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8-(2-Phenylethylamino)quinoline

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The structure of the title compound, $C_{17}H_{16}N_2$, (I), comprises twisted molecules that contain a single intramolecular N—H···N hydrogen-bonding interaction. The dihedral angle between the two ring systems is 65.72 (4)°.

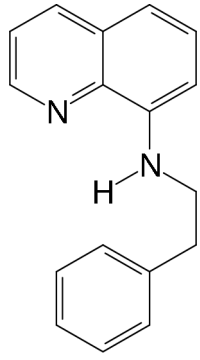
Key indicators

Single-crystal X-ray study
T = 151 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.126
Data-to-parameter ratio = 17.0

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

Experimental

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



(I)

Crystal data

$C_{17}H_{16}N_2$
M_r = 248.32
Monoclinic, $P2_1/n$
a = 10.1202 (3) Å
b = 9.9645 (3) Å
c = 13.8592 (5) Å
β = 110.7743 (11)°
V = 1306.73 (7) Å^3
Z = 4
D_x = 1.262 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11683 reflections
θ = 2.9–38.6°
μ = 0.08 mm^{-1}
T = 150 (2) K
Plate, colourless
0.30 × 0.15 × 0.08 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.978, T_{max} = 0.994
18 654 measured reflections
2989 independent reflections
2065 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 18$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.126
S = 1.03
2989 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11···N1	0.929 (15)	2.277 (15)	2.6961 (15)	106.8 (12)

All H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.95 (Ar–H) and 0.99 Å (CH_2), except for the amine H atom, which was located on difference syntheses and both positional and thermal parameters refined.

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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