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# 2-(1*H*-1,2,3-Benzotriazol-1-yl)-1-benzoylethyl 2-chlorobenzoate

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.046
*wR* factor = 0.116
Data-to-parameter ratio = 14.4

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



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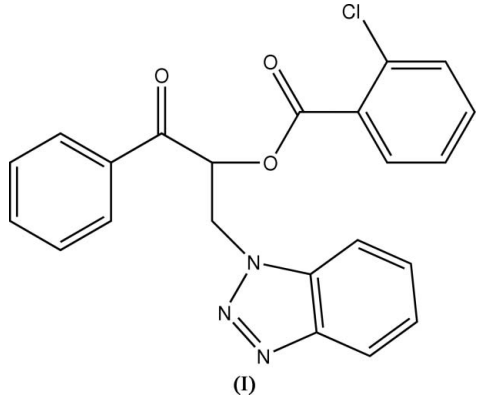
In the crystal structure of the title compound, $C_{22}H_{16}ClN_3O_3$, weak intermolecular C—H···N hydrogen bonds link the molecules into chains extended along the *c* axis. The packing is further stabilized by weak C—H···O interactions.

## Comment

We have recently reported the structure of 2-(1*H*-1,2,3-benzotriazol-1-yl)-1-benzoylethyl 4-chlorobenzoate, (II) (Wan *et al.*, 2005). In order to investigate the effect of the substituent Cl atom on the conformation and biological activities, the title compound, (I), has been synthesized.




(I)

All bond lengths (Table 1) and angles in (I) are within normal ranges (Allen *et al.*, 1987) and in good agreement with those in (II). The benzotriazole system is essentially planar, with a dihedral angle of 0.5 (1)° between the triazole and benzene (C10–C15) rings, comparable to 1.9 (1)° in (II). The mean plane of the benzotriazole system makes dihedral angles of 41.6 (1) and 78.4 (1)° with the phenyl (C1–C6) and benzene (C17–C22) rings, respectively. The dihedral angle between the C1–C6 and C17–C22 rings is 70.7 (7)°. In the crystal structure, weak intermolecular C—H···N hydrogen bonds (Table 2) link the molecules into chains extended along the *c* axis. The packing (Fig. 2) is further stabilized by weak C—H···O interactions (Table 2).

## Experimental

Bromine (3.2 g, 0.02 mol) was added dropwise to a solution of 3-(benzotriazol-1-yl)-1-phenylpropan-1-one (5.0 g, 0.02 mol) and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml). The reaction proceeded for 13 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 the chloroform solution filtered. It was cooled

with ice–water, and then an acetone solution (10 ml) of 2-chlorobenzoic acid (3.1 g, 0.02 mol) and triethylamine (2.8 ml) was added. The mixture was stirred at room temperature for about 2 h. The solution was then filtered and concentrated. Single crystals were obtained by slow evaporation of an acetone–ethyl acetate (1:3 *v*/*v*) solution at room temperature over a period of one week.

*Crystal data*

$C_{22}H_{16}ClN_3O_3$
$M_r$ = 405.83
Monoclinic, $P2_1/c$
$a$ = 12.9341 (9) Å
$b$ = 9.4562 (7) Å
$c$ = 18.1878 (9) Å
$\beta$ = 120.441 (3)°
$V$ = 1917.9 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.406 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3073 reflections
$\theta$ = 2.5–24.9°
$\mu$ = 0.23 mm$^{-1}$
$T$ = 293 (2) K
Column, colourless
0.40 × 0.23 × 0.10 mm

*Data collection*

Siemens SMART 1000 CCD area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.914, $T_{max}$ = 0.978
10521 measured reflections
3769 independent reflections
2894 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022
$\theta_{max}$ = 26.0°
$h = -15 \rightarrow 15$
$k = -9 \rightarrow 11$
$l = -16 \rightarrow 22$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.116
$S$ = 1.03
3769 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.4844P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cl1—C18 | 1.741 (2) | O3—C16 | 1.201 (2) |
| O1—C7 | 1.211 (2) | C7—C8 | 1.524 (3) |
| O2—C16 | 1.339 (2) | C8—C9 | 1.520 (3) |
| O2—C8 | 1.442 (2) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8$A$···N3$^{i}$ | 0.98 | 2.48 | 3.296 (3) | 140 |
| C21—H21$A$···O1$^{ii}$ | 0.93 | 2.53 | 3.330 (3) | 144 |

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

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) = 1.2 $U_{eq}$(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).

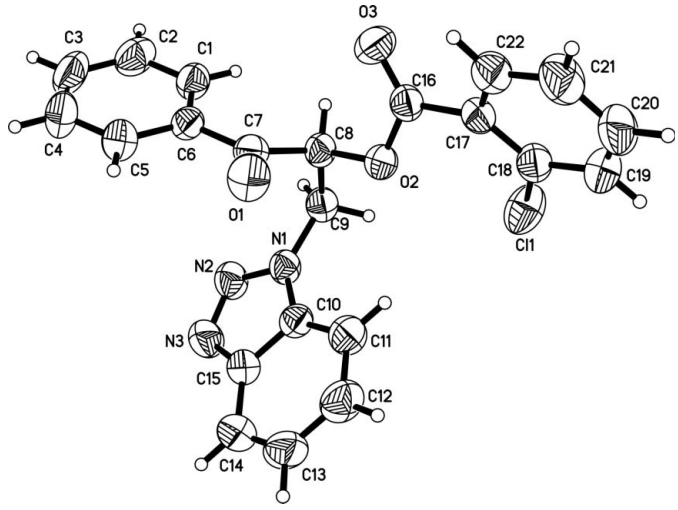



**Figure 1**
View of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

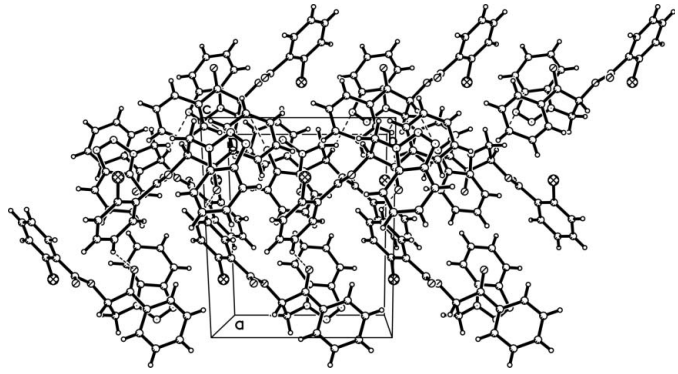



**Figure 2**
A perspective view of the crystal packing down the *c* axis. Hydrogen bonds are indicated by dashed lines.

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