

Crystal structure of $\{(1E)-1-isobutyl-4-(2-(1-phenylethylidene)hydrazinyl)-1H-imidazo[4,5-c]quinoline\}$ Chethan Prathap K. N.¹, Lokanath N. K.¹, Naveen S.²¹Department of Studies In Physics, University of Mysore, Mysuru, India, ²Institution of Excellence, University of Mysore, Mysuru, India

E-mail: cpforphysics@gmail.com

Imidazo-quinolone have been demonstrated to possess antiviral, antitumor, antiallergic, human toll like reception, and immune response modification activities. Imidazo quinolone derivative, (1E)-1-isobutyl-4-(2-(1-phenylethylidene)hydrazinyl)-1H-imidazo[4,5-c] quinolone hydrate (C₂₂H₂₁N₅.H₂O) was synthesized by condensation of 4-hydrazino-1-isobutyl-1H-imidazo[4,5-c]quinolone with acetophenone. The title compound was characterized by FT-IR, NMR spectroscopic techniques and finally the structure was confirmed by X-ray diffraction studies. The structure adopts an E conformation with respect to the C=N. The compound exhibits both inter and intramolecular hydrogen bonds of type O—H...N, C—H...O and C—H...N. The intermolecular interaction studies were carried out using Hirshfeld surface analysis. The intermolecular contacts H...H (60%) play a prominent role in the stabilization of crystal and molecular structure of the title molecule. The packing diagram indicates that the molecules exhibit layered stacking and are inter connected by the intermolecular hydrogen bonds.

[1] Shukla and Nikunj, M. et al., (2011). Bioorganic & medicinal chemistry letters, 21, 3232-3236.

[2] Sheldrick, G. M. (2008). Acta Cryst., A64, 112.

[3] Spackman, M. A. and Jayatilaka, D. (2009). CrystEngComm., 11, 1932.

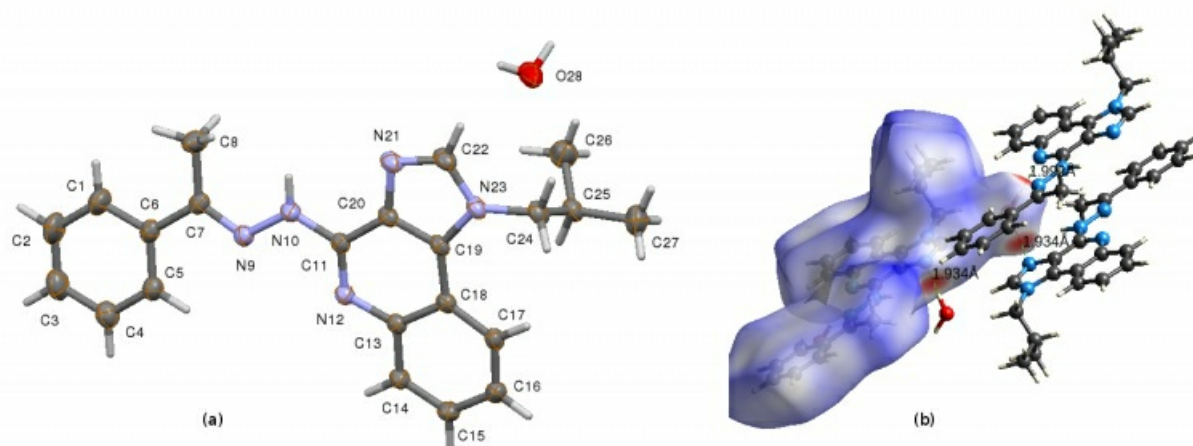


Figure: (a) ORTEP diagram of the title molecule with 30% probability. (b) Visualization of intermolecular interactions in the crystal lattice.

Keywords: [Imidazo-quinolone](#), [Single crystal X-ray diffraction](#), [Hirshfeld surface analysis](#)