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2-(4-Pyridyl)pyrrolo[3,2-*h*]quinoline

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Key indicators

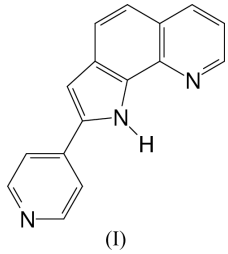
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.109
Data-to-parameter ratio = 11.8

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

The structure of the title compound, $C_{32}H_{22}N_6$, comprises two unique molecules that associate *via* N—H···N interactions to form a single convoluted hydrogen-bonded polymer chain. The dihedral angles between the indole rings and the substituted pyridyl rings are 13.43 (14) and 22.34 (12) Å.

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from an ethanol solution.



(I)

Crystal data

$C_{32}H_{22}N_6$
M_r = 490.56
Monoclinic, $P2_1/n$
a = 19.3539 (8) Å
b = 6.8609 (3) Å
c = 19.3579 (8) Å
β = 112.325 (2)°
V = 2377.77 (17) Å^3
Z = 4
D_x = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8137 reflections
θ = 2.9–30.5°
μ = 0.08 mm^{-1}
T = 150 (2) K
Prism, colourless
0.28 × 0.12 × 0.04 mm

Data collection

Enraf–Nonius KappaCCD area detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.977, T_{max} = 0.997
11 617 measured reflections
4179 independent reflections
3199 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 25.0°
$h = -22 \rightarrow 22$
$k = -8 \rightarrow 8$
$l = -23 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 0.89
4179 reflections
353 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.0087 (13)

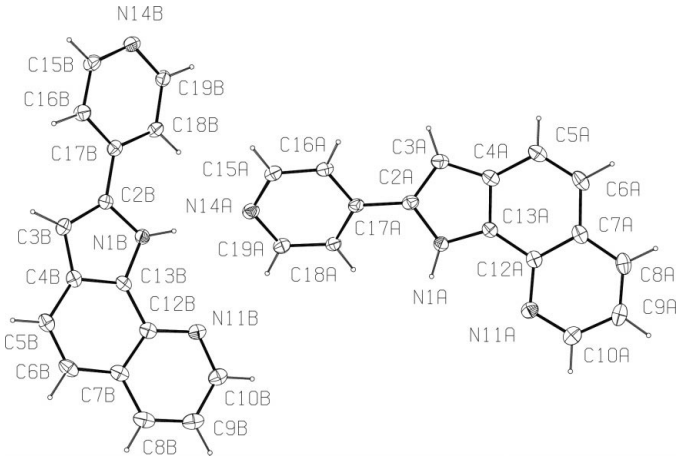


Figure 1
The mlecular configuration and atom-numbering scheme for (I), showing 30% probability ellipsoids.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···N14*B*	0.92 (3)	2.18 (3)	3.100 (3)	173 (3)
N1*B*—H1*B*···N14*A*^{i}	0.87 (3)	2.12 (3)	2.982 (3)	171 (3)
C18*A*—H18*A*···N14*B*	0.95	2.61	3.376 (3)	138
C18*B*—H18*B*···N14*A*^{i}	0.95	2.57	3.350 (3)	139
C19*B*—H19*B*···N11*A*	0.95	2.55	3.289 (4)	135

Symmetry code: (i) $x-\frac{1}{2},\frac{1}{2}-y,z-\frac{1}{2}$.

All H atoms were included in the refinement at calculated positions as riding models, with C—H set to 0.95 Å, except for the indole NH group, which was located on difference syntheses and for which both positional and displacement parameters were refined. The unit cell for (I) was initially determined as orthorhombic C [a = 21.5564 (8), b = 32.161 (1), c = 6.8627 (4) Å], but it was not possible to obtain a solution in this setting. The structure was eventually solved as primitive monoclinic in $P2_1/n$. However, the refinement was poor, $R1$ was around 26% and the ellipsoids were unreasonable. It was noted that a and c were approximately equal in length and the structure was refined as a pseudo-merohedral twin (twin law: 001, 010, 100). This resulted in a final $R1$ value of 4.4%, sensible ellipsoids and a twin component of 0.46 (1).

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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