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

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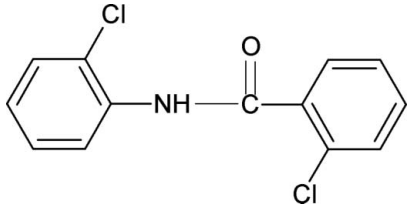
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.007 Å; R factor = 0.078; wR factor = 0.156; data-to-parameter ratio = 16.2.

The conformation of the N—H bond in the structure of the title compound, $C_{13}H_9Cl_2NO$, is *syn* to the *ortho*-Cl substituent in the aniline ring, similar to that observed in *N*-(2,3-dichlorophenyl)benzamide with respect to both the *ortho*-Cl and *meta*-Cl substituents, but in contrast to the *anti* conformation observed with respect to the *ortho*-Cl substituent in *N*-(2-chlorophenyl)benzamide. The bond parameters are similar to those in 2-chloro-*N*-phenylbenzamide and other benzanilides. The molecules are linked into chains in the direction of the *b* axis through N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2003, 2007*a*,*b*).



Experimental

Crystal data

$C_{13}H_9Cl_2NO$
M_r = 266.11
Orthorhombic, *Pbca*
a = 5.9466 (5) Å
b = 9.8323 (8) Å
c = 41.559 (3) Å
V = 2429.9 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 299 (2) K
0.50 × 0.50 × 0.40 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.777, T_{max} = 0.824
28151 measured reflections
2489 independent reflections
2116 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.156
S = 1.29
2489 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.86	2.04	2.896 (4)	172

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2470).

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supplementary materials

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

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Comment

In the present work, as part of a study of the substituent effects on the structures of N-aromatic amides (Gowda, Jyothi *et al.*, 2003; Gowda, Sowmya *et al.*, 2007*a*, *b*), the structure of *N*-(2-chlorophenyl)- 2-chlorobenzamide has been determined. The conformation of the N—H bond is *syn* to the *ortho*-Cl substituent in the aniline ring (Fig. 1), similar to that observed in *N*-(2,3-dichlorophenyl)-benzamide (Gowda, Sowmya *et al.*, 2007*b*) with respect to both the *ortho*-Cl and *meta*-Cl substituents, but in contrast to the *anti* conformation observed with respect to the *ortho*-Cl substituent in *N*-(2-chlorophenyl)-benzamide (Gowda, Sowmya *et al.*, 2007*a*). The bond parameters are similar to those in *N*-(phenyl)-2-chlorobenzamide (Gowda, Jyothi *et al.*,2003) and other benzanilides. The crystal packing is characterized by N—H¨¨O hydrogen bonds (Table 1) leading to chains in the direction of the *b* axis (Fig. 2).

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.

Refinement

The H atoms were positioned geometrically and including in the refinement in the riding-model approximation, with C—H = 0.93 Å, N—H = 0.86 Å and with U_{iso}(H) = 1.2 U_{eq} of the parent atom.

Figures

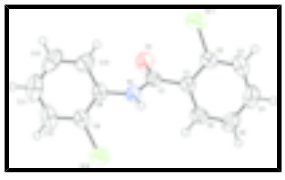

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

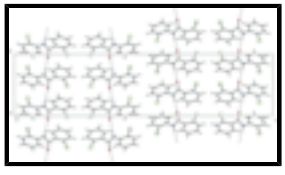

Fig. 2. Molecular packing of the title compound with hydrogen bonds shown as dashed lines.

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

Crystal data

$C_{13}H_9Cl_2NO$	F_{000} = 1088
M_r = 266.11	D_x = 1.455 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 6575 reflections
a = 5.9466 (5) Å	θ = 3.0–27.6º
b = 9.8323 (8) Å	μ = 0.52 mm^{-1}
c = 41.559 (3) Å	*T* = 299 (2) K
V = 2429.9 (3) Å^3	Prism, colourless
Z = 8	0.50 × 0.50 × 0.40 mm

Data collection

Oxford Diffraction Xcalibur single-crystal X-ray diffractometer with Sapphire CCD detector	2489 independent reflections
Radiation source: fine-focus sealed tube	2116 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 299(2) K	θ_{max} = 26.4º
Rotation method data acquisition using ω and phi scans.	θ_{min} = 4.1º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	*h* = −7→7
T_{min} = 0.777, T_{max} = 0.824	*k* = −12→12
28151 measured reflections	*l* = −51→51

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.078	H-atom parameters constrained
$wR(F^2)$ = 0.156	$w = 1/[\sigma^2(F_o^2) + (0.0123P)^2 + 6.6653P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.29	$(\Delta/\sigma)_{max} < 0.001$
2489 reflections	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
154 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.0524 (7)	0.1362 (4)	0.15997 (9)	0.0383 (9)
C2	0.0696 (7)	0.0990 (4)	0.19211 (9)	0.0440 (10)
C3	−0.0719 (9)	0.1534 (5)	0.21502 (11)	0.0616 (13)
H3	−0.0573	0.1287	0.2365	0.074*
C4	−0.2344 (10)	0.2444 (6)	0.20579 (12)	0.0677 (14)
H4	−0.3306	0.2805	0.2212	0.081*
C5	−0.2581 (9)	0.2836 (5)	0.17411 (12)	0.0629 (13)
H5	−0.3690	0.3452	0.1681	0.076*
C6	−0.1136 (8)	0.2293 (4)	0.15167 (10)	0.0504 (11)
H6	−0.1274	0.2557	0.1303	0.061*
C7	0.1937 (7)	0.0726 (4)	0.13436 (9)	0.0419 (9)
C8	0.4467 (7)	0.1213 (4)	0.08982 (9)	0.0400 (9)
C9	0.4116 (8)	0.1720 (4)	0.05922 (9)	0.0457 (10)
C10	0.5503 (10)	0.1354 (6)	0.03421 (12)	0.0685 (15)
H10	0.5260	0.1703	0.0137	0.082*
C11	0.7245 (12)	0.0472 (6)	0.03968 (16)	0.0831 (19)
H11	0.8175	0.0215	0.0227	0.100*
C12	0.7632 (10)	−0.0038 (5)	0.07010 (16)	0.0742 (16)
H12	0.8824	−0.0631	0.0738	0.089*
C13	0.6235 (8)	0.0338 (4)	0.09495 (12)	0.0560 (12)
H13	0.6491	−0.0004	0.1155	0.067*
Cl1	0.2734 (3)	−0.01613 (14)	0.20427 (3)	0.0688 (4)
Cl2	0.1935 (2)	0.28517 (14)	0.05234 (3)	0.0700 (4)
N1	0.3050 (6)	0.1613 (3)	0.11571 (7)	0.0430 (8)
H1N	0.2899	0.2467	0.1196	0.052*
O1	0.2008 (6)	−0.0508 (3)	0.13050 (7)	0.0597 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.050 (2)	0.0260 (17)	0.0387 (19)	−0.0059 (17)	0.0031 (18)	−0.0024 (15)
C2	0.051 (2)	0.038 (2)	0.043 (2)	−0.008 (2)	−0.0042 (19)	0.0003 (18)
C3	0.080 (4)	0.064 (3)	0.041 (2)	−0.012 (3)	0.013 (2)	0.000 (2)
C4	0.070 (3)	0.063 (3)	0.071 (3)	0.000 (3)	0.026 (3)	−0.013 (3)
C5	0.063 (3)	0.049 (3)	0.077 (3)	0.010 (3)	0.010 (3)	−0.005 (3)
C6	0.067 (3)	0.035 (2)	0.049 (2)	0.002 (2)	0.000 (2)	0.0049 (19)
C7	0.055 (3)	0.035 (2)	0.036 (2)	−0.0010 (19)	−0.0031 (18)	0.0005 (16)

C8	0.050 (2)	0.0297 (19)	0.041 (2)	−0.0057 (18)	0.0048 (18)	−0.0046 (16)
C9	0.055 (3)	0.041 (2)	0.041 (2)	−0.010 (2)	0.0023 (19)	−0.0036 (17)
C10	0.085 (4)	0.072 (3)	0.048 (3)	−0.021 (3)	0.020 (3)	−0.011 (2)
C11	0.083 (4)	0.079 (4)	0.088 (4)	−0.013 (4)	0.038 (4)	−0.031 (3)
C12	0.060 (3)	0.049 (3)	0.114 (5)	0.007 (3)	0.013 (3)	−0.020 (3)
C13	0.059 (3)	0.038 (2)	0.071 (3)	0.002 (2)	−0.001 (2)	−0.004 (2)
Cl1	0.0846 (9)	0.0649 (8)	0.0569 (7)	0.0116 (7)	−0.0214 (7)	0.0030 (6)
Cl2	0.0795 (9)	0.0737 (8)	0.0568 (7)	0.0097 (7)	−0.0141 (6)	0.0075 (6)
N1	0.062 (2)	0.0271 (15)	0.0403 (17)	0.0003 (16)	0.0064 (16)	−0.0027 (14)
O1	0.090 (3)	0.0259 (14)	0.0635 (19)	−0.0028 (16)	0.0167 (18)	−0.0053 (13)

Geometric parameters (Å, °)

C1—C2	1.389 (5)	C8—C13	1.375 (6)
C1—C6	1.389 (6)	C8—C9	1.382 (5)
C1—C7	1.493 (5)	C8—N1	1.422 (5)
C2—C3	1.379 (6)	C9—C10	1.375 (6)
C2—Cl1	1.734 (4)	C9—Cl2	1.733 (5)
C3—C4	1.372 (7)	C10—C11	1.370 (8)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.379 (7)	C11—C12	1.379 (8)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.376 (6)	C12—C13	1.376 (7)
C5—H5	0.9300	C12—H12	0.9300
C6—H6	0.9300	C13—H13	0.9300
C7—O1	1.225 (5)	N1—H1N	0.8600
C7—N1	1.341 (5)		
C2—C1—C6	117.7 (4)	C13—C8—C9	118.9 (4)
C2—C1—C7	122.3 (4)	C13—C8—N1	120.6 (4)
C6—C1—C7	119.9 (4)	C9—C8—N1	120.5 (4)
C3—C2—C1	121.1 (4)	C10—C9—C8	120.7 (5)
C3—C2—Cl1	118.6 (3)	C10—C9—Cl2	119.5 (4)
C1—C2—Cl1	120.3 (3)	C8—C9—Cl2	119.8 (3)
C4—C3—C2	119.3 (4)	C11—C10—C9	119.6 (5)
C4—C3—H3	120.3	C11—C10—H10	120.2
C2—C3—H3	120.3	C9—C10—H10	120.2
C3—C4—C5	121.4 (5)	C10—C11—C12	120.5 (5)
C3—C4—H4	119.3	C10—C11—H11	119.7
C5—C4—H4	119.3	C12—C11—H11	119.7
C6—C5—C4	118.3 (5)	C13—C12—C11	119.3 (5)
C6—C5—H5	120.8	C13—C12—H12	120.3
C4—C5—H5	120.8	C11—C12—H12	120.3
C5—C6—C1	122.1 (4)	C8—C13—C12	120.9 (5)
C5—C6—H6	119.0	C8—C13—H13	119.6
C1—C6—H6	119.0	C12—C13—H13	119.6
O1—C7—N1	123.5 (4)	C7—N1—C8	123.3 (3)
O1—C7—C1	121.8 (4)	C7—N1—H1N	118.3
N1—C7—C1	114.7 (3)	C8—N1—H1N	118.3
C6—C1—C2—C3	−0.5 (6)	C13—C8—C9—C10	0.3 (6)

C7—C1—C2—C3	−176.1 (4)	N1—C8—C9—C10	178.9 (4)
C6—C1—C2—Cl1	−179.8 (3)	C13—C8—C9—Cl2	−178.7 (3)
C7—C1—C2—Cl1	4.6 (5)	N1—C8—C9—Cl2	0.0 (5)
C1—C2—C3—C4	0.9 (7)	C8—C9—C10—C11	0.3 (7)
Cl1—C2—C3—C4	−179.8 (4)	Cl2—C9—C10—C11	179.2 (4)
C2—C3—C4—C5	−0.6 (8)	C9—C10—C11—C12	−0.7 (8)
C3—C4—C5—C6	−0.2 (8)	C10—C11—C12—C13	0.6 (9)
C4—C5—C6—C1	0.6 (7)	C9—C8—C13—C12	−0.4 (6)
C2—C1—C6—C5	−0.2 (6)	N1—C8—C13—C12	−179.1 (4)
C7—C1—C6—C5	175.5 (4)	C11—C12—C13—C8	0.0 (8)
C2—C1—C7—O1	54.3 (6)	O1—C7—N1—C8	−1.2 (7)
C6—C1—C7—O1	−121.2 (5)	C1—C7—N1—C8	−179.4 (4)
C2—C1—C7—N1	−127.5 (4)	C13—C8—N1—C7	−56.3 (6)
C6—C1—C7—N1	57.0 (5)	C9—C8—N1—C7	125.0 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O1^{i}	0.86	2.04	2.896 (4)	172

Symmetry codes: (i) −*x*+1/2, *y*+1/2, *z*.

Fig. 1

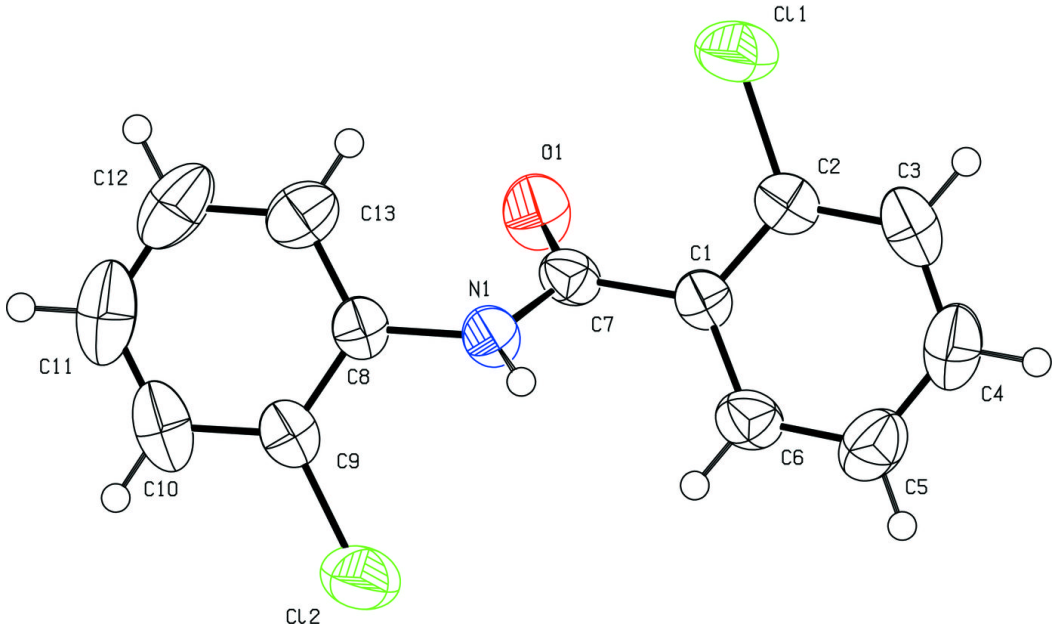

Fig. 2