(E)-N'-(4-nitrobenzylidene)-2-(1-(4-methoxyphenyl)-5-oxo-1H-1,2,4-triazol-4(5H)-yl)acetohydrazide acetohydrazide: Synthesis, Crystal structure, DFT and Hirshfeld surface analysis

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(*E*)-*N'*-(4-nitrobenzylidene)-2-(1-(4-methoxyphenyl)-5-oxo-1*H*-1,2,4-triazol-4(5*H*)-yl)acetohydrazide acetohydrazide: Synthesis, Crystal structure, DFT and Hirshfeld surface analysis

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A B S T R A C T

A new Schiff base (*E*)-*N'*-(4-nitrobenzylidene)-2-(1-(4-methoxyphenyl)-5-oxo-1*H*-1,2,4-triazol-4(5*H*)-yl)acetohydrazide acetohydrazide (**3**) was synthesized and characterized by IR, ^{1}H NMR, ^{13}C NMR, Mass spectral data, elemental analysis, TGA/DTA and finally by single crystal X–ray crystallography. X–ray diffraction study indicates that the title compound crystallizes in the monoclinic crystal system (space group $P2_1/n$) with unit cell dimensions a = 11.2265(3) Å, b = 8.8051(2) Å, c = 18.6200(6) Å, β = 90.772(2)°, Z = 4, and V= 1840.43(9) Å^3. The crystal structure is stabilized by intermolecular hydrogen bonds (C–H···O and N–H···O) and short contacts of the type C–O···π. Theoretical calculations of the compound **3** are carried out using density functional theory (DFT) at B3LYP/6–31+G level. Intermolecular interactions in the crystal structures were quantified using the Hirshfeld surface analysis. The majority contribution to the Hirshfeld surface is H···O (34.6%) contacts.

Key words: Crystal structure, Schiff base, X–ray diffraction, Interactions, DFT calculations, Hirshfeld surface analysis, Fingerprint plots.

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