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Crystal Structure and Hirshfeld Surface Analysis of a *β*-Carboline Derivative

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ABSTRACT

The title compound was synthesized in redox neutral C–H functionalization method. The resultant compound was characterized by ^{1}H NMR and X-ray diffraction. The X-ray diffraction study reveals that the sample has crystallized in the triclinic crystal system with the space group $P\bar{1}$. The asymmetric 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) Å^3. 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.

Keywords: *β*-carbolines, *P. Harmala*, Hirshfeld surface analysis, Fingerprint plots.