



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 06:54 AM 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 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/ValidationPDFNotes.html>

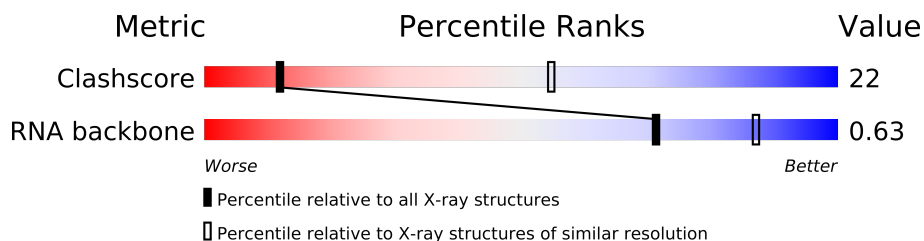
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1039 (3.66-3.34)
RNA backbone	1838	1007 (4.22-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59940 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

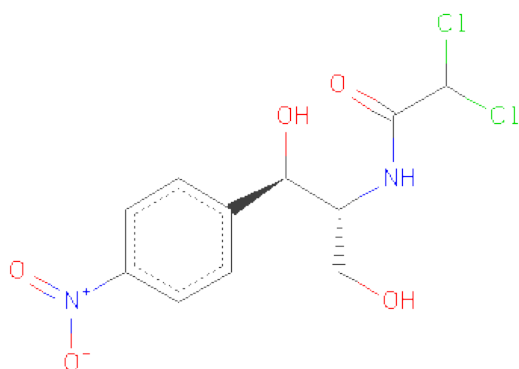
- Molecule 4 is a protein called Ribosomal Protein L32.

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

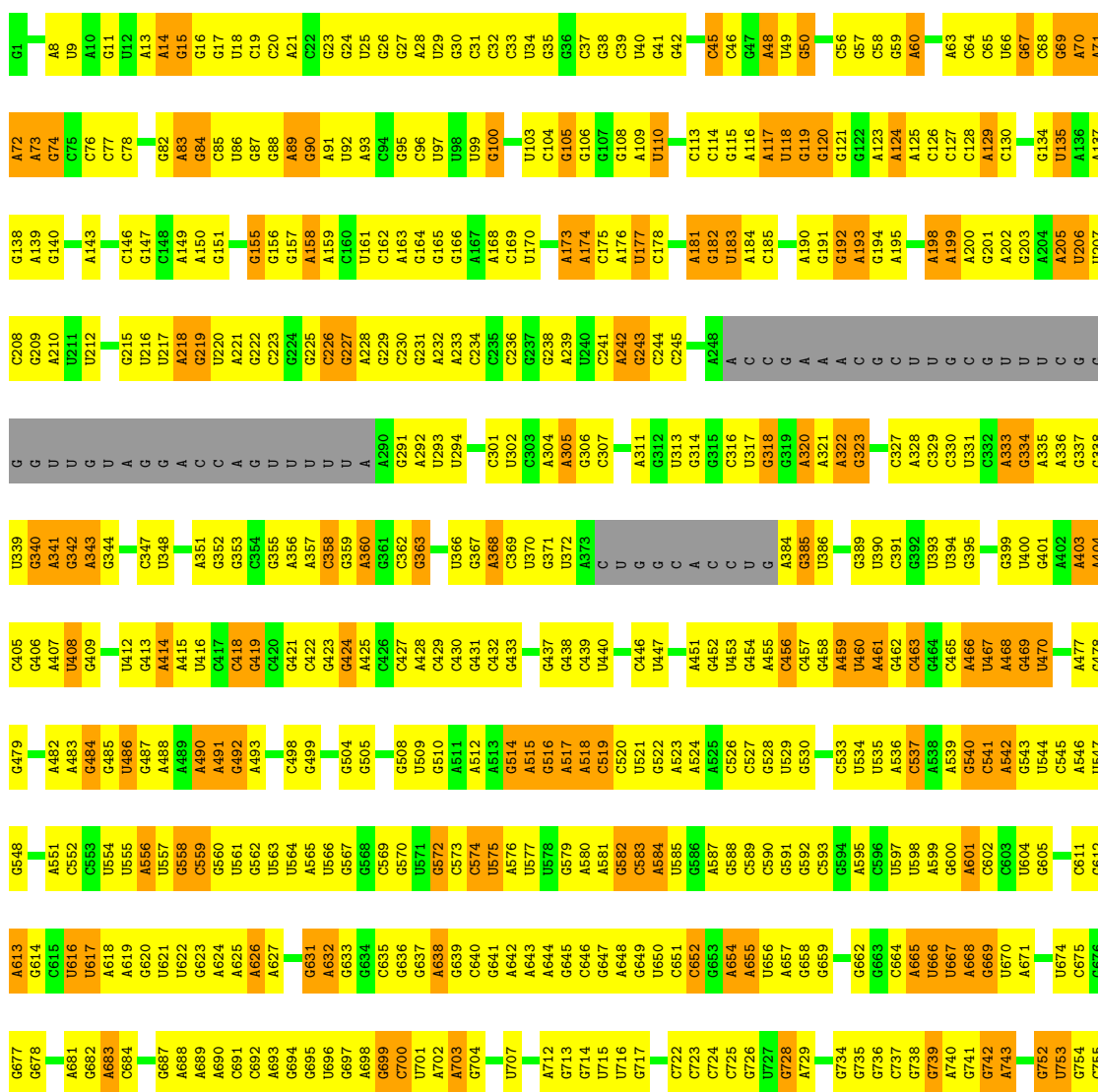
3 Residue-property plots

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.

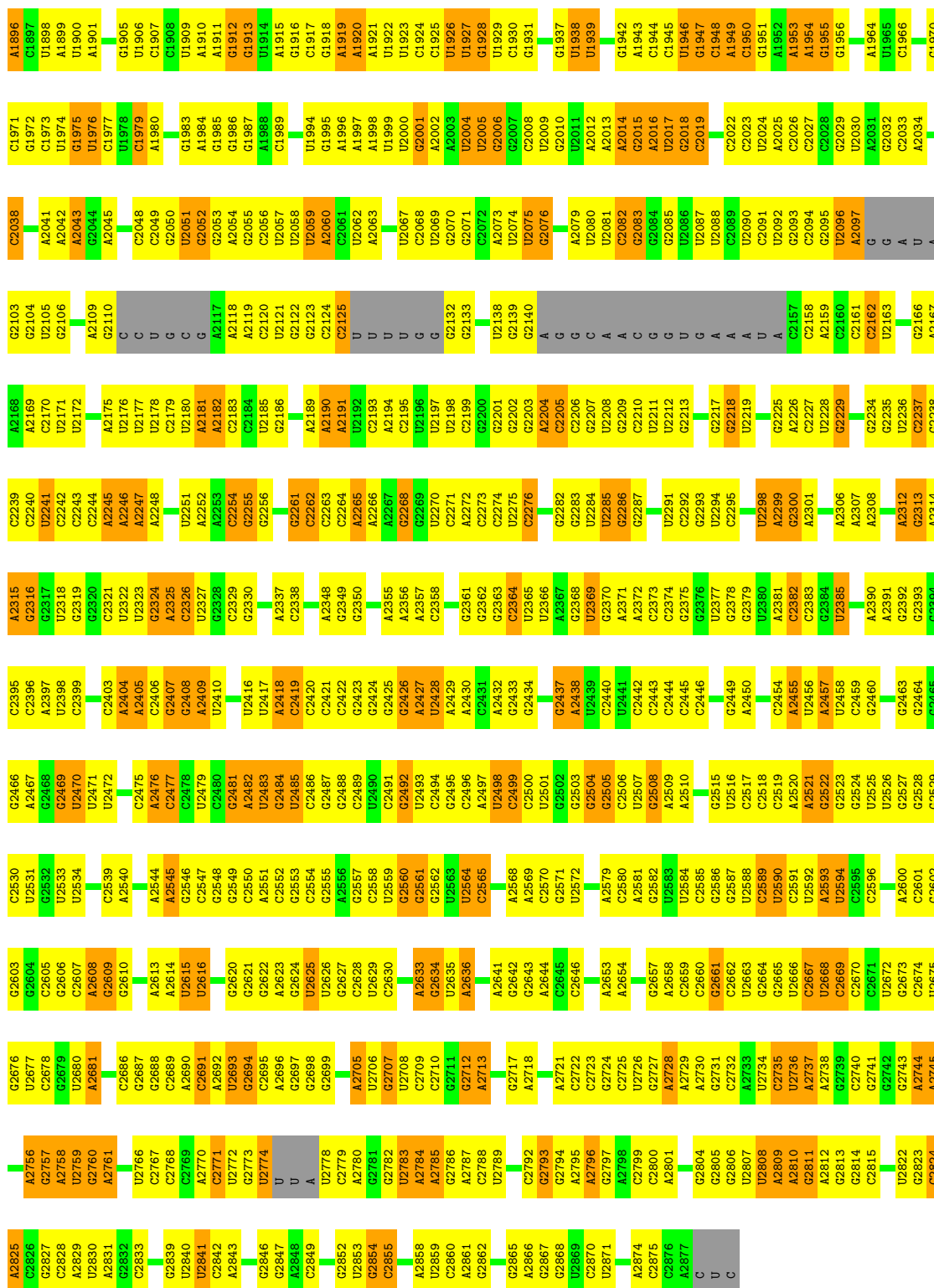
Note EDS was not executed.

• Molecule 1: 23S rRNA

Chain A:

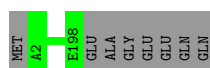


A1807	C1665	U1592	A1525	A1457	G1387	A1321	G1251	U1170	U1101	A1032	G958	G	U823	C756
C1808	G1666	C1593	U1526	A1458	A1391	G1322	C1261	A1171	G1102	A1033	C959	G	U824	U757
C1809	A1667	U1594	C1527	U1459	A1392	G1323	C1262	U1172	G1103	U1034	C960	C	C825	C758
U1810	G1668	A1595	G1528	G1460	G1393	G1324	G1258	G1173	G1104	G1035	U964	C	U826	C759
A1811	A1669	A1596	C1529	G1465	G1394	U1325	A1259	G1174	U1105	U1036	A964	U	C827	U760
U1812	G1670	A1597	U1530	C1466	G1394	U1326	A1260	A1175	A1106	U1037	U968	A	C828	G761
A1813	A1671	G1598	C1531	C1467	A1397	C1327	A1261	G1183	A1107	U1038	U969	C	C829	A762
U1817	A1672	G1599	A1532	U1467	A1398	G1328	G1262	G1184	U1108	A1039	U970	C	C830	A763
G1818	C1673	U1600	G1533	A1468	G1399	U1329	U1263	A1187	A1109	U1040	A970	C	C831	A764
U1819	A1674	A1534	C1534	U1469	A1400	G1330	G1264	A1188	G1110	G1041	A832	A	A832	C765
A1820	C1675	G1602	A1535	G1470	A1401	G1331	G1265	G1189	C1111	C972	A971	A	A833	A766
G1820	A1603	A1603	G1536	G1471	G1401	G1332	G1266	G1190	U1112	U1044	U973	C	U833	G767
A1821	U1537	A1604	U1537	C1472	G1402	G1333	A1267	C1190	C1113	U1045	U974	U	A838	U768
C1822	G1678	A1605	A1538	U1473	U1403	A1334	A1267	G1191	G1118	U1046	C975	U	U839	
G1823	U1679	C1606	U1539	A1474	C1404	G1337	U1268	A1192	A1192	U1047	C976	A	U840	G772
C1824	A1607	U1607	C1540	U1475	A1405	U1338	G1269	G1193	U1119	G1048	C977	C909	G841	G773
U1825	U1608	U1608	G1541	G1476	A1406	U1339	C1270	U1194	U1194	C1049	U978	C910	A842	A774
A1826	G1542	G1543	G1542	G1480	U1409	U1340	C1271	U1195	G1121	U1054	A979	A911	G843	U775
G1827	U1611	U1612	A1544	U1481	U1410	C1340	G1272	G1196	A1122	U1055	C980	A912	G844	G776
C1828	U1613	C1614	A1545	U1482	C1411	G1341	G1273	U1197	G1123	A1056	C981	A913		A777
C1829	A1685	C1614	U1547	U1483	C1412	U1342	C1274	C1198	U1124	A1057	C982	C914		G778
U1830	A1686	C1614	U1548	G1484	C1415	C1343	A1275	U1199	A1126	U1058	A984	C915		
G1831	C1687	U1617	U1549	U1485	A1416	G1345	G1276	U1201	C1127	A1059	G985	A918		U784
U1834	U1690	G1617	C1549	G1486	C1417	C1346	A1277	U1202	G1128	U1060	A986	U919		U785
C1835	U1691	A1618	C1550	A1487	C1417	G1347	G1278	U1203	A1129	A1061	G987			U786
U1836	C1692	U1619	U1551	C1488	A1420	C1348	G1279	A1203	U1130					A787
A1840	G1693	C1623	C1552	G1489	A1421	U1349	A1281	G1205	A1065	A994	A994	A922		G788
U1851	A1694	A1624	U1554	U1490	G1435	G1350	C1282	G1209	G1066	A995	A995	A923		U789
U1854	U1697	A1626	A1556	A1493	U1424	G1351	C1283	C1210	C1135	G1067	C996	U925		A790
G1855	C1698	C1627	G1557	G1494	U1426	G1352	A1284	G1211	G1136	A1068	C997	C926		G791
U1856	A1699	C1631	U1558	G1495	U1427	A1353	A1285	U1212	A1137	G1069	C998	C927		A794
C1857	C1703	A1632	G1559	G1496	G1428	A1355	U1286	U1213	A1138	G1070	A999	G928		A795
U1867	G1704	A1633	A1561	G1498	A1429	U1356	A1288	C1214	A1139	U1071	G1000	A929		A796
U1870	A1707	G1635	U1563	U1500	U1431	U1357	A1289	A1215	A1141	G1073	A865	A930		A797
C1871	C1708	C1640	U1564	C1501	G1432	G1358	A1292	G1216	G1142	C1002	G1003	G931		G798
U1874	U1709	G1641	G1565	G1502	A1433	U1364	A1293	U1217	A1143	C1004	A1004	G932		C799
C1876	C1710	G1642	G1571	G1503	U1434	U1365	A1298	C1218	U1144	U1005	U1006	G933		U800
U1877	U1711	U1645	C1572	G1504	G1436	U1366	G1299	C1219	C1145	G1079	A1006	G934		A801
G1879	G1713	U1648	A1574	U1506	A1437	G1367	U1300	C1221	G1146	A1080	C870	C937		A802
U1880	A1714	C1648	C1575	C1507	G1438	G1368	C1302	A1224	U1151	A1081	U871	G938		C803
U1881	G1716	U1651	G1576	G1508	G1439	U1370	U1306	U1225	C1152	C1083	G872	C939		C804
A1883	A1717	U1652	U1579	A1510	C1442	G1372	U1307	A1226	A1153	C1086	A874	U941		G805
U1884	G1720	C1653	C1580	A1511	G1443	G1373	C1308	A1227	G1155	A1087	C877	G945		A806
C1885	G1721	A1654	C1581	A1512	C1444	G1374	G1309	U1233	U1160	C1089	A879	U1019		A807
U1886	U1722	C1655	A1582	U1513	A1445	U1377	C1310	C1234	U1161	C1090	C880	C948		G808
C1887	G1723	U1656	C1583	C1514	U1446	G1380	C1312	G1240	U1162	C1091	A1021	G949		C809
U1888	C1724	A1657	G1584	U1515	U1447	C1381	G1313	G1241	C1163	U1092	A1022	G950		A813
G1889	C1725	G1660	A1585	G1519	G1450	G1382	U1301	U1244	C1164	U1093	U1023	G951		A814
U1890	C1726	C1661	U1588	U1520	C1451	G1383	U1302	G1245	G1165	A1096	G1024	A952		A815
C1891	G1727	C1662	A1589	U1521	U1452	C1384	C1303	G1316	A1167	A1097	G1028	A953		U816
U1894	A1728	C1663	U1590	C1522	A1453	C1385	C1319	G1249	A1166	U1098	C1029	G955		A817
A1895	G1730	U1664	U1591	C1524	C1456	A1386	A1320	A1250	G1168	A1099	U1030	A956		G818
									C1169	G1100	C1031	G957		G819
													G	G822



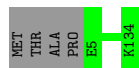
- Molecule 2: Ribosomal Protein L4

Chain K:



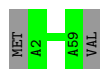
- Molecule 3: Ribosomal Protein L22

Chain L: 



- Molecule 4: Ribosomal Protein L32

Chain M: 



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	171.10Å 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 ⓘ

5.1 Standard geometry ⓘ

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 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

The worst 5 of 1942 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	20,20,20	3.49	9 (45%)	27,27,27	2.35	9 (33%)

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 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2884	CLM	O9A-N9	-7.51	1.11	1.25
6	A	2884	CLM	C7-C6	7.08	1.51	1.39
6	A	2884	CLM	O9B-N9	6.74	1.34	1.23
6	A	2884	CLM	C1-C2	5.10	1.60	1.53
6	A	2884	CLM	C5-C3	3.91	1.58	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2884	CLM	C10-C9-N9	-7.29	112.22	118.96
6	A	2884	CLM	C8-C9-N9	5.41	123.97	118.96
6	A	2884	CLM	O9A-N9-C9	3.40	120.94	114.42
6	A	2884	CLM	O2-C2-N2	2.94	128.59	122.93
6	A	2884	CLM	O5-C5-C6	-2.61	105.34	111.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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