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1-(3-Methylphenyl)-3-{5-[4-(trifluoromethyl)phenyl]-1,3,4-thiadiazol-2-yl}urea

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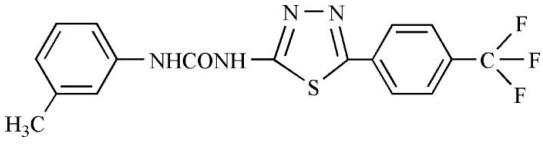
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.069; wR factor = 0.204; data-to-parameter ratio = 10.9.

The molecule of the title compound, $C_{17}H_{13}F_3N_4OS$, assumes a planar conformation except for the F atoms and methyl H atoms. Intermolecular N—H···N hydrogen bonding between the urea and thiadiazole groups links neighbouring molecules into centrosymmetric supramolecular $R_2^2(8)$ dimers. The F atoms are disordered over two positions with a site occupancy ratio of 2:1.

Related literature

For general background, see: Du *et al.* (2000); Song *et al.* (2005); Wang *et al.* (2004); Zou *et al.* (2002); Bernstein *et al.* (1995). For synthesis, see: Song, Wang *et al.* (2007); Song, Tan & Wang (2007).



Experimental

Crystal data

$C_{17}H_{13}F_3N_4OS$
M_r = 378.38
Triclinic, $P\overline{1}$
a = 5.478 (1) Å
b = 8.0133 (14) Å
c = 19.351 (3) Å
α = 99.972 (3)°
β = 92.435 (4)°
γ = 94.290 (3)°
V = 832.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 292 (2) K
0.20 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
4221 measured reflections
2889 independent reflections
2203 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.204
S = 1.10
2889 reflections
264 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N3^{i}	0.87	1.99	2.829 (4)	162

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2300).

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supplementary materials

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1-(3-Methylphenyl)-3-{5-[4-(trifluoromethyl)phenyl]-1,3,4-thiadiazol-2-yl}urea

Z.-W. Tan, X.-H. Tan and X.-J. Song

Comment

1,3,4-Thiadiazole derivatives have been reported to possess broad spectrum bioactivities, such as insecticidal, fungicidal and plant-growth regulating activities (Zou *et al.*, 2002; Song *et al.*, 2005). Urea derivatives have attracted much attention owing to their diverse biological effects (Du *et al.*, 2000; Wang *et al.*, 2004). Furthermore, considerable interest has been shown in fluorine-containing compounds in the field of modern agrochemistry and medicinal chemistry. In our continuing search for biological active urea derivatives as plant-growth regulators, we would like to investigate substituted ureas incorporating both 1,3,4-thiadiazole and CF_3 groups, including the title compound.

The crystal structure (Fig. 1) revealed that the three rings in the molecule are essentially coplanar, the dihedral angles formed by the thiadiazole ring with methylbenzene and trifluoromethylbenzene moieties being only 1.4 (2)° and 4.8 (2)°. It is obvious that the molecule is nearly planar, as can be attributed to the presence of the extended π conjugated system throughout the whole molecule. Bond lengths and angles are as expected. In the crystal structure, neighbouring molecules are linked by complementary N—H···N hydrogen bonding into an $R_2^2(8)$ motif (Bernstein *et al.*, 1995), as shown in Fig. 2 and Table 1.

Experimental

The required 2-amino-5-(4-trifluoromethyl-phenyl)-1,3,4-thiadiazole was obtained by dehydration-cyclization of 4-trifluoromethyl-benzoic acid and thiosemicarbozide in presence of phosphorus oxychloride according to a literature method (Song, Wang *et al.*, 2007). The title compound was then prepared according to the procedure reported by Song, Tan & Wang (2007). Suitable crystals were obtained from a methanol–DMF (1:3) solution at room temperature. Elemental analysis: analysis calculated for $C_{17}H_{13}F_3N_4OS$: C 53.96, H 3.46, N 14.81%; found: C 54.03, H 3.59, N 14.67%.

Refinement

Imino H atoms were located in a difference Fourier map and refined as riding in as-found relative positions, U_{iso}(H) = 1.2U_{eq}(N). The methyl H atoms were placed in calculated positions with C—H = 0.96 Å and torsion angle was refined to fit the electron density, U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were positioned geometrically and constrained to ride on their parent atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The F atoms of trifluoromethyl group are disordered over two sites, occupancies were initialy refined and fixed at 0.67 and 1/3, respectively; geometry constrains were applied for the disordered group.

Figures

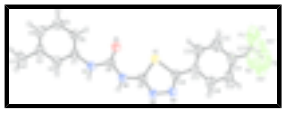

Fig. 1. View of the molecule of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

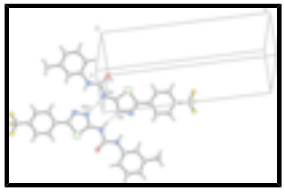

Fig. 2. A partial packing diagram for (I) [symmetry code: (*a*) 2 − *x*, 2 − *y*, −*z*]. Hydrogen bonds are indicated by dashed lines.

1-(3-Methylphenyl)-3-{5-[4-(trifluoromethyl)phenyl]-1,3,4-thiadiazol-2-yl}urea

Crystal data

$C_{17}H_{13}F_3N_4OS$	$Z = 2$
$M_r = 378.38$	$F_{000} = 388$
Triclinic, $P\overline{1}$	$D_x = 1.509$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.4780$ (10) Å	Cell parameters from 1187 reflections
$b = 8.0133$ (14) Å	$\theta = 2.6$–22.1°
$c = 19.351$ (3) Å	$\mu = 0.24$ mm^{-1}
$\alpha = 99.972$ (3)°	$T = 292$ (2) K
$\beta = 92.435$ (4)°	Block, colourless
$\gamma = 94.290$ (3)°	0.20 × 0.10 × 0.06 mm
$V = 832.9$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2203 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.027$
Monochromator: graphite	$\theta_{max} = 25.0^\circ$
$T = 292(2)$ K	$\theta_{min} = 2.1^\circ$
φ and ω scans	$h = -6 \rightarrow 6$
Absorption correction: none	$k = -6 \rightarrow 9$
4221 measured reflections	$l = -22 \rightarrow 19$
2889 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.069$	H-atom parameters constrained

$wR(F^2) = 0.204$	$w = 1/[\sigma^2(F_o^2) + (0.1058P)^2 + 0.1695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
2889 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
264 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3164 (11)	0.3797 (7)	−0.3256 (2)	0.0919 (18)	
H1A	0.4439	0.3032	−0.3295	0.138*	
H1B	0.3728	0.4827	−0.3411	0.138*	
H1C	0.1747	0.3273	−0.3544	0.138*	
C2	0.4087 (7)	0.5277 (5)	−0.2014 (2)	0.0517 (10)	
H2	0.5538	0.5741	−0.2163	0.062*	
C3	0.2499 (9)	0.4203 (5)	−0.2499 (2)	0.0604 (12)	
C4	0.0373 (9)	0.3538 (6)	−0.2259 (3)	0.0676 (12)	
H4	−0.0733	0.2815	−0.2572	0.081*	
C5	−0.0134 (8)	0.3925 (5)	−0.1569 (2)	0.0642 (11)	
H5	−0.1593	0.3465	−0.1423	0.077*	
C6	0.1433 (7)	0.4969 (5)	−0.1082 (2)	0.0503 (9)	
H6	0.1076	0.5197	−0.0611	0.060*	
C7	0.3573 (7)	0.5676 (4)	−0.13140 (18)	0.0423 (8)	
C8	0.5228 (6)	0.7434 (5)	−0.01756 (18)	0.0424 (8)	
C9	0.7631 (7)	0.9361 (5)	0.07428 (18)	0.0438 (9)	
C10	0.7901 (6)	1.0522 (4)	0.19476 (18)	0.0428 (9)	
C11	0.7676 (7)	1.1034 (5)	0.27066 (18)	0.0463 (9)	
C12	0.5630 (9)	1.0524 (6)	0.3030 (2)	0.0731 (13)	
H12	0.4356	0.9858	0.2758	0.088*	
C13	0.5405 (10)	1.0969 (6)	0.3743 (2)	0.0795 (14)	
H13	0.3998	1.0615	0.3948	0.095*	
C14	0.7283 (9)	1.1941 (5)	0.4146 (2)	0.0638 (12)	
C15	0.9277 (10)	1.2474 (7)	0.3834 (2)	0.0781 (14)	

H15	1.0533	1.3154	0.4107	0.094*	
C16	0.9507 (9)	1.2039 (6)	0.3120 (2)	0.0706 (12)	
H16	1.0903	1.2428	0.2918	0.085*	
C17	0.7119 (15)	1.2439 (9)	0.4920 (3)	0.096 (2)	
F1	0.4700 (19)	1.2214 (17)	0.5122 (9)	0.121 (4)	0.67
F2	0.829 (2)	1.1386 (11)	0.5265 (4)	0.126 (3)	0.67
F3	0.788 (3)	1.3979 (13)	0.5189 (5)	0.147 (6)	0.67
F1'	0.552 (5)	1.180 (4)	0.5166 (18)	0.138 (9)	0.33
F2'	0.907 (4)	1.252 (4)	0.5279 (10)	0.181 (12)	0.33
F3'	0.672 (5)	1.410 (3)	0.5021 (11)	0.163 (12)	0.33
N1	0.5294 (5)	0.6798 (4)	−0.08729 (15)	0.0476 (8)	
H1	0.6555	0.7089	−0.1080	0.057*	
N2	0.7195 (5)	0.8563 (4)	0.00599 (14)	0.0492 (8)	
H2A	0.8396	0.8756	−0.0201	0.059*	
N3	0.9620 (5)	1.0398 (4)	0.09270 (15)	0.0494 (8)	
N4	0.9775 (6)	1.1066 (4)	0.16332 (15)	0.0495 (8)	
O1	0.3635 (5)	0.7090 (3)	0.02018 (13)	0.0579 (7)	
S1	0.57658 (17)	0.91409 (12)	0.14109 (5)	0.0467 (3)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.139 (5)	0.089 (4)	0.044 (2)	0.022 (3)	−0.004 (3)	−0.004 (2)
C2	0.058 (2)	0.046 (2)	0.053 (2)	0.0083 (18)	0.0051 (18)	0.0107 (18)
C3	0.083 (3)	0.053 (2)	0.044 (2)	0.022 (2)	−0.011 (2)	0.0009 (19)
C4	0.065 (3)	0.059 (3)	0.071 (3)	−0.002 (2)	−0.021 (2)	−0.001 (2)
C5	0.052 (3)	0.061 (3)	0.078 (3)	0.003 (2)	−0.002 (2)	0.011 (2)
C6	0.048 (2)	0.048 (2)	0.054 (2)	−0.0001 (17)	0.0043 (17)	0.0054 (18)
C7	0.049 (2)	0.0362 (18)	0.0413 (19)	0.0059 (16)	0.0018 (16)	0.0049 (15)
C8	0.0359 (19)	0.049 (2)	0.0427 (19)	−0.0027 (16)	0.0104 (15)	0.0098 (16)
C9	0.045 (2)	0.046 (2)	0.0398 (19)	0.0003 (16)	0.0062 (15)	0.0078 (16)
C10	0.045 (2)	0.0402 (19)	0.0433 (19)	0.0026 (16)	0.0040 (16)	0.0078 (16)
C11	0.060 (2)	0.039 (2)	0.0401 (19)	0.0041 (17)	0.0046 (17)	0.0079 (16)
C12	0.090 (3)	0.080 (3)	0.043 (2)	−0.016 (3)	0.009 (2)	−0.001 (2)
C13	0.103 (4)	0.086 (4)	0.046 (2)	−0.013 (3)	0.017 (2)	0.007 (2)
C14	0.092 (3)	0.052 (2)	0.046 (2)	0.003 (2)	0.010 (2)	0.0050 (19)
C15	0.089 (4)	0.086 (3)	0.049 (2)	−0.013 (3)	−0.003 (2)	−0.008 (2)
C16	0.074 (3)	0.076 (3)	0.054 (3)	−0.007 (2)	0.002 (2)	−0.003 (2)
C17	0.142 (6)	0.090 (5)	0.049 (3)	−0.017 (4)	0.012 (4)	0.000 (3)
F1	0.121 (6)	0.167 (9)	0.061 (5)	0.004 (5)	0.036 (5)	−0.019 (5)
F2	0.184 (9)	0.154 (7)	0.044 (4)	0.017 (6)	−0.002 (4)	0.031 (5)
F3	0.243 (13)	0.112 (8)	0.059 (5)	−0.074 (9)	0.024 (7)	−0.026 (4)
F1'	0.18 (2)	0.165 (15)	0.057 (8)	−0.019 (15)	0.022 (15)	0.008 (10)
F2'	0.167 (18)	0.29 (4)	0.066 (9)	0.09 (2)	−0.046 (11)	−0.047 (18)
F3'	0.29 (3)	0.109 (14)	0.073 (11)	0.067 (18)	−0.005 (13)	−0.047 (8)
N1	0.0454 (18)	0.0529 (19)	0.0420 (17)	−0.0085 (14)	0.0128 (14)	0.0044 (14)
N2	0.0479 (18)	0.060 (2)	0.0366 (16)	−0.0112 (15)	0.0137 (13)	0.0021 (14)
N3	0.0477 (19)	0.0543 (19)	0.0424 (17)	−0.0063 (15)	0.0092 (13)	0.0008 (14)

N4	0.0540 (19)	0.0483 (18)	0.0426 (17)	−0.0028 (15)	0.0055 (14)	0.0006 (14)
O1	0.0574 (17)	0.0684 (18)	0.0435 (14)	−0.0139 (13)	0.0116 (13)	0.0038 (13)
S1	0.0495 (6)	0.0502 (6)	0.0390 (5)	−0.0053 (4)	0.0075 (4)	0.0068 (4)

Geometric parameters (Å, °)

C1—C3	1.511 (6)	C10—C11	1.468 (5)
C1—H1A	0.9600	C10—S1	1.726 (4)
C1—H1B	0.9600	C11—C16	1.372 (6)
C1—H1C	0.9600	C11—C12	1.376 (6)
C2—C7	1.383 (5)	C12—C13	1.378 (6)
C2—C3	1.385 (6)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.369 (7)
C3—C4	1.377 (7)	C13—H13	0.9300
C4—C5	1.364 (6)	C14—C15	1.348 (7)
C4—H4	0.9300	C14—C17	1.490 (7)
C5—C6	1.369 (6)	C15—C16	1.379 (6)
C5—H5	0.9300	C15—H15	0.9300
C6—C7	1.389 (5)	C16—H16	0.9300
C6—H6	0.9300	C17—F1'	1.15 (3)
C7—N1	1.402 (4)	C17—F2'	1.24 (2)
C8—O1	1.208 (4)	C17—F3	1.284 (12)
C8—N1	1.360 (4)	C17—F2	1.344 (12)
C8—N2	1.363 (4)	C17—F3'	1.35 (2)
C9—N3	1.316 (5)	C17—F1	1.405 (14)
C9—N2	1.367 (5)	N1—H1	0.8513
C9—S1	1.706 (3)	N2—H2A	0.8663
C10—N4	1.300 (5)	N3—N4	1.375 (4)
C3—C1—H1A	109.5	C11—C12—C13	122.2 (5)
C3—C1—H1B	109.5	C11—C12—H12	118.9
H1A—C1—H1B	109.5	C13—C12—H12	118.9
C3—C1—H1C	109.5	C14—C13—C12	119.1 (5)
H1A—C1—H1C	109.5	C14—C13—H13	120.5
H1B—C1—H1C	109.5	C12—C13—H13	120.5
C7—C2—C3	121.7 (4)	C15—C14—C13	119.3 (4)
C7—C2—H2	119.2	C15—C14—C17	120.0 (5)
C3—C2—H2	119.2	C13—C14—C17	120.7 (5)
C4—C3—C2	117.5 (4)	C14—C15—C16	121.9 (5)
C4—C3—C1	123.0 (4)	C14—C15—H15	119.0
C2—C3—C1	119.5 (5)	C16—C15—H15	119.0
C5—C4—C3	120.9 (4)	C11—C16—C15	119.9 (4)
C5—C4—H4	119.5	C11—C16—H16	120.0
C3—C4—H4	119.5	C15—C16—H16	120.0
C4—C5—C6	122.2 (4)	F1'—C17—F2'	111.9 (18)
C4—C5—H5	118.9	F3—C17—F2	108.7 (8)
C6—C5—H5	118.9	F1'—C17—F3'	105.1 (14)
C5—C6—C7	117.9 (4)	F2'—C17—F3'	99.8 (14)
C5—C6—H6	121.0	F3—C17—F1	105.8 (8)
C7—C6—H6	121.0	F2—C17—F1	102.3 (7)

C2—C7—C6	119.8 (4)	F1'—C17—C14	116.7 (18)
C2—C7—N1	116.8 (3)	F2'—C17—C14	116.0 (12)
C6—C7—N1	123.5 (3)	F3—C17—C14	116.4 (7)
O1—C8—N1	125.8 (3)	F2—C17—C14	110.9 (6)
O1—C8—N2	122.5 (3)	F3'—C17—C14	104.9 (11)
N1—C8—N2	111.7 (3)	F1—C17—C14	111.7 (8)
N3—C9—N2	120.0 (3)	C8—N1—C7	129.2 (3)
N3—C9—S1	114.8 (3)	C8—N1—H1	117.4
N2—C9—S1	125.2 (3)	C7—N1—H1	113.4
N4—C10—C11	121.7 (3)	C8—N2—C9	124.2 (3)
N4—C10—S1	115.1 (3)	C8—N2—H2A	122.7
C11—C10—S1	123.2 (3)	C9—N2—H2A	112.7
C16—C11—C12	117.6 (4)	C9—N3—N4	112.1 (3)
C16—C11—C10	121.0 (4)	C10—N4—N3	111.6 (3)
C12—C11—C10	121.4 (4)	C9—S1—C10	86.44 (17)
C7—C2—C3—C4	−0.1 (6)	C13—C14—C17—F2'	144.9 (19)
C7—C2—C3—C1	−179.4 (4)	C15—C14—C17—F3	40.9 (12)
C2—C3—C4—C5	−0.1 (6)	C13—C14—C17—F3	−137.9 (10)
C1—C3—C4—C5	179.2 (4)	C15—C14—C17—F2	−84.0 (8)
C3—C4—C5—C6	−0.6 (7)	C13—C14—C17—F2	97.2 (9)
C4—C5—C6—C7	1.6 (6)	C15—C14—C17—F3'	72.7 (14)
C3—C2—C7—C6	1.1 (5)	C13—C14—C17—F3'	−106.1 (13)
C3—C2—C7—N1	−179.0 (3)	C15—C14—C17—F1	162.5 (7)
C5—C6—C7—C2	−1.8 (5)	C13—C14—C17—F1	−16.3 (10)
C5—C6—C7—N1	178.3 (3)	O1—C8—N1—C7	2.1 (6)
N4—C10—C11—C16	−3.4 (6)	N2—C8—N1—C7	−176.8 (3)
S1—C10—C11—C16	175.3 (3)	C2—C7—N1—C8	178.2 (3)
N4—C10—C11—C12	176.6 (4)	C6—C7—N1—C8	−1.9 (6)
S1—C10—C11—C12	−4.7 (5)	O1—C8—N2—C9	2.9 (6)
C16—C11—C12—C13	−1.1 (7)	N1—C8—N2—C9	−178.1 (3)
C10—C11—C12—C13	178.9 (4)	N3—C9—N2—C8	178.1 (3)
C11—C12—C13—C14	−0.4 (8)	S1—C9—N2—C8	−2.1 (5)
C12—C13—C14—C15	1.6 (8)	N2—C9—N3—N4	−179.2 (3)
C12—C13—C14—C17	−179.6 (5)	S1—C9—N3—N4	1.0 (4)
C13—C14—C15—C16	−1.4 (8)	C11—C10—N4—N3	178.8 (3)
C17—C14—C15—C16	179.8 (5)	S1—C10—N4—N3	0.0 (4)
C12—C11—C16—C15	1.3 (7)	C9—N3—N4—C10	−0.6 (4)
C10—C11—C16—C15	−178.7 (4)	N3—C9—S1—C10	−0.8 (3)
C14—C15—C16—C11	−0.1 (8)	N2—C9—S1—C10	179.4 (3)
C15—C14—C17—F1'	−171.5 (17)	N4—C10—S1—C9	0.4 (3)
C13—C14—C17—F1'	9.7 (18)	C11—C10—S1—C9	−178.4 (3)
C15—C14—C17—F2'	−36 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N3^{i}	0.87	1.99	2.829 (4)	162

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*.

Fig. 1

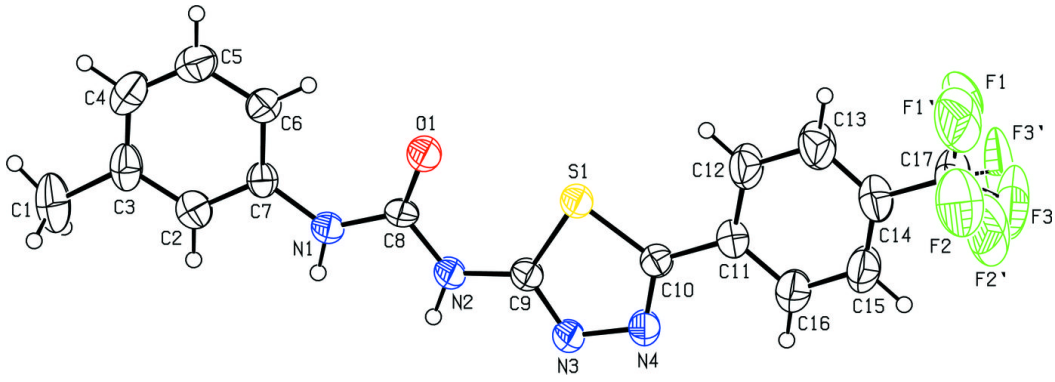
C5
C4
C6
O1
C13
F1
F1'
F3'
C12
C17
S1
C1
C3
C7
C8
C14
F3
F2
C2
N1
C11
F2'
N2
C9
C10
C15
C16
N3
N4

Fig. 2