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

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.126
Data-to-parameter ratio = 14.1

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

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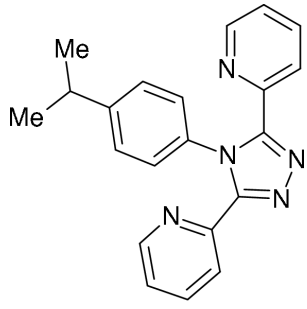
In the title compound, $C_{21}H_{19}N_5$, the pyridyl groups and the benzene ring lie in a propeller arrangement around the central 1,2,4-triazole ring, minimizing the steric effects among these rings.

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 work on the structural characterization of triazole derivatives, the crystal structure of the title compound, (I), is reported here.



(I)

In (I), the pyridyl groups and the benzene ring lie in a propeller arrangement around the central 1,2,4-triazole ring (Fig. 1), thereby minimizing the steric effects among these rings. The dihedral angles between the 4-isopropylphenyl ring and the two pyridyl rings (N1/C1–C5 and N4/C8–C12) are 55.0 (2) and 64.3 (2)°, respectively. The dihedral angle between the two pyridyl rings is 72.7 (2)°, the two pyridyl rings form dihedral angles of 43.7 (2) and 29.8 (2)° with the triazole ring, and the dihedral angle between the triazole ring and the 4-isopropylphenyl ring is 58.2 (2)°. The crystal structure is shown in Fig. 2. Intermolecular C—H···N short contacts are not observed, the H···N distances being longer than 2.70 Å.

Experimental

Compound (I) was synthesized by the reaction of equivalent amounts of *p*-isopropylphenylphosphazoanilide and *N,N′*-dipyridylhydrazine in *N,N′*-dimethylaniline for 3 h at 483–493 K (yield 72%). Colourless block-shaped crystals of (I) were obtained by slow evaporation of an acetone solution.

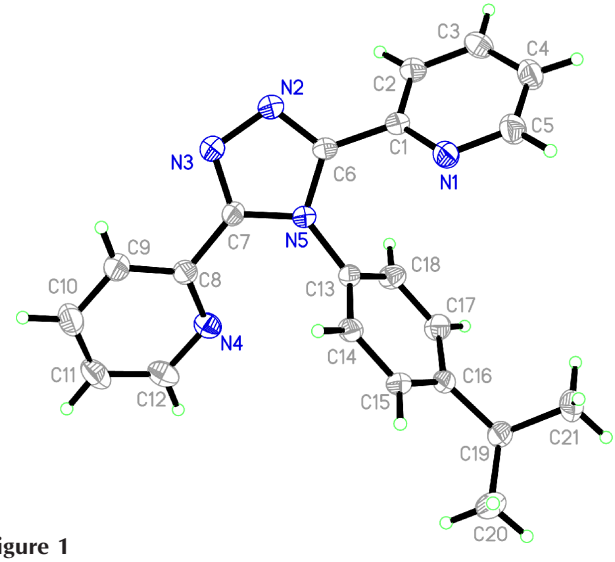


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

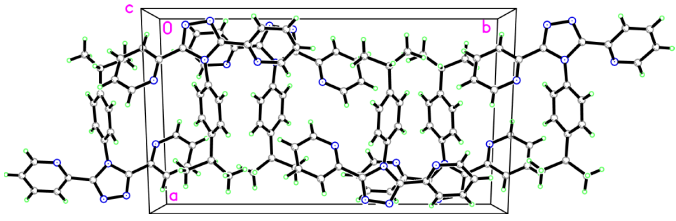


Figure 2
The crystal packing of (I), viewed along the *c* axis.

Crystal data

$C_{21}H_{19}N_5$
M_r = 341.41
Monoclinic, $P2_1/c$
a = 11.704 (1) Å
b = 19.935 (2) Å
c = 8.181 (1) Å
β = 107.580 (2)°
V = 1819.7 (3) Å^3
Z = 4
D_x = 1.246 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1463 reflections
θ = 2.9–21.2°
μ = 0.08 mm^{-1}
T = 298 (2) K
Block, colourless
0.23 × 0.21 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.986
7778 measured reflections
3336 independent reflections
2245 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.5°
$h = -14 \rightarrow 12$
$k = -21 \rightarrow 24$
$l = -6 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.126
S = 1.00
3336 reflections
237 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N2—C6	1.310 (2)	N5—C6	1.367 (2)
N2—N3	1.381 (2)	N5—C7	1.368 (2)
N3—C7	1.312 (2)		
C6—N2—N3	107.21 (14)	N2—C6—N5	110.55 (16)
C7—N3—N2	107.49 (14)	N3—C7—N5	110.22 (16)
C6—N5—C7	104.53 (14)		
N1—C1—C6—N5	−44.3 (3)	C7—N5—C13—C14	−60.4 (3)
N3—C7—C8—C9	−29.2 (3)		

All 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_{iso}(H) = 1.2 or 1.5U_{eq}(C). The structure contains solvent-accessible voids of 35 Å^3, which might accommodate a disordered water molecule.

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*.

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