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4-Chloro-*N*-(2,4-dimethylphenyl)-benzamide

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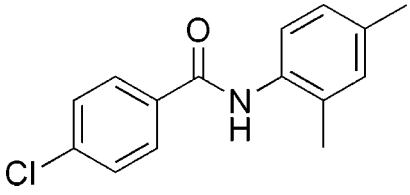
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.128; data-to-parameter ratio = 14.0.

Molecules of the title compound, $C_{15}H_{14}ClNO$, are linked into chains along the c axis by intermolecular N—H···O hydrogen bonds. The xylene and chlorobenzene rings deviate from the amide plane [C(=O)—N] by 77.8 (1) and 29.7 (1)°, respectively.

Related literature

For arylamides, see: Jackson *et al.* (2002); Gowda, Sowmya, Kožíšek *et al.* (2007); Gowda, Sowmya, Tokarčík *et al.* (2007*a*,*b*); Gowda, Foro *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{14}ClNO$
M_r = 259.72
Monoclinic, $P2_1/c$
a = 22.918 (6) Å
b = 6.4588 (17) Å
c = 9.261 (3) Å
β = 99.654 (4)°
V = 1351.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 294 (2) K
0.30 × 0.26 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.924, T_{max} = 0.948
4885 measured reflections
2367 independent reflections
1861 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.128
S = 1.05
2367 reflections
169 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.892 (10)	2.027 (12)	2.886 (2)	161 (2)

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2319).

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supplementary materials

Acta Cryst. (2007). E**63**, o4630 [**doi:10.1107/S1600536807054256**]

4-Chloro-*N*-(2,4-dimethylphenyl)benzamide

B. Zhou and P.-W. Zheng

Comment

The bonds to nitrogen of the title amide (I), Fig.1, lie in the same plane (C7—N1—C8 123.92 (17), C7—N1—H1A 121.5 (16), C8—N1—H1A 114.5 (16)), unlike the pyramidal arrangement of bonds in ammonia and amines. The C7—N1 bond has considerable double-bond character, at 1.344 (3) Å, is substantially shorter than the normal C—N single-bond distance observed in amines. The dihedral angle between the xylene and chlorobenzene ring is 73.27 (11)°.

In the crystal of (I), the intermolecular N—H···O H-bonds (Table 1) linked molecules to chains along the *c* axis (Fig.2).

Experimental

The title compound was prepared, in a 90% yield, by reaction of 2,4-xylidine (1.21 g, 10 mmol) with 4-chlorobenzoyl chloride (1.92 g, 11 mmol) in CH_2Cl_2 (20 ml)in the presence of aqueous $NaHCO_3$ (1.68 g, 20 mmol). Colorless blocks of (I) were grown by natural evaporation of a MeOH solution.

Refinement

The N-bound H atoms were refined freely while the other H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

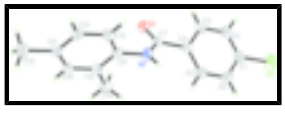

Fig. 1. The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids for the non-hydrogen atoms.

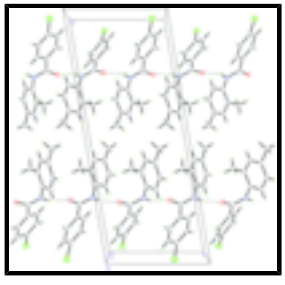

Fig. 2. A partial packing diagram for (1). The dashed lines indicate intermolecular hydrogen bonds.

4-Chloro-*N*-(2,4-dimethylphenyl)benzamide

Crystal data

$C_{15}H_{14}ClNO$ F_{000} = 544

M_r = 259.72	D_x = 1.277 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2688 reflections
a = 22.918 (6) Å	θ = 3.1–26.3º
b = 6.4588 (17) Å	μ = 0.27 mm^{-1}
c = 9.261 (3) Å	T = 294 (2) K
β = 99.654 (4)º	Block, colorless
V = 1351.4 (6) Å^3	0.30 × 0.26 × 0.20 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2367 independent reflections
Radiation source: fine-focus sealed tube	1861 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −20→27
T_{min} = 0.924, T_{max} = 0.948	k = −7→5
4885 measured reflections	l = −11→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.128	$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.7152P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.002
2367 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
169 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl1	0.03364 (4)	1.33583 (14)	0.65684 (12)	0.1027 (4)
O1	0.23813 (7)	0.5885 (2)	0.72579 (15)	0.0473 (4)
N1	0.25229 (8)	0.6922 (3)	0.96238 (18)	0.0454 (5)
C1	0.08899 (11)	1.1520 (4)	0.7080 (3)	0.0592 (7)
C2	0.08721 (11)	0.9683 (5)	0.6315 (3)	0.0646 (7)
H2	0.0567	0.9420	0.5539	0.077*
C3	0.13137 (10)	0.8242 (4)	0.6718 (3)	0.0519 (6)
H3	0.1306	0.7005	0.6202	0.062*
C4	0.17688 (9)	0.8604 (3)	0.7879 (2)	0.0389 (5)
C5	0.17761 (11)	1.0476 (4)	0.8624 (3)	0.0544 (6)
H5	0.2079	1.0747	0.9402	0.065*
C6	0.13392 (13)	1.1936 (4)	0.8224 (3)	0.0648 (7)
H6	0.1349	1.3188	0.8723	0.078*
C7	0.22494 (9)	0.7027 (3)	0.8224 (2)	0.0388 (5)
C8	0.30162 (9)	0.5585 (3)	1.0128 (2)	0.0393 (5)
C9	0.35792 (10)	0.6094 (3)	0.9857 (2)	0.0409 (5)
C10	0.40452 (10)	0.4800 (4)	1.0444 (2)	0.0453 (5)
H10	0.4424	0.5121	1.0278	0.054*
C11	0.39697 (10)	0.3051 (4)	1.1265 (2)	0.0480 (6)
C12	0.34021 (10)	0.2593 (4)	1.1516 (2)	0.0504 (6)
H12	0.3339	0.1436	1.2068	0.061*
C13	0.29303 (10)	0.3851 (4)	1.0947 (2)	0.0449 (5)
H13	0.2552	0.3529	1.1117	0.054*
C14	0.36859 (12)	0.7973 (4)	0.8979 (3)	0.0594 (7)
H14A	0.4104	0.8208	0.9065	0.089*
H14B	0.3503	0.9157	0.9343	0.089*
H14C	0.3519	0.7754	0.7969	0.089*
C15	0.44913 (13)	0.1704 (5)	1.1882 (3)	0.0760 (9)
H15A	0.4766	0.1661	1.1205	0.114*
H15B	0.4355	0.0328	1.2035	0.114*
H15C	0.4684	0.2268	1.2798	0.114*
H1A	0.2396 (10)	0.765 (3)	1.033 (2)	0.062 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0736 (6)	0.0776 (6)	0.1499 (9)	0.0316 (4)	−0.0017 (5)	0.0127 (5)
O1	0.0544 (9)	0.0523 (9)	0.0344 (7)	0.0066 (8)	0.0053 (6)	−0.0048 (7)
N1	0.0505 (11)	0.0548 (12)	0.0307 (9)	0.0119 (9)	0.0064 (8)	−0.0029 (8)

C1	0.0461 (14)	0.0566 (15)	0.0749 (17)	0.0100 (12)	0.0105 (12)	0.0102 (13)
C2	0.0425 (14)	0.0704 (18)	0.0750 (17)	0.0028 (13)	−0.0070 (12)	0.0000 (15)
C3	0.0430 (13)	0.0528 (15)	0.0577 (14)	−0.0018 (11)	0.0023 (11)	−0.0071 (11)
C4	0.0379 (11)	0.0446 (12)	0.0350 (10)	−0.0015 (9)	0.0080 (8)	0.0023 (9)
C5	0.0602 (15)	0.0515 (14)	0.0473 (13)	0.0038 (12)	−0.0033 (11)	−0.0055 (11)
C6	0.0759 (19)	0.0464 (15)	0.0713 (17)	0.0099 (13)	0.0100 (14)	−0.0054 (13)
C7	0.0419 (12)	0.0420 (12)	0.0330 (10)	−0.0031 (9)	0.0078 (9)	−0.0006 (9)
C8	0.0447 (12)	0.0442 (12)	0.0278 (9)	0.0026 (10)	0.0025 (8)	−0.0043 (9)
C9	0.0467 (13)	0.0441 (12)	0.0320 (10)	−0.0026 (10)	0.0065 (9)	0.0005 (9)
C10	0.0394 (12)	0.0551 (14)	0.0414 (11)	−0.0040 (10)	0.0061 (9)	−0.0005 (10)
C11	0.0516 (14)	0.0462 (13)	0.0448 (12)	0.0038 (11)	0.0038 (10)	0.0012 (10)
C12	0.0598 (15)	0.0402 (12)	0.0508 (12)	−0.0046 (11)	0.0079 (11)	0.0071 (11)
C13	0.0442 (12)	0.0497 (13)	0.0415 (11)	−0.0067 (11)	0.0089 (9)	−0.0015 (10)
C14	0.0628 (16)	0.0573 (16)	0.0587 (14)	−0.0036 (13)	0.0120 (12)	0.0147 (12)
C15	0.0644 (18)	0.074 (2)	0.085 (2)	0.0148 (15)	0.0009 (15)	0.0197 (16)

Geometric parameters (Å, °)

Cl1—C1	1.744 (3)	C8—C9	1.395 (3)
O1—C7	1.236 (2)	C9—C10	1.393 (3)
N1—C7	1.344 (3)	C9—C14	1.503 (3)
N1—C8	1.437 (3)	C10—C11	1.388 (3)
N1—H1A	0.892 (10)	C10—H10	0.9300
C1—C6	1.374 (4)	C11—C12	1.391 (3)
C1—C2	1.379 (4)	C11—C15	1.511 (3)
C2—C3	1.380 (3)	C12—C13	1.384 (3)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.387 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—H14A	0.9600
C4—C5	1.390 (3)	C14—H14B	0.9600
C4—C7	1.495 (3)	C14—H14C	0.9600
C5—C6	1.380 (4)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600
C6—H6	0.9300	C15—H15C	0.9600
C8—C13	1.386 (3)		
C7—N1—C8	123.92 (17)	C10—C9—C8	117.4 (2)
C7—N1—H1A	121.5 (16)	C10—C9—C14	120.8 (2)
C8—N1—H1A	114.5 (16)	C8—C9—C14	121.8 (2)
C6—C1—C2	121.2 (2)	C11—C10—C9	123.0 (2)
C6—C1—Cl1	119.5 (2)	C11—C10—H10	118.5
C2—C1—Cl1	119.3 (2)	C9—C10—H10	118.5
C1—C2—C3	119.0 (2)	C10—C11—C12	118.1 (2)
C1—C2—H2	120.5	C10—C11—C15	120.8 (2)
C3—C2—H2	120.5	C12—C11—C15	121.1 (2)
C2—C3—C4	121.2 (2)	C13—C12—C11	120.3 (2)
C2—C3—H3	119.4	C13—C12—H12	119.9
C4—C3—H3	119.4	C11—C12—H12	119.9
C3—C4—C5	118.4 (2)	C12—C13—C8	120.6 (2)
C3—C4—C7	118.81 (19)	C12—C13—H13	119.7

C5—C4—C7	122.64 (19)	C8—C13—H13	119.7
C6—C5—C4	120.9 (2)	C9—C14—H14A	109.5
C6—C5—H5	119.6	C9—C14—H14B	109.5
C4—C5—H5	119.6	H14A—C14—H14B	109.5
C1—C6—C5	119.3 (2)	C9—C14—H14C	109.5
C1—C6—H6	120.3	H14A—C14—H14C	109.5
C5—C6—H6	120.3	H14B—C14—H14C	109.5
O1—C7—N1	122.50 (19)	C11—C15—H15A	109.5
O1—C7—C4	120.87 (17)	C11—C15—H15B	109.5
N1—C7—C4	116.63 (18)	H15A—C15—H15B	109.5
C13—C8—C9	120.7 (2)	C11—C15—H15C	109.5
C13—C8—N1	119.17 (19)	H15A—C15—H15C	109.5
C9—C8—N1	120.08 (19)	H15B—C15—H15C	109.5
C6—C1—C2—C3	0.3 (4)	C7—N1—C8—C13	−106.9 (2)
Cl1—C1—C2—C3	179.5 (2)	C7—N1—C8—C9	76.4 (3)
C1—C2—C3—C4	0.5 (4)	C13—C8—C9—C10	−0.2 (3)
C2—C3—C4—C5	−0.9 (4)	N1—C8—C9—C10	176.43 (18)
C2—C3—C4—C7	−177.3 (2)	C13—C8—C9—C14	−179.6 (2)
C3—C4—C5—C6	0.4 (4)	N1—C8—C9—C14	−3.0 (3)
C7—C4—C5—C6	176.7 (2)	C8—C9—C10—C11	0.4 (3)
C2—C1—C6—C5	−0.8 (4)	C14—C9—C10—C11	179.8 (2)
Cl1—C1—C6—C5	180.0 (2)	C9—C10—C11—C12	−0.5 (3)
C4—C5—C6—C1	0.4 (4)	C9—C10—C11—C15	−179.8 (2)
C8—N1—C7—O1	4.1 (3)	C10—C11—C12—C13	0.4 (3)
C8—N1—C7—C4	−176.16 (19)	C15—C11—C12—C13	179.7 (2)
C3—C4—C7—O1	27.6 (3)	C11—C12—C13—C8	−0.3 (3)
C5—C4—C7—O1	−148.7 (2)	C9—C8—C13—C12	0.2 (3)
C3—C4—C7—N1	−152.1 (2)	N1—C8—C13—C12	−176.50 (19)
C5—C4—C7—N1	31.6 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.892 (10)	2.027 (12)	2.886 (2)	161 (2)

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

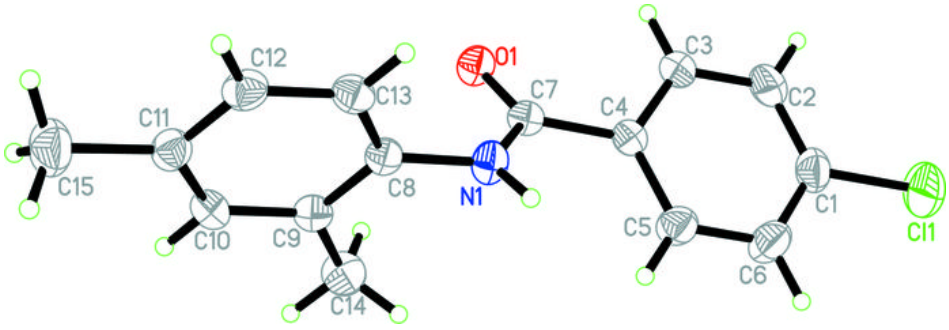

Fig. 2