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5,7-Di-*tert*-butyl-2-(2-pyridyl)benzo[*d*]oxazole

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The multiple-bond character of the C—C bond connecting the pyridine and benzoxazole ring systems results in an overall planarity of the central aromatic part of the title compound, $C_{20}H_{24}N_2O$. The crystal structure is stabilized by intermolecular C—H···N close contacts, linking molecules into layers.

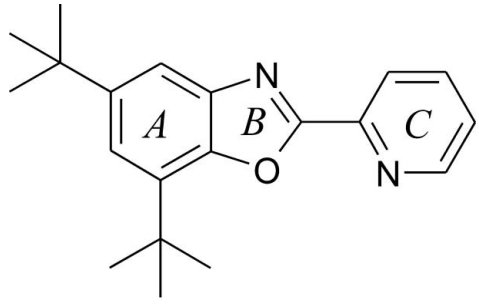
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.106
Data-to-parameter ratio = 14.3

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

Comment

The benzoxazole skeleton is an essential structural unit of several antibacterial (Temiz *et al.*, 1998), anticancer (Kumar *et al.*, 2002) and anti-HIV-1 agents (*e.g.* Hoffman *et al.*, 1993). We recently prepared and studied the antituberculotic activity of several benzoxazole derivatives (Vinšová *et al.*, 2005). With the aim of studying the complexation behaviour of benzoxazoles, we prepared the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. Most of the bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). An exception is C7—C8 [1.461 (2) Å]; comparison with the analogous bond lengths in 2-(2-quinolyl)-benzoxazole (1.48 Å; Klyuyev *et al.*, 1982) and (2,6-bis(benzoxazol-2-yl)pyridine) (1.471–1.507 Å; Drew *et al.*, 2004) indicates its weak multiple-bond character. This is in good agreement with the overall planarity of the central aromatic part of (I), where the dihedral angles between planar rings *A*/*B* and *B*/*C* (see scheme) are 4.08 (4) and 8.85 (5)°, respectively (*PARST*; Nardelli, 1995).

In the crystal structure, intermolecular C—H···N close contacts (Table 1) link the molecules into layers.

Experimental

Crystals of (I) were prepared by a recently described method (Lodyato *et al.*, 2003, Vinšová *et al.*, 2006). Purification was by column chromatography on silica gel using ethyl acetate–petroleum ether (1:9 *v*/*v*) as eluent.

Crystal data

$C_{20}H_{24}N_2O$
M_r = 308.41
Monoclinic, $P2_1/n$
a = 9.7224 (13) Å
b = 6.0174 (8) Å
c = 30.103 (4) Å
β = 99.019 (13)°
V = 1739.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 120 (2) K
0.50 × 0.30 × 0.20 mm

Data collection

Kuma KM-4-Plus CCD diffractometer
Absorption correction: none
8261 measured reflections
3066 independent reflections
2403 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.106
S = 1.02
3066 reflections
214 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···N1^{i}	0.95	2.65	3.355 (2)	132
C12—H12···N2^{ii}	0.95	2.69	3.323 (2)	125
C19—H19A···N1^{iii}	0.98	2.66	3.630 (2)	170

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, y+1, z$.

All H atoms were located in a difference map and refined as riding, with C—H = 0.95 (CH) or 0.98 Å (CH_3), and with U_{iso}(H) = 1.2U_{eq}(aromatic C) or 1.5U_{eq}(methyl C).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Johnson & Burnett, 1996); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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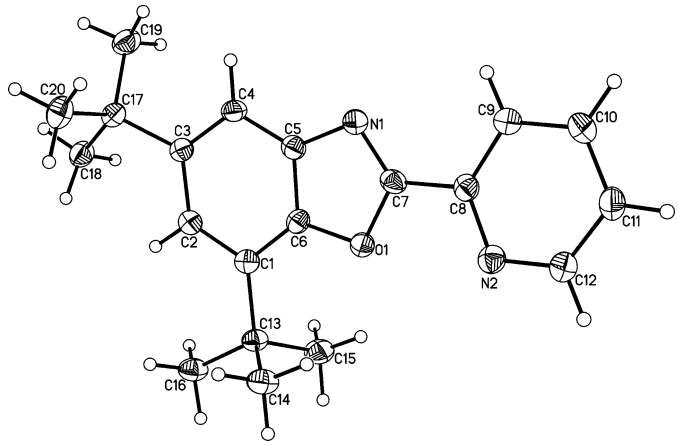

Figure 1
The molecular structure of the title compound. The non-H atoms are drawn as 50% probability displacement ellipsoids, and H atoms as small spheres of arbitrary radius.

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