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3-(3*H*-Benzotriazol-1-yl)-1-(2,5-dichlorophenyl)-2-oxopropyl nicotinate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.070
wR factor = 0.171
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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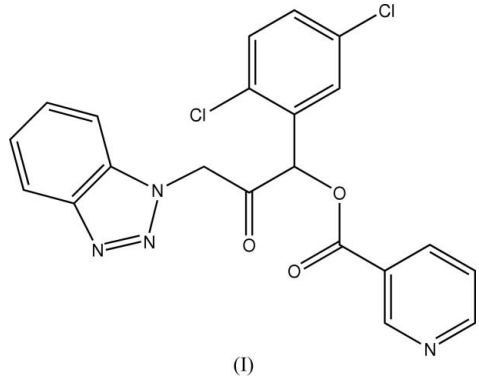
Molecules of the title compound, $C_{21}H_{14}Cl_2N_4O_3$, are linked into chains along the *b* axis by intermolecular C—H···O hydrogen bonds. C—H···N interactions connect these chains into a two-dimensional layer. The packing is further stabilized by π–π interactions involving the triazole rings.

Comment

We have recently reported the 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 studies of triazole derivatives, the title compound, (I), was synthesized and its structure is reported here.



(I)

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable with those in the related compound, (II). The benzotriazole system is essentially planar, with a dihedral angle of 0.8 (2)° between the triazole (N2–N4/C16/C21) and benzene (C16–C21) rings. The mean plane of the benzotriazole group makes dihedral angles of 44.38 (1) and 66.90 (2)° with the pyridine (N1/C10–C14) and (C1–C6) benzene rings, respectively. The dihedral angle between the planes of the latter two aromatic rings is 81.0 (2)°.

In the crystal structure, molecules are linked into chains along the *b* axis by intermolecular C—H···O hydrogen bonds. C—H···N interactions connect the chains into a two-dimensional layer (Table 1 and Fig. 2). The packing is further stabilized by π–π interactions involving the triazole rings: $Cg1\cdots Cg1^{i}$ = 3.494 Å [symmetry code: (i) 3 − *x*, 1 − *y*, 1 − *z*; *Cg*1 is the centroid of the triazole ring].

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 one week.

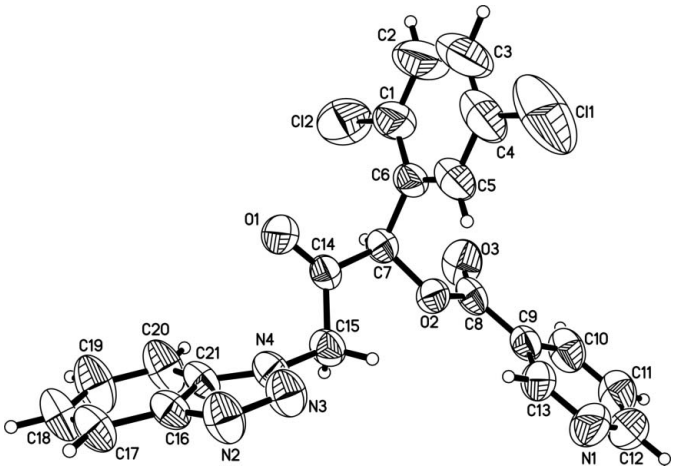


Figure 1
The molecular structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_{21}H_{14}Cl_2N_4O_3$
M_r = 441.26
Triclinic, $P\overline{1}$
a = 6.1578 (14) Å
b = 10.779 (3) Å
c = 16.166 (4) Å
α = 105.048 (4)°
β = 93.677 (4)°
γ = 99.606 (4)°
V = 1015.2 (4) Å^3
Z = 2
D_x = 1.444 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 293 (2) K
Column, colourless
0.36 × 0.12 × 0.11 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.884, T_{max} = 0.962
5721 measured reflections
3902 independent reflections
1932 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.171
S = 1.00
3902 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.3295P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 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
C7—H7A···N3^{i}	0.98	2.59	3.327 (5)	132
C11—H11A···O1^{ii}	0.93	2.51	3.427 (6)	169
C20—H20A···N2^{i}	0.93	2.46	3.346 (6)	160

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1, y-1, z$.

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).

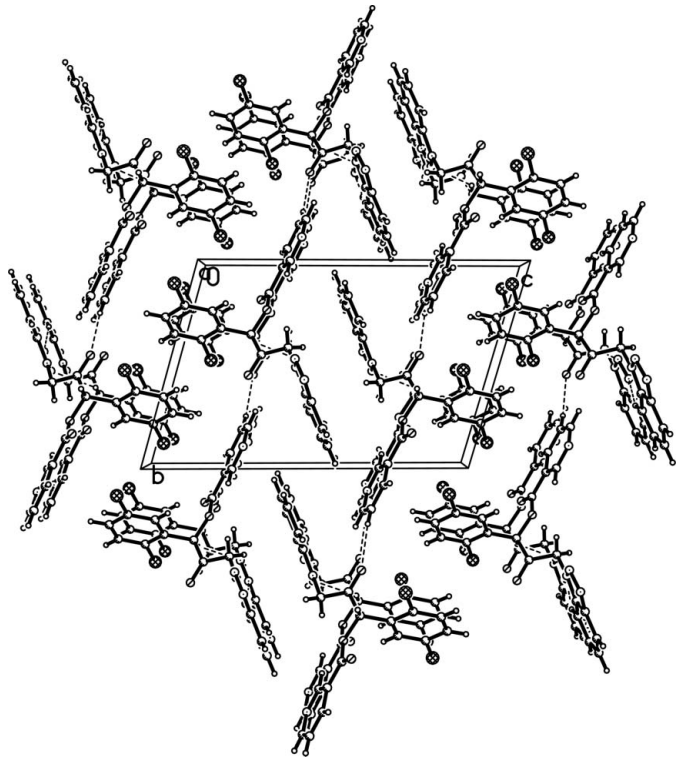


Figure 2
Packing diagram of (I), viewed down the a axis, showing the intermolecular hydrogen bonds (dashed lines).

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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