

2-(1*H*-1,2,3-Benzotriazol-1-yl)-1-benzoyl-ethyl 2,4-dichlorobenzoateJun Wan, Xue-Mei Li,
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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.041
 wR factor = 0.103
Data-to-parameter ratio = 14.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.In the crystal structure of the title compound, $\text{C}_{22}\text{H}_{15}\text{Cl}_2\text{N}_3\text{O}_3$, molecules are linked into dimers by $\text{C}-\text{H} \cdots \text{O}$ intermolecular hydrogen bonds. The packing is further stabilized by $\pi-\pi$ interactions.Received 9 February 2006
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Comment

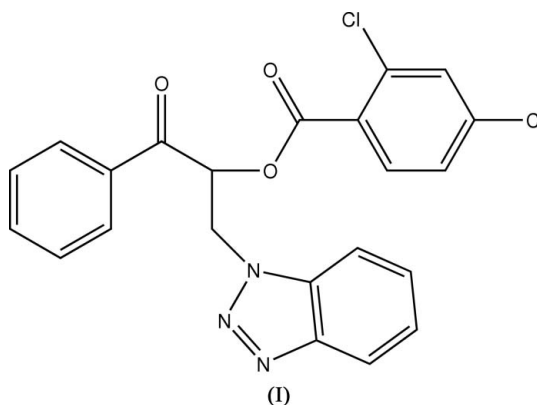
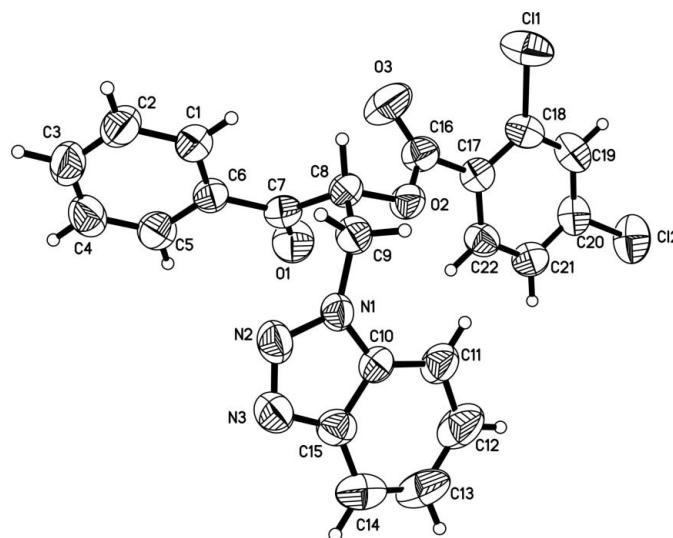
We have recently reported the structure of 2-(1*H*-1,2,3-benzotriazol-1-ylmethyl)-1-benzoyl-ethyl 4-ethylbenzoate, (II) (Wan, Peng *et al.*, 2005). As part of our ongoing studies, the title compound, (I), was synthesized and its structure is presented here.The bond lengths and angles (Table 1) in (I) are within normal ranges (Allen *et al.*, 1987) and are comparable with the corresponding ones in (II).

Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

In (I), the benzotriazole system is almost planar, with a dihedral angle of 1.52 (8)° between triazole ring A (N1–N3/C10/C15) and benzene ring B (C10–C15). The dihedral angles between the mean planes of the benzotriazole system and rings C (C1–C6) and D (C17–C22) are 43.82 (8) and 6.47 (8)°, respectively. The dihedral angle between rings C and D is 38.96 (9)°.

In the crystal structure, molecules of (I) are linked into dimers by C–H···O hydrogen bonds (Table 2 and Fig. 2). The packing is further stabilized by π – π interactions between ring D at (x, y, z) and ring D at (–x, –y, 1–z), with a distance of 3.721 (2) Å between the centroids of the two rings.

Experimental

The title compound was prepared according to the literature method of Wan, Li *et al.* (2005). Single crystals suitable for X-ray measurements were obtained by slow evaporation of an acetone/petroleum ether (1:1) (yield 4.0 g, 46%; m.p. 443.5–444.3 K).

Crystal data

C ₂₂ H ₁₅ Cl ₂ N ₃ O ₃	$D_x = 1.460 \text{ Mg m}^{-3}$
$M_r = 440.27$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3057 reflections
$a = 9.1235 (12) \text{ \AA}$	$\theta = 2.2\text{--}23.6^\circ$
$b = 9.4228 (12) \text{ \AA}$	$\mu = 0.35 \text{ mm}^{-1}$
$c = 23.307 (3) \text{ \AA}$	$T = 296 (2) \text{ K}$
$\beta = 90.916 (2)^\circ$	Block, colorless
$V = 2003.4 (4) \text{ \AA}^3$	$0.33 \times 0.17 \times 0.12 \text{ mm}$
$Z = 4$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3943 independent reflections
ω scans	2846 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.024$
$T_{\text{min}} = 0.892$, $T_{\text{max}} = 0.959$	$\theta_{\text{max}} = 26.0^\circ$
11397 measured reflections	$h = -10 \rightarrow 11$
	$k = -11 \rightarrow 7$
	$l = -27 \rightarrow 28$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.3548P]$
$R[F^2 > 2\sigma(F^2)] = 0.041$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.103$	$(\Delta\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
3943 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
271 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

C11–C18	1.729 (2)	O2–C16	1.351 (2)
C12–C20	1.739 (2)	O2–C8	1.435 (2)
O1–C7	1.212 (2)	O3–C16	1.193 (2)
O2–C8–C9	107.04 (14)	C9–C8–C7	112.38 (16)
O2–C8–C7	109.34 (15)		

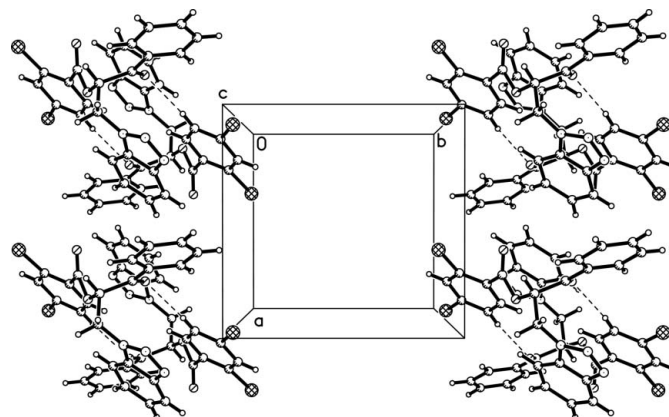


Figure 2

Part of the packing of (I). Hydrogen bonds are shown as dashed lines.

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
C21–H21A···O1 ⁱ	0.93	2.46	3.371 (2)	166

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

H atoms were positioned geometrically, with C–H = 0.93, 0.97 and 0.98 Å for aromatic, methylene and methine H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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

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