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N-(8-Quinolylamino)phthalimide

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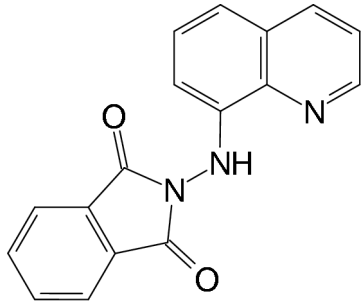
The structure of the title compound, $C_{17}H_{11}N_3O_2$, (I), comprises twisted molecules that associate *via* a single N—H···O intermolecular interaction, forming a linear one-dimensional hydrogen-bonded chain. The dihedral angle between the two ring systems is 89.9 (1)°.

Experimental

Crystals of (I) were obtained from Spa Contract Synthesis.



(I)

Crystal data

$C_{17}H_{11}N_3O_2$
M_r = 289.29
Orthorhombic, $Pca2_1$
a = 16.397 (3) Å
b = 10.819 (2) Å
c = 7.6737 (15) Å
V = 1361.4 (5) Å^3
Z = 4
D_x = 1.411 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4257 reflections
θ = 1.0–27.5°
μ = 0.10 mm^{-1}
T = 150 (2) K
Needle, yellow
0.26 × 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} = 0.976, T_{max} = 0.996
8737 measured reflections
1676 independent reflections
1350 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 27.5°
$h = -21 \rightarrow 19$
$k = -14 \rightarrow 13$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.099
S = 1.18
1676 reflections
204 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0490P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.060 (5)

Key indicators

Single-crystal X-ray study
T = 151 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.099
Data-to-parameter ratio = 8.2

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N81—H81···O11^{i}	0.90 (3)	2.50 (3)	3.081 (3)	123 (2)
N81—H81···N1^{ii}	0.90 (3)	2.28 (3)	2.712 (3)	109 (2)
C17—H17···N1^{iii}	0.95	2.39	3.316 (4)	166

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

All H atoms were included in the refinement at calculated positions as riding models, with C—H set to 0.95 Å (Ar-H), except for the amine H atom, which was located on the difference syntheses and for which both positional and displacement parameters were refined. The number of Friedal pairs is 1341.

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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