Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

2-(*o*-Tolyloxy)-*N*-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]acetamide

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Received 11 March 2007
Accepted 25 March 2007

Key indicators

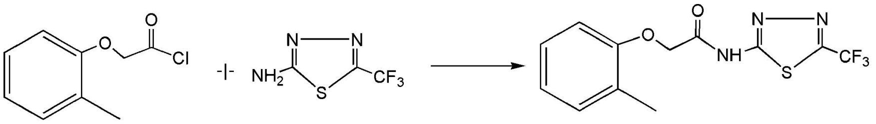
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.063
wR factor = 0.171
Data-to-parameter ratio = 11.6

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

In the title compound, $C_{12}H_{10}F_3N_3O_2S$, the molecules are linked into two-dimensional networks parallel to $(1\bar{1}0)$ through a mixture of π–π stacking and N—H···N hydrogen-bond interactions.

Comment

1,3,4-Thiadiazole derivatives exhibit many important bioactivities (Wang *et al.*, 2004; Castro *et al.*, 1996) and considerable interest has been shown in fluorine-containing compounds. Therefore, it is worth investigating fluoro derivatives incorporating 1,3,4-thiadiazole. In view of this, a number of new compounds have been synthesized in our laboratory, including the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The molecules are linked into a two-dimensional structure (Fig. 2) by a combination of N—H···N hydrogen bonds (Table 1) and π–π stacking between the rings S1/N2/N3/C10/C11 (centroid *Cg*1) and C2–C7 (centroid *Cg*2). The relevant centroid–centroid and (mean) perpendicular distances defining these interactions are 3.945 (2) and 3.77 (12) Å, respectively, for $Cg1\cdots Cg2^{i}$ [symmetry code: (i) $2 - x, -y, 1 - z$]. The trifluoromethyl group exhibits rotational disorder (Fig. 1), as previously observed in similar compounds (see, for example, Tan *et al.*, 2005).

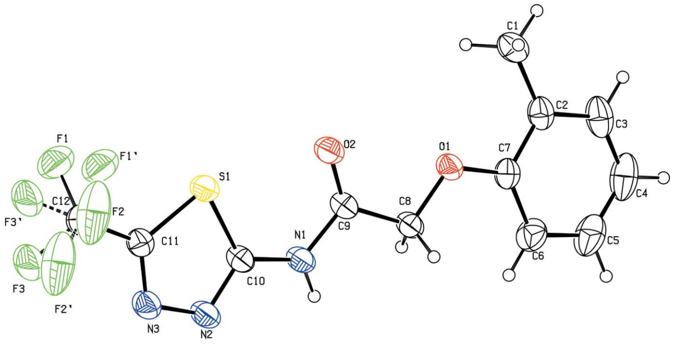


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Both disordered components of the CF_3 group are shown.

doi:10.1107/S1600536807014389

Experimental

2-Amino-5-[4-(trifluoromethyl)]-1,3,4-thiadiazole (0.68 g, 4.0 mmol) was prepared according to the reported procedure of Song *et al.* (2005). It (0.68 g, 4.0 mmol) was then treated with *o*-tolyloxyacetyl chloride (0.88 g, 4.5 mmol). The title compound was isolated in 63% yield. Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a solution in a mixture of methanol and dimethylformamide (1:5 *v*/*v*) at room temperature.

Crystal data

$C_{12}H_{10}F_3N_3O_2S$
$M_r = 317.29$
Triclinic, $P\overline{1}$
$a = 8.347$ (2) Å
$b = 9.430$ (2) Å
$c = 9.493$ (2) Å
$\alpha = 108.030$ (4)°
$\beta = 101.762$ (4)°
$\gamma = 94.381$ (4)°
$V = 687.8$ (3) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.28$ mm^{-1}
$T = 298$ (2) K
0.30 × 0.26 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
3448 measured reflections
2385 independent reflections
2061 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.171$
$S = 1.03$
2385 reflections
205 parameters
22 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max} = 0.33$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.31$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2$^{\rm i}$	0.856 (10)	2.037 (12)	2.885 (4)	171 (3)

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

Carbon-bound H atoms were positioned geometrically and refined using a riding model, with Csp^2—H = 0.93 Å, methyl C—H = 0.96 Å and methylene 0.97 Å; $U_{\rm iso}$(H) = $xU_{\rm eq}$(C), where x = 1.5 for methyl and 1.2 for methylene and Csp^2. The H atom attached to N was located in a difference map and refined with a restrained distance N—H = 0.86 (1) Å and a free $U_{\rm iso}$(H). The occupancies of the disordered trifluoromethyl group refined to 0.884 (16):0.116 (16). The disorder was refined using the commands DFIX and SADI.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

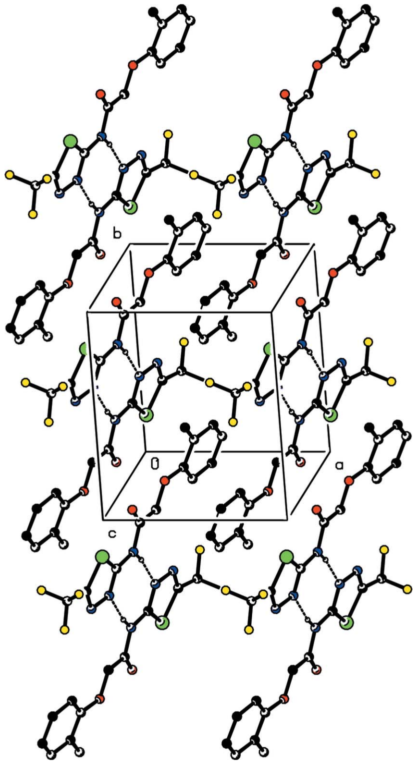


Figure 2
A packing view of (I). Dashed lines indicate hydrogen bonds. Only one disorder component is shown, and H atoms not involved in hydrogen bonding have been omitted.

This work was supported financially by the National Natural Science Foundation of China (No. 20602015), Program for Distinguished Young Scientist of Hubei Province and Program for Chenguang Young Scientist for Wuhan (No. 200750731283).

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