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6-Chloro-2-(4-fluorophenyl)imidazo[1,2-*b*]-pyridazine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.131
Data-to-parameter ratio = 14.7

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

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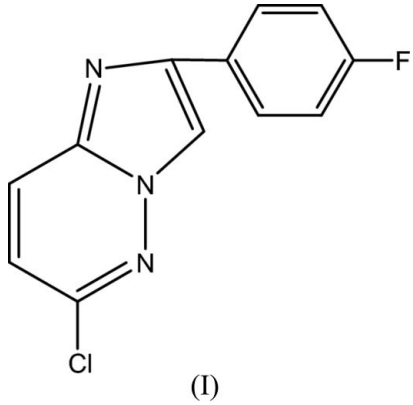
The title compound, $C_{12}H_7ClFN_3$, is of pharmacological interest. Both substituents lie close to the plane of the heterocycle. C—H···F and C—H···N hydrogen bonds stabilize the structure.

Comment

Derivatives of imidazo[1,2-*b*]pyridazine are active in a wide spectrum of biological and therapeutic areas (Moreau *et al.*, 1994; Sacchi *et al.*, 1999; Ishikawa *et al.*, 2000). Research findings indicate that imidazo[1,2-*b*]pyridazines exhibit high biological activity as selective cyclin-dependent kinase (CDK) inhibitors (Byth *et al.*, 2004) and potential antirhinoviral agents (Hamdouchi *et al.*, 2003). In view of this, we have recently focused on the preparation of new imidazo[1,2-*b*]pyridazine derivatives.



(I)

The title compound, (I), has been synthesized by mixing 6-chloropyridazin-3-amine and 2-bromo-1-(4-fluorophenyl)-ethanone in dry ethanol (Enguehard *et al.*, 2001). Both substituents lie close to the plane of the heterocycle (Fig. 1), with a dihedral angle of 3.09 (9)° between the plane of the heterocycle and that of the fluorobenzene ring. The structure is stabilized by weak C—H···F hydrogen bonds linking molecules in a head-to-tail fashion. C—H···N interactions, forming centrosymmetric rings, also contribute to the packing (Fig. 2 and Table 1).

Experimental

A solution of 6-chloropyridazin-3-amine (5.87 g, 55.7 mmol) and 2-bromo-1-(4-fluorophenyl)ethanone (15.7 g, 72.4 mmol) in dry ethanol (60 ml) was refluxed for 12 h. After cooling, ethanol was removed in a vacuum and the residue was taken up in H_2O. The mixture was made basic with Na_2CO_3 and extracted with CH_2Cl_2. The organic layers were dried (Na_2SO_4), filtered, and evaporated to

dryness. The residue was chromatographed on silica gel (CH_2Cl_2). A white powder was obtained (yield 50.2%) and single crystals of (I), suitable for crystallographic analysis, were obtained by slow evaporation of an ethyl acetate solution.

Crystal data

$C_{12}H_7ClFN_3$
M_r = 247.66
Triclinic, $P\overline{1}$
a = 5.6051 (7) Å
b = 7.4946 (10) Å
c = 13.2471 (17) Å
α = 101.308 (2)°
β = 91.883 (2)°
γ = 100.565 (2)°
V = 535.06 (12) Å^3
Z = 2
D_x = 1.537 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1324 reflections
θ = 5.7–52.4°
μ = 0.35 mm^{-1}
T = 293 (2) K
Block, colourless
0.47 × 0.33 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.685, T_{max} = 0.910
3153 measured reflections
2260 independent reflections
1695 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 27.0°
$h = -6 \rightarrow 7$
$k = -9 \rightarrow 6$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.131
S = 0.96
2260 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 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
C7—H7···F1^{i}	0.93	2.64	3.470 (3)	149
C8—H8···N1^{ii}	0.93	2.68	3.573 (2)	161

Symmetry codes: (i) $x, y, z+1$; (ii) $-x-1, -y+1, -z+2$.

All H atoms were refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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

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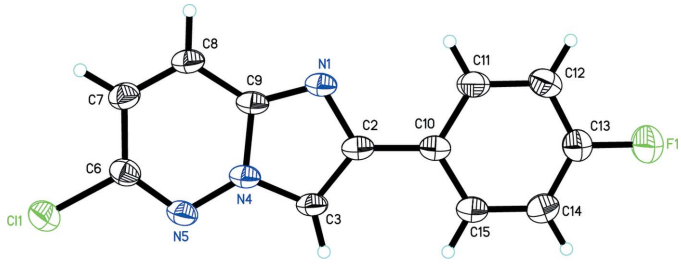

Figure 1
The molecular structure of (I), drawn with 30% probability ellipsoids.

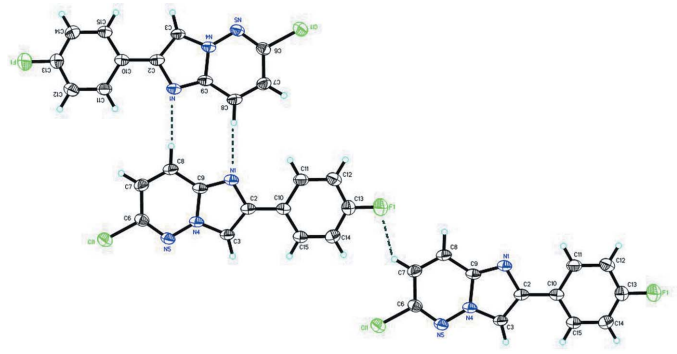

Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines) in (I).

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