

tert-Butyl 3-phenylcarbazateBin Zhou,^a Wen-Yuan Gao,^a
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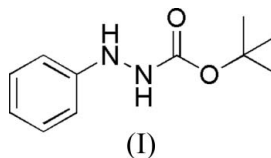
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Key indicatorsSingle-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.053
 wR factor = 0.145
Data-to-parameter ratio = 16.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the molecule of the title compound, $\text{C}_{11}\text{H}_{16}\text{N}_2\text{O}_2$, the amide unit has the usual *trans* conformation. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules, forming infinite chains. Acylhydrazines are an important synthon used to construct hydrogen-bond networks.

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We report here the molecular structure (Fig. 1) of the title compound, (I). The coordination of atom N2 is almost planar, while that of N1 is markedly pyramidal, similar to that reported by Wardell *et al.* (2006). Atom N1 is at a distance of 0.101 (6) Å from the plane of the phenyl ring, and thus it is nearly coplanar. The four atoms of the carbazate, N2/C7/O1/O2, are essentially coplanar. The C1–N1 [1.399 (4)-Å] and C7–N2 [1.340 (3)-Å] bond lengths are within the ranges of normal C–N single (1.47–1.50-Å) and double (1.34–1.38-Å) bonds (Allen *et al.*, 1987), which indicates that atoms N1 and N2 are conjugated with the aryl plane and carbonyl group, respectively. Based on the relative torsion angles, the amide unit has the usual *trans*-planar conformation (Table 1).



As can be seen from the packing diagram (Fig. 2), intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) link the molecules, forming infinite chains which may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

The title compound was prepared from di-*tert*-butyl dicarbonate and phenylhydrazine by the method of Kisseljova *et al.* (2006) (yield 90%, m.p. 362–363 K). Suitable single crystals were grown from an ethyl acetate–*n*-hexane (1:3) solution.

Crystal data $\text{C}_{11}\text{H}_{16}\text{N}_2\text{O}_2$
 $M_r = 208.26$
Monoclinic, $P2_1/c$
 $a = 10.236$ (4) Å
 $b = 13.662$ (6) Å
 $c = 8.628$ (3) Å
 $\beta = 101.814$ (7)°
 $V = 1180.9$ (8) Å³ $Z = 4$
 $D_x = 1.171$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 294$ (2) K
Block, colourless
0.20 × 0.14 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.984$, $T_{\max} = 0.992$

6439 measured reflections
 2400 independent reflections
 1102 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.068$
 $\theta_{\text{max}} = 26.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.145$
 $S = 1.03$
 2400 reflections
 146 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.1989P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.004$
 $\Delta\rho_{\text{max}} = 0.15 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.14 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.011 (2)

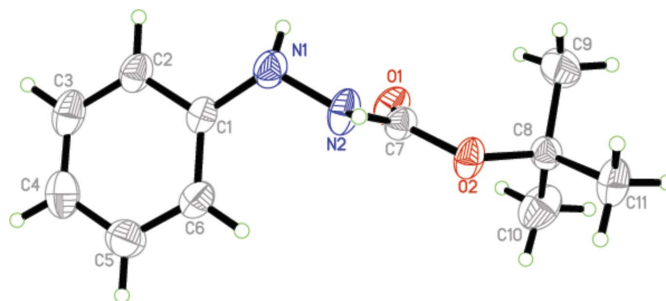


Figure 1
 The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Table 1

Selected geometric parameters (\AA , $^\circ$).

O1—C7	1.204 (3)	N1—N2	1.389 (3)
O2—C7	1.343 (3)	N1—C1	1.399 (4)
O2—C8	1.471 (3)	N2—C7	1.340 (3)
N2—N1—C1	118.4 (3)	O1—C7—N2	125.5 (2)
C7—N2—N1	122.2 (2)	N2—C7—O2	108.9 (2)
C1—N1—N2—C7	94.2 (3)	N1—N2—C7—O2	173.2 (3)
N1—N2—C7—O1	-6.2 (5)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2 \cdots O1 ⁱ	0.85 (3)	2.05 (3)	2.900 (3)	171 (3)
N1—H1 \cdots O2 ⁱⁱ	0.85 (3)	2.40 (3)	3.237 (3)	167 (3)

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

The N-bound H atoms were refined freely, with both N—H = 0.85 (3) \AA , while the other H atoms were positioned geometrically, with C—H = 0.93 and 0.96 \AA for aromatic and methyl H atoms, respectively, and were constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{N})$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H atoms.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

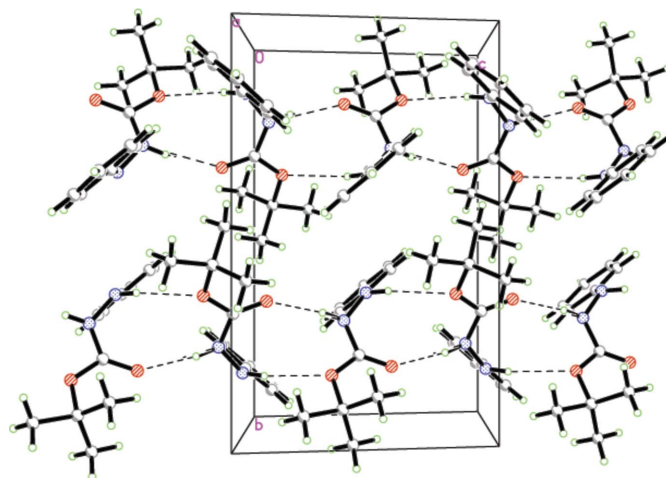


Figure 2
 A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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