



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 02:04 AM EDT

PDB ID : 1JZY  
Title : Structural Basis for the Interaction of Antibiotics with the Peptidyl Transferase Center in Eubacteria  
Authors : Schluenzen, 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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) : 2.36.2

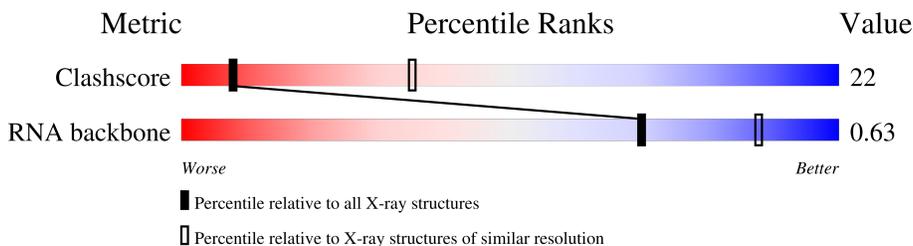
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

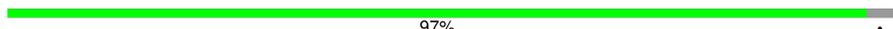
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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% 48% 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
5	ERY	A	2881	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 59970 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
			Total	C	N	O	P			
1	A	2774	59532	26556	10982	19221	2773	0	0	0

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
			Total	C			
2	K	197	197	197	0	0	197

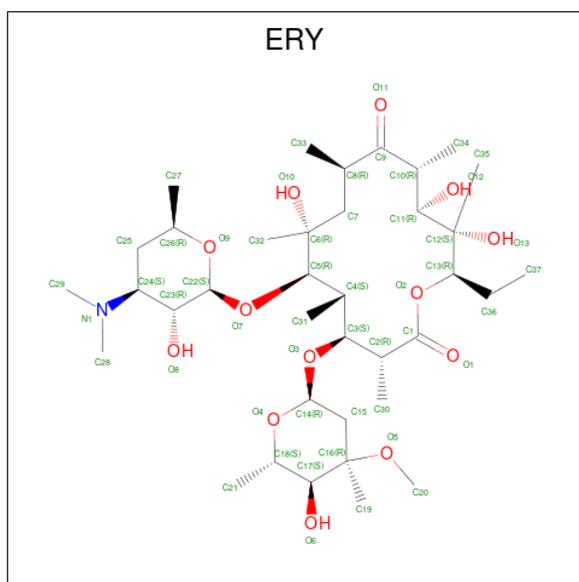
- Molecule 3 is a protein called Ribosomal Protein L22.

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

- Molecule 4 is a protein called Ribosomal Protein L32.

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

- Molecule 5 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	51	37	1	13	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

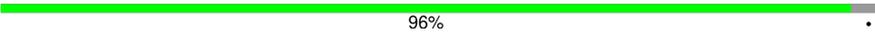
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0

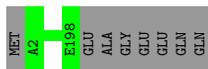


A1746	C827	C	A964	U1038	U1105	G1174	C1252	A1321	G1460	C1529	G1599	A1672	A1746
G1747	C828	U	C968	A1039	A1106	A1175	C1285	G1322	G1465	U1530	U1600	C1673	G1747
U1748	C829	A	U969	A1040	U1107	U1176	G1258	G1323	G1466	C1531	G1601	C1674	U1748
G1749	C830	C	A970	G1041	U1108	C1178	G1259	G1324	U1467	A1532	G1602	C1675	G1749
A1750	G831	C	A971	U1042	G1109	C1179	A1259	U1325	A1468	G1533	A1603	C1676	A1750
G1751	C832	A	A972	U1043	G1110	C1180	A1260	U1326	U1469	A1534	A1604	C1677	G1751
U1752	G833	C	C972	G1044	C1111	C1181	G1261	C1327	U1470	C1535	A1605	C1678	U1752
A1753	U834	C	U973	U1045	U1112	C1182	G1262	G1328	G1471	G1536	G1606	C1679	A1753
G1754	A835	U	U974	U1046	U1113	A1187	U1263	U1329	U1472	U1537	U1607	C1680	G1754
U1755	U836	U	C975	U1047	G1118	A1188	G1264	G1330	U1473	A1538	U1608	C1681	U1755
G1756	U837	A	C976	C1048	G1119	G1189	A1265	G1331	U1474	U1539	A1609	C1682	G1756
C1757	G838	C	C977	U1049	G1120	A1190	G1266	G1332	U1475	U1540	G1541	C1683	C1757
U1758	A839	C	U977	G1050	C1121	G1191	A1267	A1333	G1476	G1541	U1541	C1684	U1758
A1759	G840	C	U978	G1051	C1122	G1192	U1268	A1334	G1477	U1542	U1542	A1685	A1759
G1760	U841	C	A979	A1052	G1123	A1193	G1269	G1337	G1480	U1547	U1547	A1686	G1760
U1761	G842	C	A980	U1053	A1124	U1194	C1270	U1338	U1481	U1548	U1548	A1687	U1761
G1762	C843	C	G981	A1054	U1125	U1195	U1271	G1339	U1482	C1549	G1549	C1688	G1762
A1763	G844	C	U982	U1055	G1126	U1196	G1272	U1340	U1483	C1550	U1550	U1689	G1763
U1764	C845	C	G983	A1056	U1127	G1197	U1273	G1341	U1484	U1551	A1619	U1690	A1764
G1765	C846	C	A984	C1060	C1128	C1198	C1274	U1342	U1485	C1552	C1623	G1691	G1765
U1766	U847	C	G985	A1061	G1129	U1199	A1275	C1343	A1486	G1553	U1624	C1692	U1766
U1767	C848	C	A995	A1062	A1129	G1200	U1276	C1344	U1487	A1554	A1625	A1693	A1767
U1768	G849	C	U996	G1063	U1130	G1201	G1277	G1345	G1488	A1555	A1626	A1694	U1768
U1769	C850	C	C997	U1064	U1131	U1202	A1278	C1346	C1489	U1556	A1627	U1697	U1769
U1770	U851	C	U998	G1065	C1132	A1203	U1279	C1347	U1490	G1557	G1627	U1697	U1770
A1771	C852	C	C999	U1066	C1133	G1204	U1280	C1348	G1491	C1558	C1628	C1698	A1771
G1772	U853	C	C999	G1067	G1134	G1205	A1281	A1349	U1492	U1559	C1629	A1699	G1772
U1773	C854	C	A999	U1068	U1135	G1206	A1282	A1349	U1493	G1560	A1630	A1699	C1773
U1774	G855	C	U999	G1069	G1136	G1209	A1283	A1350	G1494	U1561	G1631	G1703	A1774
A1775	U856	C	A999	U1070	U1137	G1210	C1283	G1351	G1495	U1562	G1632	G1704	A1775
U1776	C857	C	U1001	G1071	A1138	C1211	C1284	G1352	G1496	G1563	A1633	G1705	U1776
A1777	U858	C	A1002	U1072	A1139	G1212	A1285	U1353	C1497	U1564	G1635	U1710	A1777
U1778	C859	C	U1003	G1073	A1140	U1212	U1286	A1354	G1498	U1565	C1640	C1711	U1778
U1779	U860	C	A1004	U1074	U1141	U1213	A1287	A1355	A1499	U1566	G1641	G1712	U1779
A1780	G861	C	U1005	U1075	G1142	U1214	A1288	U1356	U1500	U1430	C1642	G1713	G1780
U1781	C862	C	U1006	U1076	U1143	G1215	A1289	G1357	U1431	U1433	G1643	A1714	U1781
C1782	U863	C	A1007	U1077	U1144	G1216	A1290	U1358	U1432	U1434	U1574	G1715	C1782
U1783	C864	C	U1008	U1078	C1145	G1217	A1291	G1359	G1433	G1435	U1575	G1716	U1783
U1784	U865	C	G1008	A1080	G1146	U1218	A1292	C1364	U1434	G1436	C1576	A1717	U1784
G1785	C866	C	A1012	A1081	U1149	C1219	A1293	U1365	U1435	U1437	U1506	G1722	G1785
C1786	U867	C	G1013	G1082	C1150	G1220	A1298	U1366	G1436	G1438	A1507	U1723	C1786
U1787	G868	C	U1014	A1083	U1151	C1221	G1298	A1366	G1437	G1439	U1508	U1724	U1787
U1788	C869	C	U1015	U1084	C1152	G1222	A1299	A1367	U1438	U1439	G1509	C1725	U1788
G1789	U869	C	C1016	G1085	A1153	G1223	U1300	G1368	G1440	G1441	A1510	C1726	U1789
C1790	C869	C	U1019	U1087	A1154	U1224	U1301	U1369	A1441	C1442	A1511	U1727	C1790
U1800	U870	C	A1020	A1088	G1185	G1225	C1302	U1370	U1442	U1443	A1512	U1728	A1800
C1801	C871	C	A1021	C1089	C1160	A1226	U1306	A1371	U1443	C1444	U1513	C1729	C1801
A1802	U872	C	A1022	U1092	U1161	G1227	U1307	A1372	U1444	U1445	C1514	U1730	A1802
G1803	C873	C	G1024	U1093	C1162	C1234	G1309	G1374	U1446	U1447	U1515	G1731	G1803
U1807	U874	C	U1028	U1096	C1164	G1240	C1310	G1377	U1447	G1450	G1519	U1732	U1807
C1808	C875	C	C1029	A1096	G1165	G1241	C1311	C1380	U1448	G1451	G1520	U1733	C1808
G1809	U876	C	U1030	A1097	A1166	G1242	G1312	C1381	U1449	U1452	U1521	G1734	G1809
U1810	C877	C	C1031	G1098	A1167	G1243	U1313	C1382	U1450	U1453	C1522	U1735	U1810
A1811	U878	C	A891	A1099	G1168	U1244	U1314	G1383	U1451	A1453	A1523	C1736	A1811
U1812	C878	C	A1032	A1100	C1169	G1245	U1315	G1384	U1452	U1456	C1524	U1737	U1812
A1813	U879	C	G1033	U1101	U1170	G1249	U1316	U1385	U1457	A1458	A1525	U1738	A1813
U1817	C879	C	U1034	U1102	A1171	G1250	C1319	C1386	U1458	U1459	U1526	G1742	U1817
G1818	U880	C	G1035	G1102	U1172	A1251	A1320	G1387	U1459	U1459	C1528	C1743	G1818
U826	C	C	U1037	G1104	U1173								U826

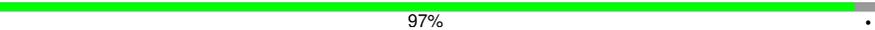


- Molecule 2: Ribosomal Protein L4

Chain K:  96%

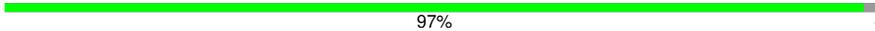


- Molecule 3: Ribosomal Protein L22

Chain L:  97%



- Molecule 4: Ribosomal Protein L32

Chain M:  97%



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	169.20Å 410.00Å 695.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.268 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	59970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	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: ERY, 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	3/103976 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1746	A	C2'-C3'-O3'	6.01	123.32	113.70
1	A	777	A	C2'-C3'-O3'	5.45	122.42	113.70
1	A	2588	U	C2'-C3'-O3'	5.12	121.89	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	1926	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	51	0	67	22	0
6	A	2	0	0	0	0
All	All	59970	0	30071	1944	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 1944 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'	1.30	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''	1.34	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	1.06

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%)	147 (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 147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2261	G
1	A	2760	G
1	A	2418	A
1	A	2564	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 monosaccharides 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	ERY	A	2881	-	53,53,53	1.63	11 (20%)	82,82,82	3.06	45 (54%)

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	ERY	A	2881	-	-	7/72/107/107	1/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	ERY	C7-C8	4.91	1.60	1.54
5	A	2881	ERY	O2-C13	-3.41	1.40	1.46
5	A	2881	ERY	C7-C6	3.36	1.59	1.54
5	A	2881	ERY	C35-C12	3.17	1.58	1.52
5	A	2881	ERY	C15-C14	2.99	1.58	1.51

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	ERY	O3-C3-C4	7.41	116.97	108.23
5	A	2881	ERY	C33-C8-C7	6.94	122.79	109.88
5	A	2881	ERY	C19-C16-C17	6.93	124.81	111.19
5	A	2881	ERY	O5-C16-C17	6.65	113.50	103.86
5	A	2881	ERY	C6-C5-C4	6.45	123.24	113.89

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	ERY	C17-C16-O5-C20
5	A	2881	ERY	O4-C14-O3-C3
5	A	2881	ERY	C1-C2-C3-O3
5	A	2881	ERY	C6-C7-C8-C33
5	A	2881	ERY	C1-C2-C3-C4

All (1) ring outliers are listed below:

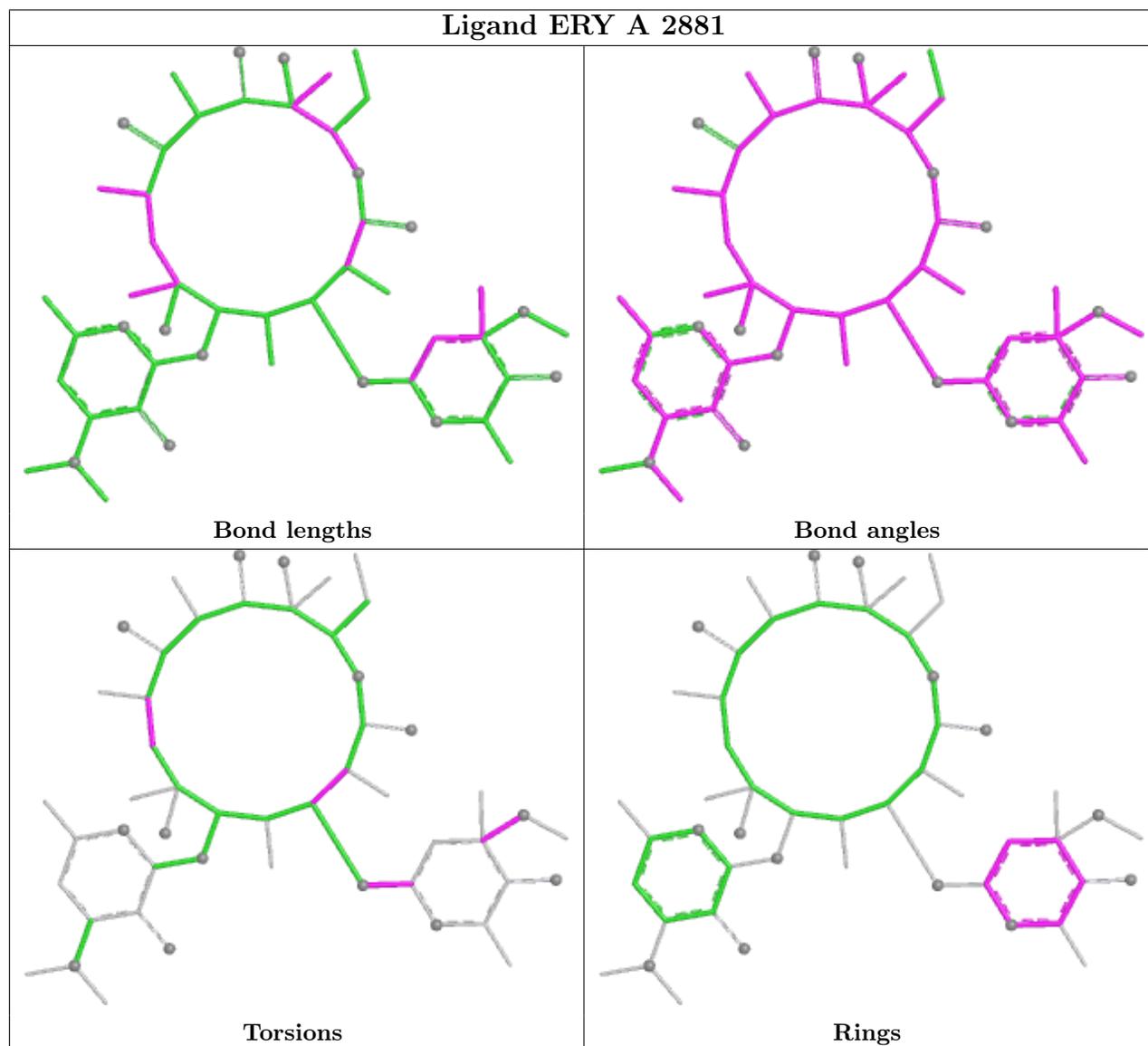
Mol	Chain	Res	Type	Atoms
5	A	2881	ERY	C14-C15-C16-C17-C18-O4

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	ERY	22	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.