



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 11:24 pm BST

PDB ID : 1K01
Title : Structural Basis for the Interaction of Antibiotics with the Peptidyl Transferase Center in Eubacteria
Authors : Schlutzen, 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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) : 2.11

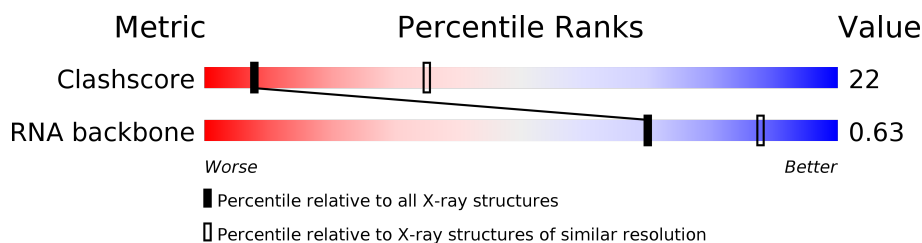
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.



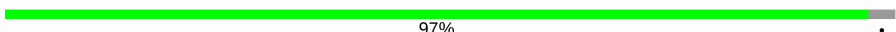
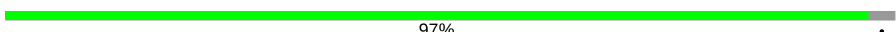
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	
2	K	205	
3	L	134	
4	M	60	

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

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
1	A	2774	Total	C	N	O	P	0	0	0
			59532	26556	10982	19221	2773			

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
2	K	197	Total	C	0	0	197
			197	197			

- Molecule 3 is a protein called Ribosomal Protein L22.

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

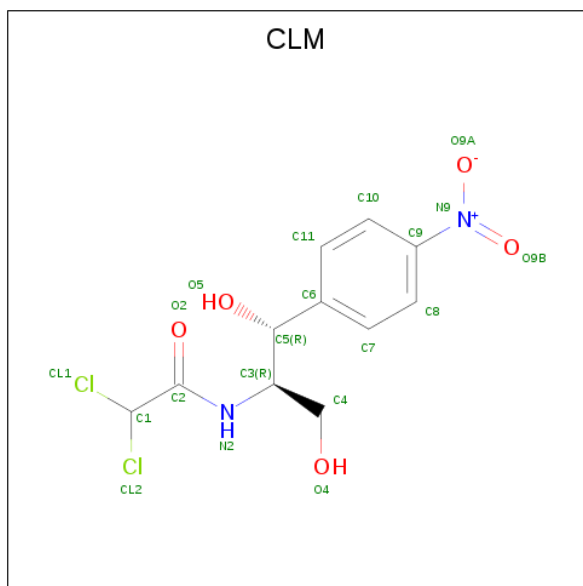
- Molecule 4 is a protein called Ribosomal Protein L32.

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

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

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

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



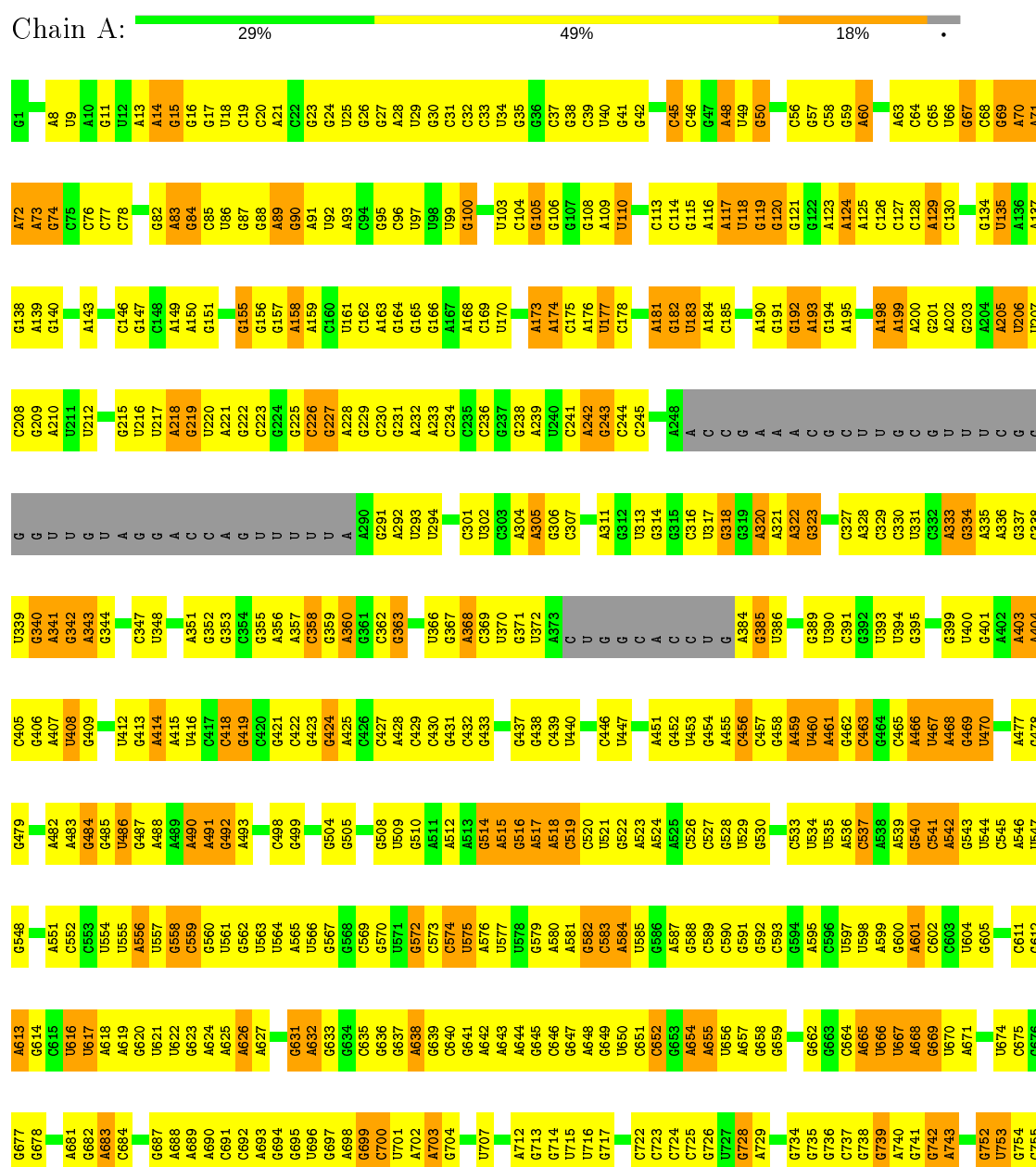
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
6	A	1	20	11	2	2	5	0	0

3 Residue-property plots

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.

Note EDS was not executed.

• Molecule 1: 23S rRNA

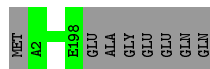


U1733	C1685	U1592	A1525	A1457	G1387	A1321	G1251	U1170	U1101	A1032	G958	G	U823	C756
U1734	C1686	C1593	U1526	A1458	A1391	G1322	C1252	A1171	G1102	G1033	C959	G	U824	U757
G1735	G1687	U1594	G1527	U1459	U1392	G1323	C1253	G1172	C1103	U1034	U960	C	C825	G758
A1699	A1595	C1528	C1528	G1460	G1393	G1324		G1173	G1104	G1035		C	U826	C759
A1699	A1596	C1529	C1529	G1465	G1393	U1325	G1258	G1174	U1105	G1036	A964	C	C827	U760
U1737	U1597	U1530	U1530	G1466	G1394	U1326	A1259	A1175	A1106	U1037		U	G828	G761
A1671	C1598	C1598	C1591	U1466		C1327	A1260		A1107	C968		A	C829	A762
C1672	A1532	U1467	A1532	U1467	A1397	G1328	G1261	C1183	U1108	U1038	U969	C	C830	A763
U1600	G1533	A1468	G1398	A1468	G1398	U1329	U1262		U1109	A1039	A970	C	G831	A764
A1674	A1534	U1469	C1399	U1469	G1399	G1330	G1263	A1187	G1110	G1040		A	A832	C765
C1675	C1535	G1470	A1400	G1470	A1400	G1331	G1264	A1188	C1111	G1041	C972	A	A833	A766
A1603	G1536	G1471	G1401	G1471	G1401	G1332	G1265	G1189	U1112		U973	C		G767
C1677	U1537	C1472	G1402	G1472	G1402	G1333	G1266	G1190	C1113	U1044	U974	U	A838	U768
A1604	A1538	U1473	U1403	U1473	U1403	A1334	A1267	G1191		U1045			U839	
G1678	U1539	U1474	C1404	U1474	C1404	G1337	U1268	A1192	G1118	G1047	C976	A	U840	G772
U1679	C1540	U1475	A1405	U1475	A1405	G1338	G1269	A1193	U1119	U1048	C977		U841	G773
A1681	G1541	G1476		G1476		U1339	G1270	U1194	G1120	C1049	U978		A842	A774
A1682	U1542		U1409		U1409	G1340	C1271	U1195	G1121		A979		A843	A775
G1683	G1543	U1480	U1410	U1480	U1410	G1341	G1272	G1196	A1122	C1054	G980		A844	G776
G1684	A1544	U1481	C1411	U1481	C1411	G1342	G1273	U1197	G1123	A1055	C981			G777
A1685		U1482	C1412	U1482		U1341	G1274	C1198	U1124	A1056	C982			A778
A1686	U1547	G1483	C1415	G1483	C1415	C1343	A1275	U1199	G1125	A1057	G983			
C1687	U1548	U1484	C1416	U1484	C1416	G1344	U1276	G1200	A1126	U1058	G984			
	U1549	U1485	A1416	U1485	A1416	G1345	G1277	G1201	G1127	A1059	G985			U784
U1618	C1550	C1487	C1417	C1487	C1417	C1346	A1278	U1202	G1128	U1060	A986			U785
A1619	U1551	G1488		G1488		C1347	G1279	A1203	A1129	A1061	G987			U786
	C1552	G1489	A1420	G1489	A1420	C1348	U1280	G1204	U1130					A787
A1690	G1553	U1490	U1421	U1490	U1421	G1349	A1281	G1205		A1065	A994			G788
G1691	U1554					G1350	A1282		C1134	U1066	A995			G789
C1692	A1555	U1493	U1424	U1493	U1424	G1351	C1283	G1209	G1135	G1067	C996			A790
A1693	A1556	G1494	G1425	G1494	G1425	G1352	U1284	G1210	G1136	A1068	C997			G791
C1694	U1557	G1495	U1426	G1495	U1426	A1353	A1285	G1211	A1137	G1069	C998			A794
U1697	C1558	G1496	G1427	G1496	G1427	U1354	U1286	U1212	A1138	G1070	A999			A795
A1698	U1559	G1497	A1429	G1497	A1429	G1355	A1287	U1213	A1139	U1071	C1000			A796
C1703	A1560	U1498	G1430	U1498	G1430	G1356	A1288	G1214	U1140	U1072	A1001			A797
G1704	U1561	A1499	U1431	A1499	U1431	U1357	A1289	A1215	U1141	G1073	A865			G798
	G1562	U1500	G1432	U1500	G1432	C1358		G1216	G1142	G1074	U866			C799
U1707	U1563	G1501	A1433	G1501	A1433	G1359	A1282	U1217	A1143	C1075	G1003			U800
C1708	G1564	G1502	U1434	G1502	U1434	C1364	A1283	C1218	U1144		A1004			A801
U1709	U1565	G1503	G1435	G1503	G1435	U1365		C1219	C1145	G1079	U1005			A802
C1710		G1504	G1436	G1504	G1436	A1366	G1298	G1220	G1146	A1080	A1007			C803
A1711	G1571	U1505	A1437	U1505	A1437	A1367	A1299	C1221		A1081	G1008			C804
G1712	G1572	C1506	G1438	C1506	G1438	G1368	U1301	G1222	G1149	G1082	C939			G805
U1713	A1574	A1507	G1439	A1507	G1439	G1369	C1302	G1223	C1150	A1083	U873			A806
	C1575	G1508	G1440	G1508	G1440	U1370		A1224	U1151	A1084	U941			A807
A1714	C1576	A1510	A1441	A1510	A1441	G1371	U1306	G1225	C1152	G1085	U942			C808
U1717		G1442	G1442	G1442	G1442	A1372	U1307	A1226	A1153	C1086	U943			C809
G1720	G1579	A1511	G1443	A1511	G1443	G1373	C1308	A1227	A1154	C1087	U944			U810
C1721	C1580	A1512	C1444	A1512	C1444	G1374	C1309		G1155	A1088	G945			G811
A1715	C1581	U1513	A1445	U1513	A1445			C1233		C1089				G812
A1717	A1582	U1515	U1446	U1515	U1446	G1377	C1311	C1234		G1090	U1019			A813
	U1584	G1519	U1447	G1519	U1447	C1380	C1312	G1240	U1161	C1091	A1020			A814
U1789	A1585	U1520	G1450	U1520	G1450	U1381	U1313	G1241	C1163	U1092	A1021			A815
G1790	C1586	U1521	A1451	U1521	A1451	G1382	A1314		C1164	U1093	A886			U816
C1791	A1588	U1522	U1452	U1522	U1452	C1383	A1315	U1244	G1165		G887			A817
A1793	A1589	A1523	A1453	A1523	A1453	C1384	G1316	G1245	A1166	A1096	G888			A818
C1794	U1591	C1524	C1456	C1524	C1456	G1385	C1319	G1249	A1167	A1097	U890			G819
						G1386			U1168	A1098	A891			U820
A1800	C1726	G1660		G1660		A1386	A1320		C1169	G1100	G892			A821
C1801	C1727	C1661		C1661							G			G822
A1802	G1589	G1662		G1662										
G1803	C1728	C1663		C1663										
	U1738	G1664		G1664										



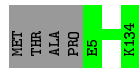
- Molecule 2: Ribosomal Protein L4

Chain K:  96% .



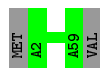
- Molecule 3: Ribosomal Protein L22

Chain L:  97% .



- Molecule 4: Ribosomal Protein L32

Chain M:  97% .



4 Data and refinement statistics

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	171.10 Å 409.30 Å 696.90 Å 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($^{\circ}$)	Ideal($^{\circ}$)
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	1279	G
1	A	1623	C
1	A	2633	A
1	A	1301	U
1	A	1355	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 carbohydrates 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(°)	Ideal(°)
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:

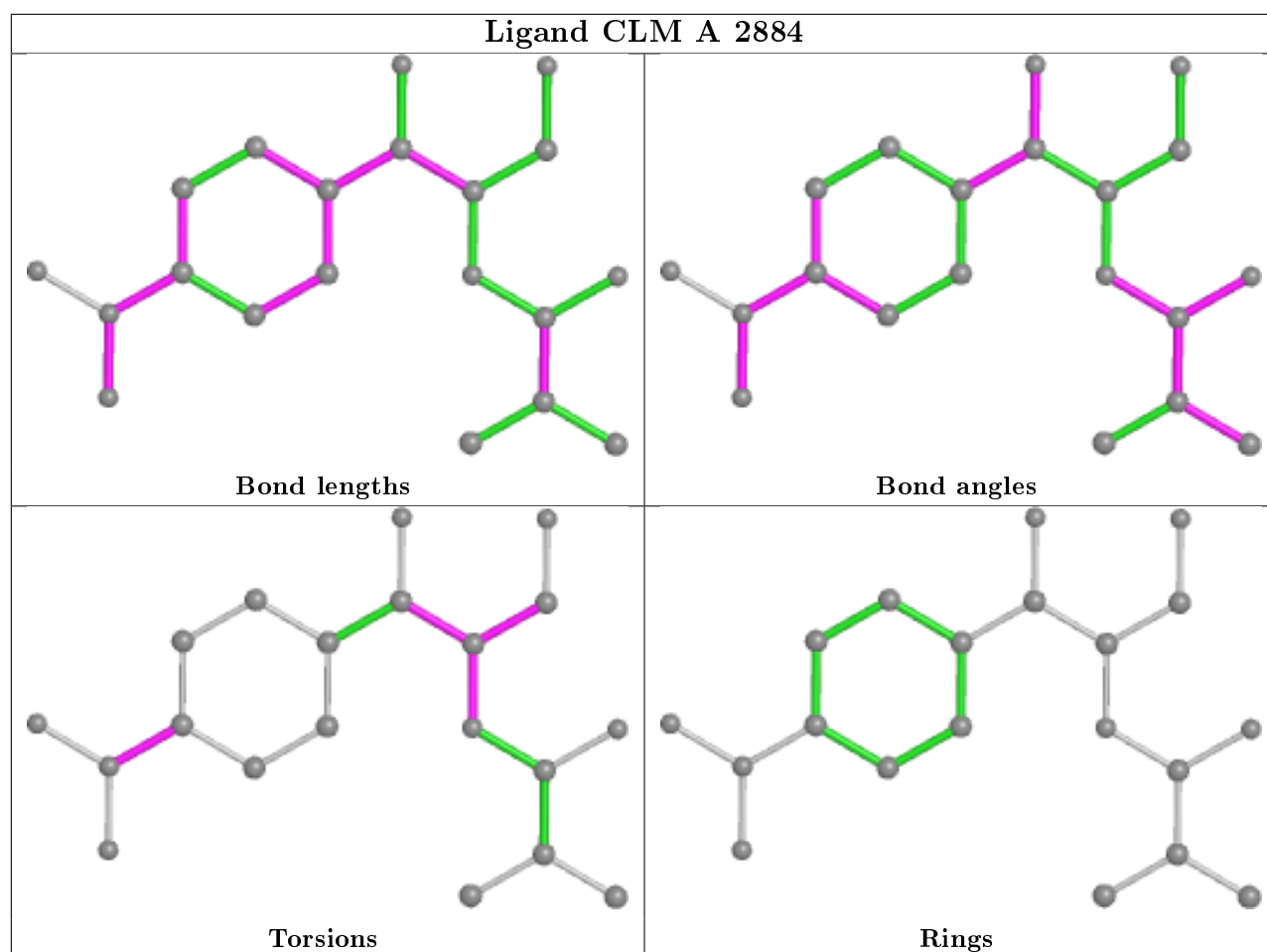
Mol	Chain	Res	Type	Atoms
6	A	2884	CLM	C4-C3-N2-C2
6	A	2884	CLM	N2-C3-C5-O5
6	A	2884	CLM	N2-C3-C5-C6
6	A	2884	CLM	C4-C3-C5-O5
6	A	2884	CLM	C4-C3-C5-C6

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 than 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.



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.