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4-(3-Methylphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.064
wR factor = 0.136
Data-to-parameter ratio = 12.4

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

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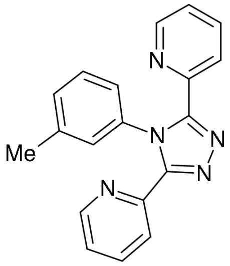
In the title compound, $C_{19}H_{15}N_5$, the pyridyl groups and the benzene ring lie in a propeller arrangement around the central 1,2,4-triazole ring, thereby minimizing the steric crowding of these rings.

Comment

Triazole derivatives play an important role in the development of coordination chemistry related to antibacterial and enzymatic reactions (Gupta & Bhargava, 1978; Cornelissen *et al.*, 1992; Kunkeler *et al.*, 1996). As an extension of our work on the structural characterization of triazole derivatives, the crystal structure of the title compound, (I), is reported here.



(I)

Compound (I) is a triazole derivative (Fig. 1). Some selected bond lengths and angles are listed in Table 1. The dihedral angle between the two pyridyl rings is 71.8 (3)°. The dihedral angles between the benzene ring and the two pyridyl rings (C1/C2/C3/C4/C5/N1 and C8/C9/C10/C11/C12/N4) are 72.5 (3) and 74.5 (3)°, respectively. The two pyridyl rings form dihedral angles of 35.9 (3) and 36.8 (3)°, respectively, with the triazole ring. The dihedral angle between the triazole ring and the benzene ring is 75.7 (3)°. The pyridyl groups and the benzene ring lie in a propeller arrangement around the central 1,2,4-triazole ring, thereby minimizing the steric crowding of these rings. The crystal packing is shown in Fig. 2.

Experimental

The title compound was synthesized according to a literature method (Zhang *et al.*, 2004). Equivalent amounts of *m*-tolylphosphazoanilide and *N*,*N*′-dipyridoylhydrazine were reacted in *N*,*N*′-dimethylaniline for 3 h at 483–493 K, with stirring. Colourless block-shaped crystals were obtained by slow evaporation of an acetone solution. The crystals were collected and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 68%).

Crystal data

$C_{19}H_{15}N_5$
$M_r = 313.36$
Monoclinic, $P2_1/c$
$a = 11.229\ (1)$ Å
$b = 9.207\ (1)$ Å
$c = 19.086\ (1)$ Å
$\beta = 125.40\ (1)^\circ$
$V = 1608.5\ (3)$ Å^3
$Z = 4$

$D_x = 1.294$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 581 reflections
$\theta = 2.2$–23.1°
$\mu = 0.08$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.32 × 0.28 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.974$, $T_{\max} = 0.982$
6850 measured reflections

2896 independent reflections
1601 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$
$\theta_{\max} = 25.5^\circ$
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 10$
$l = -11 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.136$
$S = 1.01$
2896 reflections
234 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N2—C6	1.304 (3)	N4—C8	1.340 (3)
N2—N3	1.388 (3)	N5—C7	1.368 (3)
N3—C7	1.320 (3)	N5—C6	1.377 (3)
N4—C12	1.331 (4)	N5—C13	1.444 (3)
C6—N2—N3	107.7 (2)	C7—N5—C6	104.7 (2)
C7—N3—N2	107.1 (2)	C7—N5—C13	127.1 (2)
C12—N4—C8	116.5 (3)	C6—N5—C13	128.1 (2)

There is a orientational disorder of one of the pyridyl groups, and atoms N1 and C2 share their positions with C2′ and N1′, respectively. The occupation factors of these atoms were assumed to 50% each. Positional parameters of the atoms H2(—C2), H2′(—N1), H3(—C3) and H5(—C5) were refined isotropically, the C—H distances being restrained to 0.93 (1) Å. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.96 Å and with $U_{\rm iso}({\rm H}) = 1.2$ or $1.5U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

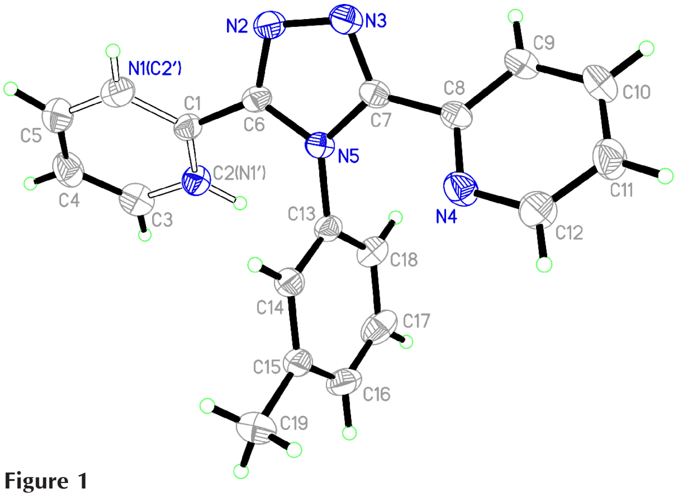


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. One of the pyridyl groups has two possible orientations, and atoms N1 and C2 share their positions with C2′ and N1′, respectively.

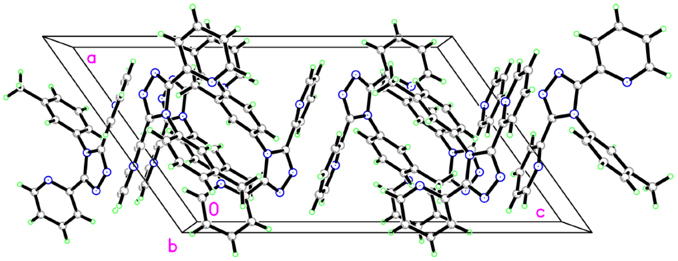


Figure 2
The crystal packing of (I), viewed along the *b* axis.

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