



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:53 pm BST

PDB ID : 1J5A
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 : 2002-03-06
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.11

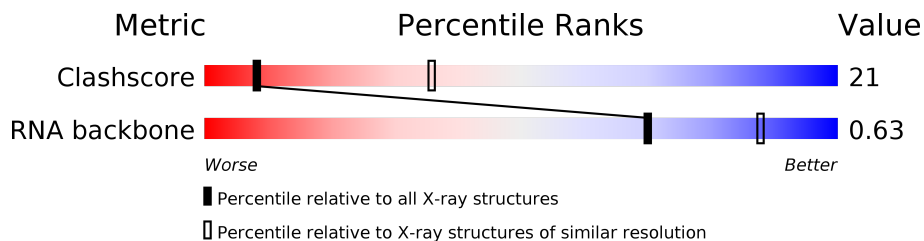
1 Overall quality at a glance

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 on 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	CTY	A	2881	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 59971 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

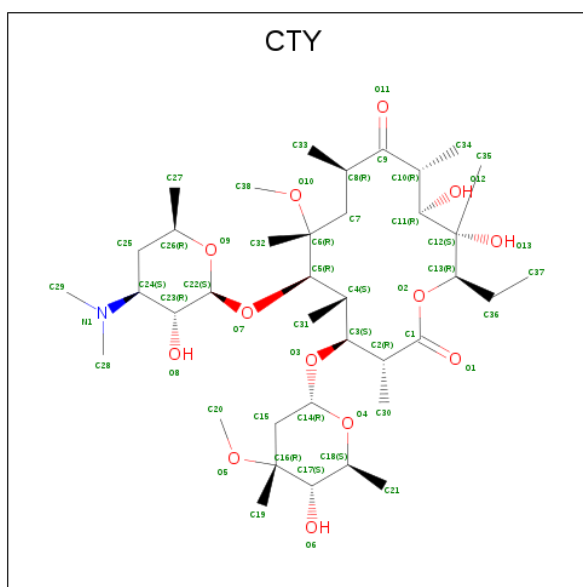
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

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 CLARITHROMYCIN (three-letter code: CTY) (formula: C₃₈H₆₉NO₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	52	38	1	13	0	0

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

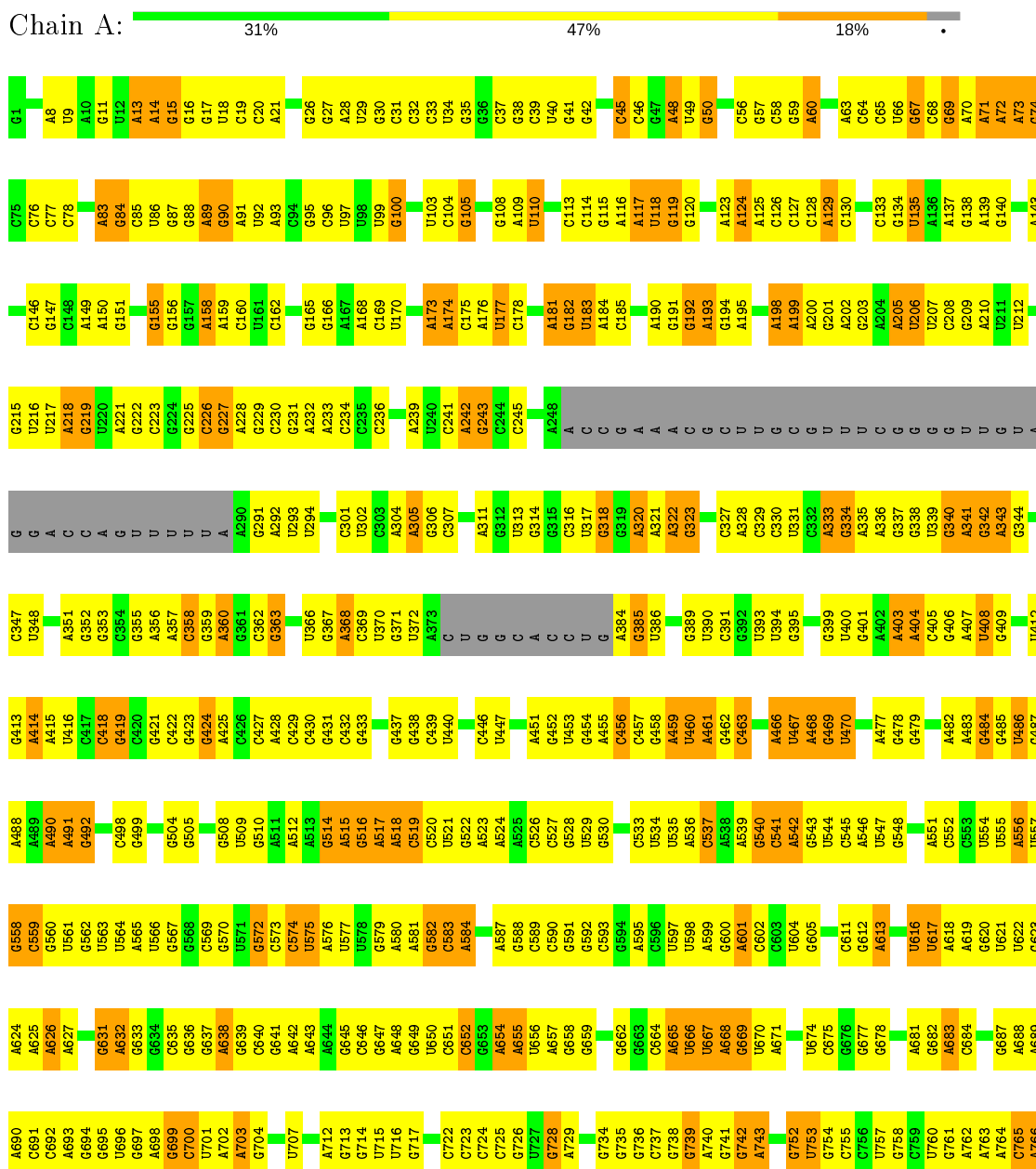
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0

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 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.

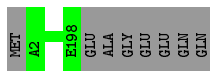
- Molecule 1: 23S rRNA



G1752	G1683	G1612	G1542	G1480	G1338	G1269	G1193	U1124	A1055	G997	C909	U840	G773
A1753	G1684	G1613	G1543	G1481	U1339	C1270	U1194	G1125	U1056	U978	C910	G841	A1774
G1754	A1685	C1614	A1544	U1482	C1340	G1271	U1195	A1126	A1057	A979	A10125	A842	U775
G1755	A1686	C1615	U1483	U1482	G1341	C1272	G1196	G1127	G1058	G980	A911	G843	G776
G1756	C1687	U1548	U1548	G1483	U1342	G1273	U1197	G1128	C981	C981	A912	G844	A777
G1757	U1688	G1484	U1484	U1484	U1343	C1274	C1198	A1129	C1060	C982	C914	U845	A778
G1758	U1689	U1618	C1445	U1485	C1344	A1275	U1199	U1130	A1061	G983	C915	A846	G778
C1762	U1690	A1619	A1446	A1486	G1345	U1276	G1200	C1134	A1065	A984	A918	C850	U784
G1763	C1552	C1552	C1417	G1487	C1346	G1277	G1201	G1135	U1066	G985	U919	C851	U785
G1764	G1553	G1553	U1420	G1488	C1347	A1278	U1202	C1136	G1067	A994	U919	C852	U786
A1765	G1554	U1420	A1420	G1489	C1348	G1279	G1203	G1137	A1068	A995	A922	U857	A787
A1694	U1421	U1421	U1421	U1490	A1349	A1280	G1204	A1138	G1069	C996	A923	G858	G788
U1697	A1483	U1484	U1484	U1493	G1350	A1281	G1205	A1139	G1070	C997	C924	G859	G789
C1698	G1494	U1494	U1494	G1494	G1351	A1282	G1209	A1140	U1071	C998	U925	U859	A790
A1699	G1495	U1495	U1495	G1495	G1352	C1283	C1210	U1141	U1072	A999	C926	U860	G791
C1699	G1496	U1496	U1496	G1496	A1353	A1284	G1211	U1142	U1073	G999	C927	G861	G792
C1702	G1497	G1497	G1497	G1497	A1354	A1285	G1212	A1143	G1074	A1001	C928	G862	A794
C1703	G1498	G1498	G1498	G1498	A1355	A1286	U1212	A1144	G1075	A1002	G929	C863	A795
G1704	A1499	G1499	G1499	G1499	G1356	A1287	U1213	U1145	C1003	C1003	A930	C864	A796
A1707	U1500	U1500	U1500	U1500	U1357	A1288	G1214	G1146	G1079	C1004	A931	C865	A797
A1708	C1501	G1432	G1432	G1432	C1358	A1289	A1215	C1150	A1080	U1005	G932	U866	G798
U1709	G1502	A1433	A1433	A1433	G1359	A1290	U1216	G1149	A1081	U1006	G933	U867	C799
U1710	G1503	U1434	U1434	U1434	C1364	A1292	G1217	C1150	A1082	A1007	G934	U868	U800
C1711	G1504	G1435	G1435	G1435	U1365	A1293	C1218	U1151	G1083	G1008	G934	C869	A801
G1712	U1505	G1436	G1436	U1505	A1366	A1294	G1220	C1152	A1084	C1008	C937	C870	A802
C1575	C1506	A1437	A1437	C1506	A1367	G1298	C1221	A1153	G1085	A1012	G938	U871	C803
C1576	A1507	G1438	G1438	A1507	C1368	A1299	G1222	G1154	A1086	G1013	C939	G872	C804
G1579	G1508	G1439	G1439	G1508	A1369	A1300	G1223	G1155	C1087	G1014	G940	U873	G805
U1580	A1509	G1440	G1440	U1509	U1370	U1301	A1224	U1015	A1088	U941	G941	A874	A806
C1581	A1510	A1441	A1441	A1510	G1371	C1302	G1225	C1160	C1089	C1016	U942	G875	A807
A1582	C1442	C1442	C1442	A1511	A1372	A1302	A1226	U1161	C1090	C1017	U943	C876	C808
A1583	G1443	G1443	G1443	A1512	G1373	U1306	A1227	U1162	G1091	U1019	A944	G877	C809
C1584	A1444	A1444	A1444	C1513	G1374	U1307	A1233	C1163	U1092	A1020	G945	C878	U810
A1585	U1446	U1446	U1446	C1514	G1375	G1308	G1234	G1165	U1093	A1021	G946	C879	G811
U1588	U1447	U1447	U1447	C1515	G1377	G1310	G1240	A1166	A1096	A1022	C948	C880	G812
G1589	G1450	G1450	G1450	G1519	C1380	G1311	G1241	A1167	A1097	G1024	G950	A886	G814
C1590	C1451	C1451	C1451	U1521	G1381	G1312	G1242	G1168	G1098	G1030	G951	G887	U816
U1592	U1452	U1452	U1452	C1522	G1382	U1313	U1244	C1169	A1099	U1031	A952	G888	U817
C1593	A1523	A1453	A1453	A1523	G1383	A1314	G1245	U1170	G1100	A1032	G953	C889	G818
U1594	C1524	A1454	A1454	C1524	G1384	A1315	G1246	A1171	U1101	G1033	U954	U890	G819
U1594	A1525	C1456	C1456	A1525	G1385	G1316	G1249	G1173	G1102	U1034	G955	A891	C819
A1595	U1526	A1457	A1457	U1526	A1386	C1316	A1250	G1174	C1103	U1034	A956	U820	A821
A1596	G1527	A1458	A1458	G1527	G1387	G1322	G1251	A1175	U1105	G1036	G957	G822	A822
A1597	C1528	U1459	U1459	C1528	A1391	G1323	C1252	U1176	A1106	G1037	G958	U823	U824
G1599	C1529	G1460	G1460	C1529	U1392	G1324	C1253	U1177	A1107	U1038	U960	U824	U824
U1600	U1530	U1530	U1530	U1530	G1393	U1325	G1258	C1178	U1108	A1039	A964	C825	C825
U1601	G1531	G1465	G1465	G1531	G1394	U1326	G1258	U1180	U1109	A1040	U964	U826	U826
A1602	A1532	C1466	C1466	A1532	A1397	C1328	A1259	C1183	G1110	G1041	C968	C827	C827
A1603	G1533	U1467	U1467	G1533	A1398	U1329	A1260	G1184	C1111	U1044	C969	C828	C828
A1604	A1534	A1468	A1468	A1534	C1399	G1330	G1261	C1185	U1112	G1045	U969	C829	C829
A1605	G1470	U1469	U1469	C1399	G1400	G1330	U1262	G1186	C1113	C830	C970	C830	C830
A1606	U1537	G1470	G1470	G1400	A1401	G1333	C1264	A1187	G1118	A1046	A971	C831	G831
A1607	U1538	U1473	U1473	G1402	G1402	G1334	G1266	A1188	G1119	G1047	C972	A832	A832
U1608	A1539	U1474	U1474	G1403	G1403	A1335	G1266	G1189	U1119	U1048	U973	A833	A833
C1540	C1540	U1475	U1475	U1404	U1404	G1336	A1267	C1190	A1122	C1049	U974	U838	A838
A1541	A1405	G1476	G1476	A1405	A1405	G1337	U1268	G1192	G1123	C1054	C976	U839	U839

- 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, α , β , γ	169.90Å 412.70Å 697.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.273 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	59971	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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, CTY

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(°)	Ideal(°)
1	A	1746	A	C2'-C3'-O3'	5.89	123.12	113.70
1	A	777	A	C2'-C3'-O3'	5.52	122.53	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	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	52	0	69	32	0
6	A	2	0	0	0	0
All	All	59971	0	30073	1896	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 1896 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:2042:A:C2	5:A:2881:CTY:H383	1.63	1.30
1:A:2042:A:N3	5:A:2881:CTY:H383	1.62	1.14
1:A:1747:G:H4'	1:A:1749:G:H1'	1.29	1.12
1:A:940:G:H3'	1:A:941:U:H5''	1.34	1.09
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.08

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%)	555 (20%)	142 (5%)

5 of 555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	45	C
1	A	48	A

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1278	A
1	A	1563	U
1	A	2633	A
1	A	1285	A
1	A	1354	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 carbohydrates 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	CTY	A	2881	-	54,54,54	1.64	10 (18%)	83,83,83	3.07	42 (50%)

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	CTY	A	2881	-	-	11/75/110/110	1/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	CTY	C7-C6	5.09	1.60	1.52
5	A	2881	CTY	C7-C8	4.75	1.60	1.54
5	A	2881	CTY	O2-C13	-3.26	1.40	1.46
5	A	2881	CTY	C35-C12	3.02	1.58	1.52
5	A	2881	CTY	C15-C14	2.89	1.58	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	CTY	O5-C16-C19	-7.63	98.20	110.92
5	A	2881	CTY	O3-C3-C4	7.26	116.97	108.22
5	A	2881	CTY	C33-C8-C7	7.06	122.79	109.81
5	A	2881	CTY	C19-C16-C17	6.65	124.84	111.24
5	A	2881	CTY	O5-C16-C17	6.56	113.53	103.81

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C4-C5-C6-C32
5	A	2881	CTY	C7-C6-O10-C38
5	A	2881	CTY	C32-C6-O10-C38
5	A	2881	CTY	C17-C16-O5-C20
5	A	2881	CTY	O4-C14-O3-C3

All (1) ring outliers are listed below:

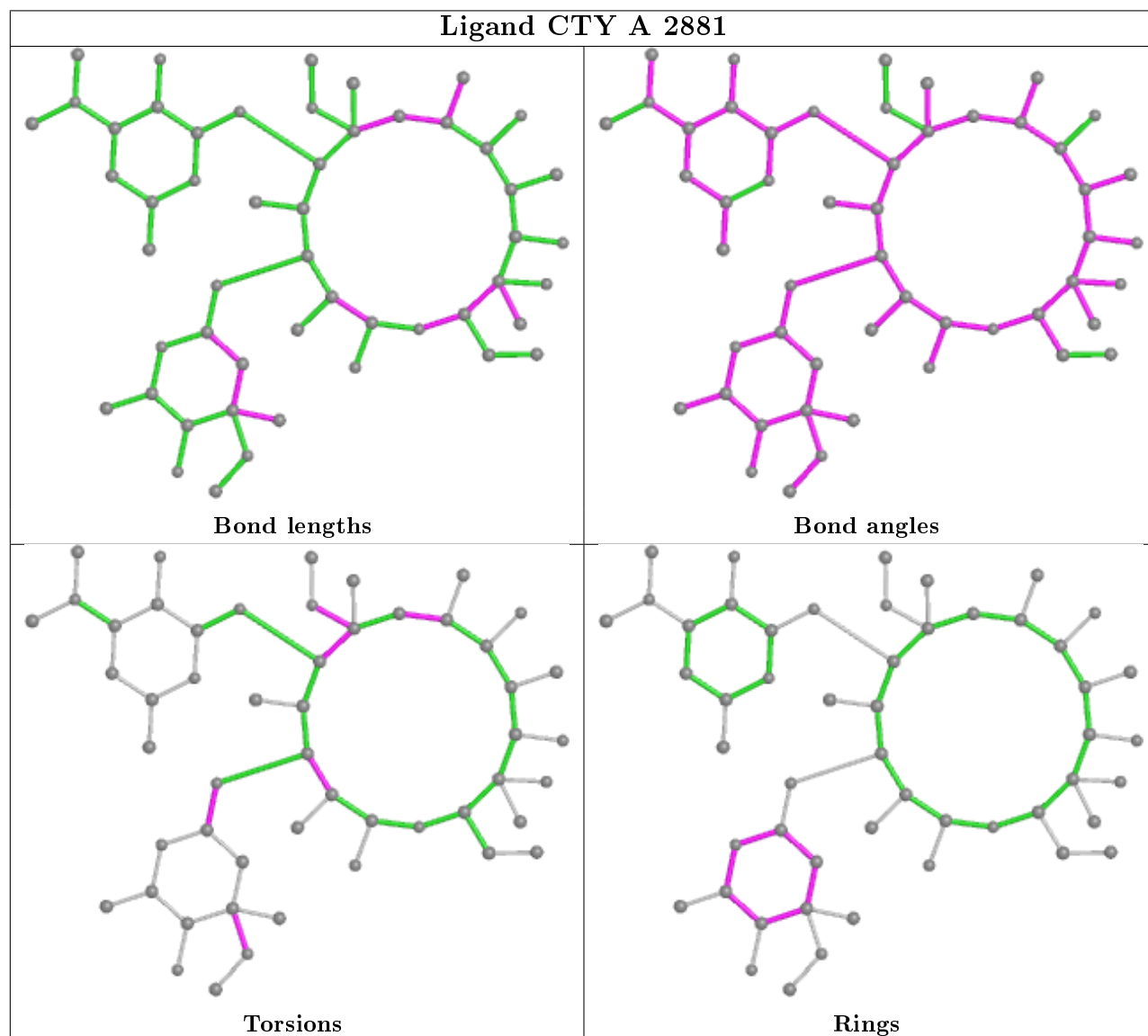
Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C14-C15-C16-C17-C18-O4

1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	CTY	32	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.