wwPDB EM Validation Summary Report

Oct 2, 2024 – 12:18 PM JST

PDB ID	:	8Y36
EMDB ID	:	EMD-38873
Title	:	cryo-EM structure of Staphylococcus aureus(ATCC 29213) 50S ribosome in complex with MCX-190.
Authors	:	Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on	:	2024-01-28
Resolution	:	2.65 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

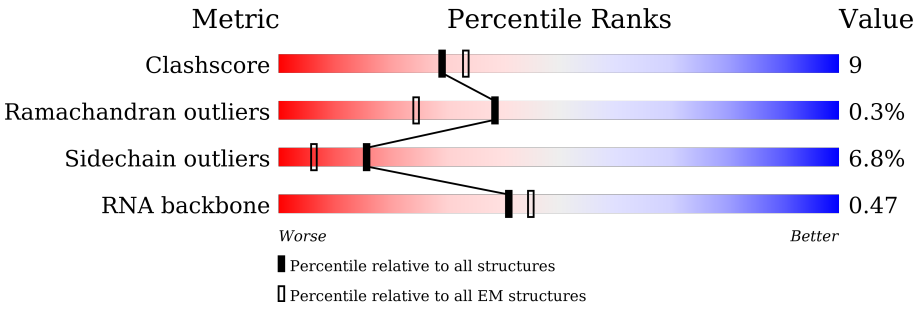
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	A	2921	49% 39% 11% .
2	1	47	64% 32% .
3	2	43	79% 21%
4	3	64	73% 27%
5	4	37	62% 35% .
6	B	115	43% 44% 13%
7	C	274	77% 22% .
8	D	215	72% 27% .

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Mol	Chain	Length	Quality of chain
9	E	206	
10	F	175	
11	G	175	
12	H	145	
13	I	122	
14	J	146	
15	K	137	
16	L	120	
17	M	119	
18	N	114	
19	O	116	
20	P	102	
21	Q	117	
22	R	89	
23	S	103	
24	T	94	
25	U	82	
26	V	58	
27	W	67	
28	X	58	
29	Y	59	
30	Z	48	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 88318 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
			Total	C	N	O	P		
1	A	2885	61864	27621	11316	20042	2885	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	47	390	238	78	70	4	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	43	367	225	89	52	1	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	521	324	113	82	2	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	296	186	60	45	5	0	0

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	115	2445	1094	436	801	114	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1315	832	224	253	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	175	Total	C	N	O	S	0	0
			1259	788	239	229	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	N	114	Total	C	N	O	0	0
			889	563	175	151		

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	112	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	T	94	Total	C	N	O	0	0
			715	459	128	128		

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	U	82	Total	C	N	O	0	0
			615	380	121	114		

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	V	58	Total	C	N	O	0	0
			445	277	96	72		

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	W	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	58	Total 449	C 280	N 85	O 84	0	0

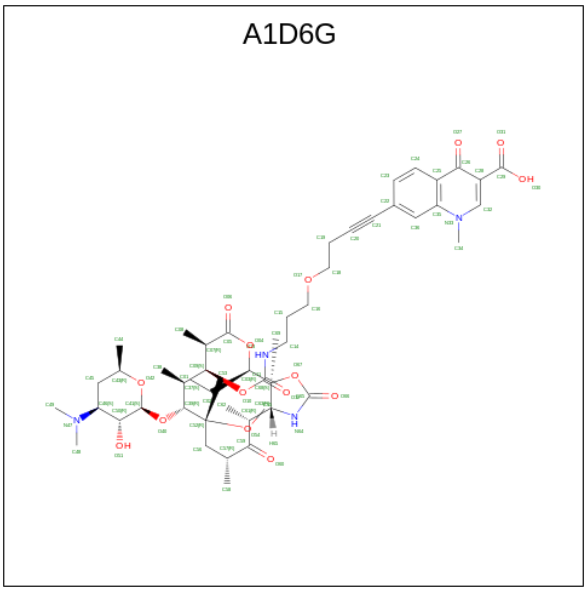
- Molecule 29 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	59	Total 363	C 219	N 68	O 75	S 1	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	48	Total 361	C 222	N 77	O 59	S 3	0	0

- Molecule 31 is 7-[4-[3-[[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxa-15-azabicyclo[12.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (three-letter code: A1D6G) (formula: $C_{50}H_{72}N_4O_{15}$).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total 69	C 50	N 4	O 15	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	11	Total	Mg	0
			11	11	

- Molecule 33 is water.

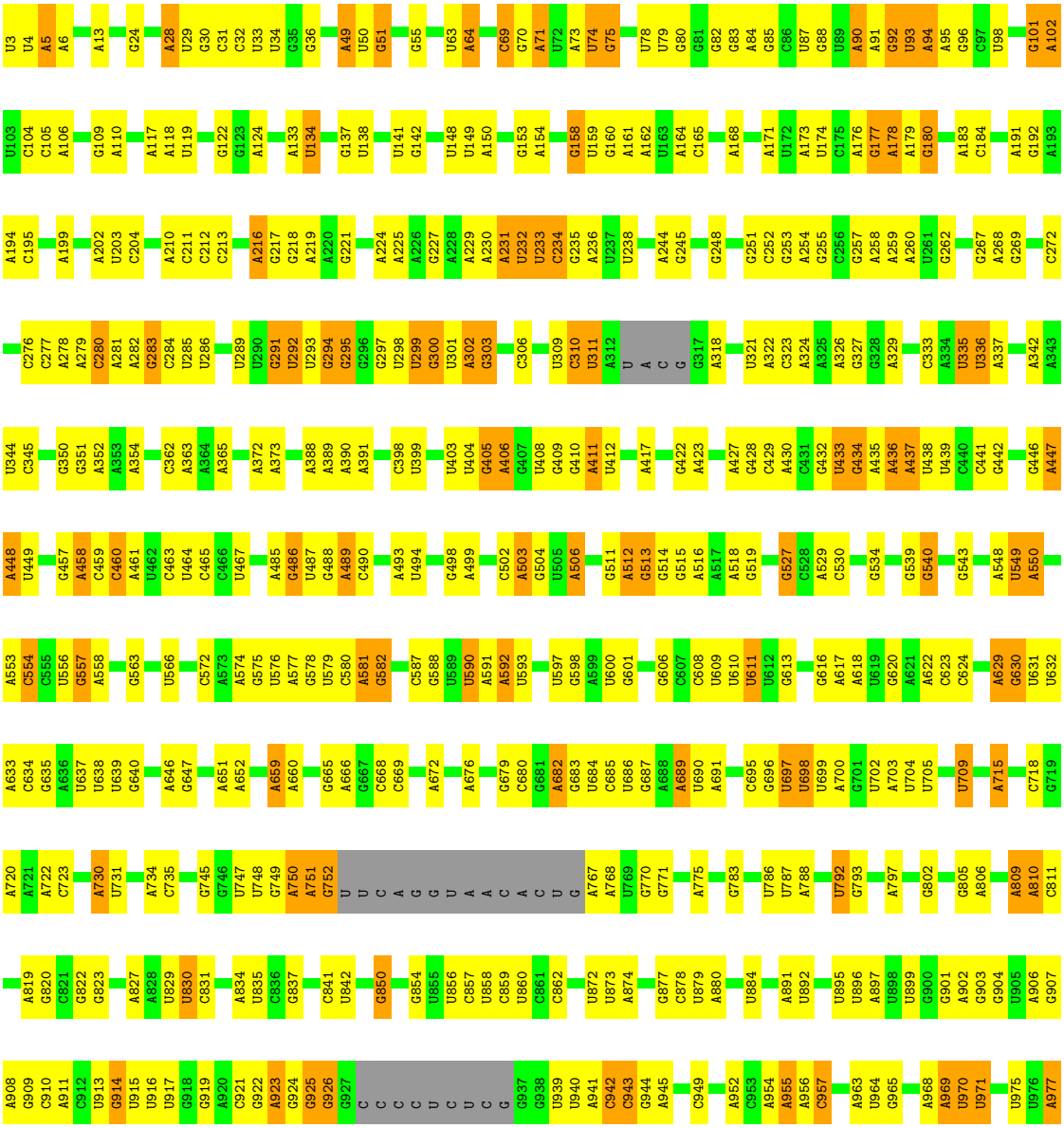
Mol	Chain	Residues	Atoms		AltConf
33	A	3	Total	O	0
			3	3	

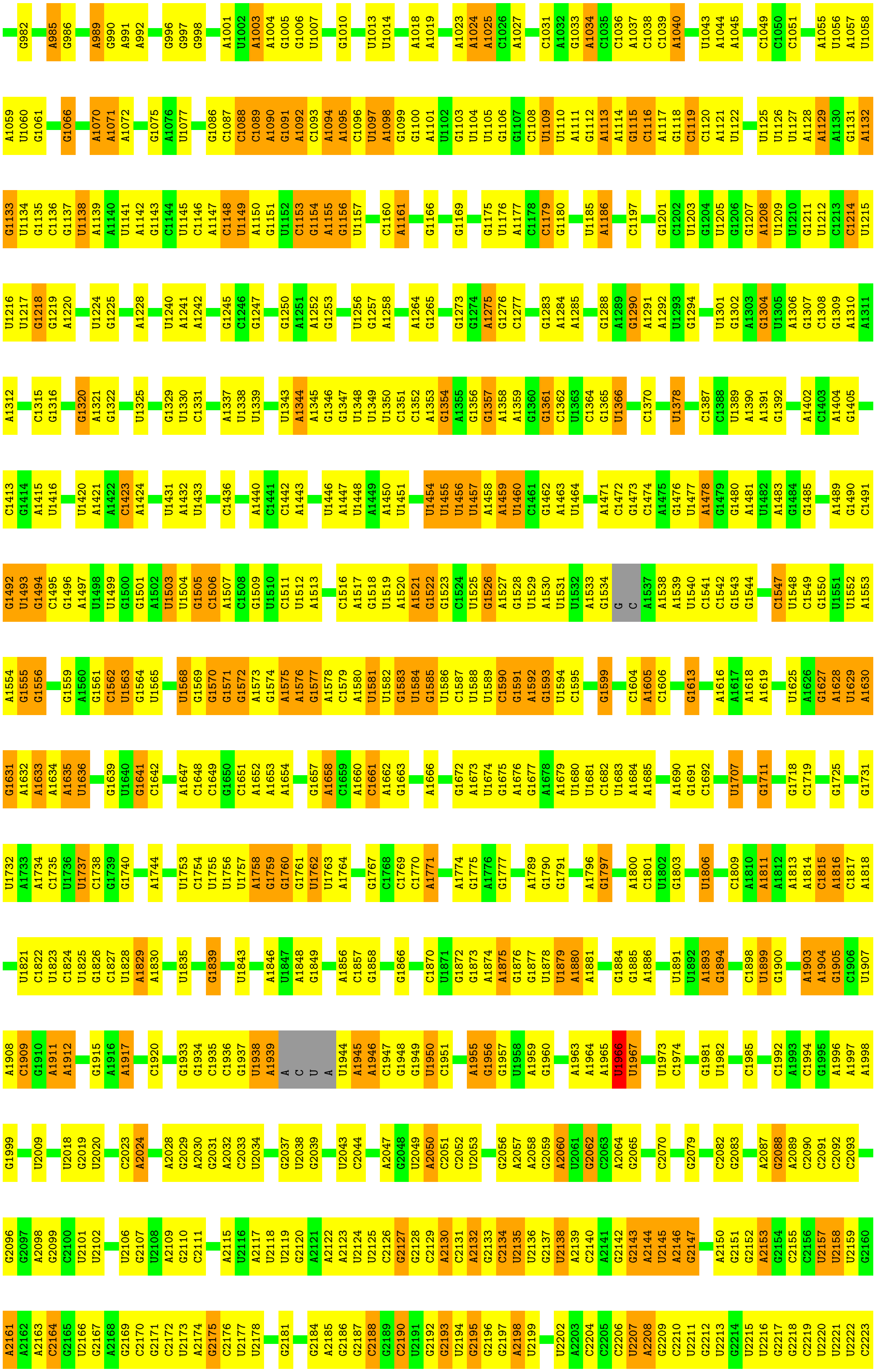
3 Residue-property plots (i)

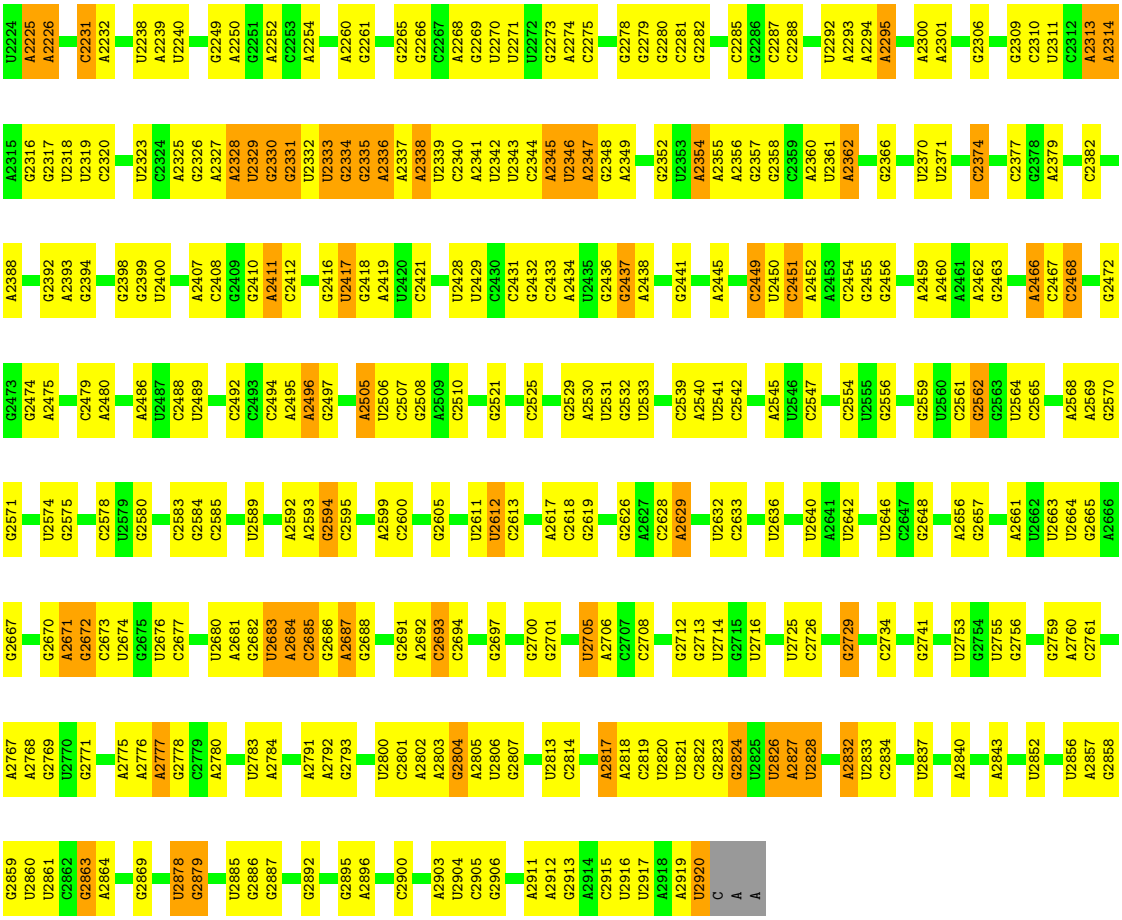
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: 23S ribosomal RNA

Chain A:




G982 A985 G986 A989 G990 A991 A992 G996 G997 G998 A1001 U1002 A1003 A1004 G1005 G1006 U1007 G1010 U1013 U1014 A1018 A1019 A1023 A1024 A1025 C1026 A1027 C1031 A1032 G1033 A1034 C1035 C1036 A1037 C1038 C1039 A1040 U1043 A1044 A1045 C1049 C1050 C1051 A1055 U1056 A1057 U1058
A1059 U1060 G1061 G1066 A1070 A1071 A1072 G1075 A1076 U1077 G1086 C1087 C1088 C1089 A1090 G1091 A1092 C1093 A1094 A1095 C1096 U1097 A1098 G1099 G1100 A1101 U1102 G1103 U1104 U1105 U1106 G1107 C1108 U1109 U1110 A1111 G1112 A1113 A1114 G1115 C1116 A1117 G1118 C1119 C1120 A1121 U1122 U1125 U1126 U1127 A1128 A1129 A1130 G1131 A1132
G1133 U1134 G1135 C1136 G1137 U1138 A1139 A1140 U1141 A1142 G1143 C1144 U1145 C1146 A1147 C1148 U1149 A1150 G1151 U1152 C1153 G1154 A1155 G1156 U1157 C1160 A1161 G1166 G1169 G1175 U1176 A1177 C1178 C1179 G1180 U1185 A1186 C1197 G1201 C1202 U1203 G1204 U1205 G1206 G1207 A1208 U1209 U1210 G1211 U1212 C1213 C1214 U1215
U1216 U1217 G1218 G1219 A1220 U1224 G1225 A1228 U1240 A1241 A1242 G1245 C1246 G1247 G1250 A1251 A1252 G1253 U1256 G1257 A1258 A1264 G1265 G1273 G1274 A1275 G1276 C1277 G1283 A1284 A1285 G1288 A1289 G1290 A1291 A1292 U1293 G1294 U1301 G1302 A1303 G1304 U1305 A1306 G1307 C1308 G1309 A1310 A1311
A1312 C1315 G1316 G1320 A1321 G1322 U1325 G1329 U1330 C1331 A1337 U1338 U1339 U1343 A1344 A1345 G1346 G1347 U1348 U1349 U1350 C1351 C1352 A1353 G1354 A1355 G1356 G1357 A1358 A1359 G1360 G1361 C1362 U1363 C1364 G1365 U1366 C1370 U1378 C1387 C1388 U1389 A1390 A1391 G1392 A1402 C1403 A1404 G1405
C1413 G1414 A1415 U1416 U1420 A1421 A1422 C1423 A1424 U1431 A1432 U1433 C1436 A1440 C1441 C1442 A1443 U1446 A1447 U1448 A1449 A1450 U1451 U1454 U1455 U1456 U1457 A1458 A1459 U1460 C1461 G1462 A1463 U1464 A1471 C1472 G1473 C1474 A1475 G1476 U1477 A1478 G1479 G1480 A1481 U1482 A1483 G1484 G1485 A1489 G1490 C1491
G1492 U1493 G1494 C1495 G1496 A1497 U1498 U1499 G1500 G1501 A1502 U1503 U1504 G1505 C1506 A1507 C1508 G1509 U1510 C1511 U1512 A1513 C1516 A1517 G1518 U1519 A1520 A1521 G1522 G1523 C1524 U1525 G1526 A1527 G1528 U1529 A1530 U1531 U1532 A1533 G1534 G C A1537 A1538 A1539 U1540 C1541 C1542 G1543 G1544 C1547 U1548 C1549 G1550 U1551 U1552 A1553
A1554 G1555 G1556 G1559 A1560 G1561 C1562 U1563 G1564 U1565 U1568 G1569 G1570 G1571 G1572 A1573 G1574 A1575 A1576 G1577 A1578 C1579 A1580 U1581 U1582 G1583 U1584 G1585 U1586 C1587 U1588 U1589 C1590 G1591 A1592 G1593 U1594 C1595 G1599 C1604 A1605 C1606 G1613 A1616 A1617 A1618 A1619 U1625 A1626 G1627 A1628 U1629 A1630
G1631 A1632 A1633 A1634 A1635 U1636 G1639 U1640 G1641 C1642 A1647 C1648 C1649 G1650 C1651 A1652 A1653 A1654 G1657 A1658 C1659 A1660 C1661 A1662 G1663 A1666 G1672 A1673 U1674 G1675 A1676 G1677 A1678 A1679 U1680 U1681 C1682 U1683 A1684 A1685 A1690 G1691 C1692 U1707 G1711 G1718 C1719 G1725 G1731
U1732 A1733 A1734 C1735 U1736 U1737 C1738 G1739 G1740 A1744 U1753 C1754 U1755 U1756 U1757 A1758 G1759 G1760 G1761 U1762 U1763 A1764 G1767 C1768 C1769 C1770 A1771 A1774 G1775 A1776 G1777 A1789 G1790 G1791 A1796 G1797 A1800 C1801 U1802 G1803 U1806 C1809 A1810 A1811 A1812 A1813 A1814 C1815 A1816 C1817 A1818
U1821 C1822 U1823 C1824 U1825 G1826 C1827 U1828 A1829 A1830 U1835 G1839 U1843 A1846 U1847 A1848 G1849 A1856 C1857 G1858 G1866 C1870 U1871 G1872 G1873 A1874 A1875 G1876 G1877 U1878 U1879 A1880 A1881 G1884 G1885 A1886 U1891 U1892 A1893 G1894 C1898 U1899 G1900 A1903 A1904 G1905 C1906 U1907
A1908 C1909 G1910 A1911 A1912 G1915 A1916 A1917 C1920 G1933 G1934 C1935 C1936 G1937 U1938 A1939 A C U A U1944 A1945 A1946 C1947 G1948 G1949 U1950 C1951 A1955 G1956 G1957 U1958 A1959 G1960 A1963 A1964 A1965 U1966 U1967 U1973 C1974 G1981 U1982 C1985 C1992 A1993 C1994 G1995 A1996 A1997 A1998
G1999 U2009 U2018 G2019 U2020 C2023 A2024 A2028 G2029 A2030 G2031 A2032 C2033 U2034 G2037 U2038 G2039 U2043 C2044 A2047 G2048 U2049 A2050 C2051 C2052 U2053 G2056 A2057 A2058 G2059 A2060 U2061 G2062 C2063 A2064 G2065 C2070 G2079 C2082 G2083 A2087 G2088 A2089 C2090 C2091 C2092 C2093
G2096 G2097 A2098 G2099 C2100 U2101 U2102 U2106 G2107 U2108 A2109 G2110 C2111 A2115 U2116 A2117 U2118 U2119 G2120 A2121 A2122 A2123 U2124 U2125 C2126 G2127 G2128 C2129 A2130 C2131 A2132 G2133 C2134 U2135 U2136 G2137 U2138 A2139 C2140 A2141 G2142 G2143 A2144 U2145 A2146 G2147 A2150 G2151 G2152 A2153 G2154 C2155 C2156 U2157 U2158 U2159 G2160
A2161 A2162 A2163 C2164 G2165 U2166 G2167 A2168 G2169 C2170 G2171 C2172 U2173 A2174 G2175 C2176 U2177 U2178 G2181 G2184 A2185 G2186 G2187 C2188 G2189 C2190 U2191 G2192 G2193 U2194 G2195 G2196 G2197 A2198 U2199 U2202 A2203 C2204 C2205 C2206 U2207 A2208 G2209 C2210 U2211 G2212 U2213 G2214 U2215 U2216 G2217 G2218 C2219 U2220 U2221 U2222 C2223



• Molecule 2: Large ribosomal subunit protein bL33B

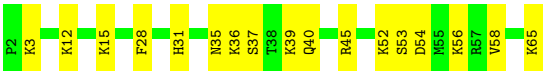
Chain 1:

• Molecule 3: Large ribosomal subunit protein bL34

Chain 2:

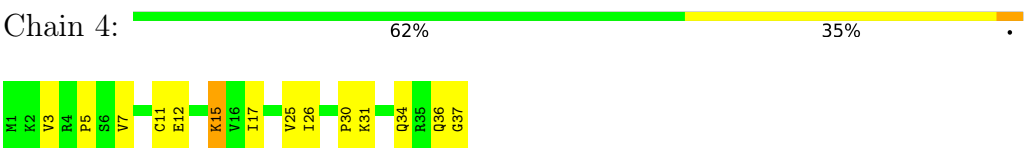
• Molecule 4: Large ribosomal subunit protein bL35

Chain 3:



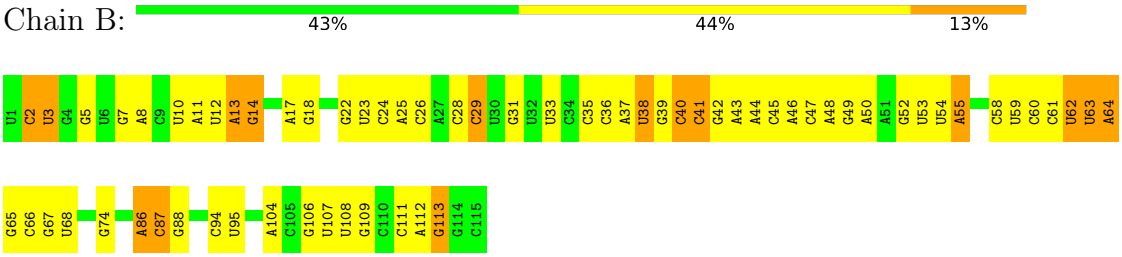
• Molecule 5: Large ribosomal subunit protein bL36

Chain 4:



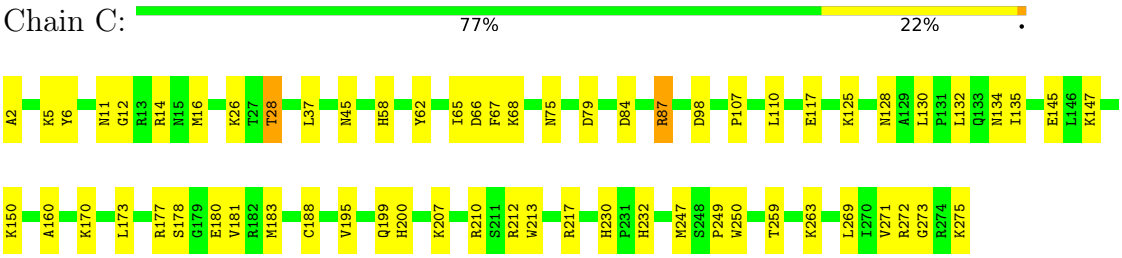
• Molecule 6: 5S ribosomal RNA

Chain B:



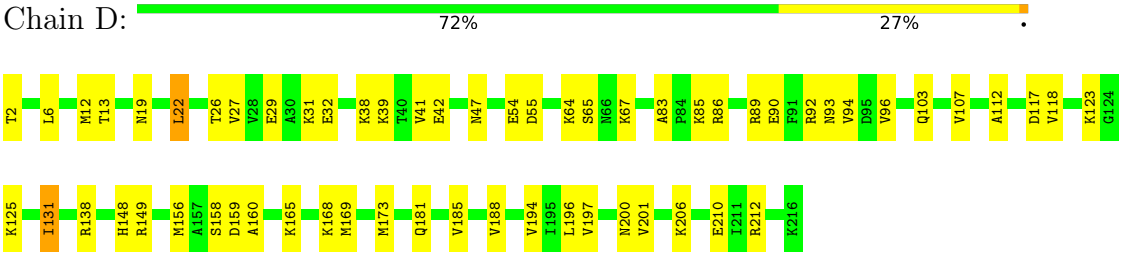
• Molecule 7: Large ribosomal subunit protein uL2

Chain C:



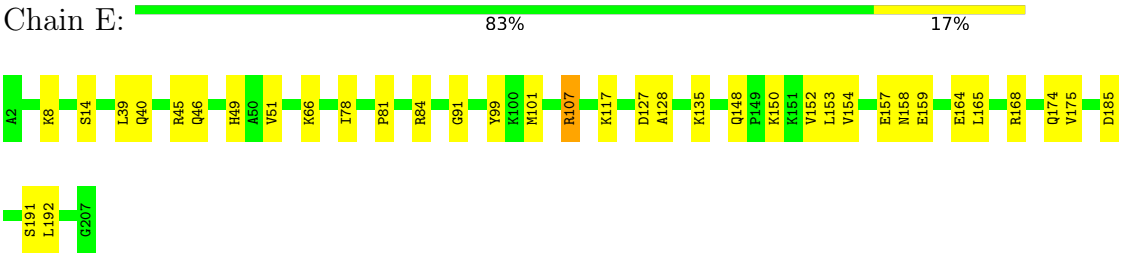
• Molecule 8: Large ribosomal subunit protein uL3

Chain D:



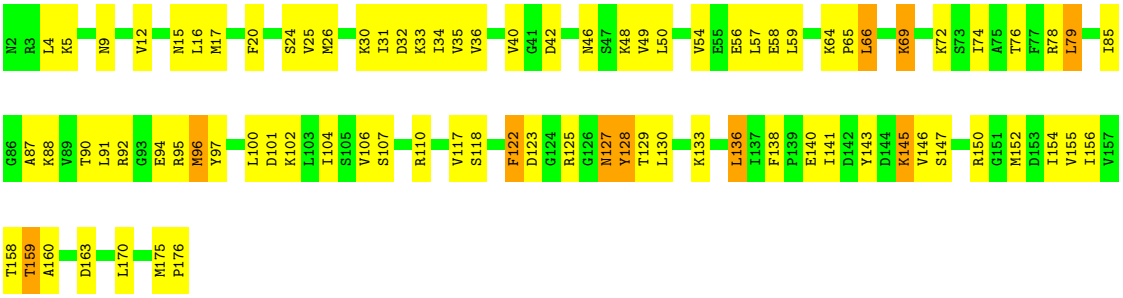
• Molecule 9: Large ribosomal subunit protein uL4

Chain E:

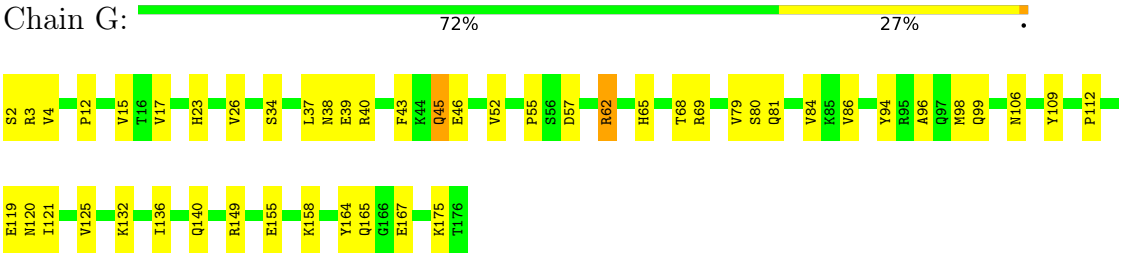


• Molecule 10: Large ribosomal subunit protein uL5

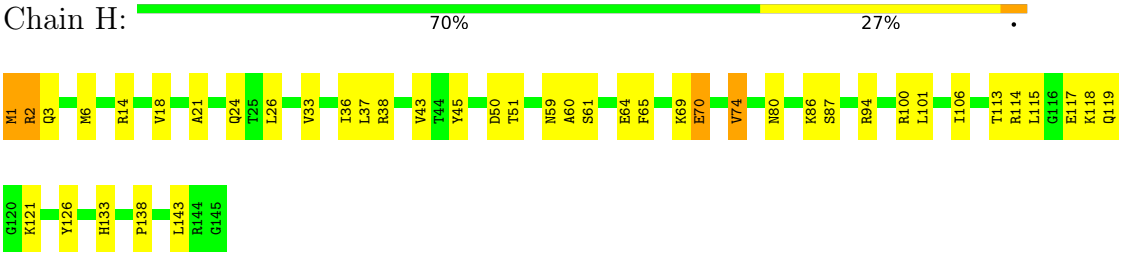
Chain F:



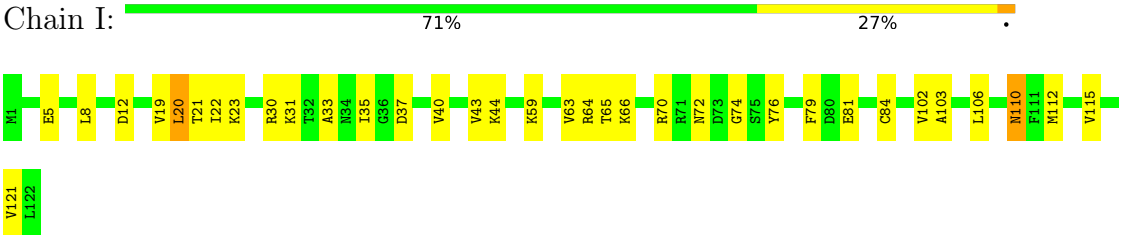
• Molecule 11: Large ribosomal subunit protein uL6



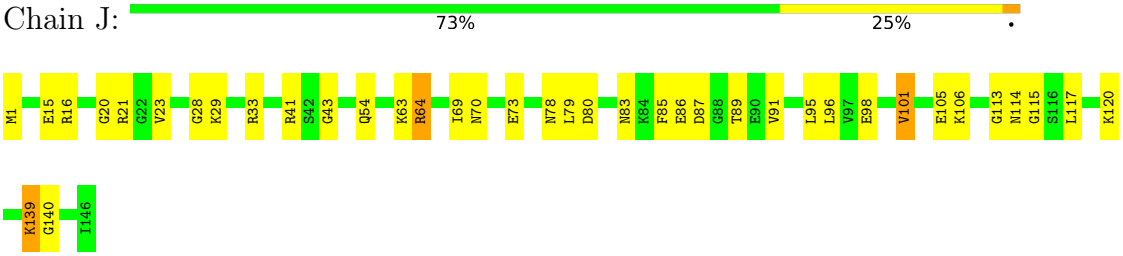
• Molecule 12: Large ribosomal subunit protein uL13



• Molecule 13: Large ribosomal subunit protein uL14

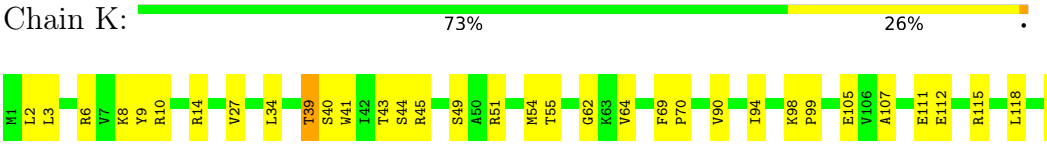


• Molecule 14: Large ribosomal subunit protein uL15



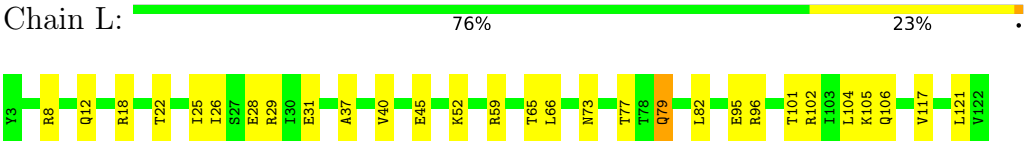
• Molecule 15: Large ribosomal subunit protein uL16

Chain K:



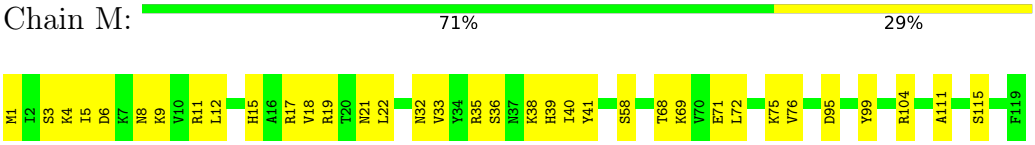
• Molecule 16: Large ribosomal subunit protein bL17

Chain L:



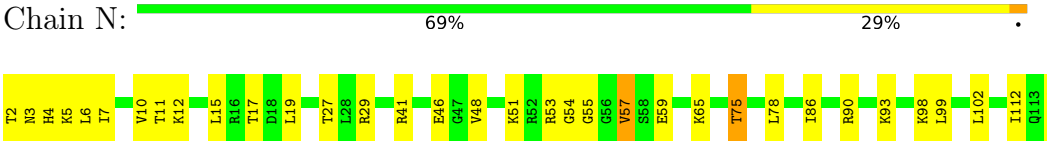
• Molecule 17: Large ribosomal subunit protein uL18

Chain M:



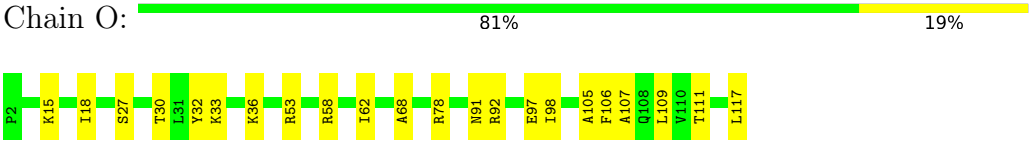
• Molecule 18: Large ribosomal subunit protein bL19

Chain N:



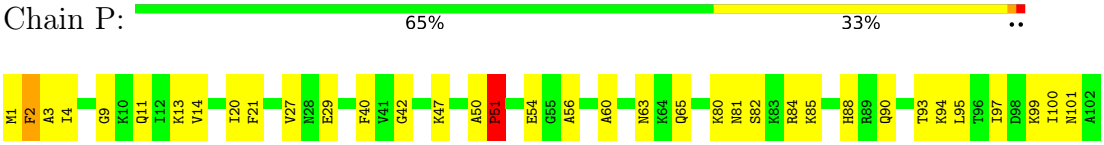
• Molecule 19: Large ribosomal subunit protein bL20

Chain O:



• Molecule 20: Large ribosomal subunit protein bL21

Chain P:

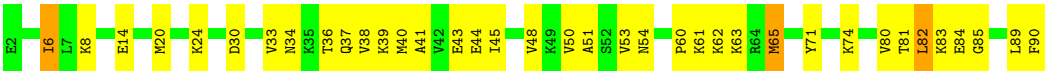


• Molecule 21: Large ribosomal subunit protein uL22

Chain Q:

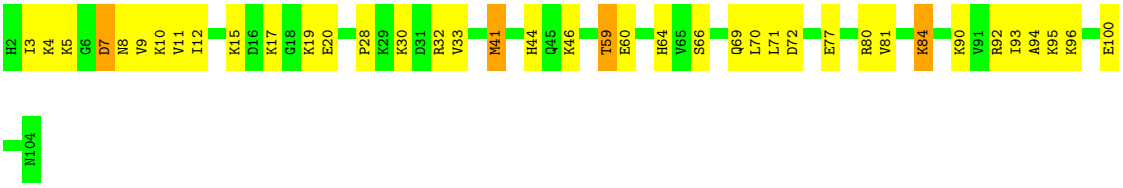
• Molecule 22: Large ribosomal subunit protein uL23

Chain R:



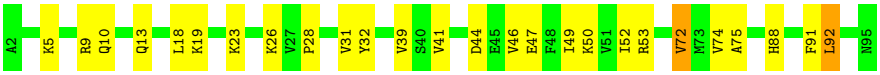
• Molecule 23: Large ribosomal subunit protein uL24

Chain S:



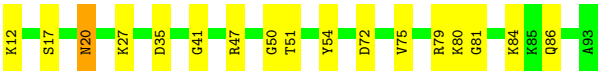
• Molecule 24: Large ribosomal subunit protein bL25

Chain T:



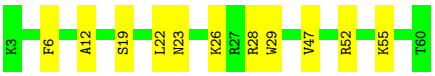
• Molecule 25: Large ribosomal subunit protein bL27

Chain U:



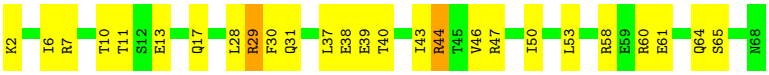
• Molecule 26: Large ribosomal subunit protein bL28

Chain V:

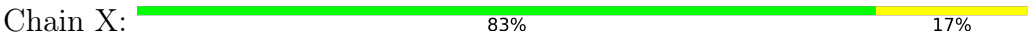


• Molecule 27: Large ribosomal subunit protein uL29

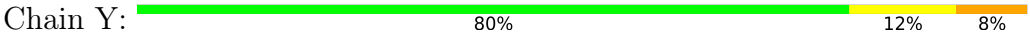
Chain W:

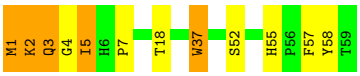


• Molecule 28: Large ribosomal subunit protein uL30

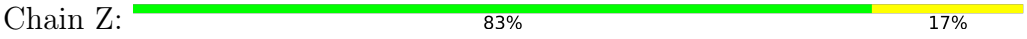


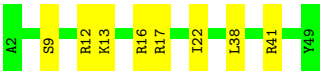
• Molecule 29: Large ribosomal subunit protein bL31B





• Molecule 30: Large ribosomal subunit protein bL32





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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: OMG, 2MG, MG, 2MA, 5MU, A1D6G

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	0.67	0/69155	0.86	14/107848 (0.0%)
2	1	0.40	0/395	0.63	0/530
3	2	0.35	0/371	0.69	0/484
4	3	0.35	0/526	0.64	0/690
5	4	0.37	0/299	0.60	0/393
6	B	0.50	0/2733	0.82	0/4257
7	C	0.39	0/2125	0.60	0/2853
8	D	0.41	0/1651	0.60	0/2215
9	E	0.35	0/1595	0.55	0/2154
10	F	0.33	0/1329	0.61	0/1793
11	G	0.35	0/1277	0.58	0/1731
12	H	0.41	0/1165	0.58	0/1570
13	I	0.40	0/925	0.67	0/1242
14	J	0.38	0/1100	0.64	0/1467
15	K	0.39	0/1095	0.61	0/1472
16	L	0.40	0/936	0.66	0/1253
17	M	0.35	0/900	0.60	0/1205
18	N	0.37	0/901	0.65	0/1209
19	O	0.40	0/954	0.60	0/1264
20	P	0.42	0/800	0.69	1/1070 (0.1%)
21	Q	0.35	0/861	0.58	0/1161
22	R	0.35	0/723	0.58	0/966
23	S	0.37	0/779	0.61	0/1043
24	T	0.32	0/723	0.55	0/973
25	U	0.41	0/621	0.62	0/825
26	V	0.32	0/451	0.61	0/603
27	W	0.32	0/542	0.59	0/722
28	X	0.32	0/451	0.63	0/606
29	Y	0.38	0/370	0.66	0/510
30	Z	0.41	0/367	0.61	0/490
All	All	0.60	0/96120	0.81	15/144599 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1760	G	O4'-C1'-N9	7.27	114.02	108.20
1	A	557	G	O4'-C1'-N9	7.01	113.81	108.20
1	A	1760	G	C3'-C2'-C1'	-6.93	95.95	101.50
1	A	1760	G	C1'-O4'-C4'	-6.42	104.77	109.90
1	A	1351	C	C2-N1-C1'	6.12	125.53	118.80

There are no chirality outliers.

There are no planarity outliers.

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	A	61864	0	31099	785	0
2	1	390	0	394	12	0
3	2	367	0	415	6	0
4	3	521	0	586	10	0
5	4	296	0	342	9	0
6	B	2445	0	1240	49	0
7	C	2090	0	2201	42	0
8	D	1627	0	1667	36	0
9	E	1572	0	1619	25	0
10	F	1315	0	1327	77	0
11	G	1259	0	1221	27	0
12	H	1143	0	1134	33	0
13	I	918	0	981	20	0
14	J	1086	0	1125	25	0
15	K	1071	0	1123	25	0
16	L	932	0	983	17	0
17	M	891	0	925	25	0
18	N	889	0	937	26	0
19	O	942	0	1014	17	0
20	P	790	0	830	29	0
21	Q	853	0	905	24	0
22	R	715	0	748	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	S	770	0	809	29	0
24	T	715	0	751	17	0
25	U	615	0	622	12	0
26	V	445	0	466	9	0
27	W	541	0	563	16	0
28	X	449	0	491	7	0
29	Y	363	0	236	17	0
30	Z	361	0	361	7	0
31	A	69	0	0	1	0
32	A	11	0	0	0	0
33	A	3	0	0	1	0
All	All	88318	0	57115	1295	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 9.

The worst 5 of 1295 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)
10:F:54:VAL:O	10:F:58:GLU:HB3	1.78	0.83
13:I:63:VAL:HG12	13:I:106:LEU:HD11	1.62	0.81
1:A:2421:C:H42	1:A:2449:C:H41	1.27	0.81
27:W:11:THR:OG1	27:W:60:ARG:NH1	2.14	0.81
1:A:1570:G:N2	1:A:1571:G:O6	2.15	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	45/47 (96%)	43 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
4	3	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
5	4	35/37 (95%)	35 (100%)	0	0	100	100
7	C	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
8	D	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	25	40
9	E	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
10	F	173/175 (99%)	152 (88%)	20 (12%)	1 (1%)	22	35
11	G	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	22	35
12	H	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
13	I	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
14	J	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
15	K	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	L	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
17	M	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
18	N	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
19	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
20	P	100/102 (98%)	92 (92%)	5 (5%)	3 (3%)	3	5
21	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
22	R	87/89 (98%)	82 (94%)	5 (6%)	0	100	100
23	S	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
24	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
25	U	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
26	V	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
27	W	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
28	X	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
29	Y	57/59 (97%)	48 (84%)	7 (12%)	2 (4%)	3	4
30	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	3071/3132 (98%)	2898 (94%)	165 (5%)	8 (0%)	38	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	160	ALA

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Mol	Chain	Res	Type
11	G	55	PRO
20	P	51	PRO
20	P	56	ALA
10	F	76	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1	44/45 (98%)	40 (91%)	4 (9%)	7 12
3	2	39/39 (100%)	37 (95%)	2 (5%)	20 34
4	3	55/55 (100%)	51 (93%)	4 (7%)	11 19
5	4	35/35 (100%)	31 (89%)	4 (11%)	4 7
7	C	220/221 (100%)	210 (96%)	10 (4%)	23 39
8	D	173/173 (100%)	163 (94%)	10 (6%)	17 29
9	E	168/168 (100%)	159 (95%)	9 (5%)	18 32
10	F	139/154 (90%)	120 (86%)	19 (14%)	3 4
11	G	123/153 (80%)	114 (93%)	9 (7%)	11 19
12	H	122/123 (99%)	115 (94%)	7 (6%)	17 29
13	I	100/100 (100%)	88 (88%)	12 (12%)	4 6
14	J	109/112 (97%)	100 (92%)	9 (8%)	9 15
15	K	108/114 (95%)	102 (94%)	6 (6%)	17 30
16	L	96/101 (95%)	93 (97%)	3 (3%)	35 55
17	M	86/95 (90%)	83 (96%)	3 (4%)	31 50
18	N	93/100 (93%)	87 (94%)	6 (6%)	14 24
19	O	96/96 (100%)	92 (96%)	4 (4%)	25 42
20	P	84/86 (98%)	81 (96%)	3 (4%)	30 48
21	Q	89/94 (95%)	82 (92%)	7 (8%)	10 17
22	R	78/80 (98%)	70 (90%)	8 (10%)	6 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	S	81/88 (92%)	74 (91%)	7 (9%)	8 13
24	T	76/82 (93%)	72 (95%)	4 (5%)	19 33
25	U	60/64 (94%)	56 (93%)	4 (7%)	13 22
26	V	44/49 (90%)	43 (98%)	1 (2%)	45 67
27	W	58/60 (97%)	51 (88%)	7 (12%)	4 6
28	X	52/52 (100%)	50 (96%)	2 (4%)	28 47
29	Y	22/56 (39%)	18 (82%)	4 (18%)	1 1
30	Z	36/44 (82%)	36 (100%)	0	100 100
All	All	2486/2639 (94%)	2318 (93%)	168 (7%)	16 22

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	N	75	THR
23	S	80	ARG
19	O	78	ARG
21	Q	108	SER
25	U	20	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
20	P	81	ASN
21	Q	61	ASN
8	D	33	ASN
8	D	19	ASN
23	S	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2878/2921 (98%)	779 (27%)	32 (1%)
6	B	114/115 (99%)	33 (28%)	0
All	All	2992/3036 (98%)	812 (27%)	32 (1%)

5 of 812 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	13	A
1	A	28	A
1	A	34	U
1	A	36	G

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2449	C
1	A	2466	A
1	A	872	U
1	A	809	A
1	A	2783	U

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

5 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	OMG	A	2278	1	18,26,27	0.99	1 (5%)	19,38,41	1.03	2 (10%)
1	2MG	A	2472	1	18,26,27	0.98	1 (5%)	16,38,41	1.22	3 (18%)
1	2MA	A	2530	32,1	17,25,26	1.05	0	17,37,40	1.25	3 (17%)
1	5MU	A	1966	1	19,22,23	1.39	5 (26%)	28,32,35	2.16	6 (21%)
1	5MU	A	792	1	19,22,23	1.43	5 (26%)	28,32,35	2.12	9 (32%)

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
1	OMG	A	2278	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	2472	1	-	2/5/27/28	0/3/3/3
1	2MA	A	2530	32,1	-	3/3/25/26	0/3/3/3
1	5MU	A	1966	1	-	2/7/25/26	0/2/2/2
1	5MU	A	792	1	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	5MU	C4-N3	-3.16	1.33	1.38
1	A	2278	OMG	C6-N1	-3.02	1.33	1.37
1	A	2472	2MG	C6-N1	-2.93	1.33	1.37
1	A	1966	5MU	C4-N3	-2.84	1.33	1.38
1	A	792	5MU	C2-N3	-2.66	1.33	1.38

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1966	5MU	C4-N3-C2	-5.43	120.32	127.35
1	A	792	5MU	N3-C2-N1	5.35	121.99	114.89
1	A	1966	5MU	N3-C2-N1	5.21	121.81	114.89
1	A	792	5MU	C4-N3-C2	-4.84	121.08	127.35
1	A	1966	5MU	C5-C4-N3	4.46	119.12	115.31

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1966	5MU	C3'-C4'-C5'-O5'
1	A	2530	2MA	O4'-C4'-C5'-O5'
1	A	1966	5MU	O4'-C4'-C5'-O5'
1	A	2472	2MG	C3'-C4'-C5'-O5'
1	A	2530	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1966	5MU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 11 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	$\#\|Z\| > 2$
31	A1D6G	A	3001	32	70,73,73	2.35	22 (31%)	96,107,107	1.68	19 (19%)

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
31	A1D6G	A	3001	32	-	8/82/113/113	0/5/5/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	3001	A1D6G	C65-N64	8.47	1.45	1.33
31	A	3001	A1D6G	C11-N13	7.34	1.50	1.34
31	A	3001	A1D6G	O10-C11	5.06	1.43	1.35
31	A	3001	A1D6G	C22-C21	4.58	1.55	1.44
31	A	3001	A1D6G	O67-C65	4.56	1.43	1.36

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	3001	A1D6G	C02-C03-C68	-5.64	107.46	115.23
31	A	3001	A1D6G	O10-C11-N13	5.22	120.27	111.11
31	A	3001	A1D6G	O04-C05-C07	3.77	119.83	111.56
31	A	3001	A1D6G	C52-C39-C37	-3.58	108.13	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	3001	A1D6G	O66-C65-N64	-3.41	125.23	129.22

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	3001	A1D6G	N13-C14-C15-C16
31	A	3001	A1D6G	O10-C11-N13-C14
31	A	3001	A1D6G	O12-C11-N13-C14
31	A	3001	A1D6G	O17-C18-C19-C20
31	A	3001	A1D6G	C19-C20-C21-C22

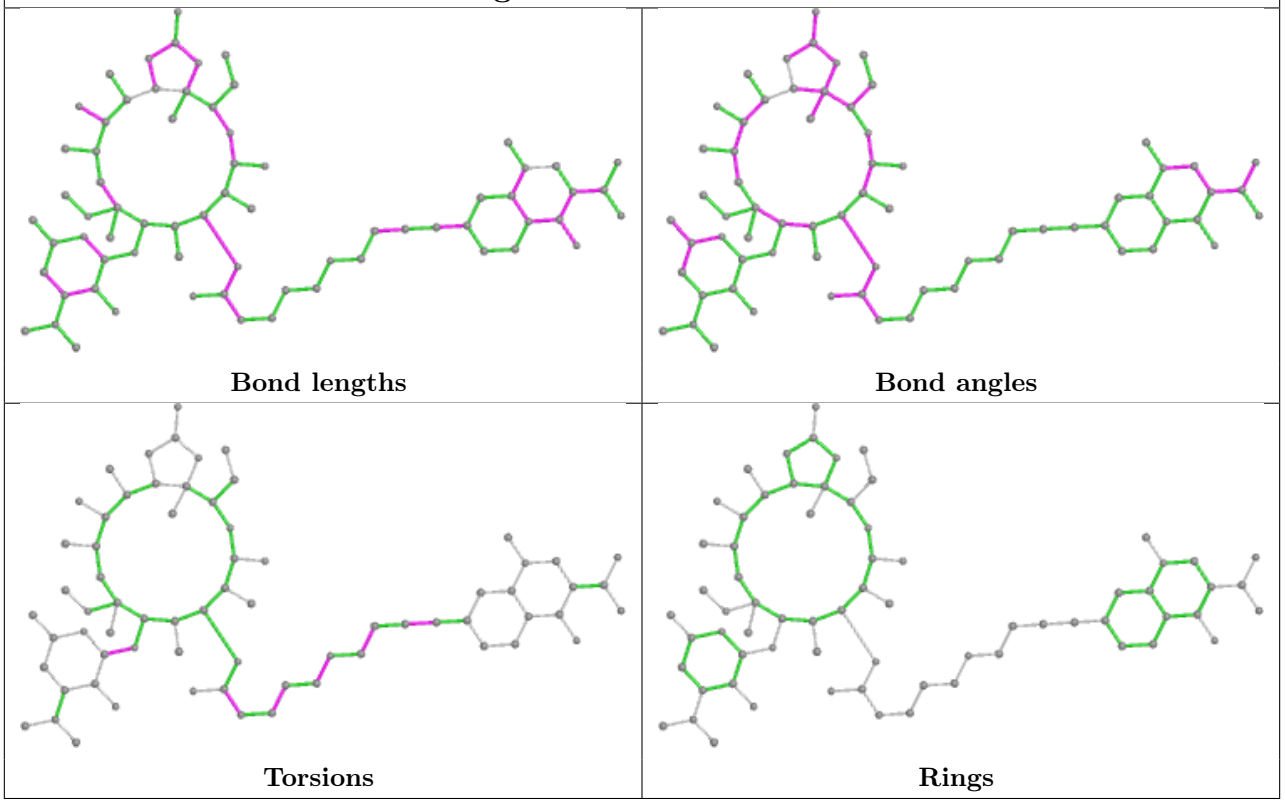
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	3001	A1D6G	1	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 A1D6G A 3001



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.