

## 6-Bromoquinoline-8-carbonitrile

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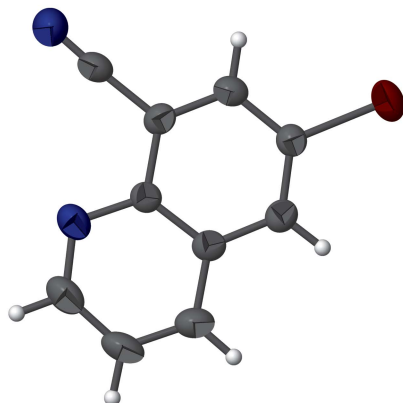
Keywords: crystal structure; quinoline ring;  $\pi$ - $\pi$  stacking interactions; synthesis.

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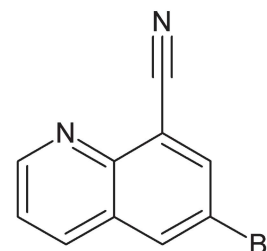
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>10</sub>H<sub>5</sub>BrN<sub>2</sub>, the whole molecule is essentially planar (r.m.s. deviation = 0.005 Å). The crystal packing features face-to-face  $\pi$ - $\pi$  stacking interactions [centroid-centroid distance = 3.755 (3) Å] between the pyridine and benzene rings of the quinoline ring systems of adjacent molecules, along the *a*-axis direction. Short Br...Br contacts of 3.5908 (12) Å (compared to a van der Waals separation of 3.70 Å) are also observed.

### 3D view



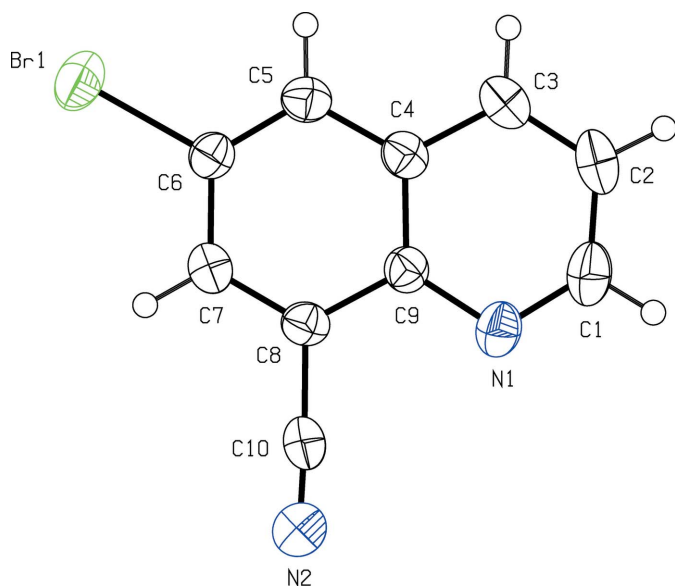
### Chemical scheme



### Structure description

The asymmetric syntheses of 2-cyano-substituted dihydro and tetrahydroquinolines have been achieved using the Reissert reaction (Pauvert *et al.*, 2005) while 8-cyano substituted quinolines have been prepared by the treatment of cyano substituted aniline with several ketones in polar solvents (Ekiz *et al.*, 2016). As the cyclization methods using cyano-substituted benzene or cyclohexane allow only the synthesis of mono cyano-substituted quinolines, the synthesis of two or more cyano-substituted quinolines has been limited (Ökten & Çakmak, 2015). As part of our studies in this area, the crystal structure of the title compound is now reported.

The title molecule (Fig. 1) is essentially planar, with a maximum deviation of 0.063 (1) Å for atom Br1. All bond lengths and angles are in normal ranges and are comparable with those reported for similar compounds: 2-chloro-8-methyl-3-[(pyrimidin-4-yloxy)methyl]quinoline (Khan *et al.*, 2010), 6,8-dibromoquinoline (Çelik *et al.*, 2010a), 3,6,8-tribromoquinoline (Çelik *et al.*, 2010b) and 5,7-dibromo-8-methoxyquinoline (Çelik *et al.*, 2017).

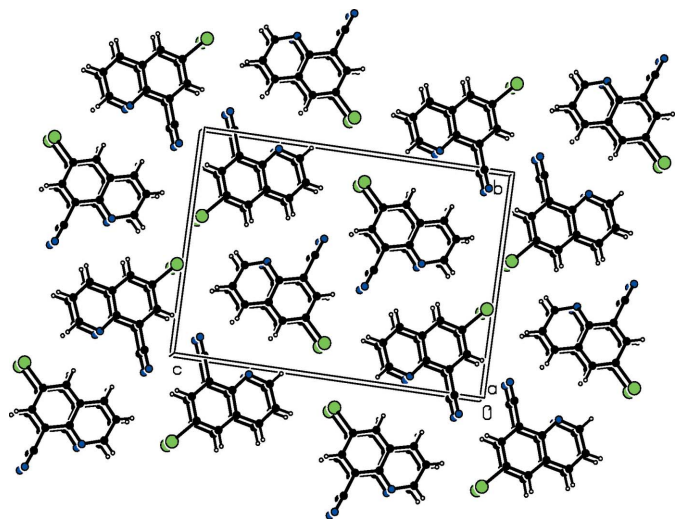


**Figure 1**  
View of the title compound, with displacement ellipsoids drawn at the 50% probability level.

In the crystal, the packing features face-to-face  $\pi$ - $\pi$  stacking interactions [ $Cg1 \cdots Cg2^i = 3.755(3) \text{ \AA}$ ; symmetry code: (i)  $-1 + x, y, z$ ] between the pyridine (N1/C1-C4/C9; centroid  $Cg1$ ) and benzene (C4-C9; centroid  $Cg2$ ) rings of the quinoline ring systems of adjacent molecules, along the  $a$ -axis direction. Short  $Br \cdots Br$  contacts [ $3.5908(12) \text{ \AA}$  compared to a van der Waals separation of  $3.70 \text{ \AA}$ ] are also observed. The packing viewed down the  $a$ -axis direction is shown in Fig. 2.

### Synthesis and crystallization

The title compound was prepared according to the reported method (Ökten *et al.*, 2013). Colourless prisms were obtained by recrystallization from mixed solvents of AcOEt/hexane (1:2).



**Figure 2**  
View of the packing of the title compound down the  $a$  axis.

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_5BrN_2$
$M_r$	233.07
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
$a, b, c$ (Å)	3.8484 (8), 12.634 (3), 18.042 (4)
$\beta$ (°)	92.918 (7)
$V$ (Å <sup>3</sup> )	876.0 (3)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	4.64
Crystal size (mm)	0.15 × 0.12 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Sheldrick, 2003)
$T_{\min}$ , $T_{\max}$	0.565, 0.746
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	26227, 2203, 1501
$R_{\text{int}}$	0.073
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.672
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.058, 0.120, 1.22
No. of reflections	2203
No. of parameters	118
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.53, -0.61

Computer programs: APEX2 and SAINT (Bruker, 2007), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), ORTEP3for Windows (Farrugia, 2012) and PLATON (Spek, 2009).

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

### Acknowledgements

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## full crystallographic data

*IUCrData* (2017). 2, x170930 [https://doi.org/10.1107/S2414314617009300]

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*Crystal data*

$C_{10}H_5BrN_2$	$F(000) = 456$
$M_r = 233.07$	$D_x = 1.767 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 3.8484 (8) \text{ \AA}$	Cell parameters from 9362 reflections
$b = 12.634 (3) \text{ \AA}$	$\theta = 3.2\text{--}25.3^\circ$
$c = 18.042 (4) \text{ \AA}$	$\mu = 4.64 \text{ mm}^{-1}$
$\beta = 92.918 (7)^\circ$	$T = 296 \text{ K}$
$V = 876.0 (3) \text{ \AA}^3$	Prism, colourless
$Z = 4$	$0.15 \times 0.12 \times 0.10 \text{ mm}$

*Data collection*

Bruker APEXII CCD diffractometer	2203 independent reflections
$\varphi$ and $\omega$ scans	1501 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$R_{\text{int}} = 0.073$
$T_{\text{min}} = 0.565$ , $T_{\text{max}} = 0.746$	$\theta_{\text{max}} = 28.5^\circ$ , $\theta_{\text{min}} = 3.2^\circ$
26227 measured reflections	$h = -4 \rightarrow 5$
	$k = -16 \rightarrow 16$
	$l = -24 \rightarrow 24$

*Refinement*

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.0088P)^2 + 3.5104P]$
$wR(F^2) = 0.120$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.22$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2203 reflections	$\Delta\rho_{\text{max}} = 0.53 \text{ e \AA}^{-3}$
118 parameters	$\Delta\rho_{\text{min}} = -0.61 \text{ e \AA}^{-3}$
0 restraints	

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0305 (16)	0.4253 (5)	0.8151 (3)	0.0491 (15)

H1	-0.0601	0.4759	0.8462	0.059*
C2	0.1004 (16)	0.3254 (5)	0.8451 (3)	0.0482 (15)
H2	0.0526	0.3104	0.8940	0.058*
C3	0.2403 (15)	0.2500 (5)	0.8014 (3)	0.0449 (14)
H3	0.2927	0.1832	0.8206	0.054*
C4	0.3047 (14)	0.2741 (4)	0.7272 (3)	0.0346 (11)
C5	0.4372 (14)	0.1998 (4)	0.6781 (3)	0.0375 (12)
H5	0.4966	0.1322	0.6948	0.045*
C6	0.4792 (14)	0.2268 (4)	0.6057 (3)	0.0339 (11)
C7	0.3995 (14)	0.3287 (4)	0.5793 (3)	0.0371 (12)
H7	0.4317	0.3460	0.5300	0.045*
C8	0.2738 (14)	0.4027 (4)	0.6266 (3)	0.0337 (11)
C9	0.2174 (13)	0.3781 (4)	0.7021 (2)	0.0332 (10)
C10	0.1862 (16)	0.5105 (5)	0.5988 (3)	0.0438 (14)
N1	0.0822 (12)	0.4542 (4)	0.7461 (2)	0.0412 (11)
N2	0.1305 (16)	0.5879 (4)	0.5762 (3)	0.0606 (15)
Br1	0.63809 (18)	0.12498 (5)	0.53862 (3)	0.0525 (2)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.052 (4)	0.058 (4)	0.038 (3)	-0.006 (3)	0.006 (3)	-0.015 (3)
C2	0.049 (4)	0.068 (4)	0.028 (3)	-0.008 (3)	0.006 (2)	-0.003 (3)
C3	0.049 (4)	0.050 (3)	0.035 (3)	-0.003 (3)	0.002 (2)	0.008 (2)
C4	0.035 (3)	0.036 (3)	0.031 (2)	-0.005 (2)	-0.004 (2)	0.000 (2)
C5	0.039 (3)	0.033 (3)	0.040 (3)	-0.002 (2)	0.001 (2)	0.002 (2)
C6	0.033 (3)	0.033 (3)	0.035 (2)	-0.002 (2)	0.001 (2)	-0.003 (2)
C7	0.037 (3)	0.043 (3)	0.031 (2)	-0.001 (2)	0.003 (2)	0.001 (2)
C8	0.037 (3)	0.030 (3)	0.034 (2)	-0.004 (2)	-0.004 (2)	0.0005 (19)
C9	0.036 (3)	0.033 (2)	0.031 (2)	-0.003 (2)	0.0006 (19)	-0.002 (2)
C10	0.056 (4)	0.047 (3)	0.029 (2)	0.002 (3)	0.007 (2)	-0.001 (2)
N1	0.043 (3)	0.043 (3)	0.038 (2)	-0.004 (2)	0.004 (2)	-0.0097 (19)
N2	0.085 (5)	0.047 (3)	0.051 (3)	0.010 (3)	0.011 (3)	-0.001 (2)
Br1	0.0572 (4)	0.0517 (4)	0.0490 (3)	0.0076 (3)	0.0052 (2)	-0.0145 (3)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

C1—N1	1.321 (7)	C5—H5	0.9300
C1—C2	1.394 (8)	C6—C7	1.401 (7)
C1—H1	0.9300	C6—Br1	1.889 (5)
C2—C3	1.364 (8)	C7—C8	1.371 (7)
C2—H2	0.9300	C7—H7	0.9300
C3—C4	1.408 (7)	C8—C9	1.425 (6)
C3—H3	0.9300	C8—C10	1.484 (7)
C4—C5	1.404 (7)	C9—N1	1.366 (6)
C4—C9	1.425 (7)	C10—N2	1.077 (7)
C5—C6	1.368 (7)		

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N1—C1—C2	125.5 (5)	C5—C6—C7	121.3 (5)
N1—C1—H1	117.3	C5—C6—Br1	120.0 (4)
C2—C1—H1	117.3	C7—C6—Br1	118.7 (4)
C3—C2—C1	118.8 (5)	C8—C7—C6	119.5 (4)
C3—C2—H2	120.6	C8—C7—H7	120.2
C1—C2—H2	120.6	C6—C7—H7	120.2
C2—C3—C4	119.5 (5)	C7—C8—C9	121.5 (4)
C2—C3—H3	120.3	C7—C8—C10	119.8 (4)
C4—C3—H3	120.3	C9—C8—C10	118.7 (4)
C5—C4—C3	122.9 (5)	N1—C9—C8	118.9 (4)
C5—C4—C9	120.2 (4)	N1—C9—C4	123.7 (4)
C3—C4—C9	116.8 (5)	C8—C9—C4	117.4 (4)
C6—C5—C4	120.0 (5)	N2—C10—C8	177.0 (6)
C6—C5—H5	120.0	C1—N1—C9	115.7 (5)
C4—C5—H5	120.0		
N1—C1—C2—C3	1.4 (10)	C7—C8—C9—N1	-178.1 (5)
C1—C2—C3—C4	-1.1 (9)	C10—C8—C9—N1	0.5 (7)
C2—C3—C4—C5	-177.9 (5)	C7—C8—C9—C4	1.5 (8)
C2—C3—C4—C9	0.0 (8)	C10—C8—C9—C4	-179.9 (5)
C3—C4—C5—C6	177.0 (5)	C5—C4—C9—N1	178.9 (5)
C9—C4—C5—C6	-0.8 (8)	C3—C4—C9—N1	1.0 (8)
C4—C5—C6—C7	1.5 (8)	C5—C4—C9—C8	-0.6 (7)
C4—C5—C6—Br1	-177.2 (4)	C3—C4—C9—C8	-178.6 (5)
C5—C6—C7—C8	-0.6 (8)	C2—C1—N1—C9	-0.4 (9)
Br1—C6—C7—C8	178.0 (4)	C8—C9—N1—C1	178.8 (5)
C6—C7—C8—C9	-0.9 (8)	C4—C9—N1—C1	-0.8 (8)
C6—C7—C8—C10	-179.5 (5)		

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