



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:26 AM UTC

PDB ID : 1K01 / pdb_00001k01
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 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

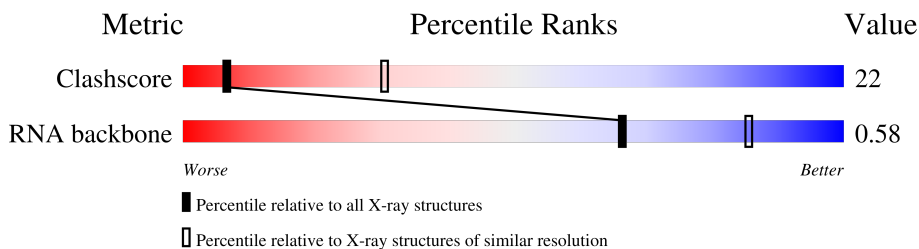
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

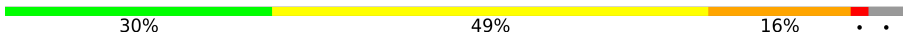
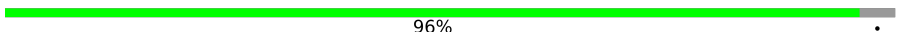
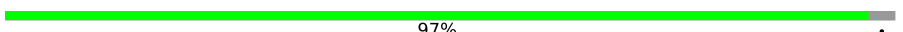
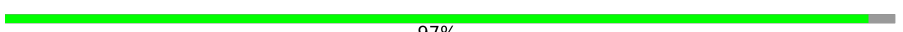
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	 30% 49% 16% . .
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			

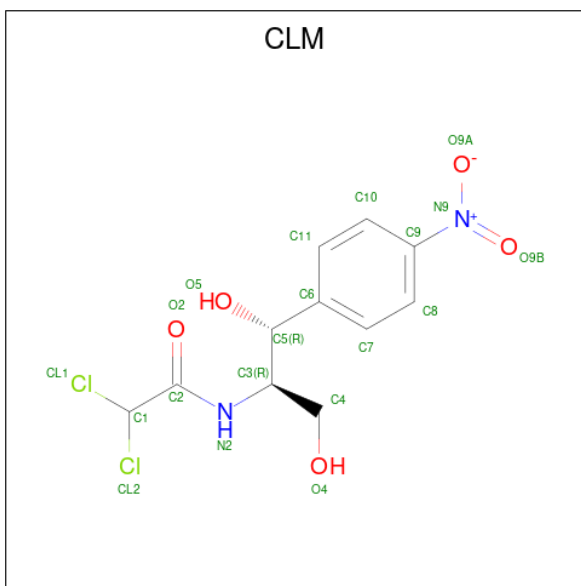
- Molecule 4 is a protein called Ribosomal Protein L32.

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $\text{C}_{11}\text{H}_{12}\text{Cl}_2\text{N}_2\text{O}_5$).



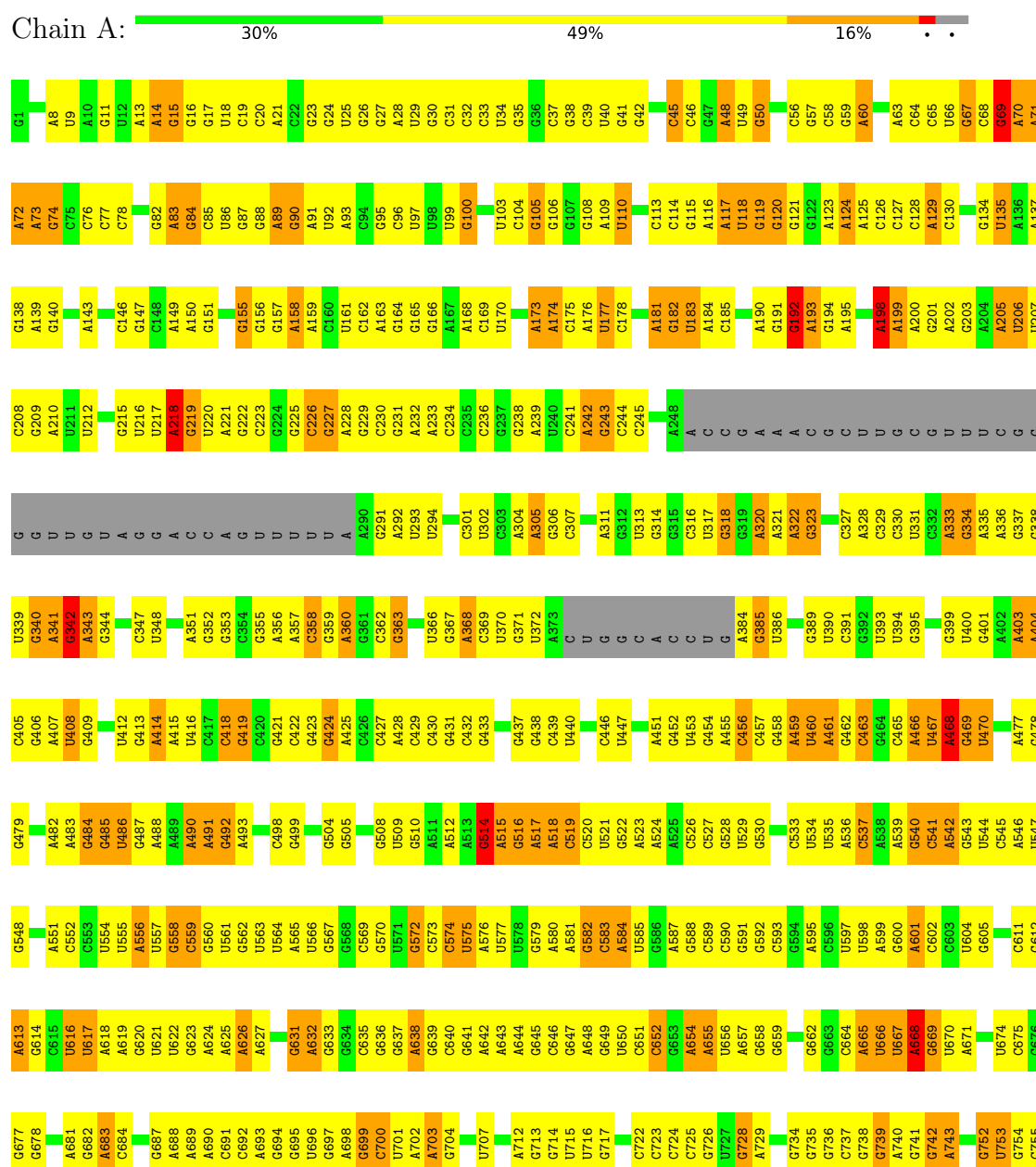
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 20	C 11	Cl 2	N 2	O 5	0	0

3 Residue-property plots

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

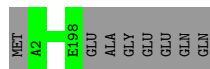


C1685	U1592	G1387	A1321	G1251	U1170	U1101	A1032	G958	G	U823	C756
G1666	C1593	G1391	G1322	C1252	A1171	G1102	G1033	C959	G	U824	U757
G1667	A1594	A1392	G1323	C1253	U1172	C1103	U1034	C959	C	C825	G758
G1668	A1595	G1392	G1324	G1258	G1173	G1104	G1035	U960	C	U826	C759
A1669	C1529	G1393	U1325	G1259	G1174	U1105	G1036	A964	C	C827	U760
G1670	U1530	G1394	U1326	A1259	A1175	A1106	U1037	U964	U	C828	G761
A1671	C1597	G1397	C1327	A1260	G1183	A1107	U1038	C968	A	C829	A762
A1672	A1532	A1397	G1328	G1261	G1188	U1108	U1039	U969	C	C830	A763
C1673	G1533	G1398	U1329	U1262	A1187	U1109	A1040	A970	C	G831	A764
A1674	A1534	C1399	G1330	G1263	A1188	C1110	G1041	A971	A	A832	C765
C1675	C1535	A1400	G1331	C1264	G1189	C1111	U1044	C972	G	A833	A766
G1676	A1603	G1401	G1332	G1265	G1190	U1112	U1045	U973	C	G767	G767
C1677	U1537	G1402	G1333	G1266	C1190	C1113	U1046	U974	U	U768	U768
A1605	A1538	U1403	A1334	A1267	G1191	G1118	U1047	C975	U	U838	G772
C1606	U1539	C1404	G1337	U1268	A1192	U1119	G1048	C976	A	U840	G773
A1607	C1540	A1405	U1338	G1269	G1193	G1120	C1049	G977	C909	U841	G774
U1608	G1541	G1406	G1339	C1270	U1194	G1121	U1050	U978	C910	A842	U775
U1611	A1542	U1409	U1340	G1271	U1195	G1122	C1054	G980	A911	G843	U776
U1612	G1543	U1410	G1341	G1272	G1196	A1123	A1055	C981	A912	G844	A777
G1613	A1544	C1411	U1342	G1273	U1197	G1124	A1056	C982	A913	G778	G778
C1614	G1547	C1412	G1343	C1274	C1198	U1125	A1057	G983	C914	C850	U784
U1548	U1548	C1415	C1344	A1275	U1199	A1126	G1058	A984	C915	C851	U785
C1549	C1549	A1416	G1345	G1277	G1201	G1127	A1059	G985	A918	C852	U786
C1550	C1550	C1417	G1346	A1278	U1202	G1128	U1060	A986	U919	G853	U787
U1551	U1551	C1417	G1347	G1279	A1203	A1129	A1061	G987	U919	G854	A787
C1552	C1552	A1420	C1348	U1280	G1204	U1130	U1065	A994	A922	A856	G788
G1553	G1553	U1421	A1349	A1281	G1205	C1134	G1066	A995	A923	U857	G789
A1554	A1554	C1411	G1350	C1282	G1209	C1135	G1067	C996	C924	G858	A790
U1555	U1555	C1412	G1351	C1283	G1210	G1136	A1068	C997	U925	U859	G791
A1556	A1556	U1424	G1352	G1284	G1211	A1137	G1069	C998	C926	U860	U794
G1557	G1557	U1426	A1353	A1285	U1212	A1138	G1070	A999	C927	G861	A794
C1558	C1558	G1427	A1354	U1286	U1213	A1139	G1071	C999	G928	A862	A795
G1559	G1559	G1429	A1355	A1287	U1214	A1140	U1072	A1000	A929	C863	A796
A1560	A1560	A1429	G1356	A1288	G1215	U1141	G1073	A1001	A930	C864	A797
G1561	G1561	G1430	U1357	A1289	A1216	G1142	G1074	C1002	G931	A865	G798
G1562	G1562	U1431	C1358	A1289	G1217	A1143	C1075	A1004	G932	U866	C799
U1563	U1563	G1432	G1359	A1292	U1218	U1144	U1075	U1005	G933	G867	U800
U1564	U1564	A1433	C1364	A1293	C1219	G1145	G1079	U1006	G934	U868	A801
G1565	G1565	U1434	U1365	A1298	G1220	C1146	A1080	A1007	C937	C869	A802
U1571	U1571	G1435	A1366	G1298	G1221	G1149	A1081	U1008	G938	C870	C803
C1572	C1572	A1437	A1367	A1299	G1222	C1150	A1082	G1083	G939	U871	C804
G1573	G1573	G1438	G1368	U1300	G1223	U1151	C1083	U1012	C940	G872	G805
A1574	A1574	G1439	G1369	C1302	A1224	C1152	A1084	G1013	U941	A874	A806
C1575	C1575	G1440	U1370	C1302	G1225	C1153	G1085	G1014	U942	G875	A807
G1576	G1576	A1441	G1371	U1306	A1226	A1154	C1087	U1015	U943	A876	C808
U1579	U1579	C1442	A1372	U1307	A1227	G1155	A1088	C1016	G944	G877	C809
C1580	C1580	G1443	G1373	C1308	C1233	U1156	A1089	U1019	U945	C878	G811
C1581	C1581	A1444	G1381	G1309	C1234	C1160	C1090	A1020	C948	A879	C812
A1582	A1582	U1446	G1382	C1310	C1234	U1161	G1091	A1021	G949	C880	A813
U1583	U1583	U1447	G1383	C1311	G1240	A1162	U1092	A1022	G949	A886	G814
G1584	G1584	G1447	G1384	C1312	G1241	C1163	U1093	U1023	G950	G887	A815
A1585	A1585	U1448	G1385	U1313	C1241	C1164	G1094	G1024	G951	U816	U816
U1588	U1588	G1450	G1386	A1314	U1244	G1165	A1096	U1028	A952	G888	A817
C1589	C1589	U1451	C1387	A1315	G1245	A1166	A1097	C1029	G953	C889	A818
C1590	C1590	A1453	G1388	G1316	G1245	A1167	G1098	A891	U954	U890	C819
A1591	A1591	C1456	C1389	C1319	G1249	A1168	A1099	A956	G955	G892	U820
U1592	U1592	G1456	A1386	A1320	A1250	C1169	G1100	G	G957	G	G822



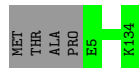
- Molecule 2: Ribosomal Protein L4

Chain K:  96% .



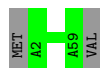
- Molecule 3: Ribosomal Protein L22

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: MG, CLM

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	0.27	0/66661	0.59	53/103976 (0.1%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	A	C2'-C3'-O3'	7.71	121.07	109.50
1	A	1715	A	C2'-C3'-O3'	7.33	120.50	109.50
1	A	2608	A	C2'-C3'-O3'	7.26	120.38	109.50
1	A	813	A	C2'-C3'-O3'	7.21	120.32	109.50
1	A	2693	U	C2'-C3'-O3'	7.04	120.06	109.50

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	1935	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59940	0	30015	1940	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 1940 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

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Mol	Chain	Res	Type
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 oligosaccharides 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	20,20,20	3.30	10 (50%)	23,27,27	2.55	8 (34%)

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 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2884	CLM	C7-C6	7.69	1.51	1.39
6	A	2884	CLM	O9B-N9	6.71	1.34	1.22
6	A	2884	CLM	C1-C2	5.24	1.60	1.53
6	A	2884	CLM	C10-C9	4.19	1.46	1.38
6	A	2884	CLM	C5-C3	4.13	1.58	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2884	CLM	C10-C9-N9	-8.15	112.22	119.34
6	A	2884	CLM	C8-C9-N9	5.30	123.97	119.34
6	A	2884	CLM	O2-C2-N2	3.15	128.59	122.96
6	A	2884	CLM	O5-C5-C6	-2.70	105.34	111.20
6	A	2884	CLM	C10-C9-C8	2.45	123.82	119.88

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

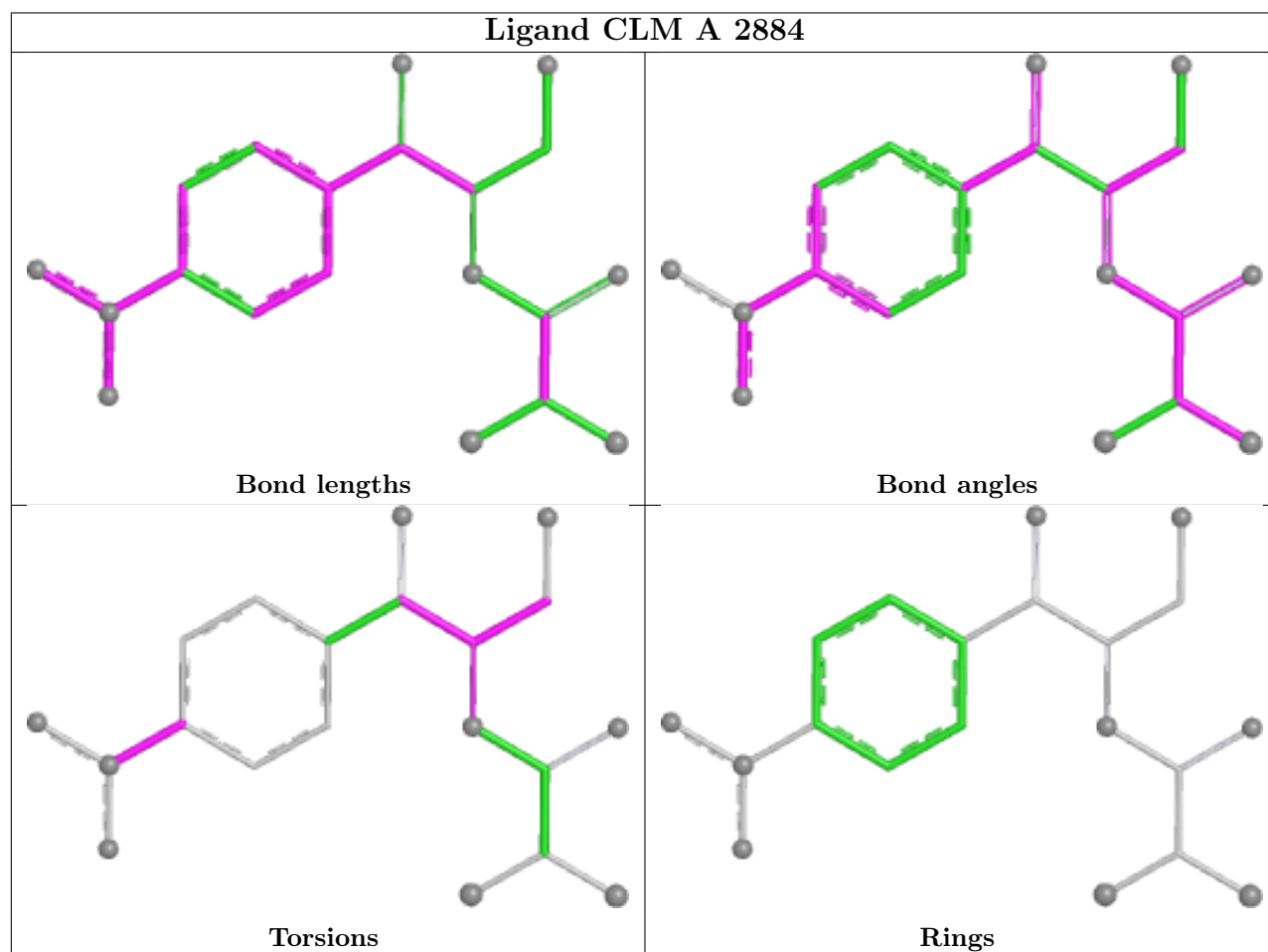
There are no ring outliers.

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 [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.