

## 2-(4-Fluoroanilino)-4,5-dimethyl-1,3-thiazole

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## Key indicators

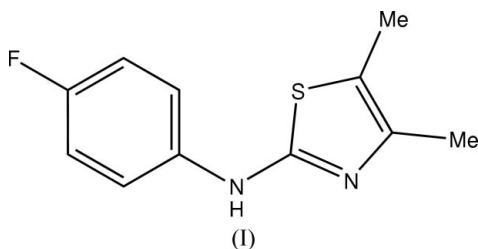
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.064  
 $wR$  factor = 0.152  
Data-to-parameter ratio = 13.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{11}\text{H}_{11}\text{FN}_2\text{S}$ , the dihedral angle between the least-squares planes of the fluoroaniline and 1,3-thiazole fragments is  $46.47(17)^\circ$ . The molecules form dimers by  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds. There are no significant  $\pi-\pi$  interactions in the crystal structure.

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## Comment

In a previous study, we found the molecule of 2-anilino-4,5-dimethyl-1,3-thiazole, (II), to be essentially planar except for the methyl H atoms (Jumal & Yamin, 2006). However, compound (I), which has an F atom at the 4-position of the aniline group (Fig. 1), shows a non-planar conformation, with an angle of  $46.47(17)^\circ$  between the least-squares planes of the fluoroaniline ( $\text{F1}/\text{C1}-\text{C6}/\text{N1}$ ) and 1,3-thiazole ( $\text{S1}/\text{N2}/\text{C7}-\text{C9}$ ) fragments. The maximum deviation from the mean plane of the fluoroaniline fragment is  $0.031(3)\text{ \AA}$  for atom N1. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987).



In the crystal structure, the molecules are linked by  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds (Table 2), forming dimers, as observed in (II), and are stacked parallel to the  $b$  axis without significant  $\pi-\pi$  interactions (Fig. 2).

It seems that the driving force for the non-planar conformation of (I) is the intramolecular  $\text{H1B}\cdots\text{S1}$  short contact of  $2.72\text{ \AA}$  (Table 2), which is nearly the sum of the van der Waals radii of H (aromatic) and S atoms ( $2.80\text{ \AA}$ ; Bondi, 1964). The corresponding  $\text{H}\cdots\text{S}$  distance in (II) is  $2.49\text{ \AA}$ , suggesting intramolecular strain which may be compensated by the intermolecular  $\pi-\pi$  interactions (Jumal & Yamin, 2006).

## Experimental

A solution of 4-fluoroaniline (2.20 g, 0.02 mol) in acetone (40 ml) was added dropwise to an acetone solution (40 ml) containing equimolar amounts of 3-chloro-2-butanone (2.14 g, 0.02 mol) and ammonium thiocyanate (1.52 g, 0.02 mol) in a two-necked round-bottomed flask. The mixture was refluxed for 3 h. The resulting solution was poured into a beaker containing ice cubes. The white precipitate was filtered off, washed with distilled water and ethanol, and then dried.

Recrystallization from acetone yielded crystals of (I) (3.1 g, 70%) suitable for X-ray analysis.

Crystal data

$C_{11}H_{11}FN_2S$   
 $M_r = 222.28$   
 Monoclinic,  $P2_1/c$   
 $a = 11.915 (5) \text{ \AA}$   
 $b = 4.0811 (17) \text{ \AA}$   
 $c = 22.546 (9) \text{ \AA}$   
 $\beta = 100.151 (7)^\circ$   
 $V = 1079.2 (8) \text{ \AA}^3$

$Z = 4$   
 $D_x = 1.368 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.28 \text{ mm}^{-1}$   
 $T = 298 (2) \text{ K}$   
 Slab, colourless  
 $0.50 \times 0.24 \times 0.09 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scan  
 Absorption correction: multi-scan  
 SADABS (Bruker, 2000)  
 $T_{\min} = 0.872, T_{\max} = 0.975$

5081 measured reflections  
 1887 independent reflections  
 1423 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.041$   
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.064$   
 $wR(F^2) = 0.152$   
 $S = 1.14$   
 1887 reflections  
 138 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.3409P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

Table 1

Selected torsion angles ( $^\circ$ ).

C7–N1–C6–C1	41.3 (5)	C6–N1–C7–S1	9.0 (5)
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Table 2

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1–H1B $\cdots$ S1	0.93	2.72	3.124 (4)	107
N1–H1A $\cdots$ N2 <sup>i</sup>	0.86	2.18	3.038 (4)	172

Symmetry code: (i)  $-x, -y + 1, -z + 1$ .

After their location in difference maps, all H-atoms were positioned geometrically and allowed to ride on their parent atoms with  $C-H = 0.93-0.96 \text{ \AA}$  and  $N-H = 0.86 \text{ \AA}$ , and with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C,N)$  or  $1.5U_{\text{eq}}(C)$  for methyl groups.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

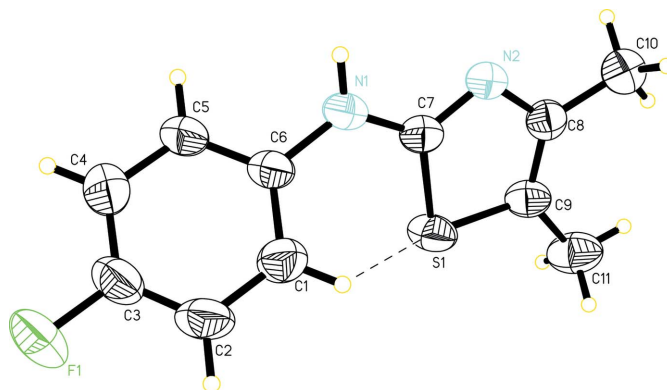


Figure 1

Molecular structure of (I), with 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

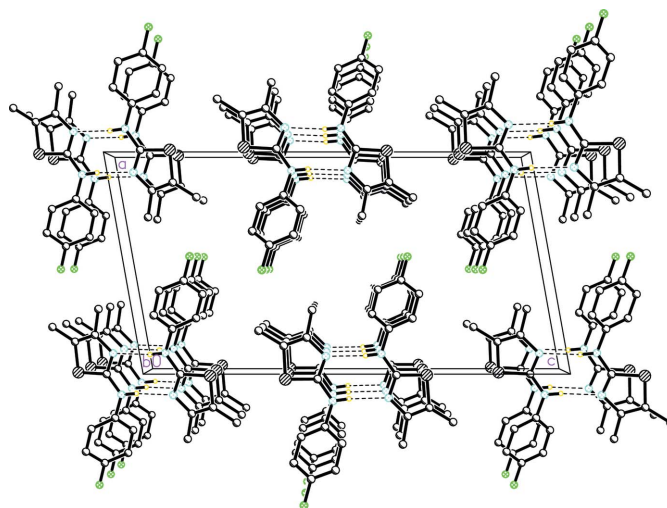


Figure 2

Packing diagram of (I), viewed down the  $b$  axis. H atoms have been omitted unless they are involved in hydrogen bonds (dashed lines).

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