wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 08:14 am BST

PDB ID	:	2OGM
Title	:	The crystal structure of the large ribosomal subunit from Deinococcus radiodurans complexed with the pleuromutilin derivative SB-571519
Authors	:	Davidovich, C.; Bashan, A.; Auerbach-Nevo, T.; Yonath, A.
Deposited on	:	2007-01-07
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

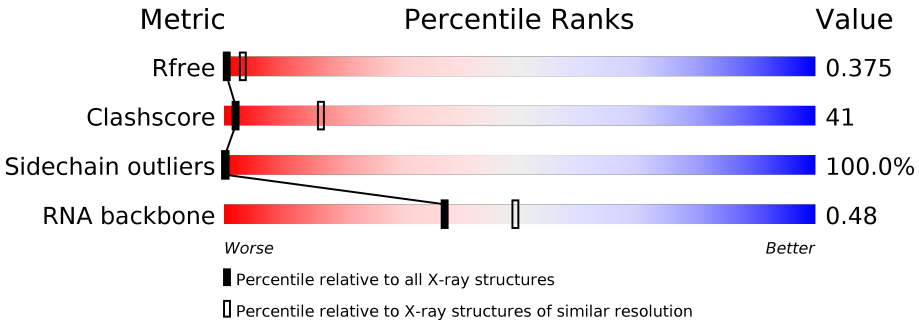
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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)
Sidechain outliers	138945	1006 (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 <=5%

Mol	Chain	Length	Quality of chain
1	0	2880	18% 55% 20%
2	B	211	95%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 59610 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.

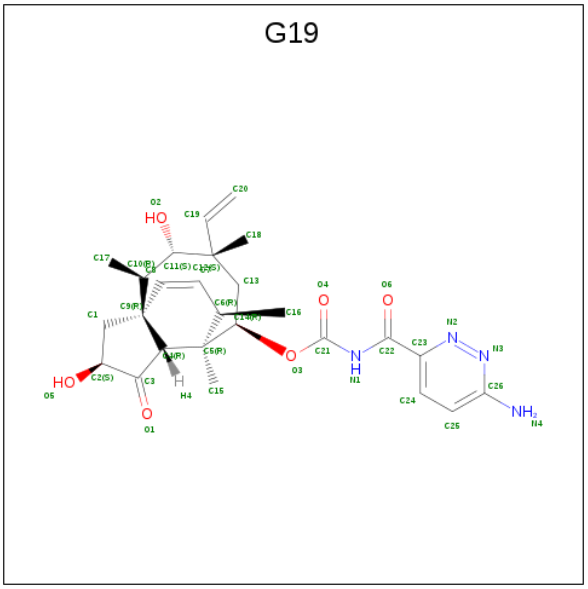
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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 protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	205	215	210	4	1	0	0	204

- Molecule 3 is (2S,3AR,4R,5S,6S,8R,9R,9AR,10R)-2,5-DIHYDROXY-4,6,9,10-TETRAMETHYL-1-OXO-6-VINYLDECAHYDRO-3A,9-PROP[1]ENOCYCLOPENTA[8]ANNULEN-8-YL [(6-AMINOPYRIDAZIN-3-YL)CARBONYL]CARBAMATE (three-letter code: G19) (formula: $C_{26}H_{34}N_4O_6$).



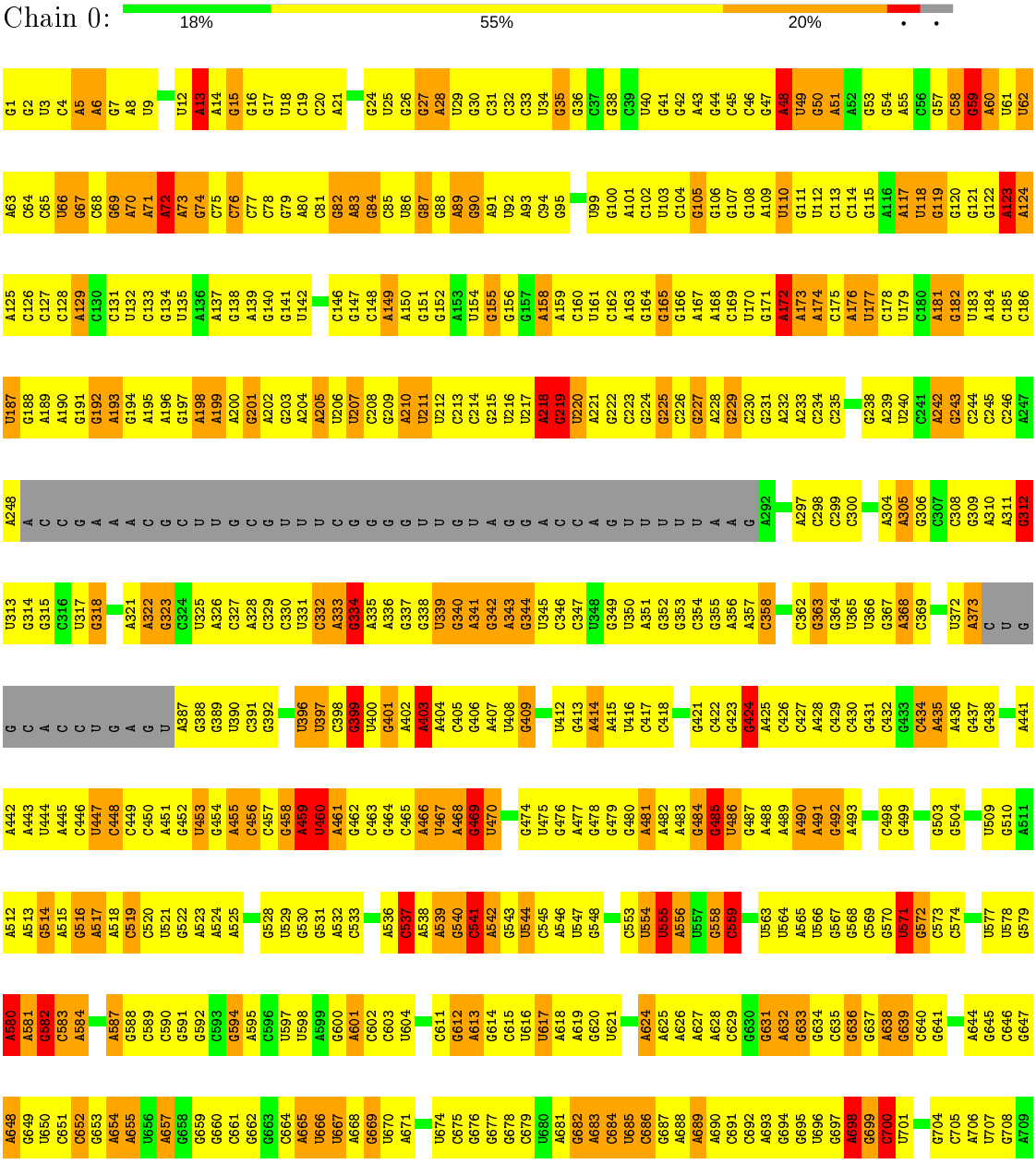
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	0	1	36	26	4	6	0	0

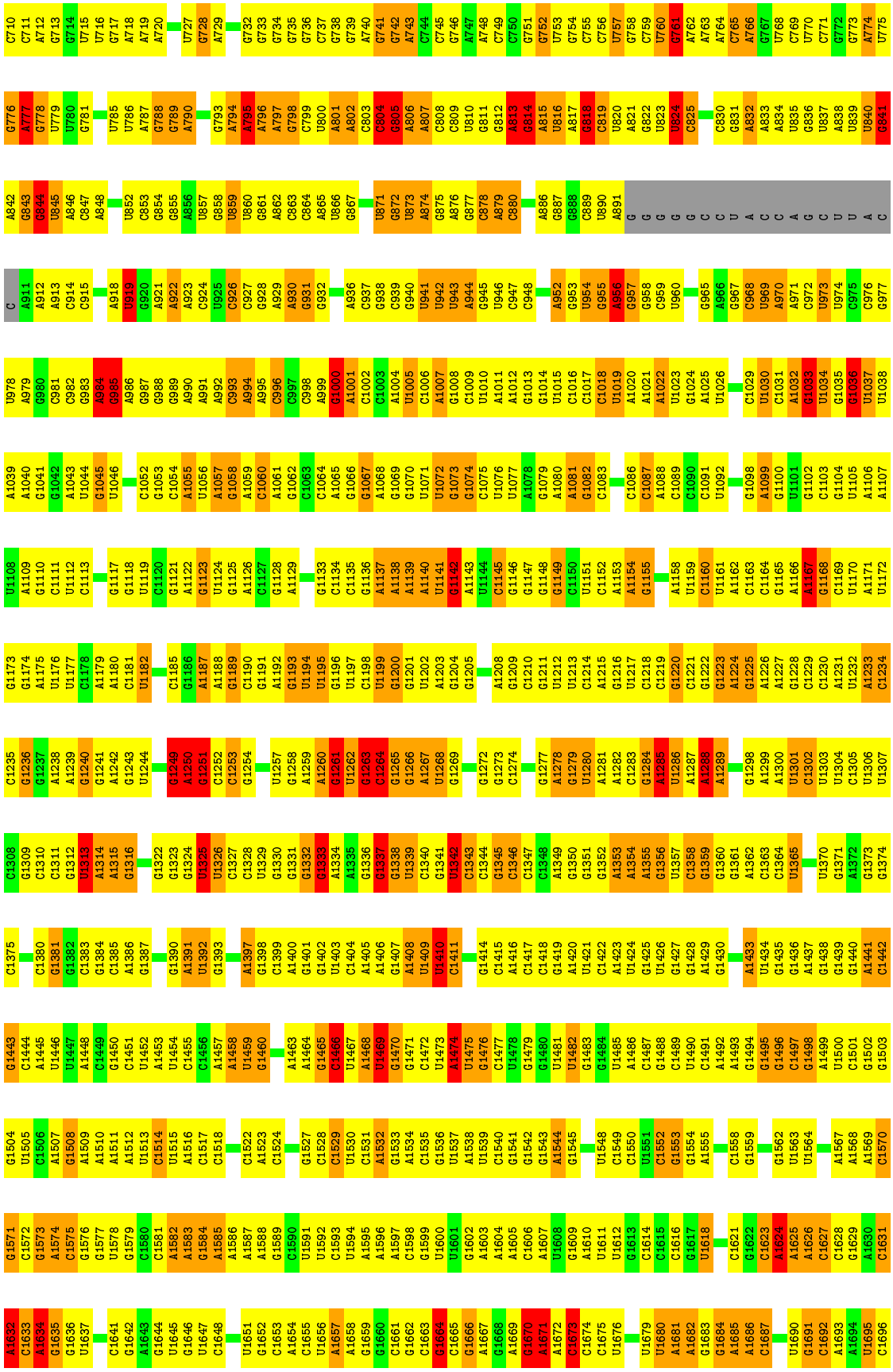
3 Residue-property plots (i)

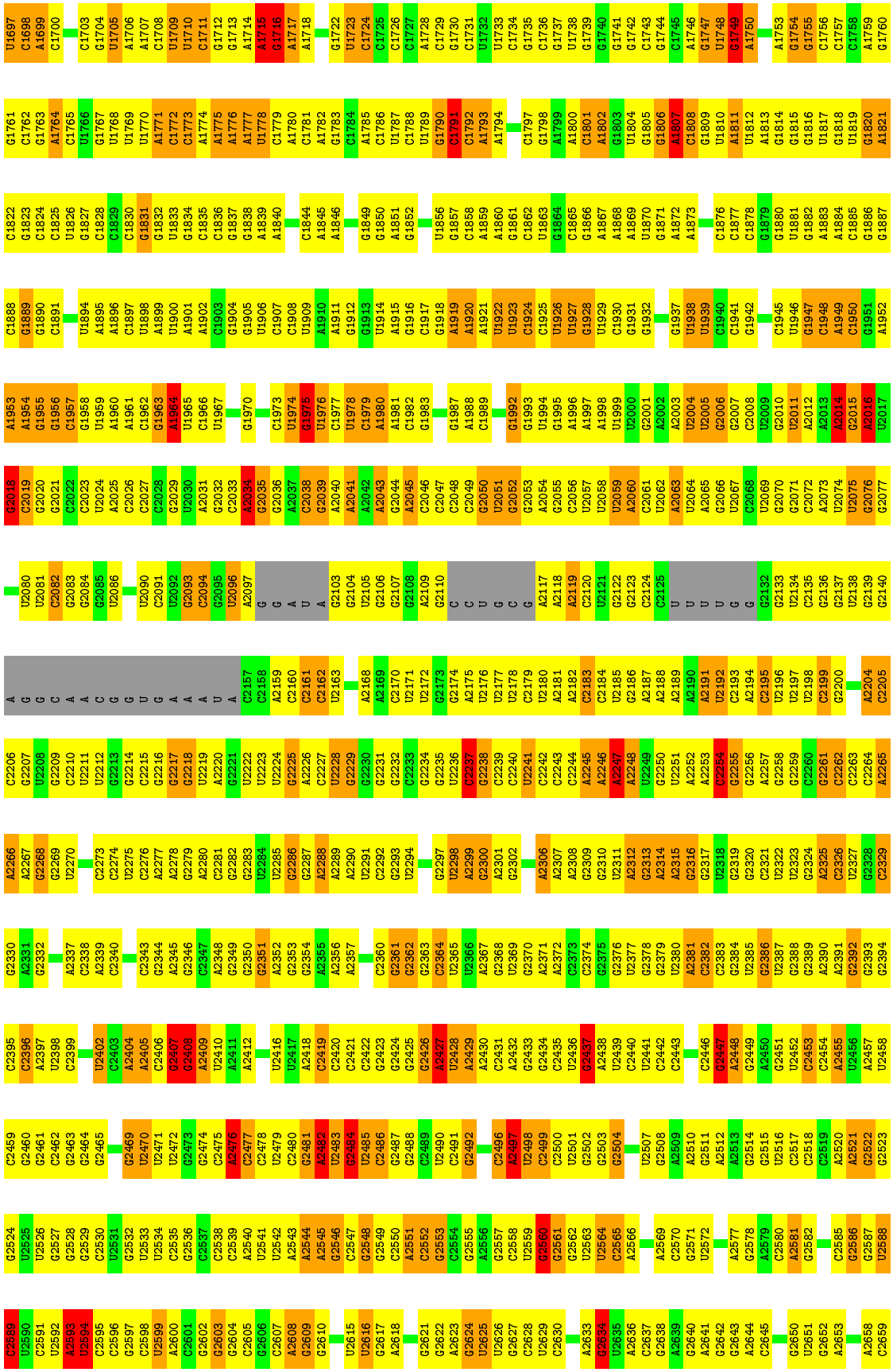
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

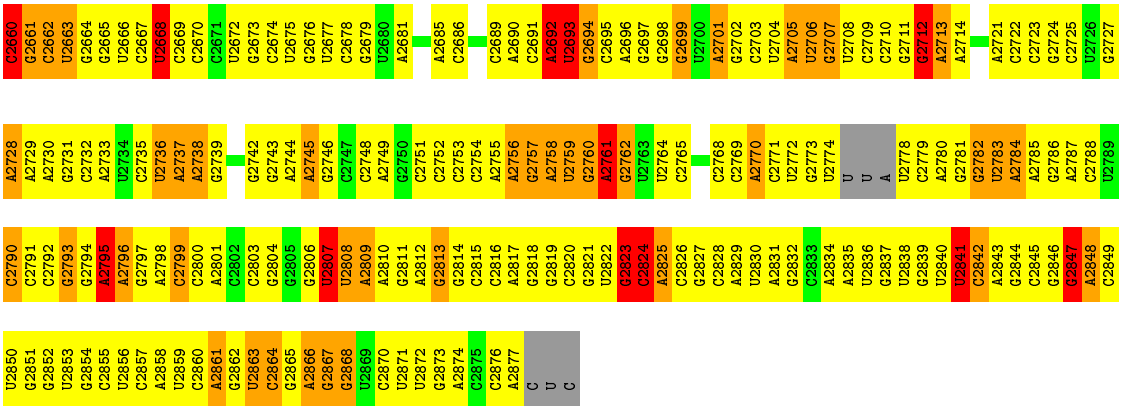
- Molecule 1: 23S ribosomal RNA

Chain 0:



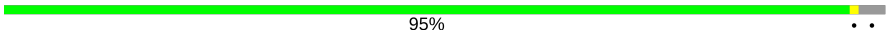

C710 C711 A712 G713 G714 U715 U716 G717 A718 A719 A720 U727 G728 A729 G732 G733 G734 G735 G736 C737 G738 G739 A740 G741 G742 A743 C744 C745 G746 A747 A748 C749 C750 G751 G752 U753 G754 C755 C756 U757 G758 C759 U760 G761 A762 A763 A764 C765 A766 G767 U768 C769 U770 C771 G772 G773 A774 U775
G776 A777 G778 U779 U780 G781 U785 U786 A787 G788 G789 A790 G793 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 C830 G831 A832 A833 A834 U835 G836 U837 A838 U839 U840 G841
A842 G843 G844 U845 A846 C847 A848 U852 C853 G854 G855 A856 U857 G858 U859 U860 G861 A862 C863 C864 A865 U866 G867 U871 G872 U873 A874 G875 A876 G877 C878 A879 C880 A886 G887 G888 C889 U890 A891 G A952 G953 U954 G955 A956 G957 G958 C959 U960 G965 A966 G967 G968 U969 A970 A971 G972 U973 U974 C975 C976 G977
C A911 A912 A913 C914 C915 A918 U919 G920 A921 A922 A923 C924 U925 C926 C927 G928 A929 A930 G931 G932 A936 C937 G938 C939 G940 U941 U942 U943 A944 G945 U946 C947 C948 U978 A979 G980 C981 C982 C983 A984 G985 A986 G987 G988 G989 A990 A991 A992 C993 A994 A995 C996 G997 C998 A999 G1000 A1001 C1002 C1003 A1004 U1005 C1006 A1007 G1008 C1009 U1010 A1011 A1012 G1013 G1014 U1015 C1016 C1017 C1018 U1019 A1020 A1021 A1022 U1023 G1024 A1025 U1026 C1029 U1030 C1031 A1032 G1033 U1034 G1035 G1036 U1037 U1038
A1039 A1040 G1041 G1042 A1043 U1044 G1045 U1046 C1052 G1053 C1054 A1055 U1056 A1057 G1058 A1059 C1060 A1061 G1062 C1063 C1064 A1065 G1066 G1067 A1068 G1069 G1070 U1071 U1072 G1073 G1074 C1075 U1076 U1077 A1078 G1079 A1080 A1081 G1082 C1083 C1086 C1087 A1088 C1089 C1090 C1091 U1092 G1098 A1099 G1100 U1101 G1102 C1103 G1104 U1105 A1106 A1107
U1108 A1109 C1110 C1111 U1112 C1113 G1117 G1118 U1119 C1120 G1121 A1122 G1123 U1124 G1125 A1126 C1127 G1128 A1129 G1133 C1134 A1135 G1136 A1137 A1138 A1139 A1140 U1141 G1142 A1143 U1144 C1145 G1146 G1147 G1148 G1149 C1150 U1151 C1152 A1153 A1154 G1155 A1158 U1159 C1160 U1161 A1162 C1163 C1164 G1165 A1166 A1167 G1168 C1169 U1170 A1171 U1172
G1173 G1174 A1175 U1176 U1177 C1178 A1179 A1180 C1181 U1182 C1185 G1186 A1187 A1188 G1189 C1190 G1191 A1192 G1193 U1194 U1195 G1196 U1197 C1198 U1199 G1200 G1201 U1202 A1203 G1204 G1205 A1208 G1209 C1210 G1211 U1212 U1213 C1214 A1215 G1216 U1217 C1218 C1219 G1220 C1221 G1222 G1223 A1224 G1225 A1226 A1227 G1228 C1229 C1230 A1231 U1232 A1233 C1234
C1235 G1236 G1237 A1238 A1239 G1240 G1241 A1242 G1243 U1244 G1249 A1250 G1251 C1252 C1253 G1254 U1257 G1258 A1259 A1260 G1261 U1262 G1263 C1264 G1265 G1266 A1267 U1268 G1269 G1272 G1273 C1274 G1277 A1278 G1279 U1280 A1281 A1282 C1283 G1284 A1285 U1286 A1287 A1288 A1289 G1298 A1299 A1300 U1301 C1302 U1303 U1304 C1305 U1306 U1307
C1308 G1309 C1310 C1311 G1312 U1313 A1314 A1315 G1316 G1322 G1323 G1324 U1325 U1326 C1327 C1328 U1329 G1330 G1331 G1332 G1333 A1334 A1335 G1336 G1337 G1338 U1339 C1340 G1341 U1342 C1343 C1344 G1345 C1346 C1347 C1348 A1349 G1350 G1351 G1352 A1353 A1354 A1355 G1356 U1357 C1358 G1359 G1360 G1361 A1362 C1363 C1364 U1365 U1370 G1371 A1372 G1373 G1374
C1375 C1380 G1381 G1382 C1383 G1384 C1385 A1386 G1387 G1390 A1391 U1392 G1393 A1397 G1398 C1399 A1400 G1401 G1402 U1403 C1404 A1405 A1406 G1407 A1408 U1409 U1410 C1411 G1414 C1415 A1416 C1417 C1418 G1419 A1420 U1421 C1422 A1423 A1424 G1425 U1426 G1427 G1428 A1429 G1430 A1433 U1434 G1435 C1436 A1437 G1438 G1439 G1440 A1441 C1442
G1443 C1444 A1445 U1446 U1447 A1448 C1449 G1450 C1451 U1452 A1453 U1454 C1455 C1456 A1457 A1458 U1459 G1460 A1463 A1464 G1465 C1466 U1467 A1468 U1469 G1470 G1471 C1472 U1473 A1474 U1475 G1476 C1477 U1478 G1479 G1480 U1481 U1482 G1483 G1484 U1485 A1486 A1487 G1488 C1489 U1490 C1491 A1492 A1493 G1494 G1495 G1496 C1497 G1498 A1499 U1500 C1501 G1502 G1503
G1504 U1505 C1506 A1507 G1508 A1509 A1510 A1511 A1512 U1513 C1514 U1515 A1516 C1517 C1518 C1522 A1523 C1524 G1527 C1528 C1529 U1530 C1531 A1532 G1533 A1534 C1535 G1536 U1537 A1538 U1539 C1540 G1541 G1542 G1543 A1544 G1545 U1548 C1549 C1550 U1551 C1552 G1553 G1554 A1555 C1558 G1559 G1562 U1563 U1564 A1567 A1568 A1569 C1570
G1571 C1572 G1573 A1574 C1575 G1576 G1577 U1578 G1579 C1580 C1581 A1582 A1583 G1584 A1585 A1586 A1587 A1588 G1589 C1590 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 C1621 G1622 C1623 A1624 A1625 A1626 C1627 C1628 G1629 A1630 C1631
A1632 C1633 A1634 G1635 G1636 U1637 C1641 G1642 A1643 G1644 U1645 G1646 U1647 C1648 U1651 C1652 C1653 A1654 C1655 U1656 A1657 A1658 G1659 G1660 C1661 G1662 C1663 G1664 C1665 G1666 A1667 G1668 A1669 G1670 A1671 A1672 C1673 C1674 C1675 U1676 U1679 U1680 A1681 A1682 G1683 G1684 A1685 A1686 C1687 U1690 G1691 C1692 A1693 A1694 U1695 C1696

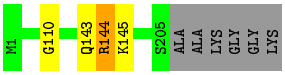




- Molecule 2: 50S ribosomal protein L3

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	170.40Å 405.83Å 703.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 3.50 29.92 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.93-3.50) 92.8 (29.92-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.334 0.356 , 0.375	Depositor DCC
R_{free} test set	14021 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	86.3	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 81.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	59610	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: G19

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	0.61	6/66467 (0.0%)	0.82	100/103673 (0.1%)
2	B	0.11	0/10	0.42	0/11
All	All	0.61	6/66477 (0.0%)	0.82	100/103684 (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	121

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	700	C	N1-C2	9.14	1.49	1.40
1	0	788	G	N9-C4	7.37	1.43	1.38
1	0	1664	G	N9-C4	-5.84	1.33	1.38
1	0	1681	A	C5-C6	-5.47	1.36	1.41
1	0	2799	C	N1-C2	-5.33	1.34	1.40

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	985	G	N9-C1'-C2'	11.62	129.11	114.00
1	0	460	U	N1-C1'-C2'	10.14	127.18	114.00
1	0	1264	C	N1-C1'-C2'	10.06	127.08	114.00
1	0	788	G	N9-C1'-C2'	10.03	127.04	114.00
1	0	984	A	N9-C1'-C2'	9.21	125.98	114.00

There are no chirality outliers.

5 of 121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	13	A	Sidechain
1	0	15	G	Sidechain
1	0	48	A	Sidechain
1	0	67	G	Sidechain
1	0	82	G	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	3642	0
2	B	215	0	12	5	0
3	0	36	0	34	2	0
All	All	59610	0	29963	3646	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 41.

The worst 5 of 3646 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)
1:0:1280:U:C5	1:0:1995:G:C2	2.04	1.44
1:0:1440:G:H3'	1:0:1441:A:C5'	1.66	1.25
1:0:699:G:N2	1:0:801:A:H2	1.40	1.18
1:0:1440:G:C3'	1:0:1441:A:H5"	1.75	1.16
1:0:2205:C:O2'	1:0:2206:C:H5'	1.42	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	1/157 (1%)	0	1 (100%)	0 0

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	144	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	618 (22%)	184 (6%)

5 of 618 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	5	A
1	0	6	A
1	0	13	A
1	0	28	A
1	0	35	G

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1263	G
1	0	1474	A
1	0	2594	U
1	0	1265	G
1	0	1325	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 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	$\#\|Z\| > 2$
3	G19	0	2881	-	35,39,39	4.35	15 (42%)	47,62,62	2.69	21 (44%)

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
3	G19	0	2881	-	-	0/15/79/79	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	2881	G19	C7-C8	17.53	1.58	1.32
3	0	2881	G19	C12-C11	9.50	1.64	1.55
3	0	2881	G19	C5-C14	9.04	1.63	1.56
3	0	2881	G19	C10-C11	7.83	1.63	1.56
3	0	2881	G19	O3-C21	5.69	1.45	1.35

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2881	G19	C18-C12-C11	8.97	113.29	108.06
3	0	2881	G19	O3-C21-N1	6.18	117.46	108.02
3	0	2881	G19	O3-C21-O4	-5.34	116.49	124.53
3	0	2881	G19	C6-C7-C8	-4.70	115.16	125.22
3	0	2881	G19	C9-C10-C11	4.68	116.85	112.56

There are no chirality outliers.

There are no torsion outliers.

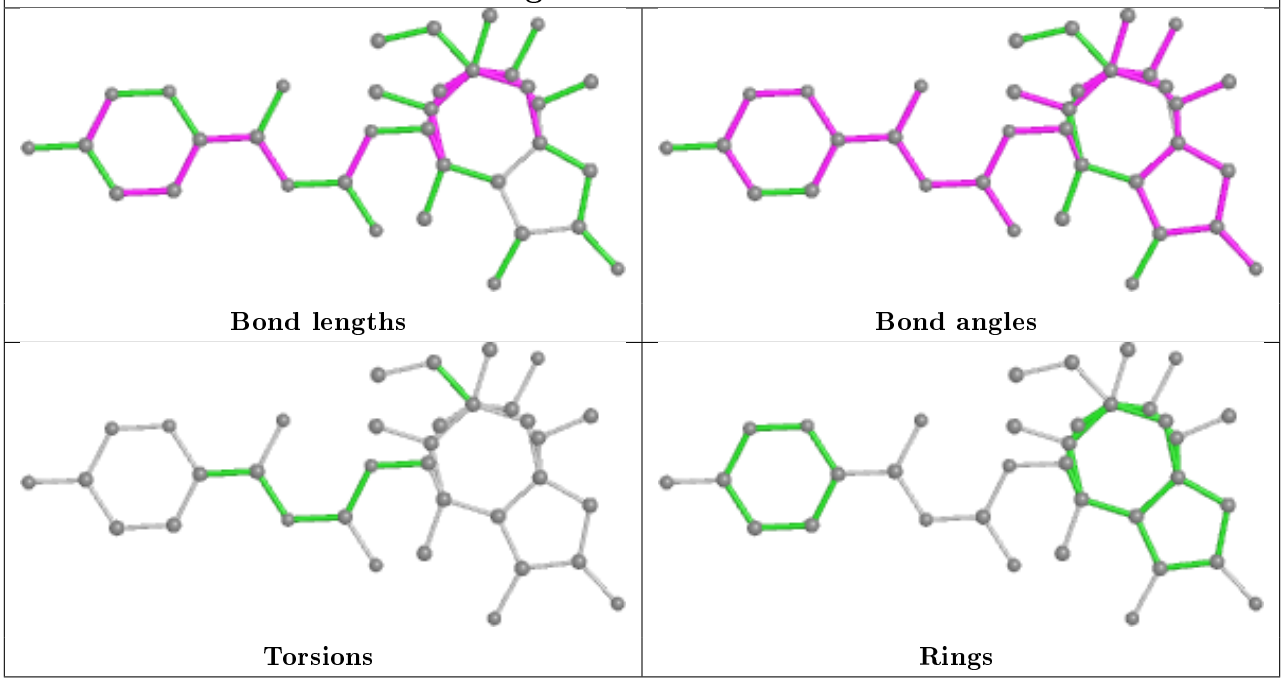
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	0	2881	G19	2	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 G19 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

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.

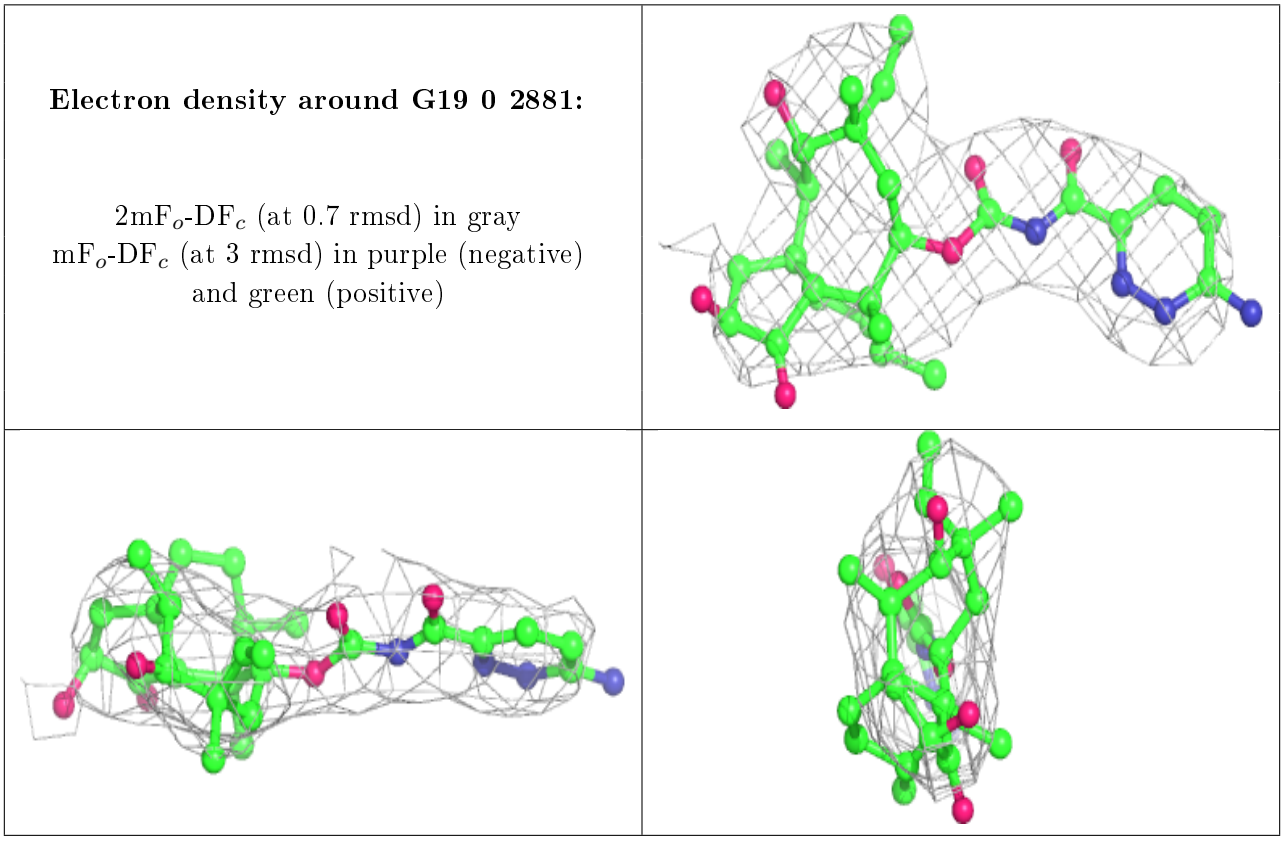
6.4 Ligands

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G19 0 2881:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

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