organic papers

2-(1H-Benzotriazol-1-yl)-1-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-yl)ethanone

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Key indicators

Single-crystal X-ray study

$T = 293$ K

Mean σ(C–C) = 0.004 Å

R factor = 0.053

wR factor = 0.130

Data-to-parameter ratio = 14.2

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

In the title compound, $C_{16}H_{10}Cl_2N_6O$, molecules are linked into ribbons along the b axis by C—H···N intermolecular hydrogen bonds. The packing is further stabilized by a π–π interaction.
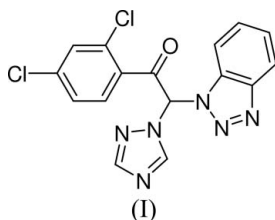
Comment

Triazole derivatives exhibit growth-inhibiting activities against some microorganisms (Xu *et al.*, 2002). In order to search for new triazole compounds with higher bioactivity, the title compound, (I), which contains both triazole and benzotriazole, was synthesized.

(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and comparable to those reported in the related compound 2-(1H-1,2,3-benzotriazol-1-yl)-1-(4-methylphenyl)-2-(1H-1,2,4-triazol-1-yl)ethanone (Wan *et al.*, 2005). The benzotriazole group is essentially planar, with a dihedral angle of 1.9 (1)° between the benzene and triazole rings. The mean plane of the benzotriazole group makes dihedral angles of 74.3 (1) and 33.9 (1)° with the other triazole (N4/N5/C16/N6/C15) ring and the benzene (C1–C6) ring, respectively. The dihedral angle between the planes of the latter two aromatic rings is 69.9 (1)°. In the crystal structure, molecules are linked into ribbons by intermolecular C—H···N hydrogen bonds (Fig. 2 and Table 2). The packing is further stabilized by a π–π interaction between the benzene (C1–C6) rings, the distance between the centroids $[Cg···Cg(\frac{1}{2} - x, \frac{3}{2} - y, -z)]$ being 3.883 (2) Å.

Experimental

The title compound was prepared according to the method of Wan *et al.* (2005).

Crystal data

$C_{16}H_{10}Cl_2N_6O$	$D_x = 1.518$ Mg m^{-3}
$M_r = 373.20$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2583
$a = 21.950$ (3) Å	reflections
$b = 9.9632$ (15) Å	$\theta = 2.3–24.0°$
$c = 15.538$ (2) Å	$\mu = 0.42$ mm^{-1}
$\beta = 106.028$ (2)°	$T = 293$ (2) K
$V = 3266.0$ (8) Å^3	Column, colorless
$Z = 8$	$0.40 \times 0.23 \times 0.12$ mm
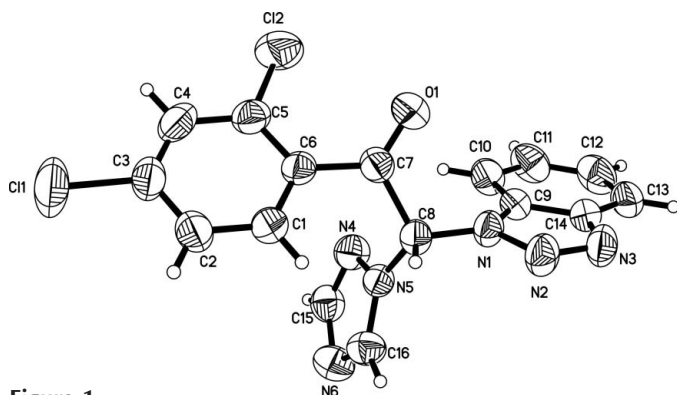
Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Figure 2
A view down the c axis. Hydrogen bonds are indicated by dashed lines.

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3199 independent reflections
ω scans	2500 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.023$
	$\theta_{max} = 26.0°$
$T_{min} = 0.851$, $T_{max} = 0.952$	$h = -27 \rightarrow 22$
8949 measured reflections	$k = -11 \rightarrow 12$
	$l = -18 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 3.9871P]$
$R[F^2 > 2\sigma(F^2)] = 0.053$	
$wR(F^2) = 0.130$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
3199 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
226 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cl1—C3	1.731 (3)	N1—C8	1.445 (3)
Cl2—C5	1.723 (3)	N5—C8	1.447 (3)
O1—C7	1.201 (3)	C7—C8	1.549 (3)
N1—C8—N5	111.83 (19)	N5—C8—C7	110.26 (18)
N1—C8—C7	112.21 (19)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C1—H1$A\cdots$N3^i	0.93	2.54	3.465 (3)	172
C8—H8$A\cdots$N3^i	0.98	2.54	3.455 (3)	156

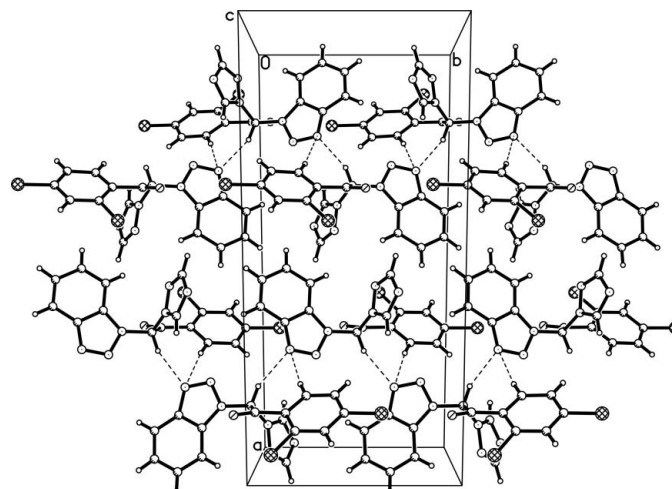Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z - \frac{1}{2}$.

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 Å and with U_{iso}(H) = $1.2U_{eq}$(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* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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