



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:41 PM UTC

PDB ID : 1JZX / pdb_00001jzx
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 : 3.10 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)
Xtrriage (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

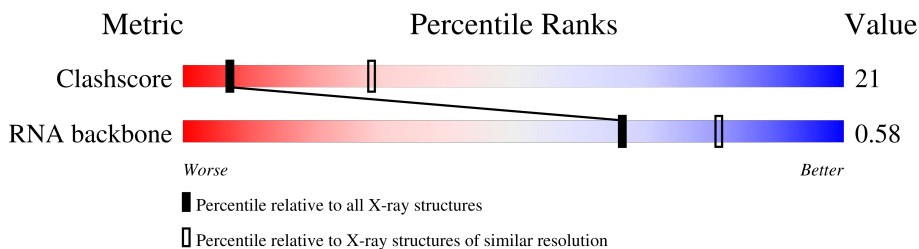
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	
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 59946 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			

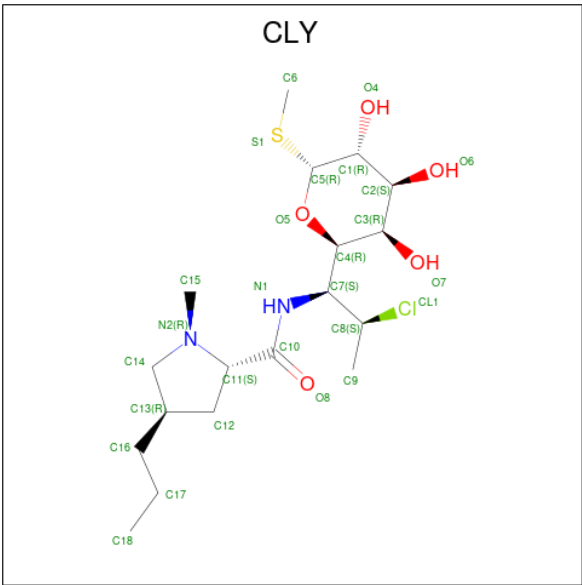
- Molecule 3 is a protein called Ribosomal Protein L22.

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 CLINDAMYCIN (CCD ID: CLY) (formula: C₁₈H₃₃ClN₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	Cl	N	O	S	0	0
			27	18	1	2	5	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

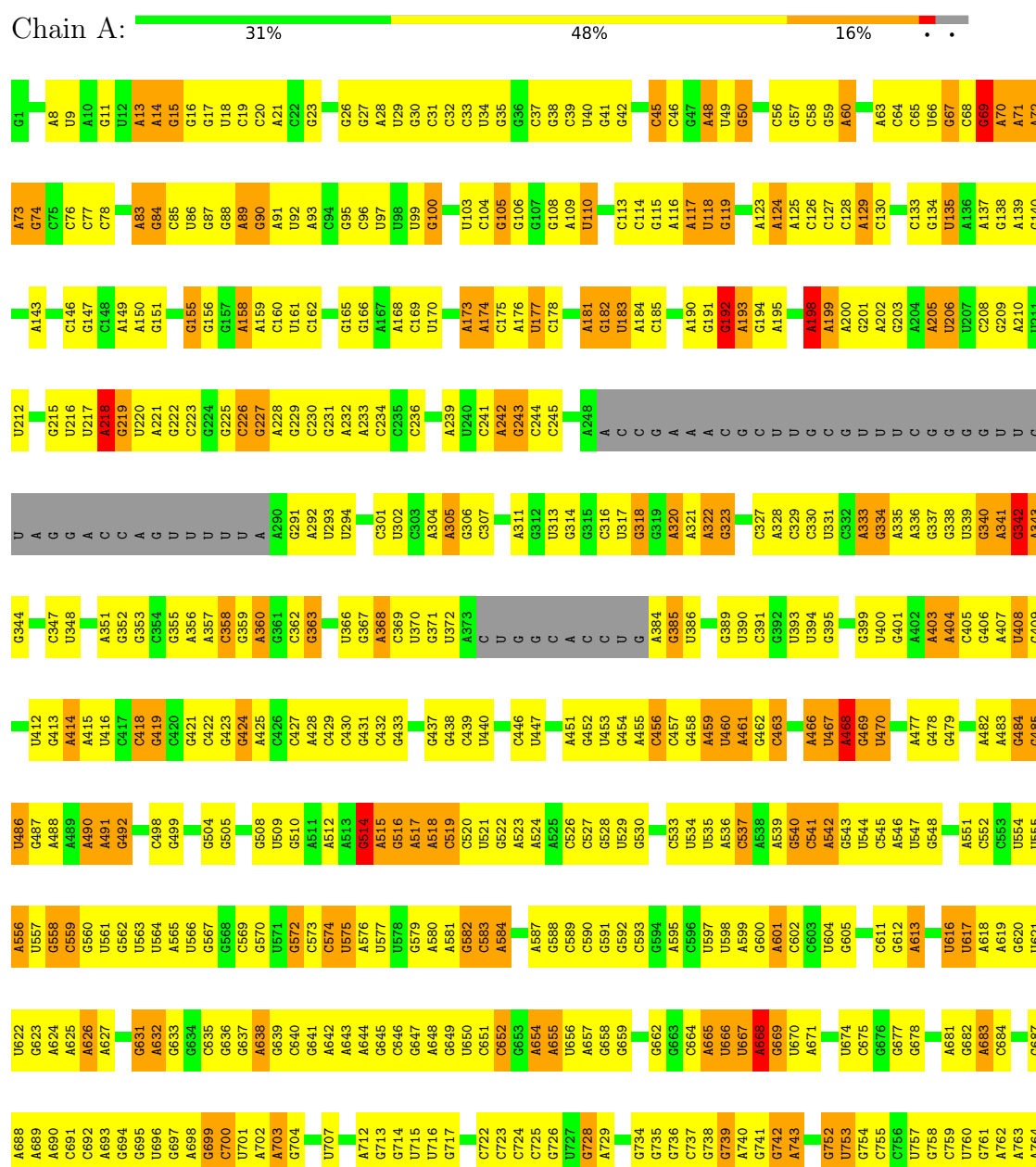
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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

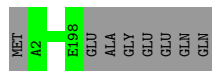


A1753	G1683	U1611	U1539	A1474	U1403	G1285	G1189	G1118	G1047	U974	G	A833	C765
G1754	G1684	U1612	C1540	U1475	C1404	G1286	C1190	U1119	U1048	C975	C	A838	A766
G1755	A1685	G1613	G1541	G1476	A1405	A1287	G1191	C1120	C1049	C976	U	U839	G767
C1756	A1686	C1614	G	G	G	U1288	A1192	G1121	G	G977	U	U768	U768
C1757	U1688	G1617	U1547	G1480	U1409	G1289	G1193	A1122	C1055	U978	A	G840	G773
C1758	U1689	U1618	U1548	U1481	U1410	G1290	U1194	G1123	A1054	A979	C909	G841	G773
C1762	G1690	A1619	C1549	U1482	C1411	G1271	U1195	A1124	U1056	G980	C910	A842	A774
G1763	G1691	G1623	U1551	G1483	C1412	G1272	U1196	G1125	A1057	C981	A911	G843	U775
A1764	C1692	C1552	C1552	G1484	C1415	G1273	U1197	A1126	G1058	C982	A912	G844	G776
C1765	A1693	A1485	G1553	U1485	C1416	G1274	C1198	G1127	A1059	G983	A913	G	A777
U1766	A1625	A1486	G1554	A1486	C1417	A1275	U1199	C1128	U1060	A984	A918	C850	G778
G1767	A1626	C1487	A1555	G1488	G1417	G1276	G1200	A1129	A1061	G985	U919	C851	U784
U1768	C1627	G1489	A1556	G1489	A1420	A1278	U1202	U1130	G	G	C	C852	U785
U1769	C1698	U1490	G1557	U1490	U1421	G1279	A1203	C1134	A1065	A994	A922	C853	U786
A1770	C1558	G	C1558	G	G	G1280	G1204	C1135	G1066	A995	A923	G854	U786
A1771	A1632	A1493	A1559	A1493	U1424	A1281	G1205	U1136	G1067	C996	A924	G855	A787
C1772	C1633	G1494	A1560	G1494	G1425	A1282	G1206	A1137	U1068	C997	C925	A856	G788
G1773	A1634	G1495	U1561	U1496	U1426	G1283	G1209	A1138	G1069	C998	U925	U857	G789
C1774	G1635	G1496	G1562	G1496	G1427	G1284	C1210	A1139	G1070	A999	C926	G858	A790
A1775	G1635	C1497	U1563	C1497	G1428	G1285	C1211	A1140	U1071	G1000	C927	U859	G791
A1776	C1640	G1498	U1564	G1498	A1429	U1286	U1212	U1141	G1073	A929	G928	U860	A794
A1777	C1641	A1499	U1564	A1499	G1430	A1287	U1213	G1142	U1074	A930	A929	G861	A795
U1778	G1642	U1500	G1571	U1500	U1431	A1288	U1214	A1143	C1075	G931	A1004	C863	A796
A1782	G	G1501	G1572	G1501	G1432	A1289	C1215	U1144	U1065	U1005	A1006	C864	A797
U1787	U1645	G1502	G1573	G1502	A1433	A1290	G1216	C1145	G1079	C1006	G933	A865	G798
C1788	C1648	G1503	A1574	G1503	U1434	A1291	U1217	G1146	A1080	A1007	G934	U866	U800
C1789	G	U1504	C1575	G1504	G1435	A1292	C1218	G	A1081	G1008	C937	U868	U800
G1790	U1651	U1505	G1576	U1505	A1436	A1293	C1219	G1149	G1082	A1012	G938	C869	A801
C1791	G1652	G1506	G	G1506	G1437	G1298	C1220	U1151	C1083	G1013	C939	C870	C803
C1792	C1653	A1507	C1580	G1508	G1438	A1299	C1221	U1152	A1084	G1014	G940	U871	C804
A1793	A1654	A1509	C1581	A1509	G1439	G1299	C1222	A1153	C1086	G1015	U941	G872	G805
A1794	C1655	A1510	U1582	A1510	G1440	A1300	G1223	U1154	C1087	C1016	U942	U873	A806
C1795	U1656	A1511	A1583	A1511	C1442	U1301	A1224	G1155	U1088	G1017	U943	A874	A807
G1796	A1657	A1512	G1584	U1512	G1443	C1302	G1225	G	C1089	A944	A944	G875	C808
C1797	G	U1513	A1585	U1513	C1444	G1371	A1226	G1160	C1090	A1019	G945	A876	C809
A1799	U1660	C1514	G	C1514	A1445	A1372	U1227	U1161	U1091	A1020	G877	G877	U810
C1800	C1661	U1515	A1588	U1515	U1446	G1373	G	U1162	U1092	A1021	C948	C878	G811
A1801	G1662	G	G1589	G	G1447	G1374	A1233	C1163	U1093	A1022	G949	A879	G812
C1802	C1663	G1519	C1590	G1519	U1447	G1377	C1234	C1164	G	G1024	G950	C880	A813
G1803	G1664	U1520	U1591	U1520	G1450	G1311	G1240	G1165	A1096	G951	G951	A866	G814
A1807	C1665	C1521	C1592	U1521	U1451	G1312	G1241	A1167	A1097	A952	A952	G867	A815
C1808	A1667	C1522	C1593	C1522	U1452	U1313	G	A1168	G1098	C1029	G953	G868	U816
G1809	G1668	A1523	U1594	A1523	A1453	G1381	U1244	G1169	A1099	U1030	U954	G869	A817
U1810	A1669	C1524	A1595	C1524	G	G1382	G1245	G1170	G	A1031	G955	G868	G818
A1811	G1670	A1525	A1596	A1525	C1456	C1383	G	U1171	U1101	A1032	A956	U890	C819
U1812	A1671	U1526	G	U1526	A1457	G1384	G1249	A1172	G1102	G1033	G957	A891	U820
A1813	G1672	C1528	C1598	G1527	A1458	C1385	C1250	U1173	C1103	U1034	G958	G892	A821
G1814	A1673	U1529	U1600	C1529	U1459	G1387	G1251	G1174	G1104	G1035	C959	G	G822
G	C1674	U1530	U1601	C1529	G1460	G1387	C1252	U1105	U1036	G1036	U960	G	U823
C1743	G1675	G1531	G1602	C1531	G1465	A1391	C1253	A1175	A1106	U1037	A964	G	U824
G1744	U1676	A1532	A1603	A1532	C1466	U1392	G1258	U1176	A1107	U1038	C	C	C825
A1746	C1677	G1533	G1604	G1533	U1467	A1397	G1259	U1177	U1108	A1039	C	C	U826
U1819	G1678	A1605	A1605	A1534	A1468	G1397	A1260	C1178	A1109	A1040	U968	U	C827
G1749	U1679	G1686	C1686	G1535	U1469	C1327	G1261	G	A1112	G1041	A970	A	C828
A1821	U1680	A1607	A1607	G1536	G1470	C1328	U1262	C1183	C1111	U1044	A971	C	G829
C1824	A1751	U1608	U1608	U1537	G	C1329	G1263	A1187	C1113	G1045	C972	C	C830
C1825	U1752	A1682	G	A1538	U1473	G1402	C1264	U1188	G	U1046	U973	A	A832



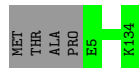
- Molecule 2: Ribosomal Protein L4

Chain K:  96% .



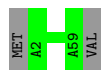
- Molecule 3: Ribosomal Protein L22

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	170.30Å 410.10Å 697.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.268 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59946	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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, CLY

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	52/103976 (0.1%)

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	A	C2'-C3'-O3'	7.63	120.95	109.50
1	A	1715	A	C2'-C3'-O3'	7.33	120.50	109.50
1	A	2608	A	C2'-C3'-O3'	7.31	120.47	109.50
1	A	813	A	C2'-C3'-O3'	7.24	120.36	109.50
1	A	2693	U	C2'-C3'-O3'	7.01	120.02	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	1877	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	27	0	32	2	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59946	0	30036	1877	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 21.

The worst 5 of 1877 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:1747:G:H4'	1:A:1749:G:H1'	1.29	1.14
1:A:2668:U:H4'	1:A:2669:C:H5'	1.32	1.12
1:A:940:G:H3'	1:A:941:U:H5''	1.34	1.09
1:A:367:G:H2'	1:A:368:A:H5''	1.34	1.08
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.07

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%)	556 (20%)	144 (5%)

5 of 556 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 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2312	A
1	A	2854	G
1	A	2426	G
1	A	2592	U
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 3 ligands modelled in this entry, 2 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	$\# Z > 2$
5	CLY	A	2881	-	26,28,28	1.79	6 (23%)	31,40,40	1.22	3 (9%)

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
5	CLY	A	2881	-	-	4/21/53/53	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	CLY	C7-N1	4.74	1.53	1.45
5	A	2881	CLY	C12-C11	-3.27	1.48	1.53
5	A	2881	CLY	C10-N1	2.97	1.40	1.34
5	A	2881	CLY	C4-C7	2.85	1.56	1.53
5	A	2881	CLY	O5-C4	2.28	1.47	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	CLY	C11-C10-N1	-3.02	109.89	116.52
5	A	2881	CLY	O8-C10-N1	2.75	127.89	122.96
5	A	2881	CLY	C12-C11-C10	2.45	116.05	111.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	CLY	C8-C7-N1-C10
5	A	2881	CLY	C12-C13-C16-C17
5	A	2881	CLY	C14-C13-C16-C17
5	A	2881	CLY	C4-C7-N1-C10

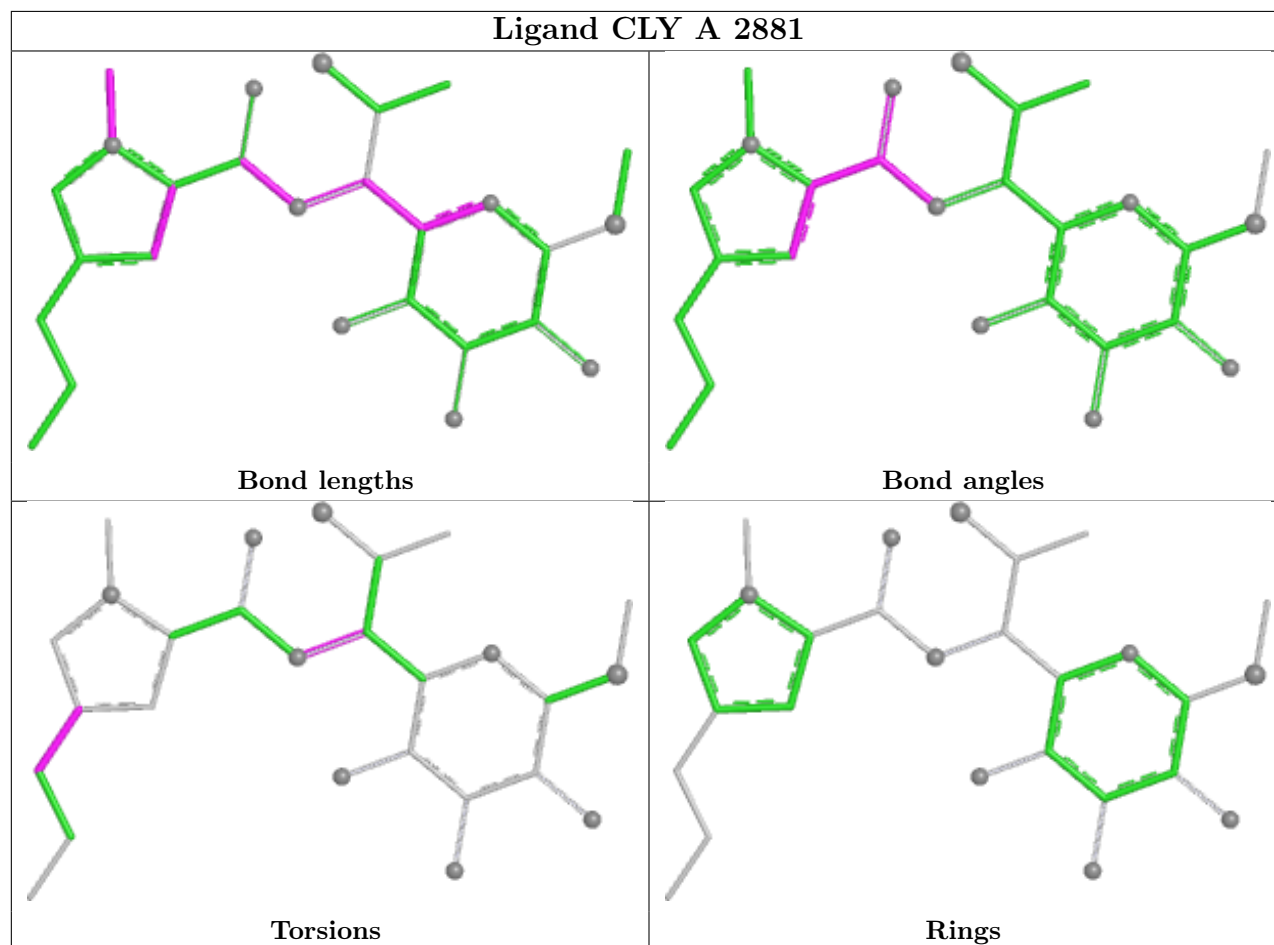
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	CLY	2	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.