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2-(1*H*-Benzotriazol-1-yl)-1-(2,5-dichlorophenyl)-2-(1*H*-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) = 0.005 Å
R factor = 0.060
wR factor = 0.124
Data-to-parameter ratio = 13.2

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

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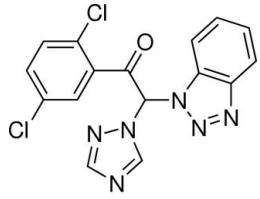
In the title compound, $C_{16}H_{10}Cl_2N_6O$, molecules are linked into a dimer by a pair of C—H···N hydrogen bonds. The packing is further stabilized by a π–π interaction.

Comment

We have recently reported the structure of 2-(1*H*-benzotriazol-1-yl)-1-(2,4-dichlorophenyl)-2-(1*H*-1,2,4-triazol-1-yl)-ethanone, (II) (Wan *et al.*, 2005). In order to investigate the effect of the substituted Cl atoms on the conformation and biological activities, the title compound, (I), was synthesized.



(I)

All bond lengths in (I) are in good agreement with those in (II). The benzotriazole group is planar; the dihedral angle between the C9–C14 benzene ring and the N1–N3/C14/C9 triazole ring is 1.2 (2)° in (I), comparable to 1.9 (1)° in (II). The mean plane of the benzotriazole group is nearly parallel to the C1–C6 benzene ring, with a dihedral angle of 3.2 (1)°, in contrast to 33.9 (1)° in (II). The other triazole ring (N4/N5/C15/N6/C16) makes dihedral angles of 63.2 (2) and 60.4 (2)° with the C1–C6 ring and the benzotriazole group, respectively.

In the crystal structure, molecules are linked into a dimer by a pair of weak C—H···N hydrogen bonds (Fig. 2 and Table 2). The packing is further stabilized by a π–π interaction between the N1–N3/C14/C9 ring (centroid *Cg*1) and the C1–C6 ring (centroid *Cg*2), the distance between the centroids [*Cg*1···*Cg*2(x, $-1+y$, z)] being 3.742 (2) Å.

Experimental

Bromine (3.2 g, 0.02 mol, 50 ml) was added dropwise to a solution of 1-(2,5-dichlorophenyl)-2-(1*H*-1,2,4-triazol-1-yl)ethanone (5.1 g, 0.02 mol) and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml). The reaction was maintained for 5 h. 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 with ice–water, and then an acetone solution (10 ml) of benzotriazole (2.4 g, 0.02 mol) and triethylamine (2.8 ml) was added. The mixture was stirred at room temperature for about 3 h. The solution was then filtered, concentrated and purified by flash column chromatography (silica gel, petroleum ether–ethyl acetate, 2:1 *v*/*v*) to

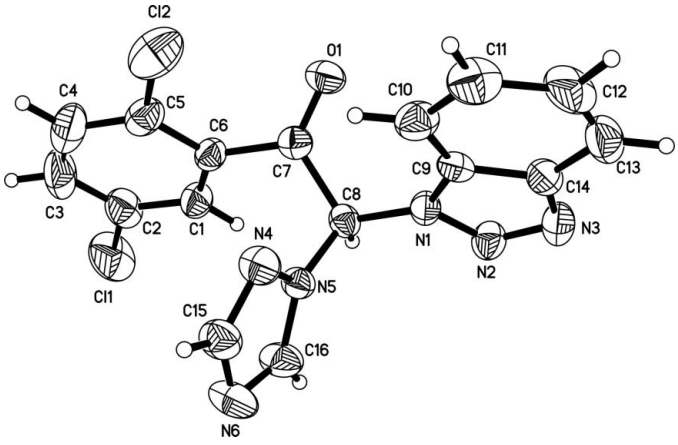


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

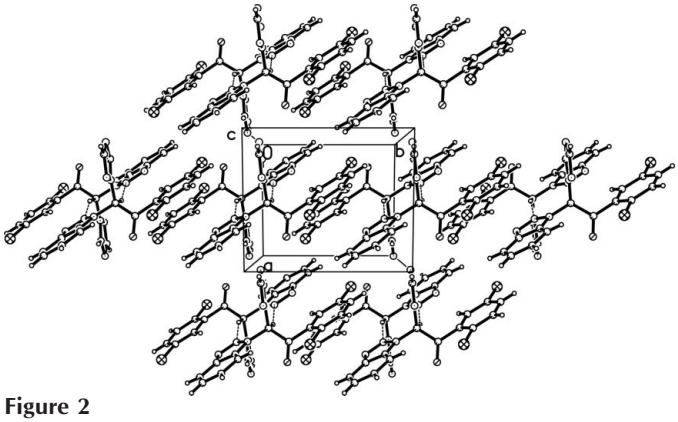


Figure 2
A view down the *c* axis. Hydrogen bonds are indicated by dashed lines.

afford the title compound. Single crystals were obtained by slow evaporation of an ethyl acetate–cyclohexane (3:1 *v*/*v*) solution at room temperature over a period of 6 d.

Crystal data

$C_{16}H_{10}Cl_2N_6O$
M_r = 373.20
Monoclinic, $P2_1/c$
a = 7.6217 (6) Å
b = 8.6107 (8) Å
c = 25.5989 (19) Å
β = 107.322 (2)°
V = 1603.8 (2) Å^3
Z = 4
D_x = 1.546 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 984 reflections
θ = 2.5–19.6°
μ = 0.42 mm^{-1}
T = 293 (2) K
Needle, colourless
0.34 × 0.07 × 0.06 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.870, T_{max} = 0.975
8418 measured reflections
2983 independent reflections
2004 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 25.5°
$h = -9 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -22 \rightarrow 30$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.124
S = 1.07
2983 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.0033P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C2	1.730 (3)	N1—C8	1.442 (3)
Cl2—C5	1.726 (3)	N5—C8	1.451 (3)
O1—C7	1.200 (3)	C7—C8	1.537 (4)
N1—C8—N5	111.6 (2)	N5—C8—C7	110.1 (2)
N1—C8—C7	113.2 (2)		
O1—C7—C8—N1	10.1 (4)	O1—C7—C8—N5	135.8 (3)
C6—C7—C8—N1	−171.2 (2)	C6—C7—C8—N5	−45.6 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···N2^{i}	0.98	2.33	3.259 (4)	158

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

All H atoms were located in a difference Fourier map 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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