

Chain A: 99%



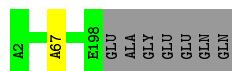
- Molecule 4: ribosomal protein L3

Chain B: 96%



- Molecule 5: ribosomal protein L4

Chain C: 96%



- Molecule 6: ribosomal protein L5

Chain D: 98%

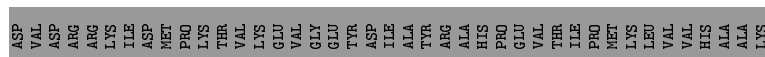
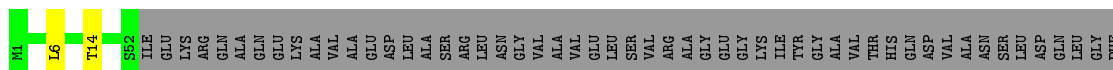


- Molecule 7: ribosomal protein L6

Chain E: 95%



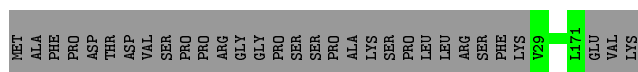
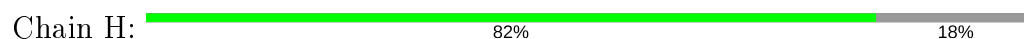
- Molecule 8: ribosomal protein L9



- Molecule 9: ribosomal protein L11



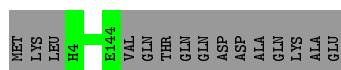
- Molecule 10: ribosomal protein L13



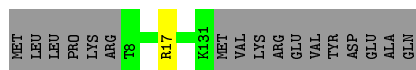
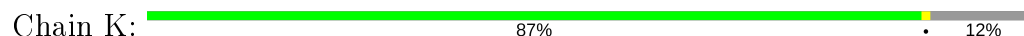
- Molecule 11: ribosomal protein L14



- Molecule 12: ribosomal protein L15



- Molecule 13: ribosomal protein L16



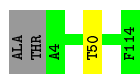
- Molecule 14: ribosomal protein L17

Chain L:  97% ..



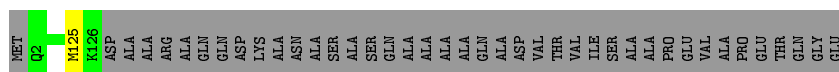
- Molecule 15: ribosomal protein L18

Chain M:  97% ..



- Molecule 16: ribosomal protein L19

Chain N:  75% . 25%



- Molecule 17: ribosomal protein L20

Chain O:  99% .



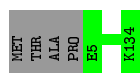
- Molecule 18: ribosomal protein L21

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: ribosomal protein L22

Chain Q:  97% .



- Molecule 20: ribosomal protein L23

Chain R:  99% .



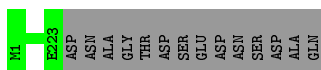
- Molecule 21: ribosomal protein L24

Chain S:  98% .



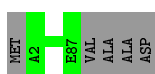
- Molecule 22: general stress protein Ctc

Chain T: 94% 6%



- Molecule 23: ribosomal protein L27

Chain U: 95% 5%



- Molecule 24: ribosomal protein L29

Chain W: 97% .



- Molecule 25: ribosomal protein L30

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 26: ribosomal protein L31

Chain Y: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: ribosomal protein L32

Chain Z: 97% ..



- Molecule 28: ribosomal protein L33

Chain 1: 96% .



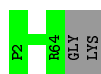
- Molecule 29: ribosomal protein L34

Chain 2:  98% .



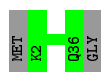
- Molecule 30: ribosomal protein L35

Chain 3:  97% .



- Molecule 31: ribosomal protein L36

Chain 4:  95%  5%



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	170.80 Å 409.50 Å 695.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65404	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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: ZIT

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	0.23	0/66467	0.67	0/103673
2	9	0.59	0/2816	0.81	1/4388 (0.0%)
All	All	0.26	0/69283	0.67	1/108061 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	9	94	G	N9-C1'-C2'	-6.58	104.76	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1342	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	2160	0
2	9	2519	0	1285	147	0
3	A	270	0	0	0	0
4	B	205	0	0	3	0
5	C	197	0	0	1	0
6	D	178	0	0	1	0
7	E	177	0	0	1	0
8	F	52	0	0	1	0
9	G	143	0	0	0	0
10	H	143	0	0	0	0
11	I	132	0	0	0	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	1	0
15	M	111	0	0	1	0
16	N	125	0	0	1	0
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	130	0	0	0	0
20	R	93	0	0	0	0
21	S	113	0	0	0	0
22	T	223	0	0	0	0
23	U	86	0	0	0	0
24	W	65	0	0	0	0
25	X	55	0	0	0	0
26	Y	73	0	0	0	0
27	Z	58	0	0	1	0
28	1	53	0	0	0	0
29	2	46	0	0	0	0
30	3	63	0	0	0	0
31	4	35	0	0	0	0
32	0	104	0	144	47	0
All	All	65404	0	31346	2342	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 24.

The worst 5 of 2342 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)
32:0:2882:ZIT:H6A1	32:0:2882:ZIT:C6B	1.61	1.30
32:0:2881:ZIT:H6A1	32:0:2881:ZIT:C6B	1.61	1.29
1:0:1679:U:H2'	1:0:1680:U:H5''	1.27	1.16
1:0:2058:U:H1'	1:0:2576:G:H21	1.10	1.14
1:0:2548:G:H2'	1:0:2549:G:H5''	1.26	1.14

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%)	485 (17%)	43 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	508 (17%)	44 (1%)

5 of 508 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
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	1410	U
1	0	1685	A

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Mol	Chain	Res	Type
1	0	2633	A
1	0	1495	G
1	0	1651	U

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
32	ZIT	0	2882	-	54,54,54	0.84	2 (3%)	82,83,83	1.27	5 (6%)
32	ZIT	0	2881	-	54,54,54	0.84	1 (1%)	82,83,83	1.27	6 (7%)

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
32	ZIT	0	2882	-	-	5/72/107/107	0/3/3/3
32	ZIT	0	2881	-	-	3/72/107/107	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	ZIT	C3A-N3A	-2.32	1.42	1.48
32	0	2882	ZIT	C3A-N3A	-2.23	1.42	1.48
32	0	2882	ZIT	C1A-C2A	2.04	1.58	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2882	ZIT	C1A-O1A-C5	-7.16	103.82	116.25
32	0	2881	ZIT	C1A-O1A-C5	-7.09	103.94	116.25
32	0	2881	ZIT	C4A-C3A-C2A	-3.16	105.42	109.97
32	0	2882	ZIT	C4A-C3A-C2A	-3.12	105.47	109.97
32	0	2882	ZIT	O1B-C3-C4	2.68	111.45	108.22

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	2882	ZIT	C13-C14-C15-C16
32	0	2882	ZIT	O5A-C1A-O1A-C5
32	0	2881	ZIT	O5A-C1A-O1A-C5
32	0	2882	ZIT	O14-C14-C15-C16
32	0	2882	ZIT	C4-C5-O1A-C1A

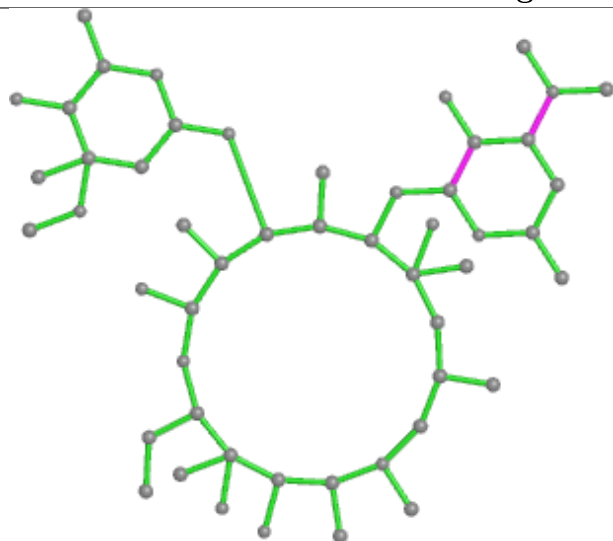
There are no ring outliers.

2 monomers are involved in 47 short contacts:

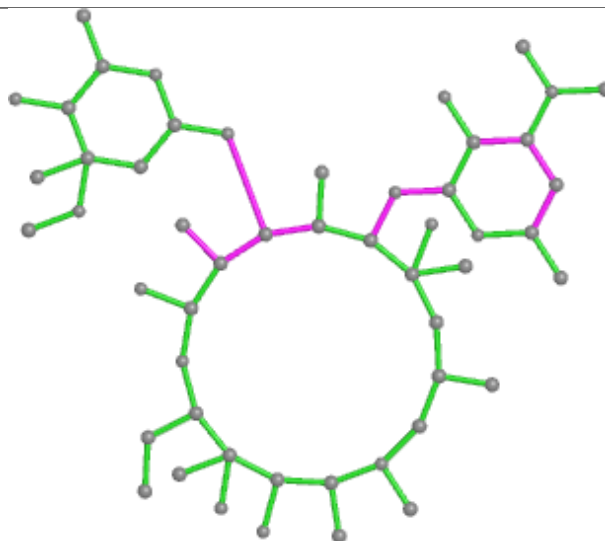
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2882	ZIT	26	0
32	0	2881	ZIT	21	0

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.

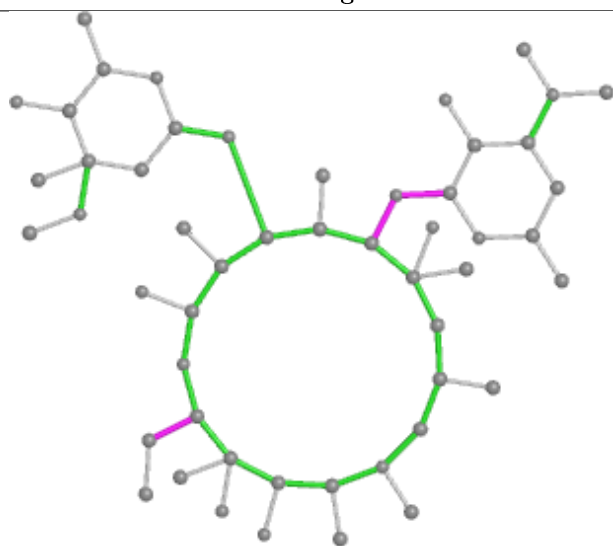
Ligand ZIT 0 2882



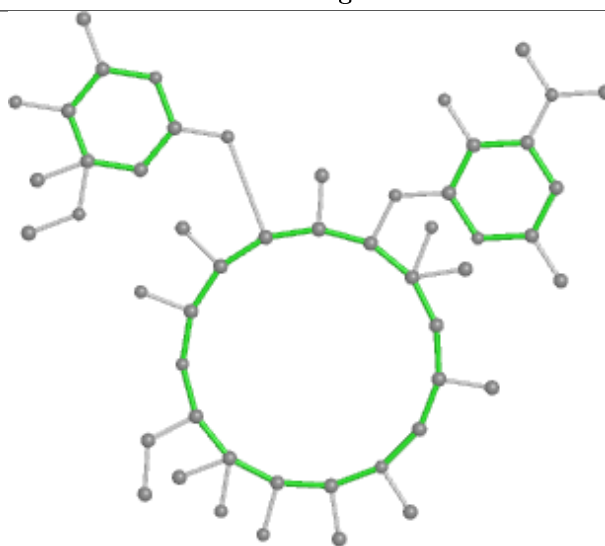
Bond lengths



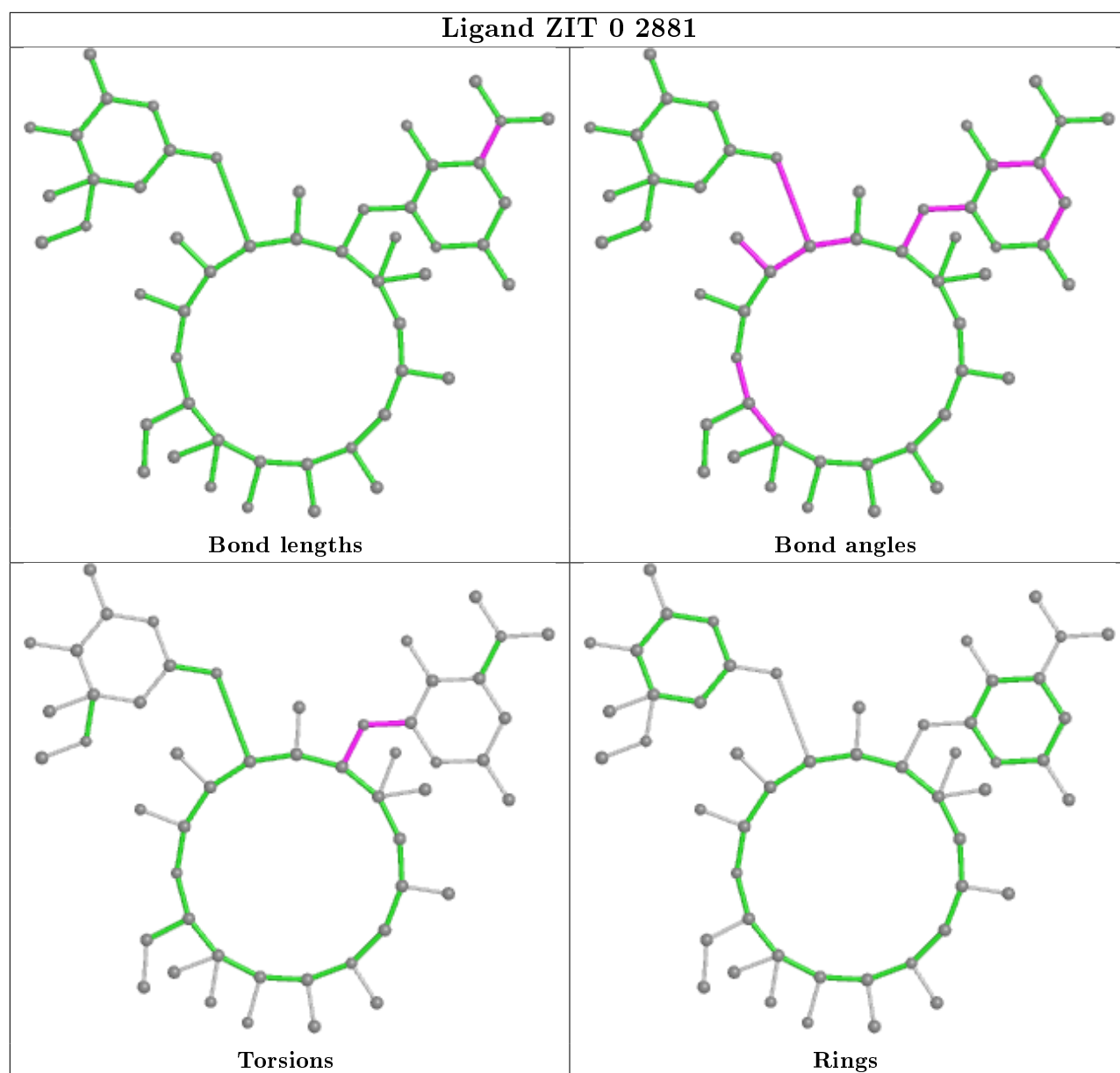
Bond angles



Torsions



Rings



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.