N-(3-Chlorophenyl)-2-methylbenzamide

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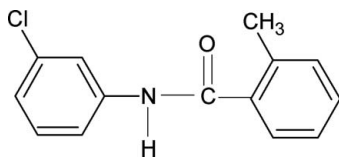
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The conformation of the N—H bond in the structure of the title compound, $C_{14}H_{12}ClNO$, is *anti* to the *meta*-chloro substituent in the aniline ring, while the C=O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring. The conformations of the N—H and C=O bonds are *anti* to each other, similar to those observed in 2-methyl-*N*-(3-methyl-phenyl)benzamide (N3MP2MBA). The –NHC(=O)– group makes a dihedral angle of 55.8 (7)° with the benzoyl ring, while the angle between the benzoyl and aniline rings is 37.5 (1)°; the respective values for N3MP2MBA are 55.2 (7) and 36.2 (1)°. N—H⋯O hydrogen bonds link the molecules into infinite chains running along the *c* axis.

Related literature

For related literature, see: Gowda *et al.* (2003, 2008*a*,*b*).

Experimental

Crystal data

$C_{14}H_{12}ClNO$	c = 15.977 (2) Å
M_r = 245.70	V = 1243.9 (2) Å^3
Tetragonal, $P4_3$	Z = 4
a = 8.8237 (8) Å	Cu $K\alpha$ radiation

μ = 2.57 mm^{-1}	0.60 × 0.10 × 0.07 mm
T = 299 (2) K	

Data collection

Enraf–Nonius CAD-4 diffractometer	2173 independent reflections
Absorption correction: ψ scan (North *et al.*, 1968)	1844 reflections with $I > 2\sigma(I)$
T_{min} = 0.308, T_{max} = 0.841	R_{int} = 0.036
4144 measured reflections	3 standard reflections frequency: 120 min intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.120	
S = 1.07	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
2173 reflections	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
159 parameters	Absolute structure: Flack (1983), 1020 Friedel pairs
1 restraint	Flack parameter: 0.00 (2)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1N⋯O1^i	0.83 (4)	2.12 (4)	2.900 (3)	157 (3)

Symmetry code: (i) $-y + 1, x, z - \frac{1}{4}$.

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

References

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supporting information

N-(3-Chlorophenyl)-2-methylbenzamide

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S1. Comment

In the present work, the structure of 2-methyl-*N*-(3-chlorophenyl)- benzamide (N3CP2MBA) has been determined as part of substituent effect studies on the solid state structures of benzanilides (Gowda *et al.*, 2003; Gowda *et al.* (2008a, 2008b). The conformation of the N—H bond in N3CP2MBA (Fig. 1) is *anti* to the *meta*-chloro substituent in the aniline ring, while the C=O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring and the conformations of the N—H and C=O bonds are *anti* to each other, identical to that observed in 2-methyl-*N*-(3-methylphenyl)-benzamide (N3MP2MBA). The bond parameters in N3CP2MBA are similar to those in 2-methyl-*N*-(phenyl)-benzamide (Gowda *et al.*, 2008a), N3MP2MBA (Gowda *et al.*, 2008b) and other benzanilides (Gowda *et al.*, 2003). The amide group, –NHCO– makes a dihedral angle of 55.8 (7)° with the benzoyl ring, while that between benzoyl and aniline rings is 37.5 (1)°, compared to the respective values of 55.2 (7)° and 36.2 (1)° for N3MP2MBA. The packing diagram of N3CP2MBA showing the hydrogen bonds N1—H1N···O1 (Table 1) is given in Fig. 2.

S2. Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

S3. Refinement

The H on N1 was located in difference map and its position freely refined. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å and were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).
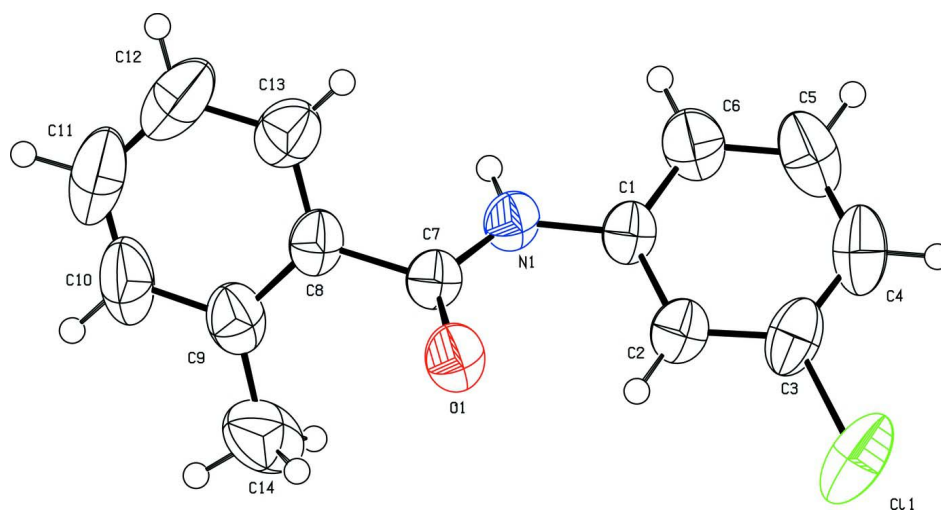
Figure 1

Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids drawn at the 50% probability level.
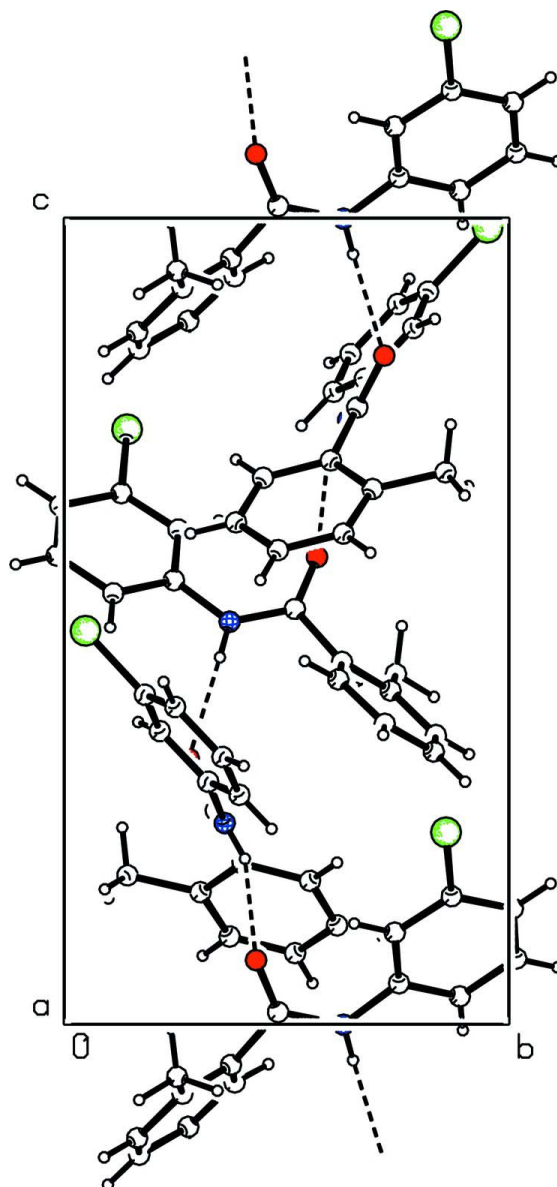
Figure 2

Molecular packing of the title compound as viewed down a and with hydrogen bonding shown as dashed lines.

N-(3-Chlorophenyl)-2-methylbenzamide

Crystal data

$C_{14}H_{12}ClNO$	$D_x = 1.312$ Mg m^{-3}
$M_r = 245.70$	Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Tetragonal, $P4_3$	Cell parameters from 25 reflections
Hall symbol: P 4cw	$\theta = 5.7–21.9°$
$a = 8.8237 (8)$ Å	$\mu = 2.57$ mm^{-1}
$c = 15.977 (2)$ Å	$T = 299$ K
$V = 1243.9 (2)$ Å^3	Rod, colourless
$Z = 4$	$0.60 \times 0.10 \times 0.07$ mm
$F(000) = 512$	

Data collection

Enraf–Nonius CAD-4 diffractometer	2173 independent reflections
Radiation source: fine-focus sealed tube	1844 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.036$
$\omega/2\theta$ scans	$\theta_{max} = 66.9°$, $\theta_{min} = 5.0°$
Absorption correction: psi-scan (North *et al.*, 1968)	$h = -10 \rightarrow 10$
	$k = -10 \rightarrow 1$
	$l = -19 \rightarrow 16$
$T_{min} = 0.308$, $T_{max} = 0.841$	3 standard reflections every 120 min
4144 measured reflections	intensity decay: none

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0774P)^2 + 0.019P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.120$	
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.025$
2173 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
159 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
1 restraint	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Primary atom site location: structure-invariant direct methods	
	Extinction coefficient: 0.0079 (12)
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 1020 Friedel pairs
Hydrogen site location: inferred from neighbouring sites	Absolute structure parameter: 0.00 (2)

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	0.6762 (3)	0.7532 (3)	0.05087 (15)	0.0463 (6)
C2	0.7849 (3)	0.7433 (3)	0.11372 (17)	0.0528 (6)
H2	0.8336	0.6521	0.1249	0.063*
C3	0.8186 (4)	0.8716 (4)	0.15884 (17)	0.0627 (8)
C4	0.7505 (5)	1.0087 (4)	0.1436 (2)	0.0763 (10)
H4	0.7762	1.0940	0.1747	0.092*
C5	0.6440 (5)	1.0169 (4)	0.0815 (2)	0.0831 (11)
H5	0.5963	1.1088	0.0705	0.100*
C6	0.6061 (4)	0.8896 (3)	0.0346 (2)	0.0673 (8)
H6	0.5337	0.8965	−0.0075	0.081*
C7	0.6591 (3)	0.4810 (3)	0.01510 (14)	0.0452 (5)
C8	0.5994 (3)	0.3752 (3)	−0.05047 (17)	0.0516 (6)

C9	0.6935 (4)	0.2659 (3)	−0.08605 (18)	0.0644 (8)
C10	0.6279 (6)	0.1643 (4)	−0.1412 (2)	0.0887 (12)
H10	0.6885	0.0897	−0.1650	0.106*
C11	0.4808 (7)	0.1690 (4)	−0.1617 (3)	0.0992 (14)
H11	0.4415	0.0984	−0.1991	0.119*
C12	0.3864 (5)	0.2793 (5)	−0.1272 (3)	0.0955 (13)
H12	0.2841	0.2826	−0.1411	0.115*
C13	0.4472 (4)	0.3834 (4)	−0.0721 (2)	0.0695 (8)
H13	0.3863	0.4591	−0.0495	0.083*
C14	0.8575 (5)	0.2539 (5)	−0.0653 (3)	0.0923 (12)
H14A	0.8693	0.2414	−0.0059	0.111*
H14B	0.9088	0.3444	−0.0828	0.111*
H14C	0.9003	0.1680	−0.0936	0.111*
N1	0.6388 (3)	0.6279 (2)	−0.00053 (14)	0.0488 (5)
H1N	0.594 (4)	0.650 (3)	−0.045 (2)	0.059*
O1	0.7197 (2)	0.4315 (2)	0.07953 (11)	0.0598 (5)
Cl1	0.95205 (13)	0.85850 (13)	0.23813 (6)	0.0996 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0581 (14)	0.0483 (13)	0.0324 (12)	−0.0062 (11)	0.0045 (10)	0.0009 (10)
C2	0.0615 (15)	0.0546 (14)	0.0421 (13)	−0.0076 (11)	0.0013 (11)	0.0021 (11)
C3	0.0766 (18)	0.0721 (19)	0.0394 (15)	−0.0252 (15)	0.0044 (13)	−0.0071 (13)
C4	0.115 (3)	0.0605 (18)	0.0538 (19)	−0.0194 (18)	0.0127 (18)	−0.0145 (15)
C5	0.125 (3)	0.0505 (15)	0.074 (2)	0.0089 (18)	0.012 (2)	−0.0043 (16)
C6	0.092 (2)	0.0568 (16)	0.0532 (17)	0.0043 (14)	−0.0034 (16)	0.0023 (13)
C7	0.0528 (13)	0.0500 (13)	0.0327 (13)	−0.0022 (10)	0.0041 (10)	0.0020 (10)
C8	0.0721 (17)	0.0465 (13)	0.0361 (13)	−0.0069 (11)	−0.0036 (11)	0.0030 (10)
C9	0.094 (2)	0.0559 (15)	0.0434 (15)	0.0070 (15)	−0.0037 (14)	−0.0022 (12)
C10	0.149 (4)	0.0572 (18)	0.059 (2)	0.006 (2)	−0.020 (2)	−0.0159 (15)
C11	0.162 (4)	0.064 (2)	0.071 (2)	−0.034 (3)	−0.034 (3)	−0.0049 (18)
C12	0.103 (3)	0.095 (3)	0.089 (3)	−0.039 (2)	−0.039 (2)	0.009 (2)
C13	0.0712 (19)	0.0665 (17)	0.071 (2)	−0.0106 (15)	−0.0094 (15)	0.0044 (15)
C14	0.099 (3)	0.109 (3)	0.069 (2)	0.035 (2)	0.0100 (19)	−0.012 (2)
N1	0.0627 (13)	0.0512 (11)	0.0324 (10)	0.0005 (9)	−0.0063 (10)	0.0014 (9)
O1	0.0893 (13)	0.0559 (10)	0.0342 (10)	0.0054 (9)	−0.0073 (9)	0.0033 (8)
Cl1	0.1114 (7)	0.1195 (8)	0.0678 (6)	−0.0442 (6)	−0.0276 (5)	−0.0081 (5)

Geometric parameters (Å, º)

C1—C6	1.377 (4)	C8—C13	1.388 (4)
C1—C2	1.391 (4)	C8—C9	1.394 (4)
C1—N1	1.416 (3)	C9—C10	1.384 (5)
C2—C3	1.374 (4)	C9—C14	1.488 (5)
C2—H2	0.9300	C10—C11	1.339 (7)
C3—C4	1.373 (5)	C10—H10	0.9300
C3—Cl1	1.734 (3)	C11—C12	1.394 (7)

C4—C5	1.368 (6)	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.382 (5)
C5—C6	1.392 (5)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—H14A	0.9600
C7—O1	1.240 (3)	C14—H14B	0.9600
C7—N1	1.332 (3)	C14—H14C	0.9600
C7—C8	1.499 (3)	N1—H1N	0.83 (4)
C6—C1—C2	120.0 (2)	C10—C9—C8	117.3 (3)
C6—C1—N1	117.9 (2)	C10—C9—C14	120.2 (3)
C2—C1—N1	122.0 (2)	C8—C9—C14	122.5 (3)
C3—C2—C1	118.4 (3)	C11—C10—C9	122.8 (4)
C3—C2—H2	120.8	C11—C10—H10	118.6
C1—C2—H2	120.8	C9—C10—H10	118.6
C4—C3—C2	122.6 (3)	C10—C11—C12	120.3 (3)
C4—C3—Cl1	119.1 (2)	C10—C11—H11	119.9
C2—C3—Cl1	118.4 (3)	C12—C11—H11	119.9
C5—C4—C3	118.4 (3)	C13—C12—C11	118.9 (4)
C5—C4—H4	120.8	C13—C12—H12	120.5
C3—C4—H4	120.8	C11—C12—H12	120.5
C4—C5—C6	120.8 (3)	C12—C13—C8	120.0 (4)
C4—C5—H5	119.6	C12—C13—H13	120.0
C6—C5—H5	119.6	C8—C13—H13	120.0
C1—C6—C5	119.7 (3)	C9—C14—H14A	109.5
C1—C6—H6	120.1	C9—C14—H14B	109.5
C5—C6—H6	120.1	H14A—C14—H14B	109.5
O1—C7—N1	123.8 (2)	C9—C14—H14C	109.5
O1—C7—C8	120.8 (2)	H14A—C14—H14C	109.5
N1—C7—C8	115.3 (2)	H14B—C14—H14C	109.5
C13—C8—C9	120.7 (3)	C7—N1—C1	128.3 (2)
C13—C8—C7	118.8 (3)	C7—N1—H1N	117 (2)
C9—C8—C7	120.5 (3)	C1—N1—H1N	115 (2)
C6—C1—C2—C3	0.5 (4)	C7—C8—C9—C10	174.9 (3)
N1—C1—C2—C3	177.7 (2)	C13—C8—C9—C14	179.4 (3)
C1—C2—C3—C4	−0.8 (4)	C7—C8—C9—C14	−3.6 (4)
C1—C2—C3—Cl1	179.1 (2)	C8—C9—C10—C11	0.9 (5)
C2—C3—C4—C5	0.7 (5)	C14—C9—C10—C11	179.5 (4)
Cl1—C3—C4—C5	−179.2 (3)	C9—C10—C11—C12	0.0 (6)
C3—C4—C5—C6	−0.4 (5)	C10—C11—C12—C13	0.3 (6)
C2—C1—C6—C5	−0.3 (5)	C11—C12—C13—C8	−1.4 (6)
N1—C1—C6—C5	−177.5 (3)	C9—C8—C13—C12	2.3 (5)
C4—C5—C6—C1	0.2 (6)	C7—C8—C13—C12	−174.7 (3)
O1—C7—C8—C13	121.7 (3)	O1—C7—N1—C1	−1.7 (4)
N1—C7—C8—C13	−56.8 (3)	C8—C7—N1—C1	176.9 (2)
O1—C7—C8—C9	−55.2 (3)	C6—C1—N1—C7	−160.9 (3)
N1—C7—C8—C9	126.2 (3)	C2—C1—N1—C7	21.9 (4)

C13—C8—C9—C10	−2.0 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1[i]	0.83 (4)	2.12 (4)	2.900 (3)	157 (3)

Symmetry code: (i) −*y*+1, *x*, *z*−1/4.