wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 02:13 AM EDT

PDB ID	:	1JZZ
Title	:	Structural Basis for the Interaction of Antibiotics with the Peptidyl Transferase Center in Eubacteria
Authors	:	Schluenzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.; Yonath, A.; Franceschi, F.
Deposited on	:	2001-09-17
Resolution	:	3.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

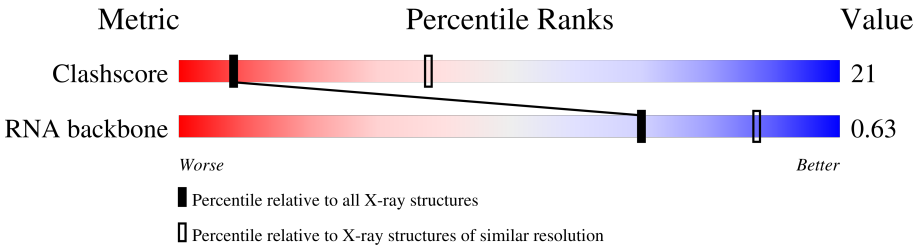
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	30% 48% 18% .
2	K	205	96% .
3	L	134	97% .
4	M	60	97% .

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
5	ROX	A	2881	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 59977 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2774	59532	26556	10982	19221	2773	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1526	U	Y	SEE REMARK 999	GB 15805042

- Molecule 2 is a protein called Ribosomal Protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
2	K	197	197	197	0	0	197

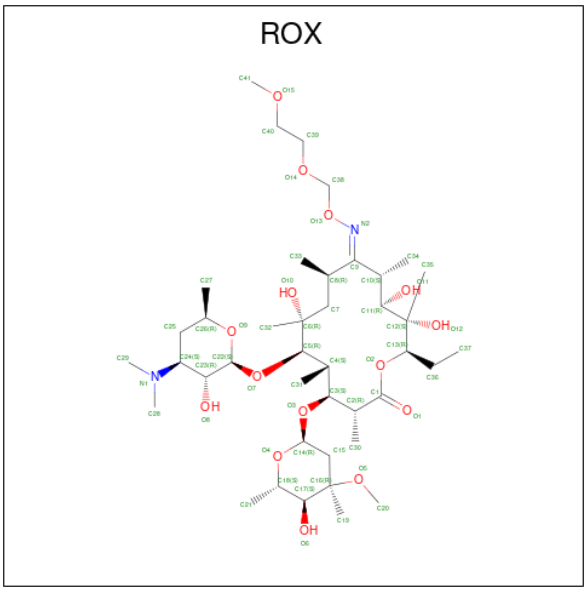
- Molecule 3 is a protein called Ribosomal Protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	L	130	130	130	0	0	130

- Molecule 4 is a protein called Ribosomal Protein L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	M	58	58	58	0	0	58

- Molecule 5 is ROXITHROMYCIN (three-letter code: ROX) (formula: $C_{41}H_{76}N_2O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 58 41 2 15	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0

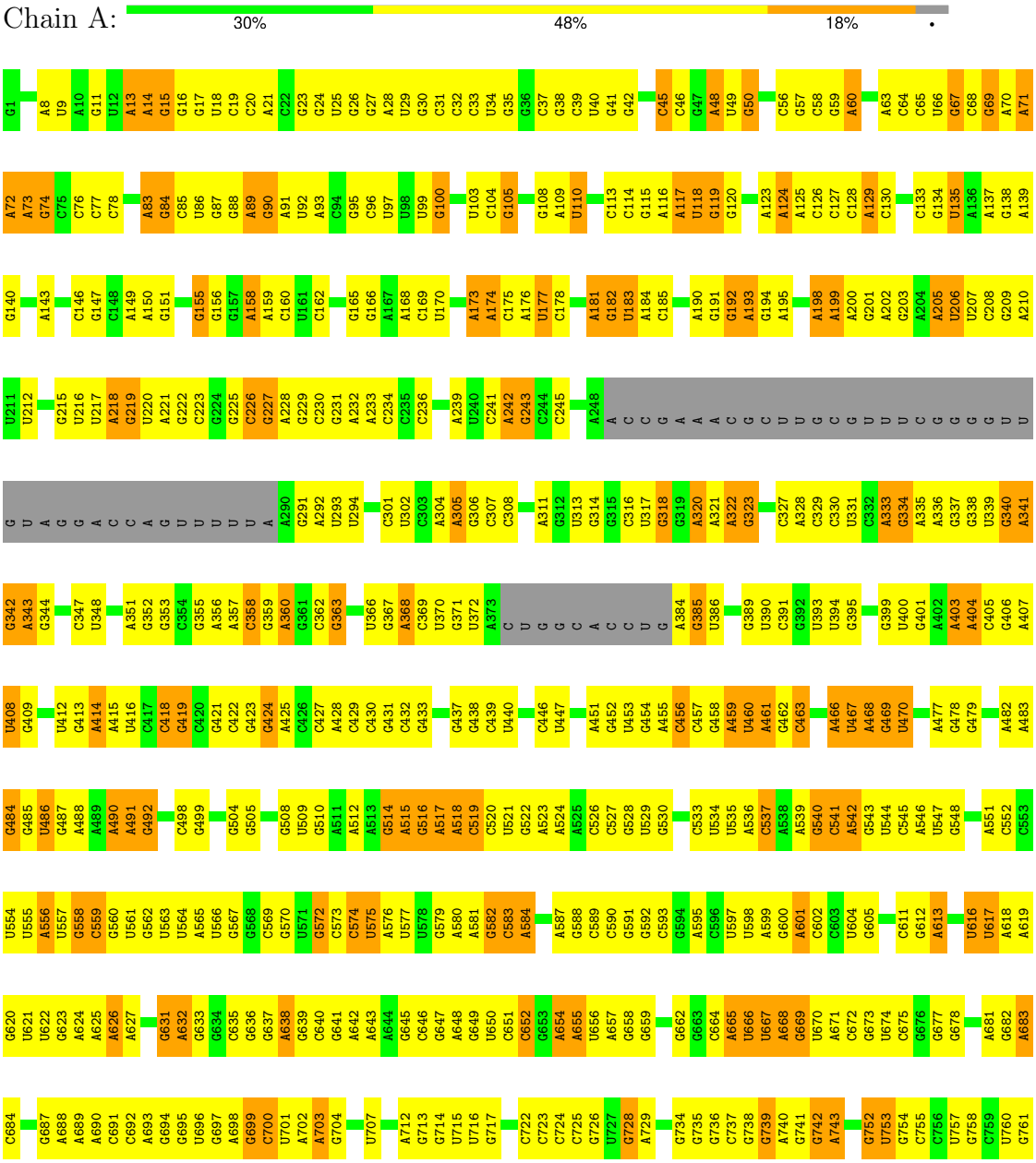
3 Residue-property plots (i)

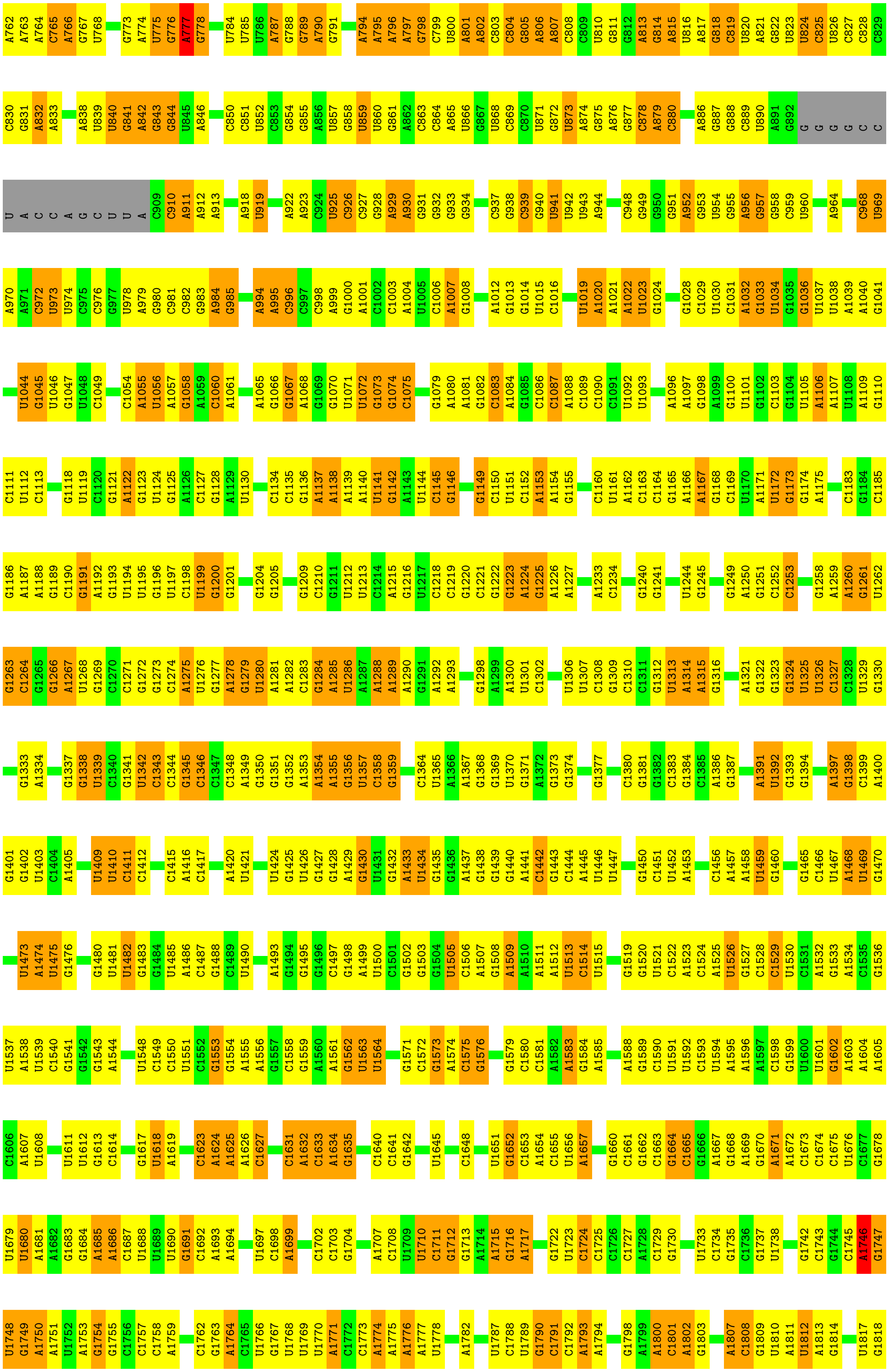
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

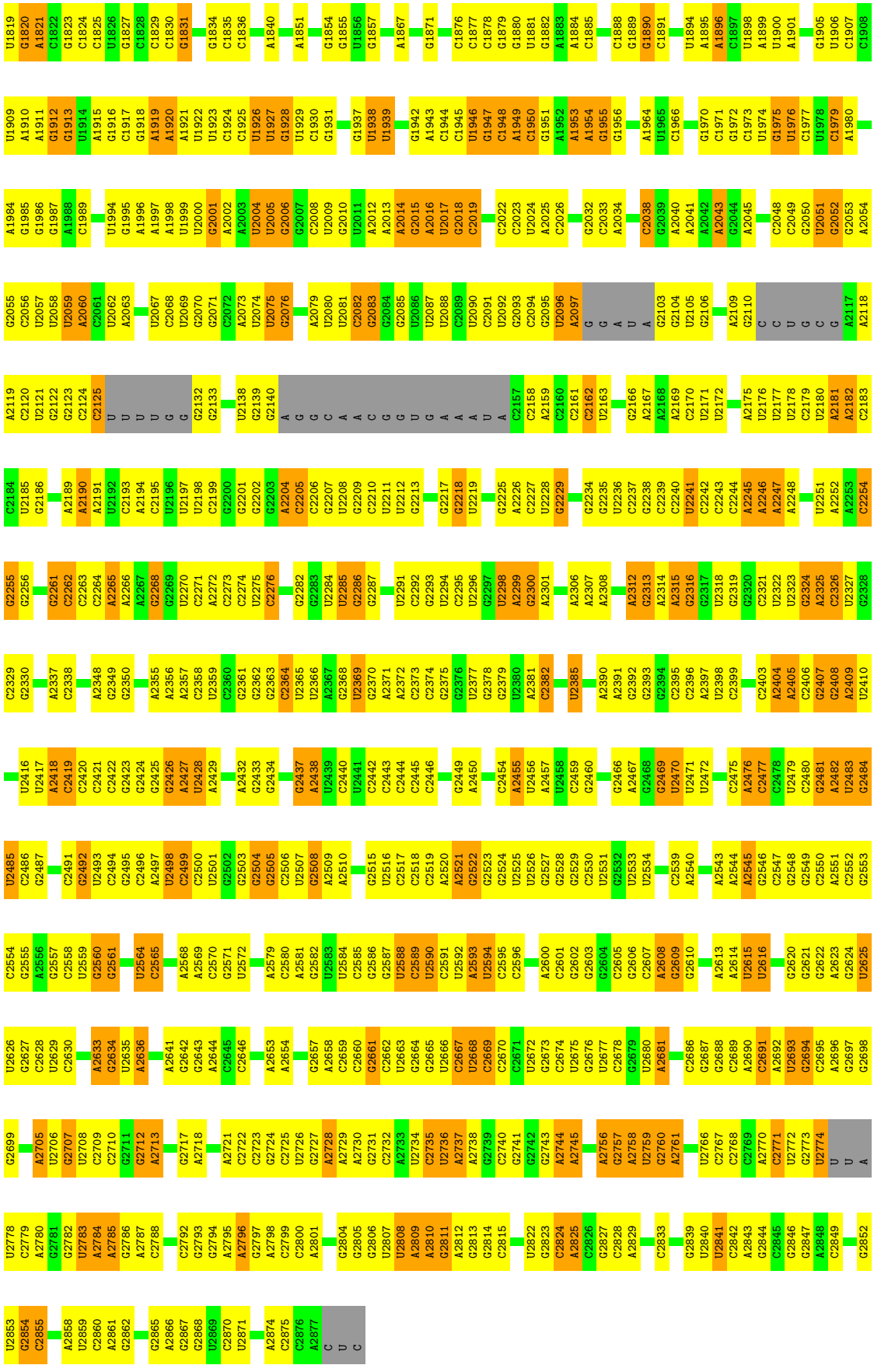
Note EDS was not executed.

- Molecule 1: 23S rRNA

Chain A:

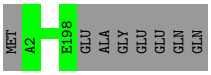



A762 A763 A764 C765 A766 G767 U768 G773 A774 U775 G776 A777 G778 U784 U785 U786 A787 G788 G789 A790 G791 A794 A795 A796 A797 G798 C799 U800 A801 A802 C803 C804 G805 A806 A807 C808 C809 U810 G811 G812 A813 G814 A815 U816 A817 G818 C819 U820 A821 G822 U823 U824 C825 U826 C827 C828 C829
C830 G831 A832 A833 A838 U839 U840 G841 A842 G843 G844 U845 A846 C850 C851 U852 C853 G854 G855 A856 U857 G858 U859 U860 G861 A862 C863 C864 A865 U866 G867 U868 C869 C870 U871 G872 U873 A874 G875 A876 G877 C878 A879 C880 A886 G887 G888 C889 U890 A891 G892 G G G G C C
U A C C A G C U U A C909 C910 A911 A912 A913 A918 U919 A922 A923 C924 U925 C926 C927 G928 A929 A930 G931 G932 G933 G934 C937 G938 C939 G940 U941 U942 U943 A944 C948 G949 G950 G951 A952 G953 U954 G955 A956 G957 G958 C959 U960 A964 C968 U969
A970 A971 C972 U973 U974 C975 C976 G977 U978 A979 G980 C981 C982 G983 A984 G985 A994 A995 C996 C997 C998 A999 G1000 A1001 C1002 C1003 A1004 U1005 C1006 A1007 G1008 A1012 G1013 G1014 U1015 C1016 U1019 A1020 A1021 A1022 U1023 G1024 G1028 C1029 U1030 C1031 A1032 G1033 U1034 G1035 G1036 U1037 U1038 A1039 A1040 G1041
U1044 G1045 U1046 G1047 U1048 C1049 C1054 A1055 U1056 A1057 G1058 A1059 C1060 A1061 A1065 G1066 G1067 A1068 G1069 G1070 U1071 U1072 G1073 G1074 C1075 G1079 A1080 A1081 G1082 C1083 A1084 G1085 C1086 C1087 A1088 C1089 C1090 C1091 U1092 U1093 A1096 A1097 G1098 A1099 G1100 U1101 G1102 C1103 G1104 U1105 A1106 A1107 U1108 A1109 G1110
C1111 U1112 C1113 G1118 U1119 C1120 G1121 A1122 G1123 U1124 G1125 A1126 C1127 G1128 A1129 U1130 C1134 C1135 G1136 A1137 A1138 A1139 A1140 U1141 G1142 A1143 U1144 C1145 G1146 G1149 C1150 U1151 C1152 A1153 A1154 G1155 C1160 U1161 A1162 C1163 C1164 G1165 A1166 A1167 G1168 C1169 U1170 A1171 U1172 G1173 G1174 A1175 C1183 G1184 C1185
G1186 A1187 A1188 G1189 C1190 G1191 A1192 G1193 U1194 U1195 G1196 U1197 C1198 U1199 G1200 G1201 G1204 G1205 G1209 C1210 G1211 U1212 U1213 C1214 A1215 G1216 U1217 C1218 C1219 G1220 C1221 G1222 G1223 A1224 G1225 A1226 A1227 A1233 C1234 G1240 G1241 U1244 G1245 G1249 A1250 G1251 C1252 C1253 G1258 A1259 A1260 G1261 U1262
G1263 C1264 G1265 G1266 A1267 U1268 G1269 C1270 C1271 G1272 G1273 C1274 A1275 U1276 G1277 A1278 G1279 U1280 A1281 A1282 C1283 G1284 A1285 U1286 A1287 A1288 A1289 A1290 G1291 A1292 A1293 G1298 A1299 A1300 U1301 C1302 U1306 U1307 C1308 G1309 C1310 C1311 G1312 U1313 A1314 A1315 G1316 A1321 G1322 G1323 G1324 U1325 U1326 C1327 C1328 U1329 G1330
G1333 A1334 G1337 G1338 U1339 C1340 G1341 U1342 C1343 C1344 G1345 C1346 C1347 C1348 A1349 G1350 G1351 G1352 A1353 A1354 A1355 G1356 U1357 C1358 G1359 C1364 U1365 A1366 A1367 G1368 G1369 U1370 G1371 A1372 G1373 G1374 G1377 C1380 G1381 G1382 C1383 G1384 C1385 A1386 G1387 A1391 U1392 G1393 G1394 A1397 G1398 C1399 A1400
G1401 G1402 U1403 C1404 A1405 U1409 U1410 C1411 C1412 C1415 A1416 C1417 A1420 U1421 U1424 G1425 U1426 G1427 G1428 A1429 G1430 U1431 G1432 A1433 U1434 G1435 G1436 A1437 G1438 G1439 G1440 A1441 C1442 G1443 C1444 A1445 U1446 U1447 G1450 C1451 U1452 A1453 C1456 A1457 A1458 U1459 G1460 G1465 C1466 U1467 A1468 U1469 G1470
U1473 A1474 U1475 G1476 G1480 U1481 U1482 G1483 G1484 U1485 A1486 C1487 G1488 C1489 U1490 A1493 G1494 G1495 G1496 C1497 G1498 A1499 U1500 C1501 G1502 G1503 G1504 U1505 C1506 A1507 G1508 A1509 A1510 A1511 A1512 U1513 C1514 U1515 G1519 G1520 U1521 C1522 A1523 C1524 A1525 U1526 G1527 C1528 C1529 U1530 C1531 A1532 G1533 A1534 C1535 G1536
U1537 A1538 U1539 C1540 G1541 G1542 G1543 A1544 U1548 C1549 C1550 U1551 C1552 G1553 G1554 A1555 A1556 G1557 C1558 G1559 A1560 A1561 G1562 U1563 U1564 G1571 C1572 G1573 A1574 C1575 G1576 G1579 C1580 C1581 A1582 A1583 G1584 A1585 A1588 G1589 C1590 U1591 U1592 C1593 U1594 A1595 A1596 A1597 C1598 G1599 U1600 U1601 G1602 A1603 A1604 A1605
C1606 A1607 U1608 U1611 U1612 G1613 C1614 G1617 U1618 A1619 C1623 A1624 A1625 A1626 C1627 C1631 A1632 C1633 A1634 G1635 C1640 C1641 G1642 U1645 C1648 U1651 G1652 C1653 A1654 C1655 U1656 A1657 G1660 C1661 G1662 C1663 G1664 C1665 G1666 A1667 G1668 A1669 G1670 A1671 A1672 C1673 C1674 C1675 U1676 C1677 G1678
U1679 U1680 A1681 A1682 G1683 G1684 A1685 A1686 C1687 U1688 U1689 U1690 G1691 C1692 A1693 A1694 U1697 C1698 A1699 C1702 C1703 G1704 A1707 C1708 U1709 U1710 C1711 G1712 G1713 A1714 A1715 G1716 A1717 G1722 U1723 C1724 C1725 C1726 C1727 A1728 C1729 G1730 U1733 C1734 G1735 C1736 G1737 U1738 G1742 C1743 G1744 C1745 A1746 G1747
U1748 G1749 A1750 A1751 U1752 A1753 G1754 G1755 C1756 C1757 C1758 A1759 C1762 G1763 A1764 C1765 U1766 G1767 U1768 U1769 U1770 A1771 C1772 C1773 A1774 A1775 A1776 A1777 U1778 A1782 U1787 C1788 U1789 G1790 C1791 C1792 A1793 A1794 G1798 A1799 A1800 C1801 A1802 G1803 A1807 C1808 G1809 U1810 A1811 U1812 A1813 G1814 U1817 G1818



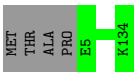
• Molecule 2: Ribosomal Protein L4

Chain K:



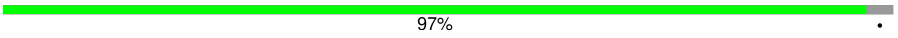
• Molecule 3: Ribosomal Protein L22

Chain L:



• Molecule 4: Ribosomal Protein L32

Chain M:



4 Data and refinement statistics (i)

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	170.40Å 410.70Å 694.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.209 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59977	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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: ROX, MG

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	A	0.23	0/66661	0.66	2/103976 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	777	A	C2'-C3'-O3'	5.48	122.47	113.70
1	A	1746	A	C2'-C3'-O3'	5.31	122.19	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59532	0	30004	1878	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	58	0	76	22	0
6	A	2	0	0	0	0
All	All	59977	0	30080	1896	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 21.

The worst 5 of 1896 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:A:1747:G:H4'	1:A:1749:G:H1'	1.31	1.13
1:A:940:G:H3'	1:A:941:U:H5"	1.35	1.09
1:A:367:G:H2'	1:A:368:A:H5"	1.34	1.08
1:A:1199:U:H3'	1:A:1200:G:H5"	1.35	1.07
5:A:2881:ROX:H211	5:A:2881:ROX:H71	1.36	1.06

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	A	2765/2880 (96%)	557 (20%)	142 (5%)

5 of 557 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	45	C

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2404	A
1	A	2437	G
1	A	2615	U
1	A	929	A
1	A	925	U

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
5	ROX	A	2881	-	60,60,60	1.60	12 (20%)	87,89,89	3.42	48 (55%)

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
5	ROX	A	2881	-	-	12/80/115/115	1/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	ROX	C7-C8	4.91	1.60	1.54
5	A	2881	ROX	C7-C6	3.45	1.60	1.54
5	A	2881	ROX	O2-C13	-3.34	1.40	1.46
5	A	2881	ROX	C35-C12	3.21	1.58	1.52
5	A	2881	ROX	C10-C9	-3.20	1.50	1.53

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2881	ROX	C8-C9-N2	-9.35	119.32	126.21
5	A	2881	ROX	C34-C10-C9	-7.99	101.01	110.58
5	A	2881	ROX	O3-C3-C4	7.39	116.94	108.23
5	A	2881	ROX	C19-C16-C17	6.95	124.86	111.19
5	A	2881	ROX	C33-C8-C7	6.94	122.80	109.88

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C17-C16-O5-C20
5	A	2881	ROX	O4-C14-O3-C3
5	A	2881	ROX	C1-C2-C3-O3
5	A	2881	ROX	O13-C38-O14-C39
5	A	2881	ROX	C6-C7-C8-C33

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C14-C15-C16-C17-C18-O4

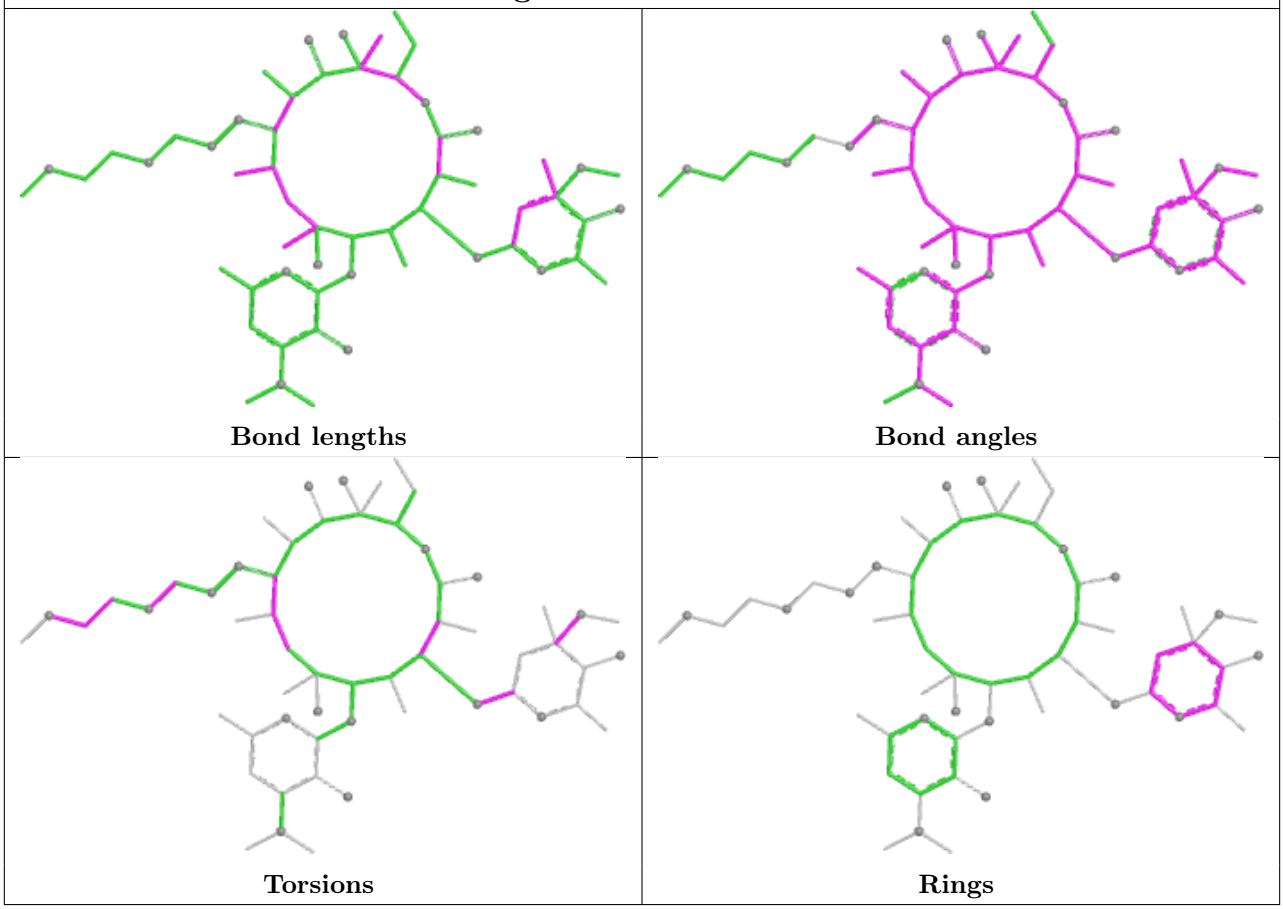
1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	ROX	22	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ROX A 2881



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.