



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:15 PM GMT

PDB ID : 1NWX
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOC-
CUS RADIODURANS WITH ABT-773
Authors : Schlutzen, F.; Harms, J.; Franceschi, F.; Hansen, H.A.S.; Bartels, H.; Zari-
vach, R.; Yonath, A.
Deposited on : 2003-02-07
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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

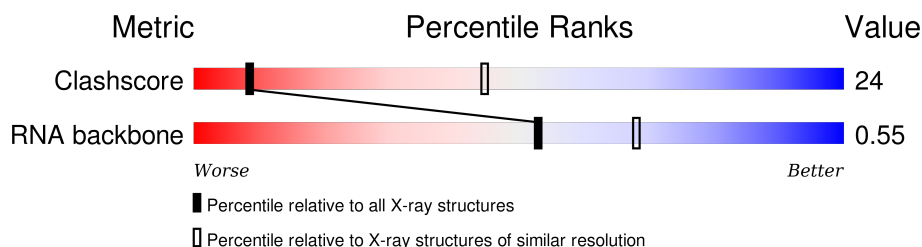
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

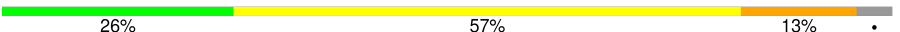
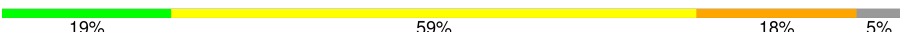
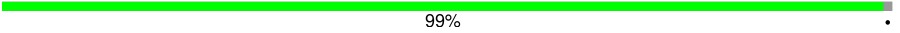
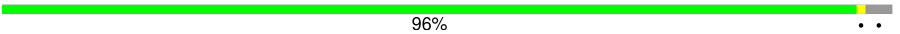
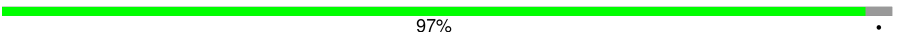
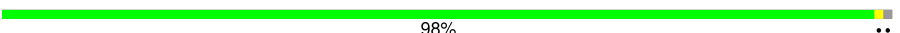


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

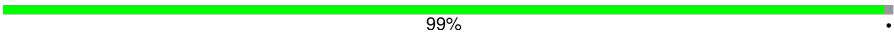

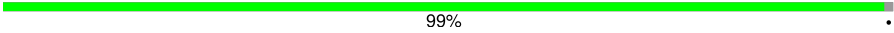


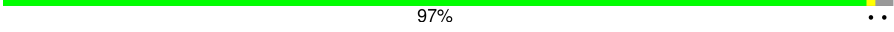
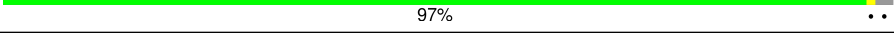

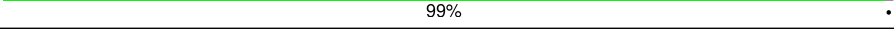
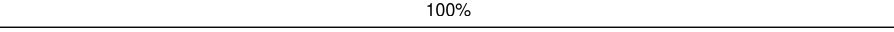
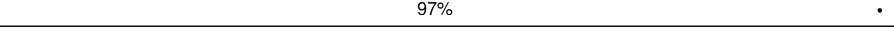
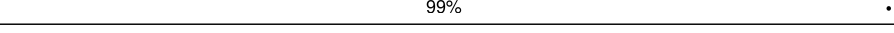
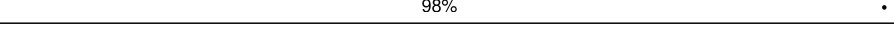
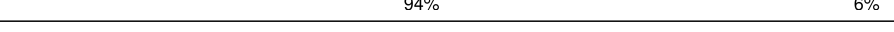
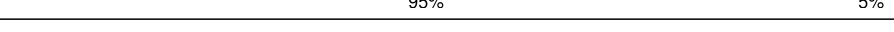
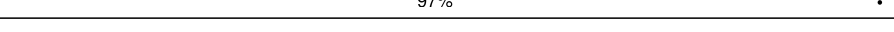
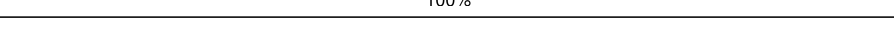
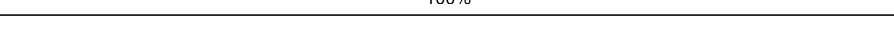
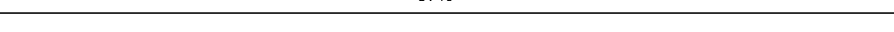
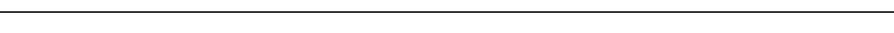


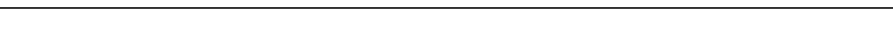
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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	 26% 57% 13% .
2	9	124	 19% 59% 18% 5%
3	A	274	 99% .
4	B	211	 96% . .
5	C	204	 97% .
6	D	180	 98% . .
7	E	185	 95% . .
8	F	146	 34% 64%

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Mol	Chain	Length	Quality of chain
9	G	144	 99% .
10	H	174	 82% 18%
11	I	134	 99% .
12	J	156	 90% 10%
13	K	141	 87% . 12%
14	L	116	 97% ..
15	M	113	 97% ..
16	N	166	 75% . 25%
17	O	118	 99% .
18	P	100	 100%
19	Q	134	 97% .
20	R	94	 99% .
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	 97% ..
28	1	55	 96% .
29	2	47	 98% .
30	3	65	 97% .
31	4	37	 95% 5%

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 65355 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
			2519	1124	464	813	118			

- Molecule 3 is a protein called 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 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 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 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 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 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 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 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 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 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 ribosomal protein L17.

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

- Molecule 15 is a protein called ribosomal protein L18.

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

- Molecule 16 is a protein called ribosomal protein L19.

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

- Molecule 17 is a protein called ribosomal protein L20.

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

- Molecule 18 is a protein called ribosomal protein L21.

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

- Molecule 19 is a protein called ribosomal protein L22.

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

- Molecule 20 is a protein called ribosomal protein L23.

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

- Molecule 21 is a protein called 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 general stress protein Ctc.

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

- Molecule 23 is a protein called 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 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 ribosomal protein L30.

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

- Molecule 26 is a protein called 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 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 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 ribosomal protein L34.

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

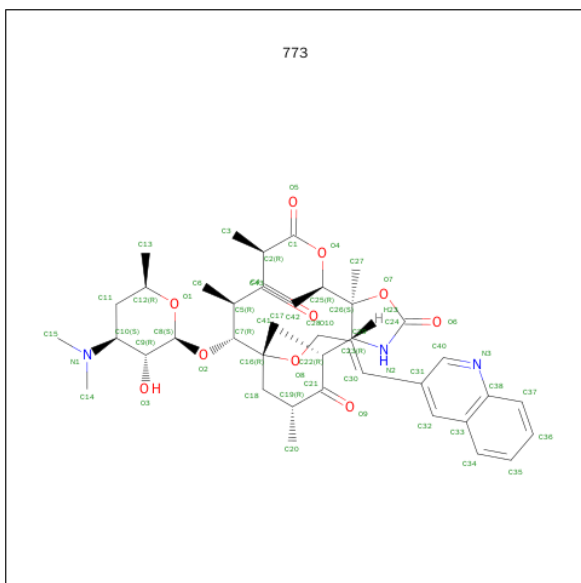
- Molecule 30 is a protein called ribosomal protein L35.

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

- Molecule 31 is a protein called ribosomal protein L36.

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

- Molecule 32 is CETHROMYCIN (three-letter code: 773) (formula: $C_{42}H_{59}N_3O_{10}$).



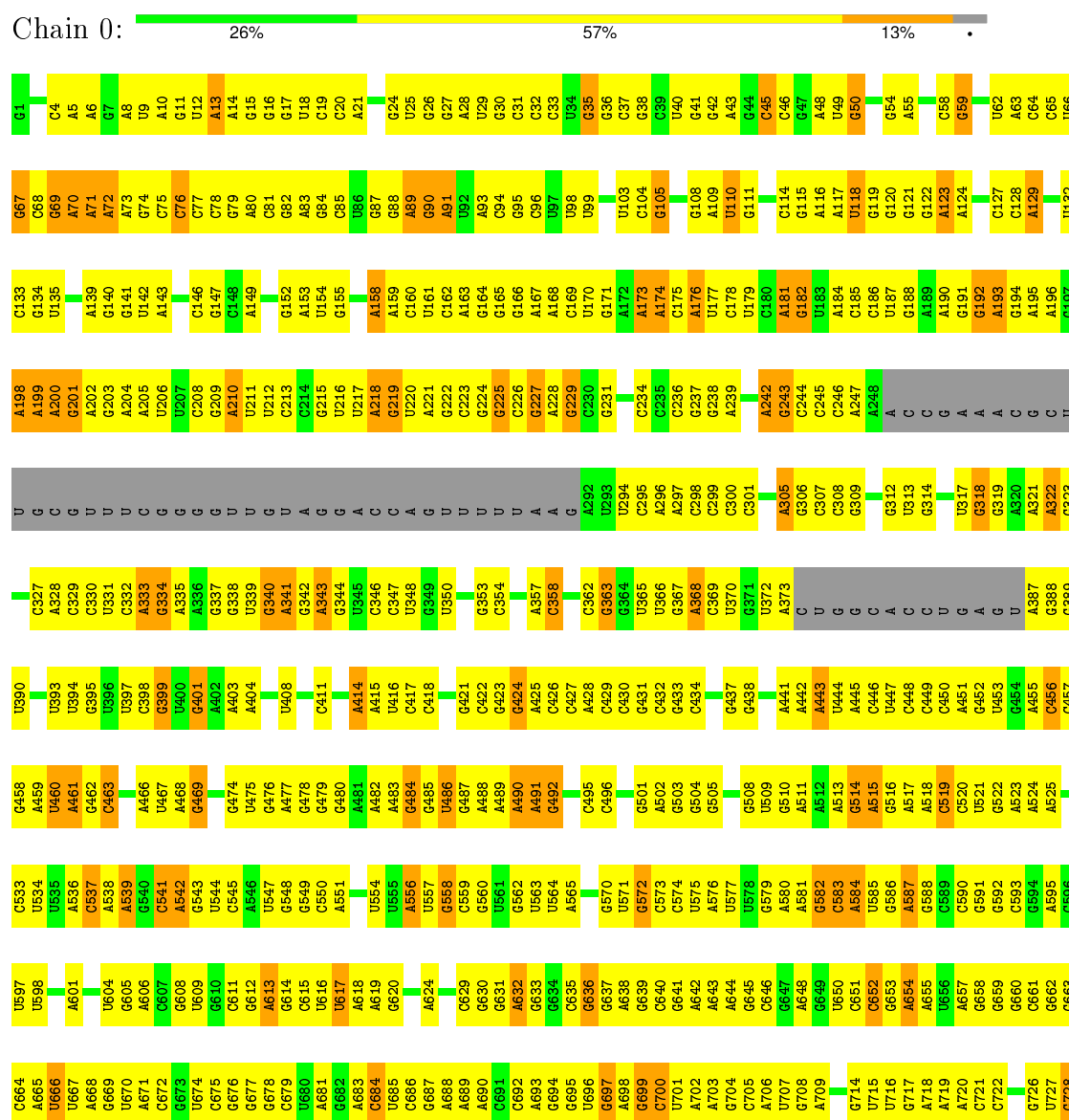
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C N O 55 42 3 10	0	0

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 errors 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.

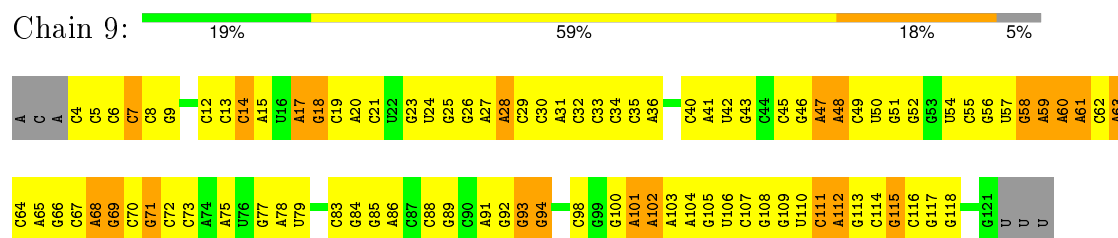
• Molecule 1: 23S RIBOSOMAL RNA



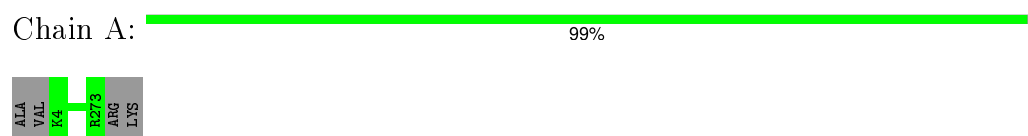
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G1761	C1692	G1622	G1559	G1489	G1427	C1358	A1297	A1233	U1156	C1083	C1003	A936	C865	A795	G733
G1762	A1693	C1623	A1560	C1490	G1428	G1359	G1298	A1234	A1162	C1086	U1005	C937	U866	A796	G734
G1763	C1694	A1624	A1561	C1491	A1429	C1363	U1300	C1235	C1163	C1087	U1006	G938	U867	A797	G735
G1764	C1695	A1625	G1562	A1492	G1430	C1364	U1301	A1238	G1165	A1088	U1007	G939	U868	C799	G736
G1765	C1696	A1626	G1566	A1493	G1431	U1365	C1302	A1238	A1166	C1089	U1008	G940	C869	U800	C737
U1766	U1697	C1627	A1567	G1494	G1432	U1365	U1303	A1238	A1167	C1090	U1009	U941	A801	A801	G738
G1767	C1698	A1630	G1568	G1495	A1433	G1368	U1304	G1241	G1168	C1091	U1010	U942	C803	A740	G739
U1768	U1699	A1631	A1568	G1496	G1436	G1368	U1305	G1242	C1169	U1092	A1011	U943	C804	A741	G740
C1703	C1703	A1632	U1569	U1500	A1437	G1371	U1306	G1243	A1170	A1095	C1016	U944	G805	A742	G741
U1770	G1704	C1633	C1570	C1501	G1438	A1372	U1307	U1244	A1171	A1096	U1017	U945	G806	A743	G742
U1771	U1705	A1634	C1571	G1502	G1439	G1373	C1308	G1245	U1172	A1099	C1017	U946	A807	C744	G743
C1772	A1706	G1635	G1572	G1503	G1440	G1374	G1309	G1246	U1173	A1099	C1018	U947	C808	C745	G744
G1773	C1707	A1636	G1573	G1504	A1441	G1375	C1310	U1247	U1174	A1099	U1019	U948	C809	C746	G745
U1774	C1708	G1638	A1574	U1505	A1442	C1376	C1311	U1248	A1179	A1099	U1019	U949	C810	C746	G746
A1775	U1709	A1639	G1575	U1506	G1443	C1377	C1312	G1249	A1180	A1099	U1020	U950	C811	C746	G746
A1776	U1710	G1641	G1576	U1507	C1444	A1378	U1313	G1250	A1181	A1099	U1021	U951	C812	C746	G746
U1777	C1711	G1642	U1577	A1509	C1445	A1379	A1314	G1251	U1182	C1103	U1022	U952	C813	C746	G746
U1778	G1712	A1643	G1578	A1512	U1446	C1380	A1315	C1252	C1183	C1103	U1023	U953	C814	C746	G746
C1781	G1713	G1644	G1579	U1513	U1447	C1381	A1316	C1253	C1184	G1110	G1024	U954	C815	C746	G746
A1782	A1714	U1645	C1581	C1514	A1448	C1382	G1317	G1254	C1185	C1111	A1025	U955	C816	C746	G746
G1783	A1715	U1646	A1582	U1515	C1449	C1383	A1318	A1255	C1186	U1112	U1026	U956	C817	C746	G746
C1784	G1716	C1648	A1583	A1516	G1450	C1384	C1319	G1256	C1187	C1113	G1027	U957	C818	C746	G746
A1785	A1717	U1651	G1584	C1517	C1451	C1385	A1320	U1257	C1188	C1114	C1028	U958	C819	C746	G746
C1786	U1718	U1652	A1585	C1518	U1452	A1386	A1321	G1258	A1192	C1115	C1029	U959	C820	C746	G746
G1787	G1719	G1653	A1586	G1519	C1453	G1387	G1322	A1259	G1193	C1116	U1030	U960	C821	C746	G746
C1788	C1720	C1654	C1587	G1520	C1454	C1388	G1323	A1260	C1194	C1117	C1031	U961	C822	C746	G746
U1789	A1721	A1654	A1588	C1521	A1455	C1389	G1324	G1261	U1195	C1118	A1032	U962	C823	C746	G746
G1790	C1722	C1655	G1589	G1522	A1456	C1390	U1325	U1262	C1196	C1119	U1033	U963	C824	C746	G746
C1791	U1723	U1656	C1590	U1523	A1457	C1391	U1326	G1263	C1197	C1120	U1034	U964	C825	C746	G746
G1792	C1724	A1657	U1591	G1524	A1458	U1392	U1327	C1264	C1198	C1121	G1035	U965	C826	C746	G746
C1793	C1725	U1658	U1592	G1525	U1459	U1393	G1328	G1265	C1199	C1122	G1036	U966	C827	C746	G746
A1794	C1726	C1661	C1593	C1526	G1460	C1394	U1329	G1266	C1201	C1123	U1037	U967	C828	C746	G746
C1795	G1727	G1662	U1594	U1530	C1461	A1395	G1330	A1267	C1202	C1124	U1038	U968	C829	C746	G746
G1796	A1728	C1663	A1595	C1531	A1462	A1400	U1331	U1268	C1203	C1125	A1039	U969	C830	C746	G746
C1797	C1729	G1664	G1596	A1532	A1463	C1399	G1332	G1269	A1204	C1126	U1040	U970	C831	C746	G746
G1798	U1730	C1665	A1597	G1533	G1465	A1401	A1333	G1270	C1205	C1127	G1041	U971	C832	C746	G746
A1799	G1731	G1666	G1598	C1534	C1466	A1402	U1334	C1271	C1206	C1128	C1042	U972	C833	C746	G746
C1800	C1732	A1667	G1599	C1535	U1467	G1403	G1335	G1272	G1207	C1129	U1043	U973	C834	C746	G746
G1801	C1733	G1668	U1600	G1536	U1468	U1404	G1336	G1273	C1208	C1130	C1043	U974	C835	C746	G746
C1802	G1734	A1669	U1601	U1537	A1469	C1405	U1337	U1274	C1209	C1131	A1044	U975	C836	C746	G746
G1803	U1735	C1670	G1602	A1538	G1470	A1406	U1338	G1275	U1212	C1132	C1044	U976	C837	C746	G746
U1804	C1736	G1671	A1603	U1539	G1471	A1407	G1339	A1278	U1213	C1133	C1045	U977	C838	C746	G746
G1805	G1737	A1672	A1604	C1540	C1472	G1408	C1340	G1279	C1214	C1134	U1046	U978	C839	C746	G746
G1806	G1741	C1673	G1541	G1542	U1473	U1409	U1341	U1280	A1215	C1135	U1047	U979	C840	C746	G746
C1807	G1742	U1674	U1605	G1543	U1474	A1410	U1342	G1281	G1216	C1136	C1048	U980	C841	C746	G746
G1808	C1743	G1675	U1606	A1544	U1475	U1411	C1343	U1282	U1217	C1137	U1049	U981	C842	C746	G746
U1810	G1744	U1676	G1607	A1545	G1476	C1412	C1344	G1283	C1218	C1138	C1049	U982	C843	C746	G746
A1811	U1745	U1677	U1611	C1546	C1477	C1412	C1345	U1284	C1219	C1139	C1050	U983	C844	C746	G746
U1812	U1746	U1680	U1612	U1547	U1478	A1416	C1346	U1285	G1220	C1140	C1051	U984	C845	C746	G746
G1813	G1747	A1681	U1613	U1548	G1479	A1417	C1347	U1286	G1221	C1141	C1052	U985	C846	C746	G746
A1814	A1750	C1682	G1613	U1549	G1480	C1418	U1348	A1287	C1222	G1146	G1053	U986	C847	C746	G746
G1815	G1751	G1683	C1614	U1550	U1481	C1419	G1349	A1288	G1223	G1147	G1054	U987	C848	C746	G746
U1816	U1752	A1684	C1615	U1551	U1482	G1419	U1350	A1289	U1224	C1148	C1055	U988	C849	C746	G746
G1817	A1753	G1685	G1616	C1552	U1483	G1420	G1351	A1290	C1225	G1149	C1056	U989	C850	C746	G746
U1818	G1754	A1686	G1617	G1553	G1484	C1422	G1352	G1291	A1226	C1150	C1057	U990	C851	C746	G746
G1819	U1755	C1687	U1618	G1554	G1485	A1423	G1353	U1292	G1227	U151	C1058	U991	C852	C746	G746
C1820	C1756	U1688	A1619	U1555	U1486	U1424	A1354	A1293	A1228	C1152	U1059	U992	C853	C746	G746
G1820	C1757	U1690	C1620	G1557	C1487	G1425	G1355	U1295	C1229	A1154	A1061	U993	C854	C746	G746



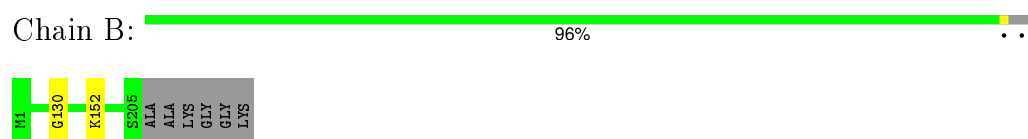
- Molecule 2: 5S RIBOSOMAL RNA



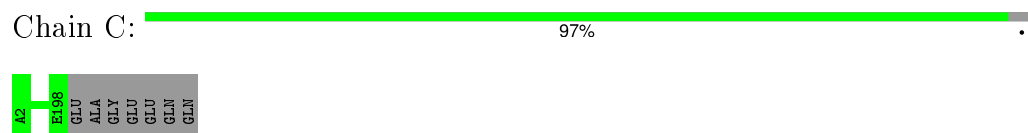
- Molecule 3: ribosomal protein L2



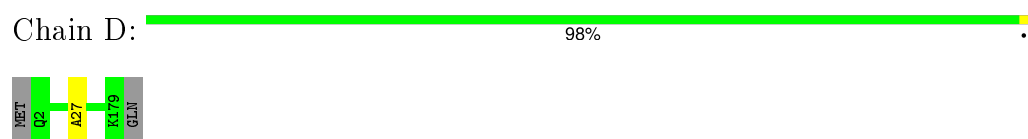
- Molecule 4: ribosomal protein L3



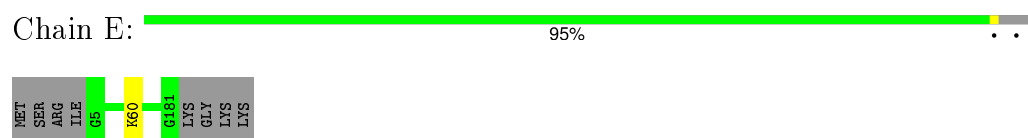
- Molecule 5: ribosomal protein L4



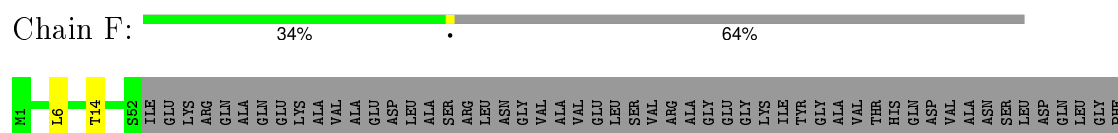
- Molecule 6: ribosomal protein L5



- Molecule 7: ribosomal protein L6



- Molecule 8: ribosomal protein L9




ASP VAL ASP ARG ARG LYS ILE ASP MET PRO LYS THR VAL LYS GLU VAL GLY TYR ASP ILE ALA TYR ARG ALA HIS PRO GLU VAL THR ILE PRO MET LYS LEU VAL VAL HIS ALA ALA LYS

- Molecule 9: ribosomal protein L11

Chain G:  99% .

H1 H43 ALA

- Molecule 10: ribosomal protein L13

Chain H:  82% 18%


MET ALA PHE PRO ASP THR ASP VAL SER PRO ARG GLY GLY PRO SER PRO ALA LYS SER PRO LEU ARG SER PHE LYS V29 L171 GLU VAL LYS

- Molecule 11: ribosomal protein L14

Chain I:  99% .


MET I2 V133 LEU

- Molecule 12: ribosomal protein L15

Chain J:  90% 10%

MET LYS LEU H4 E144 VAL GLN THR GLN ASP ALA GLN LYS ALA GLU

- Molecule 13: ribosomal protein L16

Chain K:  87% 12%

MET LEU LEU PRO LYS ARG T8 R17 K131 MET VAL LYS ARG GLU TYR ASP GLU ALA GLN

- Molecule 14: ribosomal protein L17

Chain L:  97% ..

MET ARG E3 S15 V116

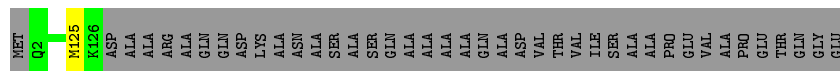
- Molecule 15: ribosomal protein L18

Chain M:  97% ..

ALA THR A4 T50 F114

- Molecule 16: ribosomal protein L19

Chain N:  75% 25%



- Molecule 17: ribosomal protein L20

Chain O:  99%



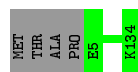
- Molecule 18: ribosomal protein L21

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: ribosomal protein L22

Chain Q:  97%



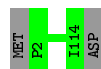
- Molecule 20: ribosomal protein L23

Chain R:  99%



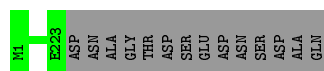
- Molecule 21: ribosomal protein L24

Chain S:  98%



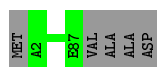
- Molecule 22: general stress protein Ctc

Chain T:  94% 6%



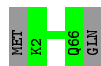
- Molecule 23: ribosomal protein L27

Chain U:  95% 5%



- Molecule 24: ribosomal protein L29

Chain W:  97%



- Molecule 25: ribosomal protein L30

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: ribosomal protein L31

Chain Y:  100%

There are no outlier residues recorded for this chain.

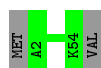
- Molecule 27: ribosomal protein L32

Chain Z:  97%



- Molecule 28: ribosomal protein L33

Chain 1:  96%



- Molecule 29: ribosomal protein L34

Chain 2:  98%



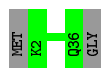
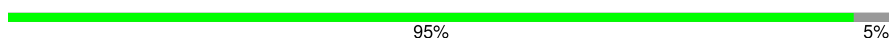
- Molecule 30: ribosomal protein L35

Chain 3:  97%



- Molecule 31: ribosomal protein L36

Chain 4:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	171.00 Å 409.50 Å 695.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.285 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65355	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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: 773

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	0.23	0/66467	0.67	0/103673
2	9	0.59	0/2816	0.81	1/4388 (0.0%)
All	All	0.25	0/69283	0.67	1/108061 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	9	94	G	N9-C1'-C2'	-6.58	104.76	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1342	U	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	2141	0
2	9	2519	0	1285	147	0
3	A	270	0	0	0	0
4	B	205	0	0	2	0
5	C	197	0	0	0	0
6	D	178	0	0	1	0
7	E	177	0	0	1	0
8	F	52	0	0	1	0
9	G	143	0	0	0	0
10	H	143	0	0	0	0
11	I	132	0	0	0	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	1	0
15	M	111	0	0	1	0
16	N	125	0	0	1	0
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	130	0	0	0	0
20	R	93	0	0	0	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
27	Z	58	0	0	1	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	55	0	59	9	0
All	All	65355	0	31261	2286	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 24.

The worst 5 of 2286 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)
1:0:2041:A:N6	32:0:2881:773:H143	1.54	1.19
1:0:2548:G:H2'	1:0:2549:G:H5''	1.21	1.17
1:0:1679:U:H2'	1:0:1680:U:H5''	1.27	1.16
1:0:2041:A:H61	32:0:2881:773:C14	1.58	1.16
1:0:2058:U:H1'	1:0:2576:G:H21	1.11	1.14

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%)	482 (17%)	41 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	505 (17%)	42 (1%)

5 of 505 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1313	U
1	0	1651	U

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Mol	Chain	Res	Type
1	0	2633	A
1	0	1354	A
1	0	1495	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	773	0	2881	-	57,59,59	1.74	11 (19%)	72,88,88	1.36	12 (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	773	0	2881	-	-	0/67/98/98	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	773	C35-C34	-5.26	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	773	C5-C4	-5.09	1.44	1.52
32	0	2881	773	C37-C38	-4.86	1.33	1.41
32	0	2881	773	C22-C21	-2.91	1.47	1.52
32	0	2881	773	C6-C5	-2.49	1.47	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2881	773	C41-C22-C21	-2.28	104.05	108.21
32	0	2881	773	C26-C23-N2	-2.26	96.79	101.59
32	0	2881	773	O8-C16-C7	-2.15	103.28	107.76
32	0	2881	773	C43-C42-C25	2.33	119.58	113.22
32	0	2881	773	C32-C31-C30	2.37	123.53	119.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	773	9	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.