



**Crystal Structure and Hirshfeld Surfaces of
5-(3-Bromophenyl)-3-(4-methoxyphenyl) Isoxazole**

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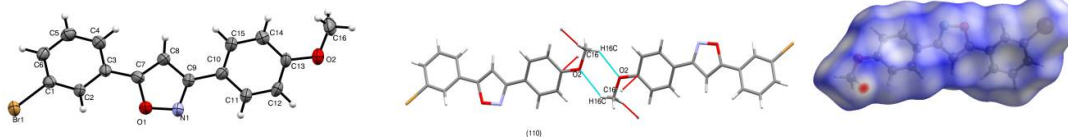
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ABSTRACT

The titled compound was synthesized and the structure was investigated by X-ray crystallography. The compound crystallizes into a monoclinic crystal class with space group of $P_{21/c}$ with unit cell parameters of $a=30.1197(19)\text{\AA}$, $b=5.8661(4)\text{\AA}$, $c=7.7258(5)\text{\AA}$, $\beta=96.630(3)^\circ$ and $Z=4$. The structure is solved by a direct method and it is refined to $R_1=0.053$. The dihedral angle between the terminal benzene rings are $48.3(2)^\circ$ which indicate the structure is not a planar one. The presence of C-H... π and C-H...O intermolecular interactions leads to the formation of molecular stacking parallel to (101) plane. The Hirshfeld surface studies were carried out and it is confirmed that C...H, H...H and H...Br are the significant contributions towards packing.

Graphical Abstract



Keywords: Isoxazole, Dihedral angle, C-H... π interactions, Hirshfeld surfaces.