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6-(4-Nitrobenzyloxy)quinoline

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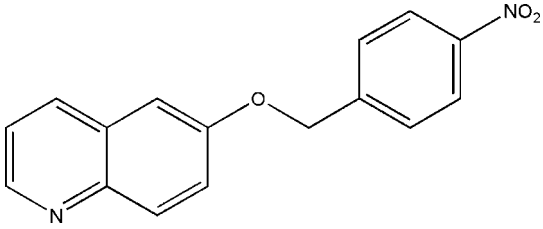
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.065; wR factor = 0.152; data-to-parameter ratio = 13.8.

In the molecule of the title compound, $C_{16}H_{12}N_2O_3$, the nitrobenzene benzene ring forms a dihedral angle of 23.8 (8)° with the plane of the quinoline ring system. The crystal structure is stabilized by an aromatic π–π stacking interaction between centrosymmetrically related benzene rings [centroid–centroid distance 3.663 (2) Å].

Related literature

For related structures, see: Fu & Zhao (2007); Li & Chen (2008); Zhao (2008); Zhao *et al.* (2009).



Experimental

Crystal data

$C_{16}H_{12}N_2O_3$
M_r = 280.28
Monoclinic, $P2_1/n$
a = 12.296 (3) Å
b = 8.9146 (18) Å
c = 13.559 (3) Å
β = 115.25 (3)°
V = 1344.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.20 × 0.18 × 0.15 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.976, T_{max} = 0.981
11965 measured reflections
2630 independent reflections
1372 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.152
S = 1.02
2630 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2340).

References

Fu, D.-W. & Zhao, H. (2007). *Acta Cryst.* E**63**, o3206.
Li, M. & Chen, X. (2008). *Acta Cryst.* E**64**, o2291.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhao, Y.-Y. (2008). *Acta Cryst.* E**64**, o761.
Zhao, M. M., Li, Y. H., Wu, D. H. & Wan, Q. (2009). *Acta Cryst.* E**65**, o1261.

supplementary materials

Acta Cryst. (2009). E**65**, o1795 [**doi:10.1107/S1600536809025823**]

6-(4-Nitrobenzyloxy)quinoline

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Comment

Recently, we have reported the synthesis and crystal structure of some benzonitrile compounds (Fu & Zhao, 2007; Li & Chen, 2008; Zhao, 2008; Zhao *et al.*, 2009). As an extension of our work on the structural characterization of benzonitrile derivatives, we present herein the synthesis and crystal structure of the title compound.

In the molecule of the title compound (Fig. 1), bond lengths and angles are within normal ranges. The C11–C16 benzene ring forms a dihedral angle of 23.8 (8)° with the plane of the quinoline ring system. No intra- or intermolecular hydrogen bonds are observed. The crystal structure is stabilized by an aromatic π-π stacking interaction involving centrosymmetrically related benzene rings at (x, y, z) and (1-x, -y, 1-z), with a centroid-centroid distance of 3.663 (2) Å.

Experimental

Quinolin-6-ol (1 g,0.0069 mol) was added to a solution of sodium hydroxide (0.276 g, 0.0069 mol) in methanol (15 ml) and stirred for one hour. Then 4-(bromomethyl)benzonitrile (1.49 g, 0.0069 mol) was added and the mixture stirred at room temperature for 1 day. The title compound was isolated by column chromatography using petroleum ether/ethyl acetate (1:1 v/v) as eluent. Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethyl acetate/tetrahydrofuran (3:1 v/v) solution.

Refinement

All H atoms were calculated geometrically allowed to ride on their parent atoms, with C—H = 0.93-0.97 Å, and with U_{iso}(H) = 1.2U_{eq} (C).

Figures

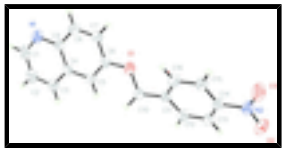

Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

6-(4-Nitrobenzyloxy)quinoline

Crystal data

$C_{16}H_{12}N_2O_3$	F_{000} = 584
M_r = 280.28	D_x = 1.385 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å

Hall symbol: -P 2yn	Cell parameters from 8689 reflections
a = 12.296 (3) Å	θ = 3.0–27.8º
b = 8.9146 (18) Å	μ = 0.10 mm^{-1}
c = 13.559 (3) Å	T = 293 K
β = 115.25 (3)º	Block, colourless
V = 1344.3 (6) $Å^3$	0.20 × 0.18 × 0.15 mm
Z = 4	

Data collection

Rigaku SCXmini diffractometer	2630 independent reflections
Radiation source: fine-focus sealed tube	1372 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.079
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 26.0º
T = 293 K	θ_{min} = 3.3º
CCD profile fitting scans	h = −15→15
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −10→10
T_{min} = 0.976, T_{max} = 0.981	l = −16→16
11965 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.065	H-atom parameters constrained
$wR(F^2)$ = 0.152	$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.1856P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
2630 reflections	$\Delta\rho_{max}$ = 0.15 e $Å^{-3}$
190 parameters	$\Delta\rho_{min}$ = −0.15 e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > \sigma(F^2)$ 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}
C1	0.3786 (4)	0.3414 (4)	−0.1994 (3)	0.0901 (11)
H1A	0.3497	0.3839	−0.2686	0.108*
C2	0.4967 (4)	0.3728 (4)	−0.1275 (3)	0.0881 (11)
H2A	0.5444	0.4336	−0.1487	0.106*
C3	0.5411 (3)	0.3132 (4)	−0.0257 (3)	0.0735 (9)
H3A	0.6202	0.3321	0.0235	0.088*
C4	0.4671 (3)	0.2230 (3)	0.0046 (2)	0.0542 (7)
C5	0.5069 (2)	0.1580 (3)	0.1090 (2)	0.0557 (7)
H5A	0.5847	0.1750	0.1616	0.067*
C6	0.4303 (3)	0.0705 (3)	0.1319 (2)	0.0555 (8)
C7	0.3126 (3)	0.0454 (3)	0.0539 (2)	0.0657 (8)
H7A	0.2613	−0.0147	0.0711	0.079*
C8	0.2730 (3)	0.1074 (3)	−0.0460 (2)	0.0650 (8)
H8A	0.1943	0.0902	−0.0967	0.078*
C9	0.3483 (3)	0.1972 (3)	−0.0747 (2)	0.0572 (8)
C10	0.5763 (2)	0.0164 (3)	0.3124 (2)	0.0597 (8)
H10A	0.5943	0.1212	0.3318	0.072*
H10B	0.6332	−0.0211	0.2861	0.072*
C11	0.5866 (2)	−0.0718 (3)	0.4102 (2)	0.0502 (7)
C12	0.6722 (3)	−0.0323 (3)	0.5119 (2)	0.0620 (8)
H12A	0.7211	0.0504	0.5189	0.074*
C13	0.6870 (3)	−0.1124 (3)	0.6032 (2)	0.0605 (8)
H13A	0.7456	−0.0855	0.6715	0.073*
C14	0.6139 (2)	−0.2321 (3)	0.5916 (2)	0.0504 (7)
C15	0.5270 (3)	−0.2749 (3)	0.4919 (2)	0.0607 (8)
H15A	0.4777	−0.3568	0.4859	0.073*
C16	0.5142 (3)	−0.1945 (3)	0.4008 (2)	0.0627 (8)
H16A	0.4565	−0.2231	0.3325	0.075*
N1	0.3048 (2)	0.2567 (3)	−0.1773 (2)	0.0782 (8)
N2	0.6285 (3)	−0.3179 (3)	0.6883 (2)	0.0655 (7)
O1	0.45682 (16)	0.0016 (2)	0.22964 (15)	0.0699 (6)
O2	0.7111 (2)	−0.2867 (3)	0.77502 (18)	0.0885 (8)
O3	0.5578 (2)	−0.4184 (3)	0.67829 (19)	0.1026 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.105 (3)	0.111 (3)	0.062 (2)	0.029 (3)	0.043 (2)	0.032 (2)
C2	0.096 (3)	0.101 (3)	0.080 (3)	0.005 (2)	0.050 (2)	0.028 (2)
C3	0.074 (2)	0.083 (2)	0.070 (2)	0.0011 (18)	0.0365 (18)	0.0121 (19)
C4	0.0594 (18)	0.0558 (17)	0.0529 (17)	0.0062 (14)	0.0293 (15)	0.0049 (15)
C5	0.0499 (17)	0.0636 (19)	0.0504 (17)	0.0014 (14)	0.0182 (14)	0.0028 (15)
C6	0.0569 (18)	0.0606 (19)	0.0488 (17)	0.0038 (15)	0.0224 (15)	0.0096 (15)
C7	0.0593 (19)	0.075 (2)	0.061 (2)	−0.0085 (16)	0.0246 (17)	0.0075 (17)

C8	0.0535 (18)	0.078 (2)	0.0564 (19)	−0.0016 (16)	0.0167 (16)	−0.0063 (17)
C9	0.0624 (19)	0.064 (2)	0.0458 (17)	0.0152 (16)	0.0241 (15)	0.0030 (15)
C10	0.0556 (18)	0.0685 (19)	0.0551 (17)	−0.0006 (15)	0.0235 (15)	0.0073 (16)
C11	0.0513 (16)	0.0530 (17)	0.0498 (17)	0.0060 (14)	0.0249 (14)	0.0037 (14)
C12	0.065 (2)	0.0585 (19)	0.0581 (19)	−0.0059 (15)	0.0220 (16)	−0.0016 (16)
C13	0.0649 (19)	0.063 (2)	0.0443 (17)	0.0002 (16)	0.0144 (15)	−0.0018 (15)
C14	0.0552 (17)	0.0486 (17)	0.0475 (17)	0.0149 (14)	0.0219 (14)	0.0077 (14)
C15	0.0610 (18)	0.0558 (18)	0.0592 (19)	−0.0042 (14)	0.0196 (16)	0.0100 (16)
C16	0.0626 (19)	0.064 (2)	0.0515 (17)	−0.0022 (16)	0.0150 (15)	0.0042 (16)
N1	0.081 (2)	0.097 (2)	0.0538 (16)	0.0222 (16)	0.0264 (15)	0.0179 (15)
N2	0.0721 (18)	0.0630 (18)	0.0608 (18)	0.0157 (15)	0.0278 (15)	0.0106 (15)
O1	0.0584 (13)	0.0896 (15)	0.0573 (13)	−0.0055 (11)	0.0204 (11)	0.0238 (11)
O2	0.0970 (18)	0.0955 (18)	0.0544 (13)	0.0180 (14)	0.0145 (13)	0.0151 (13)
O3	0.114 (2)	0.106 (2)	0.0789 (17)	−0.0218 (17)	0.0334 (15)	0.0297 (15)

Geometric parameters (Å, °)

C1—N1	1.310 (4)	C10—O1	1.425 (3)
C1—C2	1.389 (4)	C10—C11	1.500 (3)
C1—H1A	0.9300	C10—H10A	0.9700
C2—C3	1.358 (4)	C10—H10B	0.9700
C2—H2A	0.9300	C11—C12	1.377 (4)
C3—C4	1.402 (4)	C11—C16	1.382 (4)
C3—H3A	0.9300	C12—C13	1.373 (4)
C4—C5	1.410 (4)	C12—H12A	0.9300
C4—C9	1.415 (4)	C13—C14	1.360 (4)
C5—C6	1.357 (4)	C13—H13A	0.9300
C5—H5A	0.9300	C14—C15	1.372 (4)
C6—O1	1.368 (3)	C14—N2	1.461 (3)
C6—C7	1.399 (4)	C15—C16	1.378 (4)
C7—C8	1.346 (4)	C15—H15A	0.9300
C7—H7A	0.9300	C16—H16A	0.9300
C8—C9	1.399 (4)	N2—O2	1.214 (3)
C8—H8A	0.9300	N2—O3	1.215 (3)
C9—N1	1.367 (3)		
N1—C1—C2	125.1 (3)	O1—C10—H10A	110.0
N1—C1—H1A	117.5	C11—C10—H10A	110.0
C2—C1—H1A	117.5	O1—C10—H10B	110.0
C3—C2—C1	118.8 (3)	C11—C10—H10B	110.0
C3—C2—H2A	120.6	H10A—C10—H10B	108.4
C1—C2—H2A	120.6	C12—C11—C16	118.8 (3)
C2—C3—C4	119.5 (3)	C12—C11—C10	119.4 (3)
C2—C3—H3A	120.2	C16—C11—C10	121.7 (3)
C4—C3—H3A	120.2	C13—C12—C11	121.4 (3)
C3—C4—C5	122.6 (3)	C13—C12—H12A	119.3
C3—C4—C9	117.4 (3)	C11—C12—H12A	119.3
C5—C4—C9	120.0 (3)	C14—C13—C12	118.5 (3)
C6—C5—C4	119.2 (3)	C14—C13—H13A	120.8
C6—C5—H5A	120.4	C12—C13—H13A	120.8

C4—C5—H5A	120.4	C13—C14—C15	122.1 (3)
C5—C6—O1	125.3 (3)	C13—C14—N2	119.0 (3)
C5—C6—C7	120.9 (3)	C15—C14—N2	119.0 (3)
O1—C6—C7	113.8 (3)	C14—C15—C16	118.8 (3)
C8—C7—C6	120.6 (3)	C14—C15—H15A	120.6
C8—C7—H7A	119.7	C16—C15—H15A	120.6
C6—C7—H7A	119.7	C15—C16—C11	120.4 (3)
C7—C8—C9	121.1 (3)	C15—C16—H16A	119.8
C7—C8—H8A	119.5	C11—C16—H16A	119.8
C9—C8—H8A	119.5	C1—N1—C9	116.6 (3)
N1—C9—C8	119.2 (3)	O2—N2—O3	122.7 (3)
N1—C9—C4	122.6 (3)	O2—N2—C14	118.8 (3)
C8—C9—C4	118.2 (3)	O3—N2—C14	118.5 (3)
O1—C10—C11	108.5 (2)	C6—O1—C10	117.5 (2)

Fig. 1