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

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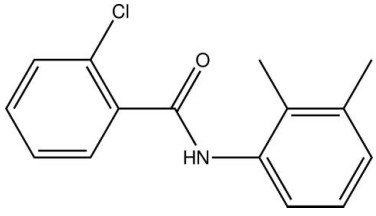
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.039; $wR$ factor = 0.102; data-to-parameter ratio = 13.8.

In the title compound, $C_{15}H_{14}ClNO$, the N—H and C═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 N—H···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

$C_{15}H_{14}ClNO$
$M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 295 K
0.54 × 0.43 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···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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# supplementary materials

*Acta Cryst.* (2010). E**66**, o1897 [ **doi:10.1107/S1600536810024943** ]

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

**B. T. Gowda, M. Tokarcík, V. Z. Rodrigues, J. Kozísek and H. Fuess**

## 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 Cl1···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.

## 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.

## 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 1.2$U_{eq}$(C aromatic, N) and 1.5$U_{eq}$(C methyl).

## Figures

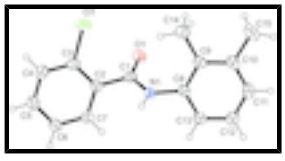

Fig. 1. Molecular structure of (I) showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radii.

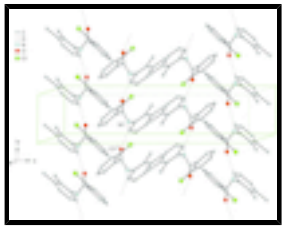

Fig. 2. View of the crystal packing of (I), showing the chains of molecules linked by intermolecular N–H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted. Symmetry code (i): *x*, *y* - 1, *z*.

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

*Crystal data*

| | |
|---|---|
| $C_{15}H_{14}ClNO$ | $F(000) = 544$ |
| $M_r = 259.72$ | $D_x = 1.335$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 11536 reflections |
| $a = 13.0108$ (5) Å | $\theta = 2.0$–$29.4°$ |
| $b = 4.9970$ (1) Å | $\mu = 0.28$ mm$^{-1}$ |
| $c = 22.6241$ (9) Å | $T = 295$ K |
| $\beta = 118.553$ (4)° | Plate, colorless |
| $V = 1292.01$ (9) Å$^3$ | 0.54 × 0.43 × 0.05 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini R CCD diffractometer | 2293 independent reflections |
| graphite | 1959 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.434 pixels mm$^{-1}$ | $R_{int} = 0.027$ |
| ω scans | $\theta_{max} = 25.1°$, $\theta_{min} = 2.1°$ |
| Absorption correction: analytical (*CrysAlis PRO*; Oxford Diffraction, 2009) | $h = -15 \rightarrow 15$ |
| $T_{min} = 0.861$, $T_{max} = 0.985$ | $k = -5 \rightarrow 5$ |
| 20701 measured reflections | $l = -26 \rightarrow 26$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.102$ | H-atom parameters constrained |
| $S = 1.06$ | $w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 0.5282P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2293 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 166 parameters | $\Delta\rho_{max} = 0.20$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.20$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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—Cl1 | 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—Cl1 | 118.23 (15) | C11—C12—H12 | 120.3 |
| C2—C3—Cl1 | 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—Cl1 | 177.75 (13) | C9—C10—C11—C12 | 0.3 (3) |
| C1—C2—C3—Cl1 | −3.9 (2) | C15—C10—C11—C12 | 179.72 (19) |
| C2—C3—C4—C5 | −0.2 (3) | C10—C11—C12—C13 | 0.9 (3) |
| Cl1—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 (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1N···O1$^{i}$ | 0.86 | 2.23 | 2.9388 (19) | 140 |

Symmetry codes: (i) *x*, *y*−1, *z*.

**Fig. 1**

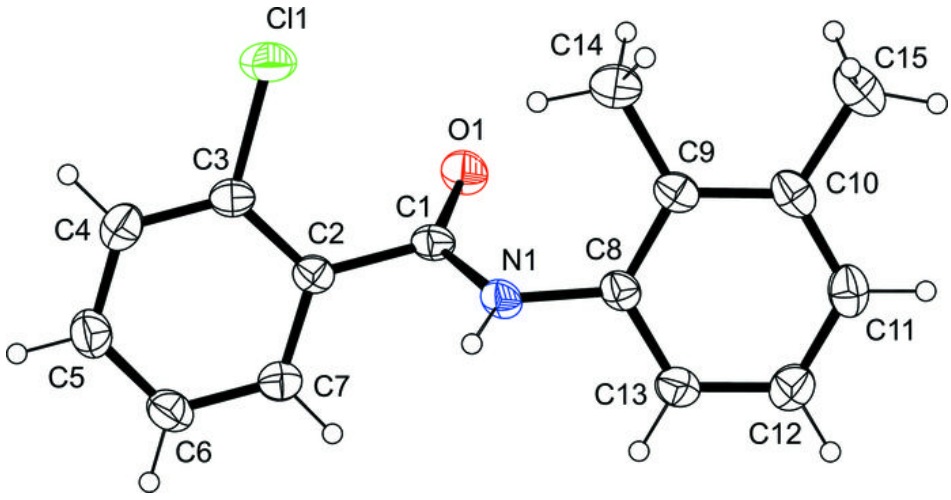

**Fig. 2**