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3-(Benzotriazol-1-yl)-1-(4-chlorophenyl)-1-oxopropan-2-yl 2-chlorobenzoate

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Key indicators

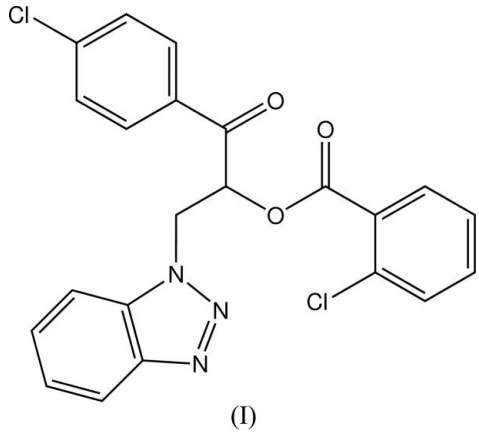
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.118
Data-to-parameter ratio = 15.1

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

In the title molecule, $C_{22}H_{15}Cl_2N_3O_3$, the benzotriazole mean plane makes dihedral angles with the two benzene rings of 11.29 (1) and 84.90 (1)°. Weak intermolecular C—H···O hydrogen bonds link the molecules into chains extended along the b axis.

Comment

Recently, we have reported the crystal structure of 2-(1*H*-1,2,3-benzotriazol-1-ylmethyl)-1-benzoylethyl 4-chlorobenzoate, (II) (Wan *et al.*, 2006). As part of our ongoing search for new benzotriazole compounds with high bioactivity, the title compound, (I), was synthesized. We present here its crystal structure.



(I)

In (I) (Fig. 1), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and comparable with those in the related compound (II). The benzotriazole mean plane makes dihedral angles with the two benzene rings, C1–C6 and C17–C22, of 11.29 (1) and 84.90 (1)°, respectively. The dihedral angle between the benzene rings is 73.63 (1)°.

In the crystal structure (Fig. 2), weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into chains along the b axis. The distance of 3.728 (2) Å between the centroids of rings N1–N3/C10/C11 and C10–C15 related by the symmetry element $(-x, -y, 1-z)$ suggests a possible π–π interaction.

Experimental

The title compound was prepared according to the literature method of Wan *et al.* (2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of 6 d.

Crystal data

$C_{22}H_{15}Cl_2N_3O_3$
M_r = 440.27
Monoclinic, $P2_1/c$
a = 10.112 (2) Å
b = 9.2772 (19) Å
c = 21.998 (5) Å
β = 92.773 (3)°
V = 2061.2 (8) Å^3
Z = 4
D_x = 1.419 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 293 (2) K
Plate, white
0.30 × 0.19 × 0.03 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.904, T_{max} = 0.990
11245 measured reflections
4081 independent reflections
2690 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.118
S = 1.02
4081 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.1582P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O1^{i}	0.98	2.49	3.455 (3)	170
C9—H9A···O3^{ii}	0.97	2.51	3.117 (3)	121

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (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 = 0.93–0.98 Å and 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: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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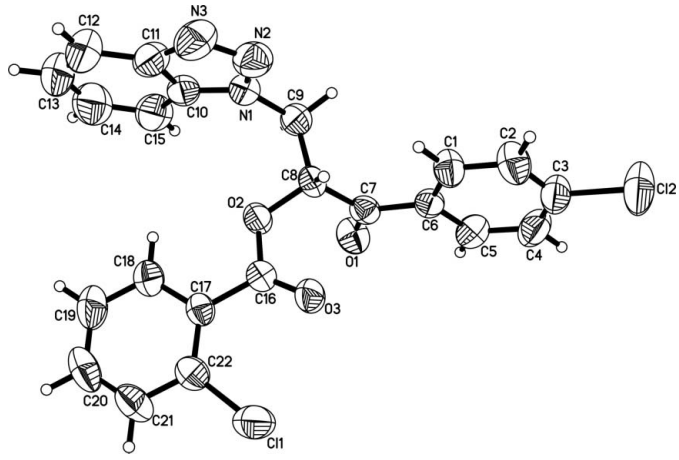

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

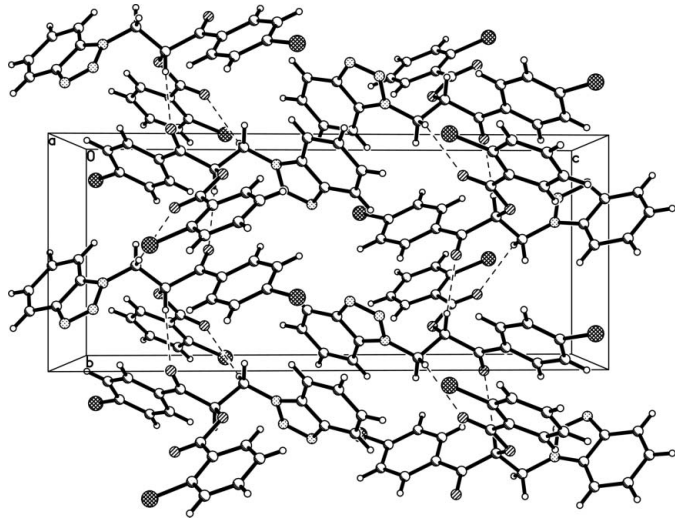

Figure 2
Packing diagram of (I), viewed down the *a* axis, showing the intermolecular hydrogen bonds as dashed lines.

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