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Crystal structure analysis of 6-amino-5-(6-fluoro-3-phenylisoxazolo[5,4-b]quinolin-4-yl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione

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Abstract: The crystal structure of 6-amino-5-(6-fluoro-3-phenylisoxazolo[5,4-b]quinolin-4-yl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione ($C_{22}H_{16}FN_5O_3$). The compound crystallizes in Monoclinic P2₁/c space group with unit cell parameters at 296(2) K as follows: $a = 13.3119(5) \text{ \AA}$, $b = 10.7033(4) \text{ \AA}$, $c = 13.8141(4) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 91.8261(12)^\circ$, $\gamma = 90^\circ$. Crystal data were collected using BRUKER SMART APEX II CCD X-ray diffractometer. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares procedures to the final R_1 of 0.0384 using SHELXL programs.

Key Words: isoxazole, quinolone, pyrimidine and crystal structure.

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