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## Structure Reports

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2-Chloro-*N*-(4-methylphenyl)benzamideVinola Z. Rodrigues,<sup>a</sup> Peter Herich,<sup>b</sup> B. Thimme Gowda<sup>a\*</sup> and Jozef Kožíšek<sup>b</sup>

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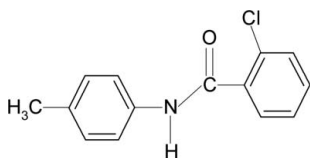
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.057;  $wR$  factor = 0.138; data-to-parameter ratio = 23.3.

In the title compound,  $\text{C}_{14}\text{H}_{12}\text{ClNO}$ , the *ortho*-Cl atom in the benzoyl ring is positioned *syn* to the  $\text{C}=\text{O}$  bond. The benzoyl and aniline benzene rings are tilted relative to each other by  $82.8(1)^\circ$ . In the crystal, intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into infinite chains running along the *c*-axis direction.

## Related literature

For the preparation of the title compound, see: Gowda *et al.* (2003). For studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Bowes *et al.* (2003); Gowda *et al.* (2000); Saeed *et al.* (2010), on *N*-(aryl)-methanesulfonamides, see: Gowda *et al.* (2007), on *N*-(aryl)-arylsulfonamides, see: Shetty & Gowda (2005) and on *N*-chloro-arylsulfonamides, see: Gowda & Shetty (2004).



## Experimental

## Crystal data

$\text{C}_{14}\text{H}_{12}\text{ClNO}$   
 $M_r = 245.70$   
Monoclinic,  $P2_1/c$   
 $a = 20.2969(14)$  Å  
 $b = 7.1850(5)$  Å  
 $c = 8.8662(5)$  Å  
 $\beta = 93.750(5)^\circ$

$V = 1290.22(15)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.28$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.92 \times 0.28 \times 0.07$  mm

## Data collection

Oxford Diffraction Xcalibur Ruby  
Gemini diffractometer  
Absorption correction: analytical  
[*CrysAlis RED* (Oxford  
Diffraction, 2009), based on  
expressions derived from Clark &  
Reid (1995)]  
 $T_{\min} = 0.911$ ,  $T_{\max} = 0.981$   
21209 measured reflections  
3594 independent reflections  
1870 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$   
 $wR(F^2) = 0.138$   
 $S = 1.03$   
3594 reflections  
154 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.35$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.42$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}^i$	0.86	2.01	2.847 (2)	165

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

PH and JK thank the VEGA Grant Agency of Slovak Ministry of Education 1/0679/11 and the Research and Development Agency of Slovakia (APVV-0202-10) for financial support and the Structural Funds, Interreg IIIA, for financial support in purchasing the diffractometer. VZR thanks the University Grants Commission, Government of India, New Delhi, for the award of an RFSMS research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5668).

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## supporting information

*Acta Cryst.* (2011). E67, o2940 [doi:10.1107/S1600536811041651]

## 2-Chloro-*N*-(4-methylphenyl)benzamide

Vinola Z. Rodrigues, Peter Herich, B. Thimme Gowda and Jozef Kožíšek

### S1. Comment

The amide and sulfonamide moieties are the constituents of many biologically significant compounds. As part of our studies on the substituent effects on the structures and other aspects of *N*-(aryl)-amides (Bowes *et al.*, 2003; Gowda *et al.*, 2000; Saeed *et al.*, 2010), *N*-(aryl)-methanesulfonamides (Gowda *et al.*, 2007), *N*-(aryl)-arylsulfonamides (Shetty & Gowda, 2005) and *N*-chloro-arylsulfonamides (Gowda & Shetty, 2004), in the present work, the crystal structure of 2-chloro-*N*-(4-methylphenyl)benzamide (I) has been determined (Fig.1).

In (I), the *ortho*-Cl atom in the benzoyl ring is positioned *syn* to the C=O bond and *anti* to the N-H bond of the C—NH—C(O)—C segment.

The central amide group —NHCO— is tilted to the anilino ring with the C9—C8—N1—C1 and C13—C8—N1—C1 torsion angles of  $-144.4(2)^\circ$  and  $35.6(3)^\circ$ . The C3—C2—C1—N1 and C7—C2—C1—N1 torsion angles are  $-118.8(2)^\circ$  and  $64.0(3)^\circ$ , respectively, while the C3—C2—C1—O1 and C7—C2—C1—O1 torsion angles are  $61.8(3)^\circ$  and  $-115.4(2)^\circ$ , respectively. But the C2—C1—N1—C8 and C8—N1—C1—O1 torsion angles are  $178.0(2)^\circ$  and  $-2.7(3)^\circ$ , respectively.

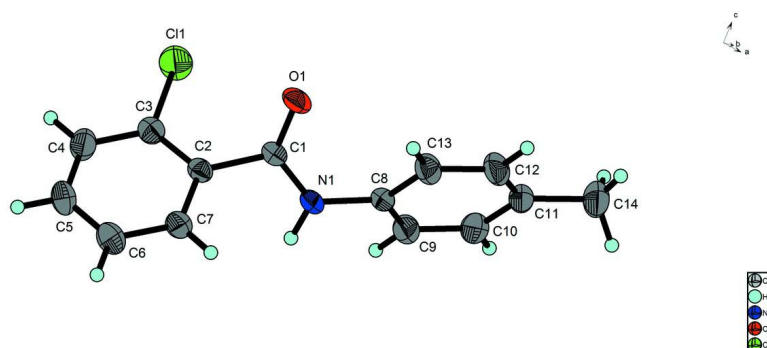
In the crystal structure, intermolecular N—H $\cdots$ O hydrogen bonds link the molecules into infinite chains running along the *c*-axis. Part of the crystal structure is shown in Fig. 2.

### S2. Experimental

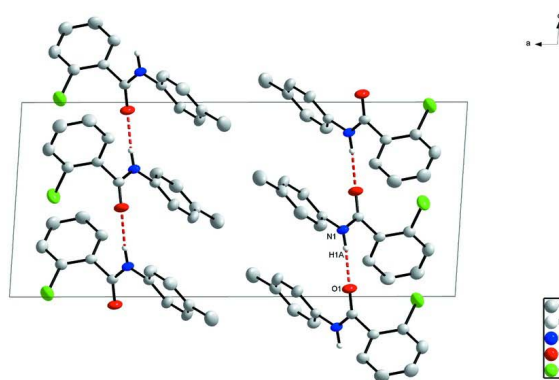
The title compound was prepared according to the method described by Gowda *et al.* (2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. Rod like colourless single crystals of the title compound used in X-ray diffraction studies were obtained by slow evaporation of an ethanol solution of the compound (0.5 g in 30 ml of ethanol) at room temperature.

### S3. Refinement

All hydrogen atoms were placed in calculated positions with C—H distances of 0.93 Å (C-aromatic), 0.96 Å (C-methyl), 0.86 Å (N-H) and constrained to ride on their parent atoms. The  $U_{\text{iso}}(\text{H})$  values were set at 1.2  $U_{\text{eq}}(\text{C-aromatic, N})$  and 1.5  $U_{\text{eq}}(\text{C-methyl})$ .

**Figure 1**

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

**Figure 2**

Part of the crystal structure of the title compound. Molecular chains are generated by N—H...O hydrogen bonds which are shown by dashed lines. H atoms not involved in intermolecular bonding have been omitted.

## 2-Chloro-*N*-(4-methylphenyl)benzamide

### Crystal data

$C_{14}H_{12}ClNO$

$M_r = 245.70$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 20.2969\ (14)\ \text{\AA}$

$b = 7.1850\ (5)\ \text{\AA}$

$c = 8.8662\ (5)\ \text{\AA}$

$\beta = 93.750\ (5)^\circ$

$V = 1290.22\ (15)\ \text{\AA}^3$

$Z = 4$

$F(000) = 512$

$D_x = 1.265\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3776 reflections

$\theta = 3.5\text{--}29.5^\circ$

$\mu = 0.28\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Rod, colorless

$0.92 \times 0.28 \times 0.07\ \text{mm}$

*Data collection*

Oxford Diffraction Xcalibur Ruby Gemini diffractometer  
 Radiation source: Enhance (Mo) X-ray Source  
 Graphite monochromator  
 Detector resolution: 10.4340 pixels mm<sup>-1</sup>  
 $\omega$  scans  
 Absorption correction: analytical  
 [CrysAlis RED (Oxford Diffraction, 2009),  
 based on expressions derived from Clark & Reid (1995)]

$T_{\min} = 0.911$ ,  $T_{\max} = 0.981$   
 21209 measured reflections  
 3594 independent reflections  
 1870 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$   
 $\theta_{\max} = 29.5^\circ$ ,  $\theta_{\min} = 3.5^\circ$   
 $h = -28 \rightarrow 28$   
 $k = -9 \rightarrow 9$   
 $l = -12 \rightarrow 12$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.057$   
 $wR(F^2) = 0.138$   
 $S = 1.03$   
 3594 reflections  
 154 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.4284P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$

*Special details*

**Experimental.** CrysAlis RED (Oxford Diffraction, 2009) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived (Clark & Reid, 1995).

**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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.22887 (10)	0.1405 (3)	0.4095 (2)	0.0490 (5)
C2	0.17841 (10)	0.0438 (3)	0.30648 (19)	0.0481 (5)
C3	0.11200 (11)	0.0438 (3)	0.3330 (2)	0.0568 (5)
C4	0.06674 (12)	-0.0529 (4)	0.2409 (3)	0.0719 (6)
H4A	0.0221	-0.0500	0.2589	0.086*
C5	0.08826 (14)	-0.1534 (4)	0.1225 (3)	0.0820 (8)
H5A	0.0581	-0.2215	0.0614	0.098*
C6	0.15356 (14)	-0.1548 (4)	0.0931 (3)	0.0808 (8)
H6A	0.1675	-0.2227	0.0118	0.097*
C7	0.19841 (11)	-0.0560 (3)	0.1836 (2)	0.0616 (6)
H7A	0.2427	-0.0559	0.1624	0.074*
C8	0.31056 (9)	0.3950 (3)	0.4145 (2)	0.0524 (5)
C9	0.31260 (12)	0.5767 (4)	0.3668 (3)	0.0693 (6)

H9A	0.2826	0.6178	0.2901	0.083*
C10	0.35880 (13)	0.6989 (4)	0.4316 (3)	0.0797 (7)
H10A	0.3590	0.8218	0.3987	0.096*
C11	0.40448 (12)	0.6430 (4)	0.5435 (3)	0.0757 (7)
C12	0.40141 (11)	0.4610 (5)	0.5898 (3)	0.0802 (8)
H12A	0.4315	0.4201	0.6664	0.096*
C13	0.35533 (11)	0.3354 (4)	0.5273 (2)	0.0668 (6)
H13A	0.3548	0.2130	0.5612	0.080*
C14	0.45614 (15)	0.7752 (5)	0.6112 (3)	0.1150 (12)
H14C	0.4833	0.7117	0.6876	0.138*
H14B	0.4349	0.8791	0.6556	0.138*
H14A	0.4831	0.8187	0.5335	0.138*
N1	0.26167 (8)	0.2768 (2)	0.34391 (17)	0.0544 (4)
H1A	0.2521	0.2947	0.2491	0.065*
O1	0.23840 (8)	0.0938 (2)	0.54154 (14)	0.0692 (5)
Cl1	0.08462 (3)	0.17186 (12)	0.48200 (8)	0.0953 (3)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0552 (11)	0.0531 (12)	0.0382 (10)	0.0015 (10)	-0.0008 (8)	-0.0014 (9)
C2	0.0600 (12)	0.0441 (11)	0.0395 (10)	-0.0023 (9)	-0.0016 (8)	0.0020 (9)
C3	0.0613 (13)	0.0547 (13)	0.0540 (11)	0.0004 (10)	0.0018 (10)	-0.0008 (10)
C4	0.0613 (14)	0.0739 (16)	0.0796 (16)	-0.0134 (12)	-0.0017 (12)	-0.0015 (14)
C5	0.0859 (19)	0.0788 (18)	0.0796 (17)	-0.0274 (15)	-0.0074 (14)	-0.0225 (14)
C6	0.096 (2)	0.0765 (18)	0.0701 (15)	-0.0153 (15)	0.0047 (14)	-0.0292 (14)
C7	0.0690 (14)	0.0618 (14)	0.0541 (12)	-0.0077 (11)	0.0048 (10)	-0.0105 (11)
C8	0.0491 (11)	0.0684 (15)	0.0396 (10)	-0.0058 (10)	0.0023 (8)	-0.0047 (10)
C9	0.0732 (15)	0.0747 (17)	0.0586 (13)	-0.0149 (13)	-0.0072 (11)	0.0063 (12)
C10	0.0863 (18)	0.0782 (18)	0.0751 (16)	-0.0268 (15)	0.0082 (14)	-0.0070 (14)
C11	0.0594 (14)	0.104 (2)	0.0648 (15)	-0.0233 (14)	0.0090 (12)	-0.0228 (15)
C12	0.0530 (14)	0.116 (2)	0.0688 (15)	0.0004 (15)	-0.0146 (11)	-0.0135 (16)
C13	0.0573 (13)	0.0780 (16)	0.0631 (13)	0.0035 (12)	-0.0111 (11)	-0.0031 (12)
C14	0.085 (2)	0.156 (3)	0.105 (2)	-0.051 (2)	0.0105 (17)	-0.046 (2)
N1	0.0606 (10)	0.0670 (11)	0.0341 (8)	-0.0105 (9)	-0.0069 (7)	0.0021 (8)
O1	0.0919 (11)	0.0781 (11)	0.0360 (7)	-0.0142 (9)	-0.0084 (7)	0.0082 (7)
Cl1	0.0758 (5)	0.1171 (6)	0.0947 (5)	0.0072 (4)	0.0185 (4)	-0.0381 (4)

*Geometric parameters (Å, °)*

C1—O1	1.221 (2)	C8—C13	1.375 (3)
C1—N1	1.339 (2)	C8—N1	1.420 (2)
C1—C2	1.498 (3)	C9—C10	1.382 (3)
C2—C3	1.383 (3)	C9—H9A	0.9300
C2—C7	1.387 (3)	C10—C11	1.373 (4)
C3—C4	1.377 (3)	C10—H10A	0.9300
C3—Cl1	1.731 (2)	C11—C12	1.373 (4)
C4—C5	1.369 (3)	C11—C14	1.510 (3)

C4—H4A	0.9300	C12—C13	1.389 (3)
C5—C6	1.368 (4)	C12—H12A	0.9300
C5—H5A	0.9300	C13—H13A	0.9300
C6—C7	1.372 (3)	C14—H14C	0.9600
C6—H6A	0.9300	C14—H14B	0.9600
C7—H7A	0.9300	C14—H14A	0.9600
C8—C9	1.374 (3)	N1—H1A	0.8600
O1—C1—N1	124.43 (18)	C8—C9—C10	120.6 (2)
O1—C1—C2	121.11 (18)	C8—C9—H9A	119.7
N1—C1—C2	114.45 (15)	C10—C9—H9A	119.7
C3—C2—C7	118.16 (18)	C11—C10—C9	121.5 (3)
C3—C2—C1	122.10 (17)	C11—C10—H10A	119.3
C7—C2—C1	119.68 (18)	C9—C10—H10A	119.3
C4—C3—C2	121.3 (2)	C10—C11—C12	116.9 (2)
C4—C3—C11	119.06 (18)	C10—C11—C14	121.5 (3)
C2—C3—C11	119.65 (16)	C12—C11—C14	121.6 (3)
C5—C4—C3	119.1 (2)	C11—C12—C13	122.8 (2)
C5—C4—H4A	120.4	C11—C12—H12A	118.6
C3—C4—H4A	120.4	C13—C12—H12A	118.6
C6—C5—C4	120.8 (2)	C8—C13—C12	118.9 (3)
C6—C5—H5A	119.6	C8—C13—H13A	120.5
C4—C5—H5A	119.6	C12—C13—H13A	120.5
C5—C6—C7	119.9 (2)	C11—C14—H14C	109.5
C5—C6—H6A	120.0	C11—C14—H14B	109.5
C7—C6—H6A	120.0	H14C—C14—H14B	109.5
C6—C7—C2	120.7 (2)	C11—C14—H14A	109.5
C6—C7—H7A	119.7	H14C—C14—H14A	109.5
C2—C7—H7A	119.7	H14B—C14—H14A	109.5
C9—C8—C13	119.2 (2)	C1—N1—C8	126.81 (15)
C9—C8—N1	117.82 (18)	C1—N1—H1A	116.6
C13—C8—N1	122.9 (2)	C8—N1—H1A	116.6
O1—C1—C2—C3	61.8 (3)	C13—C8—C9—C10	-0.4 (3)
N1—C1—C2—C3	-118.8 (2)	N1—C8—C9—C10	179.6 (2)
O1—C1—C2—C7	-115.4 (2)	C8—C9—C10—C11	0.9 (4)
N1—C1—C2—C7	63.9 (2)	C9—C10—C11—C12	-1.1 (4)
C7—C2—C3—C4	0.3 (3)	C9—C10—C11—C14	178.3 (3)
C1—C2—C3—C4	-177.0 (2)	C10—C11—C12—C13	0.8 (4)
C7—C2—C3—C11	-178.22 (16)	C14—C11—C12—C13	-178.6 (2)
C1—C2—C3—C11	4.5 (3)	C9—C8—C13—C12	0.0 (3)
C2—C3—C4—C5	1.1 (4)	N1—C8—C13—C12	-180.0 (2)
C11—C3—C4—C5	179.6 (2)	C11—C12—C13—C8	-0.2 (4)
C3—C4—C5—C6	-1.6 (4)	O1—C1—N1—C8	-2.7 (3)
C4—C5—C6—C7	0.6 (4)	C2—C1—N1—C8	178.00 (18)
C5—C6—C7—C2	0.9 (4)	C9—C8—N1—C1	-144.4 (2)
C3—C2—C7—C6	-1.3 (3)	C13—C8—N1—C1	35.6 (3)
C1—C2—C7—C6	176.0 (2)		

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*Hydrogen-bond geometry (Å, °)*

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<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—H1A $\cdots$ O1 <sup>i</sup>	0.86	2.01	2.847 (2)	165

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Symmetry code: (i)  $x, -y+1/2, z-1/2$ .