

2-(1*H*-1,2,3-Benzotriazol-1-ylmethyl)-
1-(2,4-dichlorobenzoyl)ethyl nicotinate
monohydrateJun Wan, Zheng-Zhong Peng, Sai
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Key indicators

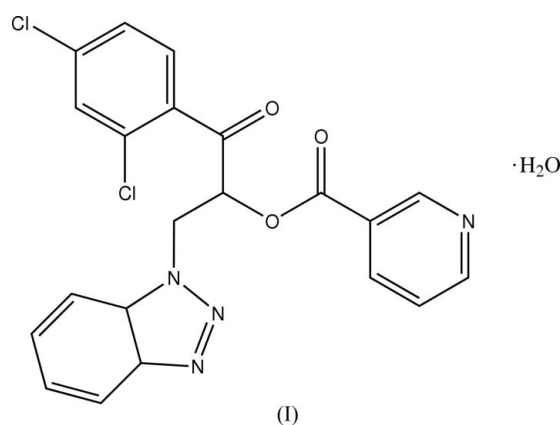
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.039
 wR factor = 0.108
Data-to-parameter ratio = 14.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The molecules of the title compound, $\text{C}_{21}\text{H}_{14}\text{Cl}_2\text{N}_4\text{O}_3 \cdot \text{H}_2\text{O}$, are linked into dimers by $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds and are linked into chains along the b axis by $\text{C}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds involving the solvent water molecule. The packing is further stabilized by $\pi-\pi$ interactions.

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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-chlorobenzoate, (II) (Wan *et al.*, 2006). As part of our ongoing studies, the title compound, (I), was synthesized and its structure was determined.



All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) (Table 1) and are comparable with those in the related compound, (II). In (I), the benzotriazole system is essentially planar, with a dihedral angle of $0.28(1)^\circ$ between triazole ring *A* (N1–N3/C9/C14) and benzene ring *B* (C9–C14). The dihedral angles between the mean planes of the benzotriazole system and rings *C* (N4/C1–C5) and *D* (C16–C21) are $36.75(8)$ and $10.73(8)^\circ$, respectively. The dihedral angle between rings *C* and *D* is $43.89(1)^\circ$. There is an intramolecular $\text{C1}-\text{H1A} \cdots \text{O2}$ hydrogen bond, forming a five-membered ring.

In the crystal structure, molecules of (I) are linked into dimers by $\text{C20}-\text{H20A} \cdots \text{O1}$ hydrogen bonds and are linked into chains along the b axis by $\text{C}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds involving the solvent water molecule (Table 2 and Fig. 2). The packing is further stabilized by $\pi-\pi$ interactions involving the benzotriazole and benzene rings, with $\text{Cg1} \cdots \text{Cg2}(1-x, -\frac{1}{2}+y, \frac{1}{2}-z)$ and $\text{Cg2} \cdots \text{Cg4}(2-x, \frac{1}{2}+y, \frac{1}{2}-z)$ distances of 3.591 and 3.961 Å, respectively (Cg1, Cg2 and Cg4 are the centroids of the rings N1–N3/C9/C14, N4/C1–C5 and C16–C21, respectively).

Experimental

The title compound was prepared according to the literature method of Wan *et al.* (2006). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of 5 d.

Crystal data

$C_{21}H_{14}Cl_2N_4O_3 \cdot H_2O$
 $M_r = 459.28$
 Monoclinic, $P2_1/c$
 $a = 11.211(3) \text{ \AA}$
 $b = 13.035(3) \text{ \AA}$
 $c = 14.231(3) \text{ \AA}$
 $\beta = 92.910(3)^\circ$
 $V = 2077.1(8) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.469 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.35 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
 Block, yellow
 $0.45 \times 0.24 \times 0.13 \text{ mm}$

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.859, T_{\max} = 0.956$

11426 measured reflections
 4118 independent reflections
 3110 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\text{max}} = 26.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.108$
 $S = 0.95$
 4118 reflections
 288 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.497P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

C11—C17	1.7325 (18)	O2—C7	1.437 (2)
C12—C19	1.7283 (19)	O3—C15	1.205 (2)
O1—C6	1.204 (2)	C7—C8	1.514 (3)
O2—C6	1.345 (2)	C7—C15	1.525 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1W-H2W1 \cdots N3^i$	0.85 (2)	2.12 (2)	2.969 (3)	174 (3)
$C1-H1A \cdots O2$	0.93	2.44	2.764 (2)	100
$C2-H2B \cdots O1W^i$	0.93	2.59	3.374 (3)	143
$C8-H8A \cdots O1W^{ii}$	0.97	2.56	3.401 (3)	145
$C8-H8B \cdots O1W$	0.97	2.44	3.382 (3)	164
$C20-H20A \cdots O1^{iii}$	0.93	2.44	3.316 (3)	157

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

All H atoms were located in a difference Fourier map. Water H atoms were refined, with $O1W-H1W1$ and $O1W-H2W1$ distance restraints of 0.85 (1) Å. The remaining H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

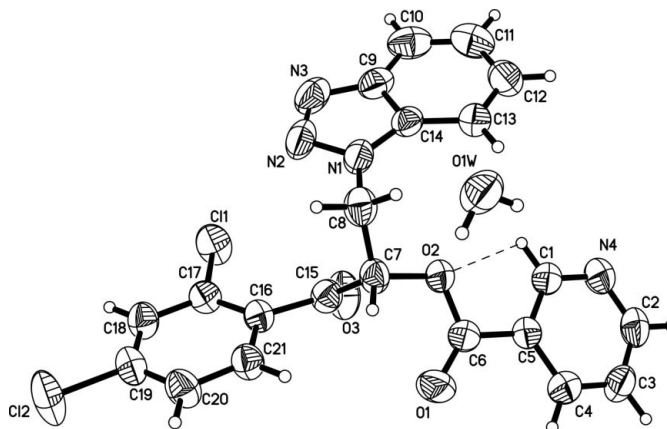


Figure 1

The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates a hydrogen bond.

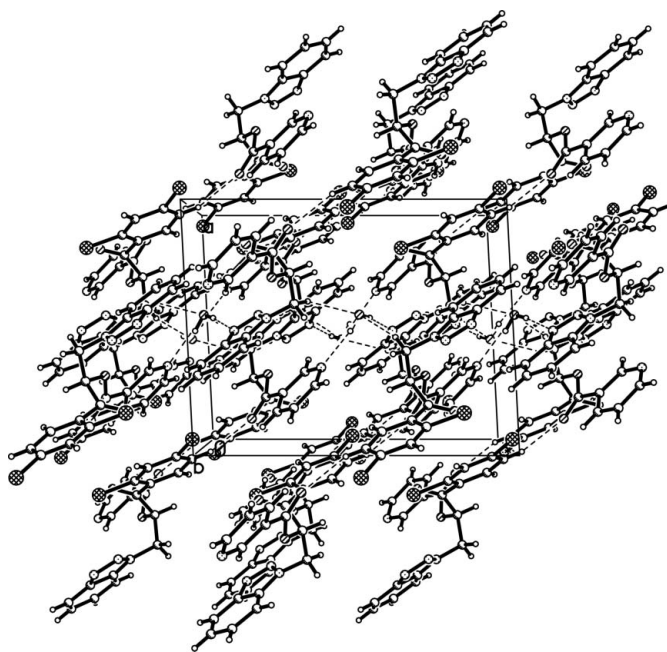


Figure 2

A packing diagram of (I), viewed down the c axis, showing the intermolecular hydrogen bonds (dashed lines), viewed down the c axis.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); 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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