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2-(4-Bromophenyl)-5-methyl-2,3-dihydro-4*H*-1,2,4-triazol-3-one

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Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.092
Data-to-parameter ratio = 20.4

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

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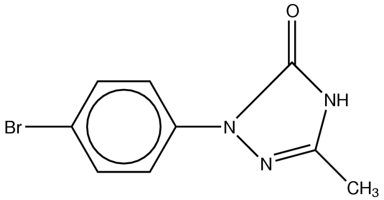
In the title compound, $C_9H_8BrN_3O$, the dihedral angle between the phenyl and triazole rings is 8.93 (14)°. In the crystal, the molecules exist as centrosymmetrically related N—H···O hydrogen-bonded dimers.

Comment

1,2,4-Triazole derivatives are found to be associated with diverse pharmacological activities, such as analgesic, anti-asthmatic, diuretic, antifungal, antibacterial, pesticidal and anti-inflammatory activities (Thamotharan *et al.*, 2003, and references therein). Triazole derivatives have been synthesized as possible anticonvulsants, antidepressants, tranquilizers and plant-growth regulators (Bradbury & Rivett, 1991; Hirota *et al.*, 1991; Walser *et al.*, 1991). In view of this, the crystal structure determination of the title triazole derivative, (I), has been carried out in order to elucidate the molecular conformation.



(I)

The bond lengths and angles in (I) are unexceptional and comparable with those reported for related structures (Chen *et al.*, 1998; Wang *et al.*, 1998; Thamotharan *et al.*, 2003). The phenyl ring is oriented at an angle of 8.93 (14)° with respect to the plane of the triazole ring, compared with a value of 30.63 (9)° reported for our previous chloro derivative of triazole (Thamotharan *et al.*, 2003). In the crystal, centrosymmetrically related molecules form dimeric pairs through N—H···O intermolecular hydrogen bonds and have a graph set motif of $R_2^2(8)$ (Bernstein *et al.*, 1995).

Experimental

The title compound was prepared by refluxing 2-(4-bromophenyl)-5-methyl-1,3,4-oxadiazolin-2-one with formamide. The solid obtained, (I), was crystallized from benzene (m.p. 503 K).

Crystal data

$C_9H_8BrN_3O$
M_r = 254.09
Monoclinic, $P2_1/c$
a = 4.0333 (1) Å
b = 10.8622 (2) Å
c = 21.1608 (4) Å
β = 93.9045 (7)°
V = 924.91 (3) Å^3
Z = 4

D_x = 1.825 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 26 468 reflections
θ = 2.0–30.0°
μ = 4.41 mm^{-1}
T = 160 (2) K
Needle, colourless
0.25 × 0.08 × 0.05 mm

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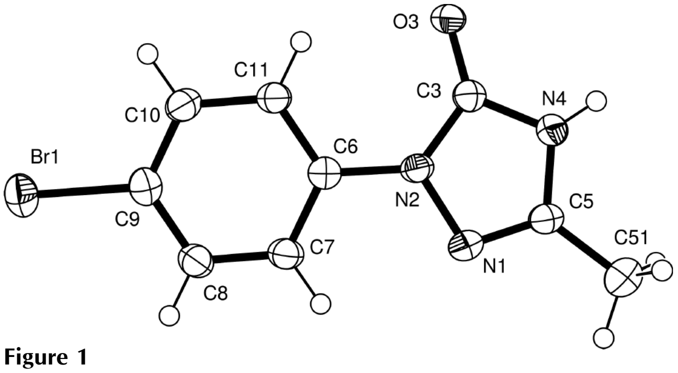

Figure 1
View of the asymmetric unit of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

Data collection

Nonius KappaCCD diffractometer
φ and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{\min} = 0.550$, $T_{\max} = 0.818$
22 923 measured reflections
2710 independent reflections
2239 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.087$
$\theta_{\max} = 30.0°$
$h = -5 \rightarrow 5$
$k = -15 \rightarrow 15$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.092$
$S = 1.07$
2710 reflections
133 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.9447P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.75$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0047 (11)

Table 1
Selected geometric parameters (Å, °).

N1—C5	1.297 (3)	N4—C5	1.363 (3)
N1—N2	1.400 (3)	N4—C3	1.372 (3)
N2—C3	1.372 (3)		
C5—N1—N2	103.8 (2)	N2—C3—N4	103.5 (2)
C3—N2—N1	111.8 (2)	N1—C5—N4	112.5 (2)
C5—N4—C3	108.4 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O3$^{\rm i}$	0.82 (3)	1.94 (3)	2.756 (3)	171 (3)

Symmetry code: (i) $-1 - x, 2 - y, -z$.

The position of the amine H atom was determined from a difference Fourier map and refined freely along with its isotropic displacement parameter. The methyl H atoms were constrained to an ideal geometry (C—H = 0.98 Å), with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$, but were allowed to rotate freely about the C—C bond. All remaining H atoms were placed in geometrically idealized positions (C—H = 0.95–0.99 Å) and constrained to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

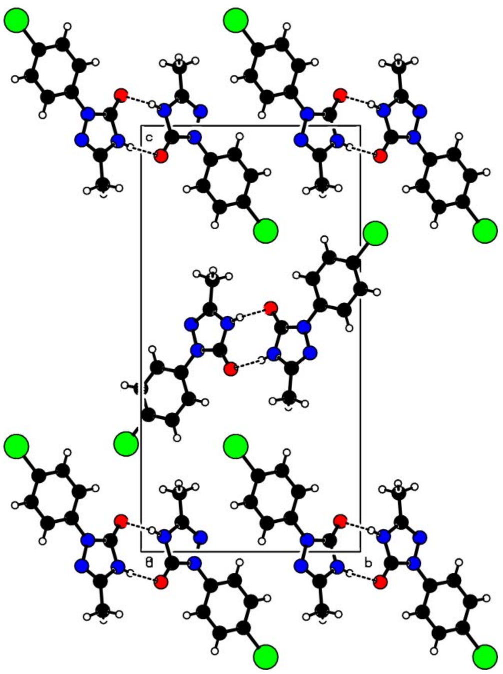

Figure 2
Packing diagram, viewed along the *a* axis..

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Version 1.07; Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2002).

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