

## 4-(4-Chlorophenyl)-2,6-diphenylpyridine

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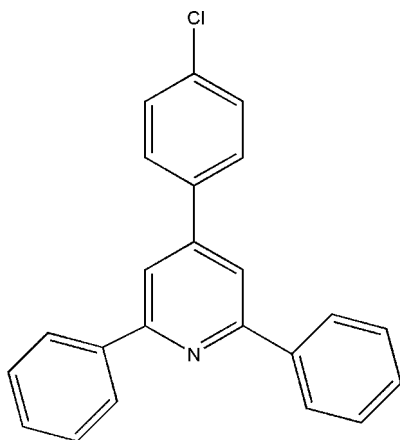
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.135; data-to-parameter ratio = 13.6.

In the title compound,  $\text{C}_{23}\text{H}_{16}\text{ClN}$ , the crystal packing exhibits no significantly short intermolecular contacts. The benzene rings show a disrotatory arrangement and the angles between them and the pyridine ring range from 20.80 (3) to 37.56 (4)°. The Cl atom deviates by 0.01 (3) Å from the plane of the benzene ring to which it is attached.

### Related literature

For the structure of 2,4,6-triphenylpyridine, see: Ondracek *et al.* (1994).



### Experimental

#### Crystal data

$\text{C}_{23}\text{H}_{16}\text{ClN}$	$V = 1756.4$ (3) Å <sup>3</sup>
$M_r = 341.82$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 9.3995$ (11) Å	$\mu = 0.22$ mm <sup>-1</sup>
$b = 20.621$ (2) Å	$T = 298$ (2) K
$c = 9.5362$ (12) Å	$0.42 \times 0.37 \times 0.15$ mm
$\beta = 108.146$ (2)°	

#### Data collection

Bruker SMART CCD area-detector diffractometer	8674 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3078 independent reflections
$T_{\min} = 0.913$ , $T_{\max} = 0.968$	1752 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.045$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	226 parameters
$wR(F^2) = 0.135$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.18$ e Å <sup>-3</sup>
3078 reflections	$\Delta\rho_{\text{min}} = -0.24$ e Å <sup>-3</sup>

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AV2004).

### References

- Ondracek, J., Novotný, J., Petru, M., Lhoták, P. & Kuthan, J. (1994). *Acta Cryst.* **C50**, 1809–1811.  
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.  
Sheldrick, G. M. (1997b). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.  
Siemens (1996). SMART and SAINT. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

**supplementary materials**

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### Comment

In this paper, we present a new crystal, 4-(4-chlorophenyl)-2,6-diphenylpyridine, (I). In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in reported the compound (Ondracek *et al.*, 1994).

The three phenyl rings display a disrotatory conformation and form different angles with the pyridine ring. The phenyl ring attached at C1 forms the smallest angle with the heterocycle, 20.8°, because there is only the free electron pair of the N atom and one H atom in the *ortho* positions. The angle formed by the phenyl ring attached at C5 is slightly larger – 22.39°. The remaining phenyl ring forms the largest angle with the heterocycle, 37.56°. Meanwhile, the crystal packing demonstrates no significantly short intermolecular contacts.

### Experimental

4-chlorobenzaldehyde (0.3 mmol) and acetophenone (0.6 mmol) under boron trifluoride ether (0.1 mmol) as a catalyst, the mixture was mixed in 50 ml flask. After irradiating for 3 min at 375 W, the mixture was cooled slowly to room temperature and the title compound was then recrystallized from ethanol, affording the title compound as a colorless crystalline solid. Elemental analysis: calculated for C<sub>23</sub>H<sub>16</sub>ClN: C 80.81, H 4.72, N 4.10%; found: C 80.68, H 4.75, N 4.14%.

### Refinement

All H atoms were positioned geometrically, with C—H=0.93–0.98 Å, and refined as riding, with  $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$ .

### Figures

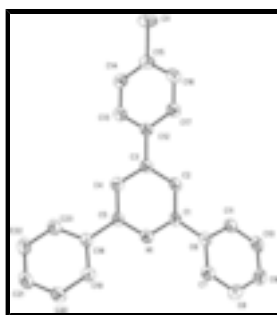


Fig. 1. ORTEP drawing of the title compound with atom numbering scheme and thermal ellipsoids at 30% probability level.

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### Crystal data

C<sub>23</sub>H<sub>16</sub>ClN

$F_{000} = 712$

# supplementary materials

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$M_r = 341.82$

Monoclinic,  $P2(1)/c$

$a = 9.3995$  (11) Å

$b = 20.621$  (2) Å

$c = 9.5362$  (12) Å

$\beta = 108.146$  (2)°

$V = 1756.4$  (3) Å<sup>3</sup>

$Z = 4$

$D_x = 1.293$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 1970 reflections

$\theta = 2.3$ – $25.2$ °

$\mu = 0.22$  mm<sup>-1</sup>

$T = 298$  (2) K

Block, colourless

$0.42 \times 0.37 \times 0.15$  mm

## Data collection

Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

phi and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.913$ ,  $T_{\max} = 0.968$

8674 measured reflections

3078 independent reflections

1752 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\text{max}} = 25.0$ °

$\theta_{\text{min}} = 2.0$ °

$h = -7 \rightarrow 11$

$k = -24 \rightarrow 24$

$l = -11 \rightarrow 11$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.135$

$S = 1.02$

3078 reflections

226 parameters

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

$$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.2473P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.18$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>

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  $F^2 > 2\sigma(F^2)$  is used only for calculat-

ing  $R$ -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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.16106 (10)	0.55491 (4)	0.64505 (11)	0.0785 (4)
N1	0.5484 (2)	0.17758 (10)	0.9845 (2)	0.0446 (6)
C1	0.4223 (3)	0.18225 (12)	0.8698 (3)	0.0416 (7)
C2	0.3630 (3)	0.24170 (13)	0.8142 (3)	0.0448 (7)
H2	0.2764	0.2434	0.7337	0.054*
C3	0.4310 (3)	0.29874 (12)	0.8770 (3)	0.0431 (7)
C4	0.5590 (3)	0.29302 (13)	0.9955 (3)	0.0480 (7)
H4	0.6078	0.3301	1.0417	0.058*
C5	0.6160 (3)	0.23244 (13)	1.0465 (3)	0.0438 (7)
C6	0.3495 (3)	0.12018 (13)	0.8094 (3)	0.0438 (7)
C7	0.4301 (3)	0.06274 (13)	0.8358 (3)	0.0527 (8)
H7	0.5311	0.0635	0.8906	0.063*
C8	0.3629 (4)	0.00434 (15)	0.7821 (4)	0.0632 (9)
H8	0.4184	-0.0338	0.8006	0.076*
C9	0.2147 (4)	0.00284 (16)	0.7020 (4)	0.0645 (9)
H9	0.1695	-0.0364	0.6656	0.077*
C10	0.1321 (3)	0.05869 (16)	0.6747 (3)	0.0624 (9)
H10	0.0312	0.0573	0.6200	0.075*
C11	0.1988 (3)	0.11723 (14)	0.7284 (3)	0.0526 (8)
H11	0.1420	0.1550	0.7100	0.063*
C12	0.3669 (3)	0.36252 (12)	0.8200 (3)	0.0427 (7)
C13	0.3699 (3)	0.41388 (13)	0.9151 (3)	0.0508 (8)
H13	0.4152	0.4085	1.0160	0.061*
C14	0.3061 (3)	0.47293 (14)	0.8612 (4)	0.0546 (8)
H14	0.3076	0.5070	0.9256	0.066*
C15	0.2407 (3)	0.48093 (13)	0.7123 (4)	0.0500 (8)
C16	0.2377 (3)	0.43147 (14)	0.6161 (3)	0.0532 (8)
H16	0.1939	0.4376	0.5152	0.064*
C17	0.3001 (3)	0.37246 (13)	0.6697 (3)	0.0491 (8)
H17	0.2973	0.3387	0.6042	0.059*
C18	0.7568 (3)	0.22443 (13)	1.1695 (3)	0.0441 (7)
C19	0.8387 (3)	0.16759 (14)	1.1839 (3)	0.0563 (8)
H19	0.8018	0.1336	1.1187	0.068*
C20	0.9737 (3)	0.16067 (15)	1.2933 (4)	0.0633 (9)
H20	1.0271	0.1221	1.3016	0.076*
C21	1.0291 (3)	0.21002 (16)	1.3893 (4)	0.0622 (9)
H21	1.1217	0.2057	1.4614	0.075*
C22	0.9486 (4)	0.26599 (16)	1.3800 (4)	0.0684 (10)
H22	0.9851	0.2993	1.4472	0.082*
C23	0.8133 (3)	0.27280 (15)	1.2707 (4)	0.0651 (9)
H23	0.7591	0.3109	1.2652	0.078*

## supplementary materials

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	0.0786 (6)	0.0582 (5)	0.1004 (8)	0.0210 (4)	0.0301 (5)	0.0221 (5)
N1	0.0400 (14)	0.0478 (14)	0.0423 (14)	0.0003 (11)	0.0075 (11)	-0.0008 (11)
C1	0.0391 (17)	0.0479 (17)	0.0373 (17)	0.0008 (13)	0.0112 (13)	-0.0030 (13)
C2	0.0404 (17)	0.0510 (17)	0.0380 (17)	0.0031 (13)	0.0050 (13)	0.0015 (13)
C3	0.0408 (17)	0.0454 (17)	0.0411 (18)	0.0035 (13)	0.0098 (14)	0.0015 (13)
C4	0.0449 (18)	0.0458 (17)	0.0489 (19)	-0.0022 (13)	0.0080 (15)	-0.0029 (13)
C5	0.0387 (17)	0.0480 (17)	0.0432 (18)	0.0008 (13)	0.0106 (13)	-0.0014 (14)
C6	0.0407 (17)	0.0517 (17)	0.0369 (17)	-0.0026 (13)	0.0091 (13)	0.0008 (13)
C7	0.0480 (18)	0.0540 (19)	0.051 (2)	-0.0004 (15)	0.0078 (14)	-0.0045 (15)
C8	0.072 (2)	0.0497 (19)	0.066 (2)	0.0011 (16)	0.0181 (19)	-0.0051 (16)
C9	0.074 (3)	0.056 (2)	0.057 (2)	-0.0182 (18)	0.0115 (18)	-0.0064 (16)
C10	0.0508 (19)	0.075 (2)	0.052 (2)	-0.0160 (18)	0.0023 (15)	0.0003 (17)
C11	0.0493 (19)	0.0562 (19)	0.0466 (19)	-0.0013 (15)	0.0069 (15)	0.0036 (14)
C12	0.0371 (16)	0.0458 (16)	0.0428 (18)	0.0012 (12)	0.0090 (13)	0.0042 (13)
C13	0.0524 (19)	0.0510 (18)	0.0454 (19)	0.0024 (14)	0.0100 (15)	-0.0012 (14)
C14	0.058 (2)	0.0468 (18)	0.061 (2)	0.0002 (14)	0.0202 (17)	-0.0057 (15)
C15	0.0457 (18)	0.0511 (18)	0.057 (2)	0.0067 (13)	0.0215 (16)	0.0108 (15)
C16	0.0532 (19)	0.063 (2)	0.0435 (19)	0.0119 (15)	0.0147 (15)	0.0077 (15)
C17	0.0497 (18)	0.0534 (18)	0.0438 (19)	0.0077 (14)	0.0140 (14)	0.0008 (14)
C18	0.0391 (17)	0.0496 (17)	0.0411 (18)	-0.0013 (13)	0.0087 (13)	-0.0008 (13)
C19	0.051 (2)	0.0526 (19)	0.057 (2)	0.0014 (14)	0.0049 (16)	-0.0033 (15)
C20	0.047 (2)	0.062 (2)	0.070 (2)	0.0055 (15)	0.0033 (17)	0.0071 (18)
C21	0.0426 (19)	0.078 (2)	0.055 (2)	-0.0050 (17)	0.0003 (15)	0.0055 (18)
C22	0.060 (2)	0.074 (2)	0.058 (2)	-0.0034 (18)	0.0004 (17)	-0.0150 (18)
C23	0.056 (2)	0.062 (2)	0.064 (2)	0.0083 (16)	0.0000 (17)	-0.0129 (17)

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

C11—C15	1.732 (3)	C11—H11	0.9300
N1—C5	1.341 (3)	C12—C17	1.389 (4)
N1—C1	1.343 (3)	C12—C13	1.389 (4)
C1—C2	1.382 (3)	C13—C14	1.384 (4)
C1—C6	1.481 (4)	C13—H13	0.9300
C2—C3	1.382 (4)	C14—C15	1.370 (4)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.375 (4)	C15—C16	1.366 (4)
C3—C12	1.478 (3)	C16—C17	1.378 (4)
C4—C5	1.386 (3)	C16—H16	0.9300
C4—H4	0.9300	C17—H17	0.9300
C5—C18	1.479 (4)	C18—C23	1.374 (4)
C6—C7	1.386 (4)	C18—C19	1.385 (4)
C6—C11	1.387 (3)	C19—C20	1.376 (4)
C7—C8	1.382 (4)	C19—H19	0.9300
C7—H7	0.9300	C20—C21	1.359 (4)
C8—C9	1.365 (4)	C20—H20	0.9300

C8—H8	0.9300	C21—C22	1.368 (4)
C9—C10	1.368 (4)	C21—H21	0.9300
C9—H9	0.9300	C22—C23	1.378 (4)
C10—C11	1.383 (4)	C22—H22	0.9300
C10—H10	0.9300	C23—H23	0.9300
C5—N1—C1	118.4 (2)	C17—C12—C3	120.8 (2)
N1—C1—C2	121.6 (2)	C13—C12—C3	121.0 (3)
N1—C1—C6	116.0 (2)	C14—C13—C12	120.7 (3)
C2—C1—C6	122.4 (2)	C14—C13—H13	119.7
C1—C2—C3	120.8 (3)	C12—C13—H13	119.7
C1—C2—H2	119.6	C15—C14—C13	119.6 (3)
C3—C2—H2	119.6	C15—C14—H14	120.2
C4—C3—C2	116.8 (2)	C13—C14—H14	120.2
C4—C3—C12	122.0 (2)	C16—C15—C14	121.0 (3)
C2—C3—C12	121.2 (2)	C16—C15—C11	119.5 (2)
C3—C4—C5	120.6 (3)	C14—C15—C11	119.5 (2)
C3—C4—H4	119.7	C15—C16—C17	119.5 (3)
C5—C4—H4	119.7	C15—C16—H16	120.3
N1—C5—C4	121.8 (3)	C17—C16—H16	120.3
N1—C5—C18	116.1 (2)	C16—C17—C12	121.1 (3)
C4—C5—C18	122.1 (2)	C16—C17—H17	119.4
C7—C6—C11	118.0 (2)	C12—C17—H17	119.4
C7—C6—C1	120.5 (2)	C23—C18—C19	117.6 (3)
C11—C6—C1	121.5 (2)	C23—C18—C5	122.0 (3)
C8—C7—C6	121.1 (3)	C19—C18—C5	120.4 (2)
C8—C7—H7	119.5	C20—C19—C18	121.0 (3)
C6—C7—H7	119.5	C20—C19—H19	119.5
C9—C8—C7	119.8 (3)	C18—C19—H19	119.5
C9—C8—H8	120.1	C21—C20—C19	120.1 (3)
C7—C8—H8	120.1	C21—C20—H20	119.9
C8—C9—C10	120.5 (3)	C19—C20—H20	119.9
C8—C9—H9	119.8	C20—C21—C22	120.0 (3)
C10—C9—H9	119.8	C20—C21—H21	120.0
C9—C10—C11	120.0 (3)	C22—C21—H21	120.0
C9—C10—H10	120.0	C21—C22—C23	119.8 (3)
C11—C10—H10	120.0	C21—C22—H22	120.1
C10—C11—C6	120.7 (3)	C23—C22—H22	120.1
C10—C11—H11	119.6	C18—C23—C22	121.4 (3)
C6—C11—H11	119.6	C18—C23—H23	119.3
C17—C12—C13	118.1 (2)	C22—C23—H23	119.3

Fig. 1

