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# 6-(4-Nitrobenzyloxy)quinoline

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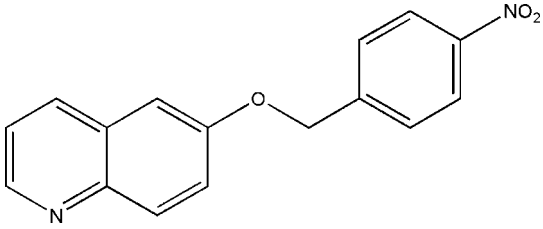
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.065; $wR$ factor = 0.152; data-to-parameter ratio = 13.8.

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 $\pi$–$\pi$ 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
$\beta$ = 115.25 (3)°
$V$ = 1344.3 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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).

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# supporting information

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

## 6-(4-Nitrobenzyloxy)quinoline

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### S1. 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 $\pi$-$\pi$ 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.

### S2. 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.

### S3. 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).

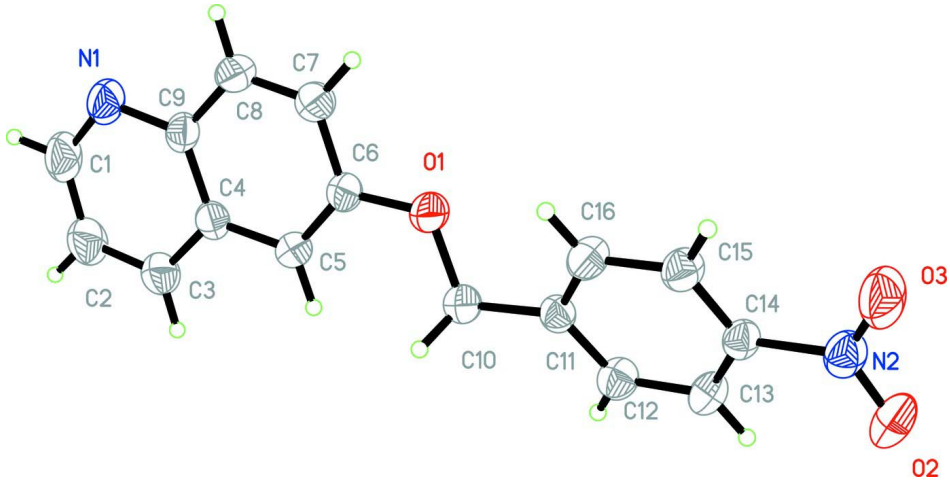


**Figure 1**

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*

$C_{16}H_{12}N_2O_3$
$M_r = 280.28$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.296$ (3) Å
$b = 8.9146$ (18) Å
$c = 13.559$ (3) Å
$\beta = 115.25$ (3)°
$V = 1344.3$ (6) Å$^3$
$Z = 4$
$F(000) = 584$
$D_x = 1.385$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8689 reflections
$\theta = 3.0$–$27.8°$
$\mu = 0.10$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.20 × 0.18 × 0.15 mm

*Data collection*

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

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.152$
$S = 1.02$
2630 reflections
190 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.1856P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ e Å$^{-3}$

*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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |