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1-(2-Chlorobenzoyl)-3-(5-trifluoromethyl-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) = 0.004 Å
Disorder in main residue
R factor = 0.045
wR factor = 0.126
Data-to-parameter ratio = 8.5

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

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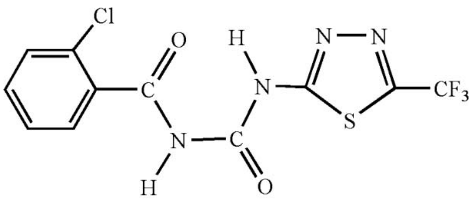
In the title compound, $C_{11}H_6ClF_3N_4O_2S$, the urea linkage adopts an essentially coplanar conformation because of the presence of an intramolecular N—H⋯O hydrogen bond. The molecules are linked by paired N—H⋯O hydrogen bonds into dimers.

Comment

1,3,4-Thiadiazole derivatives have attracted widespread attention due to their many significant bioactivities (Zou *et al.*, 2005; Song, Chen *et al.*, 2005). Aroylureas are reported to possess diverse biological effects, such as insecticidal, fungicidal, herbicidal and plant growth-regulating activities (Chen *et al.*, 2005; Wang *et al.*, 2004). In general, fluorinated compounds are the focus of considerable interest in modern agrochemistry and medicinal chemistry and are ideal for use in drug design because of the good biological activity and low toxicity of molecules containing the trifluoromethyl group (Jian *et al.*, 2006). Great interest has been shown in heterocyclic compounds containing a trifluoromethyl group. With this in mind, we have prepared the title compound, (I), and present its crystal structure here.



(I)

As shown in Fig. 1, the urea linkage unit O2—C5—N4—C4—N3—H3A adopts the most favourable conformation for the formation of an intramolecular N—H⋯O hydrogen bond, giving a planar six-membered ring, as reported previously (Tan *et al.*, 2005; Song *et al.*, 2006). Selected bond lengths and angles are listed in Table 1. In the crystal structure, the molecules are linked by paired intermolecular N—H⋯O hydrogen bonds into dimers.

Experimental

The title compound, (I), was prepared by the reaction of 2-amino-5-trifluoromethyl-1,3,4-thiadiazole with 2-chlorobenzoyl isocyanate according to the procedure of Song, Feng *et al.* (2005). Suitable crystals were obtained by vapour diffusion of methanol at room temperature (m.p. 479–480 K). Elemental analysis calculated for $C_{11}H_6ClF_3N_4O_2S$: C 36.67, H 1.72, N 15.98%; found: C 36.53, H 1.84, N 16.17%.

Crystal data

$C_{11}H_6ClF_3N_4O_2S$
$M_r = 350.72$
Monoclinic, $P2_1/c$
$a = 15.657$ (2) Å
$b = 9.6399$ (14) Å
$c = 9.5673$ (14) Å
$\beta = 95.606$ (2)°
$V = 1437.1$ (3) Å^3

$Z = 4$
$D_x = 1.621$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.46$ 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: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.875$, $T_{\max} = 0.956$

13453 measured reflections
2523 independent reflections
1753 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.063$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.126$
$S = 1.00$
2523 reflections
298 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C2—N1	1.304 (8)	C4—N3	1.350 (3)
C2—S1	1.700 (3)	C4—N4	1.389 (3)
C3—N2	1.334 (8)	C5—O2	1.161 (13)
C3—N3	1.376 (3)	C5—N4	1.358 (3)
C3—S1	1.693 (3)	N1—N2	1.339 (8)
C4—O1	1.198 (3)		
N1—C2—S1	115.8 (5)	O2—C5—N4	123.9 (7)
N2—C3—N3	120.2 (5)	O2—C5—C6	121.9 (7)
N2—C3—S1	115.2 (5)	C2—N1—N2	112.0 (8)
N3—C3—S1	124.63 (19)	C3—N2—N1	111.2 (9)
O1—C4—N3	122.38 (19)	C4—N3—C3	123.0 (2)
O1—C4—N4	121.56 (19)	C5—N4—C4	128.3 (2)
N3—C4—N4	116.0 (2)	C3—S1—C2	85.81 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1$^{\rm i}$	0.86 (1)	1.98 (1)	2.827 (2)	170 (2)
N3—H3···O2	0.86 (1)	2.01 (3)	2.650 (14)	131 (3)

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier). The F atoms in the trifluoromethyl group, the Cl atom, the O atom and the two N atoms in the thiadiazole ring are found to be disordered. The occupancies of the disordered positions were: F:F′ = 0.52:0.48; Cl:Cl' = 0.92:0.08; O2:O2*A*:O2*B* = N1:N1*A*:N1*B* = N2:N2*A*:N2*B* = 0.52:0.25:0.23. The Cl, F, O2, N1 and N2 atoms are all disordered over two or three sets of atomic sites having random occupancies.

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*.

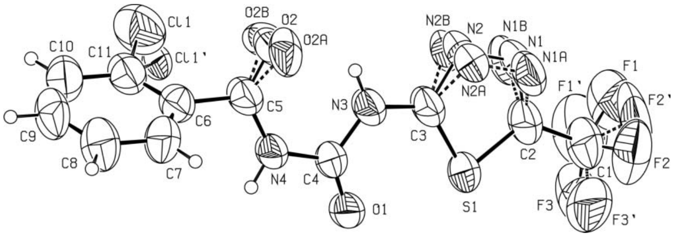


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. All disorder components are shown.

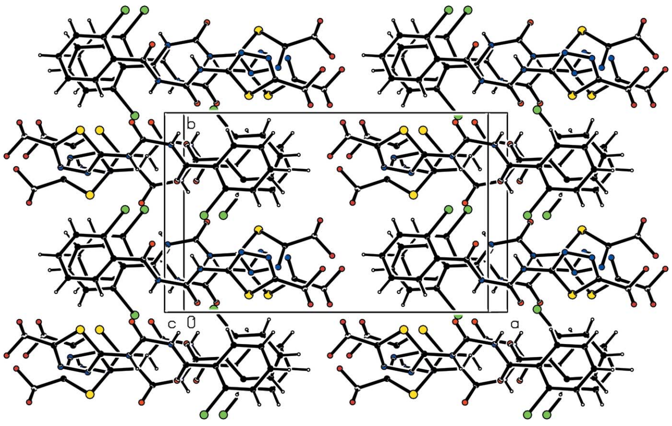


Figure 2
The packing of (I), viewed approximately along the *c* axis.

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