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# *N*-{3-[2-Chloro-4-(trifluoromethyl)phenoxy]-benzoyl}-*N*′-(4,6-dimethylpyrimidin-2-yl)thiourea

**Hao Peng and Hong-Wu He***

Key Laboratory of Pesticides and Chemical Biology, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China.

Correspondence e-mail: he1208@mail.ccnu.edu.cn

**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.058
*wR* factor = 0.163
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.



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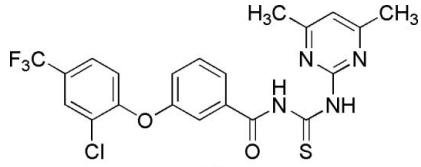
In the title molecule, $C_{21}H_{16}ClF_3N_4O_2S$, all bond lengths and angles are normal. Intermolecular N—H···S hydrogen bonds link the molecules into centrosymmetric dimers. Weak intermolecular C—H···O hydrogen bonds stabilize the crystal packing.

## Comment

Many diphenyl ether inhibitors of protoporphyrinogen oxidase contain the 3-[2-chloro-4-(trifluoromethyl)phenoxy]-benzoyl unit, which produces a class of herbicides (Dayan & Allen, 2000). The potential biological activities of acylthiourea led to comprehensive efforts in the synthesis of such classes of compounds (Venkatachalam *et al.*, 2001). The title compound, (I), has been prepared as a part our work on the design and synthesis of new herbicidal compounds.




(I)

In (I) (Fig.1), the bond lengths and angles show normal values (Allen *et al.*, 1987). An intramolecular N4—H4···N2 hydrogen bond (Table 1) contributes to the molecular geometry. The central benzene ring (C9–C14) makes dihedral angles of 11.32 (1) and 66.50 (1)° with the pyrimidine (N1/N2/C1–C4) and benzene (C15–C20) rings, respectively.

In the crystal structure, intermolecular N—H···S hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers. Weak intermolecular C—H···O hydrogen bonds (Table 1) stabilize the crystal structure (Fig. 2).

## Experimental

The title compound was prepared according to a literature procedure (Xu *et al.*, 2005). Recrystallization from dimethylformamide and water (3:1) over a period of one week gave single crystals of (I) as yellow needles.

*Crystal data*

$C_{21}H_{16}ClF_3N_4O_2S$
$M_r$ = 480.89
Monoclinic, $P2_1/c$
$a$ = 15.8533 (15) Å
$b$ = 6.9436 (7) Å
$c$ = 19.0716 (18) Å
$\beta$ = 95.648 (2)°
$V$ = 2089.2 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.529 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.34 mm$^{-1}$
$T$ = 298 (2) K
Needle, yellow
0.36 × 0.10 × 0.06 mm

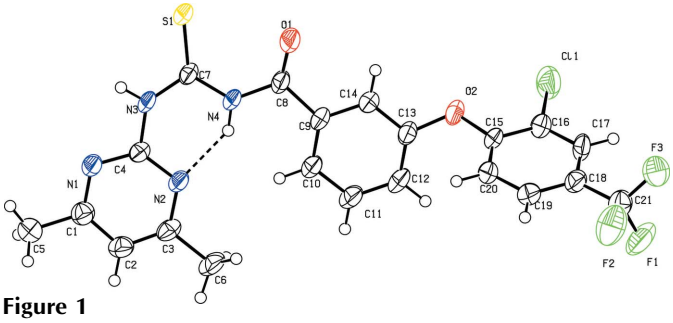



**Figure 1**
The molecular structure of (I), showing the atom-labeling scheme and 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
$\omega$ scans
Absorption correction: none
16915 measured reflections
4519 independent reflections
2763 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 27.0°$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.163$
$S = 1.02$
4519 reflections
297 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.076P)^2 + 0.4678P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H4···N2 | 0.88 (3) | 1.93 (4) | 2.671 (3) | 142 (3) |
| C19—H19···O1$^{i}$ | 0.93 | 2.55 | 3.155 (4) | 123 |
| N3—H3···S1$^{ii}$ | 0.81 (4) | 2.71 (4) | 3.522 (2) | 175 (3) |

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, -y+1, -z$.

C-bound H atoms were positioned geometrically (C—H = 0.93 or 0.96 Å) and refined as riding, with $U_{iso}$(H) = 1.2 or 1.5 times $U_{eq}$(C).

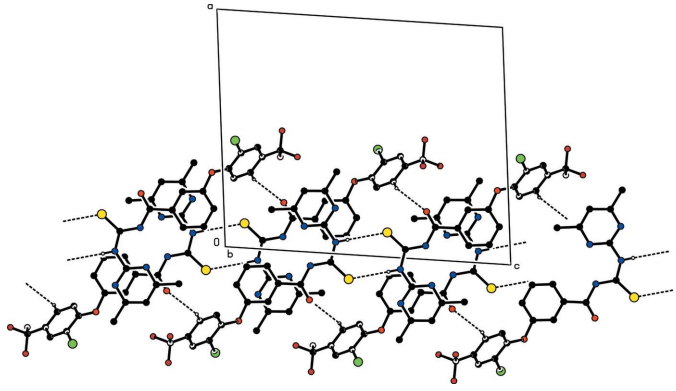



**Figure 2**
Part of the packing, viewed down the *b* axis. Dashed lines denote the intermolecular hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

The amino H atoms were located in a difference map and refined isotropically, with $U_{iso}$(H) = 1.2$U_{eq}$(N).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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