wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 11:58 PM EST

PDB ID	:	1K01
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	:	3.50 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 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:

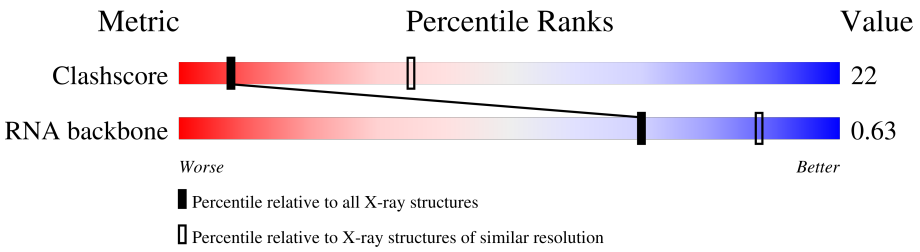
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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))
Clashscore	141614	1036 (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 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	29% 49% 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
6	CLM	A	2884	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 59940 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

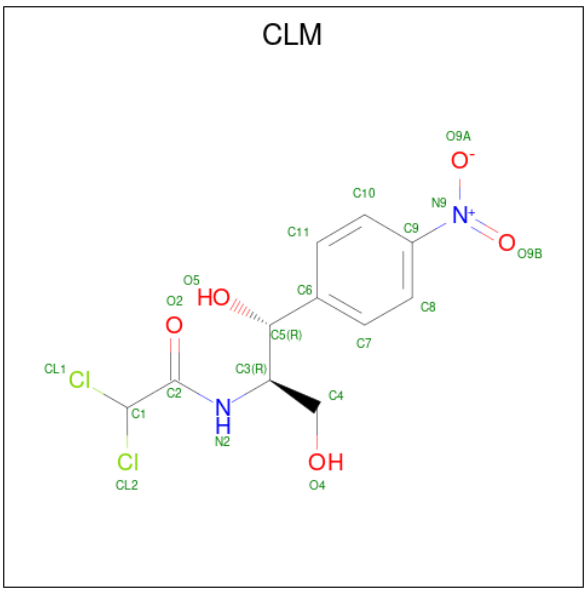
- Molecule 4 is a protein called Ribosomal Protein L32.

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	3	3	3	0	0

- Molecule 6 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
6	A	1	20	11	2	2	5	0	0

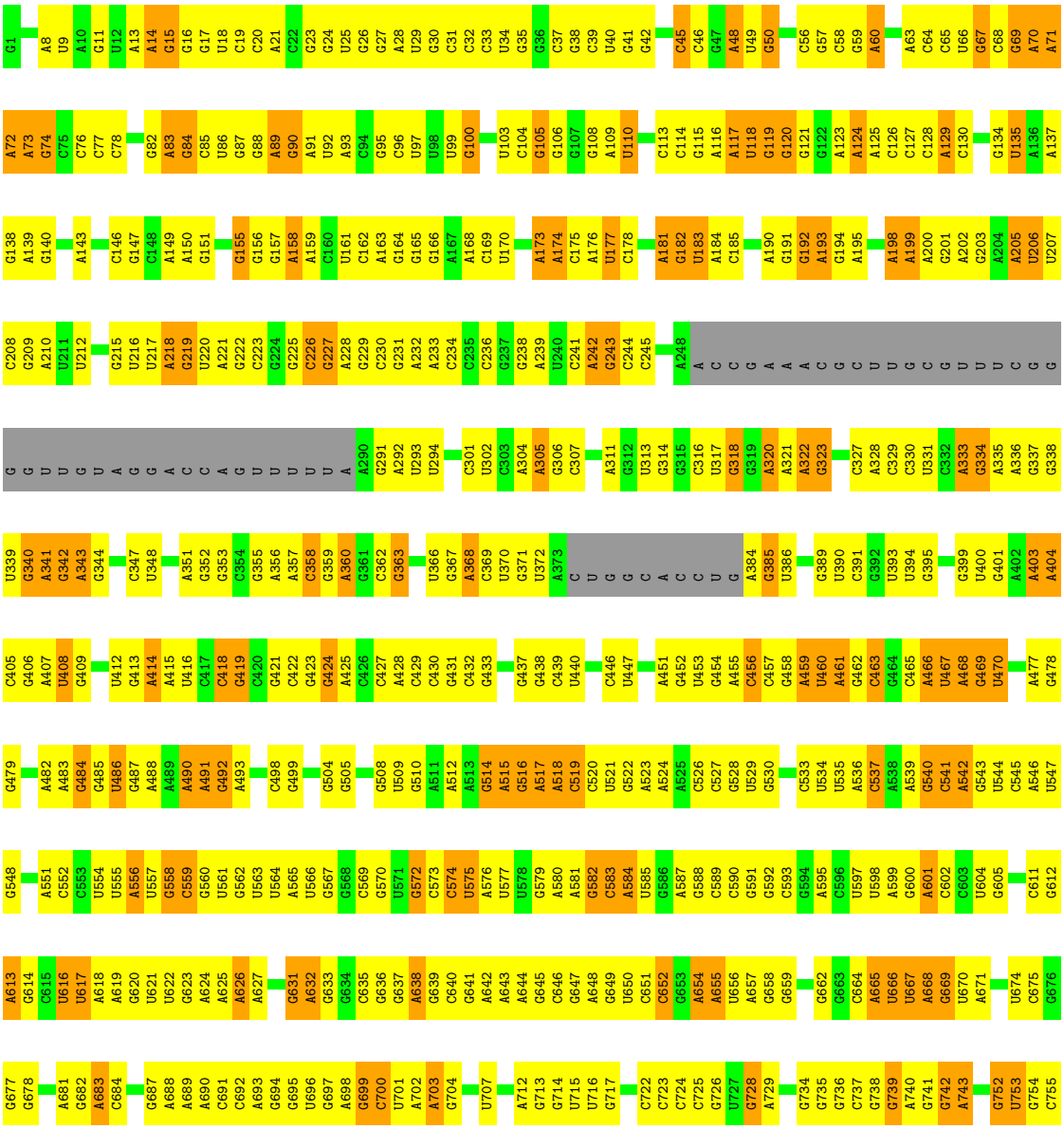
3 Residue-property plots (i)

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: 29% 49% 18% •



C756 U757 G758 C759 U760 G761 A762 A763 A764 C765 A766 G767 U768 G772 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 C850 C851 U852 C853 G854 G855 A856 U857 C858 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 C914 C915 A918 U919 A922 A923 C924 U925 C926 C927 G928 A929 A930 G931 G932 G933 G934 C937 G938 C939 G940 U941 U942 U943 A944 G945 C948 G949 G950 G951 A952 G953 U954 G955 A956 G957
G958 C959 U960 A964 C968 U969 A970 A971 C972 U973 U974 G975 G976 G977 U978 A979 G980 C981 C982 G983 A984 G985 A986 G987 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 A1187 A1188 G1189 C1190 G1191 A1192 G1193 U1194 U1195 U1196 U1197 C1198 U1199 G1200 G1201 U1202 A1203 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 A1292 A1293 G1298 A1299 A1300 U1301 C1302 U1306 U1307 C1308 G1309 C1310 C1311 G1312 U1313 A1314 A1315 G1316 C1319 A1320
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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 U1440 A1441 C1442 G1443 C1444 A1445 U1446 U1447 G1450 C1451 U1452 A1453 C1456
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C1665 G1666 A1667 G1668 A1669 G1670 A1671 A1672 C1673 C1674 C1675 U1676 C1677 G1678 U1679 U1680 A1681 A1682 G1683 G1684 A1685 A1686 C1687 U1690 G1691 C1692 A1693 A1694 C1703 G1704 A1707 C1708 U1709 U1710 C1711 G1712 G1713 A1714 A1715 G1716 A1717 G1720 G1721 G1722 U1723 C1724 C1725 C1726 C1727 A1728 C1729 G1730
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A2315 G2316 G2317 U2318 G2319 G2320 C2321 U2322 U2323 G2324 A2325 C2326 U2327 G2328 G2329 G2330 A2337 C2338 A2348 G2349 G2350 A2355 A2356 A2357 C2358 C2361 G2362 G2363 C2364 U2365 U2366 A2367 G2368 U2369 G2370 A2371 A2372 C2373 C2374 G2375 G2376 U2377 G2378 G2379 U2380 A2381 C2382 G2383 G2384 U2385 A2390 A2391 G2392 G2393 G2394
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C2038 A2041 A2042 A2043 G2044 A2045 C2048 C2049 G2050 U2051 G2052 G2053 A2054 G2055 C2056 U2057 U2058 U2059 A2060 C2061 U2062 A2063 U2067 C2068 U2069 G2070 G2071 C2072 A2073 U2074 U2075 G2076 A2079 U2080 U2081 C2082 G2083 G2084 G2085 U2086 U2087 U2088 C2089 U2090 C2091 U2092 G2093 C2094 G2095 U2096 A2097 G G A U A
C1971 G1972 C1973 U1974 G1975 U1976 C1977 U1978 C1979 A1980 G1983 A1984 G1985 G1986 G1987 A1988 C1989 U1994 G1995 A1996 A1997 A1998 U1999 U2000 G2001 A2002 A2003 U2004 U2005 G2006 G2007 C2008 U2009 G2010 U2011 A2012 A2013 A2014 G2015 A2016 U2017 G2018 C2019 C2022 C2023 U2024 A2025 C2026 C2027 C2028 G2029 U2030 A2031 G2032 C2033 A2034
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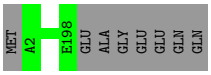
A1807 C1808 G1809 U1810 A1811 U1812 A1813 U1817 G1818 U1819 G1820 A1821 C1822 G1823 C1824 C1825 U1826 G1827 C1828 C1829 C1830 G1831 G1834 C1835 C1836 A1840 A1851 G1854 G1855 U1856 G1857 A1867 G1871 C1876 C1877 C1878 G1879 G1880 U1881 G1882 A1883 A1884 C1885 G1886 G1887 C1888 G1889 G1890 C1891 U1894 A1895

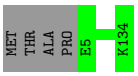
- Molecule 2: Ribosomal Protein L4

Chain K: 96%



- Molecule 3: Ribosomal Protein L22

Chain L: 97%



- Molecule 4: Ribosomal Protein L32

Chain M: 97%

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	171.10Å 409.30Å 696.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.275 , 0.321	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59940	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLM, 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	1746	A	C2'-C3'-O3'	5.91	123.15	113.70
1	A	777	A	C2'-C3'-O3'	5.45	122.42	113.70

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	59532	0	30004	1937	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	3	0	0	0	0
6	A	20	0	11	8	0
All	All	59940	0	30015	1942	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 22.

The worst 5 of 1942 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:2430:A:H2'	6:A:2884:CLM:CL2	1.51	1.48
1:A:2430:A:C2'	6:A:2884:CLM:CL2	2.23	1.22
1:A:1747:G:H4'	1:A:1749:G:H1'	1.29	1.12
1:A:2668:U:H4'	1:A:2669:C:H5'	1.33	1.11
1:A:940:G:H3'	1:A:941:U:H5"	1.35	1.09

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%)	561 (20%)	145 (5%)

5 of 561 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 145 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2261	G
1	A	2824	C
1	A	2418	A
1	A	2589	C
1	A	929	A

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 4 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
6	CLM	A	2884	5	19,20,20	3.26	9 (47%)	23,27,27	2.80	7 (30%)

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
6	CLM	A	2884	5	-	8/20/22/22	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)
6	A	2884	CLM	C7-C6	7.53	1.51	1.39
6	A	2884	CLM	O9B-N9	6.82	1.34	1.22
6	A	2884	CLM	C1-C2	5.29	1.60	1.53
6	A	2884	CLM	C5-C3	4.08	1.58	1.53
6	A	2884	CLM	C10-C9	4.01	1.46	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2884	CLM	C10-C9-N9	-9.51	112.22	119.38
6	A	2884	CLM	C8-C9-N9	6.10	123.97	119.38
6	A	2884	CLM	O2-C2-N2	3.06	128.59	122.93
6	A	2884	CLM	O5-C5-C6	-2.69	105.34	111.19
6	A	2884	CLM	C10-C9-C8	2.40	123.82	119.86

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2884	CLM	C4-C3-N2-C2
6	A	2884	CLM	N2-C3-C5-O5
6	A	2884	CLM	N2-C3-C5-C6
6	A	2884	CLM	C4-C3-C5-O5
6	A	2884	CLM	C4-C3-C5-C6

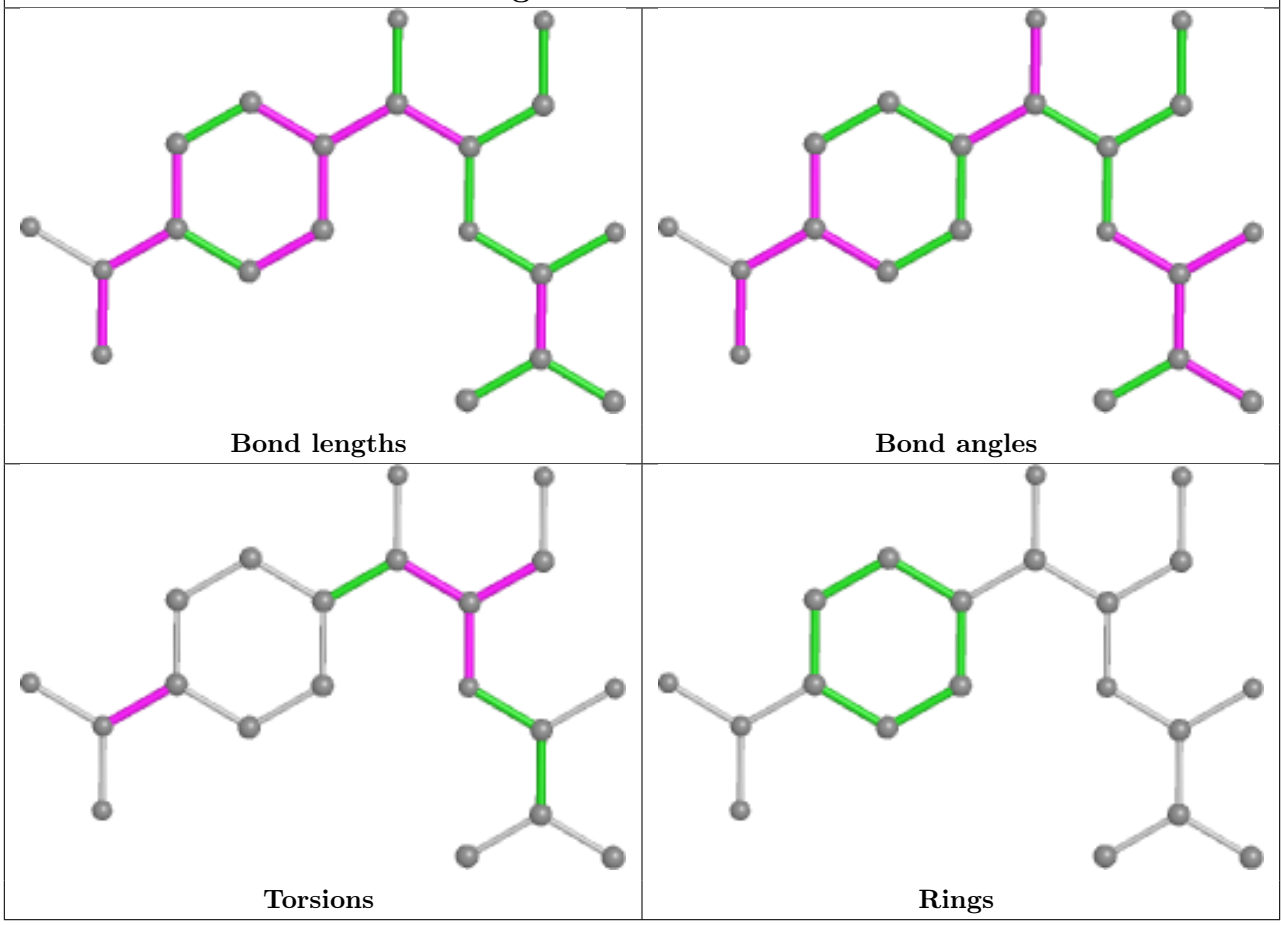
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2884	CLM	8	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 CLM A 2884



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.