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(*E*)-5-(3,5-Dimethylphenoxy)-1,3-dimethyl-1*H*-pyrazole-4-carbaldehyde *O*-(2-chloropyrimidin-4-yl)oxime

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In the title compound, $C_{18}H_{18}ClN_5O_2$, there are two independent molecules in the asymmetric unit. In both molecules, the pyrimidine ring is almost coplanar with the central pyrazole ring, while the benzene ring is almost perpendicular to it.

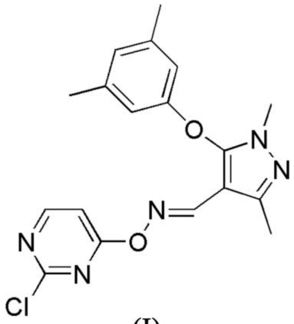
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.050
wR factor = 0.146
Data-to-parameter ratio = 13.6

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

Comment

Pyrimidine derivatives are very important molecules in biology and have many applications as pesticides and pharmaceuticals (Condon *et al.*, 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives, such as AZT, have also found use as antiviral agents (Gilchrist, 1997). In order to discover new biologically active pyrimidine compounds, the title compound, (I), was synthesized and its structure is reported here. It crystallizes with two independent molecules in the asymmetric unit (Fig. 1). All bond lengths and angles are normal.



(I)

In both independent molecules, the central pyrazole ring is almost coplanar with the pyrimidine ring and approximately perpendicular to the benzene ring. The dihedral angles formed by the pyrimidine ring and the benzene ring with the pyrazole ring in the two independent molecules are 8.35 (16) and 87.95 (10)° in one molecule and 8.30 (24) and 85.60 (9)° in the other.

Experimental

2,4-Dichloropyrimidine (2.2 mmol), anhydrous potassium carbonate (0.552 g, 4 mmol), and 5-(3,5-dimethylphenoxy)-1,3-dimethyl-1*H*-pyrazole-4-carbaldehyde oxime (2 mmol) were mixed in acetonitrile (40 ml) and refluxed for 5 h. The solvent was then evaporated *in vacuo*. The residue was recrystallized from ethanol and single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from ethyl acetate at room temperature.

Crystal data

$C_{18}H_{18}ClN_5O_2$
$M_r = 371.82$
Triclinic, $P\overline{1}$
$a = 8.217\ (2)$ Å
$b = 8.4391\ (15)$ Å
$c = 30.674\ (5)$ Å
$\alpha = 93.15\ (1)^\circ$
$\beta = 90.342\ (3)^\circ$
$\gamma = 118.958\ (3)^\circ$
$V = 1857.0\ (6)$ Å^3
$Z = 4$
$D_x = 1.330$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.23$ mm^{-1}
$T = 294\ (2)$ K
Block, colorless
$0.50 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.895$, $T_{\max} = 0.956$
9445 measured reflections
6481 independent reflections
4096 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.026$
$\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.146$
$S = 1.04$
6481 reflections
478 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.178P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.41$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0153 (15)

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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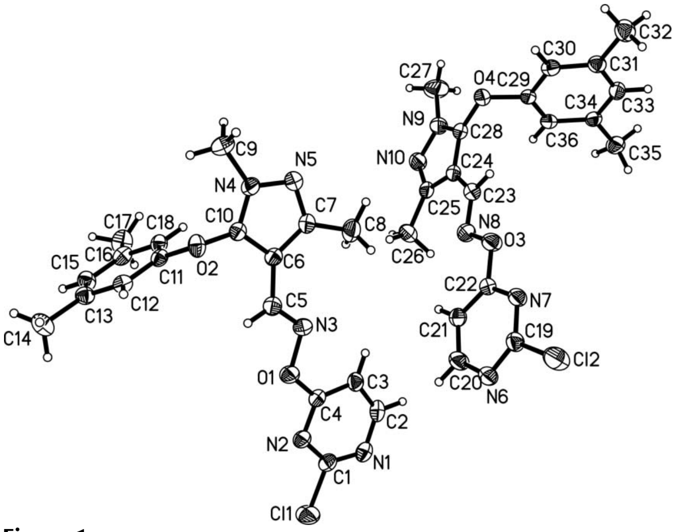

Figure 1
The asymmetric unit of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level.

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