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

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Key indicators

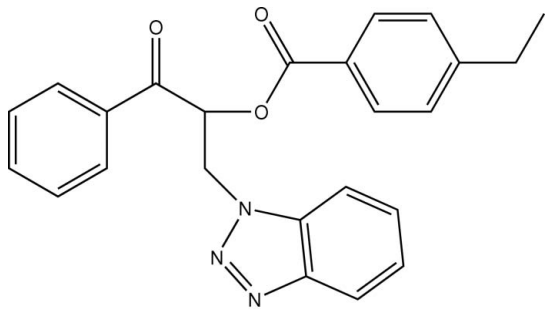
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.153
Data-to-parameter ratio = 15.1

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

In the title compound, $C_{24}H_{21}N_3O_3$, the relative orientation of the three rings is determined by the sp^3-hybridization character of the chiral atom. The molecules are linked into ribbons along the *b* axis by intermolecular C—H···O interactions.

Comment

In order to search for new benzotriazole compounds with higher bioactivity, the title compound, (I), including benzotriazole, was synthesized and its structure is presented here.



(I)

The bond lengths and angles (Table 1) in (I) are within normal ranges (Allen *et al.*, 1987). The bonds in the benzotriazole ring system show a character intermediate between single and double bonds.

In (I), the benzotriazole system is almost planar, with a dihedral angle of 1.21 (13)° between the triazole ring *A* (N1–N3/C10/C15) and benzene ring *B* (C10–C15). The dihedral angles between the mean planes of the benzotriazole system and rings *C* (C1–C6) and *D* (C17–C22) are 17.22 (10) and 60.54 (10)°, respectively. The dihedral angle between rings *C* and *D* is 76.33 (11)°. The relative orientation of the three rings is determined by the sp^3-hybridization character of the chiral atom C8.

In the crystal structure, molecules of (I) are linked into ribbons along the *b* axis by C—H···O interactions (Table 2, Fig. 2).

Experimental

The title compound was prepared according to the literature method of Wan *et al.* (2005). Single crystal suitable for X-ray measurements was obtained by slow evaporation of an ethyl acetate–petroleum ether (2:1 *v*/*v*) at room temperature over a period of one week.

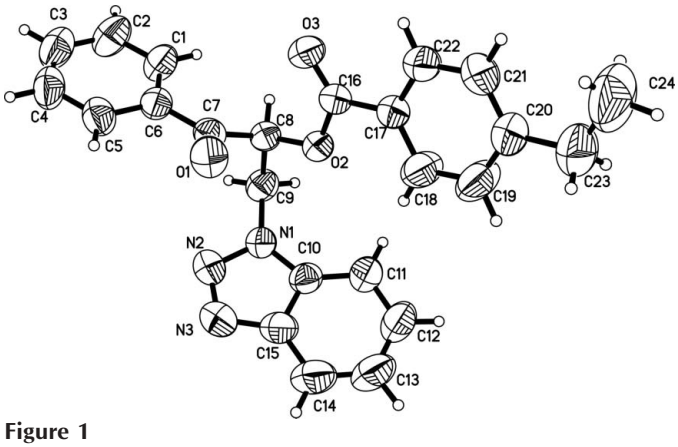


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Crystal data

$C_{24}H_{21}N_3O_3$	D_x = 1.270 Mg m^{-3}
M_r = 399.44	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3695 reflections
a = 13.9064 (9) Å	θ = 2.4–24.5°
b = 8.7793 (6) Å	μ = 0.09 mm^{-1}
c = 17.4342 (12) Å	T = 296 (2) K
β = 101.143 (1)°	Block, colourless
V = 2088.4 (2) Å^3	0.41 × 0.13 × 0.13 mm
Z = 4	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	4102 independent reflections
	2989 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.019
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 26.0°
	$h = -17 \rightarrow 16$
T_{min} = 0.966, T_{max} = 0.989	$k = -10 \rightarrow 10$
12007 measured reflections	$l = -19 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0757P)^2 + 0.4188P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.051	
$wR(F^2)$ = 0.153	
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
4102 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
271 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.208 (2)	O2—C8	1.429 (2)
O2—C16	1.359 (2)	O3—C16	1.200 (2)
O2—C8—C9	106.40 (13)	C9—C8—C7	111.98 (14)
O2—C8—C7	110.54 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O1^{i}	0.93	2.45	3.362 (2)	166

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

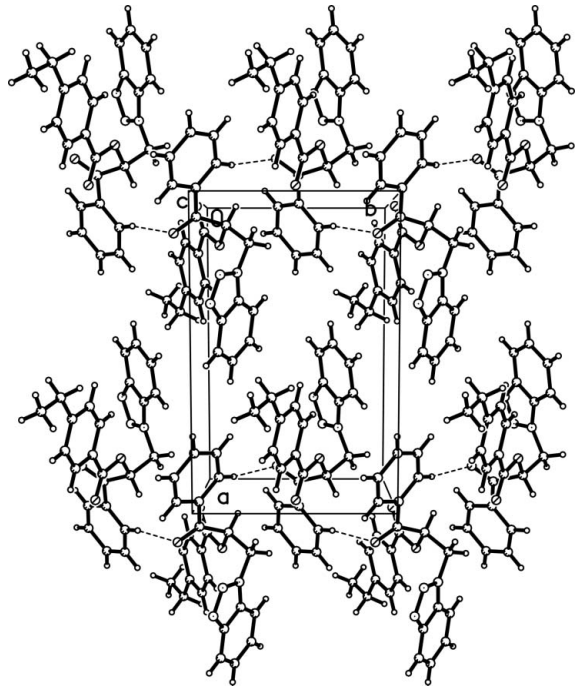


Figure 2
Packing diagram of (I). Hydrogen bonds are shown as dashed lines.

H atoms were located in a difference map and constrained to ride on their parent atoms, with C—H distances of 0.93 and 0.98 (CH), 0.97 (CH_2) and 0.96 Å (CH_3), and with U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(C) for methyl H.

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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