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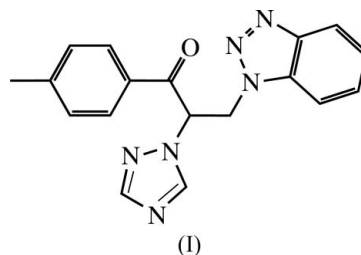
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.044
 wR factor = 0.115
Data-to-parameter ratio = 14.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.3-(Benzotriazol-1-yl)-1-(*p*-tolyl)-2-(1*H*-1,2,4-triazol-2-yl)propan-1-one

In the title molecule, $\text{C}_{18}\text{H}_{16}\text{N}_6\text{O}$, the central triazole ring is approximately perpendicular to the tolyl group [dihedral angle $85.4(1)^\circ$] and makes a dihedral angle of $46.4(1)^\circ$ with the benzotriazole group. $\text{C}-\text{H}\cdots\text{N}$, $\text{C}-\text{H}\cdots\text{O}$ and $\pi-\pi$ interactions link the molecules into a two-dimensional network parallel to the bc plane.

Comment

As part of our ongoing studies on new triazole compounds with higher bioactivity (Wan *et al.*, 2006), the title compound, (I), was synthesized.



All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The benzotriazole group is essentially planar, with a dihedral angle of $0.6(1)^\circ$ between the C10–C15 benzene and triazole rings. The mean plane of the benzotriazole group makes dihedral angles of $46.4(1)$ and $56.2(1)^\circ$ with the N4–N6/C16/C17 triazole and C1–C6 benzene rings, respectively. The dihedral angle between the N4–N6/C16/C17 and C1–C6 rings is $86.4(1)^\circ$.

In the crystal structure, molecules are linked into a two-dimensional framework parallel to the bc plane by $\text{C}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Fig. 2 and Table 1). The network structure is further stabilized by $\pi-\pi$ stacking interactions between the inversion-related benzotriazole groups. The $\text{Cg1}\cdots\text{Cg1}^{\text{iv}}$ and $\text{Cg1}\cdots\text{Cg2}^{\text{iv}}$ distances are $3.608(1)$ and $3.687(1)\text{ \AA}$, respectively, where Cg1 and Cg2 denote the centroids of the N1–N3/C10/C11 and C10–C15 rings, respectively [symmetry code: (iv) $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$].

Experimental

Bromine (3.2 g, 0.02 mol) was added dropwise to a solution of 3-(benzotriazol-1-yl)-1-(*p*-tolyl)propan-1-one (5.3 g, 0.02 mol) and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml) with stirring at 313 K. The reaction was maintained for about 20 h until the mixture turned colourless. Water (50 ml) and chloroform (20 ml) were then added. The organic layer was washed successively with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate, and filtered. The chloroform solution was cooled

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with ice-water, and then an acetone solution (10 ml) of 1,2,4-triazole (1.4 g, 0.02 mol) and triethylamine (2.8 ml, 0.02 mol) was added. The mixture was stirred at room temperature for about 2 h. The solution was then filtered, concentrated and purified by flash column chromatography (silica gel, petroleum ether-ethyl acetate, 2:1 *v/v*) to afford the title compound. Single crystals of (I) were obtained by slow evaporation of an ethanol solution at room temperature over a period of 10 d.

Crystal data

$C_{18}H_{16}N_6O$	$Z = 8$
$M_r = 332.37$	$D_x = 1.336 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 30.972 (3) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 8.1625 (8) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 14.6599 (14) \text{ \AA}$	Block, colourless
$\beta = 116.927 (1)^\circ$	$0.21 \times 0.17 \times 0.12 \text{ mm}$
$V = 3304.4 (6) \text{ \AA}^3$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	8988 measured reflections
ω scans	3249 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2396 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.982$, $T_{\max} = 0.989$	$R_{\text{int}} = 0.022$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 1.0955P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.115$	$(\Delta/\sigma)_{\text{max}} = 0.031$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
3249 reflections	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
227 parameters	
H-atom parameters constrained	

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C12-H12\cdots N6^i$	0.93	2.55	3.418 (3)	155
$C16-H16\cdots N2^{ii}$	0.93	2.44	3.328 (3)	159
$C17-H17\cdots O1^{iii}$	0.93	2.47	3.237 (3)	140

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

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with $C-H = 0.93-0.98 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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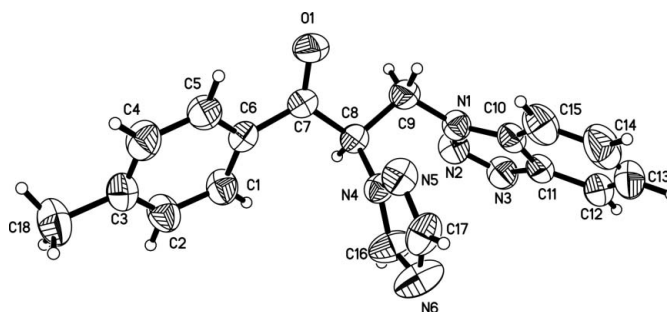


Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

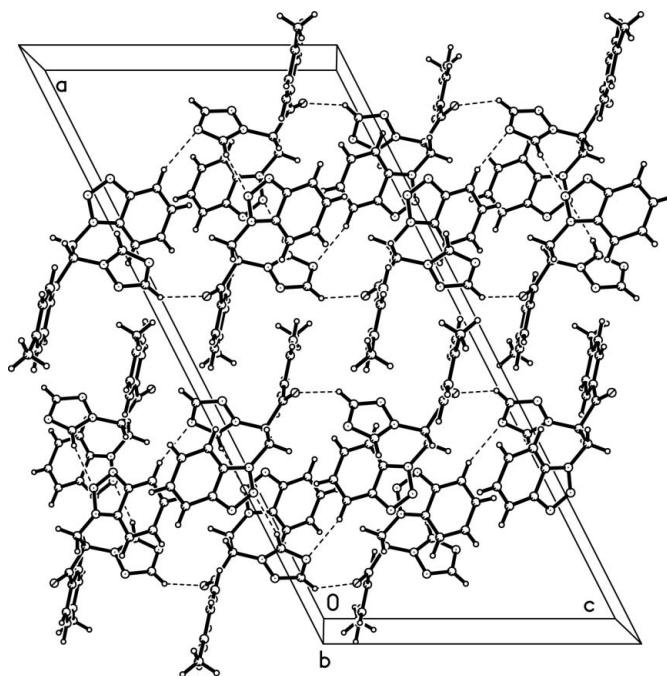


Figure 2

Packing diagram of (I), showing the hydrogen-bonded (dashed lines) network.

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