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N′-Benzoyl-4*H*-1,2,4-triazole-3-carbohydrazide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.143
Data-to-parameter ratio = 12.3

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

In the crystal structure of the title compound, $C_{10}H_9N_5O_2$, intermolecular N—H···N [H···N = 2.13 (2) Å] and N—H···O [H···O = 2.016 (18) and 2.05 (2) Å] hydrogen bonds link molecules into a two-dimensional framework.

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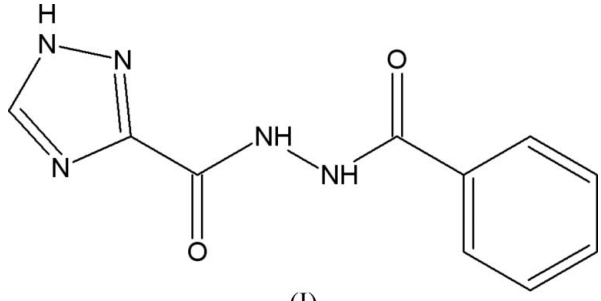
Comment

Recently, compounds containing the 1*H*-1,2,4-triazole group have aroused much interest because of their biological activities, such as fungicidal (Oita & Uchida, 1998), antifugal, antitumoural (Maravalli *et al.*, 2000), antibacterial (Zhou *et al.*, 1998*a*), and plant growth regulating activity (Zhou *et al.*, 1998*b*). In a search for new compounds with bioactivity, we have synthesized triazole compounds derived from 1*H*-1,2,4-triazole-3-carbohydrazide and have recently reported the crystal structures of two such compounds (Chen *et al.*, 2005; Pan & Yang, 2005). We report here the synthesis and crystal structure of *N*′-benzoyl-4*H*-1,2,4-triazole-3-carbohydrazide, (I).



(I)

The title compound is shown in Fig. 1 and selected bond lengths and angles are listed in Table 1. The sequence of C═O, C—N and N—N bond lengths in the central part of the molecule is consistent with the presence of a conjugated system. The bond distances and angles within the triazole and

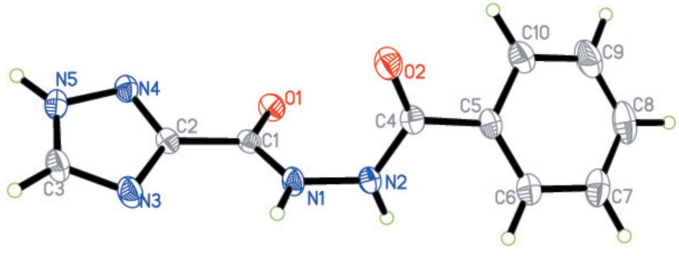


Figure 1
The structure of compound (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

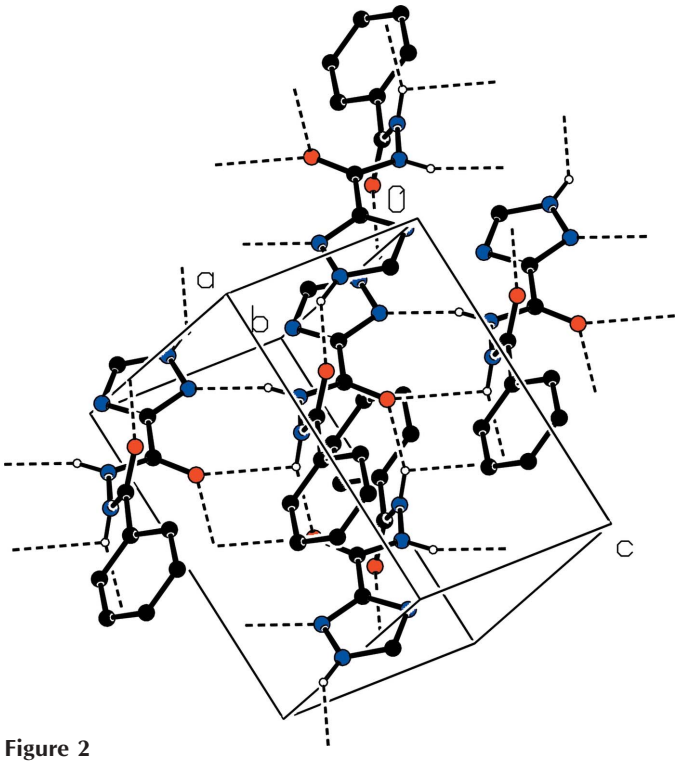


Figure 2
Packing diagram (Spek, 2003) for (I), showing hydrogen bonds as dashed lines. Colour code: red O, blue N and black C. H atoms not involved in hydrogen bonding have been omitted.

phenyl rings are normal and agree with the corresponding values found in 4-phenyl-1-(1*H*-1,2,4-triazole-3-ylcarbonyl)thiosemicarbazide (Chen *et al.*, 2005). The dihedral angle between the triazole and phenyl rings is 29.3 (1)°.

In the crystal structure, intermolecular N—H···N and N—H···O hydrogen bonds link molecules into a two-dimensional framework (Table 2 and Fig. 2).

Experimental

1*H*-1,2,4-Triazole-3-carbohydrazide (0.02 mol, 2.54 g) was dissolved in pyridine (50 ml) and benzoyl chloride (0.02 mol, 2.81 g) was added dropwise to the solution. The mixture was refluxed for 5 h and distilled. A white solid was precipitated by dilution with cold water (100 ml). This product was filtered off, washed with cold water (2 × 30 ml) and recrystallized from ethanol. (yield: 81%; m.p. 521–522 K). IR ν_{max} (KBr, cm^{-1}): 3310, 3190, 1691.5, 1649.5, 1559.3, 1527.5, 1481.2, 1268.1, 1110.0, 873.7, 722.3, 693.4. ^{1}H NMR (200 MHz, DMSO): δ 14.62 (1H), 10.40–10.60 (2H), 8.79 (1H), 7.85–7.98 (2H), 7.45–7.70 (3H).

Crystal data

$C_{10}H_9N_5O_2$
M_r = 231.22
Monoclinic, $P2_1/c$
a = 5.3572 (8) Å
b = 21.890 (3) Å
c = 9.2502 (14) Å
β = 100.082 (3)°
V = 1068.0 (3) Å^3
Z = 4
D_x = 1.438 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2517 reflections
θ = 5.8–55.9°
μ = 0.11 mm^{-1}
T = 293 (2) K
Block, colourless
0.52 × 0.35 × 0.33 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.541, T_{max} = 0.970
6209 measured reflections
2332 independent reflections
1799 reflections with $I > 2\sigma(I)$
R_{int} = 0.132
θ_{max} = 27.0°
$h = -6 \rightarrow 6$
$k = -23 \rightarrow 27$
$l = -11 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.143
S = 1.00
2332 reflections
190 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.2249 (18)	N1—N2	1.3848 (18)
O2—C4	1.2236 (19)	N2—C4	1.346 (2)
N1—C1	1.336 (2)		
C1—N1—N2	118.82 (13)	C4—N2—N1	119.99 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O2^{i}	0.88 (2)	2.02 (2)	2.7681 (18)	142 (2)
N2—H2···O1^{ii}	0.91 (2)	2.05 (2)	2.9019 (18)	156 (2)
N1—H1···N4^{iii}	0.87 (2)	2.13 (2)	2.984 (2)	164 (2)

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$; (iii) $x+1, y, z$.

All H atoms were refined independently with isotropic displacement parameters. The higher than normal R_{int} value of 0.13 may reflect the poor quality of the data and in turn the lowered precision of the structure.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, (2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02), *SADABS* (Version 2.03) and *SHELXTL*. Bruker AXS Inc., Madison, Winsonsin, USA.
Chen, D.-B., Huang, L., Pan, F.-Y. & Yang, J.-G. (2005). *Acta Cryst.* E**61**, o836–o837.
Maravalli, P. B., Gudasi, K. B. & Goudar, T. R. (2000). *Transition Met. Chem.* **25**, 411–414.
Oita, S. & Uchida, T. (1998). Jpn Patent No. 10212287 (11 August, p. 7).
Pan, F.-Y. & Yang, J.-G. (2005). *Acta Cryst.* E**61**, o63–o64.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Zhou, Z. H., Zhao, J., Peng, Y. B. & Zhao, G. F. (1998*a*). *Yingyong Huaxue*, **15**, 72–75.
Zhou, Z. H., Zhao, J., Peng, Y. B. & Zhao, G. F. (1998*b*). *Huaxue Tongbao*, **8**, 35–38.