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2-(1*H*-1,2,3-Benzotriazol-1-ylmethyl)-1-benzoylethyl 4-chlorobenzoate

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Key indicators

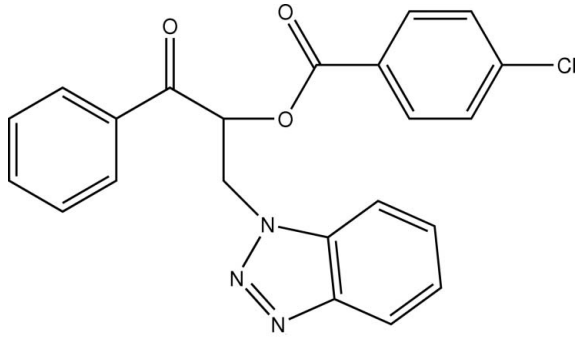
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.116
Data-to-parameter ratio = 14.8

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

In the title compound, $C_{22}H_{16}ClN_3O_3$, molecules are linked into chains along the c axis by C—H···O hydrogen bonds, while other C—H···N hydrogen bonds connect the chains into two-dimensional layers. The packing is further stabilized by π–π interactions.

Comment

Benzotriazole derivatives have been found to exhibit a broad spectrum of pharmacological activities such as anti-inflammatory, antifungal, antitumor, antineoplastic and antidepressant activities (Al-Soud *et al.*, 2003; Katarzyna *et al.*, 2004). As part of a search for new benzotriazole compounds with high bioactivity, the title compound, (I), was synthesized.



(I)

The bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are comparable to those in the related compound 2-(1*H*-1,2,3-benzotriazol-1-ylmethyl)-1-benzoylethyl 4-ethylbenzoate (Wan *et al.*, 2005). The benzotriazole system is essentially planar, with a dihedral angle of 1.9 (1)° between the triazole ring (*A*, atoms N1–N3/C10/C15) and the benzene ring (*B*, atoms C10–C15). The dihedral angles between the mean planes of the benzotriazole system and rings *C* (atoms C1–C6) and *D* (atoms C17–C22) are 38.1 (1) and 53.7 (1)°, respectively. The dihedral angle between rings *C* and *D* is 88.9 (1)°.

In the crystal structure, molecules of (I) are linked into chains along the c axis by C9—H9*A*···O1^{ii} and C11—H11*A*···O1^{ii} hydrogen bonds (see Table 2 for geometry values and symmetry codes). In addition, C3—H3*B*···N3^{i} interactions connect the chains into two-dimensional layers in the *ac* plane (Fig. 2). The packing is further stabilized by π–π interactions involving the benzotriazole system and benzene ring *D*, the distances being $Cg1\cdots Cg4^{iii}$ = 3.570 Å and $Cg3\cdots Cg4^{iii}$ = 3.654 Å [*Cg*1, *Cg*3 and *Cg*4 denote the centroids of the rings *A*, *B* and *D*, respectively; symmetry code: (iii) $x, \frac{3}{2} - y, z - \frac{1}{2}$].

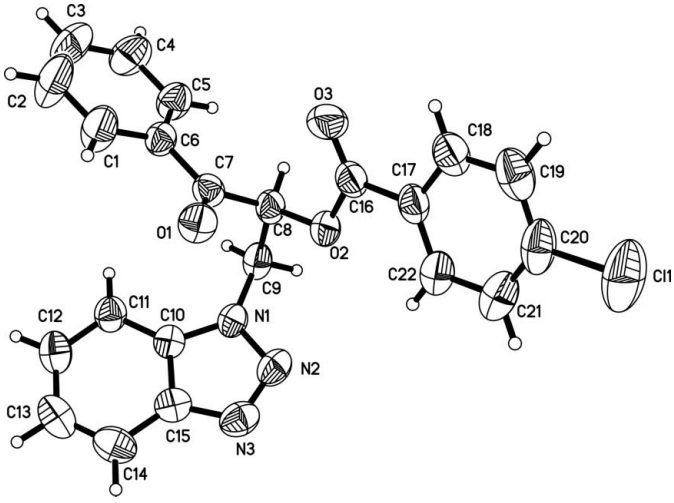


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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 was allowed to proceed 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 4-chlorobenzoic acid (3.1 g, 0.02 mol) and triethylamine (2.8 ml) were added. The mixture was stirred at room temperature for about 2 h. The solution was then filtered and concentrated (yield 62%). Crystals of (I) were obtained by slow evaporation of an acetone–water (1:1 *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 = 9.712 (3) Å
b = 20.379 (5) Å
c = 10.009 (3) Å
β = 90.392 (4)°
V = 1980.9 (9) Å^3
Z = 4
D_x = 1.361 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2380 reflections
θ = 2.3–22.3°
μ = 0.22 mm^{-1}
T = 293 (2) K
Column, colorless
0.28 × 0.11 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.941, T_{max} = 0.967
11133 measured reflections
3885 independent reflections
2719 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.0°
$h = -11 \rightarrow 10$
$k = -25 \rightarrow 19$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.116
S = 1.02
3885 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.3694P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

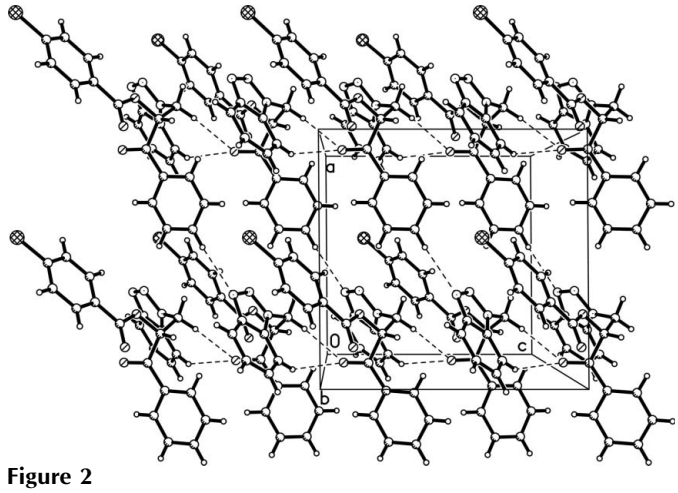


Figure 2
The two-dimensional layers of (I), viewed down the *b* axis. Dashed lines indicate C—H···O,N interactions.

Table 1
Selected bond lengths (Å).

Cl1—C20	1.743 (2)	O3—C16	1.202 (2)
O1—C7	1.218 (2)	C7—C8	1.527 (3)
O2—C16	1.357 (2)	C8—C9	1.514 (3)
O2—C8	1.436 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3B···N3^{i}	0.93	2.58	3.506 (4)	175
C9—H9A···O1^{ii}	0.97	2.49	3.453 (3)	173
C11—H11A···O1^{ii}	0.93	2.52	3.316 (3)	143

Symmetry codes: (i) $x+1, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

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) = 1.2U_{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).

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