



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

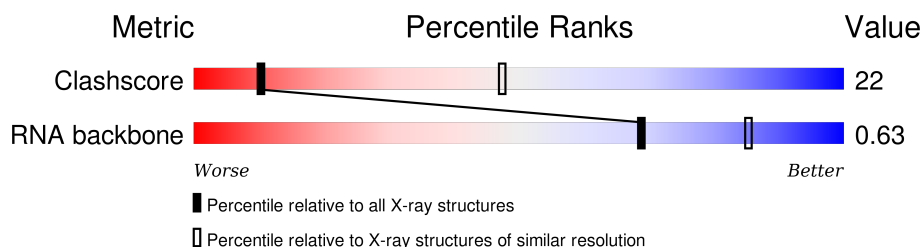
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

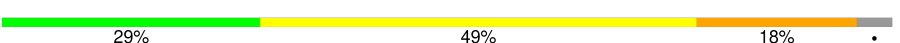
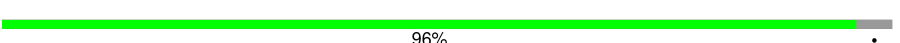
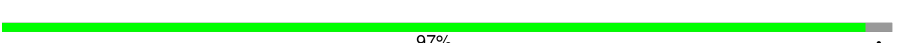

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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			

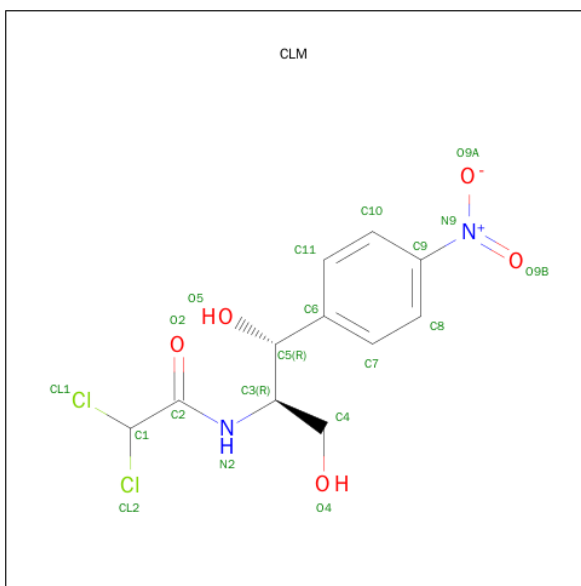
- Molecule 4 is a protein called Ribosomal Protein L32.

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: $C_{11}H_{12}Cl_2N_2O_5$).



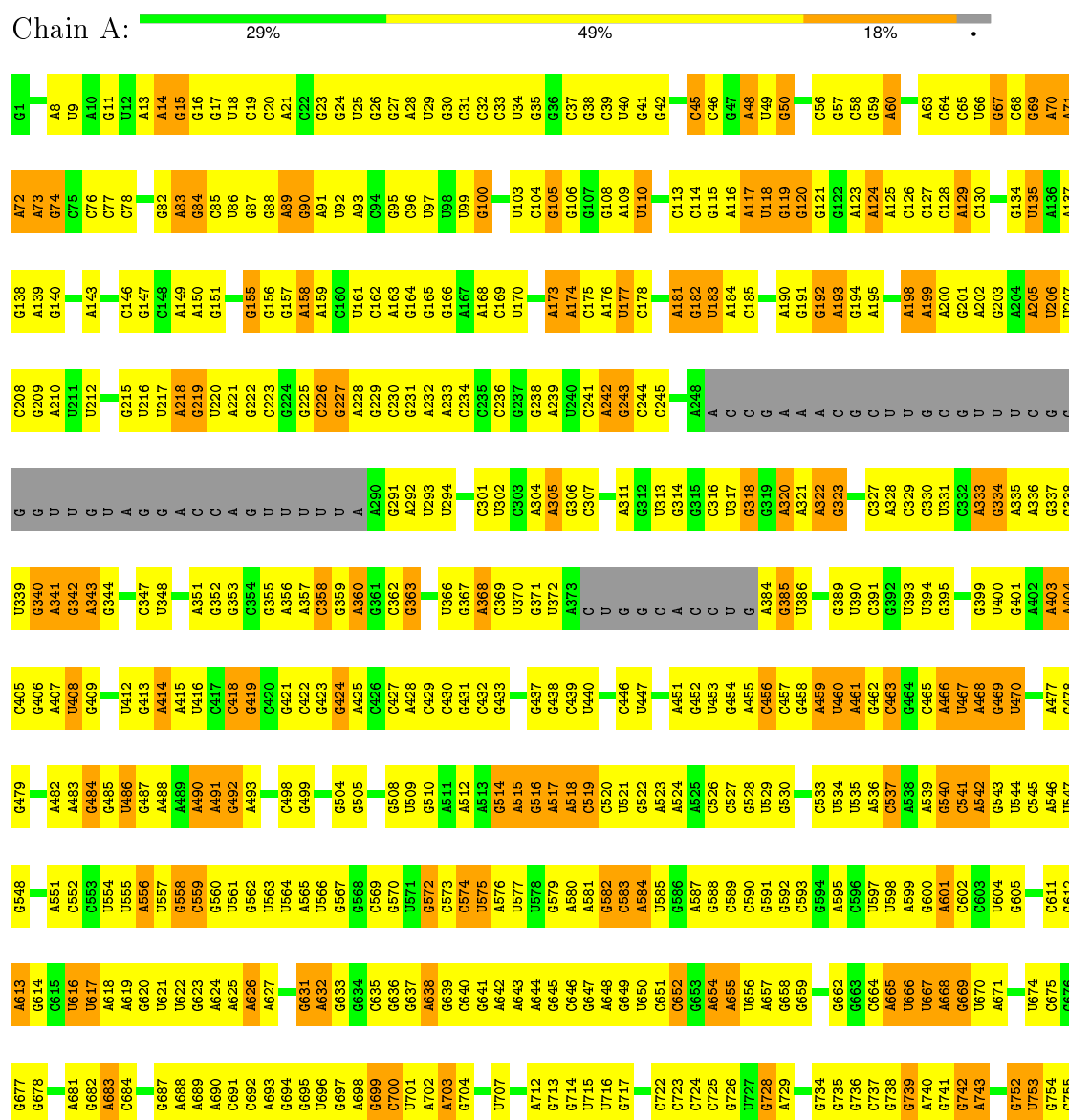
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
6	A	1	20	11	2	2	5	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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

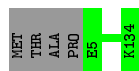


A1807	C1665	U1592	A1525	A1457	G1387	A1321	G1251	U1170	A1032	G958	G	U823	C756
C1808	G1566	C1593	U1526	A1468		G1322	C1262	A1171	G1032	C959	G	U824	U757
G1809	A1667	U1594	G1527	U1469	A1391	G1323	C1263	U1172	G1103	G768	C	C825	C759
U1810	C1668	A1595	C1528	G1460	G1392	G1324		G1173	G1104		C	U826	C759
A1811	A1669	A1596	G1529	G1465	G1393	U1325	G1258	G1174	U105	A964	C	C827	U760
U1812	G1670	C1597	U1530	G1466	U1326	U1326	A1259	A1175	U1036		U	C828	G761
A1813	A1671	C1598	G1531	C1466	C1327	C1327	A1260		U1038	C968	A	C829	A762
	A1672	G1599	A1532	U1467	A1397	U1328	G1261	G1183	U109	U969	C	C830	A763
U1817	C1673	U1600	G1533	A1468	G1398	U1329	U1262		A1039	A970	C	C831	A764
G1818	C1674	A1594	U1534	U1469	G1399	G1330	G1263	A1187	G1110	C972	A	A832	C765
U1819	C1675	G1602	G1535	G1470	A1400	G1331	C1264	A1188	G1111	A971	G	A833	C766
G1820	U1676	A1603	G1536	G1471	G1401	G1332	G1265	G1189	U1044	U973	C	U1045	A766
A1821	C1677	A1604	U1537	C1472	G1402	G1333	G1266	C1190	G1045	U974	U	G1046	G767
C1822	G1678	A1605	U1538	U1473	U1403	A1334	A1267	G1191	U1046	C975		A838	U768
G1823	U1679	C1606	U1539	U1474	C1404		U1268		G1047	C976	A	U839	
C1824	A1680	A1607	C1540	U1475	A1405	G1337	U1269	G1118	U1048	G977		U840	G772
U1825	A1681	U1608	G1541	G1476		G1338	G1270	G1119	C1049	U978	C909	G841	G773
G1826	G1682	U1611	G1542	U1480	U1409	U1339	C1271	U1195	U1049	A979		A842	A774
C1827	G1683	U1612	G1543	U1481	U1410	G1340	G1272	U1196	C1054	C980		G843	U775
G1828	A1684	G1613	A1544	U1482	C1411	U1341	G1273	U1197	U1055	C981		G844	G776
C1829	A1685	C1614		U1483	C1412	U1342	C1274	C1198	A1056	C982			
U1830	A1686	C1614	U1547	G1483	C1415	C1343	A1275	U1199	G1125	C983			
G1831	C1687		U1548	G1484	C1416	C1344	U1276	G1200	G1058	A984		C850	
			U1549	U1485	A1416	G1345	G1277	G1201	A1059	C985		C851	U784
G1834	U1690	G1617	C1549	U1486	C1417	C1346	A1278	U1202	G1060	A986		U852	U785
C1835	U1691	A1618	U1551	C1487		G1347	G1279	A1203	A1061	C987		G854	U786
G1836	C1692	U1619	C1552	G1488	A1420	C1348	U1280	U1204				G855	A787
	G1693		G1553	A1489	A1421	C1349	A1281	G1205	A1065	A994		A856	G788
A1840	A1694		U1554	U1490		G1350	C1282		G1066	A995		U857	G789
			A1555		U1424	C1351	C1283	G1209	G1067	C996		G858	A790
A1851	U1697	A1626	A1556	G1493	G1425	G1352	G1284	C1210	A1068	C997		U860	G791
	C1698	C1627	G1557	G1494	U1426	A1353	A1285	G1211	G1069	C998		C861	
G1854	C1699		C1558	G1495	U1427	A1354	U1286	U1212	G1070	A999		A862	A794
C1855	U1700	C1631	U1559	G1496	G1428	A1355	A1287	U1213	U1071	A1000		C863	A795
U1856	C1703	A1632	A1560	C1497	A1429	G1356	A1288	A1140	U1072	A1001		C864	A796
G1857	G1704	A1633	A1561	G1498	G1430	U1357	A1289	A1214	G1073	C931		A865	G798
			G1562	A1499	U1431	C1358	G1216	U1215	G1074	C1003		U866	C799
A1867	A1707	G1635	U1563	U1500	G1432	G1359	U1292	U1217	C1075	A1004		C867	U800
	C1708		U1564	C1501	A1433		A1293	C1218		U1005		U868	A801
G1871	U1709	C1640	G1565	G1502	U1434	C1364		C1219	G1079	C1006		C869	A802
	U1710		G1566	U1503	G1435	U1365	G1298	G1220	A1080	A1007		C870	C803
C1876	C1711	G1642	G1571	G1504	G1436	A1366	A1299	C1221	A1081	G1008		U871	C804
G1877	G1712	U1645	C1572	U1505	A1437	A1367	U1300	G1222	C1083	C939		G872	C805
C1878	A1714		U1573	C1506	G1438	G1368	A1301	G1223	C1083	C940		U873	A806
G1879	A1715	C1648	A1574	A1507	G1439	G1369	C1302	U1224	A1084	U941		A874	A807
U1881	G1716		C1575	G1508	G1440	U1370		G1225	G1085	G1013		G875	C808
G1882	A1717	U1651	G1576	A1509	A1441	G1371	U1306	A1226	C1086	U1015		A876	C809
				A1510	C1442	A1372	U1307	A1227	C1087	C1016		G877	U810
A1883	G1719	G1652	G1579	A1511	G1443	G1373	U1308	A1233	A1088	U1019		C878	G811
C1884	C1580	C1653	C1580	A1512	C1444	G1374	G1309	C1234	C1089	A879		A879	G812
G1885	C1581	A1654	C1581	U1513	U1445		C1310		C1090	U1020		C880	A813
C1886	G1722	C1655	A1582	C1514	U1446	G1377	C1311	U1161	C1091	A1021			A814
G1887	U1723	U1656	G1583	U1515	U1447			A1162	U1092	A1022		A886	A815
C1888	A1794	A1657	A1584	G1519	U1450	C1380	G1312	G1241	U1093	U1023		G887	U816
G1889	C1725		A1585	U1520	C1451	G1381	A1314	U1244	G1096	G1024		G888	A817
	C1726	G1660		U1521	U1452	G1382	A1315	G1245	A1097			C889	G818
C1891	C1727	C1661	A1588	U1522	U1453	C1383	G1316		A1098	G1028		U890	C819
	A1728	G1662	G1589	C1522	A1453	C1384			A1099	C1029		A891	U820
U1894	C1729	C1663	U1590	A1523	C1456	C1385	C1319	G1249	A1099	U1030		G892	A821
A1995	G1730	G1664	U1591	C1524		A1386	A1320	A1250	G1100	C1031		G	G822



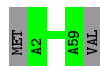
- Molecule 3: Ribosomal Protein L22

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 will therefore be 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	18,20,20	3.17	8 (44%)	22,27,27	2.68	5 (22%)

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	-	0/22/22/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2884	CLM	C8-C7	2.12	1.42	1.38
6	A	2884	CLM	C6-C5	2.71	1.55	1.51
6	A	2884	CLM	C11-C6	3.41	1.44	1.39
6	A	2884	CLM	C10-C9	3.81	1.46	1.38
6	A	2884	CLM	C5-C3	4.13	1.58	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2884	CLM	C10-C9-N9	-9.01	112.22	119.48
6	A	2884	CLM	O5-C5-C6	-2.64	105.34	111.16
6	A	2884	CLM	C10-C9-C8	2.30	123.82	119.83
6	A	2884	CLM	O2-C2-N2	2.89	128.59	122.93
6	A	2884	CLM	C8-C9-N9	5.56	123.97	119.48

There are no chirality outliers.

There are no torsion outliers.

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.