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2-(4,6-Dimethoxypyrimidin-2-yloxy)-6-fluoro-*N*-(3-methylpyridyl)benzylamine

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In the title compound, $C_{19}H_{19}FN_4O_3$, the two heterocyclic ring substituents lie on the same side of the central benzene ring.

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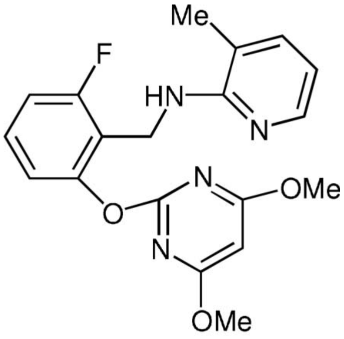
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.173
Data-to-parameter ratio = 16.0

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

Comment

Pyrimidinyloxybenzylamine derivatives have very high weed-control activity: they are highly efficient with low toxicity, and biodegradable, safe and environmentally friendly agrochemicals (Lu *et al.*, 2001). As part of a study of their structure–activity relationship (SAR), the title compound, (I), that was a product of condensation reactions of 4,6-dimethyloxy-2-methylsulfonylpyrimidine, 2-amino-3-methylpyridine and 2-fluoro-6-hydroxybenzaldehyde, was investigated.



(I)

In (I), the two heterocyclic rings lie on the same side of the benzene ring (Fig. 1); the dihedral angle between the two nitrogen-containing rings is 85.67 (10)°. This conformation allows the formation of a centrosymmetric dimer mediated by a pair of N—H···N hydrogen bonds (Table 1).

Experimental

2-Amino-3-methylpyridine (0.54 g, 5 mmol) was added dropwise to a methanol solution of 2-fluoro-6-hydroxybenzaldehyde (0.7 g, 5 mmol). At room temperature, $NaBH_4$ (0.34 g) was added with stirring to give a yellow precipitate. After extraction and distillation, and drying *in vacuo*, the product was added to a flask containing a tetrahydrofuran solution (25 ml) of 4,6-dimethyloxy-2-methylsulfonylpyrimidine (0.98 g, 4.5 mmol) and K_2CO_3 (1.17 g) and the mixture was refluxed for 5 h. After filtration, the liquor was evaporated under vacuum to give a solid (1.38 g, yield 83%), which was recrystallized from methanol and petroleum ether (3:1) to give colorless blocks (m.p. 359–360 K).

Crystal data

$C_{19}H_{19}FN_4O_3$
$M_r = 370.38$
Triclinic, $P\overline{1}$
$a = 8.8490\ (10)$ Å
$b = 10.5810\ (10)$ Å
$c = 11.3773\ (8)$ Å
$\alpha = 113.4470\ (10)^\circ$
$\beta = 98.8520\ (10)^\circ$
$\gamma = 106.364\ (2)^\circ$
$V = 893.89\ (15)$ Å^3
$Z = 2$
$D_x = 1.376$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3528 reflections
$\theta = 3.5$–27.5°
$\mu = 0.10$ mm^{-1}
$T = 295\ (1)$ K
Block, colorless
0.42 × 0.38 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.940$, $T_{\max} = 0.978$
6292 measured reflections
3991 independent reflections
2983 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 27.5^\circ$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.173$
$S = 1.06$
3991 reflections
249 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1093P)^2 + 0.0797P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.43$ e Å^{-3}
$\Delta\rho_{\min} = -0.33$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.050 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H*N*1···N3$^{\rm i}$	0.89 (2)	2.56 (2)	3.355 (2)	149 (2)

Symmetry code: (i) $-x, -y, -z$.

The H atom attached to atom N1 was located in a difference Fourier map and refined isotropically. Other H atoms were placed in calculated positions and allowed to ride on their parent atoms, with C—H = 0.98 (aromatic), 0.97 (methylene) or 0.96 Å (methyl). $U_{\rm iso}$(H) values were set at $1.2U_{\rm eq}$(C) (aromatic and methylene H) or $1.5U_{\rm eq}$(C) (methyl H).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure*; software used to prepare material for publication: *CrystalStructure*.

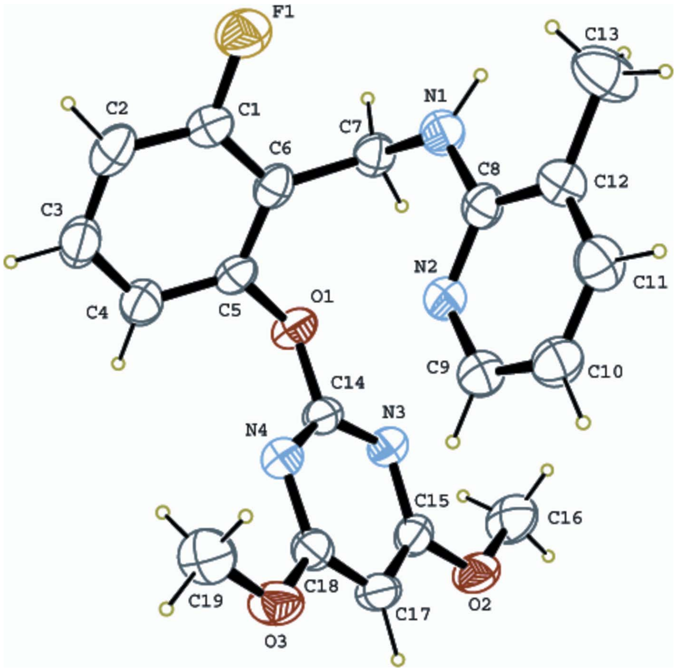


Figure 1
The structure of (I), shown with 40% probability displacement ellipsoids.

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