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1-Amino-2-anilino-4-(4-fluorobenzylidene)-1*H*-imidazol-5(4*H*)-one

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In the title compound, $C_{16}H_{13}FN_4O$, centrosymmetric hydrogen-bonded dimers are linked into one-dimensional chains along the [100] direction. The chains are further linked to give a sheet parallel to the (101) plane by C—H···F hydrogen bonds.

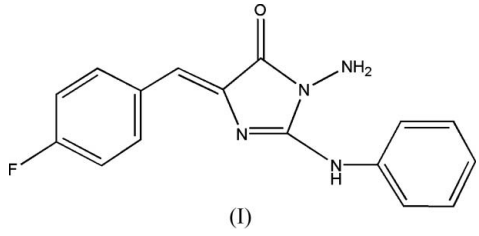
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.065
wR factor = 0.155
Data-to-parameter ratio = 15.1

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

Comment

Imidazol-4-one derivatives are important heterocycles, which have good fungicidal and antiphlogistic activities (Ding *et al.*, 2001; Trivedi & Shah, 1993). In order to find compounds presenting both low toxicity and high biological activity, we synthesized a series of new imidazol-4-ones containing 4-fluorobenzene derivatives. In this context, we have crystallized the title compound, (I), and report its crystal structure here.



(I)

The molecular conformation is illustrated in Fig. 1. In the molecular structure, two benzene rings and the imidazole ring are almost coplanar; the torsion angles C6—C7—C8—N1 and N1—C10—N4—C12 are −1.3 (5) and 1.1 (4), respectively. All other molecular geometric features are unremarkable.

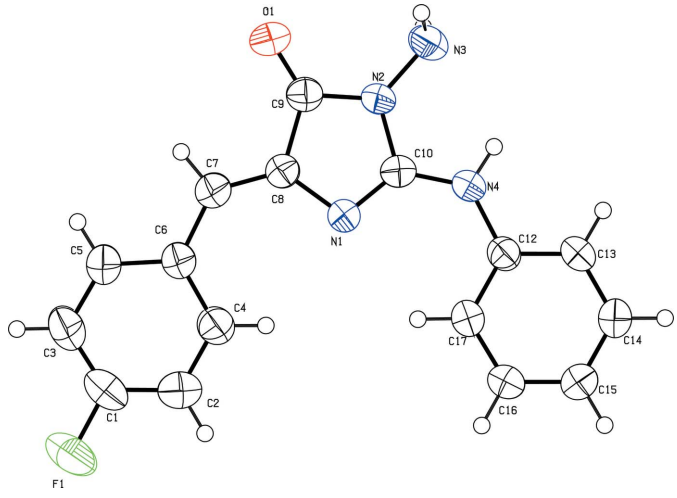


Figure 1
Molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

In the packing, the reference molecule at (x, y, z) is linked to the centrosymmetrically related molecule at $(-x, -y, 2-z)$, forming a hydrogen-bonded dimer centered at (0,0,1). These dimers are linked into a two-dimensional sheet parallel to the (101) plane by N—H···O (or ···N) and C—H···F hydrogen bonds (Fig. 2 and Table 1). Analysis using *PLATON* (Spek, 2003) shows that no specific interaction is found between the adjacent layers.

Experimental

Compound (I) was synthesized according to the procedure of Ding *et al.* (2001). Suitable crystals were obtained by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{16}H_{13}FN_4O$
$M_r = 296.30$
Monoclinic, $P2_1/n$
$a = 5.5218$ (5) Å
$b = 25.529$ (2) Å
$c = 10.0165$ (9) Å
$\beta = 100.553$ (2)°
$V = 1388.1$ (2) Å^3
$Z = 4$
$D_x = 1.418$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 292$ (2) K
Block, purple
0.20 × 0.10 × 0.04 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.980$, $T_{max} = 0.996$
9440 measured reflections
3144 independent reflections
1654 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.155$
$S = 0.98$
3144 reflections
208 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···F1^{i}	0.93	2.49	3.348 (3)	154
N3—H3B···O1^{ii}	0.862 (10)	2.52 (3)	2.973 (3)	114 (2)
N3—H3C···N1^{iii}	0.866 (10)	2.413 (11)	3.279 (3)	178 (3)
N4—H4A···N3	0.862 (10)	2.28 (2)	2.762 (3)	115 (2)

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

All C-bound H atoms were placed in idealized locations and were refined using a riding model, with C–H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C). Atoms H3*B*, H3*C* and H4*A* were located in difference maps and refined with the restraints N—H = 0.86 (1) Å and U_{iso}(H) = $1.2U_{eq}$(N).

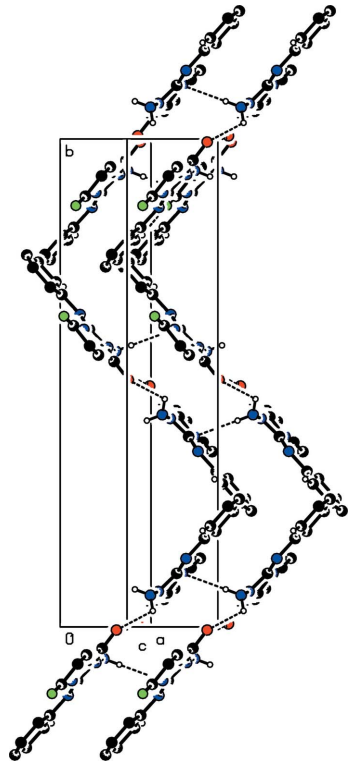


Figure 2
Packing of the molecules, with hydrogen bonds shown as dashed lines. C-bound H atoms have been omitted.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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*.

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