



wwPDB X-ray Structure Validation Summary Report ⓘ

May 12, 2020 – 11:53 pm BST

PDB ID : 2AAR
Title : Structure of trigger factor binding domain in biologically homologous complex with eubacterial ribosome.
Authors : Baram, D.; Pyetan, E.; Sittner, A.; Auerbach-Nevo, T.; Bashan, A.; Yonath, A.
Deposited on : 2005-07-14
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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

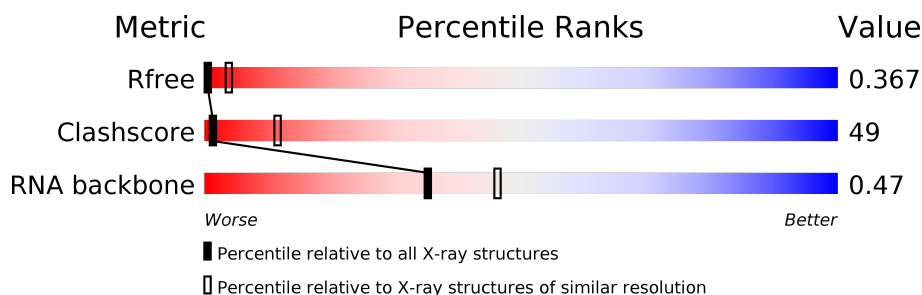
1 Overall quality at a glance

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))
R _{free}	130704	1659 (3.60-3.40)
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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	R	95	
3	W	67	
4	7	113	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 59630 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 L23.

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

- Molecule 3 is a protein called 50S ribosomal protein L29.

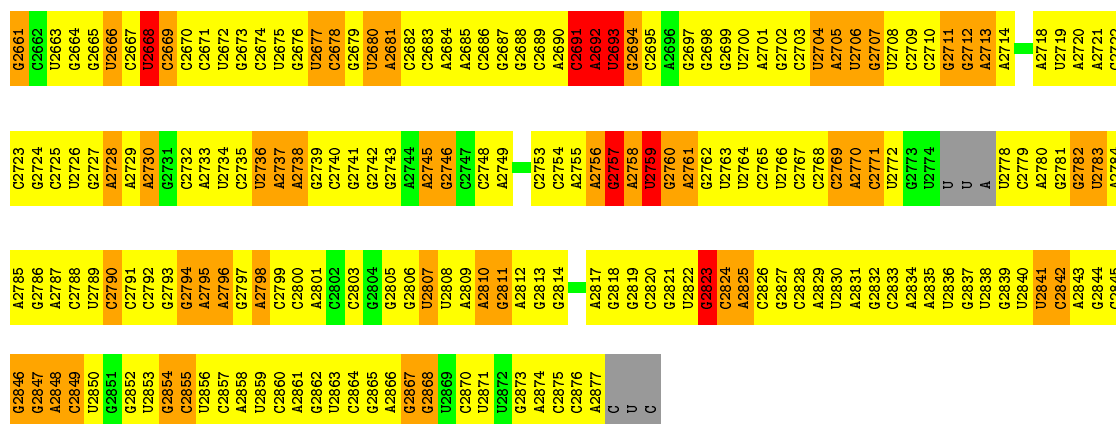
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	W	65	Total	C	0	0	65
			65	65			

- Molecule 4 is a protein called Trigger Factor.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	7	113	Total	C	0	0	113
			113	113			

G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700		A1706	A1707	A1708	A1709	U1710	C1711	C1712	C1713	A1714	A1715	C1716	A1717	A1718	G1719	C1720	G1721	G1722	U1723	C1724	C1725	C1726	C1727	A1728																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615		C1618	A1619	C1620	C1621	A1622	C1623	A1624	G1684	A1685	C1686	C1687	A1688	C1629	A1689	A1690	A1691	A1692	C1693	A1694	A1695	A1696	A1697	A1698		A1706	A1707	A1708	A1709	U1710	C1711	C1712	C1713	A1714	A1715	C1716	A1717	A1718	G1719	C1720	G1721	G1722	U1723	C1724	C1725	C1726	C1727	A1728																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	A1555	A1556	G1557	C1558	G1559	A1560	A1561	G1562	A1563	G1564	G1565	G1566	A1567	A1568	A1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	U1591	U1592	C1593	A1594	A1595	A1596	A1597	C1598	G1599	C1600	C1601	C1602	A1603	A1604																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1483		A1486	C1487	G1488	C1489	U1490	C1491	G1492	G1493	A1494	G1495	G1496	C1497	G1498	A1499	A1500	C1501	G1502	A1503	G1504	G1505	A1506	A1507	G1508	A1509	A1510	C1511	A1512	U1513	C1514	C1515	C1516	C1517	C1518	G1519	G1520	C1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	C1590	U1591	U1592	C1593	A1594	A1595	A1596	A1597	C1598	G1599	C1600	C1601	C1602	A1603	A1604																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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A1299	G1290	G1291	A1292	G1293	U1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	A1303	A1304	A1305	A1306	U1307	G1308	G1309	C1310	C1311	G1312	A1313	A1314	G1315	A1316	G1317	A1318	A1319	G1320	A1321	G1322	G1323	G1324	A1325	G1326	A1327	C1328	U1329	A1330	G1331	G1332	G1333	G1334	A1335	A1336	G1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700		A1706	A1707	A1708	A1709	U1710	C1711	C1712	C1713	A1714	A1715	C1716	A1717	A1718	G1719	C1720	G1721	G1722	U1723	C1724	C1725	C1726	C1727	A1728																																																																																																																																																																																																																								
C864	C865	U866		A807	C808	C870	U871	C880	C893	U894	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C

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G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	U2366	U2367	U2368	U2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	U2377	U2378	U2379	U2380	U2381	G2382	G2383	U2384	U2385	G2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409								
G2283	U2284	U2285	G2286	G2287	A2288	U2289	U2290	U2291	U2292	U2293	U2294	U2295	U2296	U2297	U2298	U2299	G2300	U2301	G2302	U2303	G2304	C2305	U2306	U2307	U2308	U2309	U2310	U2311	U2312	U2313	U2314	U2315	U2316	U2317	U2318	U2319	U2320	U2321	U2322	U2323	U2324	U2325	U2326	U2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348			
G2221	U2222	U2223	U2224	G2225	A2226	U2227	U2228	G2229	U2230	G2231	G2232	U2233	U2234	G2235	U2236	U2237	G2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281								
C2161	C2162	U2163	G2164	A2165	G2166	U2167	U2168	U2169	C2170	U2171	U2172	U2173	U2174	C2175	U2176	U2177	U2178	C2179	U2180	U2181	U2182	C2183	C2184	U2185	U2186	A2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	C2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220									
A	U	A	G2103	G2104	U2105	G2106	G2107	U2108	A2109	G2110	C	C	U	G	C	G	A2117	A2118	A2119	C2120	U2121	G2122	C2123	C2124	C2125	U	U	U	U	U	U	G	G2132	C2133	U2134	C2135	G2136	G2137	U2138	U2139	G2140	A	G	C	A	A	C	G	U	G	A	A	U	A	A	C2157	C2160											
A2040	A2041	A2042	A2043	G2044	A2045	C2046	C2047	C2048	C2049	G2050	U2051	G2052	G2053	A2054	G2055	C2056	U2057	U2058	U2059	A2060	C2061	U2062	A2063	U2064	A2065	C2066	U2067	C2068	U2069	U2070	G2071	C2072	A2073	U2074	U2075	U2076	U2077	G2078	A2079	U2080	U2081	G2082	U2083	C2084	G2085	U2086	U2087	U2088	C2089	U2090	C2091	U2092	G2093	C2094	U2095	U2096	A2097	G	G									
C1979	A1980	A1981	C1982	G1983	U1984	G1985	G1986	G1987	A1988	C1989	U1990	C1991	G1992	G1993	C1994	U1995	A1996	U1997	A1998	U1999	U2000	C2001	A2002	A2003	U2004	U2005	G2006	C2007	C2008	U2009	C2010	G1986	U2011	A2012	U2013	A2014	G2015	A2016	U2017	C2018	G2019	U2020	U2081	G2021	C2022	C2023	U2024	A2025	C2026	C2027	U2030	A2031	G2032	C2033	A2034	G2035	G2036	A2037	C2038	C2039								
G1917	G1918	A1919	A1920	C1921	U1922	U1923	U1924	C1925	U1926	U1927	G1928	U1929	C1930	G1931	G1932	C1933	U1934	G1937	U1938	U1999	U2000	C2001	A2002	A2003	U2004	U2005	G2006	C2007	C2008	U2009	C2010	G1986	U2011	A2012	U2013	A2014	G2015	A2016	U2017	C2018	G2019	U2020	U2081	G2021	C2022	C2023	U2024	A2025	C2026	C2027	U2030	A2031	G2032	C2033	A2034	G2035	G2036	A2037	C2038	C2039								
G1852	G1853	G1854	G1855	U1856	G1857	A1859	A1860	G1861	G1862	U1863	G1864	U1865	G1866	G1867	U1868	A1869	U1870	G1871	A1872	G1873	U1874	U2000	C2001	A2002	A2003	U2004	U2005	G2006	C2007	C2008	U2009	C2010	G1986	U2011	A2012	U2013	A2014	G2015	A2016	U2017	C2018	G2019	U2020	U2081	G2021	C2022	C2023	U2024	A2025	C2026	C2027	U2030	A2031	G2032	C2033	A2034	G2035	G2036	A2037	C2038	C2039							
C1791	C1792	A1793	A1794	C1795	A1796	C1797	U1798	A1799	A1800	C1801	A1802	G1803	G1804	U1805	G1806	A1807	C1808	U1809	A1810	A1811	U1812	U2000	C2001	A2002	A2003	U2004	U2005	G2006	C2007	C2008	U2009	C2010	G1986	U2011	A2012	U2013	A2014	G2015	A2016	U2017	C2018	G2019	U2020	U2081	G2021	C2022	C2023	U2024	A2025	C2026	C2027	U2030	A2031	G2032	C2033	A2034	G2035	G2036	A2037	C2038	C2039							
G1730	C1731	U1732	U1733	C1734	G1735	U1736	U1737	U1738	G1739	C1801	A1802	G1803	C1804	U1805	G1806	A1807	C1808	U1809	A1810	A1811	U1812	U2000	C2001	A2002	A2003	U2004	U2005	G2006	C2007	C2008	U2009	C2010	G1986	U2011	A2012	U2013	A2014	G2015	A2016	U2017	C2018	G2019	U2020	U2081	G2021	C2022	C2023	U2024	A2025	C2026	C2027	U2030	A2031	G2032	C2033	A2034	G2035	G2036	A2037	C2038	C2039							



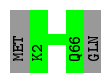
- Molecule 2: 50S ribosomal protein L23

Chain R: 98%



- Molecule 3: 50S ribosomal protein L29

Chain W: 97%



- Molecule 4: Trigger Factor

Chain 7:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.39Å 407.06Å 692.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 19.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-3.50) 100.0 (19.99-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.52Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.320 0.336 , 0.367	Depositor DCC
R_{free} test set	13451 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	98.5	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	59630	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.65	7/66467 (0.0%)	0.84	119/103673 (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	128

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	700	C	N1-C2	10.10	1.50	1.40
1	0	538	A	C5-C6	-5.66	1.35	1.41
1	0	788	G	N9-C4	5.49	1.42	1.38
1	0	2593	A	C5-C6	-5.46	1.36	1.41
1	0	774	A	C5-C6	-5.29	1.36	1.41

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1279	G	N9-C1'-C2'	10.85	128.10	114.00
1	0	1266	G	N9-C1'-C2'	10.62	127.81	114.00
1	0	765	C	O4'-C1'-N1	9.33	115.66	108.20
1	0	2237	C	N1-C1'-C2'	9.28	126.06	114.00
1	0	985	G	N9-C1'-C2'	9.24	126.01	114.00

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	123	A	Sidechain
1	0	154	U	Sidechain
1	0	67	G	Sidechain
1	0	71	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	4315	0
2	R	93	0	0	0	0
3	W	65	0	0	0	0
4	7	113	0	0	0	0
All	All	59630	0	29917	4315	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 49.

The worst 5 of 4315 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)
1:0:541:C:O2'	1:0:2018:G:N2	1.63	1.29
1:0:788:G:H22	1:0:801:A:P	1.58	1.26
1:0:1066:G:H3'	1:0:1067:G:H4'	1.23	1.20
1:0:2170:C:H2'	1:0:2171:U:H5'	1.23	1.17
1:0:1314:A:O2'	1:0:1315:A:H3'	1.42	1.15

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%)	657 (23%)	223 (8%)

5 of 657 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	14	A
1	0	34	U
1	0	45	C
1	0	48	A

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1263	G
1	0	1469	U
1	0	2608	A
1	0	1278	A
1	0	1333	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](#)

There are no ligands in this entry.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.