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#### Key indicators

Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.077  
 $wR$  factor = 0.169  
Data-to-parameter ratio = 12.6

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

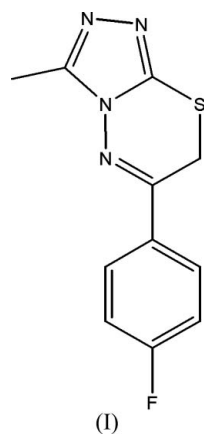
## 6-(4-Fluorophenyl)-3-methyl-7H-1,2,4-triazolo[3,4-b][1,3,4]thiadiazine

In the title compound,  $\text{C}_{11}\text{H}_9\text{FN}_4\text{S}$ , the triazole ring is planar, whereas the thiadiazine may be regarded as having a screw-boat conformation.

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#### Comment

1,2,4-Triazoles fused with six-membered ring systems are found to possess diverse applications in the fields of medicine, agriculture and industry. The commonly known systems are triazoles fused with pyridine, pyridazine, pyrimidine, pyrazines and triazines. A literature survey reveals that there are not many examples of triazoles fused with thiadiazines. Moreover, a large number of triazolothiazines have been shown to exhibit antimicrobial (Feng *et al.*, 1992) and diuretic (Mohan & Anjaneyulu, 1987) properties and act as photographic couplers (Holla *et al.*, 2001). In this paper, we report the synthesis and crystal structure of the title compound, (I).



In (I), the five-membered triazole ring (N2–N4/C9/C10) and the benzene ring (C1–C6) are each essentially planar, while the six-membered thiadiazine ring (N1/N2/C7–C9/S1) is distorted from planarity and may be regarded as having a screw-boat conformation, with atoms C8 and C7 displaced by 0.985 (5) and 0.408 (5) Å, respectively, above the N1/N2/C9/S1 plane (Fig. 1). Atoms N1 and S1 are slightly displaced away from the triazole ring plane by 0.039 (6) and 0.139 (6) Å, respectively. The benzene ring is nearly parallel to the triazole ring, with a dihedral angle between them of 5.7 (2)°. Both the S–C (mean 1.775 Å) and C–N bond lengths are in good agreement with the values observed in related complexes (Sert *et al.*, 2003; Xiang *et al.*, 2004). The C–N and N–N distances in the triazole ring indicate electron delocalization over the ring, as observed in similar compounds (Allen *et al.*, 1987; Jin *et al.*, 2004).

## Experimental

4-Amino-5-mercapto-3-methyl-1,2,4-triazole was prepared by the reaction of acetic acid and thiocarbohydrazide, following the literature method of Francesco *et al.* (1997). To a solution of 4-amino-5-mercapto-3-methyl-1,2,4-triazole (0.001 mol) in absolute ethanol (20 ml) was added 2-bromo-4'-fluoroacetophenone (0.001 mol). The mixture was refluxed for 7 h. The solid obtained on cooling was filtered, washed with cold water, dried and recrystallized from ethanol to give compound (I). The purified product was dissolved in 95% ethanol and kept at room temperature for 5 d, after which colourless single crystals of (I) were formed.

### Crystal data

$C_{11}H_9FN_4S$	$D_x = 1.517 \text{ Mg m}^{-3}$
$M_r = 248.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 1125 reflections
$a = 4.0626 (5) \text{ \AA}$	$\theta = 2.5\text{--}24.2^\circ$
$b = 25.530 (3) \text{ \AA}$	$\mu = 0.29 \text{ mm}^{-1}$
$c = 10.5576 (12) \text{ \AA}$	$T = 273 (2) \text{ K}$
$\beta = 96.909 (2)^\circ$	Block, colourless
$V = 1087.1 (2) \text{ \AA}^3$	$0.17 \times 0.14 \times 0.13 \text{ mm}$
$Z = 4$	

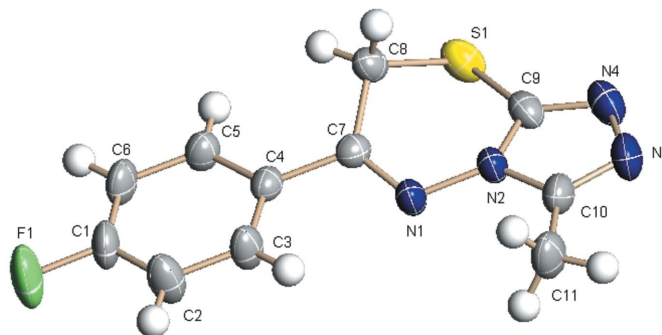
### Data collection

Bruker APEX area-detector diffractometer	1946 independent reflections
$\varphi$ and $\omega$ scans	1613 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.032$
$T_{\text{min}} = 0.956$ , $T_{\text{max}} = 0.958$	$\theta_{\text{max}} = 25.2^\circ$
5662 measured reflections	$h = -4 \rightarrow 4$
	$k = -25 \rightarrow 30$
	$l = -12 \rightarrow 11$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 0.5536P]$
$R[F^2 > 2\sigma(F^2)] = 0.077$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.169$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.25$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
1946 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
155 parameters	
H-atom parameters constrained	

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C–H = 0.93 Å (C<sub>aromatic</sub>) or 0.96 Å (C<sub>methylene</sub> and CH<sub>3</sub>), with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}_{\text{aromatic}}$ , C<sub>methylene</sub>) or  $1.5U_{\text{eq}}(\text{CH}_3)$ .



**Figure 1**

The molecular structure of (I), with the atom numbering, showing displacement ellipsoids at the 30% probability level.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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