

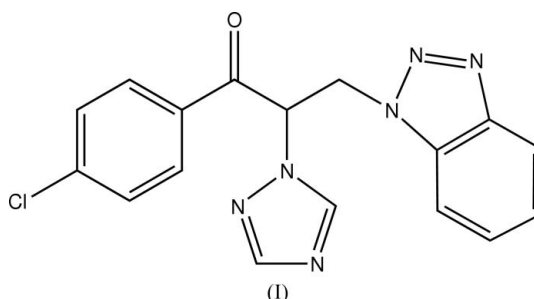
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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.041
 wR factor = 0.104
Data-to-parameter ratio = 14.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3-(Benzotriazol-1-yl)-1-(4-chlorophenyl)-
2-(1,2,4-triazol-1-yl)propan-1-oneIn the title compound, $\text{C}_{17}\text{H}_{13}\text{ClN}_6\text{O}$, molecules are linked
into a zigzag chain along the b axis by $\text{C}-\text{H}\cdots\text{N}$ hydrogen
bonds. The packing is further stabilized by $\pi-\pi$ interactions.Received 2 August 2006
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Comment

Triazole derivatives have become the most rapidly expanding
group of antifungal compounds with the advantage of low
toxicity, high oral bioavailability and broad-spectrum anti-
fungal activity which can be used against fungi including most
yeasts and filamentous fungi (Xu *et al.*, 2003). In order to
search for new triazole compound with higher bioactivity, the
title compound, (I), which contains triazole and benzotriazole
was synthesized.The 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 $0.4(1)^\circ$ between the benzene
and triazole rings. The mean plane of the benzotriazole group
makes dihedral angles of $47.6(1)$ and $57.2(8)^\circ$ with the other
triazole ($\text{N}4-\text{N}6/\text{C}16/\text{C}17$) ring and the $\text{C}1-\text{C}6$ benzene ring,
respectively. The dihedral angle between the planes of the
latter two aromatic rings is $88.6(1)^\circ$.In the crystal structure, molecules are linked into zigzag
chains along the b axis by $\text{C}15-\text{H}15\text{A}\cdots\text{N}6$ hydrogen bonds
(Fig. 2 and Table 2). The chains are further connected into a
three-dimensional framework by other $\text{C}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$
interactions (Table 2). The short distances between $\text{Cg}1\cdots\text{Cg}1^{\text{ii}}$
(3.562 \AA) and $\text{Cg}1\cdots\text{Cg}4^{\text{ii}}$ (3.748 \AA), where $\text{Cg}1$
and $\text{Cg}4$ denote the centroids of the $\text{N}1-\text{N}3/\text{C}10/\text{C}11$ and $\text{C}10-$
 $\text{C}15$ rings, respectively [symmetry code: (ii) $-1/2-x, 7/2-y, -z$]
indicate $\pi-\pi$ interactions between the benzotriazole moieties.

Experimental

Bromine (3.2 g, 0.02 mol) was added dropwise to a solution of 3-
(benzotriazol-1-yl)-1-(4-chlorophenyl)propan-1-one (5.7 g, 0.02 mol)
and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml) with stir-
ring at 313 K. The reaction was maintained for about 18 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 the chloroform solution filtered. It was cooled 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 with stirring. 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 and ethyl acetate (1:1 v/v)) to afford the title compound. Single crystals of (I) suitable for X-ray measurements were obtained by slow evaporation of an alcohol and ethyl acetate solution (1:1 v/v) at room temperature over a period of seven days.

Crystal data

$C_{17}H_{13}ClN_6O$	$Z = 8$
$M_r = 352.78$	$D_x = 1.430 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 29.914 (7) \text{ \AA}$	$\mu = 0.25 \text{ mm}^{-1}$
$b = 8.1198 (18) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 14.818 (3) \text{ \AA}$	Block, colourless
$\beta = 114.462 (3)^\circ$	$0.23 \times 0.23 \times 0.19 \text{ mm}$
$V = 3276.2 (13) \text{ \AA}^3$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	8830 measured reflections
ω scans	3216 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2506 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.944$, $T_{\max} = 0.954$	$R_{\text{int}} = 0.022$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 1.1575P]$
$R[F^2 > 2\sigma(F^2)] = 0.041$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.104$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
3216 reflections	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$
226 parameters	
H-atom parameters constrained	

Table 1

Selected bond lengths (\AA).

Cl1–C3	1.7352 (19)	N1–N2	1.3430 (19)
O1–C7	1.211 (2)	N1–C11	1.364 (2)

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15–H15A \cdots N6 ⁱ	0.93	2.59	3.461 (3)	155
C16–H16A \cdots N2 ⁱⁱ	0.93	2.43	3.316 (3)	159
C17–H17A \cdots O1 ⁱⁱⁱ	0.93	2.47	3.188 (3)	134

Symmetry codes: (i) $-x - \frac{1}{2}, y + \frac{1}{2}, -z - \frac{1}{2}$; (ii) $-x - \frac{1}{2}, -y + \frac{5}{2}, -z$; (iii) $x, -y + 3, z - \frac{1}{2}$.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C–H distances in the range 0.93–0.98 \AA , and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

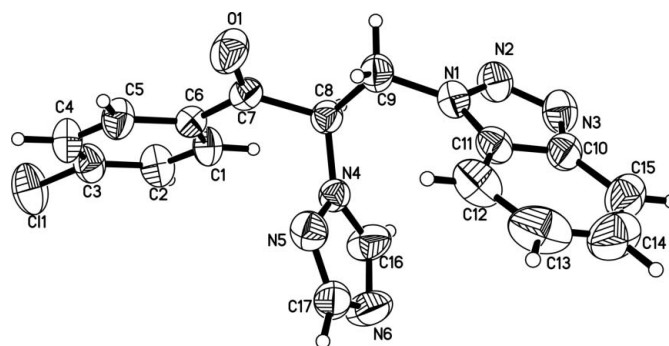


Figure 1

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

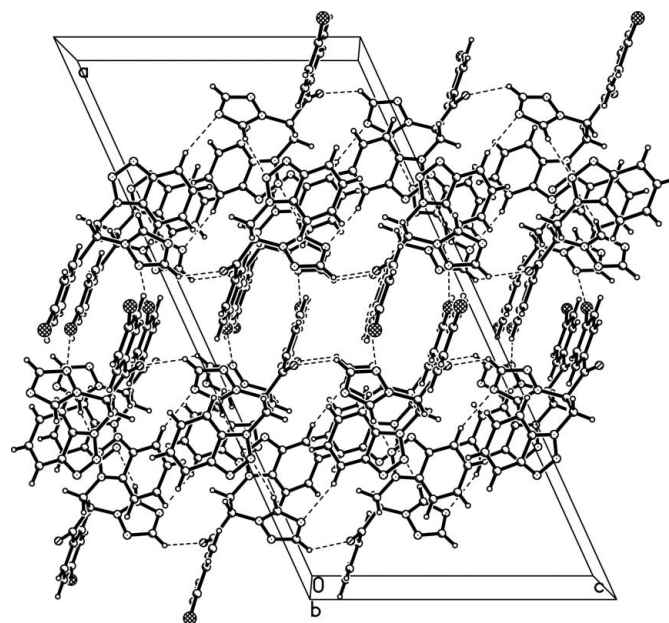


Figure 2

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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