wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 04:37 AM EDT

PDB ID	:	1NJM
Title	:	The crystal structure of the 50S Large ribosomal subunit from Deinococcus radiodurans complexed with a tRNA acceptor stem mimic (ASM) and the antibiotic sparsomycin
Authors	:	Bashan, A.; Agmon, I.; Zarivatch, R.; Schluenzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on	:	2003-01-02
Resolution	:	3.60 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:

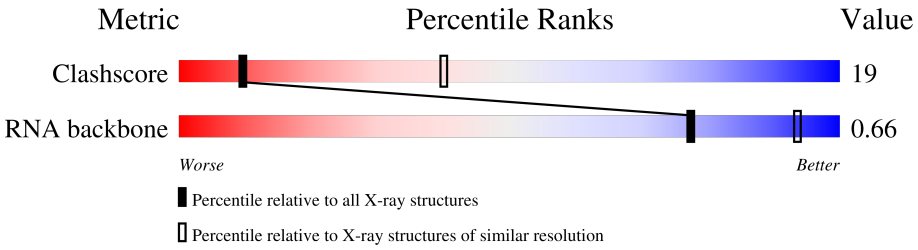
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.60 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	1353 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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	0	2880	33% 51% 11% .
2	5	35	26% 37% 9% 29%
3	K	141	88% 12%
4	T	237	94% 6%

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	SPS	0	2881	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 60271 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
			Total	C	N	O	P			
1	0	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is a RNA chain called tRNA acceptor stem mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	5	25	543	249	97	173	24	0	0	0

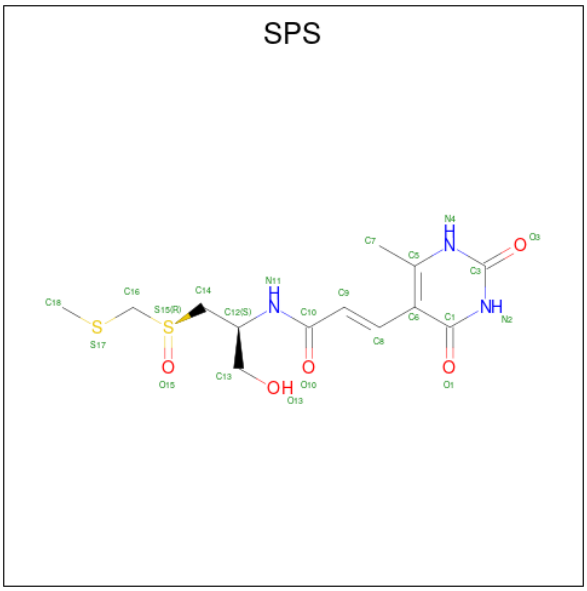
- Molecule 3 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	K	124	124	124	0	0	124

- Molecule 4 is a protein called GENERAL STRESS PROTEIN CTC.

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

- Molecule 5 is SPARSOMYCIN (three-letter code: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	0	1	Total	C	N	O	S	0	0
			22	13	3	4	2		

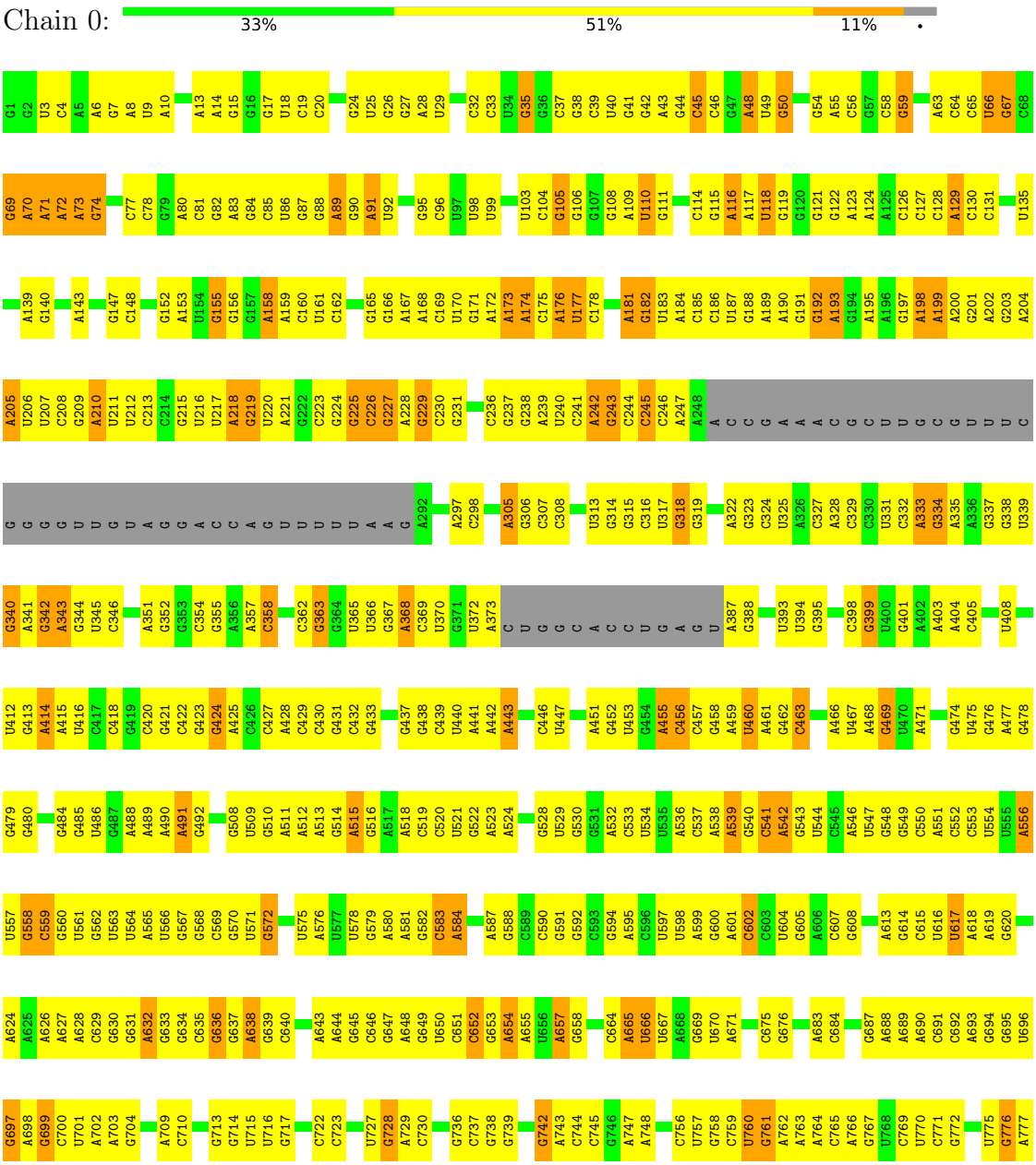
3 Residue-property plots (i)

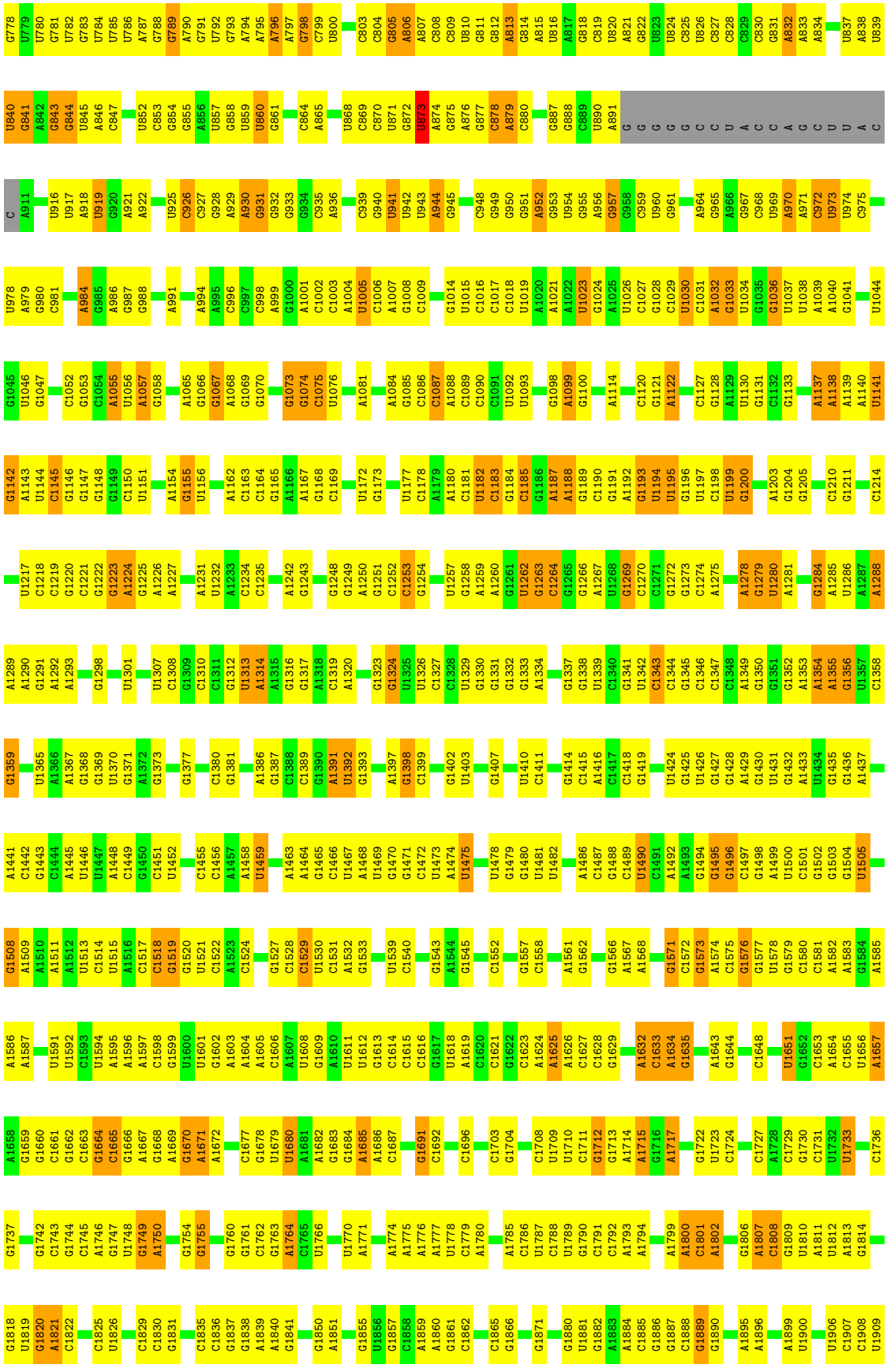
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

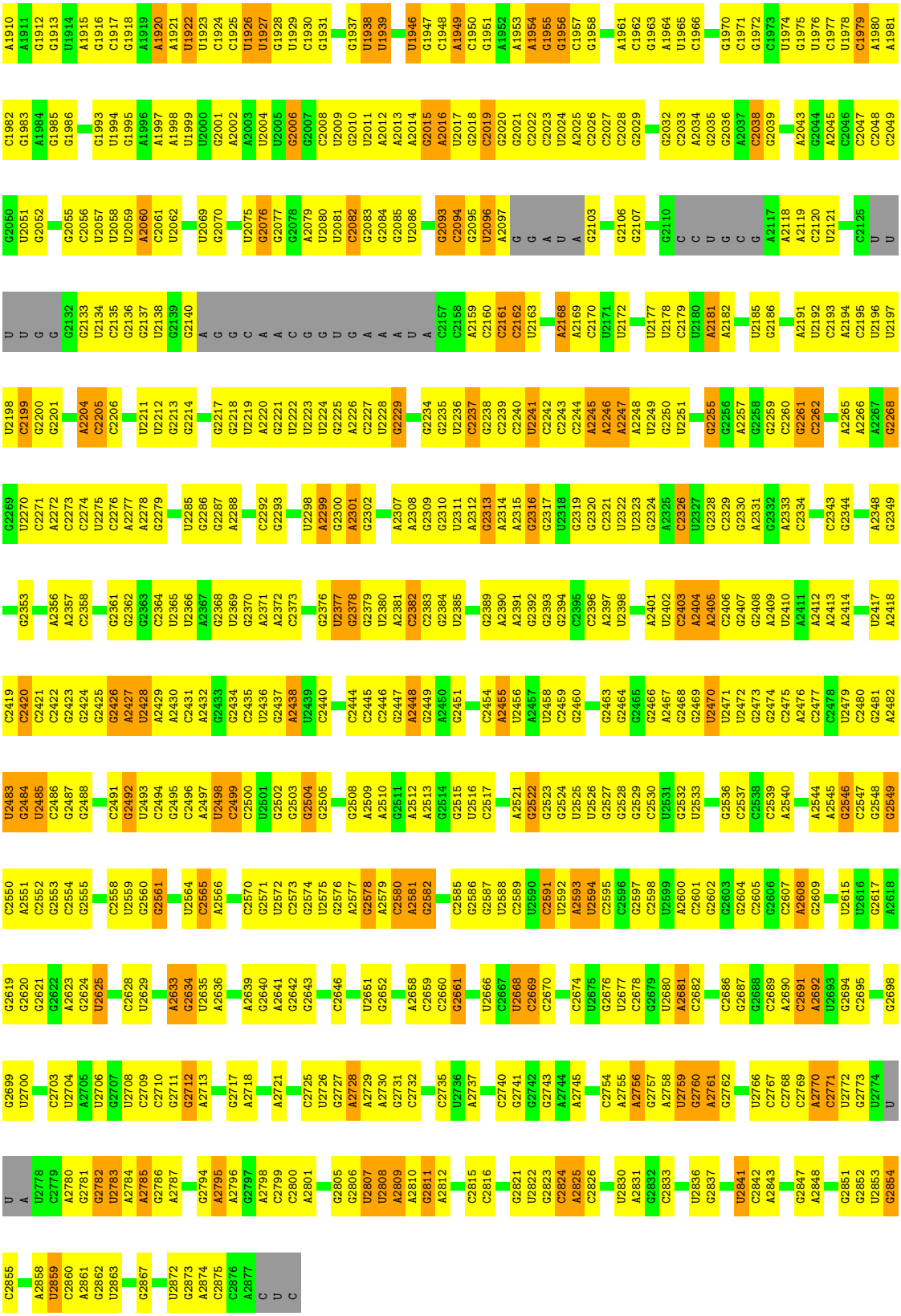
Note EDS was not executed.

- Molecule 1: 23S ribosomal RNA

Chain 0:

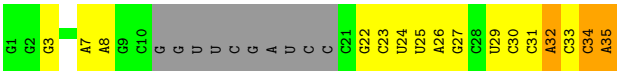



G778 U779 U780 G781 U782 G783 U784 U785 U786 A787 G788 G789 A790 G791 U792 G793 A794 A795 A796 A797 G798 C799 U800 C803 C804 G805 A806 A807 C808 C809 U810 G811 G812 A813 G814 A815 U816 A817 G818 C819 U820 A821 G822 U823 U824 C825 U826 C827 C828 C829 C830 G831 A832 A833 A834 U837 A838 U839
U840 G841 A842 G843 G844 U845 A846 C847 U852 C853 G854 G855 A856 U857 G858 U859 U860 G861 C864 A865 U868 C869 C870 U871 G872 U873 A874 G875 A876 G877 C878 A879 C880 G887 G888 C889 U890 A891 G C G G G C C U A C C A G C C U U A C
C A911 U916 U917 A918 U919 G920 A921 A922 U925 C926 C927 G928 A929 A930 G931 G932 G933 G934 C935 A936 C939 G940 U941 U942 U943 A944 G945 C948 G949 G950 G951 A952 G953 U954 G955 A956 G957 G958 C959 U960 G961 A964 G965 A966 G967 C968 U969 A970 A971 C972 U973 U974 C975
U978 A979 G980 C981 A984 G985 A986 G987 G988 A991 A994 A995 C996 G997 C998 A999 G1000 A1001 C1002 C1003 A1004 U1005 C1006 A1007 G1008 C1009 G1014 U1015 C1016 C1017 C1018 U1019 A1020 A1021 A1022 U1023 G1024 A1025 U1026 C1027 G1028 U1029 U1030 C1031 A1032 G1033 U1034 G1035 G1036 U1037 U1038 A1039 A1040 G1041 U1044
G1045 U1046 G1047 C1052 G1053 C1054 A1055 U1056 A1057 G1058 A1065 G1066 G1067 A1068 G1069 G1070 G1073 G1074 C1075 U1076 A1081 A1084 G1085 C1086 C1087 A1088 C1089 C1090 C1091 U1092 U1093 G1098 A1099 G1100 A1114 C1120 G1121 A1122 C1127 G1128 A1129 U1130 G1131 G1132 G1133 A1137 A1138 A1139 A1140 U1141
G1142 A1143 U1144 C1145 G1146 G1147 G1148 G1149 C1150 U1151 A1154 G1155 U1156 A1162 C1163 C1164 G1165 A1166 A1167 G1168 C1169 U1172 G1173 U1177 C1178 A1179 A1180 C1181 U1182 C1183 G1184 C1185 G1186 A1187 A1188 G1189 C1190 G1191 A1192 G1193 U1194 U1195 G1196 U1197 C1198 U1199 G1200 A1203 G1204 G1205 C1210 G1211 C1214
U1217 C1218 C1219 G1220 C1221 G1222 G1223 A1224 G1225 A1226 A1227 A1231 U1232 A1233 C1234 C1235 A1242 G1243 G1248 G1249 A1250 G1251 C1252 C1253 G1254 U1257 G1258 A1259 A1260 G1261 U1262 G1263 C1264 G1265 G1266 A1267 U1268 G1269 C1270 C1271 G1272 G1273 C1274 A1275 A1278 G1279 U1280 A1281 G1284 A1285 U1286 A1287 A1288
A1289 A1290 G1291 A1292 A1293 G1298 U1301 U1307 C1308 G1309 C1310 C1311 G1312 U1313 A1314 A1315 G1316 G1317 A1318 C1319 A1320 G1323 G1324 U1325 U1326 C1327 C1328 U1329 G1330 G1331 G1332 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 U1365 A1366 A1367 G1368 G1369 U1370 G1371 A1372 G1373 G1377 C1380 G1381 A1386 G1387 C1388 C1389 G1390 A1391 U1392 G1393 A1397 G1398 C1399 G1402 U1403 G1407 U1410 C1411 G1414 C1415 A1416 C1417 C1418 G1419 U1424 G1425 U1426 G1427 G1428 A1429 G1430 U1431 G1432 A1433 U1434 G1435 G1436 A1437
A1441 C1442 G1443 C1444 A1445 U1446 U1447 A1448 C1449 G1450 C1451 U1452 C1455 C1456 A1457 A1458 U1459 A1463 A1464 G1465 C1466 U1467 A1468 U1469 G1470 G1471 C1472 U1473 A1474 U1475 U1478 G1479 G1480 U1481 U1482 A1486 C1487 G1488 C1489 U1490 C1491 A1492 A1493 G1494 G1495 G1496 C1497 G1498 A1499 U1500 C1501 G1502 G1503 G1504 U1505
G1508 A1509 A1510 A1511 A1512 U1513 C1514 U1515 A1516 C1517 C1518 G1519 G1520 U1521 C1522 A1523 C1524 G1527 C1528 C1529 U1530 C1531 U1532 G1533 U1539 C1540 G1543 A1544 G1545 C1552 C1557 C1558 A1561 G1562 G1566 A1567 A1568 G1571 C1572 G1573 A1574 C1575 G1576 G1577 U1578 G1579 C1580 C1581 A1582 A1583 G1584 A1585
A1586 A1587 U1591 U1592 C1593 U1594 A1595 A1596 A1597 C1598 G1599 U1600 U1601 G1602 A1603 A1604 A1605 C1606 A1607 U1608 G1609 A1610 U1611 U1612 G1613 C1614 C1615 C1616 G1617 U1618 A1619 C1620 C1621 G1622 C1623 A1624 A1625 A1626 C1627 C1628 G1629 A1632 C1633 A1634 G1635 A1643 G1644 C1648 U1651 G1652 C1653 A1654 C1655 U1656 A1657
A1658 G1659 G1660 C1661 G1662 C1663 G1664 C1665 G1666 A1667 G1668 A1669 G1670 A1671 A1672 C1677 G1678 U1679 U1680 A1681 A1682 G1683 G1684 A1685 A1686 A1687 G1691 C1692 C1696 C1703 G1704 C1708 U1709 U1710 C1711 G1712 G1713 A1714 A1715 G1716 A1717 G1722 U1723 C1724 C1727 A1728 C1729 G1730 C1731 U1732 U1733 C1736
G1737 G1742 C1743 G1744 C1745 A1746 A1747 U1748 G1749 A1750 G1754 G1755 G1760 G1761 C1762 G1763 A1764 C1765 U1766 U1770 A1771 A1774 A1775 A1776 A1777 U1778 C1779 A1780 A1785 C1786 U1787 C1788 U1789 G1790 C1791 C1792 A1793 A1794 A1799 A1800 C1801 A1802 G1806 A1807 C1808 G1809 U1810 A1811 U1812 A1813 G1814
G1818 U1819 G1820 A1821 C1822 C1825 U1826 C1829 C1830 G1831 C1835 C1836 G1837 G1838 A1839 A1840 G1841 G1850 A1851 G1855 U1856 G1857 C1858 A1859 A1860 G1861 C1862 C1865 G1866 G1871 G1880 U1881 G1882 A1883 A1884 C1885 G1886 G1887 C1888 G1889 G1890 A1895 A1896 A1899 U1900 U1906 C1907 C1908 U1909



• Molecule 2: tRNA acceptor stem mimic

Chain 5:

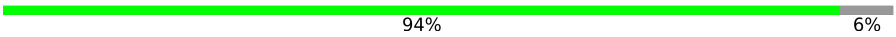


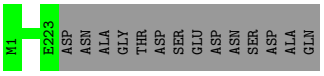
• Molecule 3: 50S ribosomal protein L16

Chain K:

• Molecule 4: GENERAL STRESS PROTEIN CTC

Chain T:





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	169.60Å 409.40Å 695.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.284 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	60271	wwPDB-VP
Average B, all atoms (Å^2)	74.0	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: SPS, PPU

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	0.14	0/66467	0.63	0/103673
2	5	0.16	0/563	0.63	0/873
All	All	0.14	0/67030	0.63	0/104546

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	873	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59359	0	29917	1742	0
2	5	543	0	290	16	0
3	K	124	0	0	0	0
4	T	223	0	0	0	0
5	0	22	0	19	0	0
All	All	60271	0	30226	1754	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 19.

The worst 5 of 1754 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)
1:0:940:G:H3'	1:0:941:U:H5"	1.22	1.14
1:0:1141:U:H3	1:0:2008:C:H5"	1.20	1.05
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.00
1:0:2548:G:H2'	1:0:2549:G:H5"	1.44	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.22	0.98

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%)	416 (15%)	44 (1%)
2	5	22/35 (62%)	2 (9%)	0
All	All	2779/2915 (95%)	418 (15%)	44 (1%)

5 of 418 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1807	A
1	0	2245	A
1	0	1820	G
1	0	2093	G
1	0	2377	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
2	PPU	5	35	2,1	32,40,41	2.81	6 (18%)	33,57,60	0.98	3 (9%)

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
2	PPU	5	35	2,1	-	0/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	C-N3'	12.63	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.96	1.27	1.42
2	5	35	PPU	C6-N1	3.86	1.38	1.33
2	5	35	PPU	CE1-CZ	3.70	1.46	1.38
2	5	35	PPU	CE2-CZ	2.70	1.44	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	35	PPU	CM-OC-CZ	2.93	123.86	117.51
2	5	35	PPU	C9-N6-C6	2.23	126.26	119.51
2	5	35	PPU	C-CA-N	2.22	117.97	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	35	PPU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
5	SPS	0	2881	-	19,22,23	4.43	9 (47%)	17,28,30	4.15	8 (47%)

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	SPS	0	2881	-	1/1/2/6	9/15/16/18	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	0	2881	SPS	O10-C10	9.82	1.43	1.24
5	0	2881	SPS	C9-C8	8.40	1.54	1.33
5	0	2881	SPS	O1-C1	7.67	1.43	1.24
5	0	2881	SPS	C10-N11	6.56	1.50	1.34
5	0	2881	SPS	C5-N4	5.43	1.42	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	0	2881	SPS	C12-N11-C10	-7.47	112.03	122.57
5	0	2881	SPS	C3-N2-C1	6.40	120.55	115.14
5	0	2881	SPS	C8-C9-C10	-6.14	109.55	121.56
5	0	2881	SPS	C14-S15-C16	6.14	109.42	101.04
5	0	2881	SPS	O10-C10-C9	-5.96	109.44	123.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	0	2881	SPS	C12

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	0	2881	SPS	C1-C6-C8-C9
5	0	2881	SPS	C9-C10-N11-C12
5	0	2881	SPS	O10-C10-N11-C12
5	0	2881	SPS	C14-C12-C13-O13
5	0	2881	SPS	N11-C12-C13-O13

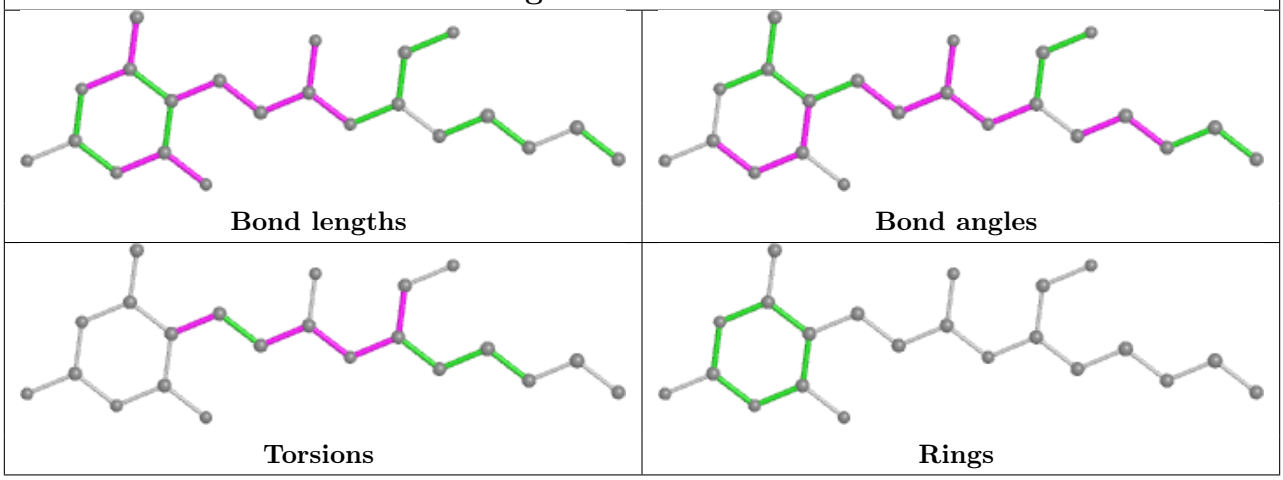
There are no ring outliers.

No monomer is involved in short contacts.

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 SPS 0 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.