

*N*-Benzoyl-*N'*-(*tert*-butylaminocarbonyl)thiourea

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The asymmetric unit of the title compound,  $C_{13}H_{17}N_3O_2$ , contains two molecules and neither of them adopts a planar conformation. The crystal structure is stabilized by the intermolecular  $N-H \cdots O$  and intramolecular  $N-H \cdots O$  and  $N-H \cdots S$  hydrogen bonds. The intermolecular hydrogen bonds link the molecules to form infinite chains along the *b* axis.

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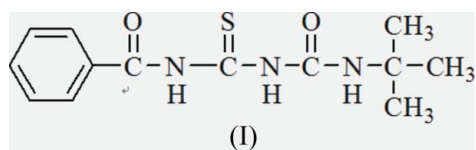
## Key indicators

Single-crystal X-ray study  
 $T = 291$  K  
Mean  $\sigma(C-C) = 0.006$  Å  
 $R$  factor = 0.075  
 $wR$  factor = 0.214  
Data-to-parameter ratio = 18.0

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

## Comment

Diacylthiourea derivatives are already known as a type of bactericide (Sarkis & Faisal, 1985) and fungicide (Bessard & Crettaz, 2000). Recently, they have attracted much interest, due to their effects against HIV (Venkatachalam & Mao, 2004) and influenza virus (Sun *et al.*, 2006). Since the structures of most biologically active small molecules play an important role in their interactions and activities, as part of further systematic studies of the relation between structure and bioactivity in these series, we report here the crystal structure of the title compound, (I), which inhibits viruses in cultured MDCK cells at concentrations of  $1.79 \mu M$  (Sun *et al.*, 2006) and has potential in structure optimization, for future drug design and development.

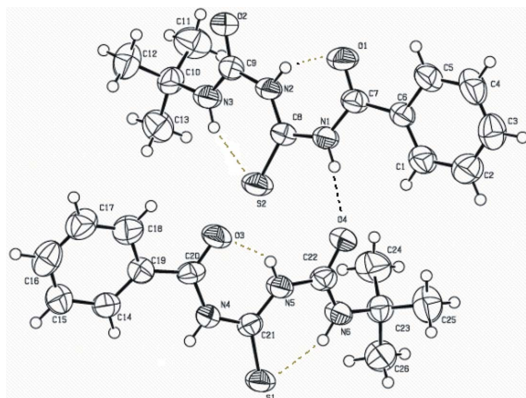


The asymmetric unit of (I) contains two molecules (Fig. 1). The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings *A* (C1–C6) and *A'* (C14–C19) are planar, while rings *B* (O1/C7/N1/C8/N2/H2A) and *B'* (O3/C20/N4/C21/N5/H5A) are nearly planar, with puckering amplitudes of  $Q_T = 0.088$  (1) and  $0.087$  (1) Å, respectively (Cremer & Pople, 1975). The dihedral angles between the rings are  $A/B = 10.58$  (2)° and  $A'/B' = 16.26$  (2)°. Thus, neither of the molecules adopts a planar conformation.

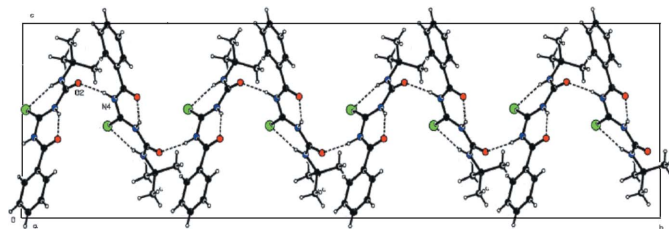
The crystal structure of (I) is stabilized by intermolecular  $N-H \cdots O$  and intramolecular  $N-H \cdots O$  and  $N-H \cdots S$  hydrogen bonds (Table 1). The intermolecular hydrogen bonds link the molecules to form infinite chains along the *b* axis (Fig. 2).

## Experimental

A mixture of benzoyl isothiocyanate (326 mg, 2.0 mmol) and *tert*-butylurea (232 mg, 2.0 mmol) in acetonitrile (10 ml) was refluxed for

**Figure 1**

The asymmetric unit, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

**Figure 2**

A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

5 h. After removal of the volatiles *in vacuo*, the solid residue was filtered and dried in a desiccator. It was recrystallized from chloroform by slow evaporation at room temperature (yield 436 mg, 78%; m.p. 438 K).

#### Crystal data

$C_{13}H_{17}N_3O_2S$   
 $M_r = 279.36$   
 Monoclinic,  $P2_1/c$   
 $a = 11.4872$  (13) Å  
 $b = 30.416$  (3) Å  
 $c = 8.3472$  (9) Å  
 $\beta = 90.317$  (2)°  
 $V = 2916.4$  (6) Å<sup>3</sup>  
 $Z = 8$

$D_x = 1.272$  Mg m<sup>-3</sup>  
 $D_m = 1.325$  Mg m<sup>-3</sup>  
 $D_m$  measured by pycnometer  
 Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 291$  (2) K  
 Block, colourless  
 $0.24 \times 0.10 \times 0.10$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: none  
 18170 measured reflections

6284 independent reflections  
 3012 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.062$   
 $\theta_{max} = 27.0^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.075$   
 $wR(F^2) = 0.214$   
 $S = 1.02$   
 6284 reflections  
 349 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0972P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.35$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.24$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ O4	0.86	2.08	2.927 (3)	170
N2—H2A $\cdots$ O1	0.86	1.85	2.586 (4)	143
N3—H3A $\cdots$ S2	0.86	2.33	3.057 (4)	142
N4—H4A $\cdots$ O2 <sup>i</sup>	0.86	2.04	2.896 (3)	171
N5—H5A $\cdots$ O3	0.86	1.87	2.598 (4)	142
N6—H6 $\cdots$ S1	0.86	2.33	3.057 (4)	142

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

H atoms were positioned geometrically, with N—H = 0.82 Å and C—H = 0.93 and 0.98 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with  $U_{iso}(H) = xU_{eq}(C,N)$ , where  $x = 1.5$  for methyl H and  $x = 1.2$  for all other H.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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