

MS10-P5 Intermolecular interactions in
4-[[[(4Z)-5-oxo-2-phenyl-4,5-dihydro-
1,3-oxazol-4-ylidene] methyl] phenyl
acetate: Insights from Crystal Structure and
Hirshfeld Surface Analysis

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The 1,3-oxazole ring is known to have the biological activity in its own right and serves as useful intermediate in the synthesis of biologically important imidazole molecules. The investigations for the title molecule (I) is the part of ongoing research on crystallographically important organic molecules. The colourless, block shape single crystals obtained by slow evaporation from ethanol solution were used for X-ray diffraction experiment. Intensity data were measured at 100 K on Agilent Technologies Super Nova diffractometer using CuK α (λ = 1.5418 Å). The structure was solved using direct methods and refined by full-matrix least-squares on F² using SHELX programs. The Hirshfeld surfaces generated using *Crystal Explorer* and the two dimensional fingerprint plots provide the visual representation of crystal packing interactions in the structure. The molecule has Z-configuration about central olefinic bond, and the overall U-shaped conformation. The crystal structure of (I) determined at 100 K shows clear distinction from that at 293 K as the intermolecular interactions can be described more precisely due to improvement in thermal as well as geometrical parameters. The collective influence of intramolecular C-H...N and C-H...O interactions with the respective S(6) and S(5) graph-set motifs, intermolecular C-H...O interaction having R²₂(14) graph-set, C-O... π and π - π stacking along b-axis stabilize the crystal structure of (I) at 100 K in contrast to the presence of only C-O... π interaction at 293 K. The intermolecular C-H...O interactions appear as bright-red spots near H7 and O3 atoms, and the inter atomic short C...C contacts as faint spots near corresponding atoms on the Hirshfeld surface mapped over d_{norm} . The C-O... π and π - π interactions in the crystal are identified from Hirshfeld surfaces mapped with shape-index and curvedness respectively. The significant features appearing in the two dimensional fingerprint plots are complementary to describe the role of intermolecular interactions in the crystal packing of title molecule (I). The intermolecular interactions were further assessed by a new descriptor enrichment ratio (ER) based on Hirshfeld surface analysis. Nearly same ER values for significantly contributing inter atomic contacts at 293 K and 100 K with the exception for C...C contacts also justify the determination of crystal structure of (I) at 100 K so as to describe the crystal packing interactions more precisely.

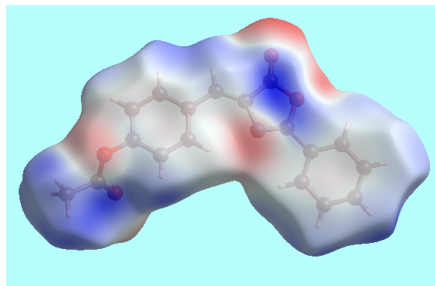


Figure 1. View of Hirshfeld surface mapped over electrostatic potential.

Keywords: Oxazoles, Intermolecular interactions, Hirshfeld surface Analysis, Fingerprint plots.