



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 3, 2024 – 02:50 PM EDT

PDB ID : 1SM1  
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOC-  
CUS RADIODURANS WITH QUINUPRISTIN AND DALFOPRISTIN  
Authors : Harms, J.M.; Schlutzen, F.; Fucini, P.; Bartels, H.; Yonath, A.  
Deposited on : 2004-03-08  
Resolution : 3.42 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](mailto: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>.

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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)	:	2.37.1

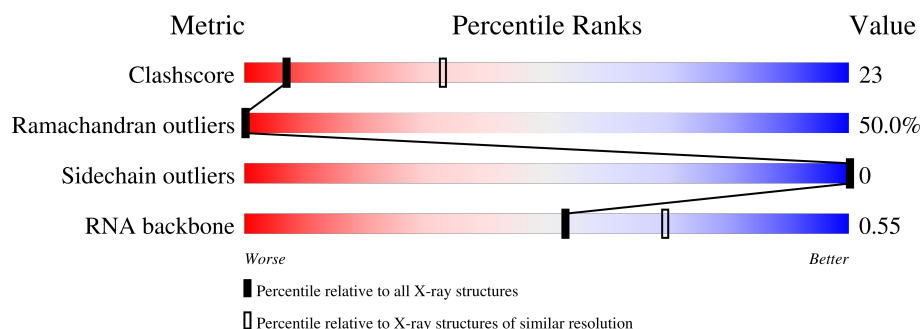
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.42 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	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)


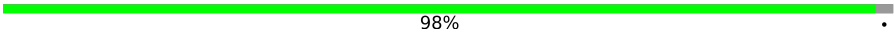
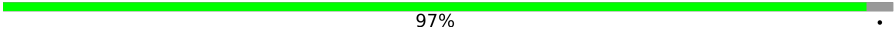
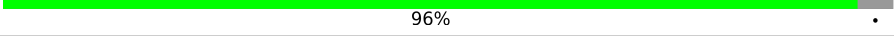
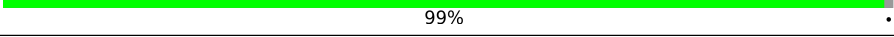


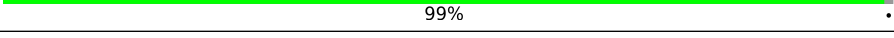
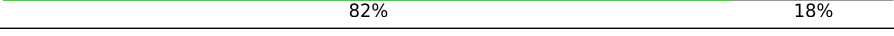
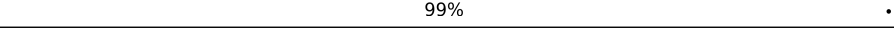
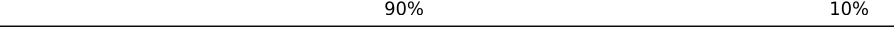
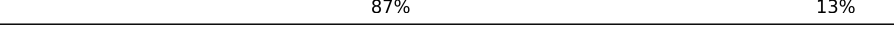
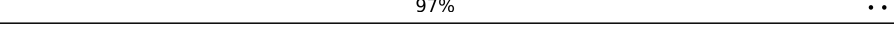
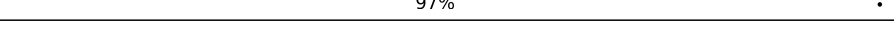

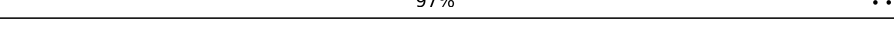
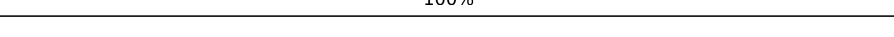
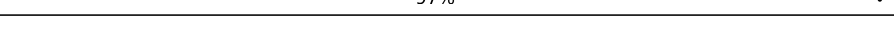
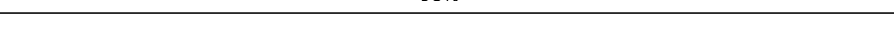






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	29% 53% 13% . .
2	1	82	65% 35%
3	2	47	98% .
4	3	66	95% 5%
5	4	37	95% 5%
6	5	8	25% 50% 12% 12%

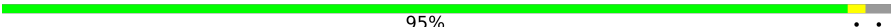
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Mol	Chain	Length	Quality of chain
7	9	124	 36%54%5%5%
8	A	275	 98%.
9	B	211	 97%.
10	C	205	 96%.
11	D	180	 99%.
12	E	212	 83%17%
13	F	146	 36%64%
14	G	144	 99%.
15	H	174	 82%18%
16	I	134	 99%.
17	J	156	 90%10%
18	K	142	 87%13%
19	L	116	 97%..
20	M	114	 97%.
21	N	166	 75%25%
22	O	118	 97%..
23	P	100	 100%
24	Q	134	 97%.
25	R	95	 98%.
26	S	115	 98%.
27	T	253	 88%12%
28	U	91	 95%5%
29	W	67	 97%.
30	X	55	 100%
31	Y	73	 100%

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Mol	Chain	Length	Quality of chain
32	Z	60	 95%

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
33	DOL	0	2882	X	-	-	-
6	DBB	5	3	-	-	X	-

## 2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 65418 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 protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	1	53	Total	C	0	0	53
			53	53			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	2	46	Total	C	0	0	46
			46	46			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	3	63	Total	C	0	0	63
			63	63			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	4	35	Total	C	0	0	35
			35	35			

- Molecule 6 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	118	Total	C	N	O	P	0	0	0
			2516	1124	464	811	117			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 27 is a protein called GENERAL STRESS PROTEIN CTC.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

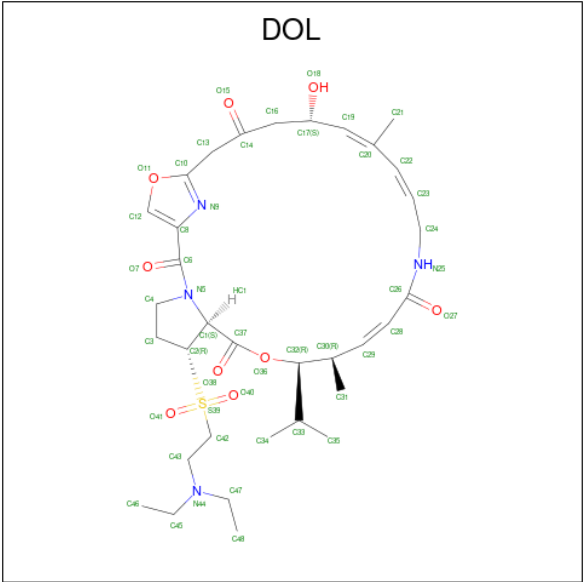
- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 33 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C<sub>34</sub>H<sub>50</sub>N<sub>4</sub>O<sub>9</sub>S).



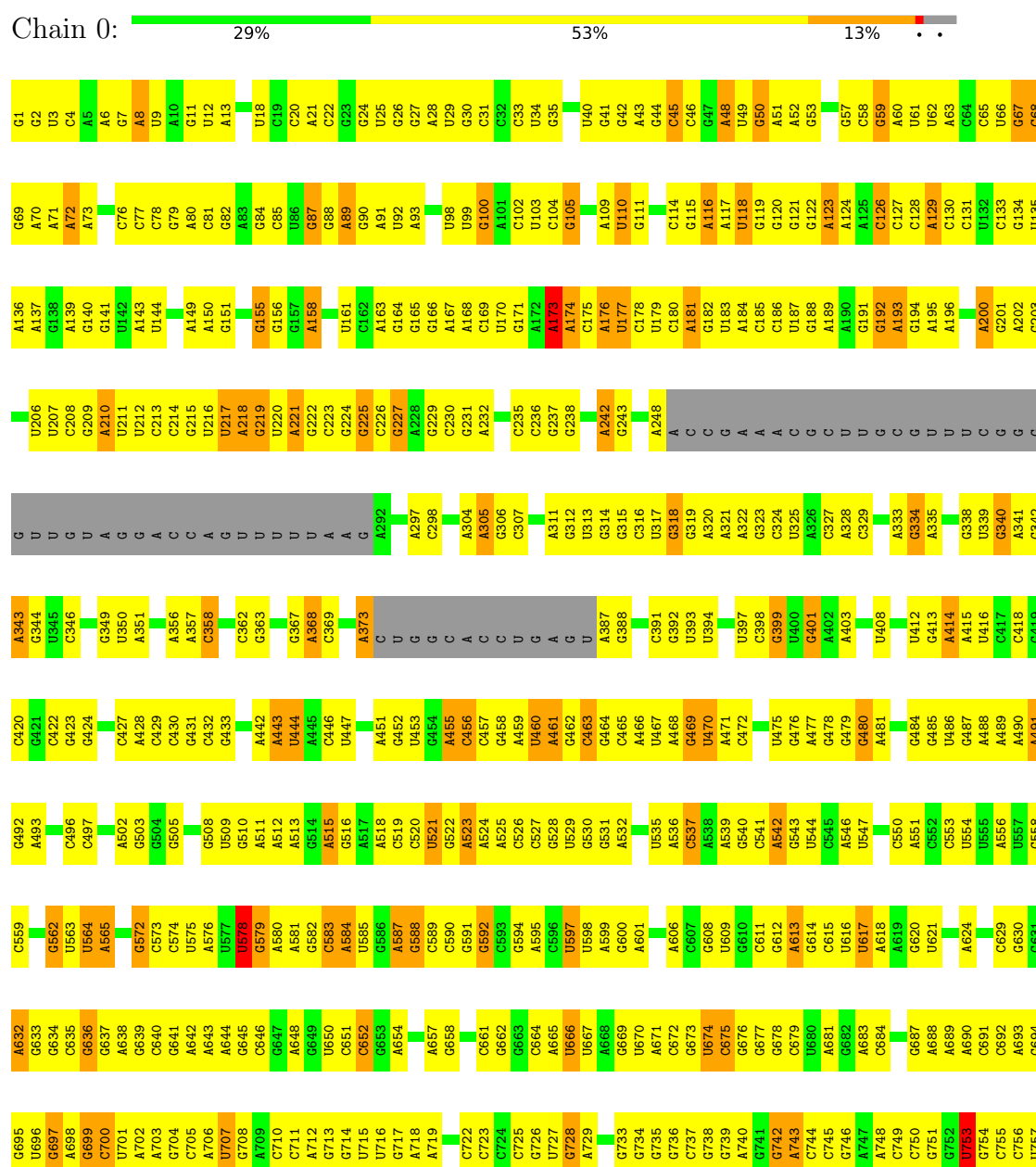
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	0	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

### 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

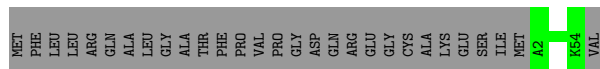


U1770	C1698	U1637	G1398	G1331	A1267	U1199	A1126	C1018	G957	G	A821	G758
A1771	A1699	G1638	C1399	G1332	U1268	G1200	G1131	A1022	G958	G	G822	C759
C1772	C1702	U1639	A1400	C1333	G1269	G1201	G1132	U1023	C959	G	U823	U760
A1773	G1702	U1473	G1401	A1334	C1270	U1202	G1133	G1024	U960	G	U824	G761
A1774	A1706	C1641	G1402	G1338	C1271	G1203	G1133	A1025	G961	G	C825	A762
A1775	A1707	U1642	U1403	U1339	G1272	G1204	G1136	U1026	C962	C	U826	A763
U1776	C1708	A1643	A1406	U1340	G1273	G1205	G1137	C1027	G963	C	C827	A764
U1777	U1709	G1644	G1407	G1341	C1274	G1206	A1137	U1028	A964	U	C828	C765
C1778	U1645	G1565	U1408	U1342	A1275	G1207	A1138	C1029	G965	A	C829	A766
U1779	G1646	U1566	U1409	C1343	U1276	A1208	A1139	U1030	A966	C	C830	
A1782	C1711	A1567	U1410	C1344	G1277	G1209	A1140	C1031	G967	C	G831	
G1783	G1712	U1647	U1411	C1345	A1278	U1212	U1341	C1032	C968	A	A832	C771
C1784	G1713	U1483	G1414	C1346	C1279	U1213	A1142	G1033	U969	G	A833	G772
A1785	A1714	G1484	G1415	C1347	U1280	U1214	A1143	G1034	A970	C	A834	A774
C1786	A1715	U1485	C1417	C1348	A1281	C1215	U1144	G1035	U975	U	U835	U775
U1787	G1716	U1486	C1418	C1349	A1282	A1215	C1145	U1036	C972	U	G836	G776
G1788	A1717	C1487	G1418	A1349	U1283	G1218	U1146	U1037	U973	A	U837	A777
U1789	G1718	G1488	G1419	G1352	C1284	U1219	G1147	C1038	U974	C	A838	G778
G1790	A1719	C1489	U1426	A1353	A1285	C1219	G1148	U1039	C975	C	U839	U779
C1791	G1720	U1490	G1427	A1354	U1286	G1222	G1149	A1040	C976	G	U840	U780
C1792	A1657	G1583	G1428	A1355	A1287	G1223	C1150	G1041	G977	G	G841	G781
A1793	G1721	G1584	A1429	G1356	A1288	G1224	U1151		U978		A842	U782
U1794	U1722	A1585	G1430	A1357	A1289	A1224	C1152		A979		G843	G783
C1795	U1723	A1586	U1431	U1357	A1290	G1225	A1153	U1044	G980		U844	U784
C1796	G1724	A1587	G1432	U1358	G1291	A1226	A1154	G1045	C981		U845	U785
A1796	C1725	A1588	G1433	G1359	A1292	A1227	G1155	U1046	C982		A846	U786
C1797	C1726	U1500	A1434	G1360	A1293	G1228		G1047	G983		A847	U787
G1798	C1727	C1501	U1435	G1361	A1294	G1229	A1158		A984		A848	G788
A1799	G1730	G1502	G1436	C1363	A1299	C1230	U1159	C1052	G985		U852	G789
U1800	C1731	G1503	A1437	C1364	A1300	A1231	C1160	G1053	A986		A790	U790
C1801	U1731	U1504	A1438	U1365	A1301	U1232	U1161	C1054	G987		G853	G791
A1802	G1736	U1505	G1438	A1366	U1302	A1233	A1162	A1055	G988		G854	U792
G1803	G1737	G1508	A1441	A1367	U1303	G1241	A1163	U1056	A991		G855	G793
U1804	U1737	A1509	C1442	G1368	A1304	C1235	C1164	A1057	C992		A856	A794
G1805	G1744	A1510	G1443	U1370	U1306	C1236	U1165	U1058	A993		U857	A795
A1807	C1745	A1511	C1444	U1371	U1307	G1242	A1166	A1059	C994		G858	G796
U1808	A1746	A1512	U1445	G1372	U1308	U1243	A1167		A994		U859	U797
C1809	G1747	U1513	U1446	A1372	C1308	U1244	G1168	G1066	G995		U860	G798
G1810	U1748	C1514	U1447	G1373	G1309	U1244		G1067	C996		C864	C799
U1811	C1749	U1515	A1448	G1374	C1310	U1247	U1172	A1068	C997		A801	U800
A1812	A1751	A1516	G1449	U1374	C1311	G1248	G1173	G1069	C998		U866	A802
U1813	U1752	G1520	G1450	A1379	G1312	U1249	G1174		A999		G867	C803
G1816	A1753	C1620	A1453	C1380	U1313	G1249	U1175	G1073	G1000		U868	C804
U1817	G1754	C1621	U1454	G1381	A1314	A1250	U1176	G1074	A1001		C804	G805
G1818	G1755	G1622	C1455	G1382	A1315	G1251	U1177		C1002		C805	A806
U1819	C1756	C1623	C1456	C1383	G1316	C1252	A1178	G1082	A1003		U871	C807
C1757	C1757	A1624	A1457	C1384	G1317	C1253	A1179	U1081	U1005		G872	C808
A1821	U1758	C1528	C1458	C1385	A1318	G1254	A1180	U1086	U1006		U873	C809
C1822	A1759	U1530	U1459	G1387	C1319	A1255	C1181	C1087	A944		A874	U810
G1823	G1760	C1627	G1460	G1388	A1320	C1256	U1182		A1007		G875	G811
C1824	U1688	C1628	C1461	C1389	G1322	U1257	C1183	C1090	G1008		A876	G812
C1825	G1629	G1629	C1462	G1390	G1323	U1258	G1184	C1091	C947		G877	A813
U1826	G1630	A1630	A1463	A1391	G1324	A1259	G1185	U1092	C948		G877	G814
A1764	G1763	G1631	A1464	A1392	A1325	G1261	A1187		G951		A883	A815
C1765	A1764	A1632	G1465	U1392	U1326	U1262	A1188	A1099	A952		C884	U816
U1766	U1766	C1633	C1466	G1393	C1327	C1263	A1189		G953			A817
G1831	C1765	A1634	U1467	G1394	C1328	G1264	U1196	G1123	U954		C889	G818
G1832	U1767	C1635	U1468	A1395	U1329	G1265	G1197	U1124	G955		U890	C808
	G1837	C1696	A1468	C1396	U1328	G1265	U1197	U1124	U955		A891	U820
G1838	U1769	U1697	U1469	A1397	G1330	G1266	C1198	G1125	C1017			

C2824	C2825	G2760	A2568	C2506	C2435	U2365	G2293	U2222	A	A2063	U1999	U1939	G1854
A2826	A2827	A2761	A2569	U2507	U2436	U2366	G2294	U2223	C	U2064	U2000	C1940	G1855
G2826	G2827	G2762	C2570	G2508	G2437	A2367	G	G2225	G	U2067	A2003	C1941	U1856
C2828	C2829	U2763	G2571	A2509	A2438	G2368	U2298	A2226	U	C2068	U2005	A1943	G1860
A2829	U2830	G2765	U2572	G2510	U2441	U2369	U2299	G2229	G	G2071	U2006	C1945	G1861
U2830	A2831	C2766	G2574	A2512	C2442	A2371	G2300	G2230	A	U2071	G2007	U1946	G1862
A2832	C2833	C2767	U2575	G2515	C2443	G2376	A2301	G2231	A	G2076	C2008	C1948	U1863
G2833	G2834	C2768	A2577	C2516	C2444	U2377	A2306	G2232	A	G2077	U2009	A1949	C1865
A2834	U2835	U2769	G2578	C2517	C2446	G2378	A2307	G2233	U	U2078	G2010	C1950	G1866
U2835	A2836	G2770	A2579	C2518	G2447	G2379	A2308	G2235	A	A2079	U2011	G1951	A1869
C2836	C2837	U2770	C2580	C2519	A2448	U2380	G2309	U2236	C2157	U2080	A2012	A1952	U1870
U2838	G2839	C2771	A2581	A2520	G2449	A2381	G2310	G2237	A2159	U2081	A2013	A1953	U1881
U2839	U2840	U	G2582	A2521	A2450	U2385	U2311	G2238	G2164	C2082	A2014	A1954	U1882
U2841	U2842	A	U2583	G2522	G2451	U2386	A2313	G2239	A2165	U2092	G2015	G1955	A1883
C2842	C2843	G2712	G2585	G2523	A2455	G2389	A2314	U2241	G2170	G2093	A2016	G1956	A1884
A2844	G2845	G2715	G2587	U2525	G2463	A2391	A2315	C2243	A2168	C2094	C2019	C1957	G1885
C2846	A2784	G2717	U2588	G2526	G2464	G2392	G2317	C2244	A2169	G2095	G2020	U1959	G1886
G2847	A2785	A2718	U2590	G2528	G2465	G2393	U2318	A2245	G2173	U2096	C2022	A1960	G1887
A2848	G2849	G2721	C2591	G2529	G2466	G2394	G2319	A2246	G2174	A2097	C2023	A1961	C1888
C2849	U2850	C2722	U2592	U2530	A2467	C2395	G2320	A2247	G	G	U2024	G1962	G1889
U2851	C2851	C2725	A2593	G2531	G2468	G2396	C2321	U2248	A	A	A2025	G1963	A1901
C2852	G2853	G2726	U2594	G2532	G2469	A2397	U2322	U2249	U	U	C2026	A1964	A1902
U2854	U2855	G2727	C2595	U2533	U2470	U2398	U2323	U2250	A	A	C2027	C1965	G1905
G2856	C2857	U2728	U2596	G2534	U2471	U2399	G2324	U2251	A	G2103	C2028	U1967	G1906
U2859	A2795	A2739	U2599	C2538	G2474	A2401	A2325	A2252	A2181	G2104	G2029	G1968	U1907
A2861	A2796	A2736	G2602	C2539	C2475	C2403	A2326	A2253	A2182	U2105	U2030	G1969	C1907
G2862	C2800	U2737	G2603	U2541	C2476	A2404	U2327	G2254	C2183	G2106	G2032	G1970	C1908
U2863	C2801	A2738	G2604	U2542	A2477	A2405	G2328	G2255	C2184	G2107	C2033	C1971	U1909
C2864	C2802	G2739	G2605	A2543	C2478	G2406	G2330	G2256	G2185	G2110	G2034	C1972	A1911
G2865	G2803	C2740	C2606	A2544	C2480	G2407	A2331	G2257	G2186	C	G2035	C1973	U1912
A2866	G2804	G2741	C2607	A2545	G2481	A2408	A2332	G2258	A2194	C	G2036	U1974	G1913
G2867	G2805	U2742	C2608	G2546	A2482	A2409	G2333	C2261	U2192	U	A2037	G1975	U1914
U2872	G2806	G2743	A2613	C2547	U2483	U2410	U2335	C2262	U2193	C	A2040	U1976	G1915
A2873	G2807	A2744	A2614	G2548	G2484	A2413	G2336	C2263	C2195	U	A2041	U1977	U1916
C2875	G2808	G2745	A2615	C2549	U2485	A2414	A2337	A2266	U2196	G	G2042	C1978	C1917
G2876	U2809	A2746	U2616	G2550	G2486	A2415	C2338	A2267	U2197	A2117	G2043	A1981	G1918
A2877	G2810	U2747	G2617	A2551	G2487	G2415	A2339	G2268	U2198	A2118	G2044	C1980	U1922
U2878	G2811	C2748	A2618	C2552	U2488	A2418	C2340	G2269	C2199	A2119	A2045	C1982	A1919
C2879	G2812	A2749	A2619	G2553	U2490	C2419	G2341	U2270	G2200	C2125	C2046	G1983	A1920
U2880	G2813	C2750	G2621	C2554	C2491	C2420	U2342	C2271	G2201	U	G2047	A1984	U1921
G2881	C2814	G2751	G2622	G2555	G2492	G2421	G2343	A2272	G2213	U	G2050	G1985	U1923
A2882	G2815	C2752	A2623	A2556	U2493	C2422	G2344	C2273	G2214	U	U2051	G1986	C1924
C2883	G2816	G2753	G2624	G2557	C2494	G2423	A2345	U2274	G2215	U	G2052	C1987	C1925
U2884	G2817	C2754	U2625	G2558	G2495	G2424	G2353	U2275	G2216	U	A2053	A1988	U1926
G2885	G2818	U2755	U2626	C2559	C2496	A2425	G2354	C2276	U2211	G	G2054	C1989	U1927
A2886	G2819	A2756	G2627	U2560	U2497	G2426	A2355	A2277	U2212	U	A2055	G1991	G1928
C2887	G2820	C2757	U2628	U2561	A2498	A2427	A2356	G2278	G2213	G2132	C2056	G1992	U1929
U2888	G2821	U2758	A2629	U2562	C2500	U2428	A2357	A2280	G2214	G2140	U2057	U1994	C1930
G2823	U2822	U2759	G2630	G2567	U2501	A2430	C2358	U2285	G2217	A	U2058	G1995	G1931
					G2502	C2431	G2362	U2286	G2218	G	U2059	A1996	A1936
					G2503	A2432	C2363	G2287	U2219	C	A2060	A1997	U1937
					G2504	G2433	C2364	A2288	G2220	G	U2062	A1998	U1938
					G2505	G2434			G2221	A			

- Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1:  65% 35%



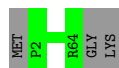
- Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:  98% .



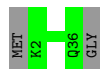
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:  95% 5%



- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4:  95% 5%



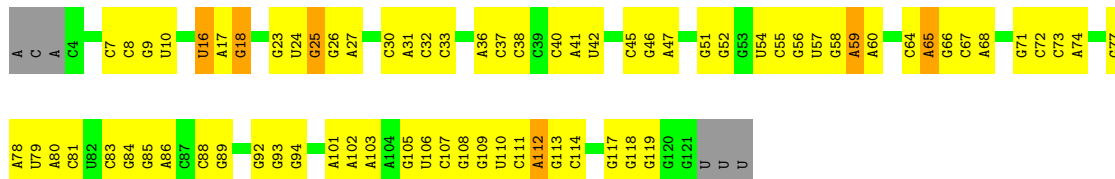
- Molecule 6: QUINUPRISTIN

Chain 5:  25% 50% 12% 12%



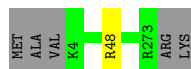
- Molecule 7: 5S RIBOSOMAL RNA

Chain 9:  36% 54% 5% 5%



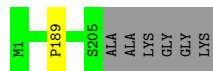
- Molecule 8: 50S RIBOSOMAL PROTEIN L2

Chain A:  98% .



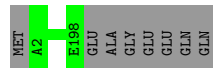
- Molecule 9: 50S RIBOSOMAL PROTEIN L3

Chain B:  97%



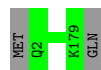
- Molecule 10: 50S RIBOSOMAL PROTEIN L4

Chain C:  96%




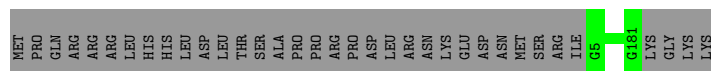
- Molecule 11: 50S RIBOSOMAL PROTEIN L5

Chain D:  99%



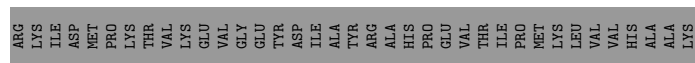
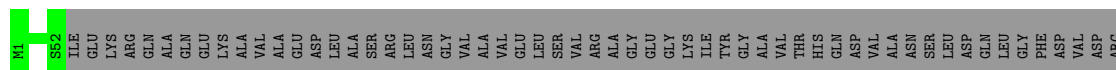
- Molecule 12: 50S RIBOSOMAL PROTEIN L6

Chain E:  83% 17%



- Molecule 13: 50S RIBOSOMAL PROTEIN L9

Chain F:  36% 64%




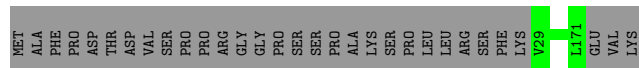
- Molecule 14: 50S RIBOSOMAL PROTEIN L11

Chain G:  99%



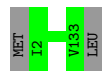
- Molecule 15: 50S RIBOSOMAL PROTEIN L13

Chain H:  82% 18%



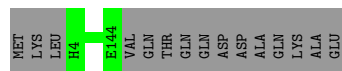
- Molecule 16: 50S RIBOSOMAL PROTEIN L14

Chain I:  99%




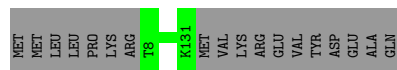
- Molecule 17: 50S RIBOSOMAL PROTEIN L15

Chain J:  90% 10%



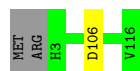
- Molecule 18: 50S RIBOSOMAL PROTEIN L16

Chain K:  87% 13%



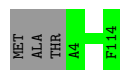
- Molecule 19: 50S RIBOSOMAL PROTEIN L17

Chain L:  97% ..



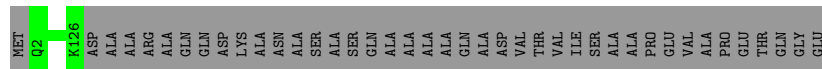
- Molecule 20: 50S RIBOSOMAL PROTEIN L18

Chain M:  97%



- Molecule 21: 50S RIBOSOMAL PROTEIN L19

Chain N:  75% 25%



- Molecule 22: 50S RIBOSOMAL PROTEIN L20

Chain O:  97% ..



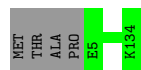
- Molecule 23: 50S RIBOSOMAL PROTEIN L21

Chain P:  100%

There are no outlier residues recorded for this chain.

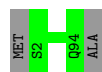
- Molecule 24: 50S RIBOSOMAL PROTEIN L22

Chain Q:  97%



- Molecule 25: 50S RIBOSOMAL PROTEIN L23

Chain R:  98%




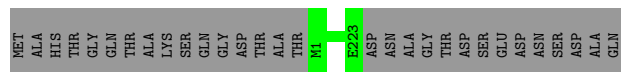
- Molecule 26: 50S RIBOSOMAL PROTEIN L24

Chain S:  98%



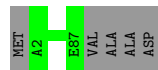
- Molecule 27: GENERAL STRESS PROTEIN CTC

Chain T:  88% 12%



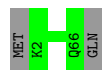
- Molecule 28: 50S RIBOSOMAL PROTEIN L27

Chain U:  95% 5%



- Molecule 29: 50S RIBOSOMAL PROTEIN L29

Chain W:  97%



- Molecule 30: 50S RIBOSOMAL PROTEIN L30

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 50S RIBOSOMAL PROTEIN L31

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S RIBOSOMAL PROTEIN L32

Chain Z:  95% ..



## 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, $\alpha$ , $\beta$ , $\gamma$	168.50 Å   406.00 Å   693.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	15.00 – 3.42	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.42)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.278 , 0.348	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	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: DOL, MHV, MHU, 004, DBB, MHT, MHW

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	0.70	16/66467 (0.0%)	0.74	12/103673 (0.0%)
6	5	0.85	0/13	0.67	0/15
7	9	0.50	0/2813	0.65	0/4384
All	All	0.70	16/69293 (0.0%)	0.73	12/108072 (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	146
6	5	1	1
7	9	0	1
All	All	1	148

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1962	C	N1-C2	-7.46	1.32	1.40
1	0	2255	G	C5-C6	-7.28	1.35	1.42
1	0	2789	U	N1-C2	6.94	1.44	1.38
1	0	868	U	N1-C2	6.93	1.44	1.38
1	0	806	A	C5-C6	6.88	1.47	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	994	A	N9-C1'-C2'	-6.36	105.00	112.00
1	0	800	U	OP2-P-O3'	6.27	119.00	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2056	C	N1-C1'-C2'	-6.04	105.36	112.00
1	0	1686	A	C5'-C4'-O4'	5.86	116.13	109.10
1	0	1938	U	C2'-C3'-O3'	5.75	122.90	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	5	8	MHT	C3

5 of 148 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	126	C	Sidechain
1	0	174	A	Sidechain
1	0	211	U	Sidechain
1	0	33	C	Sidechain
1	0	8	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	59359	0	29917	2138	0
2	1	53	0	0	0	0
3	2	46	0	0	0	0
4	3	63	0	0	0	0
5	4	35	0	0	0	0
6	5	73	0	64	6	0
7	9	2516	0	1286	66	0
8	A	270	0	0	1	0
9	B	205	0	0	1	0
10	C	197	0	0	0	0
11	D	178	0	0	0	0
12	E	177	0	0	0	0
13	F	52	0	0	0	0
14	G	143	0	0	0	0
15	H	143	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	132	0	0	0	0
17	J	141	0	0	0	0
18	K	124	0	0	0	0
19	L	114	0	0	1	0
20	M	111	0	0	0	0
21	N	125	0	0	0	0
22	O	117	0	0	2	0
23	P	100	0	0	0	0
24	Q	130	0	0	0	0
25	R	93	0	0	0	0
26	S	113	0	0	0	0
27	T	223	0	0	0	0
28	U	86	0	0	0	0
29	W	65	0	0	0	0
30	X	55	0	0	0	0
31	Y	73	0	0	0	0
32	Z	58	0	0	2	0
33	0	48	0	47	16	0
All	All	65418	0	31314	2213	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 23.

The worst 5 of 2213 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)
1:0:1463:A:H1'	1:0:1543:G:H22	1.05	1.14
1:0:128:C:H2'	1:0:129:A:H5''	1.19	1.10
1:0:1656:U:H2'	1:0:1657:A:H5''	1.34	1.10
1:0:940:G:H3'	1:0:941:U:H5''	1.23	1.09
1:0:2607:C:H3'	1:0:2608:A:H5'	1.10	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	5	2/8 (25%)	1 (50%)	0	1 (50%)	0 0

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	2	THR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	5	2/2 (100%)	2 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	433 (15%)	19 (0%)
7	9	117/124 (94%)	12 (10%)	0
All	All	2874/3004 (95%)	445 (15%)	19 (0%)

5 of 445 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	45	C
1	0	48	A
1	0	49	U
1	0	50	G
1	0	59	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2015	G
1	0	2377	U
1	0	2404	A
1	0	2261	G
1	0	1354	A

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

5 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
6	004	5	7	6	9,10,11	1.69	2 (22%)	9,12,14	1.27	1 (11%)
6	MHU	5	5	6	14,15,16	1.14	1 (7%)	18,19,21	1.11	1 (5%)
6	MHV	5	6	6	7,9,10	0.67	0	7,11,13	1.68	2 (28%)
6	MHW	5	1	6	9,9,10	0.76	0	10,11,13	1.56	1 (10%)
6	DBB	5	3	6	4,5,6	0.58	0	1,5,7	0.06	0

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
6	004	5	7	6	-	2/4/6/8	0/1/1/1
6	MHU	5	5	6	-	2/9/12/14	0/1/1/1
6	MHV	5	6	6	-	0/1/12/14	0/1/1/1
6	MHW	5	1	6	-	2/2/2/4	0/1/1/1
6	DBB	5	3	6	-	1/3/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	7	004	CB-CA	3.12	1.55	1.52
6	5	7	004	CG2-CB	-2.70	1.34	1.39
6	5	5	MHU	CZ1-NZ	-2.59	1.39	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1	MHW	O-C-CA	-4.20	120.24	124.22
6	5	6	MHV	CE-CD2-CG	3.22	117.29	111.89
6	5	5	MHU	O-C-CA	-2.83	117.37	124.78
6	5	7	004	CG2-CB-CA	2.31	124.38	120.65
6	5	6	MHV	CB-CA-N	-2.02	108.33	112.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	5	1	MHW	O-C-CA-N
6	5	1	MHW	O-C-CA-CB
6	5	3	DBB	O-C-CA-CB
6	5	5	MHU	N-CA-CB-CG
6	5	5	MHU	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	5	1	MHW	1	0
6	5	3	DBB	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	DOL	0	2882	-	43,50,50	4.58	11 (25%)	51,70,70	3.94	18 (35%)

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
33	DOL	0	2882	-	2/2/14/20	20/58/77/77	0/2/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	2882	DOL	O40-S39	18.61	1.77	1.44
33	0	2882	DOL	O41-S39	18.41	1.76	1.44
33	0	2882	DOL	C28-C29	-8.71	1.11	1.32
33	0	2882	DOL	C1-C37	4.83	1.62	1.52
33	0	2882	DOL	C8-C6	-4.51	1.42	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	2882	DOL	C4-N5-C1	-14.71	94.37	112.45
33	0	2882	DOL	O18-C17-C16	13.82	145.78	109.73
33	0	2882	DOL	C28-C26-N25	-9.38	97.30	114.97
33	0	2882	DOL	O40-S39-O41	-7.23	109.95	118.19
33	0	2882	DOL	O27-C26-C28	6.58	138.02	123.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	0	2882	DOL	C2
33	0	2882	DOL	C17

5 of 20 torsion outliers are listed below:

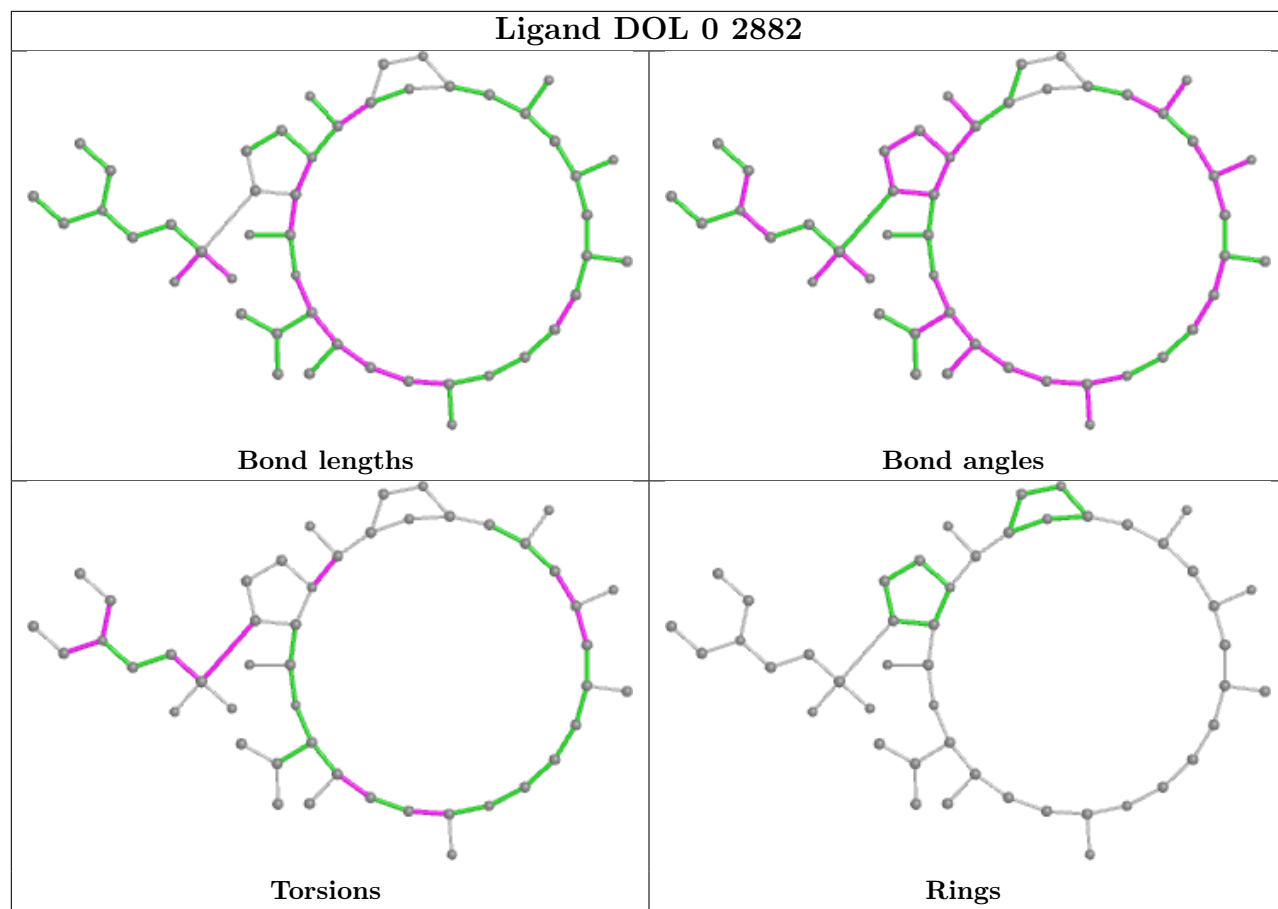
Mol	Chain	Res	Type	Atoms
33	0	2882	DOL	O7-C6-N5-C1
33	0	2882	DOL	C8-C6-N5-C1
33	0	2882	DOL	C1-C2-S39-O41
33	0	2882	DOL	C1-C2-S39-O40
33	0	2882	DOL	C1-C2-S39-C42

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	2882	DOL	16	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

### 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.