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## Key indicators

Single-crystal X-ray study

T = 297 K

Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$ 

R factor = 0.043

wR factor = 0.103

Data-to-parameter ratio = 11.7

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N,N'*-(Methylenedi-*p*-phenylene)bis(pyridine-2-carboxamide)

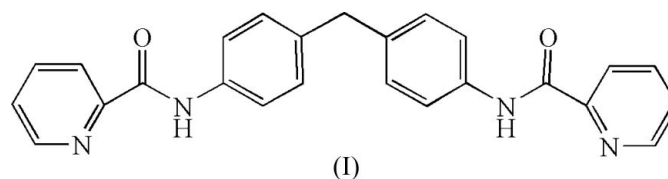
In the crystal structure of the title compound,  $\text{C}_{25}\text{H}_{20}\text{N}_4\text{O}_2$ , intramolecular  $\text{N}-\text{H}\cdots\text{N}$  and intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds may be effective in its stabilization.

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## Comment

The coordination chemistry of bispyridylamides is extremely rich. Examples of coordination *via* the pyridine N atoms, the carbonyl O atoms and the amide N atoms of the ligand in a non-, mono-, or bis-deprotonated form are known (Jubert *et al.*, 2002; Amirnasr *et al.*, 2002; Meghdadi *et al.*, 2006) and metal complexes of the ligands have been used extensively to mimic the properties of biologically active systems (Belda & Moberg, 2005). With control over the ligand properties such as donor density, the type and number of coordination sites has led to a wide variety of resultant structural motifs such as helicates (Piguet *et al.*, 1997; Lessmann & Horrocks, 2000; Albrecht, 2001). In order to develop further the supra-molecular chemistry of bispyridine-amide ligands, we synthesized the title ligand, (I), and report here its crystal structure.



In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings *A* (N1/C1–C5), *B* (C7–C12), *C* (C14–C19) and *D* (N4/C21–C25) are, of course, planar and the dihedral angles between them are  $A/B = 6.25 (4)$ ,  $A/C = 75.40 (3)$ ,  $A/D = 78.01 (4)$ ,  $B/C = 72.27 (3)$ ,  $B/D = 74.50 (3)$  and  $C/D = 4.65 (3)^\circ$ .

As can be seen from the packing diagram (Fig. 2), intramolecular  $\text{N}-\text{H}\cdots\text{N}$  and intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2) link the molecules and may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

## Experimental

A solution of 4,4'-diaminodiphenylmethane (2.97 g, 15 mmol) in pyridine (12 ml) was added to a solution of pyridine-2-carboxylic acid (3.69 g, 30 mmol) in pyridine (20 ml). The resulting solution was stirred at 313–318 K for 10 min, and then triphenyl phosphite (30 mmol, 7.9 ml) was added dropwise, and the reaction mixture was stirred at 363–373 K for 4 h, during which time a white precipitate formed. After cooling to room temperature, the reaction mixture was

left in the hood for 24 h. The white precipitate was filtered off, washed with 20 ml of acetone/water (1:1), and then dried in air. X-ray quality crystals were obtained by slow diffusion of diethyl ether into a dichloromethane solution at room temperature (yield 90.2%; m.p. 501–503 K).

#### Crystal data

$C_{25}H_{20}N_4O_2$   
 $M_r = 408.45$   
 Triclinic,  $P\bar{1}$   
 $a = 8.719$  (3) Å  
 $b = 9.877$  (3) Å  
 $c = 12.444$  (4) Å  
 $\alpha = 100.89$  (2)°  
 $\beta = 100.12$  (3)°  
 $\gamma = 102.54$  (2)°

$V = 1000.6$  (6) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.356$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 297$  (2) K  
 Prism, colorless  
 $0.45 \times 0.4 \times 0.15$  mm

#### Data collection

Stoe IPDS-II diffractometer  
 $\varphi$  scans  
 Absorption correction: numerical  
 (*X-RED32*; Stoe & Cie, 2005)  
 $T_{\min} = 0.965$ ,  $T_{\max} = 0.987$

9143 measured reflections  
 4198 independent reflections  
 3313 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$   
 $\theta_{\text{max}} = 26.8^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.103$   
 $S = 1.07$   
 4198 reflections  
 360 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.1595P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.002$   
 $\Delta\rho_{\text{max}} = 0.13$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.13$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

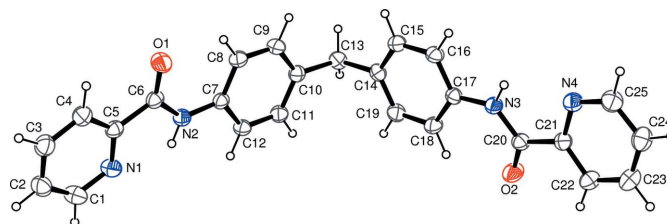
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2B\cdots N1$	0.896 (20)	2.125 (19)	2.641 (2)	115.8 (14)
$N3-H3B\cdots N4$	0.920 (19)	2.187 (14)	2.669 (2)	111.8 (13)
$N3-H3B\cdots O1^i$	0.920 (19)	2.367 (18)	3.162 (2)	144.6 (14)

Symmetry code: (i)  $-x, -y + 1, -z$ .

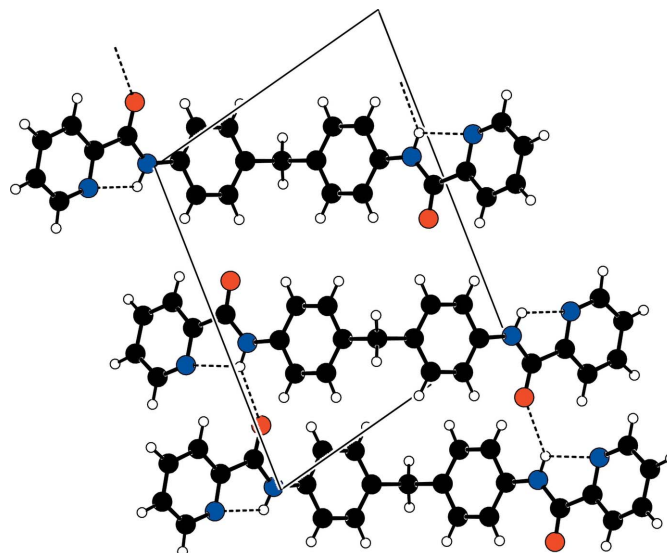
All H atoms were located in a difference synthesis and refined isotropically [ $C-H = 0.929$  (18)– $1.009$  (17) Å and  $N-H = 0.896$  (18)– $0.919$  (17) Å].

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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



**Figure 2**  
 A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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