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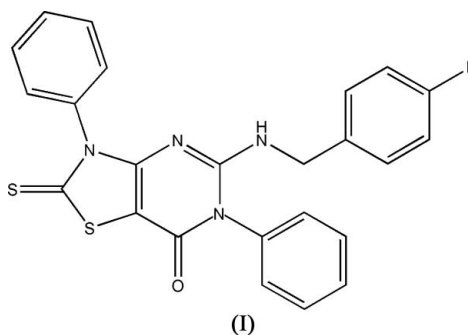
Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.053
 wR factor = 0.176
Data-to-parameter ratio = 13.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.5-(4-Fluorobenzylamino)-3,6-diphenyl-2-thioxo-
2,3-dihydro-1,3-thiazolo[4,5-*d*]pyrimidin-7(6*H*)-oneReceived 11 April 2006
Accepted 21 April 2006

In the title compound, $\text{C}_{24}\text{H}_{17}\text{FN}_4\text{OS}_2$, the three benzene rings are twisted with respect to the fused heterocyclic ring system, with dihedral angles of 76.2 (2), 90.2 (2) and 75.8 (2)°. The crystal packing is influenced by $\text{C}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{S}$ hydrogen bonds.

Comment

Thioxothiazolo[4,5-*d*]pyrimidine is an important analogue of purine, and its derivatives have shown sterilization and anti-tumour effects (Hazarika & Katakya, 2001; Abdelal *et al.*, 1999). In order to find compounds showing both low toxicity and high biological activity, we have synthesized a series of new thioxothiazolo[4,5-*d*] pyrimidines containing aminomethylbenzene derivatives. In this context, we have crystallized the title compound, (I), and report its crystal structure here.



In the crystal structure (Fig. 1), the C1–C6 and C19–C24 phenyl rings each make an approximately equal dihedral angle with the central fused heterocyclic ring system [76.2 (2) and 75.8 (8)°, respectively]. The third phenyl ring (C12–C17) is almost perpendicular to the central ring system, with a dihedral angle between the planes of 90.2 (2)°. The C19–C18–N4–C8 torsion angle is 78.2 (4). Except for this, no remarkable bonds or bond angles are observed in the molecular structure.

The crystal packing (Fig. 2) is stabilized by means of $\text{C}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{S}$ hydrogen bonds that lie along the [001] direction. Analysis using *PLATON* (Spek, 2003) shows no $\pi-\pi$ or $\text{C}-\text{H}\cdots\pi$ interactions in the crystal structure.

Experimental

Ethyl 2-isocyanoacetate (5 mmol), 1-isothiocyanatobenzene (5 mmol) and sulfur (0.16 g) were dissolved in *N,N*-dimethylformamide (20 ml), and then stirred for 8 h at 330 K. The solution

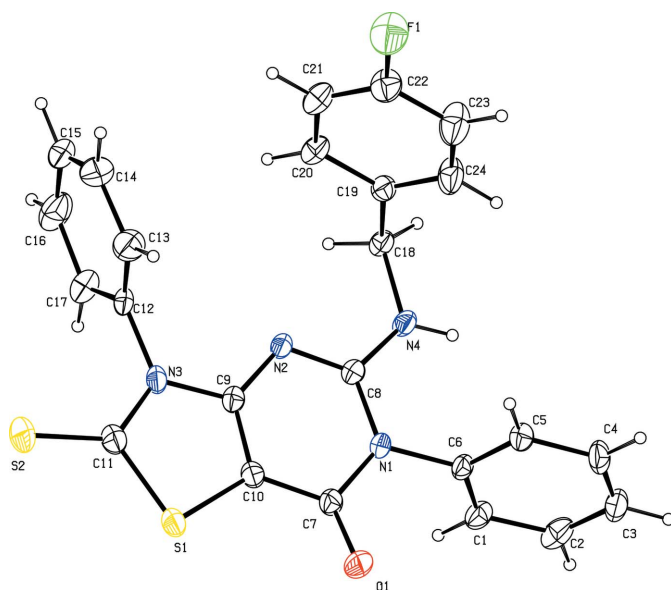


Figure 1
Molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

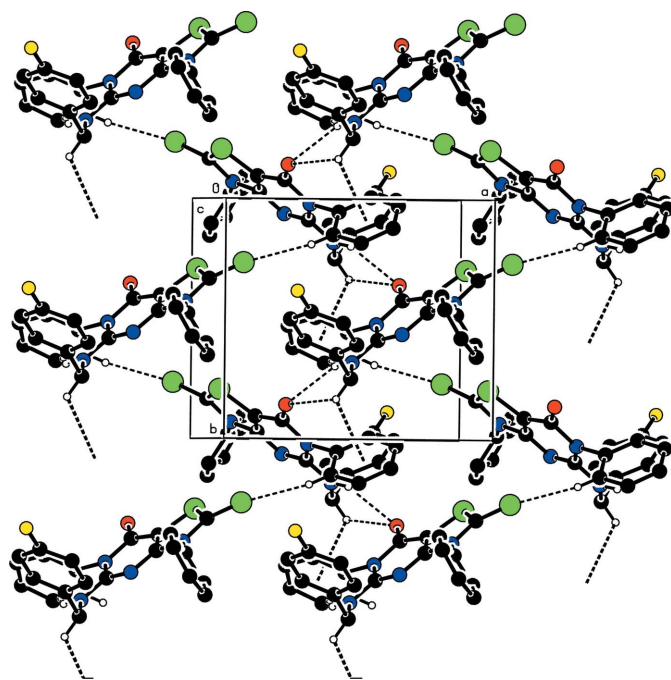


Figure 2
Packing of the molecules along the [001] direction with hydrogen bonds shown as dashed lines. H atoms not involved in the interactions shown have been omitted.

was filtered and the solvent was removed from the filtrate under reduced pressure. The solid residue was dissolved in triethylamine (30 ml), then triphenylphosphine (1.33 g), 1-isocyanatobenzene (0.60 g) and 4-fluorobenzylamine (5 mmol) were added, and the solution was stirred for 12 h at 310 K. After removal of triethylamine under reduced pressure, (I) was recrystallized from methanol. Suitable crystals were obtained by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{24}H_{17}FN_4OS_2$
 $M_r = 460.54$
Monoclinic, $P2_1$
 $a = 10.4507$ (14) Å
 $b = 9.2317$ (12) Å
 $c = 11.9817$ (16) Å
 $\beta = 104.691$ (2)°
 $V = 1118.2$ (3) Å³

$Z = 2$
 $D_x = 1.368$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.27$ mm⁻¹
 $T = 292$ (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector
diffractometer
 φ and ω scans
Absorption correction: none
6576 measured reflections

3862 independent reflections
3279 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.023$
 $\theta_{max} = 27.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.176$
 $S = 1.08$
3862 reflections
292 parameters

$w = 1/[\sigma^2(F_o^2) + (0.1174P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.25$ e Å⁻³
 $\Delta\rho_{min} = -0.31$ e Å⁻³
Absolute structure: Flack (1983),
1296 Friedel pairs
Flack parameter: 0.03 (12)

H atoms treated by a mixture of
independent and constrained
refinement

Table 1

Selected bond lengths (Å).

C8—N2	1.311 (4)	C11—S2	1.634 (4)
C8—N1	1.381 (4)	C11—S1	1.737 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C18—H18B ⁱ ⋯O1 ⁱ	0.97	2.60	3.213 (5)	122
C1—H1 ⁱ ⋯S2 ⁱⁱ	0.93	2.73	3.616 (4)	159
N4—H4A ⁱ ⋯O1 ⁱ	0.84 (2)	2.39 (5)	3.047 (5)	135 (6)

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

Atom H4 was located in a difference map and refined with the constraint $N-H = 0.86$ (1) Å; the $U_{iso}(H)$ value was set at $1.2U_{eq}(N4)$. All the other H atoms were included at calculated positions ($C-H = 0.93$ Å) and refined with a riding model with the $U_{iso}(H) = 1.2U_{eq}(C)$.

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

References

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