

2-(1*H*-1,2,3-Benzotriazol-1-ylmethyl)-1-(4-chlorobenzoyl)ethyl 2,4-dichlorobenzoateJun Wan,^a Xue-Mei Li,^b
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Key indicators

Single-crystal X-ray study

 $T = 293$ KMean $\sigma(\text{C}-\text{C}) = 0.006$ Å R factor = 0.064 wR factor = 0.150

Data-to-parameter ratio = 14.5

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

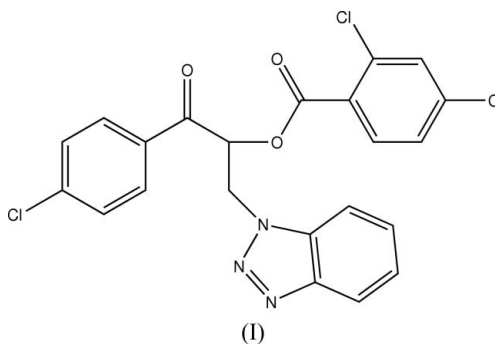
In the title compound, $\text{C}_{22}\text{H}_{14}\text{Cl}_3\text{N}_3\text{O}_3$, molecules are linked into two-dimensional layers in the ab plane by $\text{C}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds. The packing is further stabilized by $\pi-\pi$ interactions. There are two molecules in the asymmetric unit.

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Comment

In our ongoing studies of benzotriazole compounds, the title compound, (I), was obtained. The asymmetric unit of (I) contains two crystallographically independent molecules, *A* and *B* (Fig. 1). Corresponding bond lengths of these two molecules agree within two standard deviations (Table 1). In molecules *A* and *B*, the benzotriazole system is almost planar, with dihedral angles of 1.1 (2) and 1.3 (2)°, respectively, between the planes of the triazole ring and its fused benzene ring. In *A*, the dihedral angles between the mean planes of the benzotriazole system and rings *C* (C1–C6) and *D* (C17–C22) are 15.0 (2) and 18.1 (2)°, respectively. The corresponding values are 22.6 (2) and 11.0 (2)° for *B*. The dihedral angles between rings *C* and *D* are 27.4 (2) and 21.9 (2)° for *A* and *B*, respectively.



In the crystal structure, molecules of (I) are linked into two-dimensional layers in the ab plane by $\text{C}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Fig. 2 and Table 2). The packing is further stabilized by $\pi-\pi$ interactions involving the benzotriazole and benzene rings, with $\text{Cg}1\cdots\text{Cg}5^{\text{iii}}$ and $\text{Cg}2\cdots\text{Cg}7^{\text{iv}}$ distances of 3.665 and 3.590 Å, respectively [$\text{Cg}1$, $\text{Cg}2$, $\text{Cg}5$ and $\text{Cg}7$ are the centroids of the N1–N3/C10/C11, N4–N6/C32/C33, C17–C22 and C32–C37 rings, respectively; symmetry codes: (iii) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (iv) $1 - x, 1 - y, -z$].

Experimental

The title compound was prepared according to the method of Wan *et al.* (2006). Single crystals were obtained by slow evaporation of an

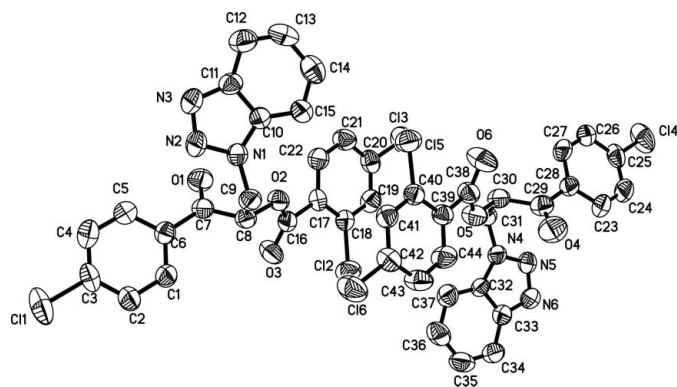


Figure 1
The structure of the asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atom numbering scheme. H atoms have been omitted for clarity.

ethyl acetate solution at room temperature over a period of one week.

Crystal data

$C_{22}H_{14}Cl_3N_3O_3$
 $M_r = 474.71$
 Monoclinic, $P2_1/c$
 $a = 11.941(3) \text{ \AA}$
 $b = 25.588(6) \text{ \AA}$
 $c = 13.780(3) \text{ \AA}$
 $\beta = 100.508(4)^\circ$
 $V = 4139.8(15) \text{ \AA}^3$

$Z = 8$
 $D_x = 1.523 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.47 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
 Column, colourless
 $0.23 \times 0.12 \times 0.09 \text{ mm}$

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.899$, $T_{\max} = 0.959$

23763 measured reflections
 8117 independent reflections
 4005 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.059$
 $\theta_{\text{max}} = 26.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.065$
 $wR(F^2) = 0.150$
 $S = 1.01$
 8117 reflections
 559 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0597P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (\AA).

C11—C3	1.734 (4)	O2—C16	1.354 (4)
C12—C18	1.736 (4)	O2—C8	1.441 (4)
C13—C20	1.737 (4)	O3—C16	1.189 (4)
C14—C25	1.735 (4)	O4—C29	1.214 (4)
C15—C40	1.737 (4)	O5—C38	1.364 (4)
C16—C42	1.733 (4)	O5—C30	1.435 (4)
O1—C7	1.211 (4)	O6—C38	1.194 (4)

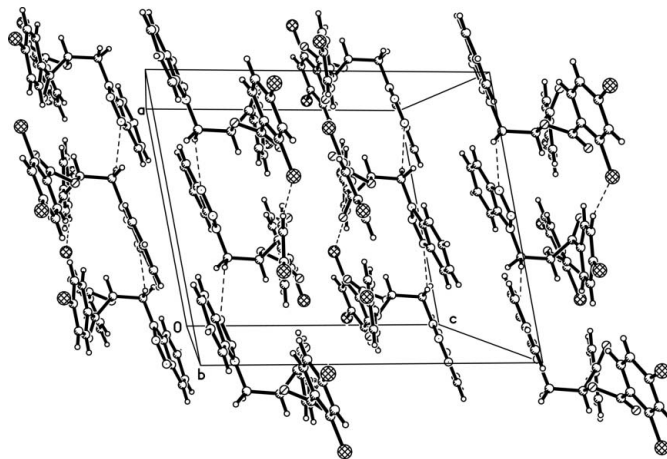


Figure 2

The two-dimensional layers of (I). Hydrogen bonds are indicated by dashed lines.

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C9—H9A \cdots N6 ⁱ	0.97	2.43	3.171 (5)	132
C31—H31B \cdots N3 ⁱⁱ	0.97	2.52	3.287 (5)	136
C36—H36A \cdots Cl4 ⁱ	0.93	2.81	3.608 (4)	144

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

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 \AA , and 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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References

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
 Siemens (1996). *SMART and SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Wan, J., Peng, Z.-Z., Li, X.-M. & Zhang, S.-S. (2006). *Acta Cryst.* **E62**, o634–o636.