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2-Chloro-*N*-(2,3-dimethylphenyl)-benzamide

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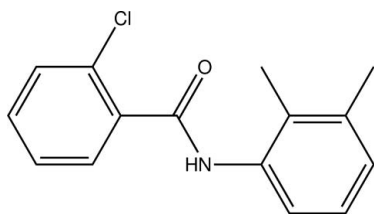
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 Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.039; wR factor = 0.102; data-to-parameter ratio = 13.8.

In the title compound, $\text{C}_{15}\text{H}_{14}\text{ClNO}$, the $\text{N}-\text{H}$ and $\text{C}=\text{O}$ bonds in the amide group are *anti* to each other. The amide group is inclined at 60.3 (1)° to the chloro-substituted benzoyl ring and at 59.2 (1)° to the dimethyl-substituted aniline ring. The mean planes through the two benzene rings make a dihedral angle of 7.7 (1)°. In the crystal structure, molecules are linked by intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming chains along $[010]$.

Related literature

For the preparation of the title compound, see: Gowda, Jyothi *et al.* (2003). For related structures, see: Gowda, Foro *et al.* (2008, 2009); Gowda, Jyothi *et al.* (2003); Gowda, Tokarčík *et al.* (2009). For a review of halogen bonding, see: Fourmigué (2009).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{14}\text{ClNO}$
 $M_r = 259.72$
 Monoclinic, $P2_1/c$

$a = 13.0108$ (5) Å
 $b = 4.9970$ (1) Å
 $c = 22.6241$ (9) Å

$\beta = 118.553$ (4)°
 $V = 1292.01$ (9) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.28$ mm⁻¹
 $T = 295$ K
 $0.54 \times 0.43 \times 0.05$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
 Absorption correction: analytical (*CrysAlis PRO*; Oxford Diffraction, 2009)
 $T_{\min} = 0.861$, $T_{\max} = 0.985$
 20701 measured reflections
 2293 independent reflections
 1959 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.102$
 $S = 1.06$
 2293 reflections
 166 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O1}^i$	0.86	2.23	2.9388 (19)	140

 Symmetry code: (i) $x, y - 1, z$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2009) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2683).

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Acta Cryst. (2010). E66, o1897 [https://doi.org/10.1107/S1600536810024943]

2-Chloro-*N*-(2,3-dimethylphenyl)benzamide

B. Thimme Gowda, Miroslav Tokarčík, Vinola Z. Rodrigues, Jozef Kožíšek and Hartmut Fuess

S1. Comment

To explore the effect of substituents on the structures of benzanilides (Gowda, Foro *et al.*, 2008, 2009; Gowda, Jyothi *et al.*, 2003; Gowda, Tokarčík *et al.*, 2009), in the present work, the structure of 2-chloro-*N*-(2,3-dimethylphenyl)-benzamide (I) has been determined. The N—H and C=O bonds in the amide group are *anti* to each other (Fig. 1), similar to that observed in 2-chloro-*N*-(phenyl)-benzamide (II) (Gowda, Jyothi *et al.*, 2003), *N*-(2,3-dimethylphenyl)-benzamide (III) (Gowda, Tokarčík *et al.*, 2009), 2-chloro-*N*-(2,3-dichlorophenyl)-benzamide (IV) (Gowda, Foro *et al.*, 2008), and 2-chloro-*N*-(3,5-dimethylphenyl)-benzamide (V) (Gowda, Foro *et al.*, 2009).

The molecular structure of (I) includes a short intramolecular C11...O1 contact of 3.1837 (16) Å, which can be interpreted within the concept of halogen bonding (Fourmigué, 2009). The central amide group —NHCO— is inclined at 60.3 (1)° to the benzoyl ring (C2–C7) and at 59.2 (1)° to the anilino ring (C8–C13). The mean planes through the two benzene rings make a dihedral angle of 7.7 (1)°. The crystal packing (Fig. 2) is dominated by intermolecular N—H...O hydrogen bonds (Table 1) which link the molecules into the chains extending along the *b* axis.

S2. Experimental

The title compound was prepared according to the literature method (Gowda, Jyothi *et al.*, 2003). Plate-like colorless single crystals of (I) were obtained from an ethanolic solution held at room temperature.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, including free rotation about the C_{aromatic}–C_{methyl} bond, with C–H = 0.93 or 0.96 Å and N–H = 0.86 Å. The $U_{iso}(H)$ values were set at $1.2U_{eq}(C \text{ aromatic}, N)$ and $1.5U_{eq}(C \text{ methyl})$.

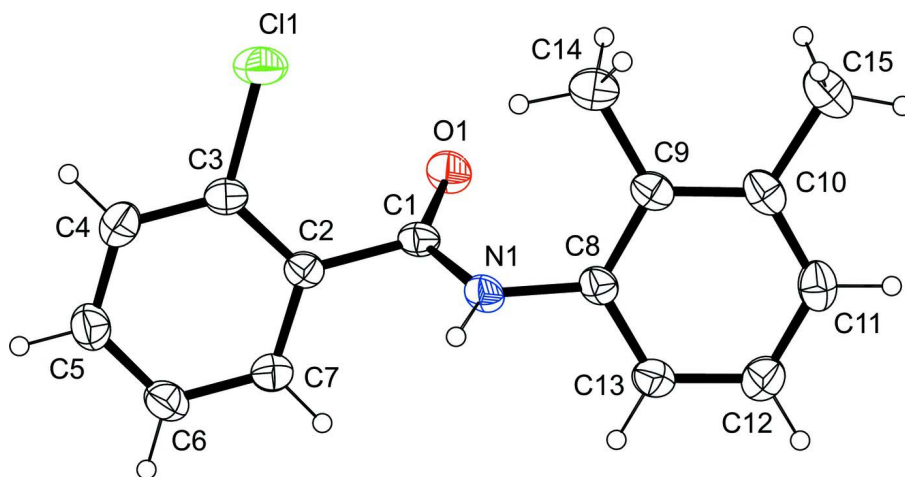


Figure 1

Molecular structure of (I) showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radii.

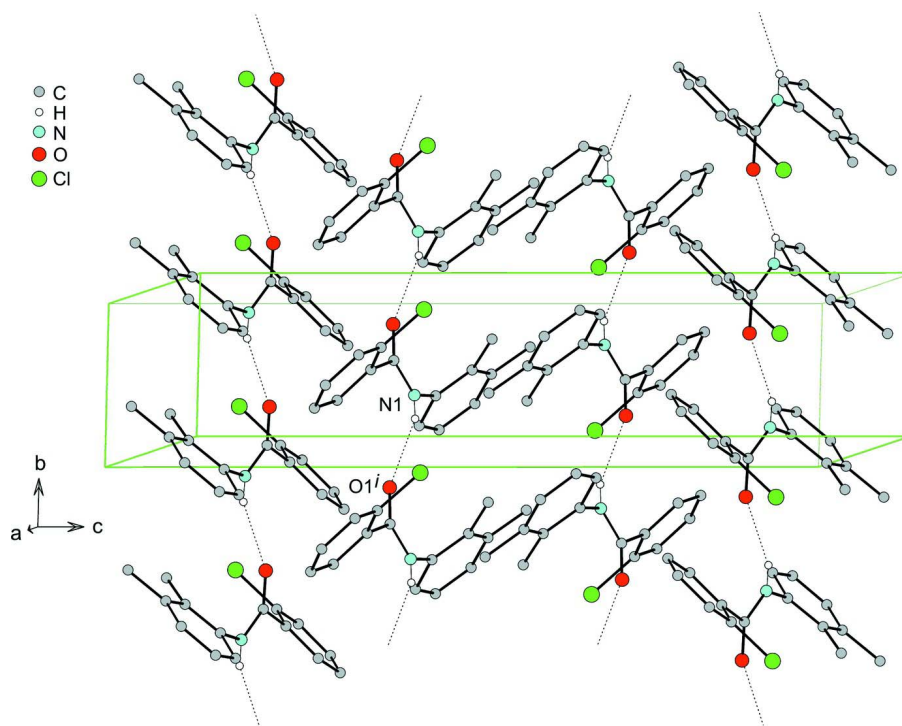


Figure 2

View of the crystal packing of (I), showing the chains of molecules linked by intermolecular N–H...O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted. Symmetry code (i): $x, y - 1, z$.

2-Chloro-*N*-(2,3-dimethylphenyl)benzamide

Crystal data

$C_{15}H_{14}ClNO$

$M_r = 259.72$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 13.0108 (5) \text{ \AA}$

$b = 4.9970 (1) \text{ \AA}$

$c = 22.6241$ (9) Å
 $\beta = 118.553$ (4)°
 $V = 1292.01$ (9) Å³
 $Z = 4$
 $F(000) = 544$
 $D_x = 1.335$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 11536 reflections
 $\theta = 2.0$ – 29.4 °
 $\mu = 0.28$ mm⁻¹
 $T = 295$ K
 Plate, colorless
 $0.54 \times 0.43 \times 0.05$ mm

Data collection

Oxford Diffraction Gemini R CCD
 diffractometer
 Graphite monochromator
 Detector resolution: 10.434 pixels mm⁻¹
 ω scans
 Absorption correction: analytical
 (*CrysAlis PRO*; Oxford Diffraction, 2009)
 $T_{\min} = 0.861$, $T_{\max} = 0.985$

20701 measured reflections
 2293 independent reflections
 1959 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\max} = 25.1$ °, $\theta_{\min} = 2.1$ °
 $h = -15 \rightarrow 15$
 $k = -5 \rightarrow 5$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.102$
 $S = 1.06$
 2293 reflections
 166 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
 $w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 0.5282P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ 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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.44821 (16)	0.5493 (3)	0.33073 (9)	0.0402 (4)
C2	0.32436 (15)	0.4698 (3)	0.28284 (9)	0.0377 (4)
C3	0.22925 (17)	0.5896 (4)	0.28448 (9)	0.0422 (4)
C4	0.11586 (17)	0.5209 (4)	0.23906 (10)	0.0525 (5)
H4	0.0534	0.6029	0.2411	0.063*
C5	0.09558 (18)	0.3309 (4)	0.19085 (11)	0.0552 (5)
H5	0.0192	0.2849	0.16	0.066*
C6	0.18775 (18)	0.2085 (4)	0.18810 (10)	0.0525 (5)
H6	0.1737	0.0797	0.1554	0.063*
C7	0.30116 (17)	0.2768 (4)	0.23385 (9)	0.0449 (4)

H7	0.3631	0.1922	0.2318	0.054*
C8	0.63848 (15)	0.3676 (3)	0.41456 (9)	0.0392 (4)
C9	0.68395 (16)	0.5350 (3)	0.47093 (9)	0.0411 (4)
C10	0.80539 (17)	0.5320 (4)	0.51345 (9)	0.0463 (5)
C11	0.87516 (17)	0.3630 (4)	0.49984 (10)	0.0523 (5)
H11	0.9555	0.3622	0.5285	0.063*
C12	0.82881 (18)	0.1955 (4)	0.44484 (11)	0.0538 (5)
H12	0.8772	0.081	0.4368	0.065*
C13	0.71009 (17)	0.1991 (4)	0.40184 (10)	0.0475 (5)
H13	0.678	0.0882	0.3642	0.057*
C14	0.6071 (2)	0.7104 (4)	0.48782 (11)	0.0550 (5)
H14A	0.6218	0.895	0.4827	0.083*
H14B	0.6242	0.6781	0.5335	0.083*
H14C	0.5264	0.6697	0.458	0.083*
C15	0.8603 (2)	0.7101 (5)	0.57434 (11)	0.0662 (6)
H15A	0.8367	0.8919	0.5611	0.099*
H15B	0.9439	0.6972	0.5947	0.099*
H15C	0.8353	0.6549	0.6061	0.099*
N1	0.51508 (13)	0.3484 (3)	0.36925 (8)	0.0424 (4)
H1N	0.4817	0.1971	0.3666	0.051*
O1	0.48384 (12)	0.7779 (3)	0.33335 (7)	0.0546 (4)
Cl1	0.25124 (5)	0.82447 (11)	0.34617 (3)	0.0650 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0486 (11)	0.0274 (9)	0.0474 (10)	-0.0033 (8)	0.0252 (9)	-0.0017 (8)
C2	0.0446 (10)	0.0279 (9)	0.0409 (9)	-0.0020 (7)	0.0206 (8)	0.0043 (7)
C3	0.0518 (11)	0.0332 (9)	0.0453 (10)	0.0006 (8)	0.0262 (9)	0.0016 (8)
C4	0.0452 (12)	0.0519 (12)	0.0599 (12)	0.0072 (9)	0.0249 (10)	0.0069 (10)
C5	0.0457 (11)	0.0538 (13)	0.0517 (12)	-0.0018 (9)	0.0117 (9)	0.0014 (10)
C6	0.0592 (13)	0.0467 (11)	0.0424 (10)	-0.0030 (10)	0.0167 (10)	-0.0061 (9)
C7	0.0496 (11)	0.0388 (10)	0.0474 (11)	0.0016 (8)	0.0241 (9)	-0.0004 (8)
C8	0.0423 (10)	0.0290 (9)	0.0431 (10)	-0.0061 (7)	0.0179 (8)	0.0023 (7)
C9	0.0521 (11)	0.0304 (9)	0.0419 (10)	-0.0070 (8)	0.0233 (9)	0.0028 (7)
C10	0.0532 (12)	0.0390 (10)	0.0389 (10)	-0.0133 (9)	0.0157 (9)	0.0054 (8)
C11	0.0420 (11)	0.0554 (12)	0.0517 (12)	-0.0055 (9)	0.0161 (9)	0.0097 (10)
C12	0.0505 (12)	0.0530 (12)	0.0619 (13)	0.0040 (10)	0.0301 (11)	0.0035 (10)
C13	0.0523 (12)	0.0400 (10)	0.0489 (11)	-0.0034 (9)	0.0232 (10)	-0.0050 (8)
C14	0.0676 (13)	0.0505 (12)	0.0531 (12)	-0.0021 (10)	0.0339 (11)	-0.0029 (10)
C15	0.0742 (16)	0.0584 (14)	0.0483 (12)	-0.0178 (12)	0.0150 (11)	-0.0045 (10)
N1	0.0448 (9)	0.0248 (7)	0.0513 (9)	-0.0071 (6)	0.0178 (7)	0.0000 (6)
O1	0.0565 (8)	0.0259 (7)	0.0734 (10)	-0.0080 (6)	0.0245 (7)	0.0035 (6)
Cl1	0.0793 (4)	0.0553 (4)	0.0724 (4)	-0.0015 (3)	0.0458 (3)	-0.0180 (3)

Geometric parameters (Å, °)

C1—O1	1.224 (2)	C9—C10	1.403 (3)
C1—N1	1.341 (2)	C9—C14	1.510 (3)
C1—C2	1.503 (3)	C10—C11	1.378 (3)
C2—C7	1.389 (3)	C10—C15	1.503 (3)
C2—C3	1.391 (3)	C11—C12	1.377 (3)
C3—C4	1.379 (3)	C11—H11	0.93
C3—C11	1.7395 (19)	C12—C13	1.377 (3)
C4—C5	1.373 (3)	C12—H12	0.93
C4—H4	0.93	C13—H13	0.93
C5—C6	1.374 (3)	C14—H14A	0.96
C5—H5	0.93	C14—H14B	0.96
C6—C7	1.380 (3)	C14—H14C	0.96
C6—H6	0.93	C15—H15A	0.96
C7—H7	0.93	C15—H15B	0.96
C8—C13	1.384 (3)	C15—H15C	0.96
C8—C9	1.398 (2)	N1—H1N	0.86
C8—N1	1.437 (2)		
O1—C1—N1	123.65 (17)	C11—C10—C9	119.96 (18)
O1—C1—C2	122.16 (16)	C11—C10—C15	119.49 (19)
N1—C1—C2	114.18 (14)	C9—C10—C15	120.54 (19)
C7—C2—C3	117.59 (17)	C12—C11—C10	121.59 (19)
C7—C2—C1	120.52 (16)	C12—C11—H11	119.2
C3—C2—C1	121.87 (16)	C10—C11—H11	119.2
C4—C3—C2	121.45 (17)	C11—C12—C13	119.30 (19)
C4—C3—C11	118.23 (15)	C11—C12—H12	120.3
C2—C3—C11	120.29 (14)	C13—C12—H12	120.3
C5—C4—C3	119.67 (19)	C12—C13—C8	120.01 (18)
C5—C4—H4	120.2	C12—C13—H13	120
C3—C4—H4	120.2	C8—C13—H13	120
C4—C5—C6	120.22 (19)	C9—C14—H14A	109.5
C4—C5—H5	119.9	C9—C14—H14B	109.5
C6—C5—H5	119.9	H14A—C14—H14B	109.5
C5—C6—C7	119.95 (19)	C9—C14—H14C	109.5
C5—C6—H6	120	H14A—C14—H14C	109.5
C7—C6—H6	120	H14B—C14—H14C	109.5
C6—C7—C2	121.11 (18)	C10—C15—H15A	109.5
C6—C7—H7	119.4	C10—C15—H15B	109.5
C2—C7—H7	119.4	H15A—C15—H15B	109.5
C13—C8—C9	121.34 (17)	C10—C15—H15C	109.5
C13—C8—N1	116.40 (16)	H15A—C15—H15C	109.5
C9—C8—N1	122.15 (16)	H15B—C15—H15C	109.5
C8—C9—C10	117.77 (17)	C1—N1—C8	124.77 (14)
C8—C9—C14	122.37 (17)	C1—N1—H1N	117.6
C10—C9—C14	119.85 (17)	C8—N1—H1N	117.6

O1—C1—C2—C7	118.6 (2)	C13—C8—C9—C14	-176.88 (17)
N1—C1—C2—C7	-60.8 (2)	N1—C8—C9—C14	-0.9 (3)
O1—C1—C2—C3	-59.7 (3)	C8—C9—C10—C11	-1.6 (2)
N1—C1—C2—C3	120.86 (19)	C14—C9—C10—C11	177.02 (17)
C7—C2—C3—C4	-0.3 (3)	C8—C9—C10—C15	179.05 (17)
C1—C2—C3—C4	178.06 (17)	C14—C9—C10—C15	-2.4 (3)
C7—C2—C3—C11	177.75 (13)	C9—C10—C11—C12	0.3 (3)
C1—C2—C3—C11	-3.9 (2)	C15—C10—C11—C12	179.72 (19)
C2—C3—C4—C5	-0.2 (3)	C10—C11—C12—C13	0.9 (3)
C11—C3—C4—C5	-178.28 (16)	C11—C12—C13—C8	-0.8 (3)
C3—C4—C5—C6	0.4 (3)	C9—C8—C13—C12	-0.5 (3)
C4—C5—C6—C7	-0.1 (3)	N1—C8—C13—C12	-176.75 (17)
C5—C6—C7—C2	-0.4 (3)	O1—C1—N1—C8	-5.1 (3)
C3—C2—C7—C6	0.6 (3)	C2—C1—N1—C8	174.31 (16)
C1—C2—C7—C6	-177.78 (17)	C13—C8—N1—C1	-119.2 (2)
C13—C8—C9—C10	1.7 (3)	C9—C8—N1—C1	64.6 (2)
N1—C8—C9—C10	177.69 (15)		

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1N \cdots O1 ⁱ	0.86	2.23	2.9388 (19)	140

Symmetry code: (i) $x, y-1, z$.