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# 6-(4-Chlorophenyl)imidazo[2,1-*b*][1,3,4]thiadiazole-2-sulfonamide

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**Key indicators**

Single-crystal X-ray study
*T* = 291 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.037
*wR* factor = 0.102
Data-to-parameter ratio = 11.5

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



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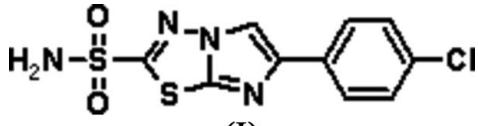
The essentially planar title compound, $C_{10}H_7ClN_4O_2S_2$, features an intramolecular C—H···N hydrogen bond. The crystal strucutre is stabilized by intermolecular N—H···O hydrogen bonds formed between sulfonyl O atoms and amino groups.

## Comment

The imidazo[2,1-*b*][1,3,4]thiadiazole ring system is the core skeleton of the well known immunomodulator levamisole (Amery & Hoerig, 1984). The anti-tumour potential of the 2-amino-1,3,4-thiadiazole skeleton was recognized in the early 1950s (Oleson *et al.*, 1955) and subsequently its fusion with the imidazo[2,1-*b*] ring system has resulted in compounds with potential anticancer (Andreani *et al.*, 1996), analgesic (Khazi *et al.*, 1996), antibacterial (Gadad *et al.*, 2000), antisectretary (Andreani *et al.*, 2000) and cytotoxic activities (Gadad *et al.*, 1999). The title compound, (I), is one of a series of sulfonamides screened for their broad-spectrum antimicrobial activity (Gadad *et al.*, 1999) and it has now been investigated in order to ascertain its structural characteristics.



(I)

The entire molecule of (I) is essentially planar (Fig. 1). The exocyclic C2—S2 distance is, as expected, longer than the other C—S bonds (Table 1). There are deviations in the bond angles around the $sp^2$ atoms C1 and C6. Thus, the S1—C1—N1 angle of 137.63 (18)° allows the 1,3 electronic repulsions to be minimized. In the same way, the C5—C6—C7 angle of 128.7 (2)° also reduces interactions between the aromatic and imidazole rings. The coplanarity of the aromatic ring with the imidazole ring is evidenced by the torsion angle of 5.2 (1)° for C5—C6—C7—C8.

An intramolecular C12—H12···N1 hydrogen bond is shown in Fig. 1. Molecules are aggregated primarily *via* intermolecular N—H···O bonds between $SO_2NH_2$ groups, as detailed in Table 2.

## Experimental

The title compound (I) was prepared by condensing 2-amino-1,3,4-thiadiazole-5-sulfonamide (0.01 *M*) with 4-chlorophenacyl bromide (0.01 *M*) in an ethanol solution (50 ml) to give the hydrobromide salt which, on neutralization with a cold saturated sodium carbonate

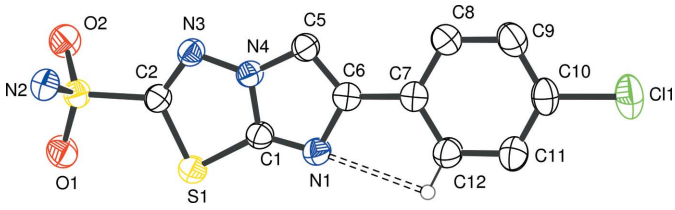



**Figure 1**
A view of (I), with displacement ellipsoids drawn at the 50% probability level. The broken line indicates the intramolecular hydrogen bond.

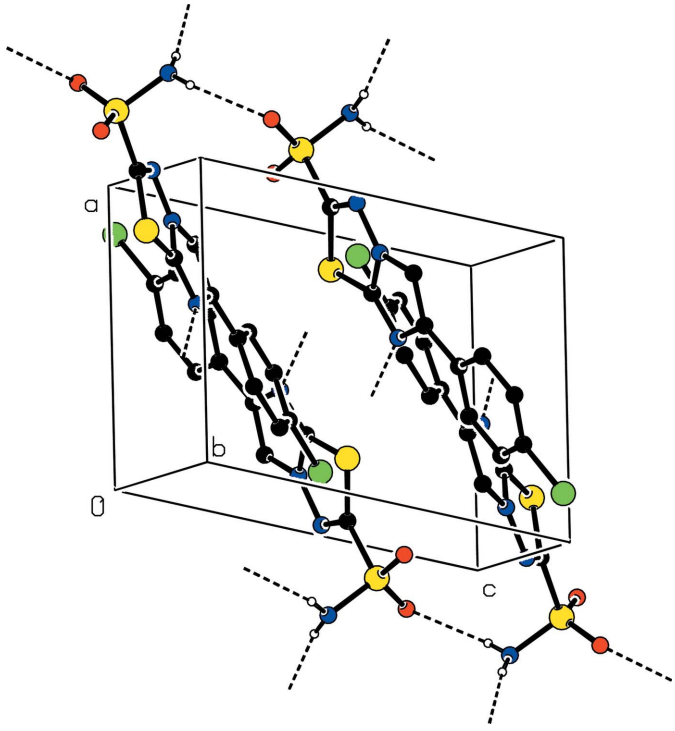



**Figure 2**
A packing diagram for (I), with N—H···O hydrogen bonds shown as dashed lines.

solution, gave compound (I). This was purified and crystallized from a solution in a mixture of ethanol and dimethylformamide (1:1 *v*/*v*).

*Crystal data*

$C_{10}H_7ClN_4O_2S_2$
$M_r$ = 314.77
Monoclinic, $P2_1/c$
$a$ = 7.469 (2) Å
$b$ = 18.640 (5) Å
$c$ = 9.156 (3) Å
$\beta$ = 103.408 (5)°
$V$ = 1239.9 (6) Å$^3$
$Z$ = 4
$D_x$ = 1.686 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.65 mm$^{-1}$
$T$ = 291 (2) K
Block, colourless
0.35 × 0.31 × 0.25 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick 1996)
$T_{min}$ = 0.796, $T_{max}$ = 0.854
9149 measured reflections
2298 independent reflections
2103 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022
$\theta_{max}$ = 25.5°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
$S$ = 1.04
2298 reflections
200 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.6933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| N2—S2 | 1.580 (2) | S1—C2 | 1.741 (2) |
| O1—S2 | 1.4232 (19) | S2—C2 | 1.778 (2) |
| O2—S2 | 1.4221 (18) | C6—C7 | 1.465 (3) |
| S1—C1 | 1.726 (2) | | |
| N1—C1—S1 | 137.63 (18) | C5—C6—C7 | 128.7 (2) |
| O2—S2—C2—N3 | 47.2 (2) | C5—C6—C7—C12 | 174.5 (2) |
| N2—S2—C2—N3 | −68.3 (2) | C5—C6—C7—C8 | −5.2 (4) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···O2$^{i}$ | 0.78 (3) | 2.23 (3) | 2.955 (3) | 155 (3) |
| N2—H2$B$···N1$^{ii}$ | 0.82 (3) | 2.04 (3) | 2.853 (3) | 167 (3) |
| C8—H8···O2$^{iii}$ | 0.93 (3) | 2.56 (3) | 3.315 (3) | 139 (2) |
| C12—H12···N1 | 0.94 (3) | 2.54 (3) | 2.876 (4) | 101 (2) |

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

All H atoms were refined without constraint, the final C—H and N—H bond lengths being in the ranges 0.84 (3)–0.94 (3) Å and 0.77 (3)–0.82 (3) Å, respectively.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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