



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:47 AM UTC

PDB ID : 1SM1 / pdb_00001sm1
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

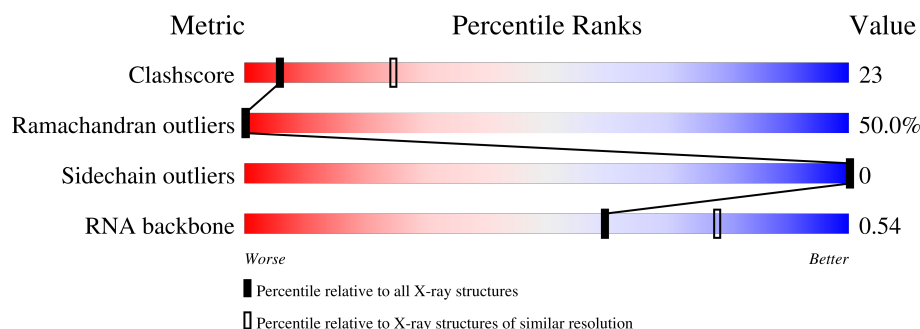
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

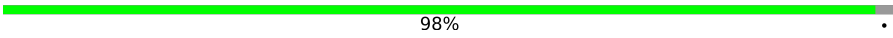
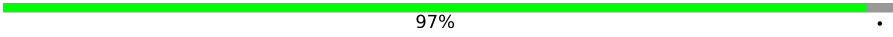
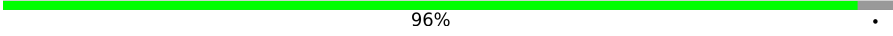
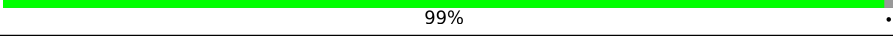
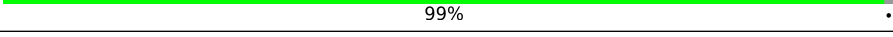
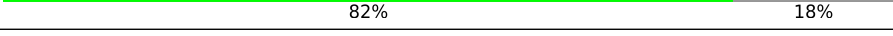
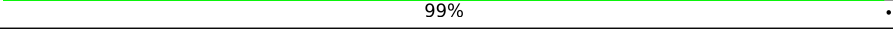
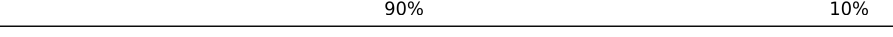
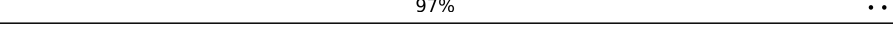
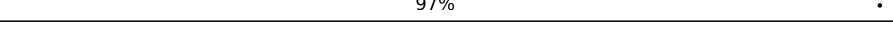
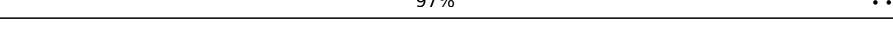
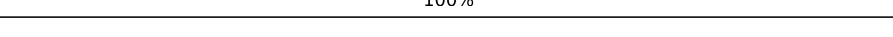
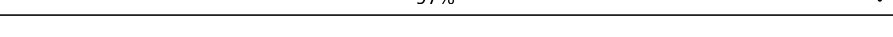
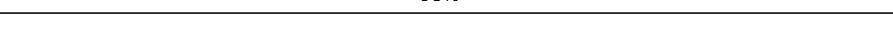
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	29% 52% 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%

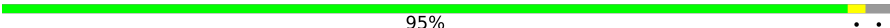
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Mol	Chain	Length	Quality of chain
7	9	124	 36%54%5%5%
8	A	275	 98%.
9	B	211	 97%.
10	C	205	 96%.
11	D	180	 99%.
12	E	212	 83%17%
13	F	146	 36%64%
14	G	144	 99%.
15	H	174	 82%18%
16	I	134	 99%.
17	J	156	 90%10%
18	K	142	 87%13%
19	L	116	 97%..
20	M	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 125	C 125	0	0	125

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

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

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

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

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

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

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

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

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

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

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

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

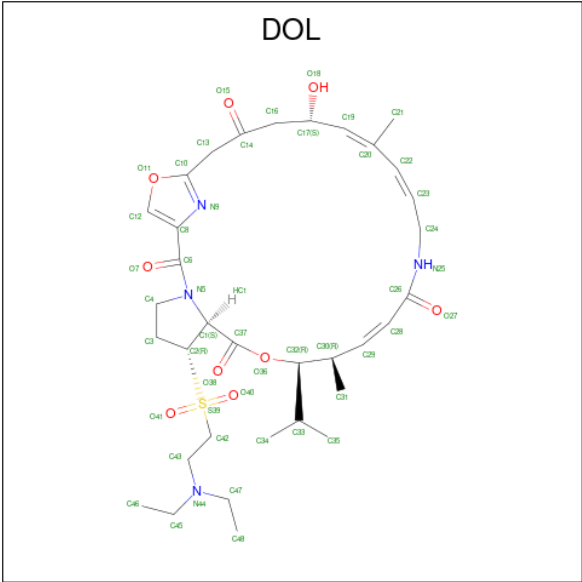
- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L31.

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 (CCD ID: DOL) (formula: $C_{34}H_{50}N_4O_9S$).



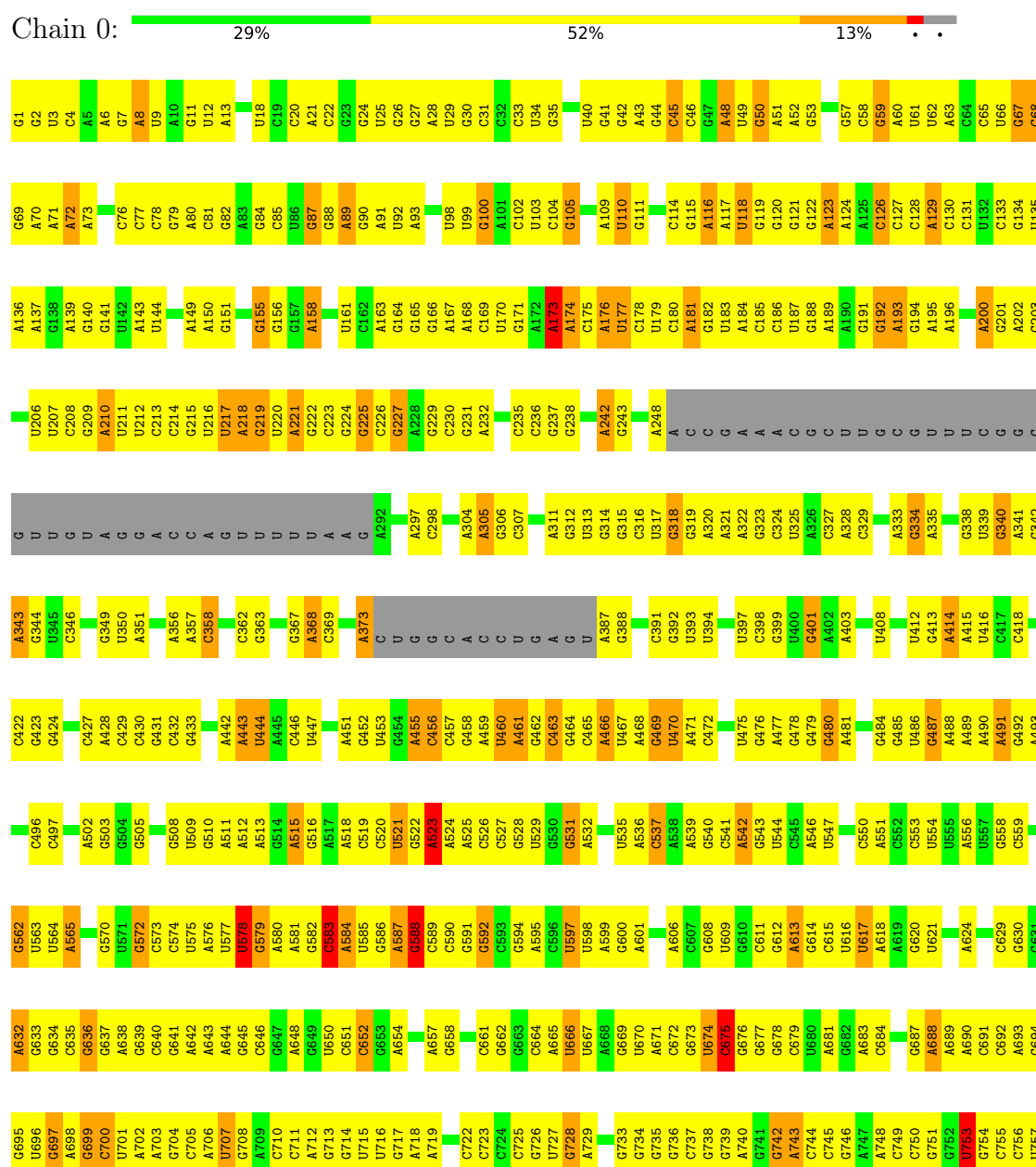
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	0	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

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

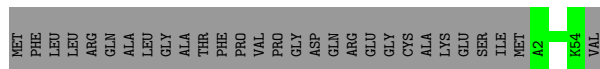


G1767	U1695	A1634	C1549	U1467	A1395	U1329	G1285	U1197	U1124	C1016	G955	U890	C819	G758
U1768	C1696	G1635	C1552	A1468	C1396	G1330	G1266	C1198	G1125	C1017	A956	A891	U820	C759
U1769	U1697	U1636	C1552	A1469	A1397	G1331	U1287	U1199	A1126	C1018	G957	G	A821	U760
C1698	U1770	U1637	C1558	G1470	G1398	G1332	U1288	G1200	G958	G	G	G	G822	G761
A1699	A1699	U1638	G1559	G1471	C1399	G1333	G1289	G1201	G1131	A1022	U960	G	U823	A762
	C1702	U1639	A1560	G1472	A1400	A1334	C1270	U1202	G1132	U1023	U961	G	U824	A763
		C1640	A1561	U1473	G1401		G1271	A1203	G1133	G1024	G961	C	C825	A764
	A1706	C1641	A1562	A1474	G1402	G1338	G1272	G1204		A1025	G962	C	U826	C765
A1707	C1708	G1642	U1475	U1476	U1403	U1339	G1273	G1205	G1136	U1026	G963	C	C827	A766
U1708	U1708	U1643	U1563	G1476	A1406	G1340	C1274	G1206		C1027	G964	U	C828	
C1779		U1644	U1564		A1407	G1341	A1275	G1207	A1137	G1028	G965	A	C829	
		G1646	G1565		G1408	U1342	U1276	A1208	A1139	C1029	A966	C	C830	
		U1647	U1409		A1408	C1343	U1277	G1209	A1140	U1030	G967	C	G831	
A1782		U1648	U1410	U1481	U1409	C1344	A1278		U1141	C1031	C968	A	A832	C771
G1783	G1783	A1649	G1571	U1482	U1410	C1345	G1279	U1212	G1142	C1032	U969	G	A833	C772
C1784	C1784	A1650	U1572	G1483	G1414	C1346	U1280	U1213	A834	G1033	A970	C	A774	C773
A1785	A1715	U1651	G1573	G1484	G1415	C1347	A1281	C1214	U1144	U1034	U	U	U835	U775
G1786	A1716	U1652	A1574	U1485	C1417	C1348	A1282	A1215	C1145	G1035	C972	U	U836	U776
U1787	G1716	G1652	A1574	U1486	C1417	A1349	C1283		G1146	G1036	U973	A	U837	A777
C1788	A1717	C1653		U1487	C1418		G1284	C1218	G1147	U1037	U974	C	A838	C778
U1789	A1718	A1654	G1577	G1488		G1352	A1285	C1219	G1148	U1038	C975	C	U839	U779
C1790	G1719	U1655		C1489	U1426	A1353	A1286		G1149	A1039	C976	G	U840	U780
C1791	G1720	U1656	A1583	U1490	G1427	A1354	A1287	G1222	C1150	A1040	G977	G	G841	G781
C1792	G1721	A1657	A1584		G1428	A1355	A1288	G1223	U1151	G1041	C978	C	A842	U782
A1793	G1722	U1658	A1585	A1493	A1429	A1356	A1289	A1224	C1152		A979	C	G843	U783
C1794	U1723	G1586	A1586		G1430	U1357	A1290	G1225	A1153	U1044	G980	C	G844	U784
C1795	C1724	G1587	A1587	G1496	U1431	C1358	G1291	A1226	A1154	G1045	C981	U	U845	U785
A1796	C1725	C1661	A1588		G1432	G1359	A1292	A1227	A1154	U1046	C982	U	U846	U786
C1797	G1726	G1662	A1493	U1500	A1433	G1360	A1293	G1228	C1155	G1047	G983	U	A847	A787
G1798	C1727	C1593	C1593	U1501	U1434		G1294	C1229	A1158		A984	C	A848	G788
A1799	A1799	G1664		G1502	G1435	C1363		G1230	U1159	C1052	G985	A	G789	
A1800	G1730	C1665	A1596	G1503	G1436	C1364	A1299	A1231	C1160	C1053	A986	C	U852	A790
C1801	C1731	U1666	A1597	G1504	A1437	U1365	A1300	U1232	U1161	C1054	G987	C	C853	G791
A1802		U1667	C1598	U1505	G1438	A1366	U1301	A1233	C1162	A1055	G988	C	G854	U792
G1803	C1736	G1668	G1599			A1367		C1234	C1163	U1056	G	C	G855	G793
U1804	G1737	U1669		G1508	A1441	G1368	U1304	C1235	G1164	A1057	A991	C	A856	A794
G1805		C1670	A1604	A1509	C1442	G1369	C1305		G1165	G1058	A992	C	U857	A795
C1806	G1744	A1671	A1605	A1510	G1443	U1370	U1306	G1241	A1166	A1059	C993	C	G858	A796
A1807	C1745	A1672		A1511	C1444	A1371	U1307	A1242	A1167		A994	C	U859	A797
C1808	U1746	C1673	G1613	A1512	A1445	G1372	U1308	G1243	G1168	G1066	A995	C	U860	G798
G1809	G1747		C1614	U1513	U1446	A1373	G1309	U1244		G1067	C996	C	C864	U800
U1810	U1748	U1676	C1615	C1514	U1447	G1374	C1310		U1172	A1068	C997	C	A865	A801
A1811	G1749	G1677	G1616	U1515	A1448	G1374	C1311	U1247	G1173	G1069	C998	C	U866	A802
U1812	A1750	U1678	G1617	A1516	C1449		G1312		G1174		A999	C	G867	C803
A1813	A1751	U1679	U1618		G1450	A1378	U1313	G1248	A1175	G1073	G1000	C	C868	C804
			A1619	G1520		A1379	A1314	G1249	U1176	G1074	A1001	C	U869	G805
G1816	A1753	A1681	C1620		A1453	C1380	A1315	A1250	U1177		A1002	C	G870	A806
U1817	G1754	A1682	C1621	C1524	U1454	G1381	G1316	G1251	C1178	A1081	C1003	C	U871	A807
G1818	G1755	G1683	G1622		C1455	G1382	G1317	G1252	A1179	G1082	A1004	C	G872	C808
U1819	C1756	G1684	C1623	G1527	C1456	G1383	A1318	G1254	A1180		U1005	C	U873	C809
			A1624	C1528	A1457	G1384	C1319	A1255	C1181	C1086	C1006	C	U874	U810
G1820	C1757	A1685	A1625	C1529	A1458	C1385	A1320	G1256	U1182	C1087	A1007	C	G875	G811
A1821	C1758	A1686	U1626	U1530	U1459	G1387	A1321	U1257	C1183	C1090	G1008	C	A876	C947
C1822	U1759	G1687	G1627		G1460	C1388	G1322	G1258	G1184	G1091	C1009	C	G877	A813
G1823	G1760	U1688	C1627	G1541	A1461	C1389	G1323	A1259	C1185	U1092	U1010	C	G878	G814
C1824	C1761	U1689	G1628	G1542	C1462	G1390	G1324	A1260	G1186		A1011	C	A883	A815
C1825	G1762	G1690	A1630	G1543	A1463	A1391	U1325	G1261	A1187		A1012	C	C884	U816
U1826	G1763		A1631	A1544	A1464	U1392	U1326	U1262	A1188	A1099	G1013	C	G885	A817
	A1764	C1765	A1632		G1465	U1393	C1327	G1263			G1014	C		G918
G1831			A1633			G1394	C1328	C1264	G1196	G1123	U1015	C	C889	

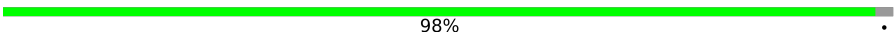
C2820	A2756	A2692	C2628	C2585	G2503	G2286	U2219	G	A2060	A1996	A1936	G1837
G2821	G2757	U2693	U2629	A2666	G2504	G2287	A2220	C	C2061	A1997	G1937	G1838
U2822	G2694	G2694	C2530	G2567	G2505	A2288	G2221	A	U2062	A1998	U1938	
G2823	C2695	C2506	C2506	A2568	C2506		G2222	A	A2063	U1999	U1939	
C2824	A2696	A2569	U2507	A2569	U2507	G2293	U2223	C	U2064	U2000	C1940	G1854
A2825	G2760	A2633	G2508	C2570	G2508	U2294	U2224	G	U2067	A2003	C1941	G1855
C2826	A2761	A2633	A2509	G2571	A2509	U2298	G2225	C	C2068	U2004	G1942	U1856
G2827	G2762	G2698	A2510	U2572	A2510		A2226	U				
C2828	U2763	U2700	G2511	U2572	G2511	U2298						
A2829	U2764	U2700	A2512	G2574	A2512	A2299	G2229	G	G2071	U2005	A1943	A1860
U2830	U2766	G2702	U2515	U2575	U2515	A2300	G2230	A		U2006	C1861	A1860
A2831	G2767	C2703	U2516	A2576	U2516	A2301	G2231	A		G2007	U1946	C1862
C2832	U2704	U2704	A2577	A2577	C2517	A2306	G2232	A		U2008	G1947	U1863
C2833	A2705	A2705	G2578	G2578	C2518	A2307	G2233	U		U2009	C1948	G1864
A2834	U2706	A2644	A2579	A2579	C2519	A2307	G2234			G2010	A1949	C1865
C2835	G2707	A2645	U2580	A2580	C2520	A2308	G2235			U2011	C1950	G1866
U2836	G2707	A2646	A2520	A2581	U2520	A2309	U2236			A2012	G1951	
G2837	U2708	C2646	A2521	U2582	G2521	A2310	G2237			A2013	A1952	A1869
C2710	C2709		A2521		G2522	U2311	G2238			A2014	A1953	U1870
G2711	G2711		G2523	C2585	G2523	U2312	C2239			G2015	A1954	
A2712	A2712		G2524	U2586	G2524	G2313	C2240			A2016	G1955	U1881
A2713	A2713		U2525	U2587	U2525	A2314	U2241				G1956	G1882
A2714	A2714		U2526	U2588	U2526	A2315	C2242			C2019	C1957	A1883
C2715	A2654		G2527	U2589	G2527	A2316	C2243			G2020	G1968	A1884
G2716	G2716		U2528	U2590	G2528	U2317	C2244			G2021	U1969	C1885
G2717	G2717		G2529	C2591	G2529	A2318	A2245			C2022	A1960	G1886
U2718	A2718		C2530	U2592	C2530	A2319	A2246			C2023	A1961	G1887
A2719	G2719		U2531	U2593	U2531	A2320	A2247			U2024	C1962	C1889
C2720	A2720		G2532	U2594	G2532	A2321	C2248			C2026	A1964	U1901
C2721	A2721		U2533	U2595	U2533	U2322	U2249			C2027	U1965	
G2722	A2722		U2534	C2596	U2534	U2323	U2250			C2028	G1966	A1902
C2725	G2725		C2535	U2597	C2535	G2324	U2251			G2029	U1967	
U2726	U2726		C2538	C2598	C2538	A2325	A2252			U2030	G1905	G1905
G2727	G2727		G2539	U2599	G2539	A2326	A2253			A2031	U1906	U1906
U2728	G2728		U2540	G2602	A2540	U2327	C2254			G2032	G1907	G1907
A2729	A2729		U2541	G2603	U2541	C2328	G2255			C2033	C1971	C1971
G2730	A2730		U2542	G2604	U2542	A2330	G2256			A2034	G1972	U1909
G2731	G2731		A2543	G2605	A2543	A2331	A2257			G2035	C1973	A1910
C2732	G2732		A2544	C2606	A2544	G2332	G2258			G2036	U1974	A1911
C2735	C2735		U2545	G2607	U2545	A2333	C2261			A2037	G1975	G1912
U2736	U2736		G2546	G2608	G2546	C2334	C2262			C2038	U1976	G1913
A2737	A2737		C2547	G2609	C2547	U2335	C2263			G2039	C1977	U1914
G2738	G2738		U2548	G2610	U2548	G2336	C2266			A2040	U1978	A1915
G2739	G2739		G2549	A2611	G2549	A2337	A2267			A2041	C1979	G1916
C2740	C2740		A2550	G2612	A2550	C2338	A2268				A1980	C1917
G2741	G2741		G2551	G2613	G2551	A2339	G2269			G2044	A1981	G1918
G2742	G2742		C2552	A2614	C2552	C2340	U2270			A2045	C1982	A1919
C2743	C2743		G2553	U2615	G2553	U2341	C2271			G2046	A1983	A1920
U2744	U2744		C2554	G2616	C2554	C2342	A2272			C2047	A1984	A1921
A2745	A2745		G2555	U2617	G2555	G2343	C2273				G1985	U1922
C2748	C2748		A2556	G2618	A2556	A2344	C2274			G2050	G1986	U1923
A2812	A2812		G2557	U2619	G2557	A2345	C2275			U2051	G1987	C1924
G2813	G2813		U2558	G2620	U2558	G2353	U2276			G2052	C1988	C1925
G2814	G2814		G2559	G2621	G2559	G2354	C2277			G2053	U1976	C1926
C2815	C2815		U2560	G2622	U2560	A2355	A2278			U1990	U1977	U1927
C2816	C2816		G2561	G2623	G2561	A2356	G2279			G2055	C1991	G1928
A2817	A2817		G2562	U2625	G2562	A2357	A2280			C2056	G1992	U1929
G2818	G2818		U2563	U2626	U2563	C2358	A2281			U2057	G1993	C1930
C2819	C2819		U2564	G2627	U2564	C2358	U2285			U2058	U1994	G1931
											G1995	

- Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1:  65% 35%

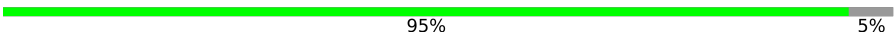


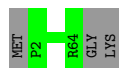
- Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:  98%

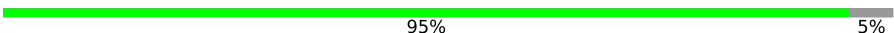


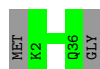
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:  95% 5%

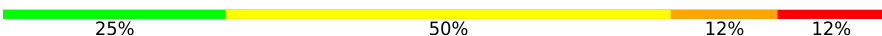


- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4:  95% 5%



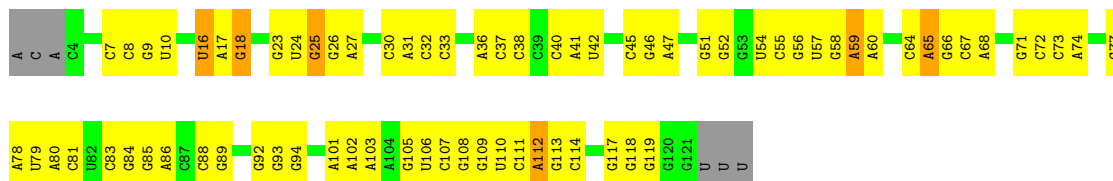
- Molecule 6: QUINUPRISTIN

Chain 5:  25% 50% 12% 12%



- Molecule 7: 5S RIBOSOMAL RNA

Chain 9:  36% 54% 5% 5%

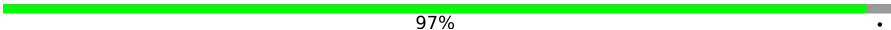


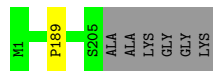
- Molecule 8: 50S RIBOSOMAL PROTEIN L2

Chain A:  98%

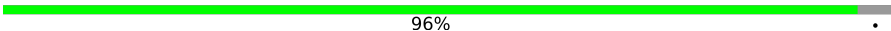


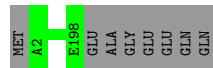
- Molecule 9: 50S RIBOSOMAL PROTEIN L3

Chain B:  97%

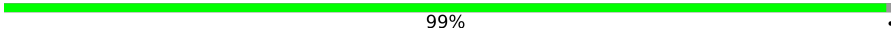


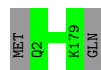
- Molecule 10: 50S RIBOSOMAL PROTEIN L4

Chain C:  96%



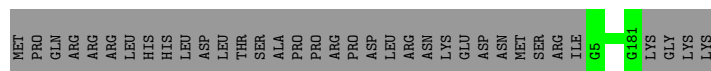
- Molecule 11: 50S RIBOSOMAL PROTEIN L5

Chain D:  99%



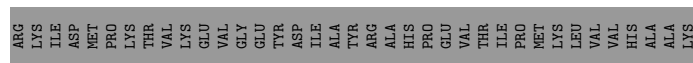
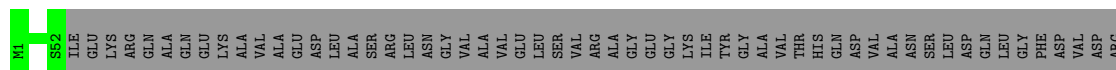
- Molecule 12: 50S RIBOSOMAL PROTEIN L6

Chain E:  83% 17%

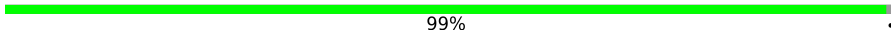


- Molecule 13: 50S RIBOSOMAL PROTEIN L9

Chain F:  36% 64%



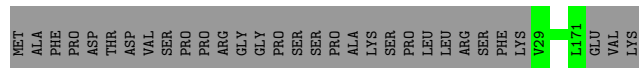
- Molecule 14: 50S RIBOSOMAL PROTEIN L11

Chain G:  99%

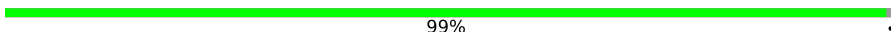
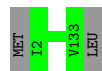


- Molecule 15: 50S RIBOSOMAL PROTEIN L13

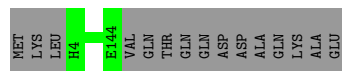
Chain H:  82% 18%



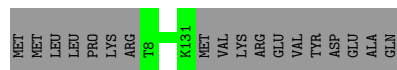
● Molecule 16: 50S RIBOSOMAL PROTEIN L14

Chain I:  99% .

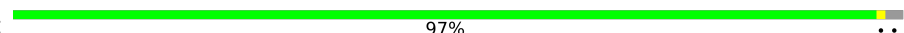
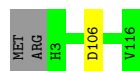
● Molecule 17: 50S RIBOSOMAL PROTEIN L15

Chain J:  90% 10%

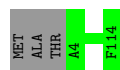
● Molecule 18: 50S RIBOSOMAL PROTEIN L16

Chain K:  87% 13%

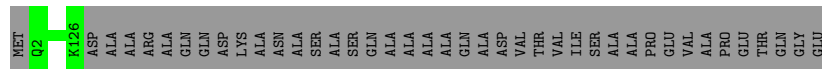
● Molecule 19: 50S RIBOSOMAL PROTEIN L17

Chain L:  97% ..

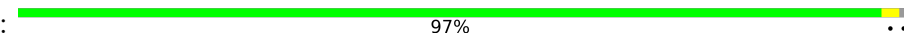
● Molecule 20: 50S RIBOSOMAL PROTEIN L18

Chain M:  97% .

● Molecule 21: 50S RIBOSOMAL PROTEIN L19

Chain N:  75% 25%

● Molecule 22: 50S RIBOSOMAL PROTEIN L20

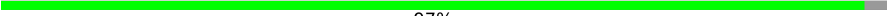
Chain O:  97% ..

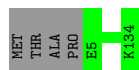
● Molecule 23: 50S RIBOSOMAL PROTEIN L21

Chain P:  100%

There are no outlier residues recorded for this chain.

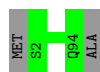
- Molecule 24: 50S RIBOSOMAL PROTEIN L22

Chain Q:  97%



- Molecule 25: 50S RIBOSOMAL PROTEIN L23

Chain R:  98%



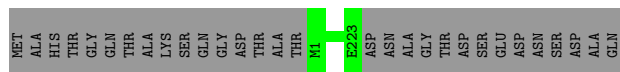
- Molecule 26: 50S RIBOSOMAL PROTEIN L24

Chain S:  98%



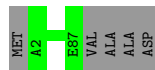
- Molecule 27: GENERAL STRESS PROTEIN CTC

Chain T:  88% 12%



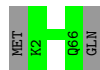
- Molecule 28: 50S RIBOSOMAL PROTEIN L27

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, α , β , γ	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 ²)	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: DBB, MHV, DOL, MHU, 004, 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	0.49	0/66467	0.77	55/103673 (0.1%)
6	5	0.88	0/13	0.98	0/15
7	9	0.40	0/2813	0.67	0/4384
All	All	0.49	0/69293	0.77	55/108072 (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	146
6	5	1	1
7	9	0	1
All	All	1	148

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	173	A	C2'-C3'-O3'	8.53	122.30	109.50
1	0	2668	U	C4'-C3'-O3'	-7.76	101.35	113.00
1	0	1264	C	C2'-C3'-O3'	-7.40	102.60	113.70
1	0	586	G	C4'-C3'-O3'	-7.16	102.26	113.00
1	0	1263	G	C2'-C3'-O3'	7.07	120.10	109.50

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	2133	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2208	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 2208 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 [i](#)

5.3.1 Protein backbone [i](#)

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 ⓘ

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	MHV	5	6	6	7,9,10	0.62	0	8,11,13	1.39	2 (25%)
6	004	5	7	6	9,10,11	1.86	3 (33%)	9,12,14	1.27	1 (11%)
6	MHU	5	5	6	14,15,16	1.20	1 (7%)	18,19,21	1.16	1 (5%)
6	DBB	5	3	6	4,5,6	0.60	0	1,5,7	0.04	0
6	MHW	5	1	6	9,9,10	0.81	0	10,11,13	1.29	1 (10%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	7	004	CB-CA	3.27	1.55	1.52
6	5	7	004	CG2-CB	-2.85	1.34	1.39
6	5	5	MHU	CZ1-NZ	-2.71	1.39	1.45
6	5	7	004	CD2-CE	-2.38	1.33	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1	MHW	O-C-CA	-3.29	120.24	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	5	MHU	O-C-CA	-2.88	117.37	124.77
6	5	6	MHV	CE-CD2-CG	2.48	117.29	111.81
6	5	7	004	CG2-CB-CA	2.41	124.38	120.64
6	5	6	MHV	CB-CA-N	-2.02	108.33	112.50

There are no chirality outliers.

All (5) 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	3	DBB	5	0
6	5	1	MHW	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DOL	0	2882	-	47,50,50	4.58	14 (29%)	57,70,70	3.87	24 (42%)

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	22/64/77/77	0/2/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	2882	DOL	O40-S39	19.25	1.77	1.44
33	0	2882	DOL	O41-S39	19.04	1.76	1.44
33	0	2882	DOL	C28-C29	-9.26	1.11	1.32
33	0	2882	DOL	C1-C37	4.47	1.62	1.52
33	0	2882	DOL	C28-C26	4.46	1.57	1.48

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	2882	DOL	C4-N5-C1	-15.46	94.37	112.51
33	0	2882	DOL	O18-C17-C16	13.82	145.78	109.24
33	0	2882	DOL	C28-C26-N25	-8.11	97.30	115.07
33	0	2882	DOL	O40-S39-O41	-7.21	109.95	118.13
33	0	2882	DOL	O27-C26-C28	6.54	138.02	122.95

All (2) chirality outliers are listed below:

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

5 of 22 torsion outliers are listed below:

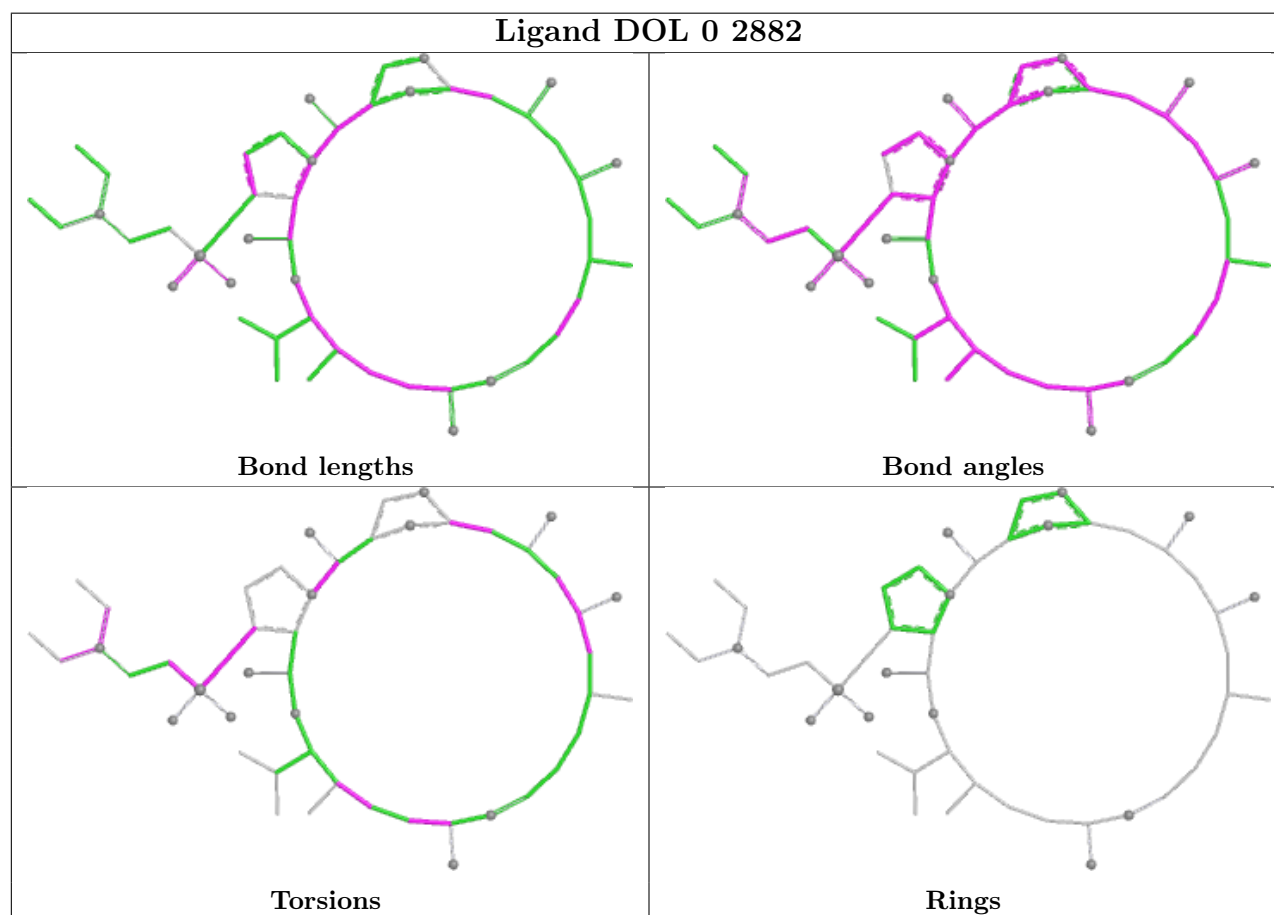
Mol	Chain	Res	Type	Atoms
33	0	2882	DOL	O7-C6-N5-C1
33	0	2882	DOL	C8-C6-N5-C1
33	0	2882	DOL	C1-C2-S39-O40
33	0	2882	DOL	C1-C2-S39-C42
33	0	2882	DOL	C43-C42-S39-O41

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 ⓘ

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

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.