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2-[3-(2-Cyano-2-propyl)-5-(1,2,4-triazol-1-yl)-phenyl]-2-methylpropiononitrile

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.063
wR factor = 0.203
Data-to-parameter ratio = 16.0

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

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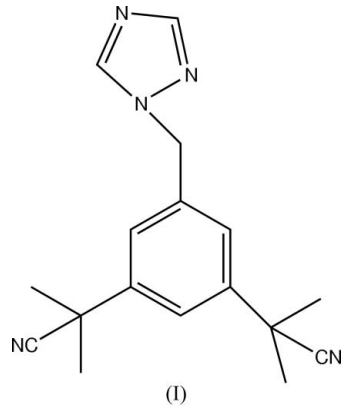
In the title compound, $C_{17}H_{19}N_5$, the almost ideally planar triazole ring forms a dihedral angle of 75.1 (1)° with the benzene ring. There are intermolecular π–π interactions.

Comment

The title compound, (I), an aromatase inhibitor, has been shown to be useful in second-line therapy of estrogen-dependent breast cancer and has recently been approved as first-line therapy in several countries (Goss & Strasser, 2001). In this paper, we report the crystal structure of (I). The bond lengths and bond angles are in agreement with those reported for other 1,2,4-triazole derivatives (Chinnakali *et al.*, 1999; Mazur *et al.*, 2004) and are within the expected ranges. The almost ideally planar triazole ring forms a dihedral angle of 75.1 (1)° with the benzene ring (Fig. 1). Atom C7 is coplanar with the triazole ring. In the crystal structure (Fig. 2), a π–π interaction is observed between the benzene ring and the symmetry-related ring at $(1 - x, y, \frac{3}{2} - z)$; the distance between the centroids of the benzene rings is 3.995 Å.



(I)

Experimental

Compound (I) was a gift from Linhai Dongdog Chemical Factory. Crystals were grown from an acetone solution by slow evaporation at room temperature.

Crystal data

$C_{17}H_{19}N_5$
M_r = 293.37
Monoclinic, $C2/c$
a = 17.9107 (8) Å
b = 11.2522 (3) Å
c = 18.9011 (7) Å
β = 121.181 (1)°
V = 3258.9 (2) Å^3
Z = 8
D_x = 1.196 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10339 reflections
θ = 2.2–27.5°
μ = 0.08 mm^{-1}
T = 295 (1) K
Prism, colorless
0.45 × 0.45 × 0.20 mm

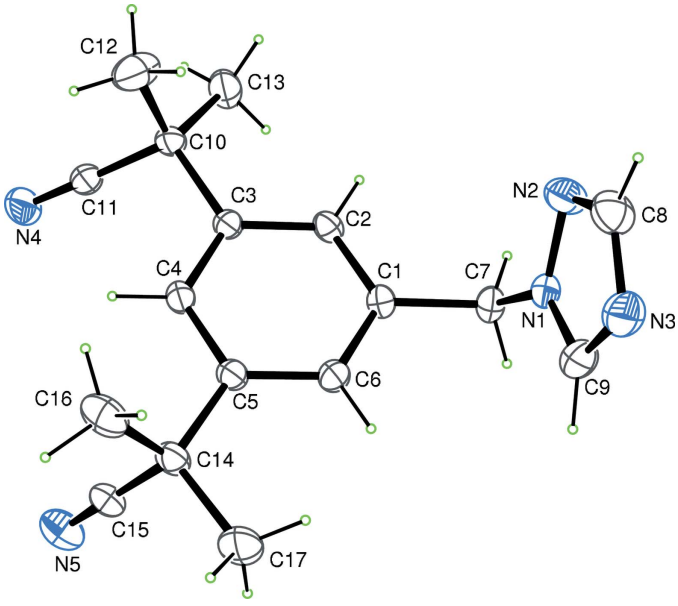


Figure 1
Molecular structure of (I), showing 30% probability displacement ellipsoids.

Data collection

Rigaku R-AXIS RAPID diffractometer	2348 reflections with $F^2 > 2\sigma(F^2)$
ω scans	$R_{int} = 0.031$
Absorption correction: none	$\theta_{max} = 27.5^\circ$
16052 measured reflections	$h = -23 \rightarrow 23$
3748 independent reflections	$k = -14 \rightarrow 14$
	$l = -23 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[0.0057F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)] = 0.063$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.203$	$\Delta\rho_{max} = 0.37$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.37$ e Å^{-3}
3197 reflections	Extinction correction: Larson (1970)
200 parameters	Extinction coefficient: 1.8 (6) $\times 10^2$
H-atom parameters constrained	

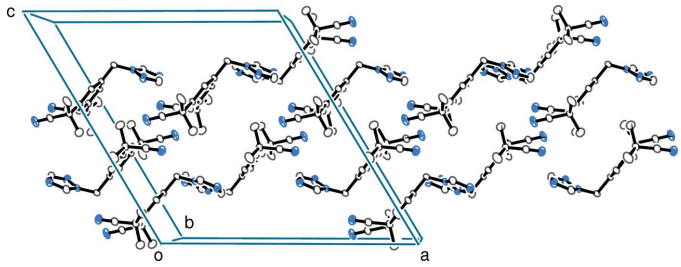


Figure 2
Packing arrangement for (I). H atoms have been omitted for clarity.

The high-angle reflections ($2\theta > 52^\circ$) were not used in the refinement, because they were weak. H atoms were placed in calculated positions, with C—H = 0.93 Å, and included in the refinement in a riding model, with $U_{iso}(H) = 1.2U_{eq}$ (carrier atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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