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Crystal structure analysis of a beta carbonyl derivative

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The title compound C30H26BrClN2O3 belongs to the class of the β-carbolines. β-carboline alkaloids are a group of natural and synthetic indole alkaloids. They are commonly present in various plants, bacteria, fungi, marine microorganisms, and in human tissues and body fluids. The compound was synthesized in redox neutral C–H functionalization method. The resultant compound was characterized by 1H NMR and X-ray diffraction. The X-ray diffraction study reveals that the sample has crystallized in the triclinic crystal system in the space group $P\bar{1}$. The asymetric unit cell contains two molecules. The lattice parameters are a = 9.6544(3) Å, b = 11.1048(4) Å, c = 14.1787(5) Å, α = 87.2370(10)°, β = 70.5310(10)°, γ = 65.3700(10)° and V = 1295.48(8) Å3. The molecule is stabilized by both intra and intermolecular interactions of the type C-H...O, C-H...N and N-H...O hydrogen bonds. The molecular conformation is stabilized by a weak intramolecular π – π stacking interaction. In the crystal, N-H..O and C-H...O hydrogen bonds connect the molecules into inversion dimers.

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