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Synthesis, Characterization, Crystal Structure and Hirshfeld Surface Analysis of (1*E*)-1-Phenylethanone (1-Isobutyl-1*H*-Imidazo [4,5-*C*] Quinolin-4-Yl)Hydrazone

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ABSTRACT

The compound (1E)-1-phenylethanone (1-isobutyl-1H-imidazo [4,5-c] quinoline-4-yl) hydrazone was synthesized by condensation of 4-hydrazino-1-isobutyl-1H-imidazo[4,5-c]quinoline with acetophenone. The resultant compound was crystallized using ethanol by slow evaporation technique. The structure was investigated by FTIR, ^{1}H NMR, ^{13}C NMR and confirmed by single crystal X-ray diffraction studies. The title compound crystallizes in the monoclinic crystal system, in the space group $P2_1/c$ with cell parameters a=10.3426(7) Å, b=18.4489(13) Å, c=11.7160(9) Å, β=115.409(4)°, Z=4 and V=2013.3(3) Å^3. The structure adopts an E-conformation with respect to C=N bond. The structure exhibits both inter and intra molecular hydrogen bonds of type N—H…N, C—H…N, O—H…N and C—H…O. The Hirshfeld surface analysis for visually analyzing intermolecular interaction in the crystal structure was carried out. H-H (57.9%) interactions play a prominent role in stabilizing the crystal structure.

Keywords: Imidazo-quinoline; Hydrazone; Crystal structure; FTIR spectrum; *E* conformation.