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N-Phenylquinoline-2-carboxamide

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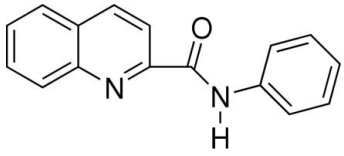
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 8.5.

In the title compound, $C_{16}H_{12}N_2O$, the dihedral angle between the quinoline ring system and the phenyl ring is 6.8 (1)°. Weak N—H···N and C—H···O intramolecular hydrogen bonds are present.

Related literature

For general background, see: Matarrese *et al.* (2001); Perlepes *et al.* (1986). For synthesis, see: Davis (1959).



Experimental

Crystal data

$C_{16}H_{12}N_2O$
M_r = 248.28
Orthorhombic, $Pna2_1$
a = 16.9856 (19) Å
b = 12.8279 (16) Å
c = 5.4455 (7) Å
V = 1186.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
0.52 × 0.30 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
11138 measured reflections
1494 independent reflections
1306 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 1.01
1494 reflections
176 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···N1	0.93 (3)	2.19 (3)	2.674 (3)	111 (2)
C17—H17···O1	0.95	2.26	2.889 (3)	123

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2426).

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supplementary materials

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N-Phenylquinoline-2-carboxamide

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Comment

Quinoline-2-carboxamide compounds are a class of important materials as metal ligands (Perlepes *et al.*, 1986) and as potential radioligands for visualization of peripheral benzodiazepine receptors (Matarrese *et al.*, 2001). We report here the crystal structure of the title compound, (I).

The O1—C11 [1.223 (3) Å], N2—C11 [1.365 (3) Å] and N2—C12 [1.412 (3) Å] bond lengths indicate extensive electron delocalization in the amide linkage. The quinoline ring system is planar within ±0.013 (2) Å. The dihedral angle between the C2/C3/C4/C9/C10/N1 and C2/C11/O1/N2 planes is 4.6 (1)° and that between C2/C11/O1/N2 and C12—C17 planes is 2.5 (1)° (Fig 1). The dihedral angle between the quinoline ring system and phenyl ring is 6.8 (1)°. Weak N—H···N and C—H···O hydrogen bonds are observed in the molecular structure (Table 1).

Experimental

The title compound was synthesized from 2-quinolinecarboxylic acid and aniline according to the general procedure of Davis (1959). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from dimethylsulfoxide.

Refinement

The N-bound H atom was located in a difference Fourier map and refined isotropically [N—H = 0.93 (3) Å]. C-bound H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

Figures

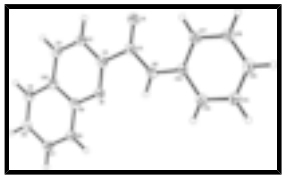

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

N-Phenylquinoline-2-carboxamide

Crystal data

$C_{16}H_{12}N_2O$	F_{000} = 520
M_r = 248.28	D_x = 1.390 Mg m^{-3}
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å

Hall symbol: P 2c -2n	Cell parameters from 8549 reflections
a = 16.9856 (19) Å	θ = 3.2–27.5º
b = 12.8279 (16) Å	μ = 0.09 mm^{-1}
c = 5.4455 (7) Å	T = 153 (2) K
V = 1186.5 (3) $Å^3$	Plate, colourless
Z = 4	0.52 × 0.30 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	1306 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	R_{int} = 0.069
Monochromator: graphite	θ_{max} = 27.5º
T = 153(2) K	θ_{min} = 3.2º
ω scans	h = −21→22
Absorption correction: none	k = −16→16
11138 measured reflections	l = −7→7
1494 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.108	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.01	$\Delta\rho_{max}$ = 0.15 e $Å^{-3}$
1494 reflections	$\Delta\rho_{min}$ = −0.20 e $Å^{-3}$
176 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.28453 (9)	0.31035 (13)	0.1870 (3)	0.0383 (4)
N1	0.37707 (10)	0.43801 (13)	0.6855 (4)	0.0289 (4)
N2	0.41118 (10)	0.29930 (14)	0.3349 (4)	0.0318 (4)
C2	0.31803 (12)	0.40935 (16)	0.5420 (4)	0.0300 (5)
C3	0.24023 (13)	0.44684 (16)	0.5661 (5)	0.0346 (5)
H3	0.1996	0.4227	0.4606	0.042*
C4	0.22498 (13)	0.51849 (17)	0.7444 (5)	0.0338 (5)
H4	0.1732	0.5453	0.7639	0.041*
C5	0.27477 (13)	0.62705 (17)	1.0899 (5)	0.0340 (5)
H5	0.2241	0.6566	1.1136	0.041*
C6	0.33486 (13)	0.65688 (16)	1.2390 (5)	0.0345 (5)
H6	0.3261	0.7070	1.3645	0.041*
C7	0.41086 (13)	0.61262 (15)	1.2059 (5)	0.0333 (5)
H7	0.4530	0.6330	1.3101	0.040*
C8	0.42357 (12)	0.54080 (16)	1.0248 (5)	0.0314 (5)
H8	0.4747	0.5118	1.0052	0.038*
C9	0.36231 (11)	0.50866 (16)	0.8660 (4)	0.0276 (4)
C10	0.28592 (12)	0.55297 (16)	0.9001 (4)	0.0303 (5)
C11	0.33541 (12)	0.33470 (16)	0.3353 (4)	0.0296 (5)
C12	0.44804 (12)	0.23178 (15)	0.1655 (4)	0.0307 (5)
C13	0.52679 (12)	0.20587 (15)	0.2071 (5)	0.0331 (5)
H13	0.5536	0.2332	0.3459	0.040*
C14	0.56576 (13)	0.14009 (17)	0.0450 (5)	0.0347 (5)
H14	0.6196	0.1235	0.0722	0.042*
C15	0.52686 (13)	0.09850 (17)	−0.1561 (5)	0.0364 (5)
H15	0.5534	0.0527	−0.2652	0.044*
C16	0.44909 (15)	0.12453 (16)	−0.1958 (5)	0.0368 (5)
H16	0.4224	0.0965	−0.3341	0.044*
C17	0.40915 (13)	0.19058 (17)	−0.0381 (4)	0.0339 (5)
H17	0.3556	0.2078	−0.0684	0.041*
H2N	0.4423 (14)	0.3254 (19)	0.462 (6)	0.043 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0378 (8)	0.0424 (9)	0.0347 (9)	−0.0023 (7)	−0.0050 (8)	−0.0061 (8)
N1	0.0326 (9)	0.0263 (8)	0.0280 (9)	−0.0012 (7)	0.0010 (8)	0.0025 (8)
N2	0.0349 (9)	0.0329 (10)	0.0275 (10)	−0.0001 (8)	−0.0023 (8)	−0.0049 (9)
C2	0.0327 (10)	0.0291 (9)	0.0283 (11)	−0.0021 (9)	0.0002 (9)	0.0023 (9)
C3	0.0330 (10)	0.0372 (12)	0.0337 (12)	−0.0027 (9)	−0.0046 (10)	0.0033 (10)
C4	0.0306 (10)	0.0364 (11)	0.0343 (12)	0.0036 (9)	0.0020 (9)	0.0049 (11)
C5	0.0358 (11)	0.0335 (11)	0.0329 (12)	0.0041 (9)	0.0045 (10)	0.0025 (10)
C6	0.0438 (12)	0.0273 (10)	0.0323 (12)	0.0010 (9)	0.0061 (10)	−0.0001 (10)
C7	0.0392 (12)	0.0312 (10)	0.0295 (12)	−0.0038 (9)	−0.0011 (9)	−0.0001 (10)

C8	0.0323 (11)	0.0304 (10)	0.0316 (12)	−0.0012 (9)	0.0012 (9)	0.0029 (10)
C9	0.0321 (10)	0.0254 (9)	0.0253 (10)	−0.0008 (8)	0.0042 (9)	0.0055 (9)
C10	0.0355 (11)	0.0262 (10)	0.0292 (11)	0.0003 (8)	0.0058 (9)	0.0036 (9)
C11	0.0343 (11)	0.0273 (11)	0.0271 (11)	−0.0026 (8)	0.0020 (9)	0.0030 (9)
C12	0.0399 (11)	0.0238 (10)	0.0285 (11)	0.0000 (9)	0.0005 (10)	0.0015 (9)
C13	0.0414 (12)	0.0299 (10)	0.0282 (12)	−0.0017 (9)	−0.0033 (10)	0.0015 (10)
C14	0.0373 (11)	0.0343 (11)	0.0326 (12)	0.0030 (9)	0.0009 (10)	0.0029 (10)
C15	0.0451 (12)	0.0323 (11)	0.0319 (13)	0.0057 (10)	0.0031 (10)	−0.0003 (10)
C16	0.0460 (13)	0.0360 (11)	0.0284 (12)	0.0014 (10)	−0.0040 (10)	−0.0029 (10)
C17	0.0375 (12)	0.0333 (11)	0.0309 (13)	−0.0013 (9)	−0.0038 (9)	0.0009 (10)

Geometric parameters (Å, °)

O1—C11	1.223 (3)	C7—C8	1.367 (3)
N1—C2	1.323 (3)	C7—H7	0.95
N1—C9	1.360 (3)	C8—C9	1.415 (3)
N2—C11	1.365 (3)	C8—H8	0.95
N2—C12	1.412 (3)	C9—C10	1.429 (3)
N2—H2N	0.93 (3)	C12—C17	1.395 (3)
C2—C3	1.412 (3)	C12—C13	1.397 (3)
C2—C11	1.507 (3)	C13—C14	1.389 (3)
C3—C4	1.362 (3)	C13—H13	0.95
C3—H3	0.95	C14—C15	1.386 (3)
C4—C10	1.409 (3)	C14—H14	0.95
C4—H4	0.95	C15—C16	1.380 (3)
C5—C6	1.359 (3)	C15—H15	0.95
C5—C10	1.417 (3)	C16—C17	1.384 (3)
C5—H5	0.95	C16—H16	0.95
C6—C7	1.422 (3)	C17—H17	0.95
C6—H6	0.95		
C2—N1—C9	118.18 (18)	N1—C9—C10	121.76 (19)
C11—N2—C12	128.57 (19)	C8—C9—C10	118.2 (2)
C11—N2—H2N	114.4 (15)	C4—C10—C5	123.5 (2)
C12—N2—H2N	117.0 (15)	C4—C10—C9	117.7 (2)
N1—C2—C3	124.0 (2)	C5—C10—C9	118.9 (2)
N1—C2—C11	117.99 (19)	O1—C11—N2	125.5 (2)
C3—C2—C11	117.96 (19)	O1—C11—C2	121.12 (19)
C4—C3—C2	118.3 (2)	N2—C11—C2	113.41 (19)
C4—C3—H3	120.9	C17—C12—C13	119.5 (2)
C2—C3—H3	120.9	C17—C12—N2	122.81 (19)
C3—C4—C10	120.1 (2)	C13—C12—N2	117.7 (2)
C3—C4—H4	120.0	C14—C13—C12	119.9 (2)
C10—C4—H4	120.0	C14—C13—H13	120.1
C6—C5—C10	121.6 (2)	C12—C13—H13	120.1
C6—C5—H5	119.2	C15—C14—C13	120.6 (2)
C10—C5—H5	119.2	C15—C14—H14	119.7
C5—C6—C7	119.6 (2)	C13—C14—H14	119.7
C5—C6—H6	120.2	C16—C15—C14	119.2 (2)
C7—C6—H6	120.2	C16—C15—H15	120.4

C8—C7—C6	120.3 (2)	C14—C15—H15	120.4
C8—C7—H7	119.9	C15—C16—C17	121.4 (2)
C6—C7—H7	119.9	C15—C16—H16	119.3
C7—C8—C9	121.4 (2)	C17—C16—H16	119.3
C7—C8—H8	119.3	C16—C17—C12	119.5 (2)
C9—C8—H8	119.3	C16—C17—H17	120.2
N1—C9—C8	120.03 (18)	C12—C17—H17	120.2
C9—N1—C2—C3	−0.7 (3)	N1—C9—C10—C5	−179.29 (19)
C9—N1—C2—C11	177.34 (17)	C8—C9—C10—C5	0.2 (3)
N1—C2—C3—C4	1.4 (3)	C12—N2—C11—O1	2.3 (4)
C11—C2—C3—C4	−176.62 (19)	C12—N2—C11—C2	−177.88 (19)
C2—C3—C4—C10	−0.4 (3)	N1—C2—C11—O1	−175.35 (19)
C10—C5—C6—C7	−0.4 (3)	C3—C2—C11—O1	2.8 (3)
C5—C6—C7—C8	0.2 (3)	N1—C2—C11—N2	4.8 (3)
C6—C7—C8—C9	0.1 (3)	C3—C2—C11—N2	−177.08 (19)
C2—N1—C9—C8	179.48 (19)	C11—N2—C12—C17	0.6 (3)
C2—N1—C9—C10	−1.1 (3)	C11—N2—C12—C13	−179.2 (2)
C7—C8—C9—N1	179.17 (19)	C17—C12—C13—C14	0.4 (3)
C7—C8—C9—C10	−0.3 (3)	N2—C12—C13—C14	−179.69 (19)
C3—C4—C10—C5	−179.9 (2)	C12—C13—C14—C15	−1.0 (3)
C3—C4—C10—C9	−1.2 (3)	C13—C14—C15—C16	1.0 (3)
C6—C5—C10—C4	178.8 (2)	C14—C15—C16—C17	−0.5 (3)
C6—C5—C10—C9	0.1 (3)	C15—C16—C17—C12	−0.1 (3)
N1—C9—C10—C4	2.0 (3)	C13—C12—C17—C16	0.1 (3)
C8—C9—C10—C4	−178.54 (19)	N2—C12—C17—C16	−179.76 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···N1	0.93 (3)	2.19 (3)	2.674 (3)	111 (2)
C17—H17···O1	0.95	2.26	2.889 (3)	123

Fig. 1