



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:14 am GMT

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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

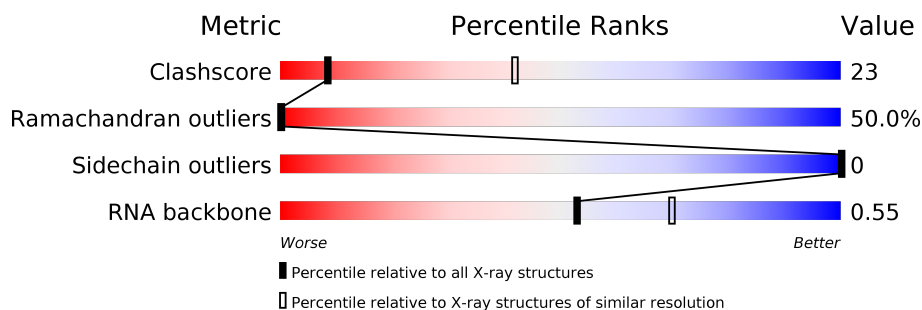
1 Overall quality at a glance

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	112137	1179 (3.50-3.34)
Ramachandran outliers	110173	1147 (3.50-3.34)
Sidechain outliers	110143	1148 (3.50-3.34)
RNA backbone	2435	1001 (3.96-2.86)


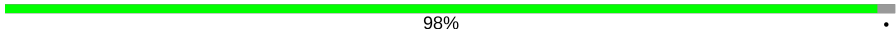
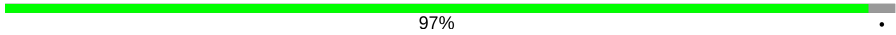
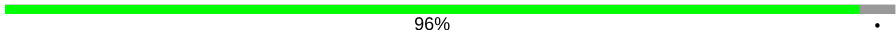
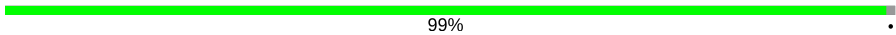


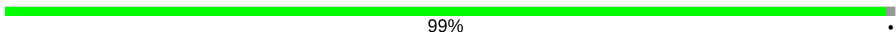

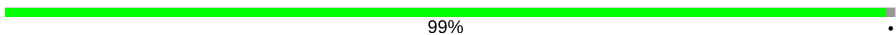


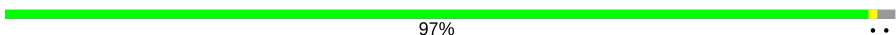
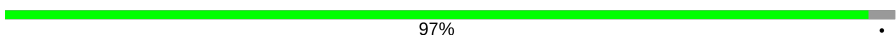

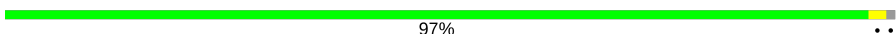

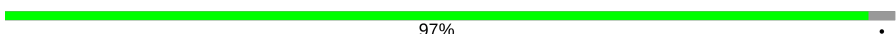
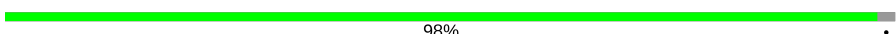
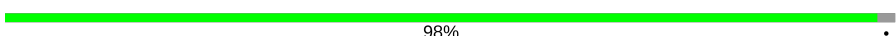



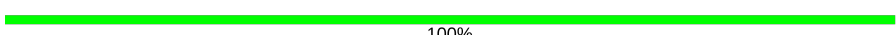

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	1	82	
3	2	47	
4	3	66	
5	4	37	
6	5	8	


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

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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

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

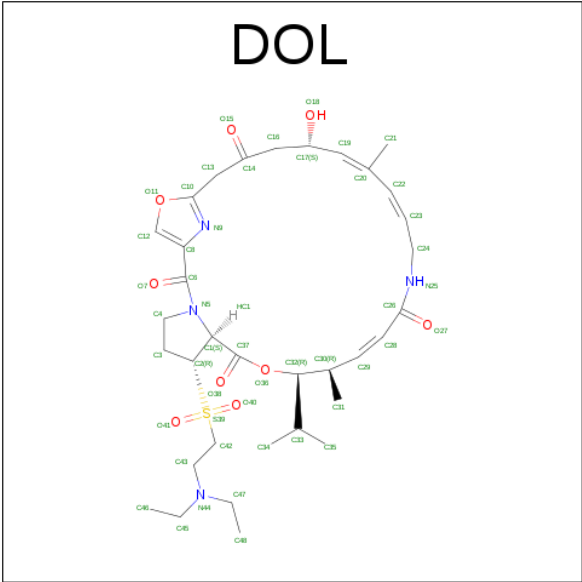
- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L31.

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 (three-letter code: DOL) (formula: C₃₄H₅₀N₄O₉S).



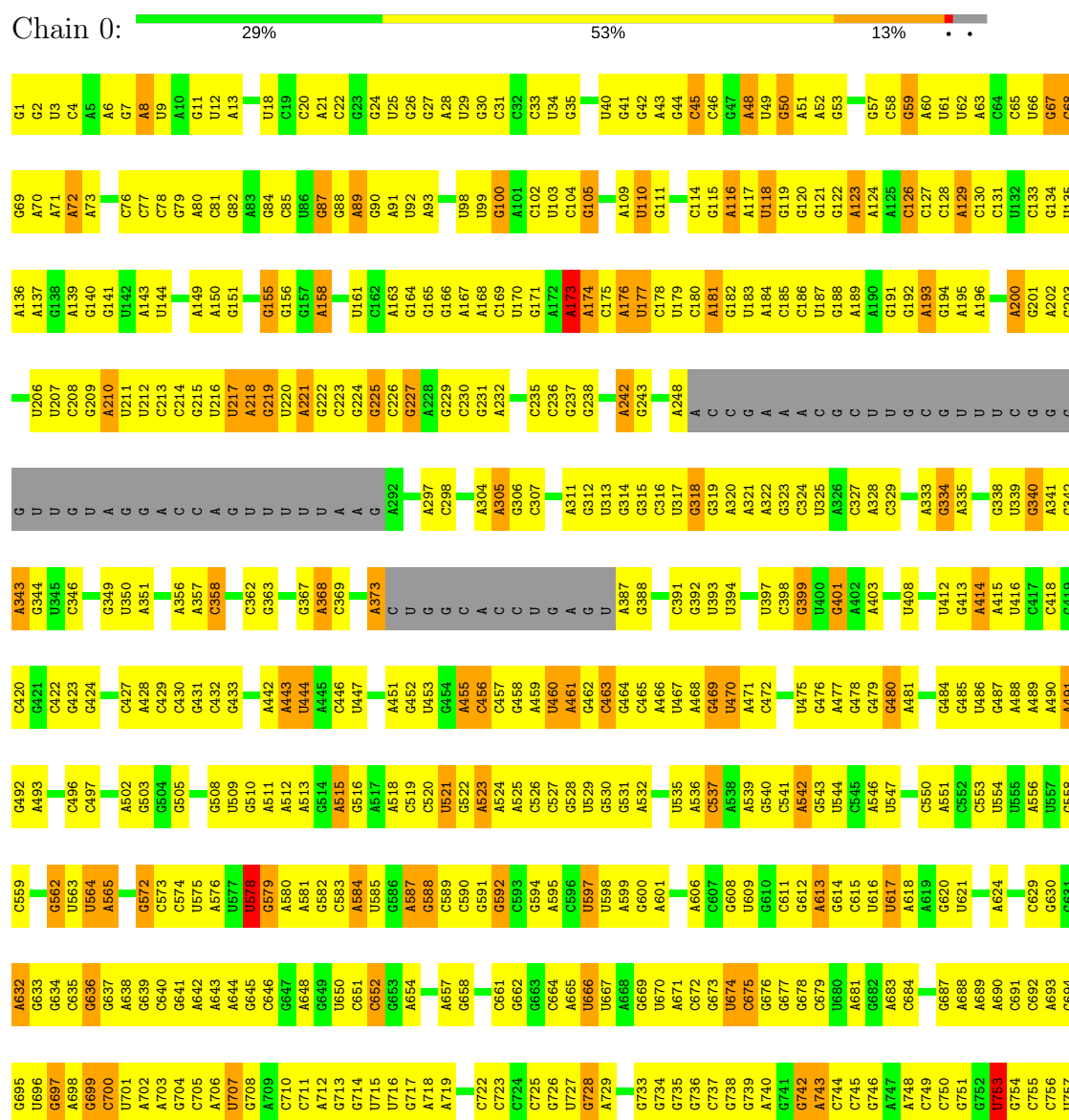
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	0	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

3 Residue-property plots

These plots are drawn for all protein, RNA 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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



G1854	U1770	C1698	U1637	C1588	G1470	G1398	G1331	U1267	U1199	C1018	G957	G	A821	G758
G1855	A1771	A1699	G1638	C1589	G1471	C1399	G1332	U1268	G1200	A1022	G958	G	G822	C759
U1856	C1772	C1702	U1639	G1559	U1472	A1400	G1333	G1269	U1201	U1023	C959	G	U823	U760
A1775	A1773	C1702	C1640	A1560	U1473	G1401	A1334	G1270	G1202	G1024	U960	G	U824	G761
A1860	A1706	A1706	G1642	G1562	A1474	U1403	G1338	C1271	G1204	A1025	G961	G	C825	A762
G1861	A1707	A1707	A1643	U1563	U1475	U1403	U1339	G1272	G1205	G1026	C962	C	U826	A763
C1862	C1708	C1708	U1644	U1564	G1476	A1406	C1340	G1273	G1206	U1027	G963	C	C827	A764
U1863	U1709	U1709	U1645	G1565	G1479	A1407	G1341	G1274	G1207	C1028	A964	U	C828	C765
C1864	C1708	C1708	U1646	U1566	G1480	A1408	U1342	A1275	G1208	G1029	G965	A	C829	
C1865	C1711	C1711	U1647	U1567	U1481	U1409	C1343	U1276	A1208	U1030	A966	C	C830	
G1866	G1712	G1712	U1648	U1567	U1482	U1410	G1344	G1277	G1209	C1031	G967	C	G831	C771
A1869	G1763	G1763	A1649	G1571	U1483	U1410	C1345	A1278	U1212	A1032	C968	A	A832	G772
U1870	C1764	C1764	A1650	C1572	G1484	G1414	G1346	G1279	U1213	G1033	U969	G	A833	G773
A1881	A1785	A1785	U1651	U1573	U1485	C1417	C1347	U1280	U1213	G1034	A970	C	A834	A774
C1882	C1786	C1786	G1652	A1574	U1486	C1418	C1348	A1281	C1214	U1035	C972	U	U835	U775
U1883	A1717	A1717	C1653	A1574	C1487	C1418	A1349	C1283	A1215	G1036	U973	A	U837	A777
C1884	G1718	G1718	U1654	G1577	G1488	U1426	G1352	G1284	C1218	U1038	C975	C	U838	G778
A1885	G1719	G1719	C1655	U1583	C1489	C1435	G1353	A1285	C1219	A1039	C976		U839	U779
C1886	U1720	U1720	U1656	G1584	U1490	G1427	A1353	U1286	C1222	G1040	G977		U840	U780
A1887	G1721	G1721	A1657	U1596	G1664	G1428	A1354	A1287	G1222	U1041	G978		G841	G781
C1888	G1722	G1722	U1658	A1596	G1502	A1429	A1355	A1288	U1223	C914	U978		A842	U782
G1889	U1723	U1723	G1659	A1586	G1503	G1436	G1356	A1289	A1224	C915	U979		G843	G783
A1890	C1724	C1724	G1660	A1587	G1496	U1431	U1357	A1290	G1225	U1044	C980		G844	U784
C1891	G1725	G1725	C1661	A1588	U1500	G1432	C1358	G1291	A1226	G1045	C981		U845	U785
U1901	C1726	C1726	G1662	C1593	U1501	A1433	G1359	A1292	A1227	U1046	C982		A846	U786
A1902	C1727	C1727	U1663	U1599	C1501	U1434	G1360	A1293	G1228	G1047	U983		C847	A787
G1905	G1730	G1730	G1665	A1596	G1502	G1435	C1363	C1229	C1229	A1052	U984		A848	G788
U1906	C1731	C1731	U1666	A1597	G1503	G1436	C1364	A1299	C1230	G1052	C985		U852	G789
C1907	G1736	G1736	A1667	C1598	G1504	G1437	U1365	A1300	U1232	C1054	C987		C853	G791
C1908	U1737	U1737	U1668	G1599	U1505	G1438	A1366	U1301	U1233	A1055	C988		G854	U792
A1910	G1744	G1744	G1670	A1604	G1508	U1441	A1367	U1304	G1241	U1056	A991		U855	G793
C1911	C1745	C1745	A1671	A1605	A1509	C1442	G1368	C1305	U1242	A1057	A992		U857	A794
U1912	A1746	A1746	U1672	G1613	A1510	G1443	U1370	U1306	G1243	G1058	C993		G858	A796
G1913	G1747	G1747	C1673	C1614	A1511	U1445	G1371	U1307	U1244	A1059	C994		U859	A797
U1914	U1748	U1748	U1676	C1615	U1512	U1446	A1372	C1308	G1243	G1066	A995		U860	G798
A1915	G1749	G1749	U1677	C1616	U1513	U1447	G1373	G1309	U1244	G1067	C996		C864	C799
C1916	U1750	U1750	U1678	U1617	C1514	A1448	G1374	C1310	U1247	A1068	C997		A865	U800
U1917	A1751	A1751	U1679	U1618	A1516	G1450	A1379	C1311	G1248	G1069	C998		U866	A801
G1918	U1752	U1752	U1680	A1619	G1520	U1453	G1380	G1312	U1249	G1073	A999		G867	A802
A1919	A1753	A1753	A1681	C1620	U1524	U1454	G1381	A1314	A1250	G1074	G1000		U868	C803
U1920	G1754	G1754	U1682	C1621	G1524	U1454	G1382	A1315	G1251	A1081	C1001		C869	C804
C1921	U1755	U1755	G1683	G1622	G1527	C1455	C1383	G1316	G1252	C1003	C1002		C870	G805
U1922	C1756	C1756	G1684	C1623	U1527	C1456	G1384	G1317	C1253	G1082	A1004		U871	A806
C1923	G1757	G1757	A1685	A1624	C1528	A1457	C1385	A1318	G1254	U1005	U1005		G872	C808
U1924	C1758	C1758	U1686	A1625	C1529	U1458	C1386	C1319	A1255	C1066	C1006		U873	C809
C1925	U1759	U1759	C1687	A1626	U1530	U1459	G1387	A1320	C1256	C1087	A1007		A874	U810
U1926	G1760	G1760	U1688	C1627	U1531	G1460	C1388	A1321	U1257	C1090	G1008		G875	G811
C1927	U1761	U1761	U1689	C1628	G1541	C1461	C1389	G1322	U1258	C1091	C947		A876	G812
U1928	G1762	G1762	U1690	G1629	G1542	C1462	G1390	G1323	A1259	C1091	U1010		G877	A813
C1929	C1763	C1763	G1691	A1630	U1543	A1463	A1391	G1324	G1260	U1092	A1011		G878	G814
U1930	A1764	A1764	C1692	C1631	A1544	U1464	C1392	U1325	G1261	A1088	A1012		A883	U816
G1931	C1765	C1765	A1693	A1632	U1545	G1465	G1393	U1326	U1262	A1099	G952		C884	A817
U1936	U1766	U1766	U1694	C1633	U1548	U1466	G1394	C1327	G1263	G1123	G953		C889	G818
C1937	U1767	U1767	C1695	A1634	C1549	U1467	A1395	C1328	G1264	U1124	U954		U890	C819
U1938	U1769	U1769	U1697	G1636	C1552	U1468	A1397	G1330	G1266	G1125	C1016		A891	U820

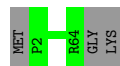
- Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2:  98%



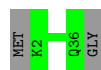
- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:  95%



- Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4:  95%

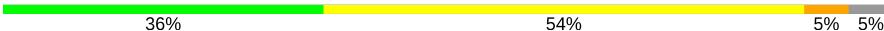


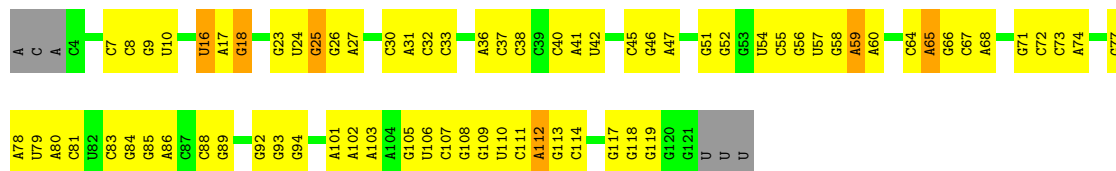
- Molecule 6: QUINUPRISTIN

Chain 5:  63%



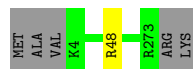
- Molecule 7: 5S RIBOSOMAL RNA

Chain 9:  36%



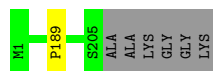
- Molecule 8: 50S RIBOSOMAL PROTEIN L2

Chain A:  98%



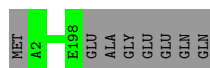
- Molecule 9: 50S RIBOSOMAL PROTEIN L3

Chain B:  97%



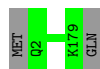
- Molecule 10: 50S RIBOSOMAL PROTEIN L4

Chain C:  96% .




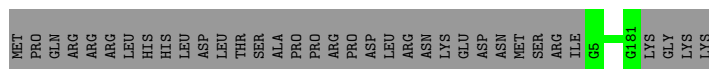
- Molecule 11: 50S RIBOSOMAL PROTEIN L5

Chain D:  99% .



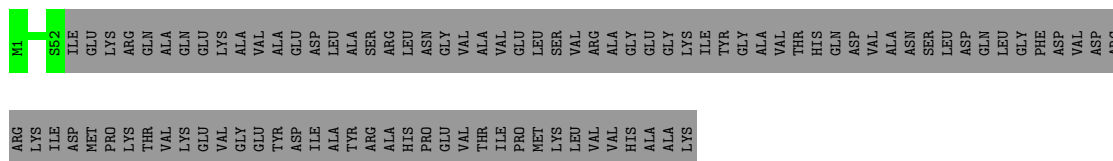
- Molecule 12: 50S RIBOSOMAL PROTEIN L6

Chain E:  83% 17%



- Molecule 13: 50S RIBOSOMAL PROTEIN L9

Chain F:  36% 64%




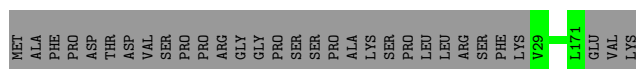
- Molecule 14: 50S RIBOSOMAL PROTEIN L11

Chain G:  99% .



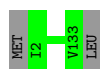
- Molecule 15: 50S RIBOSOMAL PROTEIN L13

Chain H:  82% 18%




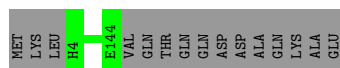
- Molecule 16: 50S RIBOSOMAL PROTEIN L14

Chain I:  99% .




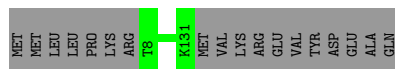
- Molecule 17: 50S RIBOSOMAL PROTEIN L15

Chain J:  90% 10%



- Molecule 18: 50S RIBOSOMAL PROTEIN L16

Chain K:  87% 13%



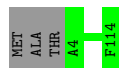
- Molecule 19: 50S RIBOSOMAL PROTEIN L17

Chain L:  97% ..



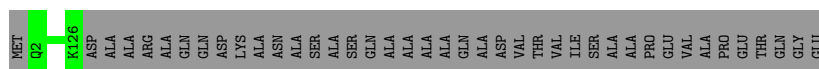
- Molecule 20: 50S RIBOSOMAL PROTEIN L18

Chain M:  97% .



- Molecule 21: 50S RIBOSOMAL PROTEIN L19

Chain N:  75% 25%



- Molecule 22: 50S RIBOSOMAL PROTEIN L20

Chain O:  97% ..



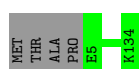
- Molecule 23: 50S RIBOSOMAL PROTEIN L21

Chain P:  100%

There are no outlier residues recorded for this chain.

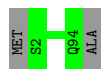
- Molecule 24: 50S RIBOSOMAL PROTEIN L22

Chain Q:  97% .



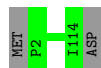
- Molecule 25: 50S RIBOSOMAL PROTEIN L23

Chain R:  98%




- Molecule 26: 50S RIBOSOMAL PROTEIN L24

Chain S:  98%



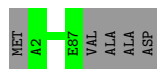
- Molecule 27: GENERAL STRESS PROTEIN CTC

Chain T:  88% 12%



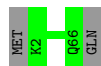
- Molecule 28: 50S RIBOSOMAL PROTEIN L27

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 1.0	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: DOL, DBB, 004, MHV, MHW, MHT, MHU

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.

Some 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%)	0
7	9	117/124 (94%)	12 (10%)	0
All	All	2874/3004 (95%)	445 (15%)	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

There are no RNA pucker outliers to report.

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	MHW	5	1	6	9,9,10	0.78	0	9,11,13	1.73	1 (11%)
6	DBB	5	3	6	5,5,6	0.93	0	3,5,7	1.23	1 (33%)
6	MHU	5	5	6	15,15,16	1.15	1 (6%)	18,19,21	1.16	1 (5%)
6	MHV	5	6	6	9,9,10	1.04	1 (11%)	9,11,13	1.53	1 (11%)
6	004	5	7	6	8,10,11	1.76	3 (37%)	11,12,14	1.45	2 (18%)

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	MHW	5	1	6	-	1/2/2/4	0/1/1/1
6	DBB	5	3	6	-	0/2/4/6	0/0/0/0
6	MHU	5	5	6	-	0/8/12/14	0/1/1/1
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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	7	004	CG2-CB	-2.70	1.34	1.39
6	5	5	MHU	CZ1-NZ	-2.51	1.39	1.45
6	5	7	004	CE-CD2	-2.12	1.33	1.38
6	5	6	MHV	CA-C	2.57	1.53	1.50
6	5	7	004	CB-CA	2.92	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1	MHW	O-C-CA	-4.71	120.24	124.32
6	5	5	MHU	O-C-CA	-3.33	117.37	125.15
6	5	3	DBB	O-C-CA	-2.12	119.18	125.02
6	5	7	004	CG2-CB-CA	2.22	124.38	120.66
6	5	7	004	C-CA-N	2.47	114.44	109.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	5	1	MHW	O-C-CA-N

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 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
33	DOL	0	2882	-	43,50,50	4.36	12 (27%)	54,70,70	4.00	18 (33%)

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	0/58/77/77	0/1/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	2882	DOL	C28-C29	-8.19	1.11	1.32
33	0	2882	DOL	C8-C6	-4.11	1.42	1.50
33	0	2882	DOL	C1-C2	-3.56	1.50	1.55
33	0	2882	DOL	C22-C23	2.56	1.38	1.31
33	0	2882	DOL	C30-C32	2.66	1.61	1.54

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	-16.26	94.37	112.33
33	0	2882	DOL	O40-S39-O41	-8.69	109.95	117.94
33	0	2882	DOL	C28-C26-N25	-8.55	97.30	114.94
33	0	2882	DOL	C23-C22-C20	-4.90	118.48	125.89
33	0	2882	DOL	C16-C17-C19	-3.96	103.99	111.20

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

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

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.