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2-[2-(*p*-Chlorophenyl)benzimidazol-1-ylmethyl]-5-(2-fluoroanilino)-1,3,4-thiadiazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.043
wR factor = 0.120
Data-to-parameter ratio = 14.3

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

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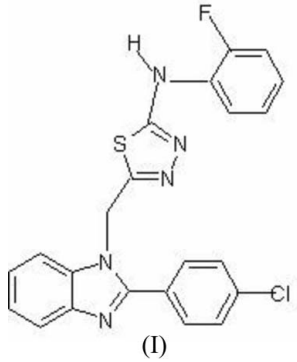
In the title compound, $C_{22}H_{15}ClFN_5S$, molecules are linked by N—H···N hydrogen bonds into chains, which in turn are linked into sheets by C—H···π interactions.

Comment

The development of resistance to current antibacterial therapy continues to drive the search for more effective agents. In addition, primary and opportunistic fungal infections continue to increase the number of immunocompromized patients, those suffering from diseases such as AIDS or cancer or who have undergone organ transplantation. It is well known that benzimidazoles exhibit antimicrobial (Göker *et al.*, 1998; Kılcıgil *et al.*, 1999), antitubercular, anticancer, anthelmintic, antiallergic, antioxidant (Can-Eke *et al.*, 1998), anticonvulsant (Demirayak *et al.*, 2002) and analgesic activities. It is also well known that thiadiazoles possess anti-inflammatory and antimicrobial activities.



(I)

In the title compound, (I), the chlorobenzene and benzimidazole ring systems are inclined at 81.91 (7)° to each other. The dihedral angle between the imidazole ring and the neighbouring benzene ring is 1.40 (9)°. The thiadiazole and fluorobenzene rings are inclined at 4.79 (11)° to each other. The dihedral angle between the benzimidazole ring system and the thiazole ring is 73.9 (1)°.

The packing consists of chains linked by hydrogen bonds between N5 and N2 (Table 1 and Fig. 2). C–H···π interactions further stabilize the structure by linking the chains into layers parallel to the *bc* plane (Table 1).

Experimental

Compound (I) was synthesized and crystallized according to Kılcıgil *et al.* (2005).

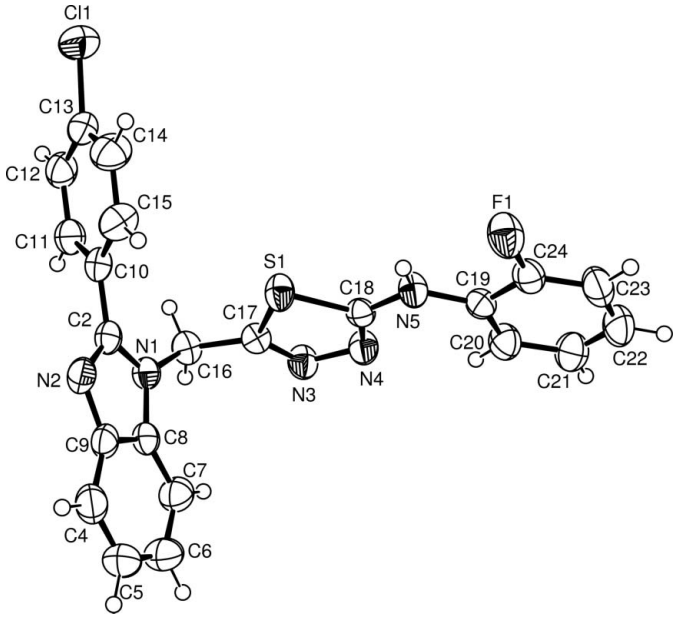


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

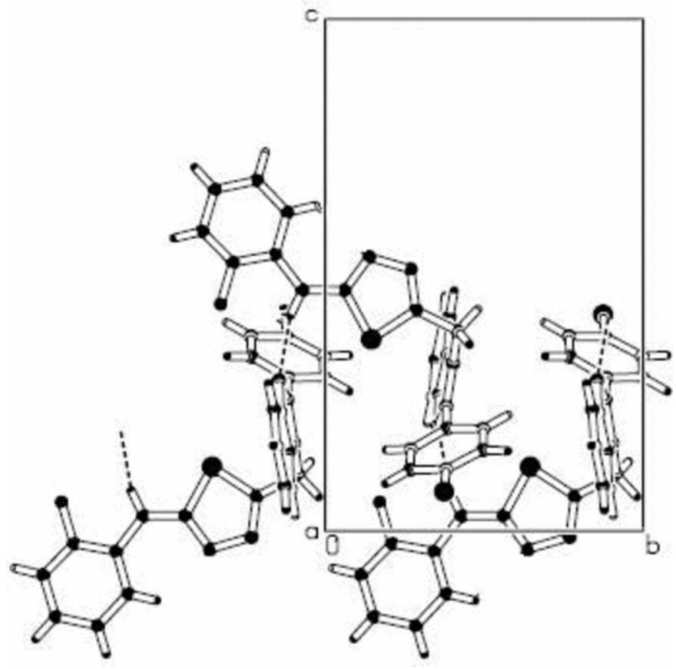


Figure 2
Crystal packing of (I), projected on to the *bc* plane. Dashed lines indicate hydrogen bonds.

Crystal data

$C_{22}H_{15}ClFN_5S$
M_r = 435.9
Monoclinic, $C2/c$
a = 25.583 (5) Å
b = 9.9377 (14) Å
c = 20.207 (3) Å
β = 127.599 (12)°
V = 4070.3 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 293 (2) K
0.36 × 0.33 × 0.24 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.894, T_{max} = 0.927
4033 measured reflections
3948 independent reflections
2473 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
3 standard reflections
frequency: 120 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.121
S = 1.03
3948 reflections
276 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···F1	0.87 (2)	2.27 (2)	2.654 (3)	106.3 (18)
C20—H20···N4	0.93	2.34	2.948 (4)	123
N5—H5···N2^{i}	0.87 (2)	2.08 (2)	2.921 (3)	161.3
C6—H6···$Cg(1)^{ii}$	0.93	3.14	3.940 (5)	145
C11—H11···$Cg(2)^{iii}$	0.93	3.00	3.806 (3)	146
C12—H12···$Cg(3)^{iii}$	0.93	2.92	3.676 (3)	140

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

The H atom attached to N5 was found in a difference map and refined freely. All other H atoms were placed in idealized positions and refined using a riding model, with U_{eq}(H) = 1.2U_{eq}(C), and fixed distances of C—H = 0.93 Å (aromatic) and 0.97 Å (ethylene).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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