



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:07 AM UTC

PDB ID : 1JZY / pdb_00001jzy
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)
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

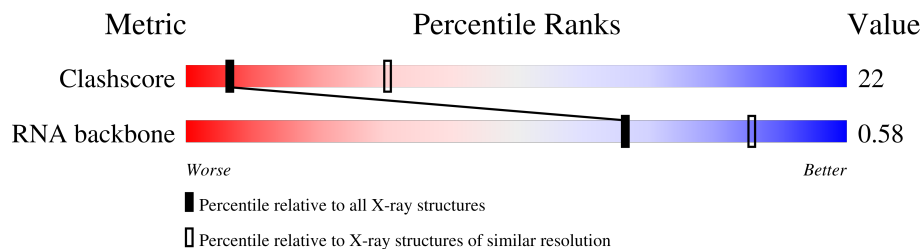
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	
2	K	205	
3	L	134	
4	M	60	

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

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
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			

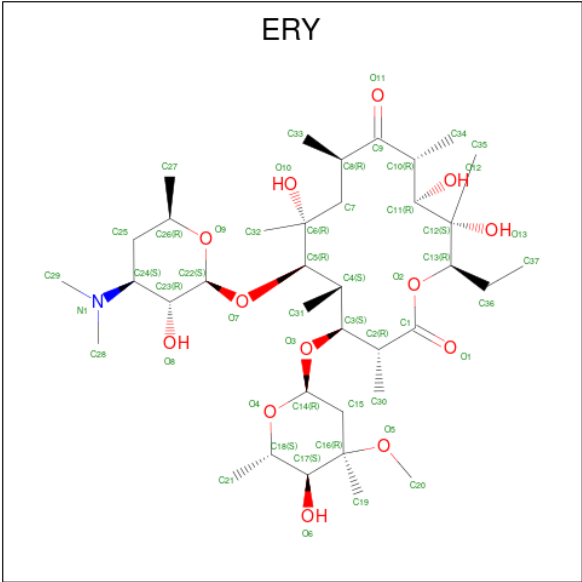
- Molecule 3 is a protein called Ribosomal Protein L22.

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 ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).



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

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

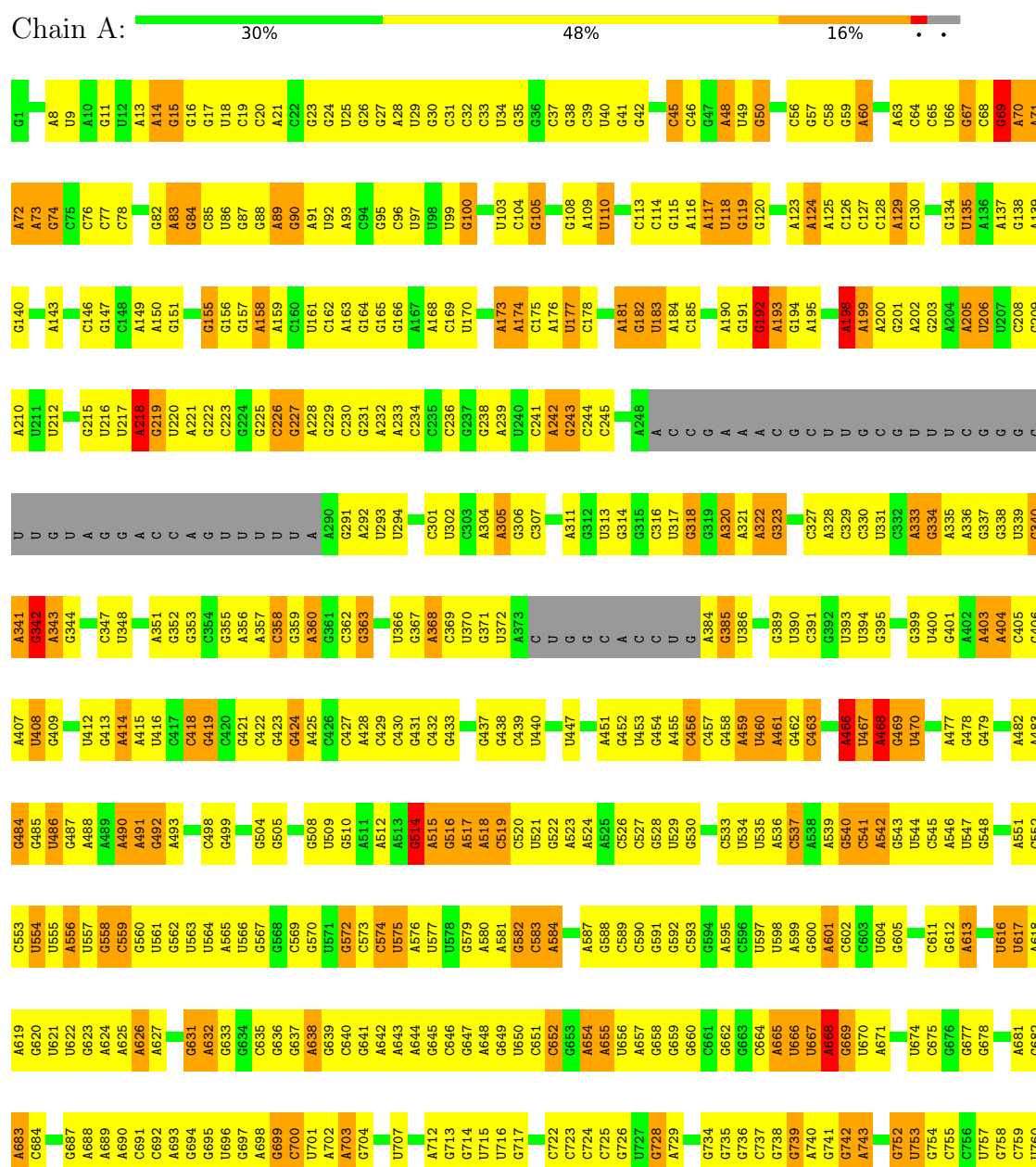
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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.

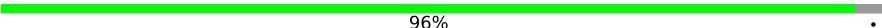
• Molecule 1: 23S rRNA

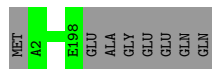


A1746	G1673	C1529	G1460	A1321	C1252	U1105	U1038	A964	C	G827	G761
G1747	C1673	U1530	G1465	G1321	C1283	A1106	A1039	A964	U	C828	A762
G1748	C1674	C1531	G1466	G1323	G1285	A1107	A1040	C968	A	C829	A763
G1749	C1675	A1532	C1467	G1324	G1288	U1108	G1041	C969	C	C830	A764
A1750	G1676	G1533	U1467	U1325	U1259	A1109	U1044	A970	C	G831	A765
A1751	C1677	A1534	A1468	U1326	A1260	G1110	U1045	A971	A	A832	A766
U1752	G1678	C1535	U1469	C1327	G1261	G1111	G1046	C972	G	G767	G767
A1753	U1679	G1536	G1470	G1328	U1262	C1112	U1047	A833	C	A833	U768
A1754	U1680	U1537	U1471	U1329	U1263	U1113	U1048	A838	U	A838	G772
G1755	U1681	U1538	U1472	G1330	G1264	G1118	C1049	U840	U	U839	G773
G1756	A1682	U1539	U1473	G1331	G1265	U1119	C976	U841	A	U840	A774
C1757	G1683	U1540	U1475	G1333	G1266	C1120	G977	A842	A	A842	U775
G1684	U1612	A1404	U1476	A1334	U1267	U1120	U978	A843	A	G843	G776
A1685	G1613	A1405	G1477	G1337	U1268	G1121	U1054	A844	A	G844	G778
A1686	C1614	U1409	G1480	G1338	U1269	A1122	A1055	C850	C909	C850	G784
A1687	U1617	U1410	U1481	G1339	G1270	A1123	A1056	U851	C910	U851	U785
G1688	G1618	C1411	U1482	U1339	C1271	G1124	A1057	U852	A911	U852	U786
G1689	U1619	C1412	G1483	U1340	G1272	U1125	U1058	U853	A912	C853	U787
U1690	A1619	G1484	U1484	G1341	C1273	G1126	A1059	U854	A913	G854	U788
G1691	C1623	C1582	U1485	U1342	C1274	A1127	C1060	A884	C915	C855	U789
C1692	A1624	G1583	U1486	U1343	U1275	G1128	U1061	U885	A918	U856	U790
A1625	G1625	U1554	U1487	G1344	U1276	A1129	A1066	A994	U919	U857	U791
A1626	A1626	A1555	G1488	G1345	G1277	U1130	G1067	A995	A922	U858	U792
C1627	U1697	A1556	U1490	C1346	U1278	U1131	U1068	C996	A923	U859	U793
U1697	C1698	G1557	G1491	G1347	G1279	C1134	G1069	C997	C924	U860	U794
C1698	A1699	C1558	G1492	U1348	U1280	C1135	U1070	C998	U925	U861	U795
A1699	C1631	G1559	U1493	A1349	A1281	G1136	G1071	A999	C926	U862	U796
C1632	U1632	A1560	G1494	G1350	A1282	U1137	U1072	U1000	C927	U863	U797
C1633	C1633	G1561	G1495	U1351	C1283	A1138	A1073	A1001	G928	U864	U798
A1634	A1634	G1496	U1496	G1352	G1284	C1139	G1074	G1002	A929	U865	U799
G1635	G1635	C1497	U1497	U1353	A1285	A1140	C1075	A1003	A930	U866	U800
U1710	C1640	U1562	U1498	A1354	U1286	U1141	U1076	U1004	G931	U867	A801
C1711	G1712	U1430	A1499	A1355	A1287	G1142	U1077	U1005	G932	U868	A802
A1715	C1642	U1431	U1500	G1356	A1288	U1143	A1078	A1006	G933	C869	C803
G1716	U1645	A1432	G1502	U1357	A1289	U1144	G1079	A1007	C937	U871	C804
A1717	G1648	G1435	G1503	C1358	U1290	C1145	A1080	G1008	C938	U872	C805
U1722	U1651	U1436	U1504	G1359	A1292	G1146	A1081	A1012	C939	U873	A806
G1723	G1652	A1437	U1506	C1364	U1293	G1149	G1082	G1013	U941	U874	C807
C1724	U1653	G1438	A1507	U1365	G1298	C1150	A1083	G1014	U942	U875	C808
A1725	A1654	G1439	G1508	A1366	A1299	U1151	G1084	G1015	U943	U876	C809
C1655	C1655	G1440	U1509	A1367	A1300	C1152	G1085	C1016	U944	U877	U810
A1582	C1656	A1441	A1510	G1368	U1301	A1153	C1086	A1019	A944	G877	G811
A1583	U1511	C1442	A1511	U1369	C1302	G1154	C1087	A1020	G945	C878	G812
G1584	U1512	U1443	G1443	U1370	U1306	C1155	A1088	A1021	C948	A879	A813
A1585	C1514	U1444	C1444	A1371	U1307	U1161	C1089	A1022	G949	C880	G814
A1588	U1515	U1445	U1446	G1373	C1308	A1162	U1092	G1024	G950	A866	A815
U1588	G1519	U1447	U1447	G1374	C1309	C1163	U1093	G1024	G951	U877	U816
C1589	G1520	G1450	G1450	G1377	C1310	C1164	A1096	G1028	A952	U878	A817
U1590	U1521	C1451	C1451	C1380	G1311	G1165	A1097	C1029	U953	U879	G818
C1592	C1522	U1452	U1452	C1381	G1312	A1166	G1098	U1030	U954	C889	C819
C1593	A1523	A1453	A1453	G1382	U1313	A1167	G1099	C1031	G955	U890	U820
U1594	C1524	G1456	G1456	G1383	A1314	G1168	A1099	A1032	A956	A891	A821
A1595	A1525	U1457	U1457	G1384	A1315	C1169	G1100	G1033	G957	G892	G822
A1596	U1526	A1458	A1458	G1385	G1316	U1170	U1101	U1034	C958	G	U823
A1597	G1527	A1459	A1459	C1386	U1317	A1171	G1102	G1035	U959	G	U824
C1598	C1528	U1459	U1459	G1387	C1319	U1172	C1103	U1037	U960	C	U825
					A1320	G1173	G1104				U826

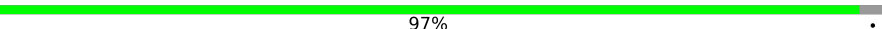


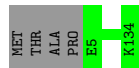
- Molecule 2: Ribosomal Protein L4

Chain K:  96% .

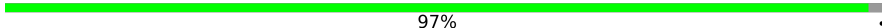


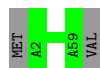
- Molecule 3: Ribosomal Protein L22

Chain L:  97% .



- Molecule 4: Ribosomal Protein L32

Chain M:  97% .



4 Data and refinement statistics

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	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.	Xtriage
Total number of atoms	59970	wwPDB-VP
Average B, all atoms (Å ²)	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	0.26	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	813	A	C2'-C3'-O3'	7.23	120.35	109.50
1	A	1715	A	C2'-C3'-O3'	7.21	120.31	109.50
1	A	2608	A	C2'-C3'-O3'	7.20	120.29	109.50
1	A	2324	G	C2'-C3'-O3'	6.91	119.86	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	1918	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59970	0	30071	1936	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 1936 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%)	144 (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 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2404	A
1	A	2854	G
1	A	2437	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	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:

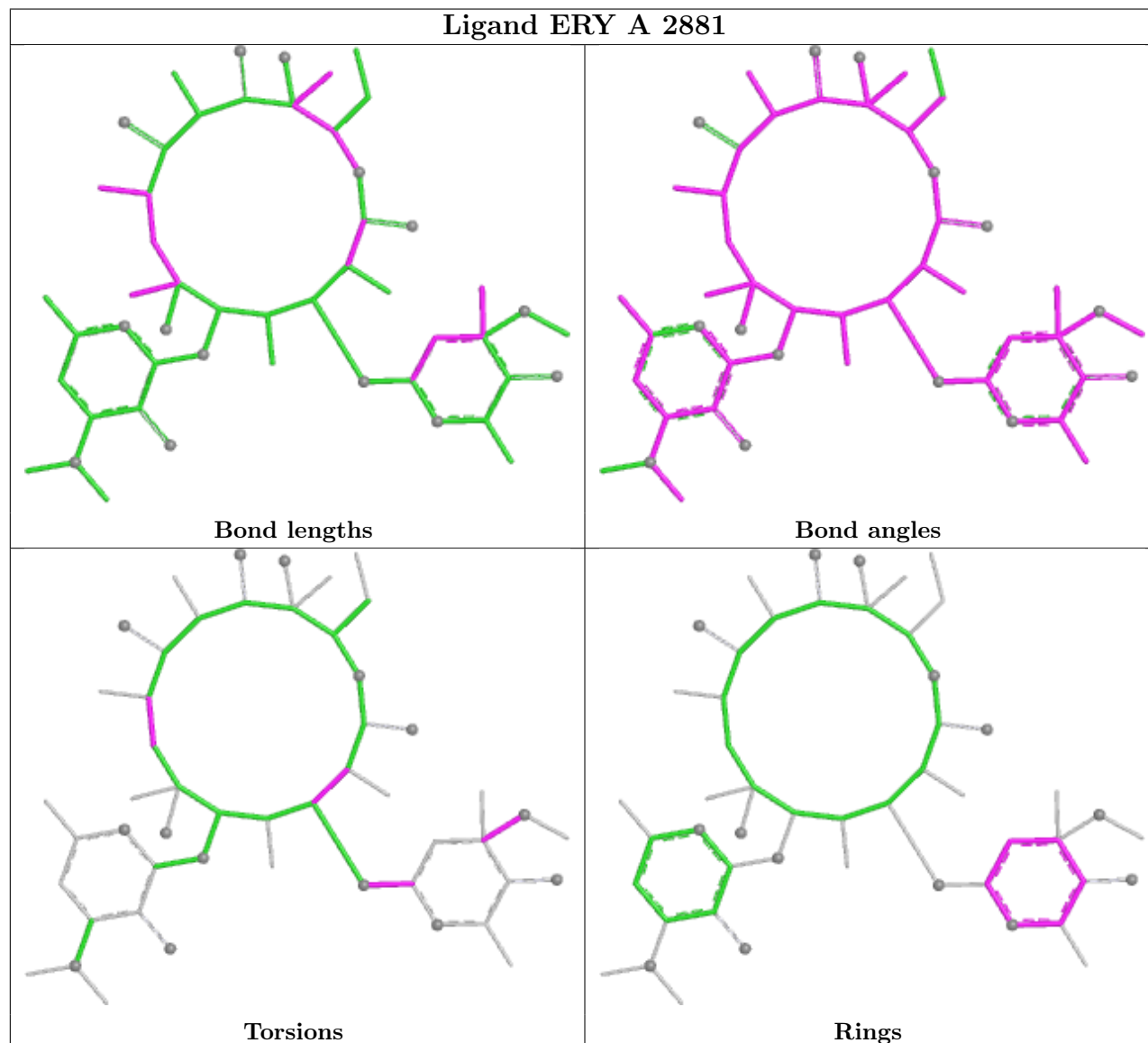
Mol	Chain	Res	Type	Atoms
5	A	2881	ERY	C14-C15-C16-C17-C18-O4

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 ⓘ

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 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.