



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:38 am BST

PDB ID : 1XBP
Title : Inhibition of peptide bond formation by pleuromutilins: The structure of the 50S ribosomal subunit from *Deinococcus radiodurans* in complex with Tiamulin
Authors : Schluenzen, F.; Pyetan, E.; Fucini, P.; Yonath, A.; Harms, J.M.
Deposited on : 2004-08-31
Resolution : 3.50 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

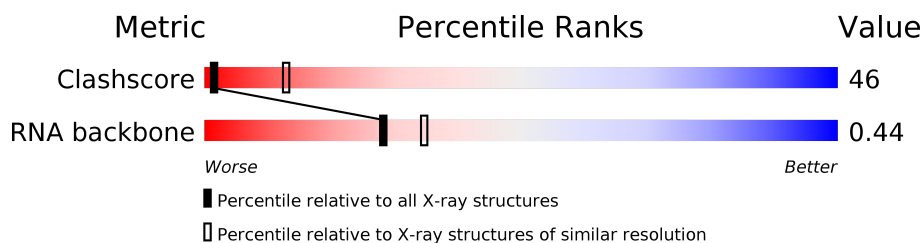
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)


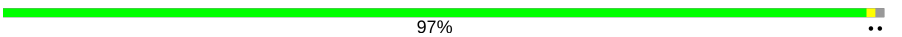



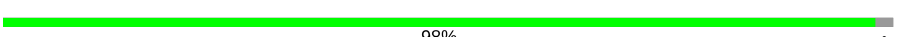




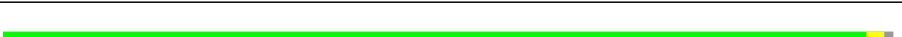


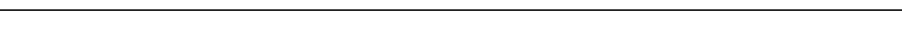

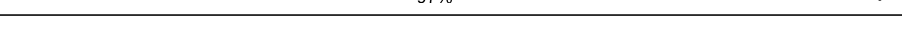
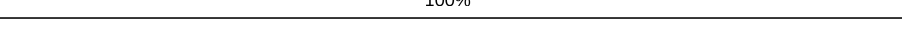
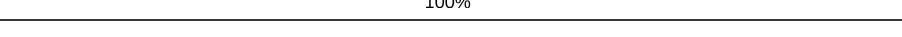
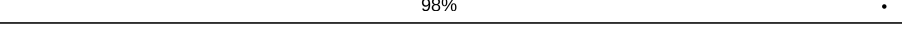
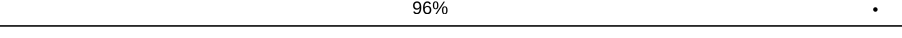
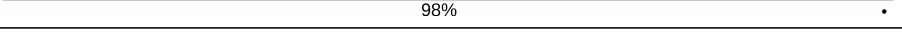
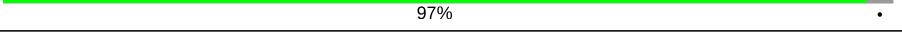
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	11% 63% 19% . .
2	9	124	13% 69% 14% 5%
3	A	274	98% ..
4	B	211	96% . .
5	C	204	97% .
6	D	180	99% .
7	E	185	95% . .
8	F	146	36% 64%
9	G	144	99% .

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Mol	Chain	Length	Quality of chain
10	H	174	 82% 18%
11	I	134	 97% ..
12	J	156	 90% 10%
13	K	141	 87% 12%
14	L	116	 97% ..
15	M	113	 98% .
16	N	166	 75% 25%
17	O	118	 99% .
18	P	100	 100%
19	Q	134	 94% 5%
20	R	94	 97% ..
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	 98% .
28	1	55	 96% .
29	2	47	 98% .
30	3	65	 97% .
31	4	37	 95% 5%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65328 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
			2516	1124	464	811	117			

- Molecule 3 is a protein called 50S 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 50S 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 50S 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 50S 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 50S 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 50S 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 50S 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 50S 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 50S 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 50S 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 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	127	Total C 127 127	0	0	127

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S 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 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S 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 50S 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 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S 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 50S 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 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

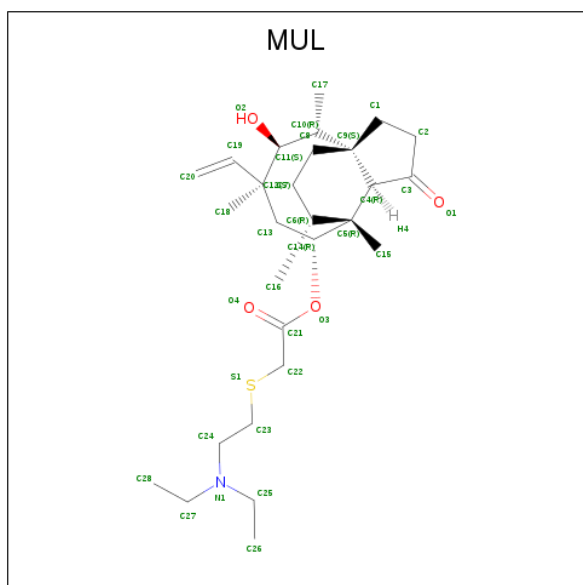
- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is TIAMULIN (three-letter code: MUL) (formula: C₂₈H₄₇NO₄S).



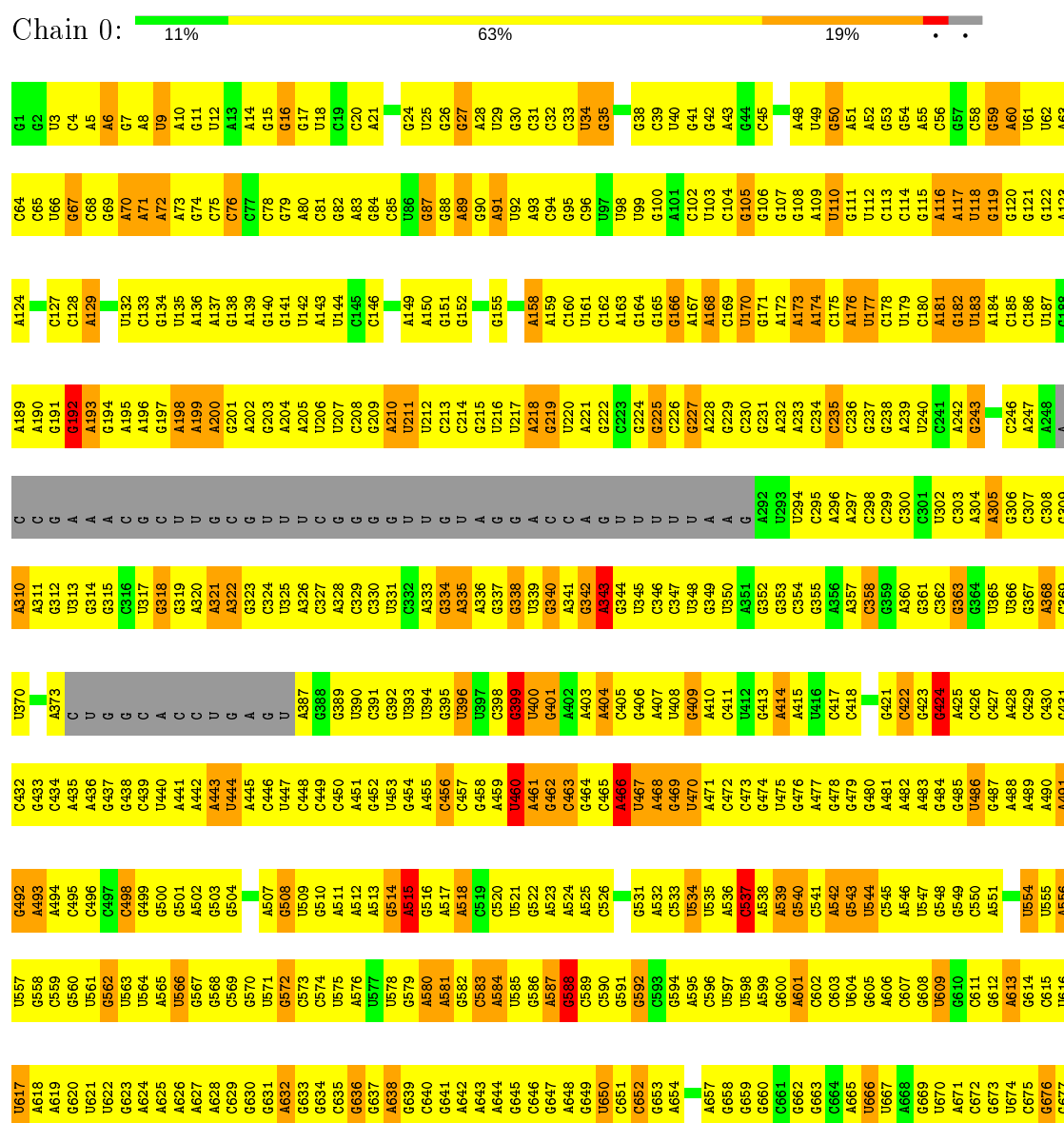
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C N O S 34 28 1 4 1	0	0

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.

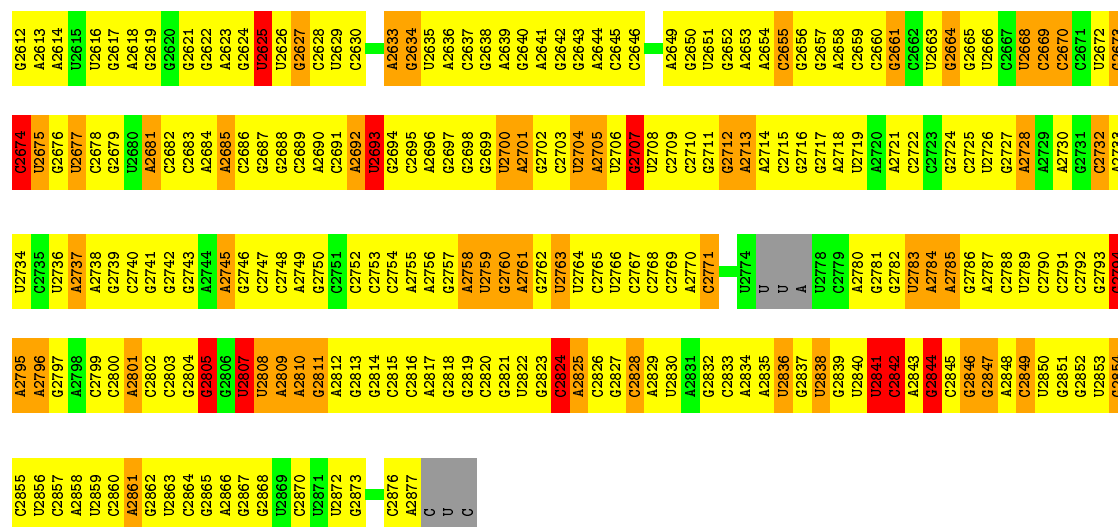
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



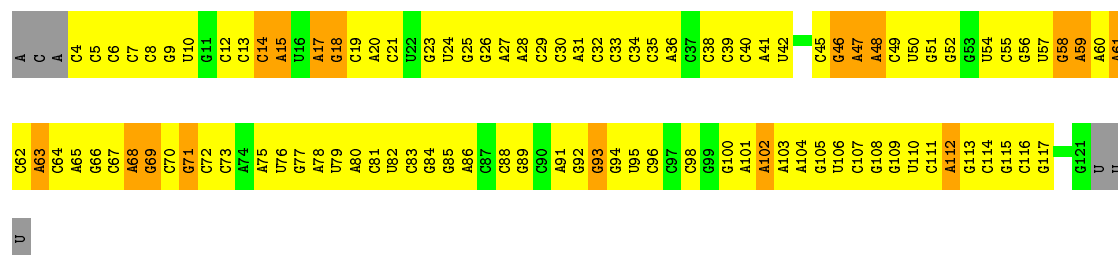
A1610	G1545	U1481	A1416	G1356	G1296	C1234	U1172	G1110	U1044	G983	A922	G861	A801	A740	G678
A1611	C1546	U1482	C1417	U1357	A1297	C1235	G1173	C1111	G1045	A984	A923	A862	A802	G741	C679
G1612	U1547	G1483		C1358	G1298	G1236	G1174	C1112	U1046	A985	G924	C863	C803	A742	U680
A1613	C1549	G1484	U1424	G1359	A1299		A1175	C1113	G1047	A986	U925	C864	C804	A743	A681
C1614		U1485	G1425	G1360	A1300	A1239	U1176	C1115	U1048	A987	G926	A865	G805	C744	G682
C1615		U1486	U1426	G1361	A1301	G1240	U1177	C1116	U1049	A988	G927	U866	A806	C745	A683
C1616		C1487	G1427	A1362	C1302	G1241		U1117		G989	G928	C867	A807	G746	C684
G1617	G1553	G1488	G1428	C1363	U1303	A1242	C1181	U1118	C1052	A990	A929	U868	C808	A747	U685
U1618	G1554	C1489	A1429	C1364	U1304	G1243	U1182	G1118	G1053	C869	A930	C869	C809	A748	C686
A1619	U1548	G1490	G1430	C1365	U1305	U1244	C1183	U1119	C1054	A991	G931	C870	U810	C749	G687
A1620	A1556	C1491	U1431	A1366	U1306	U1245	G1184	C1120	A1055	A992	G932	U871	G811	C750	A688
C1621		U1492	G1432	A1367	U1307		C1185	C1121	U1056	A993	G933	G872	G812	G751	A689
G1622	C1557		A1433	G1368	C1308	G1248	C1186		A1057	A994	G934	U873	A813	G752	A690
C1623	G1559	G1496	U1434	G1369	G1309	G1249	A1187	G1125	G1058	C996	C935	A874	G814	U753	C691
A1624	A1560	C1497	G1435	U1370	C1310	A1250	A1188	U1126	A1059	C997	A936	C875	U815	G754	C692
A1625	U1561	G1498	G1436	G1371	C1311	G1251	G1189	C1127	C1060	C998	G937	A876	U816	C755	C693
A1626	G1562	U1499	A1437	A1372	G1312	C1252	G1190	G1128	U1065	A999		C877	A817	C756	G694
C1627	U1563	U1500	G1438	G1373	U1313	C1253	G1191	G1129	C1063	G1000	G940	C878	G818	U757	G695
C1628	U1564	C1501	G1439	G1374	A1314	G1254	A1192	U1130	A1064	A1001	U941	A879	C819	G758	U696
G1629	G1565	G1502	G1440	C1375	A1315	A1255	G1193	G1131	A1065	C1002	U942	C880	U820	C759	G697
A1630	G1566	U1503	A1441	C1376	G1316	C1256	U1194	G1132	G1066	U881	U943	U881	A821	U760	A698
C1631	A1567	G1504	G1442	G1377	A1317	U1257	U1195	G1133	G1067	A982	A944	C882	U822	G761	G699
A1632	A1568	U1505	G1443	A1378	A1318	G1258	G1196	C1134	A1068	U1005	G945	A883	U823	A762	C700
C1633	A1569	C1506	C1444	A1379	C1319	A1259	U1197	G1135	G1069	C1006	U946		C825	A763	U701
A1634		A1507	U1445	C1380	A1320	A1260	C1198	U1136		A1007	C947	A886	C826	A764	A702
G1635	C1572	G1508	U1446	G1381	A1321	G1261	G1199	A1137	U1072	G1008	C948	C887	U826	C765	A703
G1636	G1573	A1509	U1447	C1382	G1322	U1262	G1200	A1138	G1073	C1009	G949	C888	C827	A766	G704
U1637	A1574	A1510	A1448	G1383	G1323	C1263	G1201	A1139	G1074	U1010	G950	C889	C828	C705	G705
G1638	C1575	A1511	G1449	G1384	C1324	C1264	U1202	A1140	C1075	A1011	G951	U890	C829	A774	A706
U1639	G1576	A1512	G1450	C1385	U1325	G1265	U1203	U1141	U1076	A1012	A952	C890	C830	U770	U707
C1640	G1577	U1513	C1451	A1386	G1326	G1266	G1204	G1142	U1077	G1013	G953	G	G831	C771	G708
C1641	U1578	C1514	U1452	G1387	C1327	A1267	G1205	A1143	A1078	G1014	U954	G	A832	C772	A709
G1642	U1579	A1515	U1453	C1388	G1328	U1268	G1206	U1144	G1079	U1015	G955	G	A833	C773	C710
A1643	C1580	A1516	U1454	C1389	U1329	G1269	G1207	C1145	A1080	A956	G957	G	U835	A774	C711
G1644	A1581	C1517	G1455	G1390	G1330	C1270	A1208	G1146	C1081	C1016	G958	G	U836	C775	A712
U1645	A1582	G1518	C1456	A1391	G1331	C1271	G1209	G1147	G1082	C1018	G959	C	U837	C776	G713
G1646	A1583	G1519	A1457	U1392	G1332	G1272	C1210	G1148	C1083	U1019	U960	U	U838	A777	G714
U1647	G1584	G1520	A1458	G1393	C1333	G1273	G1211	G1149	A1084	A1020	U961	A	A838	C778	U715
C1648	A1585	U1521	U1459	G1394	C1334	C1274	U1212	C1150	G1085	A1021	G962	C	U839	C779	U716
A1649	A1586	C1522	G1460	A1395	A1335	A1275	U1213	U1151	C1086	A1022	C962	C	U840	C780	G717
A1650	C1587	A1523	C1461	G1396	G1336	U1276	C1214	C1152	G1087	U1023	G963	C	G841	A781	A718
U1651	A1588	C1524	C1462	A1397	G1337	G1277	A1215	A1153	A1088	G1024	A964	A	A842	U782	A719
G1652			A1463	G1398	G1338	A1278	G1216	G1154	C1089	A1025	G965	C	G843	G783	A720
C1653	U1591	G1527	A1464	C1399	U1339	G1279	U1217	G1155	C1090	U1026	A966	C	G844	U784	C721
A1654	U1592	C1528	G1465	A1400	C1340	U1280	C1218	U1156	C1091	C1027	G967	U	U845	U785	C722
C1655	C1593	C1529	C1466	G1401	G1341	A1281	C1219	G1157		G1028	C968	U	A846	C786	
U1656	U1594	U1530	U1467	G1402	U1342	A1282	G1220	A1158	C1094	C1029	U969	A	C847	A787	
A1657	A1595	C1531	A1468	U1403	C1343	C1283	C1221	U1159	A1095	A970	A971	C	A848	G788	
A1658		A1532	U1469	C1404	G1344	G1284	G1222	G1160	A1096	C1031	G849	C	G849	G789	U727
G1659	C1598	G1533	G1470	A1405	G1345	A1285	G1223	U1161	A1097	A1032	C972	A911	C850	A790	G728
G1660			C1471	A1406	C1346	U1286	A1224	A1162	G1098	G1033	U973	A912	C851	G791	A729
C1661		G1536	G1407	C1347	C1347	A1287	G1225	C1163	U1099	U1034	U974	A913	U852	U792	
G1662	G1602	U1537	U1472	A1408	C1348	A1288	A1226	C1164	G1035	G1036	C975	C914	C853	G793	
C1663	A1603	A1538	A1473	U1409	A1349	A1289	A1227	G1165	G1102	G1037	C976	C915	G854	A794	G733
G1664	A1604	U1539	U1475	U1410	G1350	A1290	G1228	A1166	U1037	C1103	G977	U916	G855	A795	G734
C1665	C1605	C1540	G1476	C1411	G1351	G1291	C1229	A1167	G1104	U1038	U978	U917	A856	A796	G735
G1666	C1606	G1541	C1477	C1412	G1352	A1292	C1230	G1168	U1105	A1039	A979	A918	U857	A797	G736
A1667	U1607	U1542	U1478	U1413	A1353	A1293	U1231	C1169	A106	G980	C981	U919	G858	G798	C737
G1668	G1608	G1543	G1479	A1543	A1354	G1294	U1232	U1170	A1107	G1041	C982	A921	U859	C799	G738
A1669	G1609	A1544	G1480	C1415	A1355	U1295	A1233	A1171					U860	U800	G739

A2561	C2491	A2439	G2368	A2308	C2243	U2178	G	G2053	G1993	U1856	C1792	G1731	G1670
C2562	G2492	A2430	U2369	G2309	C2244		C	A2054	U1994	G1857	A1793	U1732	A1671
G2563	U2493	C2431	A2370	U2310	A2245	A2181	G	G2055	G1995	C1858	A1794	U1733	C1672
C2564	U2494	A2432	A2371	U2311	A2246	A2182		C2056	A1996	A1859	C1795	G1734	C1673
G2565	G2495	C2433	A2372	G2312	A2247	C2183	A2118	U2057	A1997	G1860	A1796	G1735	C1674
A2566	G2496	G2434	C2373	G2313	A2248	C2184	A2119	U2058	A1998	A1861	C1797	G1736	C1675
G2567	U2497	C2435	C2374	A2314	U2249	U2185		U2059	U1999	C1862	G1798	G1737	U1676
U2568	U2498	U2436	G2375	A2315	G2250	U2186	G2122	A2060	U2000	U1863	A1799	U1738	C1677
G2569	C2499	G2316	G2376	G2316	U2251		G2123	G2061	G2001	G1864	A1800	G1739	C1678
G2570	U2500	A2437	U2377	G2317	A2252	U2191	C2124	U2062	A2002	C1865	C1801	G1740	U1679
G2561	U2501	U2438	G2378	U2318	A2253	U2192	C2125	A2063	A2003	G1866	A1802	G1741	U1680
G2562	G2502	C2440	G2379	G2319	G2254	C2193	U	U2064	U2004	A1867		G1742	A1681
U2563	G2503	U2441	U2380	G2320	G2255	A2194	U	A2065	U2005	A1868	G1805	G1743	A1682
U2564	G2504	C2442	A2381	C2321	G2256	A2195	U	G2066	G2006	A1869	G1806	G1744	G1683
G2565	G2505	C2443	C2382	U2322		U2196	U	U2067	G2007	U1870	C1808	C1745	G1684
A2566	C2506	C2444	G2383	U2323	G2259	U2197	U	C2068	G2008	A1871	A1809	A1746	A1685
G2567	U2507	C2445	U2384	G2324	G2260	U2198	G	U2069	U2009	G1876	U1810	G1747	A1686
A2568	G2508	C2446	G2385	A2325	G2261	C2199	G2132	G2070	G2010	C1877	A1811	U1748	C1687
A2569	U2509	G2447	G2386	C2326	C2262	G2200	G2133	G2071	U2011	C1878	A1812	G1749	U1688
C2570	A2510	A2448	U2387	U2327	C2263	G2201		C2072	A2012		U1813	A1750	U1689
G2571	G2511	G2449	G2388	G2328		G2202	U2138	A2073	A2013		A1814	A1751	U1690
U2572	A2512	A2450	G2389	G2329	A2266	A2203	G2139	U2074	G2014	U1881	G1815	U1752	G1691
C2573	G2513	A2451	A2390	G2330	A2267	A2204	G2140	U2075	A2015	G1882	G1816	A1753	C1692
G2574	U2514	U2452	A2391	A2331	G2268	C2205	A	G2076	A2016	A1883	U1817	G1754	A1693
U2575	G2515	C2453	G2392	G2332	U2270	C2206	G	G2077	U2017	A1884	G1818	G1755	A1694
G2576	U2516	C2454	G2393	A2333	U2271	G2207	G	G2078	G2018	C1885	U1819	C1756	U1695
A2577	G2517	A2455	G2394	C2334	C2271	U2208	C	A2079	U2019	G1886	A1820		G1696
G2578	U2518	U2456	C2395	U2335	G2272	U2209	A	U2080	G2020	G1887	A1821	U1757	U1697
			G2396	G2336	C2274	U2210	A	C2081	G2021	C1888	A1822	G1760	G1698
A2581	G2519	U2457	C2397	A2337	U2275	U2211	C	G2082	G2022	C1889	G1823	G1761	A1699
G2582	A2520	U2458	U2398	G2338	C2276	U2212	G	C2083	C2023		G1824	G1762	C1700
U2583	G2521	C2459	G2399	A2339	A2277	G2213	U	G2084	U2024	G1892	U1825	G1763	C1701
G2584	G2522	G2460			U2278		G	G2085	A2025		G1826	A1764	C1702
G2585	U2523	G2461	A2401	C2341	G2279	G2214	G	U2086	C2026	U1900	G1827	U1766	C1703
G2586	G2524	C2462	C2402	U2342	A2280	G2215	A	U2087	C2027	G1901	G1828	G1767	G1704
G2587	U2525	U2463	C2403	G2343	C2281	U2216	A		G2028	G1968	C1829	U1705	U1705
U2588	G2526	A2464	A2404	G2344	G2282	U2217	A	U2090	G2029	G1969	G1830	U1768	A1706
C2589	U2527	G2465	A2405	A2345	G2283	A2220	U	C2091	U2030	U1909	U1769	A1707	A1707
U2590	G2528	G2466	C2406	G2346	U2284	G2221	A	U2092	A2031	A1910	G1831	U1770	C1708
C2591	U2529	U2467	G2407	U2347	U2285	U2222		G2093	G2032	A1911	U1832	A1771	U1709
U2592	G2530	U2470	A2408	A2348	G2286	U2223	G2158	C2094	C2033	G1912	U1833	C1772	U1710
A2593	U2531	U2471	G2409	G2349	G2287	U2224	G2159	U2095	A2034	G1913		C1773	G1711
G2594	U2532	U2472	A2410	G2350	A2288	G2225	C2160	U2096	U2035	U1914	G1837	A1774	G1712
C2595	U2533	G2473	U2411	G2351	A2289	G2226	C2161	A2097	G2036	A1915	G1838	A1775	G1713
G2596	U2534	G2474	A2412	C2352		C2227	C2162	G	A2037	G1916	A1839	A1776	A1714
C2597	G2535	C2475	A2413	A2353	C2292	U2228	U2163	G	G2038	C1917	A1840	A1777	A1715
U2598	G2536	A2476	A2414	G2354	G2293	U2229	G2164	A	A2039	G1918	G1841	U1778	G1716
G2599	C2537	C2477	G2415	A2355	U2294	G2230	A2165	U	A2040	A1919	U1842	C1779	A1717
A2600	U2538	U2478	G2416	A2356		G2231	G2166	A	A2041	A1920	U1843	A1780	A1718
C2601	G2539	U2479	A2418	A2357	G2297	G2232	A2167	G2103	A2042	A1921	C1844	G1781	G1719
G2602	U2540	G2480	C2419	G2358	U2298	G2233	A2168	G2104	A2043	U1922	A1845	A1782	G1720
G2603	U2541	G2481	A2420	U2359	A2299	G2234	A2169	U2105	G2044	A1923	A1846	G1783	G1721
G2604	U2542	U2482	G2421	G2360	G2300	G2235	C2170	G2106	A2045	C1924	G1847	G1784	G1722
C2605	A2543	U2483	C2422	G2361	A2301	U2236	U2171	G2107	G1985	C1925	U1848	U1785	U1723
G2606	U2544	G2484	G2423	G2362	G2302	G2237	U2172	C2108	G1986	U1926	G1849	C1786	C1724
G2607	G2545	U2485	G2424	G2363	C2303	G2238	G2173	A2109	C2047	G1927	A1851	U1787	C1725
U2608	U2546	C2486	G2425	C2364	G2304	G2239	G2174	G2110	C2048	A1928	G1852	C1788	C1726
G2609	G2547	G2487	A2426	U2365	C2305	C2240	A2175	C	C2049	G1929	C1853	U1789	G1727
G2610	U2548	U2488	G2427	U2366	A2306	U2241	U2176	G	G2050	C1930	G1854	G1790	
A2611	G2550	U2490	U2428	A2367	A2307	C2242	U2177	U	G2052	G1931	G1855	C1791	G1730



• Molecule 2: 5S RIBOSOMAL RNA

Chain 9: 13% 69% 14% 5%



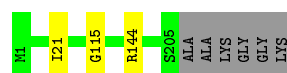
• Molecule 3: 50S ribosomal protein L2

Chain A: 98% ..



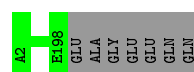
• Molecule 4: 50S ribosomal protein L3

Chain B: 96% ..



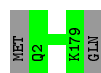
• Molecule 5: 50S ribosomal protein L4

Chain C: 97% .



• Molecule 6: 50S ribosomal protein L5

Chain D:  99% .



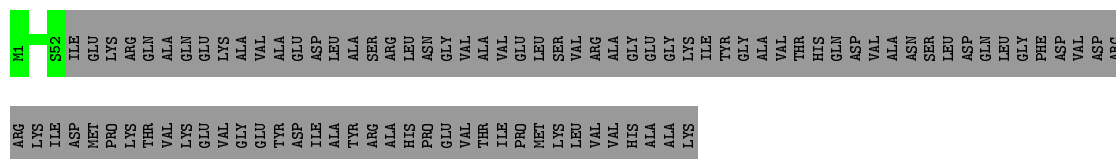
- Molecule 7: 50S ribosomal protein L6

Chain E:  95% ..



- Molecule 8: 50S ribosomal protein L9

Chain F:  36% 64%




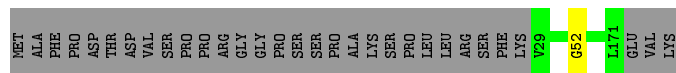
- Molecule 9: 50S ribosomal protein L11

Chain G:  99% .



- Molecule 10: 50S ribosomal protein L13

Chain H:  82% 18%




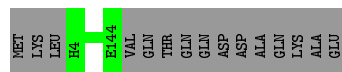
- Molecule 11: 50S ribosomal protein L14

Chain I:  97% ..




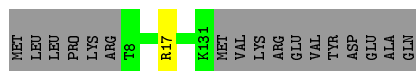
- Molecule 12: 50S ribosomal protein L15

Chain J:  90% 10%



- Molecule 13: ribosomal protein L16

Chain K:  87% 12%



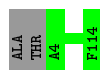
- Molecule 14: 50S ribosomal protein L17

Chain L:  97%



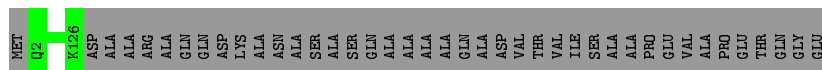
- Molecule 15: 50S ribosomal protein L18

Chain M:  98%



- Molecule 16: 50S ribosomal protein L19

Chain N:  75% 25%



- Molecule 17: 50S ribosomal protein L20

Chain O:  99%



- Molecule 18: 50S ribosomal protein L21

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L22

Chain Q:  94% 5%



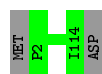
- Molecule 20: 50S ribosomal protein L23

Chain R:  97% .



- Molecule 21: 50S ribosomal protein L24

Chain S:  98%



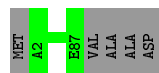
- Molecule 22: 50S ribosomal protein L25

Chain T: 94% 6%



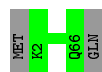
- Molecule 23: 50S ribosomal protein L27

Chain U: 95% 5%



- Molecule 24: 50S ribosomal protein L29

Chain W: 97%



- Molecule 25: 50S ribosomal protein L30

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L31

Chain Y:  100%

There are no outlier residues recorded for this chain.

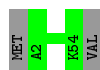
- Molecule 27: 50S ribosomal protein L32

Chain Z: 98% .



- Molecule 28: 50S ribosomal protein L33

Chain 1:  96% .



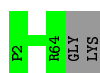
- Molecule 29: 50S ribosomal protein L34

Chain 2:  98% .



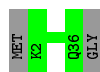
- Molecule 30: 50S ribosomal protein L35

Chain 3:  97% .



- Molecule 31: 50S 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	168.70 Å 405.00 Å 693.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	88.3 (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65328	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: MUL

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	0.79	21/66467 (0.0%)	0.82	43/103673 (0.0%)
2	9	0.44	0/2813	0.73	0/4384
All	All	0.78	21/69280 (0.0%)	0.82	43/108057 (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	260

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1646	G	C5-C6	-7.94	1.34	1.42
1	0	2570	C	N1-C2	6.85	1.47	1.40
1	0	2801	A	C5-C6	-6.62	1.35	1.41
1	0	2673	G	C5-C6	-6.49	1.35	1.42
1	0	2222	U	N3-C4	-6.45	1.32	1.38

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2482	A	N9-C1'-C2'	8.75	125.37	114.00
1	0	460	U	N1-C1'-C2'	7.48	123.72	114.00
1	0	859	U	N1-C1'-C2'	-7.43	103.83	112.00
1	0	1710	U	N1-C1'-C2'	7.14	123.28	114.00
1	0	1266	G	N9-C1'-C2'	6.48	122.43	114.00

There are no chirality outliers.

5 of 260 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	16	G	Sidechain
1	0	27	G	Sidechain
1	0	6	A	Sidechain
1	0	67	G	Sidechain
1	0	9	U	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	29916	4247	0
2	9	2516	0	1286	144	0
3	A	270	0	0	2	0
4	B	205	0	0	3	0
5	C	197	0	0	0	0
6	D	178	0	0	0	0
7	E	177	0	0	1	0
8	F	52	0	0	0	0
9	G	143	0	0	0	0
10	H	143	0	0	1	0
11	I	132	0	0	2	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	3	0
15	M	111	0	0	0	0
16	N	125	0	0	0	0
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	127	0	0	1	0
20	R	93	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Z	58	0	0	0	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	34	0	47	4	0
All	All	65328	0	31249	4383	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 46.

The worst 5 of 4383 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)
1:0:584:A:H4'	1:0:2038:C:N4	1.53	1.23
1:0:1621:C:H4'	1:0:1626:A:N6	1.57	1.19
1:0:918:A:H2'	1:0:919:U:H5''	1.24	1.18
1:0:1339:U:H5''	1:0:1994:U:H1'	1.21	1.18
1:0:1938:U:O2'	1:0:1939:U:H5'	1.42	1.18

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%)	512 (18%)	39 (1%)
2	9	117/124 (94%)	17 (14%)	1 (0%)
All	All	2874/3004 (95%)	529 (18%)	40 (1%)

5 of 529 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	34	U
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1634	A
1	0	1698	C
1	0	2482	A
1	0	1664	G
1	0	1820	G

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](#)

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
32	MUL	0	2881	-	36,36,36	1.35	4 (11%)	54,55,55	1.70	9 (16%)

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	MUL	0	2881	-	-	5/18/79/79	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	MUL	C5-C14	4.47	1.59	1.56
32	0	2881	MUL	C12-C11	3.52	1.58	1.55
32	0	2881	MUL	O3-C14	2.37	1.50	1.46
32	0	2881	MUL	C10-C11	2.31	1.58	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2881	MUL	C18-C12-C11	6.34	111.76	108.06
32	0	2881	MUL	O3-C21-C22	5.49	119.56	110.32
32	0	2881	MUL	C16-C6-C7	-2.92	105.97	110.37
32	0	2881	MUL	C9-C10-C11	2.86	115.19	112.56
32	0	2881	MUL	C17-C10-C11	-2.71	110.00	112.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	2881	MUL	C28-C27-N1-C24
32	0	2881	MUL	C28-C27-N1-C25
32	0	2881	MUL	C26-C25-N1-C27
32	0	2881	MUL	C26-C25-N1-C24
32	0	2881	MUL	C23-C24-N1-C27

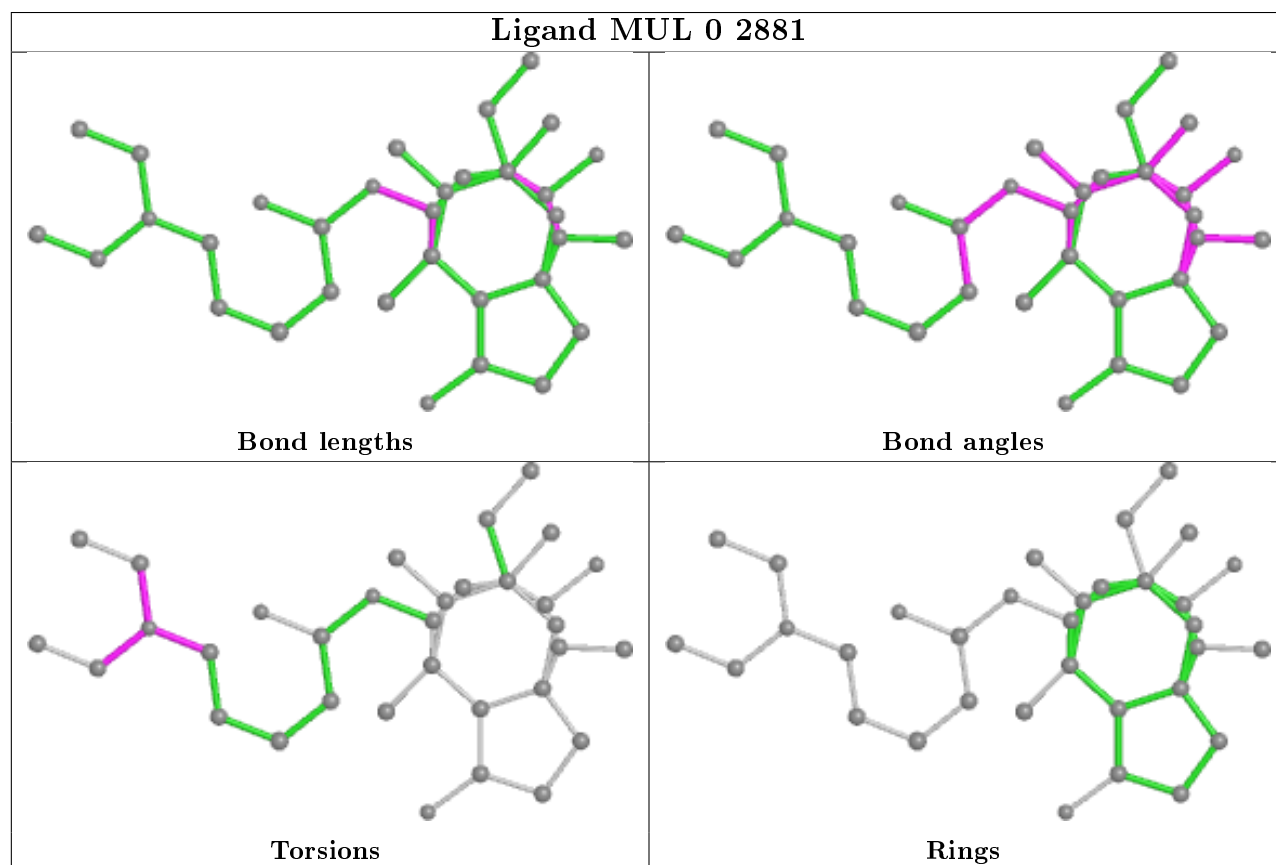
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	MUL	4	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.