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3-[5-(3,5-Dimethylphenyl)-1,3,4-thiadiazol-2-yl]-2-(4-methoxyphenyl)thiazolidin-4-one

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The title compound, $C_{20}H_{19}N_3O_2S_2$, crystallizes with C—H···O and C—H···N hydrogen bonds which form a three-dimensional network.

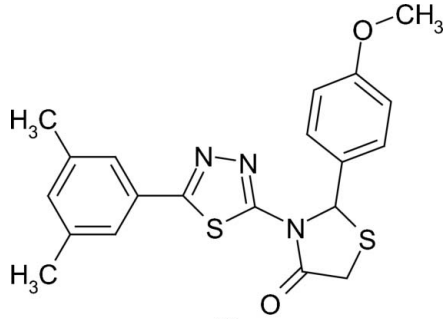
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.146
Data-to-parameter ratio = 15.2

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

Comment

Thiadiazole derivatives containing the thiazolidinone unit are of great interest because of their chemical and pharmaceutical properties. Some derivatives have fungicidal and herbicidal activities (Arun *et al.*, 1999) and others show insecticidal activities (Wasfy *et al.*, 1996). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. Intermolecular C—H···O and C—H···N hydrogen bonds form a three-dimensional network (Table 1 and Fig. 2).

Experimental

For the preparation of the title compound, [5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-yl]-(4-methoxybenzylidene)amine (5 mmol) and mercaptoacetic acid (5 mmol) were added to toluene (50 ml). The water produced by the condensation reaction was removed by distillation over a period of 5 h. The reaction mixture was then left to cool to room temperature and filtered; the filter cake was recrystallized from acetone to give pure compound (I) (m.p. 463–464 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

Crystal data

$C_{20}H_{19}N_3O_2S_2$
M_r = 397.50
Monoclinic, $P2_1/c$
a = 13.892 (3) Å
b = 7.2560 (15) Å
c = 18.912 (4) Å
β = 95.86 (3)°
V = 1896.4 (7) Å^3
Z = 4
D_x = 1.392 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

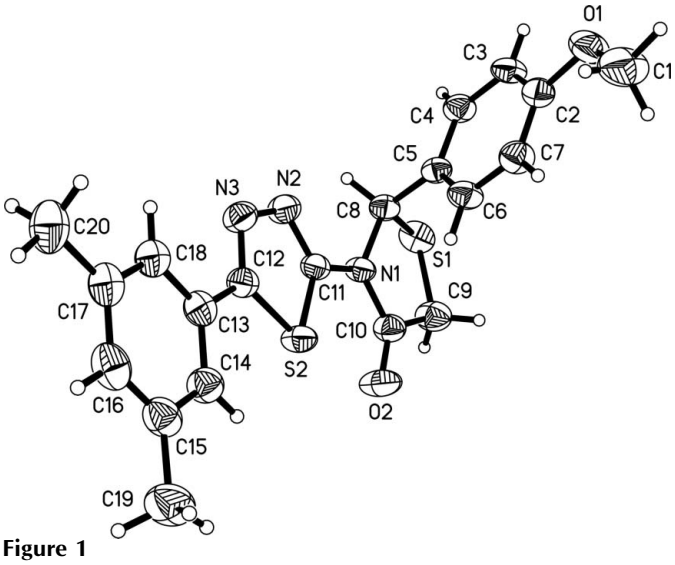


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

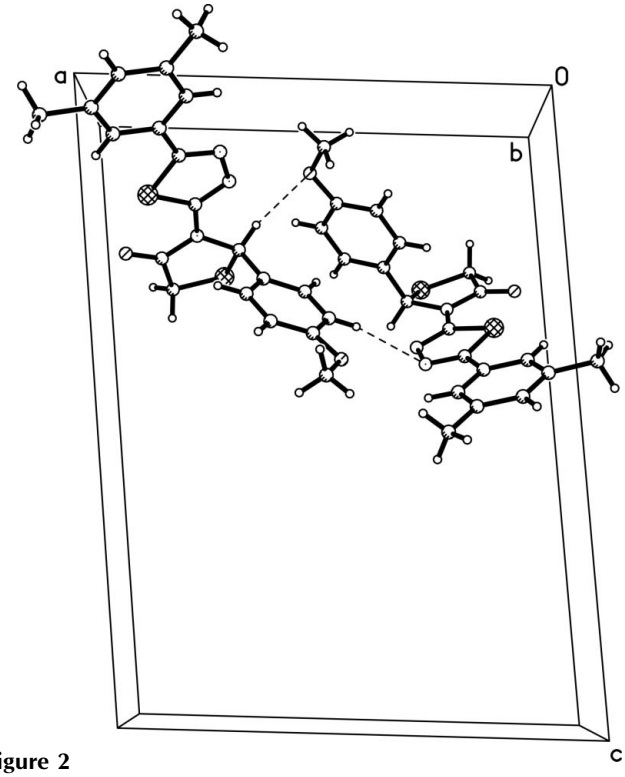


Figure 2
The hydrogen bonding in (I), with dashed lines indicating intermolecular C—H···O and C—H···N hydrogen bonds.

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.915, T_{max} = 0.971
3866 measured reflections
3709 independent reflections
2904 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.146
S = 1.03
3709 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3B···N3^{i}	0.93	2.62	3.533 (3)	169
C8—H8A···O1^{i}	0.98	2.57	3.530 (3)	166

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

All H atoms were positioned geometrically, with C—H distances in the range 0.93–0.97 Å, and included in the refinement in a riding-model approximation, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; 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: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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