



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
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Deposited on : 2002-03-06
Resolution : 3.50 Å(reported)

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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)
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

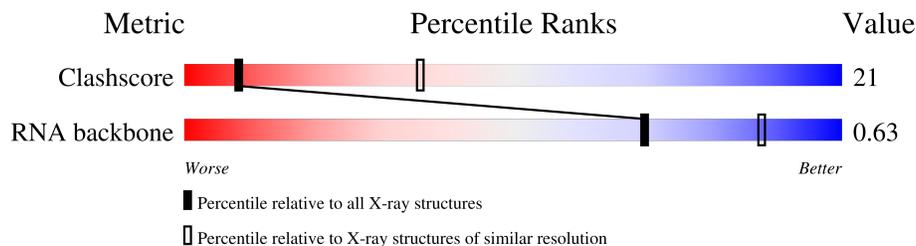
1 Overall quality at a glance

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 ≥ 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 [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

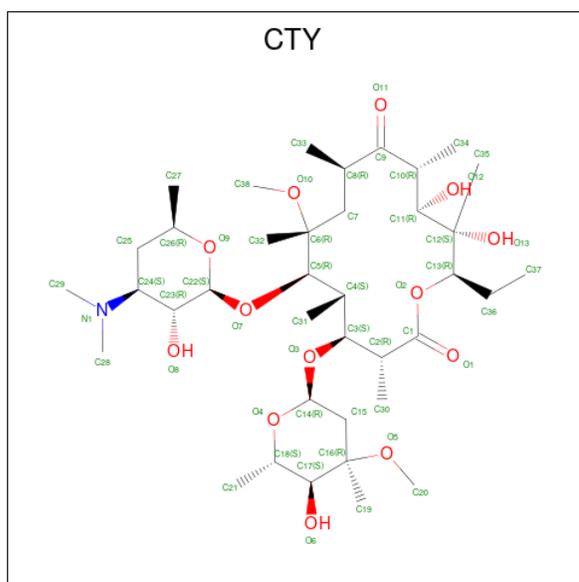
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

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).

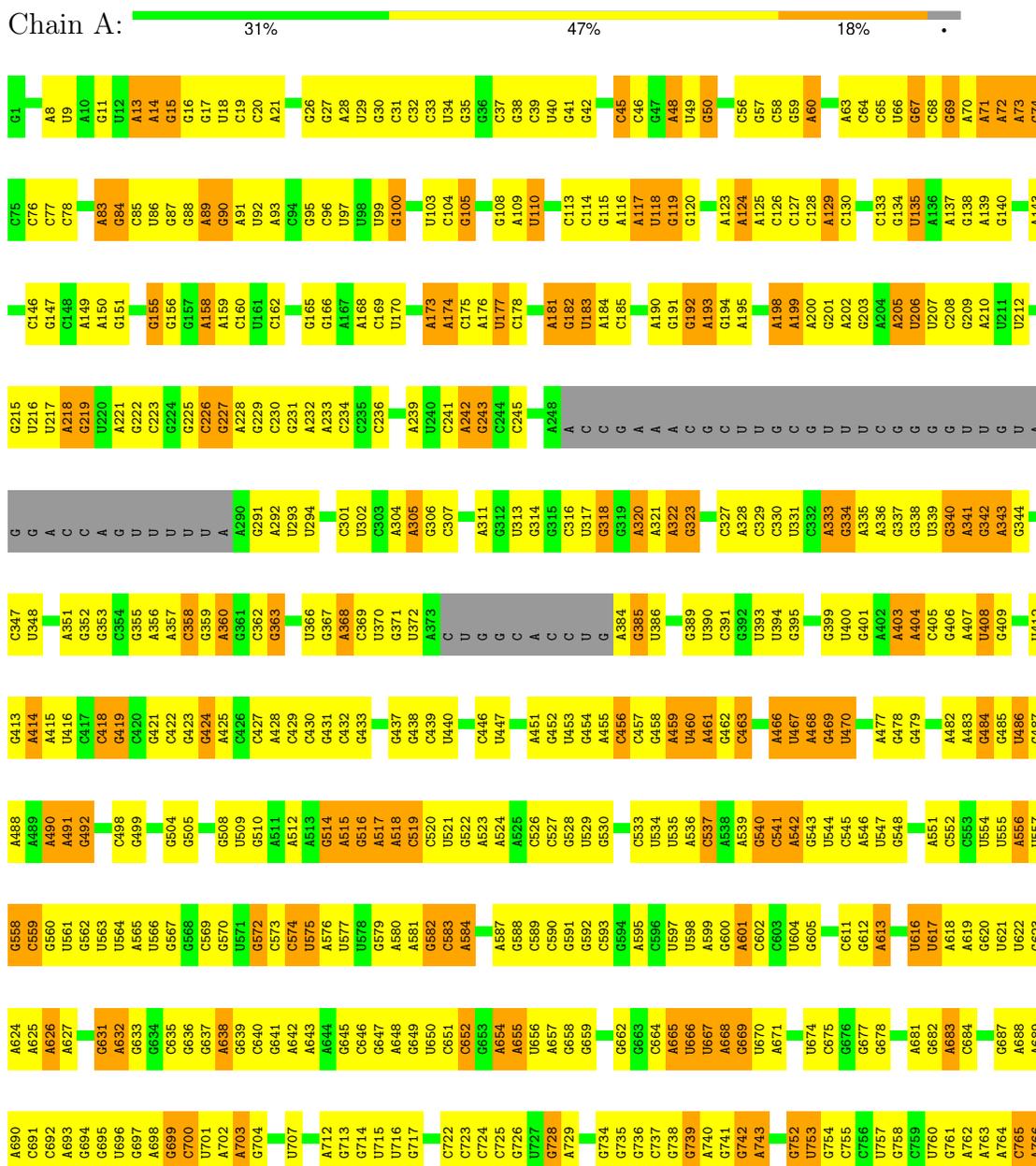
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

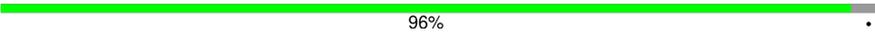
- Molecule 1: 23S RRNA



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A1753	C1763	G1613	G1543	G1481	U1410	U1339	C1270	U1194	G1125	U1056	U978	C910	G841	G774
G1754	A1686	C1614	A1544	U1482	C1411	C1340	C1271	U1195	A1126	A1057	A979	A910	A842	A775
G1755	C1686	G1615	A1545	U1483	C1412	G1341	G1272	G1196	C1127	G1058	G980	A912	G843	G776
C1756	U1548	C1616	U1548	G1484	C1413	C1342	C1273	U1197	C1128	C1060	C982	C914	G844	A777
C1757	U1549	G1617	C1549	U1485	C1414	C1343	C1274	U1198	A1129	C1061	C983	C915	U845	G778
C1758	U1550	U1618	C1550	A1486	U1416	C1344	A1275	U1199	U1130	A1061	G984	A846	C850	U784
C1762	C1552	A1619	C1552	G1487	C1417	C1346	U1277	G1200	C1134	A1065	A984	C850	C851	U785
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C1631	C1558	U1425	C1558	G1353	U1425	C1353	C1283	G1210	A1140	U1071	A999	U860	C860	A791
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A1634	C1498	A1429	C1498	G1356	U1429	G1356	A1287	U1213	U1144	G1074	A1001	U863	C863	A795
G1635	A1499	G1430	A1499	U1357	U1430	U1357	A1288	G1214	G1145	C1075	C1003	A929	C864	A796
C1640	U1500	U1431	U1500	G1358	U1431	C1358	A1289	A1215	G1146	G1079	C1003	A930	C864	A797
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A1582	C1442	C1442	C1442	A1372	U1442	A1372	C1302	G1225	C1160	C1089	C1016	U942	U875	A807
A1583	G1373	C1443	G1373	G1374	U1443	G1374	U1306	A1226	U1161	C1090	U1019	U943	U876	C808
C1514	C1444	C1444	C1444	G1374	U1444	G1374	U1307	A1227	U1162	G1091	A1022	A944	U877	C809
U1515	U1446	U1446	U1446	G1377	U1446	G1377	C1310	A1233	C1163	U1092	A1021	A945	U878	G811
G1519	G1450	U1447	G1450	C1380	U1447	C1380	C1311	G1240	A1166	A1096	A1023	C948	U879	G812
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C1522	U1452	U1452	U1452	G1382	U1452	G1382	U1313	G1242	G1168	G1098	G1030	A951	U881	G814
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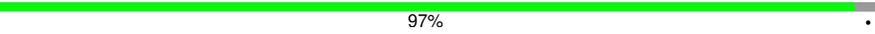
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		A2041	G2103	A2169	C2240	U2339	G2395	G2465	U2534	G2607	G2607	C2761	U2840	
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			U	U2185	G2256	G2330	U2416	U2485	C2554	U2626	U2626	U2774	U2841	
			U	G2186	G2261	A2337	U2417	G2487	C2555	G2627	G2627	U2775	U2841	
			G2122				A2418		A2556			G2782		

- Molecule 2: RIBOSOMAL PROTEIN L4

Chain K:  96%

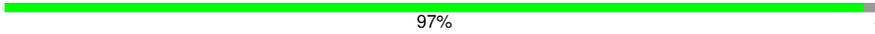


- Molecule 3: RIBOSOMAL PROTEIN L22

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	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:

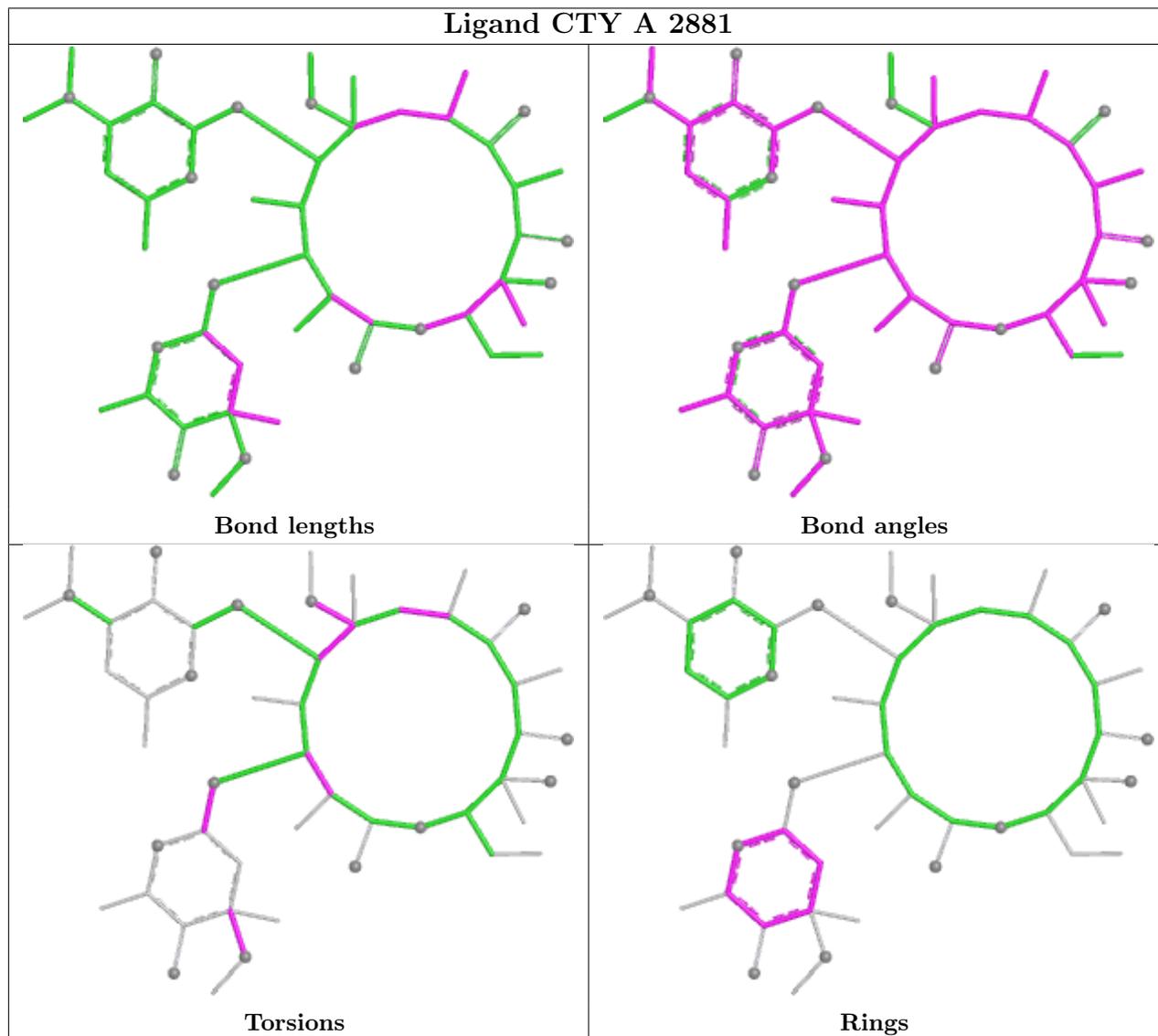
Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C14-C15-C16-C17-C18-O4

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

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.