



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 07:46 PM EDT

PDB ID : 1J5A
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.;
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Deposited on : 2002-03-06
Resolution : 3.50 Å(reported)

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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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

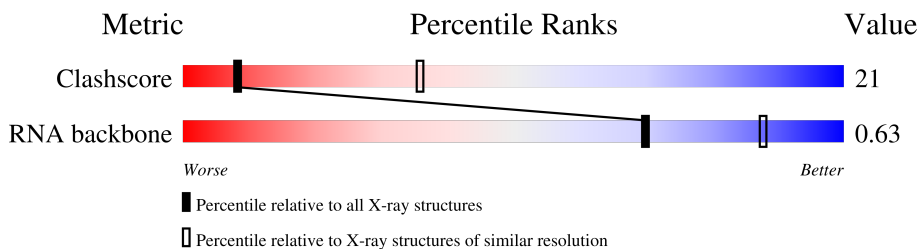
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

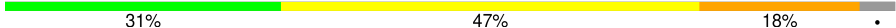
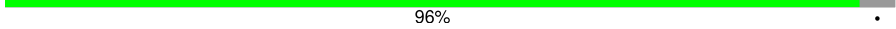
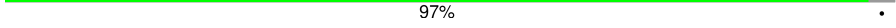
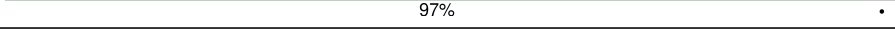
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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 ≥ 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	 31% 47% 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	CTY	A	2881	-	-	X	-

2 Entry composition

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
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			

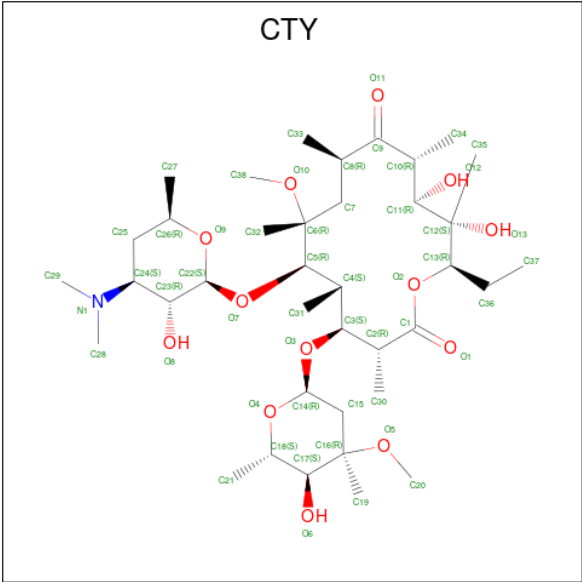
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

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



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

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

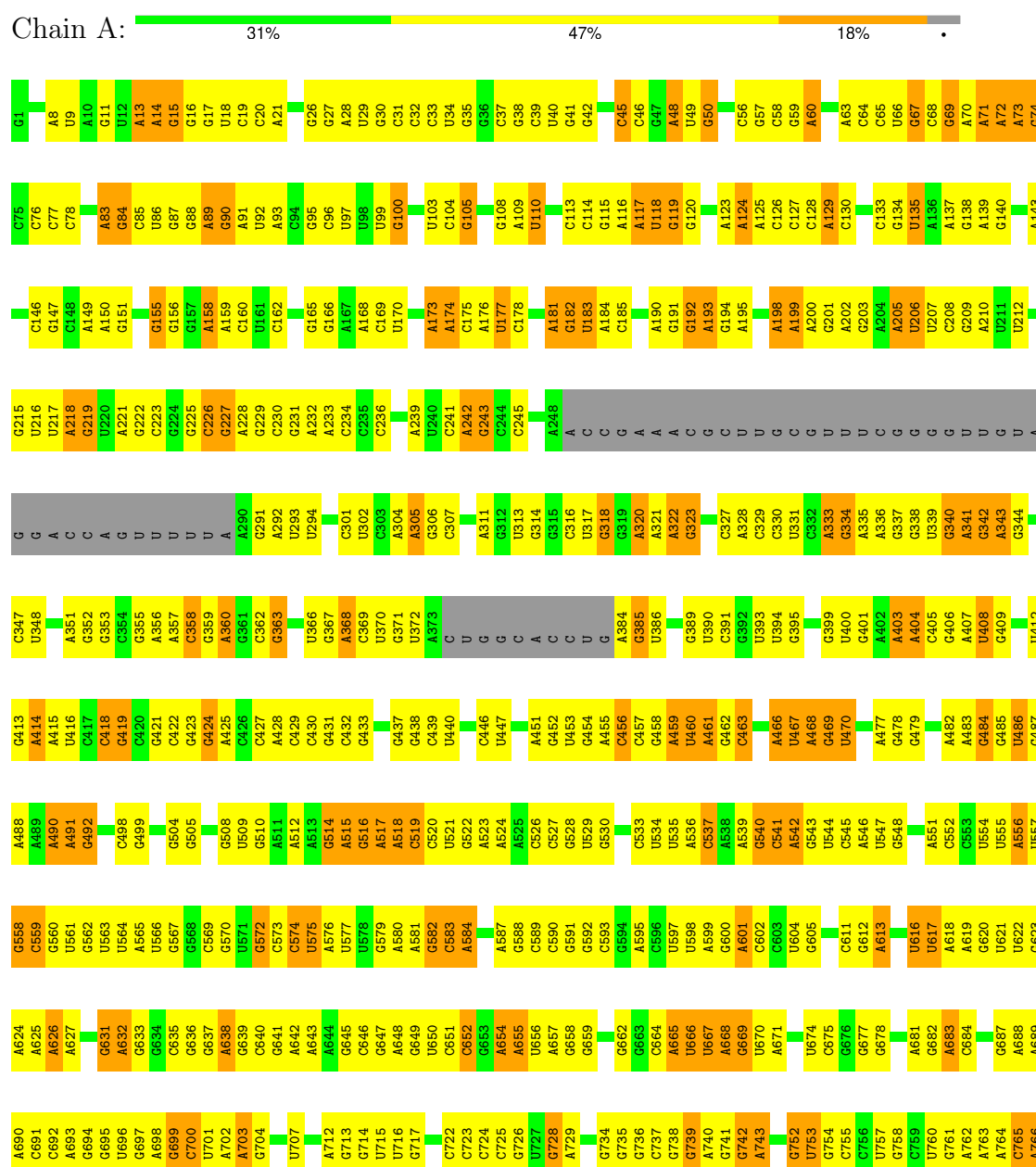
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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

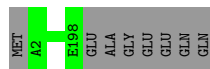


U1752	G1683	U1612	G1542	G1480	U1409	G1338	G1269	U1193	U1124	A1055	G977	C909	U840	G773
A1753	G1684	G1613	G1543	G1481	U1410	U1339	C1270	U1194	G1125	U1056	U978	C910	G841	G774
G1754	A1685	C1614	A1544	U1481	U1411	C1340	C1271	U1195	A1126	A1057	U979	A1057	A842	A775
G1755	A1686	G1615	A1545	U1482	C1411	G1341	G1272	G1196	C1127	G1058	G980	A911	G843	U776
C1756	C1687	G1616	C1548	U1483	C1412	U1342	C1273	U1197	C1128	A1059	C981	A912	G844	G776
G1757	U1688	G1617	C1549	G1484	C1413	C1343	G1274	U1198	A1129	A1060	C982	C914	U845	A777
C1758	U1689	U1618	C1550	U1485	C1415	C1344	A1275	U1199	U1130	A1061	G983	C915	A846	G778
	U1690	A1619	U1551	A1486	U1416	U1345	U1276	U1200	C1134	A1065	A984	A918	C850	U784
C1762	G1691	C1623	C1552	A1487	C1417	C1346	U1277	G1201	C1135	U1066	G985	U919	C851	U785
C1763	C1692	G1624	G1553	U1488	A1420	C1347	A1278	U1202	G1136	G1067	U994	U919	U852	U786
A1764	A1693	A1625	A1554	C1489	U1421	C1348	G1279	A1203	G1137	U1068	A995	A922	U857	A787
C1765	A1694	A1626	A1555	U1490	U1422	G1349	A1280	G1204	A1138	G1069	C996	A923	G858	G788
U1766	A1626	A1556	U1556	U1491	U1424	G1350	A1281	G1205	A1139	G1070	C997	C924	G859	G789
G1767	G1627	G1557	G1557	A1493	U1425	G1351	A1282							A790
U1768	C1628	C1558	C1558	G1494	U1426	G1352	C1283	G1209	U1140	U1071	C998	U925	U859	G791
U1769	A1698	G1559	G1559	G1495	U1427	G1353	C1284	G1210	U1141	U1072	A999	U926	G861	
U1770	C1631	A1560	A1560	G1496	G1428	A1354	A1285	G1211	U1142	U1073	G1000	C927	G862	
A1771	C1632	U1561	C1497	C1497	G1429	A1355	U1286	U1212	A1143	G1074	A1001	C928	A882	A794
C1703	A1634	G1562	G1498	A1498	A1429	G1356	A1287	U1213	U1144	C1075	C1002	A929	C863	A795
G1704	G1635	U1563	A1499	G1430	U1430	U1357	A1288	G1214	G1145		C1003	A930	C864	A796
		U1564	U1500	U1431	G1432	U1358	A1289	A1215	C1146	G1079	C1004	G931	C865	A797
C1707	C1640		C1501	G1433	A1433	G1359	G1291	G1216		A1080	U1005	G932	U866	A798
C1708	C1641	G1571	G1502	U1434	U1434	C1364	A1292	C1218	G1149	A1081	U1006	G933	C867	A799
U1709	G1642	G1572	G1503	G1435	U1435	U1365	A1293	C1219	U1151	G1082	C1007	G934	U868	U800
U1710		G1573	G1504	G1436	G1436	A1366	A1293	G1220	C1152	A1084	A1008	C937	C870	A801
C1711	U1645	A1574	U1505	A1437	A1437	G1367	G1298	C1221	A1153	G1085	A1012	G938	U871	A802
G1712		C1575	C1506	G1438	G1438	A1368	A1299	C1222	U1154	C1086	G1013	G939	C872	C803
C1713	C1648	G1576	A1507	G1439	G1439	G1369	A1300	G1223	G1155	C1087	G1014	C940	U873	C804
U1715	U1651	G1579	G1508	G1440	G1440	U1370	U1301	A1224	U1171	A1088	U1015	U941	A874	G805
A1716	G1652	C1580	A1510	A1441	A1441	G1371	C1302	G1225	C1160	C1089	C1016	U942	C875	A806
C1717	G1653	C1581	A1511	C1442	C1442	A1372		A1226	U1161	C1090		U943	A876	A807
U1789	A1654	G1592	A1512	C1443	C1443	G1373	U1306	A1227	U1162	G1091	U1019	A944	C877	C808
G1790	C1655	A1583	A1513	C1444	C1444	G1374	U1307	C1233	C1163	U1092	U1020	G945	C878	C809
C1791	U1656	G1584	C1514	U1445	C1445	U1377	C1308	A1233	C1164	U1093	A1021	G945	A879	U810
C1792	A1657	A1585	U1515	U1446	U1446		C1309	C1234	G1165		A1022	C948	C880	G811
A1793				U1447	U1447		C1310		A1166	A1096	U1023	G949	C880	G812
A1794							G1311	G1240	A1167	A1097	G1024	G950	A886	A813
G1798	G1660	C1661	A1588	U1519	G1450	C1380	G1312	G1241	G1168	G1098	U1030	G951	G887	G814
A1799	G1662	U1521	G1589	G1520	C1451	G1381	U1313		C1169	A1099	C1031	A952	G888	A815
C1800	C1663	C1522	C1590	U1521	U1452	C1382	A1314	U1244	U1170	G1100	G1032	G953	C889	U816
C1801	G1664	U1591	U1591	C1522	U1453	C1383	A1315	G1245	A1171	U1101	A1032	U954	U890	A817
A1802	C1665	C1592	C1593	C1524	A1453	C1384	A1315		U1172	G1102	G1033	G955	C819	G818
G1803	C1666	U1594	U1594	C1525	C1456	C1385	G1316	G1249	G1173	C1103	U1034	A956	A891	C819
U1733	G1667	A1595	U1595	A1526	A1457	A1386		A1250	G1174	G1104	G1035	G957	G892	U820
C1734	A1667	C1596	C1596	U1526	U1457	G1387	A1321	G1259	G1175	U1105	G1036	G958	G	A821
G1735	G1668	C1597	A1597	C1528	U1458	A1391	G1322	G1251	U1176	A1106	U1037	C959	G	A822
C1808	A1669	U1598	C1598	C1529	U1459	U1392	G1323	C1252	U1177	A1107	U1038	U960	U824	U823
G1809	G1670	G1599	U1530	U1530	G1460	G1393	U1325	C1253	C1178	U1108	A1039	U960	C	U824
U1810	A1671	U1600	C1531	G1465		G1394	U1326	G1258		U1109	A1040	A964	C	C825
A1811	C1672	U1601	A1532	C1466	C1466	U1394	C1327	A1259	C1183	G1110	G1041		U	U826
U1738	C1673	G1602	G1533	U1467	U1467	A1397	C1328	G1260	G1184	C1111	U1044	C968	C827	C827
	C1674	A1603	A1534	A1468	U1468	A1397	C1329	A1261	C1185	U1112	G1045	U969	A	C828
G1742	G1675	A1604	C1535	U1469	U1469	C1398	U1329	G1262	C1186	U1112	C829	C969	C	C829
C1743	U1676	G1536	G1536	G1470	G1470	C1399	G1330	U1262	G1187	C1113	A970	C	C	C830
G1744	C1677	A1605	U1537	U1471		G1401	G1333	G1263	A1187	U1046	C971	C	A	G831
A1745	G1678	C1606	U1537	U1472		A1401	G1334	C1264	A1188	G118	U1047	G	G	A832
C1746	U1607	A1607	A1538	U1473	U1473	G1402	A1334	G1265	G1189	U119	U1048	U973	C	A833
U1748	U1608	U1608	C1540	U1474	U1474	G1403	A1335	G1266	C1190	A1222	C1049	U974	U	A834
G1749	A1681	U1680	C1540	U1475	U1475	U1403	A1336	G1267	C1191	A1267	U1049	C975	U	A835
A1821	A1682		A1541	U1476	G1476	A1405	G1337	U1268	A1192	G1123	C1054	C976	A	U839



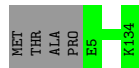
- Molecule 2: RIBOSOMAL PROTEIN L4

Chain K:  96% .



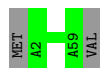
- Molecule 3: RIBOSOMAL PROTEIN L22

Chain L:  97% .



- Molecule 4: RIBOSOMAL PROTEIN L32

Chain M:  97% .



4 Data and refinement statistics

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	169.90Å 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.	Xtriage
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($^{\circ}$)	Ideal($^{\circ}$)
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	2404	A
1	A	2437	G
1	A	2615	U
1	A	929	A
1	A	925	U

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	CTY	A	2881	-	54,54,54	1.68	10 (18%)	83,83,83	3.06	43 (51%)

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	5.05	1.60	1.52
5	A	2881	CTY	C7-C8	4.91	1.60	1.54
5	A	2881	CTY	O2-C13	-3.38	1.40	1.46
5	A	2881	CTY	C35-C12	3.21	1.58	1.52
5	A	2881	CTY	C15-C14	3.00	1.58	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	CTY	O3-C3-C4	7.41	116.97	108.23
5	A	2881	CTY	C19-C16-C17	6.94	124.84	111.19
5	A	2881	CTY	C33-C8-C7	6.94	122.79	109.88
5	A	2881	CTY	O5-C16-C17	6.67	113.53	103.86
5	A	2881	CTY	C6-C5-C4	6.32	123.20	113.54

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:

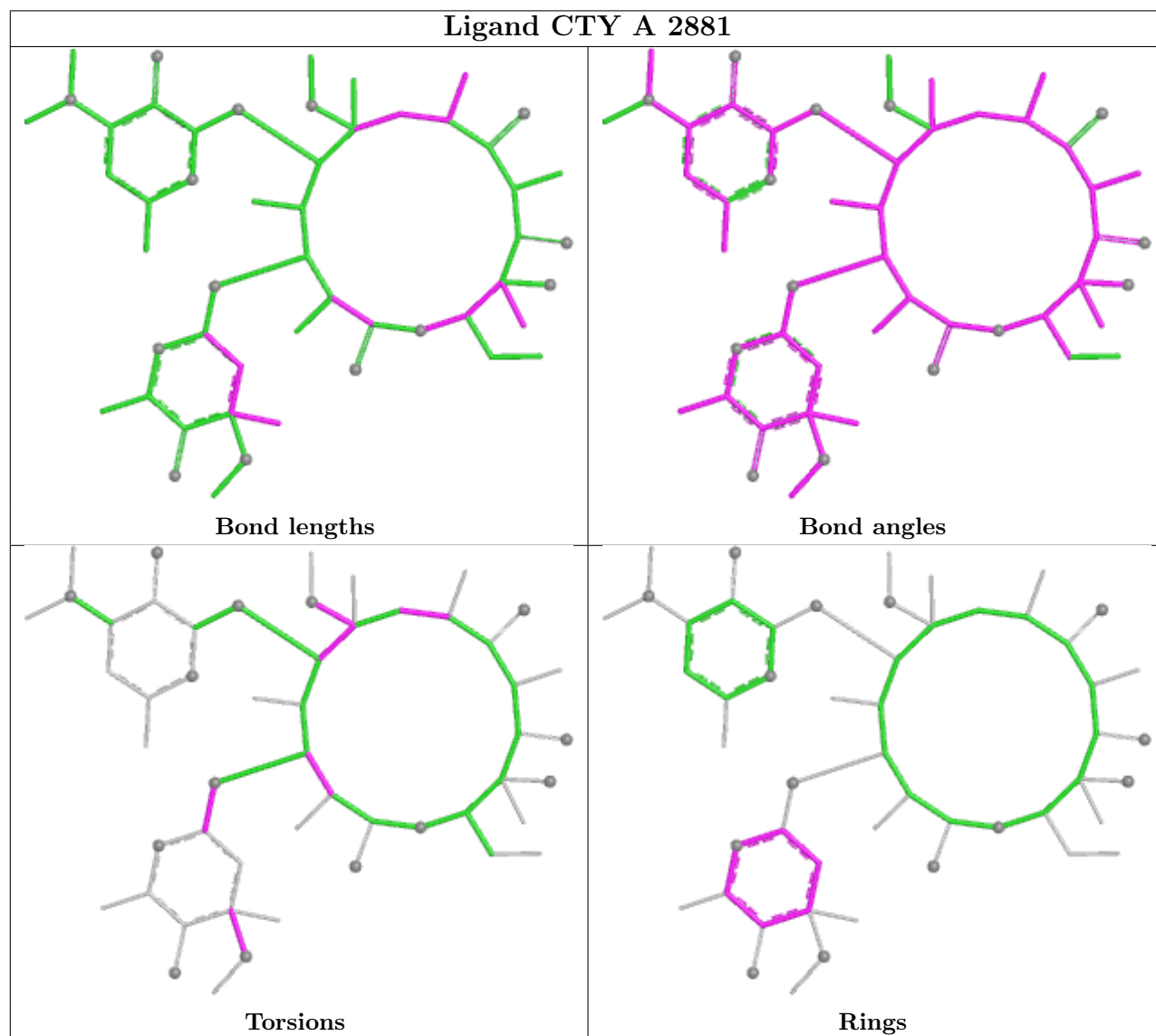
Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C14-C15-C16-C17-C18-O4

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 [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.