Structural elucidation and Hirshfeld surface analysis of a novel pyrazole derivative: 3-(Benzo[d][1,3]dioxol-5-yl)-1-(3-chlorophenyl)-5-(2,4-dichlorophenyl)-4,5-dihydro-1H-pyrazole

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Abstract

The title compound 3-(benzo[d][1,3]dioxol-5-yl)-1-(3-chlorophenyl)-5-(2,4-dichlorophenyl)-4,5-dihydro-1*H*-pyrazole was synthesized by the reaction of (*E*)-1-(benzo[d][1,3]dioxol-5-yl)-3-(2,4-dichlorophenyl)prop-2-en-1-one and (3-chlorophenyl)hydrazine hydrochloride. The synthesized compound was characterized by ^{1}H NMR, ^{13}C NMR and mass spectral analysis and finally the structure was confirmed by single crystal X-ray diffraction studies. The compound crystallizes in the triclinic crystal system with the space group *P-1*. The pyrazole ring in the chiral racemate adopts an envelope conformation with the compound possessing a chiral center at C3 with *R* conformation. The molecular structure involves C—H···π and Cg···Cg interactions. Also, the crystal structure is stabilized by both inter and intra-molecular hydrogen bonds of the type C—H...Cl and C—H…N respectively which can account for the stability of the molecule. Further, Hirshfeld surface analysis employing 3D molecular surface contours and 2D fingerprint plots have been used to analyze intermolecular interactions present in the solid state of the crystal.

Keywords: Pyrazoles, X-ray diffraction, Intermolecular Interactions, Hirshfeld surface, Electrostatic potential