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4-Chloro-*N*-(2-pyridyl)aniline

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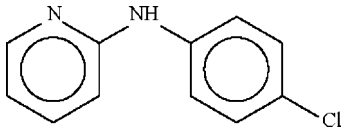
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.137; data-to-parameter ratio = 17.5.

There are two molecules in the asymmetric unit of the title compound, $C_{11}H_9ClN_2$, with dihedral angles of 41.84 (12) and 49.24 (12)° between the aromatic ring planes. The two molecules form a dimer *via* a pair of N—H···N hydrogen bonds.

Related literature

For the structures of the two modifications of *N*-(pyrazin-2-yl)aniline, see: Abdullah & Ng (2008); Wan Saffiee *et al.* (2008).



Experimental

Crystal data

$C_{11}H_9ClN_2$
M_r = 204.65
Monoclinic, $P2_1/n$
a = 15.5096 (4) Å
b = 7.5519 (2) Å
c = 17.6846 (4) Å
β = 106.284 (2)°
V = 1988.25 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 296 (2) K
0.42 × 0.06 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.870, T_{max} = 0.990
18472 measured reflections
4565 independent reflections
2369 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.137
S = 1.00
4565 reflections
261 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N4	0.87 (1)	2.16 (1)	3.018 (3)	170 (2)
N3—H3···N2	0.86 (1)	2.22 (1)	3.071 (3)	171 (2)

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2855).

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supporting information

Acta Cryst. (2008). E**64**, o2437 [doi:10.1107/S1600536808038658]

4-Chloro-*N*-(2-pyridyl)aniline

Wan Ainna Mardhiah Wan Saffiee, Azila Idris, Zaharah Aiyub, Zanariah Abdullah and Seik Weng Ng

S1. Comment

For related structures, see: Abdullah & Ng (2008); Wan Saffiee *et al.* (2008). For the molecular structure of the title compound, (I), see Fig. 1. For hydrogen bond data, see Table 1.

S2. Experimental

2-Chloropyrazine (0.11 g, 0.1 mmol) and 4-chloroaniline (0.13 g, 0.1 mmol) were heated at 423–433 K for 5 h. The mixture was cooled and dissolved in water. The solution was extracted with ether. The ether extract was dried over sodium sulfate and the solvent evaporated to yield a dark brown compound. Colourless rods of (I) were separated manually.

S3. Refinement

The carbon-bound H-atoms were placed in calculated positions (C—H = 0.95 Å) and refined as riding with U(H) = 1.2U(C). The amino H-atoms were located in a difference map, and were refined with a distance restraint of N–H = 0.88±0.01 Å.

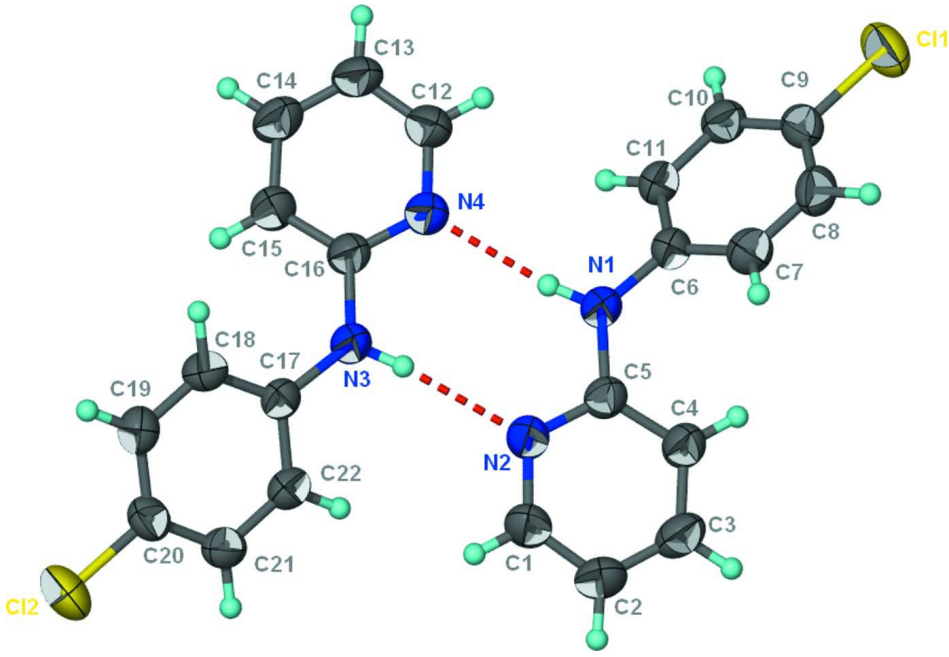

Figure 1

The molecular structure of (I) drawn at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-Chloro-*N*-(2-pyridyl)aniline

Crystal data

$C_{11}H_9ClN_2$
$M_r = 204.65$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.5096$ (4) Å
$b = 7.5519$ (2) Å
$c = 17.6846$ (4) Å
$\beta = 106.284$ (2)°
$V = 1988.25$ (9) Å^3
$Z = 8$

$F(000) = 848$
$D_x = 1.367$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2114 reflections
$\theta = 2.4$–$21.4°$
$\mu = 0.34$ mm^{-1}
$T = 296$ K
Rod, colourless
0.42 × 0.06 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.870$, $T_{max} = 0.990$

18472 measured reflections
4565 independent reflections
2369 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.6°$
$h = -20 \rightarrow 20$
$k = -9 \rightarrow 9$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.137$
$S = 1.00$
4565 reflections
261 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.3184P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.67109 (6)	0.86166 (11)	0.13818 (4)	0.0915 (3)
Cl2	0.52605 (6)	0.65436 (13)	0.94056 (4)	0.1027 (3)
N1	0.67429 (13)	0.7765 (3)	0.47124 (11)	0.0625 (5)
H1	0.6219 (9)	0.782 (3)	0.4794 (14)	0.074 (8)*
N2	0.72018 (12)	0.7057 (3)	0.60159 (11)	0.0625 (5)
N3	0.52408 (13)	0.6934 (3)	0.60693 (11)	0.0651 (6)
H3	0.5772 (9)	0.691 (3)	0.6004 (13)	0.064 (7)*
N4	0.48220 (12)	0.7816 (3)	0.47849 (11)	0.0634 (5)
C1	0.78370 (17)	0.6465 (4)	0.66437 (14)	0.0710 (7)
H1A	0.7688	0.6375	0.7116	0.085*
C2	0.86856 (17)	0.5984 (4)	0.66472 (15)	0.0743 (8)
H2	0.9099	0.5571	0.7102	0.089*
C3	0.89013 (16)	0.6137 (3)	0.59455 (15)	0.0693 (7)
H3A	0.9473	0.5828	0.5921	0.083*
C4	0.82822 (15)	0.6738 (3)	0.52878 (14)	0.0614 (6)
H4	0.8425	0.6842	0.4813	0.074*
C5	0.74264 (14)	0.7197 (3)	0.53411 (13)	0.0528 (6)
C6	0.67699 (14)	0.7960 (3)	0.39292 (12)	0.0517 (5)
C7	0.74402 (15)	0.8895 (3)	0.37290 (14)	0.0626 (6)
H7	0.7902	0.9407	0.4122	0.075*
C8	0.74268 (16)	0.9074 (3)	0.29468 (15)	0.0648 (7)
H8	0.7889	0.9670	0.2815	0.078*
C9	0.67292 (17)	0.8368 (3)	0.23664 (14)	0.0590 (6)
C10	0.60499 (15)	0.7467 (3)	0.25551 (13)	0.0571 (6)
H10	0.5576	0.7003	0.2160	0.069*
C11	0.60754 (14)	0.7255 (3)	0.33346 (13)	0.0532 (6)
H11	0.5619	0.6630	0.3463	0.064*
C12	0.41850 (17)	0.8195 (4)	0.41237 (14)	0.0756 (8)
H12	0.4368	0.8569	0.3692	0.091*
C13	0.32900 (18)	0.8074 (4)	0.40351 (15)	0.0787 (8)
H13	0.2873	0.8389	0.3565	0.094*
C14	0.30224 (16)	0.7468 (4)	0.46686 (15)	0.0747 (8)
H14	0.2415	0.7335	0.4628	0.090*

C15	0.36502 (15)	0.7066 (3)	0.53537 (14)	0.0654 (7)
H15	0.3478	0.6647	0.5784	0.078*
C16	0.45526 (14)	0.7290 (3)	0.54015 (13)	0.0546 (6)
C17	0.52001 (13)	0.6854 (3)	0.68456 (12)	0.0504 (5)
C18	0.45807 (15)	0.7767 (3)	0.71257 (13)	0.0573 (6)
H18	0.4151	0.8470	0.6784	0.069*
C19	0.45919 (16)	0.7647 (3)	0.79053 (14)	0.0614 (6)
H19	0.4161	0.8238	0.8084	0.074*
C20	0.52424 (16)	0.6652 (3)	0.84200 (13)	0.0601 (6)
C21	0.58698 (15)	0.5743 (3)	0.81581 (13)	0.0592 (6)
H21	0.6308	0.5071	0.8507	0.071*
C22	0.58459 (14)	0.5833 (3)	0.73756 (13)	0.0559 (6)
H22	0.6266	0.5205	0.7197	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1128 (6)	0.1099 (6)	0.0642 (4)	0.0274 (5)	0.0455 (4)	0.0168 (4)
Cl2	0.1127 (6)	0.1427 (8)	0.0617 (4)	0.0110 (5)	0.0395 (4)	0.0276 (4)
N1	0.0442 (11)	0.0929 (16)	0.0500 (11)	0.0058 (11)	0.0123 (10)	0.0067 (10)
N2	0.0496 (11)	0.0902 (15)	0.0470 (11)	−0.0002 (10)	0.0125 (9)	−0.0015 (10)
N3	0.0437 (11)	0.1038 (17)	0.0470 (11)	0.0070 (11)	0.0112 (9)	0.0061 (10)
N4	0.0528 (11)	0.0867 (15)	0.0499 (12)	0.0078 (10)	0.0132 (10)	0.0019 (10)
C1	0.0581 (15)	0.104 (2)	0.0467 (14)	−0.0025 (15)	0.0082 (12)	0.0000 (13)
C2	0.0530 (15)	0.101 (2)	0.0594 (16)	0.0018 (14)	0.0003 (12)	0.0038 (14)
C3	0.0453 (13)	0.0847 (19)	0.0717 (17)	0.0065 (13)	0.0062 (13)	−0.0064 (14)
C4	0.0501 (13)	0.0802 (18)	0.0535 (14)	0.0011 (12)	0.0136 (11)	−0.0050 (12)
C5	0.0437 (12)	0.0622 (14)	0.0499 (13)	−0.0034 (11)	0.0086 (11)	−0.0051 (11)
C6	0.0444 (12)	0.0614 (14)	0.0502 (13)	0.0000 (11)	0.0146 (10)	0.0030 (11)
C7	0.0509 (14)	0.0699 (16)	0.0649 (15)	−0.0099 (12)	0.0126 (12)	0.0014 (12)
C8	0.0565 (14)	0.0664 (16)	0.0782 (17)	−0.0024 (12)	0.0301 (13)	0.0124 (13)
C9	0.0627 (15)	0.0628 (16)	0.0556 (14)	0.0137 (12)	0.0231 (12)	0.0072 (11)
C10	0.0489 (13)	0.0655 (16)	0.0547 (14)	0.0020 (11)	0.0107 (11)	−0.0056 (11)
C11	0.0438 (12)	0.0596 (14)	0.0575 (14)	−0.0017 (11)	0.0162 (11)	0.0015 (11)
C12	0.0645 (17)	0.111 (2)	0.0505 (15)	0.0178 (15)	0.0148 (13)	0.0093 (14)
C13	0.0578 (16)	0.119 (2)	0.0516 (15)	0.0208 (16)	0.0031 (13)	0.0020 (15)
C14	0.0464 (14)	0.102 (2)	0.0685 (17)	0.0002 (14)	0.0049 (13)	−0.0065 (15)
C15	0.0488 (13)	0.0883 (18)	0.0560 (14)	−0.0067 (13)	0.0097 (11)	0.0019 (13)
C16	0.0478 (13)	0.0647 (15)	0.0496 (13)	0.0051 (11)	0.0106 (11)	−0.0018 (11)
C17	0.0384 (11)	0.0631 (14)	0.0489 (13)	−0.0045 (10)	0.0108 (10)	0.0009 (10)
C18	0.0499 (13)	0.0631 (15)	0.0555 (14)	0.0051 (11)	0.0094 (11)	0.0066 (11)
C19	0.0562 (14)	0.0704 (17)	0.0622 (15)	0.0023 (12)	0.0244 (12)	0.0011 (12)
C20	0.0603 (15)	0.0692 (16)	0.0526 (14)	−0.0064 (13)	0.0186 (12)	0.0107 (12)
C21	0.0486 (13)	0.0677 (16)	0.0586 (14)	−0.0023 (12)	0.0104 (11)	0.0153 (12)
C22	0.0420 (12)	0.0654 (15)	0.0585 (14)	0.0008 (11)	0.0114 (11)	0.0029 (11)

Geometric parameters (Å, º)

Cl1—C9	1.744 (2)	C8—C9	1.373 (3)
Cl2—C20	1.737 (2)	C8—H8	0.9300
N1—C5	1.372 (3)	C9—C10	1.371 (3)
N1—C6	1.405 (3)	C10—C11	1.377 (3)
N1—H1	0.865 (10)	C10—H10	0.9300
N2—C1	1.338 (3)	C11—H11	0.9300
N2—C5	1.338 (3)	C12—C13	1.356 (3)
N3—C16	1.378 (3)	C12—H12	0.9300
N3—C17	1.393 (3)	C13—C14	1.378 (3)
N3—H3	0.863 (9)	C13—H13	0.9300
N4—C12	1.333 (3)	C14—C15	1.359 (3)
N4—C16	1.333 (3)	C14—H14	0.9300
C1—C2	1.364 (3)	C15—C16	1.389 (3)
C1—H1A	0.9300	C15—H15	0.9300
C2—C3	1.378 (3)	C17—C18	1.382 (3)
C2—H2	0.9300	C17—C22	1.396 (3)
C3—C4	1.362 (3)	C18—C19	1.377 (3)
C3—H3A	0.9300	C18—H18	0.9300
C4—C5	1.400 (3)	C19—C20	1.377 (3)
C4—H4	0.9300	C19—H19	0.9300
C6—C7	1.382 (3)	C20—C21	1.373 (3)
C6—C11	1.383 (3)	C21—C22	1.376 (3)
C7—C8	1.384 (3)	C21—H21	0.9300
C7—H7	0.9300	C22—H22	0.9300
C5—N1—C6	127.0 (2)	C11—C10—H10	120.2
C5—N1—H1	115.4 (16)	C10—C11—C6	120.9 (2)
C6—N1—H1	116.6 (16)	C10—C11—H11	119.5
C1—N2—C5	116.8 (2)	C6—C11—H11	119.5
C16—N3—C17	127.9 (2)	N4—C12—C13	124.7 (2)
C16—N3—H3	115.4 (15)	N4—C12—H12	117.6
C17—N3—H3	116.0 (15)	C13—C12—H12	117.6
C12—N4—C16	117.2 (2)	C12—C13—C14	117.4 (2)
N2—C1—C2	125.3 (2)	C12—C13—H13	121.3
N2—C1—H1A	117.3	C14—C13—H13	121.3
C2—C1—H1A	117.3	C15—C14—C13	119.7 (2)
C1—C2—C3	116.8 (2)	C15—C14—H14	120.2
C1—C2—H2	121.6	C13—C14—H14	120.2
C3—C2—H2	121.6	C14—C15—C16	119.0 (2)
C4—C3—C2	120.4 (2)	C14—C15—H15	120.5
C4—C3—H3A	119.8	C16—C15—H15	120.5
C2—C3—H3A	119.8	N4—C16—N3	114.45 (19)
C3—C4—C5	118.7 (2)	N4—C16—C15	121.9 (2)
C3—C4—H4	120.7	N3—C16—C15	123.6 (2)
C5—C4—H4	120.7	C18—C17—N3	124.0 (2)
N2—C5—N1	114.34 (19)	C18—C17—C22	118.3 (2)

N2—C5—C4	122.0 (2)	N3—C17—C22	117.6 (2)
N1—C5—C4	123.7 (2)	C19—C18—C17	120.7 (2)
C7—C6—C11	118.9 (2)	C19—C18—H18	119.6
C7—C6—N1	122.6 (2)	C17—C18—H18	119.6
C11—C6—N1	118.5 (2)	C18—C19—C20	119.9 (2)
C6—C7—C8	120.3 (2)	C18—C19—H19	120.0
C6—C7—H7	119.9	C20—C19—H19	120.0
C8—C7—H7	119.9	C21—C20—C19	120.5 (2)
C9—C8—C7	119.8 (2)	C21—C20—Cl2	120.07 (18)
C9—C8—H8	120.1	C19—C20—Cl2	119.5 (2)
C7—C8—H8	120.1	C20—C21—C22	119.5 (2)
C10—C9—C8	120.6 (2)	C20—C21—H21	120.2
C10—C9—Cl1	119.87 (19)	C22—C21—H21	120.2
C8—C9—Cl1	119.55 (19)	C21—C22—C17	121.0 (2)
C9—C10—C11	119.5 (2)	C21—C22—H22	119.5
C9—C10—H10	120.2	C17—C22—H22	119.5

C5—N2—C1—C2	−0.6 (4)	C16—N4—C12—C13	−0.4 (4)
N2—C1—C2—C3	0.5 (4)	N4—C12—C13—C14	−1.9 (5)
C1—C2—C3—C4	−0.3 (4)	C12—C13—C14—C15	1.8 (4)
C2—C3—C4—C5	0.1 (4)	C13—C14—C15—C16	0.5 (4)
C1—N2—C5—N1	178.4 (2)	C12—N4—C16—N3	−179.4 (2)
C1—N2—C5—C4	0.3 (3)	C12—N4—C16—C15	2.8 (4)
C6—N1—C5—N2	−177.0 (2)	C17—N3—C16—N4	160.2 (2)
C6—N1—C5—C4	0.9 (4)	C17—N3—C16—C15	−22.0 (4)
C3—C4—C5—N2	−0.1 (4)	C14—C15—C16—N4	−2.9 (4)
C3—C4—C5—N1	−177.9 (2)	C14—C15—C16—N3	179.5 (2)
C5—N1—C6—C7	−51.1 (4)	C16—N3—C17—C18	−26.8 (4)
C5—N1—C6—C11	131.9 (3)	C16—N3—C17—C22	155.4 (2)
C11—C6—C7—C8	−1.9 (3)	N3—C17—C18—C19	−178.8 (2)
N1—C6—C7—C8	−178.9 (2)	C22—C17—C18—C19	−1.1 (3)
C6—C7—C8—C9	2.1 (4)	C17—C18—C19—C20	2.0 (4)
C7—C8—C9—C10	−0.8 (4)	C18—C19—C20—C21	−1.5 (4)
C7—C8—C9—Cl1	179.35 (19)	C18—C19—C20—Cl2	178.90 (18)
C8—C9—C10—C11	−0.7 (3)	C19—C20—C21—C22	0.1 (3)
Cl1—C9—C10—C11	179.13 (17)	Cl2—C20—C21—C22	179.70 (18)
C9—C10—C11—C6	0.9 (3)	C20—C21—C22—C17	0.8 (3)
C7—C6—C11—C10	0.4 (3)	C18—C17—C22—C21	−0.4 (3)
N1—C6—C11—C10	177.5 (2)	N3—C17—C22—C21	177.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4	0.87 (1)	2.16 (1)	3.018 (3)	170 (2)
N3—H3···N2	0.86 (1)	2.22 (1)	3.071 (3)	171 (2)