



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:59 PM UTC

PDB ID : 1J5A / pdb_00001j5a
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 : 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 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

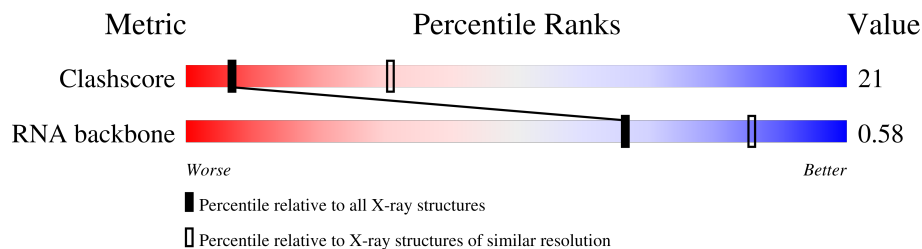
1 Overall quality at a glance

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	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			

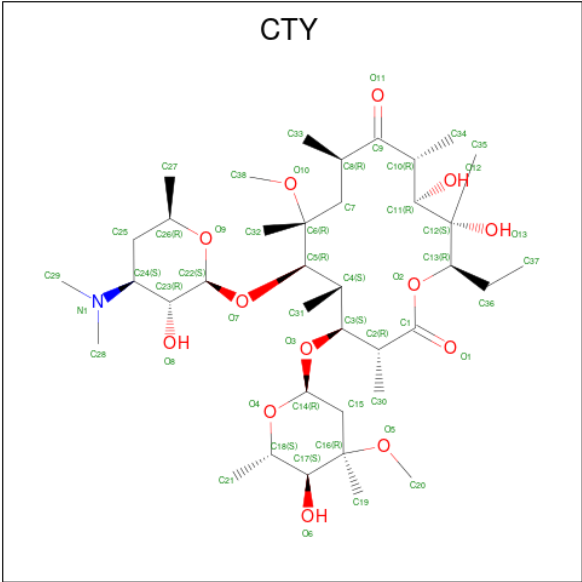
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

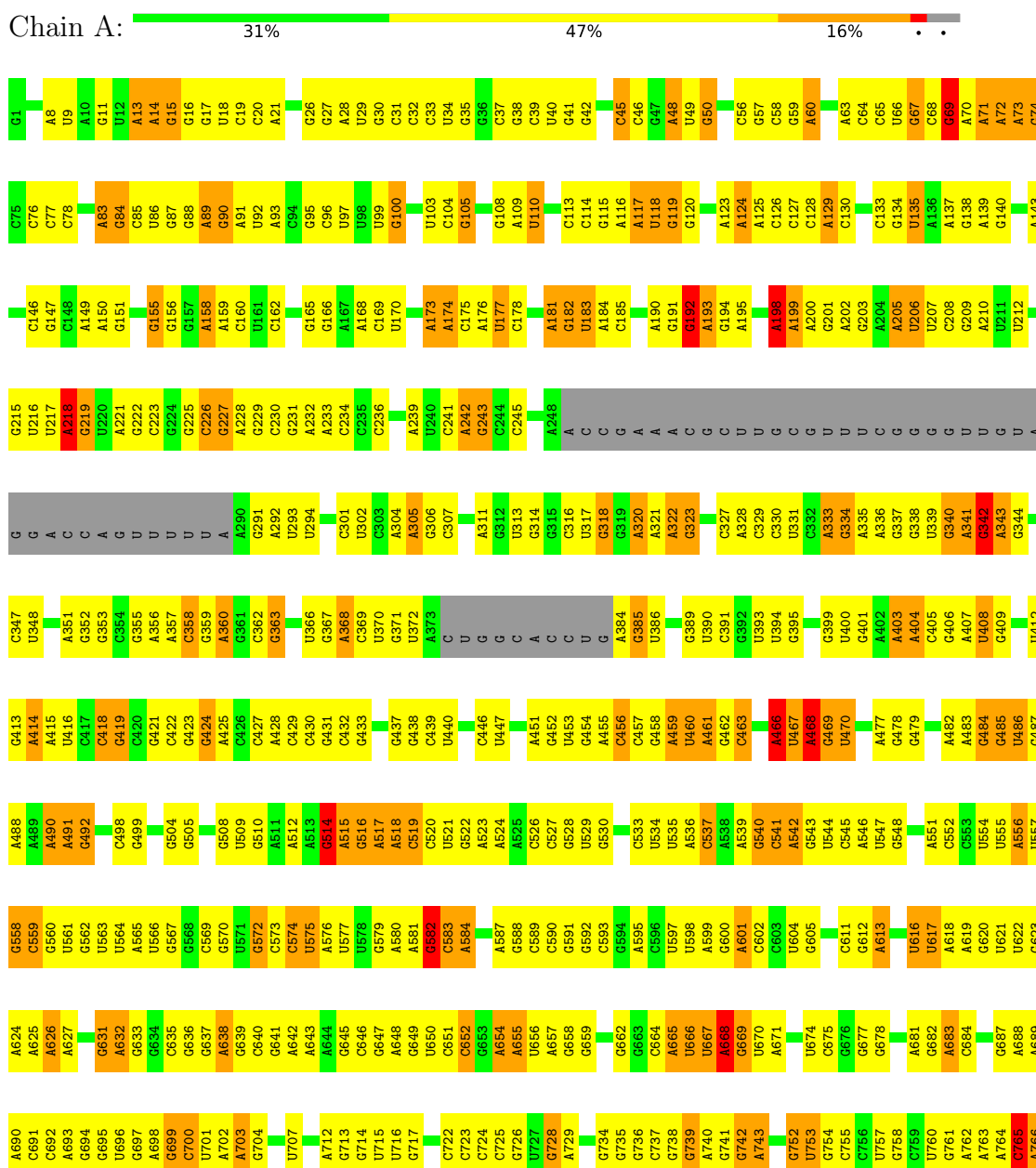
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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.

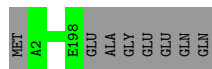
• Molecule 1: 23S rRNA



G1754	A1685	C1614	U1481	U1410	C1340	G1271	U1195	U1124	A1055	G977	C909	U840	G773
G1755	A1686	C1615	U1482	C1411	G1341	G1272	G1196	G1125	U1056	U978	C910	G841	G774
C1756	C1687	C1616	G1483	C1412	U1342	C1273	U1197	A1126	A1057	A979	A911	A842	A775
C1758	U1688	G1617	G1484		C1343	C1274	U1198	C1127	G1058	G980	A912	G843	U776
	U1689	U1618	U1485	C1415	G1344	A1275	U1199	G1128	A1059	C981	A913	G844	A777
	U1690	A1619	U1486	C1416	G1345	A1276	U1200	A1129	C1060	C982	C914	G845	G778
C1762	G1691	C1552	C1487	C1417	C1346	G1277	G1201	U1130	A1061	G983	C915	A846	
G1763	C1692	G1553	G1488		C1347	A1278	U1202		A984	A984		C850	U784
A1764	A1693	G1554	C1489	A1420	C1348	G1279	A1203	C1134	U1065	G985	A918	C851	U785
C1765	A1694	A1555	U1490	U1421	A1349	U1280	G1204	C1135	G1066	U919	U919	C852	U786
U1766	A1556	A1556			G1350	A1281	G1205	G1136	G1067		A922	U857	A787
U1768	U1557	C1558	A1493	U1424	G1351	A1282	G1209	A1138	U1068	A995	A923	U857	G788
U1769	G1559	G1495	G1496	U1426	A1353	C1283	C1210	A1139	G1070	C997	C924	G858	G789
	A1560	G1497	A1354	G1427	A1354	A1285	G1211	U1071	U1072	C998	U925	U859	A790
A1771	A1561	C1633	G1498	A1429	G1355	A1286	U1212	U1141	U1073	A999	C926	G861	G791
C1772	U1562	G1430	A1499	G1430	U1357	A1288	G1213	G1142	G1000	C999	G927	G861	
C1773	U1563	A1431	U1500	U1431	C1358	A1289	G1214	A1143	G1074	A1001	G928	A862	
A1774	U1564	G1432	G1501	G1432	G1359	A1290	U1215	U1144	C1002	A929	A929	C863	A794
A1775			G1502	A1433		G1291	G1216	G1145	C1003	A930	A930	C864	A796
A1776	G1571	U1434	G1503	U1434	C1364	A1292	U1217	G1146	A1004	G931	G931	A865	A797
U1777	C1572	G1435	G1504	G1435	U1365	A1293	C1218		U1005	U932	G932	U866	C799
	G1573	G1436	U1505	G1436	A1366	A1294	C1219	U1150	C1006	G933	G933	G867	U800
G1778	A1574	G1437	U1506	A1437	G1367	G1295	G1220	U1151	A1007	G934	G934	C869	A801
A1782	G1575	G1438	A1507	G1438	G1368	A1296	G1222	C1152	U1008		C937	C870	A802
	G1576		G1508	G1439	G1369	A1300	G1223	A1153	A1012	G938	G938	U871	C803
U1787			G1509	G1440	U1370	A1301	A1224	C1154	G1013	C939	C939	G872	C804
C1788	U1579	U1450	A1510	C1441	G1371	C1302	G1225	G1155	G1014	G805	U873	G873	G805
U1789	C1581	C1442	A1511	C1442	A1372		A1226		U941	U874	A874	A806	A806
G1790	A1582	G1443	U1512	G1443	G1373	U1306	U1227	C1160	C1016	A807	G875	A807	A807
C1791	A1583	C1444	U1513	C1444	G1374	U1307		U1161	C1090	U942	A876	C808	C808
C1792	G1584	U1445	C1514	A1445		C1308	A1233	U1162	G1091	A944	A877	C809	C809
A1793	U1514	U1446	G1515	U1446	G1377	C1309	C1234	C1163	U1092	U878	C878	U810	U810
A1794	U1515	U1447		U1447		C1310	C1234	C1164	A1021	G811	A879	G811	G811
			G1519	G1450	C1380	G1311	G1240	G1165	A1022	C948	C948	C880	G812
G1798	A1588	G1450	G1520	C1451	G1381	G1312	G1241	A1166	U1023	G949	G949	A866	A813
C1799	C1590	C1451	U1521	C1451	G1382	U1313		A1167	G1024	G950	G950	G867	G814
C1799	U1591	U1452	C1522	U1452	C1383	A1314	U1244	G1168	G1098	G951	A952	G888	A815
G1730	U1592	A1453	C1523	A1453	G1384	A1315	G1245	C1169	U1030	G953	U954	C889	A817
	C1593		C1524		C1385	G1316		U1171	G1031	U954	U954	U890	G818
	U1594	C1456	A1525	C1456	A1386		G1249	U1172	A1032	G955	G955	A891	C819
	U1595	A1457	A1526	A1457	G1387	A1321		G1173	G1102	A856	A856	G892	U820
	A1596	A1458	G1527	A1458		G1322	G1250	G1174	C1103	G957	G957	G	A821
	A1597	U1459	C1528	U1459	A1391	G1323	G1251	G1175	G1035	G958	G958	G	A822
	C1598	G1460	C1529	G1460	U1392	G1324	C1262	U1176	G1036	C959	C959	G	U824
	U1599		U1530		G1393	U1325	C1263	A1176	U1037	U1037	U960	C	U824
	U1600	G1465	C1531	G1465	G1394	C1327	G1268	C1178	U1038	U960	U960	C	C825
	G1601	C1466	A1532	C1466	A1397	C1328	A1260		U1039	A964	A964	C	U826
	G1602	U1467	G1533	U1467	G1398	U1329	G1261	C1183	A1040			U	C827
	A1603	A1468	A1534	A1468	G1399	U1330	G1262		G1041			A	C828
	A1604	U1469	C1535	U1469	C1399	G1330	U1262	U1110	U1044	C968	C968	C	C829
	G1605	G1470	G1536	G1470	A1400		G1263	C1111	G1045	A970	A970	C	C830
	C1606		U1537		A1401	G1333	C1264	C1112	A971	A971	A971	A	G831
	A1607	U1473	A1538	U1473	C1402	A1334	G1265	G1189	U1046	C872	C872	G	A832
	U1608	A1474	U1539	U1474	U1403	A1335	G1266	C1190	G1047	U973	U973	C	A833
		U1475	C1540	U1475	C1404	G1336	A1267	G1191	U1048	U974	U974	U	
		G1476	G1541	G1476	A1405	G1337	U1268	A1192	C1049	C975	C975	U	A838
			G1542		A1405	G1338	G1269	G1193	C1054	C976	C976	A	U839
		G1480	G1543	G1480	U1409	U1339	C1270	U1194	G1123				

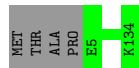
- Molecule 2: RIBOSOMAL PROTEIN L4

Chain K:  96% .



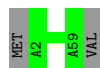
- Molecule 3: RIBOSOMAL PROTEIN L22

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	0.27	0/66661	0.59	54/103976 (0.1%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	A	C2'-C3'-O3'	7.63	120.94	109.50
1	A	1715	A	C2'-C3'-O3'	7.41	120.61	109.50
1	A	2608	A	C2'-C3'-O3'	7.28	120.42	109.50
1	A	813	A	C2'-C3'-O3'	7.27	120.40	109.50
1	A	2324	G	C2'-C3'-O3'	7.00	120.01	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	1874	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59971	0	30073	1893	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 1893 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 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	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:

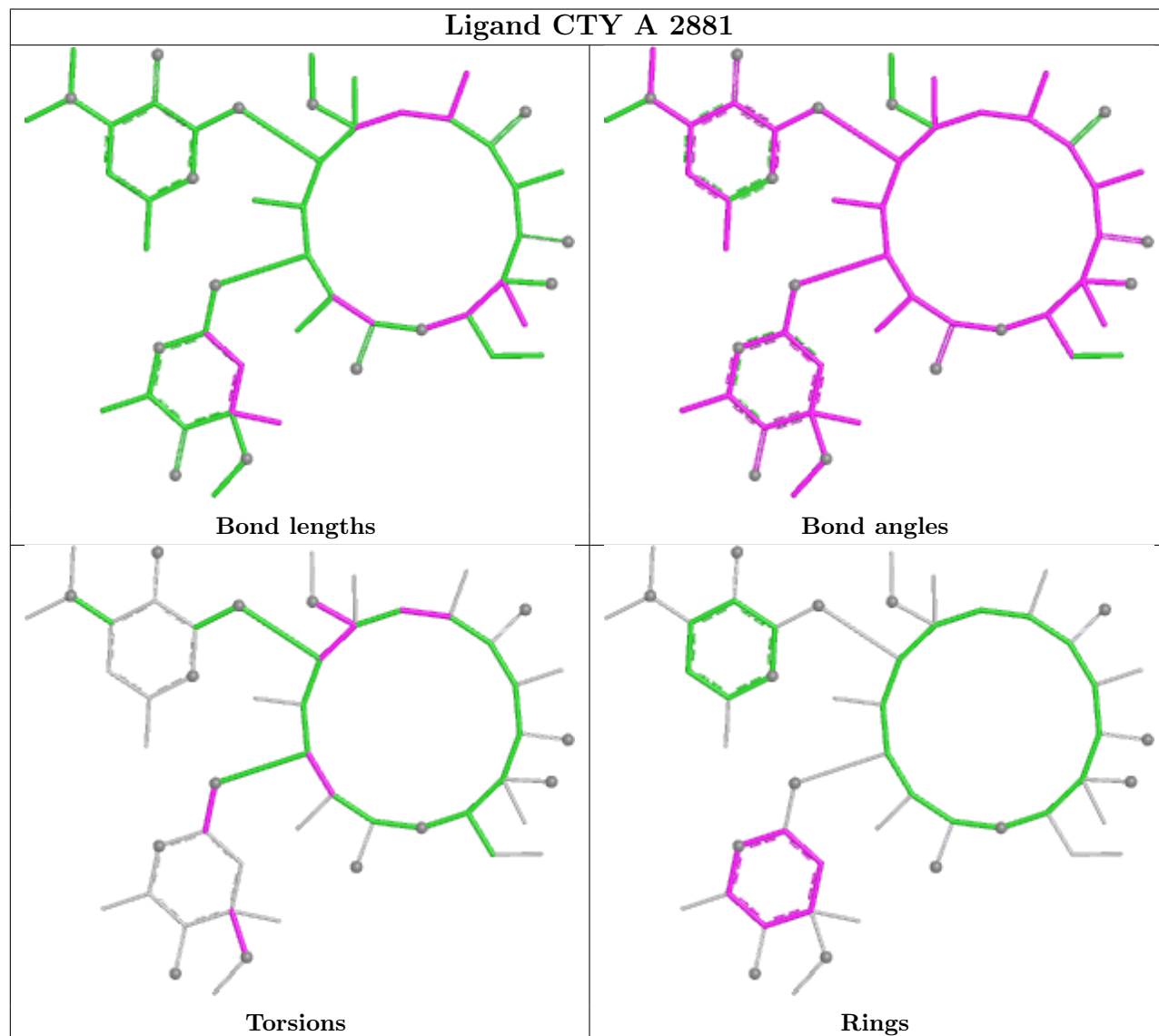
Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C14-C15-C16-C17-C18-O4

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 ⓘ

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.