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3-Chloro-*N*-(2-chlorophenyl)benzamide

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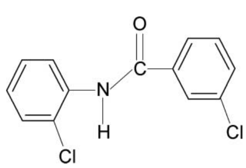
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.118; data-to-parameter ratio = 21.2.

In the title compound, $C_{13}H_9Cl_2NO$, the *meta*-Cl atom in the benzoyl ring is positioned *anti* to the C=O bond, while the *ortho*-Cl atom in the aniline ring is positioned *syn* to the N—H bond. The two aromatic rings are almost coplanar, making a dihedral angle of 4.73 (5)°. The crystal structure is stabilized by N—H···O hydrogen bonds, which link the molecules into chains along the *b* axis.

Related literature

For the preparation of the title compound, see: Gowda *et al.* (2008). For our studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Gowda *et al.* (2000, 2008); Bowes *et al.* (2003); Saeed *et al.* (2010), on *N*-(aryl)-methanesulfonamides, see: Jayalakshmi & Gowda (2004), on *N*-(aryl)-arylsulfonamides, see: Shetty & Gowda (2005) and on *N*-chloroarylamides, see: Gowda *et al.* (1996).



Experimental

Crystal data

$C_{13}H_9Cl_2NO$
M_r = 266.11
Monoclinic, $P2_1/n$
a = 11.1371 (4) Å
b = 4.85230 (17) Å
c = 21.5198 (8) Å
β = 90.142 (3)°
V = 1162.94 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 293 K
0.66 × 0.30 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2009), based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.824, T_{max} = 0.958
22845 measured reflections
3262 independent reflections
2279 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.118
S = 1.07
3262 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 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	0.86	2.14	2.9157 (17)	151

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2157).

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supplementary materials

Acta Cryst. (2012). E**68**, o49 [**doi:10.1107/S1600536811051944**]

3-Chloro-*N*-(2-chlorophenyl)benzamide

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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 (Gowda *et al.*, 2000, 2008; Bowes *et al.*, 2003; Saeed *et al.*, 2010), *N*-(aryl)-methanesulfonamides (Jayalakshmi & Gowda, 2004), *N*-(aryl)-arylsulfonamides (Shetty & Gowda, 2005) and *N*-chloro-arylamides (Gowda *et al.*, 1996), in the present work, the crystal structure of 3-Chloro-*N*-(2-chlorophenyl)benzamide (I) has been determined (Fig.1).

In (I), the *meta*-Cl atom in the benzoyl ring is positioned *anti* to the C=O bond, while the *ortho*-Cl group in the anilino ring is positioned *syn* to the N—H bond, the N—H and C=O bonds in the C—NH—C(O)—C segment being *anti* to each other.

Further, the two aromatic rings are nearly coplanar with the dihedral angle of 4.73 (5)°, compared to the values of 9.1 (2)° and 7.3 (3)° in the two independent molecules of 3-chloro-*N*-(3-chlorophenyl)benzamide (Gowda *et al.*, 2008).

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

Experimental

The title compound was prepared according to the method described by Gowda *et al.* (2008). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra.

Rod like colorless 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 about 30 ml of ethanol) at room temperature.

Refinement

All H atoms were visible in difference maps and then treated as riding atoms with C–H distances of 0.93Å (C-aromatic) and N—H = 0.86 Å. The U_{iso}(H) values were set at 1.2 U_{eq}(C-aromatic, N).

Figures

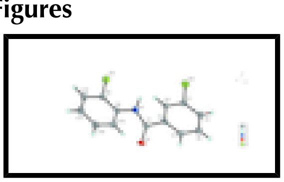

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

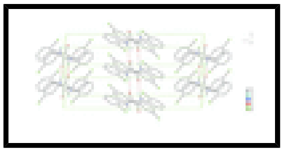

Fig. 2. Part of the crystal structure of the title compound. Molecular chains are generated by N—H···O hydrogen bonds which are shown by dashed lines.

3-Chloro-*N*-(2-chlorophenyl)benzamide

Crystal data

$C_{13}H_9Cl_2NO$	$F(000) = 544$
$M_r = 266.11$	$D_x = 1.520$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 11869 reflections
$a = 11.1371$ (4) Å	$\theta = 3.4$–29.6°
$b = 4.85230$ (17) Å	$\mu = 0.54$ mm^{-1}
$c = 21.5198$ (8) Å	$T = 293$ K
$\beta = 90.142$ (3)°	Rod, colorless
$V = 1162.94$ (7) Å^3	0.66 × 0.30 × 0.08 mm
$Z = 4$	

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer	3262 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2279 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.034$
Detector resolution: 10.4340 pixels mm^{-1}	$\theta_{max} = 29.6°$, $\theta_{min} = 3.4°$
ω scans	$h = -15 \rightarrow 15$
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2009), based on expressions derived by Clark & Reid (1995)]	$k = -6 \rightarrow 6$
$T_{min} = 0.824$, $T_{max} = 0.958$	$l = -29 \rightarrow 29$
22845 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.038$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.118$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0694P)^2 + 0.1106P]$ where $P = (F_o^2 + 2F_c^2)/3$
3262 reflections	$(\Delta/\sigma)_{max} < 0.001$
154 parameters	$\Delta\rho_{max} = 0.31$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.26$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.28710 (14)	0.3142 (3)	0.01071 (8)	0.0380 (4)
C2	0.34075 (14)	0.4188 (3)	−0.04824 (7)	0.0375 (3)
C3	0.28456 (14)	0.6171 (3)	−0.08504 (7)	0.0376 (3)
H3A	0.2115	0.6930	−0.0731	0.045*
C4	0.33904 (15)	0.6991 (3)	−0.13953 (7)	0.0389 (4)
C5	0.44901 (16)	0.5933 (4)	−0.15784 (8)	0.0454 (4)
H5A	0.4854	0.6537	−0.1942	0.055*
C6	0.50336 (16)	0.3967 (4)	−0.12103 (9)	0.0476 (4)
H6A	0.5772	0.3240	−0.1327	0.057*
C7	0.44943 (15)	0.3067 (3)	−0.06703 (8)	0.0421 (4)
H7A	0.4860	0.1705	−0.0432	0.050*
C8	0.16652 (14)	0.4468 (3)	0.10141 (7)	0.0363 (3)
C9	0.05966 (15)	0.5829 (3)	0.11471 (7)	0.0380 (4)
C10	−0.00095 (17)	0.5387 (4)	0.16973 (9)	0.0498 (4)
H10A	−0.0719	0.6328	0.1778	0.060*
C11	0.04410 (19)	0.3552 (4)	0.21236 (9)	0.0553 (5)
H11A	0.0032	0.3235	0.2493	0.066*
C12	0.15079 (18)	0.2166 (4)	0.20030 (9)	0.0518 (5)
H12A	0.1816	0.0925	0.2292	0.062*
C13	0.21073 (16)	0.2639 (4)	0.14537 (8)	0.0450 (4)
H13A	0.2823	0.1713	0.1376	0.054*
N1	0.22659 (12)	0.5014 (3)	0.04507 (6)	0.0378 (3)
H1A	0.2245	0.6679	0.0314	0.045*
O1	0.29906 (12)	0.0726 (2)	0.02617 (6)	0.0521 (3)
Cl1	−0.00096 (4)	0.81078 (10)	0.06110 (2)	0.05256 (16)
Cl2	0.26902 (4)	0.94011 (10)	−0.18730 (2)	0.05402 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1	0.0412 (8)	0.0296 (8)	0.0432 (9)	−0.0022 (6)	0.0019 (7)	0.0005 (6)
C2	0.0435 (8)	0.0289 (7)	0.0400 (8)	−0.0024 (6)	0.0023 (7)	−0.0034 (6)
C3	0.0408 (8)	0.0315 (7)	0.0406 (8)	0.0012 (6)	0.0042 (7)	−0.0026 (6)
C4	0.0462 (9)	0.0320 (8)	0.0384 (8)	−0.0015 (7)	−0.0005 (7)	−0.0016 (6)
C5	0.0499 (9)	0.0456 (9)	0.0409 (9)	−0.0042 (8)	0.0093 (7)	−0.0007 (7)
C6	0.0416 (9)	0.0484 (10)	0.0529 (10)	0.0025 (8)	0.0084 (8)	−0.0044 (8)
C7	0.0432 (9)	0.0381 (9)	0.0448 (9)	0.0036 (7)	0.0002 (7)	−0.0020 (7)
C8	0.0407 (8)	0.0285 (7)	0.0397 (8)	−0.0044 (6)	0.0024 (6)	0.0018 (6)
C9	0.0422 (8)	0.0317 (8)	0.0402 (8)	0.0002 (7)	0.0001 (7)	0.0034 (6)
C10	0.0500 (10)	0.0503 (10)	0.0492 (10)	0.0021 (8)	0.0120 (8)	0.0012 (8)
C11	0.0672 (12)	0.0553 (11)	0.0435 (10)	−0.0023 (10)	0.0150 (9)	0.0090 (8)
C12	0.0654 (12)	0.0467 (10)	0.0433 (10)	−0.0013 (9)	0.0004 (8)	0.0110 (8)
C13	0.0477 (9)	0.0392 (8)	0.0481 (10)	0.0041 (7)	0.0003 (7)	0.0070 (7)
N1	0.0467 (7)	0.0268 (6)	0.0398 (7)	0.0008 (5)	0.0065 (6)	0.0043 (5)
O1	0.0702 (8)	0.0258 (6)	0.0603 (8)	0.0037 (5)	0.0152 (6)	0.0042 (5)
Cl1	0.0524 (3)	0.0506 (3)	0.0547 (3)	0.0111 (2)	0.0019 (2)	0.01349 (19)
Cl2	0.0654 (3)	0.0488 (3)	0.0479 (3)	0.0055 (2)	0.0006 (2)	0.01029 (19)

Geometric parameters (Å, °)

C1—O1	1.2257 (19)	C8—C13	1.387 (2)
C1—N1	1.352 (2)	C8—C9	1.391 (2)
C1—C2	1.493 (2)	C8—N1	1.411 (2)
C2—C7	1.388 (2)	C9—C10	1.381 (2)
C2—C3	1.393 (2)	C9—Cl1	1.7337 (16)
C3—C4	1.380 (2)	C10—C11	1.373 (3)
C3—H3A	0.9300	C10—H10A	0.9300
C4—C5	1.386 (2)	C11—C12	1.390 (3)
C4—Cl2	1.7404 (16)	C11—H11A	0.9300
C5—C6	1.379 (3)	C12—C13	1.378 (3)
C5—H5A	0.9300	C12—H12A	0.9300
C6—C7	1.380 (3)	C13—H13A	0.9300
C6—H6A	0.9300	N1—H1A	0.8600
C7—H7A	0.9300		
O1—C1—N1	123.23 (15)	C13—C8—C9	117.77 (15)
O1—C1—C2	120.84 (15)	C13—C8—N1	122.54 (15)
N1—C1—C2	115.93 (13)	C9—C8—N1	119.69 (14)
C7—C2—C3	119.73 (15)	C10—C9—C8	121.52 (15)
C7—C2—C1	117.73 (14)	C10—C9—Cl1	118.63 (13)
C3—C2—C1	122.53 (14)	C8—C9—Cl1	119.84 (12)
C4—C3—C2	118.95 (15)	C11—C10—C9	119.68 (17)
C4—C3—H3A	120.5	C11—C10—H10A	120.2
C2—C3—H3A	120.5	C9—C10—H10A	120.2
C3—C4—C5	121.70 (15)	C10—C11—C12	120.00 (17)
C3—C4—Cl2	119.88 (13)	C10—C11—H11A	120.0
C5—C4—Cl2	118.41 (13)	C12—C11—H11A	120.0
C6—C5—C4	118.66 (16)	C13—C12—C11	119.71 (17)
C6—C5—H5A	120.7	C13—C12—H12A	120.1
C4—C5—H5A	120.7	C11—C12—H12A	120.1

C5—C6—C7	120.75 (16)	C12—C13—C8	121.31 (17)
C5—C6—H6A	119.6	C12—C13—H13A	119.3
C7—C6—H6A	119.6	C8—C13—H13A	119.3
C6—C7—C2	120.17 (16)	C1—N1—C8	125.58 (13)
C6—C7—H7A	119.9	C1—N1—H1A	117.2
C2—C7—H7A	119.9	C8—N1—H1A	117.2

O1—C1—C2—C7	−34.2 (2)	N1—C8—C9—C10	−178.97 (16)
N1—C1—C2—C7	145.40 (15)	C13—C8—C9—Cl1	−179.20 (13)
O1—C1—C2—C3	144.21 (17)	N1—C8—C9—Cl1	1.8 (2)
N1—C1—C2—C3	−36.2 (2)	C8—C9—C10—C11	−0.5 (3)
C7—C2—C3—C4	−0.4 (2)	Cl1—C9—C10—C11	178.75 (15)
C1—C2—C3—C4	−178.75 (14)	C9—C10—C11—C12	0.6 (3)
C2—C3—C4—C5	−1.3 (2)	C10—C11—C12—C13	−0.2 (3)
C2—C3—C4—Cl2	178.43 (11)	C11—C12—C13—C8	−0.3 (3)
C3—C4—C5—C6	1.5 (3)	C9—C8—C13—C12	0.4 (3)
Cl2—C4—C5—C6	−178.26 (14)	N1—C8—C13—C12	179.35 (16)
C4—C5—C6—C7	0.0 (3)	O1—C1—N1—C8	−2.0 (3)
C5—C6—C7—C2	−1.7 (3)	C2—C1—N1—C8	178.39 (14)
C3—C2—C7—C6	1.8 (2)	C13—C8—N1—C1	37.2 (2)
C1—C2—C7—C6	−179.71 (15)	C9—C8—N1—C1	−143.89 (16)
C13—C8—C9—C10	0.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.86	2.14	2.9157 (17)	151.

Symmetry codes: (i) *x*, *y*+1, *z*.

Fig. 1

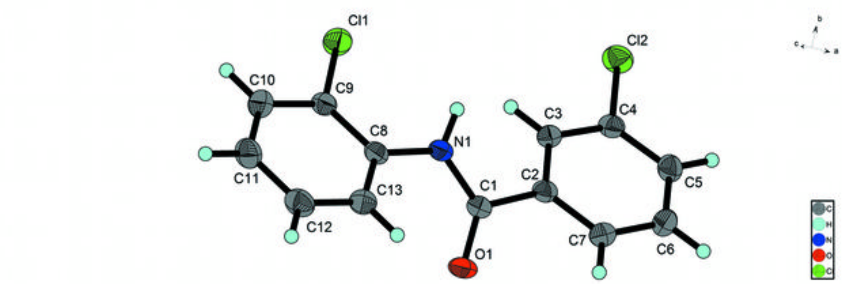

Fig. 2