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2-[1-(4,6-Dimethoxypyrimidin-2-yl)-1*H*-pyrazol-3-yl]phenol

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In the crystal structure of the title compound, $C_{15}H_{14}N_4O_3$, there are an intramolecular O—H···N hydrogen bond and intermolecular π–π stacking interactions.

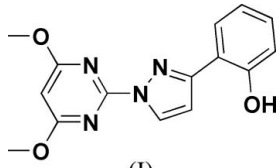
Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.128
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, (I) (Fig. 1), is a di-substituted pyrazole derivative. In this paper, we report the result of an X-ray diffraction study of this compound.



(I)

The pyrimidine, pyrazole and benzene rings are approximately coplanar; the dihedral angles between the pyrimidine and pyrazole, pyrimidine and benzene, and pyrazole and benzene rings are 3.50 (8), 11.84 (7) and 9.09 (8)°, respectively. The pyrazole rings at (x, y, z) and $(2-x, 2-y, 1-z)$, and the pyrimidine rings at (x, y, z) and $(1-x, 2-y, 1-z)$, form π–π stacking interactions; the interplanar spacing and the centroid–centroid distance between the pyrazole rings are 3.464 (4) and 3.917 (2) Å, respectively, while those between the pyrimidine rings are 3.418 (2) and 3.810 (2) Å, respectively (Fig. 2).

Experimental

To a solution of 2-(1*H*-pyrazol-3-yl)-phenol (1.60 g, 10 mmol), which was prepared according to the reported method (Pleier *et al.*, 2001), and anhydrous K_2CO_3 (1.80 g, 13 mmol) in acetone (20 ml), 2-methanesulfonyl-4,6-dimethoxypyrimidine (2.18 g, 10 mmol) was added. The mixture was stirred at 329 K for 6 h. The resulting precipitate was purified by chromatography on silica gel with petroleum ether/acetone (15:1 *v*/*v*) as eluant to give (I) as a white solid (yield 2.47 g, 83%). Single crystals suitable for X-ray diffraction were obtained by crystallization from an ethanol solution at room temperature.

Crystal data

$C_{15}H_{14}N_4O_3$
M_r = 298.30
Monoclinic, $P2_1/c$
a = 8.1971 (9) Å
b = 11.1416 (12) Å
c = 16.0917 (17) Å
β = 98.538 (2)°
V = 1453.3 (3) Å^3
Z = 4
D_x = 1.363 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 297 (2) K
Block, colorless
0.40 × 0.20 × 0.04 mm

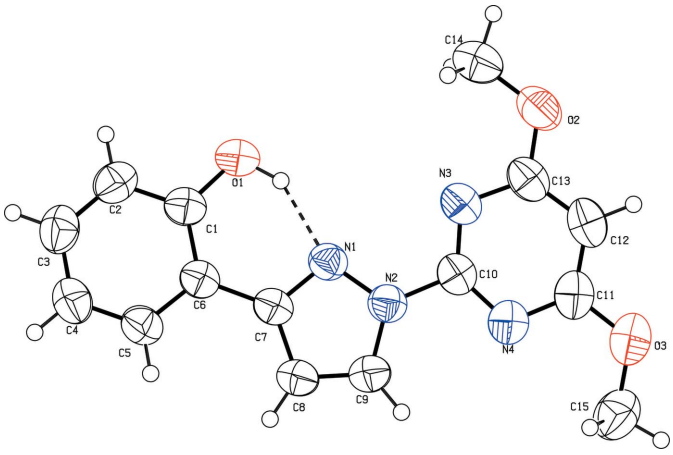


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates the intramolecular hydrogen bond.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.962, T_{max} = 0.996
8620 measured reflections
3162 independent reflections
2470 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
S = 1.02
3162 reflections
204 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 0.1123P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.92 (2)	1.78 (2)	2.6143 (16)	148 (2)

The O-bound H atom was located in a difference Fourier map and refined with a distance restraint of O—H = 0.92 (2) Å, and with U_{iso}(H) = 1.5U_{eq}(O). All other H atoms were positioned geometrically (C—H = 0.93 or 0.96 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

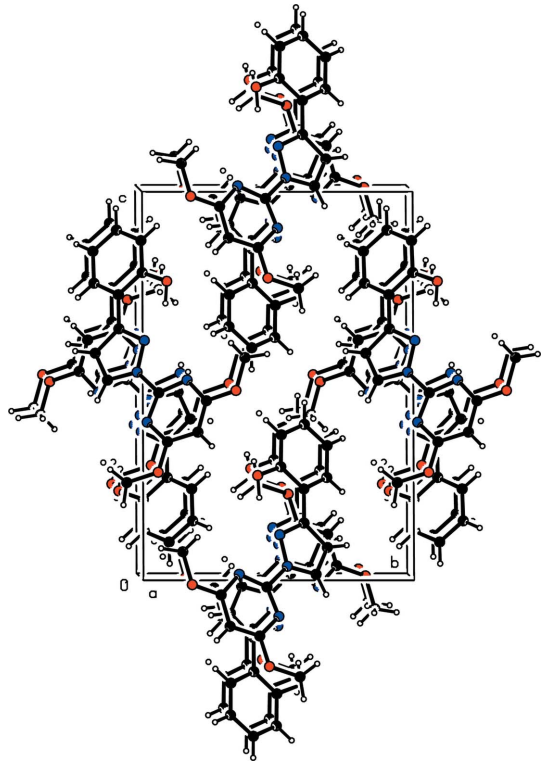


Figure 2
A packing diagram of (I), viewed down the *a* axis, showing π–π stacking interactions.

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