

N-(3,5-Dichlorophenyl)benzamide

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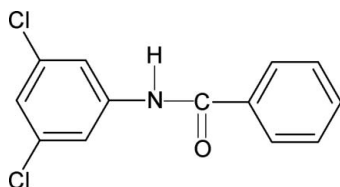
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Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.037; wR factor = 0.133; data-to-parameter ratio = 13.8.

The conformation of the $\text{H}-\text{N}-\text{C}=\text{O}$ unit in the title compound, $\text{C}_{13}\text{H}_9\text{Cl}_2\text{NO}$, is *trans*, similar to the conformation observed in *N*-(3-chlorophenyl)benzamide, *N*-(2,3-dichlorophenyl)benzamide, *N*-(2,4-dichlorophenyl)benzamide, *N*-(2,6-dichlorophenyl)benzamide and *N*-(3,4-dichlorophenyl)benzamide. The amide group makes dihedral angles of 14.3 (8) and 44.4 (4)° with the benzoyl and aniline rings, respectively, while the benzoyl and aniline rings form a dihedral angle of 58.3 (1)°. The molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into infinite chains running along the c axis.

Related literature

For related literature, see: Gowda *et al.* (2003, 2007, 2008*a,b*).



Experimental

Crystal data

$\text{C}_{13}\text{H}_9\text{Cl}_2\text{NO}$
 $M_r = 266.11$
Monoclinic, $P2_1/c$
 $a = 13.520$ (1) Å

$b = 9.9929$ (8) Å
 $c = 9.4447$ (7) Å
 $\beta = 106.357$ (9)°
 $V = 1224.37$ (16) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.51$ mm⁻¹

$T = 299$ (2) K
 $0.48 \times 0.36 \times 0.26$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford)

Diffraction, 2007)
 $T_{\min} = 0.792$, $T_{\max} = 0.879$
7774 measured reflections
2493 independent reflections
1837 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.133$
 $S = 1.12$
2493 reflections

181 parameters
Only H-atom coordinates refined
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O1}^i$	0.83 (3)	2.18 (3)	2.964 (2)	157 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2720).

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supplementary materials

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Comment

In the present work, the structure of *N*-(3,5-dichlorophenyl)-benzamide (N35DCPBA) has been determined to explore the effect of substituents on the solid state geometries of benzanilides (Gowda *et al.*, 2003, 2007, 2008*a*, 2008*b*). The conformation of the H-N-C=O unit in is *trans* (Fig. 1), similar to that observed in *N*-(3-chlorophenyl)-benzamide (Gowda *et al.*, 2008*a*), *N*-(2,3-dichlorophenyl)-benzamide and *N*-(3,4-dichlorophenyl)- benzamide (Gowda *et al.*, 2007), *N*-(2,4-dichlorophenyl)-benzamide and *N*-(2,6-dichlorophenyl)-benzamide(Gowda *et al.*, 2008*b*). The amide group –NHCO– makes the dihedral angles of 14.3 (8)° and 44.4 (4)° with the benzoyl and aniline rings, respectively, while the benzoyl and aniline rings form the dihedral angle of 58.3 (1)°. Part of the crystal structure of the title compound with infinite molecular chains running along the *c* axis is shown in Fig. 2. The chains are generated by N—H···O hydrogen bonds (Table 1)

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 located in a difference map, and their positional parameters were refined freely with U(H) set to 1.2U_{eq} of the parent atom.

Figures

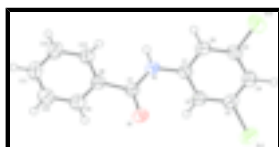


Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

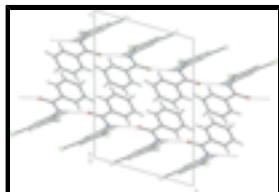


Fig. 2. Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

N-(3,5-Dichlorophenyl)benzamide

Crystal data

$C_{13}H_9Cl_2NO$	$F_{000} = 544$
$M_r = 266.11$	$D_x = 1.444 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 13.520 (1) \text{ \AA}$	Cell parameters from 3450 reflections
$b = 9.9929 (8) \text{ \AA}$	$\theta = 2.4\text{--}28.1^\circ$
$c = 9.4447 (7) \text{ \AA}$	$\mu = 0.51 \text{ mm}^{-1}$
$\beta = 106.357 (9)^\circ$	$T = 299 (2) \text{ K}$
$V = 1224.37 (16) \text{ \AA}^3$	Prism, colourless
$Z = 4$	$0.48 \times 0.36 \times 0.26 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector	2493 independent reflections
Radiation source: fine-focus sealed tube	1837 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.013$
$T = 299(2) \text{ K}$	$\theta_{\text{max}} = 26.4^\circ$
Rotation method data acquisition using ω and φ scans	$\theta_{\text{min}} = 2.6^\circ$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$h = -12 \rightarrow 16$
$T_{\text{min}} = 0.792$, $T_{\text{max}} = 0.879$	$k = -12 \rightarrow 12$
7774 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Only H-atom coordinates refined
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.5267P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
2493 reflections	$(\Delta/\sigma)_{\text{max}} = 0.010$
181 parameters	$\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$
	Extinction correction: none

Special details

Experimental. (CrysAlis RED; Oxford Diffraction, 2007) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.18869 (16)	0.6454 (2)	0.5651 (2)	0.0370 (5)
C2	0.11990 (16)	0.6605 (2)	0.4259 (2)	0.0389 (5)
H2	0.1002 (18)	0.753 (2)	0.384 (3)	0.047*
C3	0.07367 (17)	0.5473 (2)	0.3519 (2)	0.0412 (5)
C4	0.09118 (18)	0.4206 (2)	0.4131 (3)	0.0452 (5)
H4	0.0558 (19)	0.332 (3)	0.354 (3)	0.054*
C5	0.15740 (19)	0.4104 (2)	0.5533 (3)	0.0446 (5)
C6	0.20746 (18)	0.5197 (2)	0.6309 (2)	0.0429 (5)
H6	0.2544 (19)	0.506 (3)	0.726 (3)	0.051*
C7	0.29164 (16)	0.8484 (2)	0.5806 (2)	0.0357 (4)
C8	0.34903 (16)	0.9572 (2)	0.6776 (2)	0.0358 (5)
C9	0.4140 (2)	1.0369 (3)	0.6232 (3)	0.0525 (6)
H9	0.419 (2)	1.022 (3)	0.530 (4)	0.063*
C10	0.4693 (2)	1.1390 (3)	0.7066 (3)	0.0628 (7)
H10	0.509 (2)	1.189 (3)	0.663 (3)	0.075*
C11	0.4590 (2)	1.1653 (3)	0.8447 (3)	0.0601 (7)
H11	0.497 (2)	1.235 (3)	0.898 (3)	0.072*
C12	0.3940 (2)	1.0892 (3)	0.8994 (3)	0.0573 (7)
H12	0.379 (2)	1.110 (3)	0.989 (3)	0.069*
C13	0.33965 (19)	0.9850 (2)	0.8168 (2)	0.0450 (5)
H13	0.296 (2)	0.942 (3)	0.852 (3)	0.054*
N1	0.24216 (15)	0.75725 (18)	0.64286 (19)	0.0395 (4)
H1N	0.2559 (19)	0.753 (2)	0.734 (3)	0.047*
O1	0.29162 (14)	0.84106 (17)	0.45101 (16)	0.0518 (4)
Cl1	-0.00774 (6)	0.56249 (7)	0.17406 (7)	0.0640 (2)
Cl2	0.18142 (6)	0.25339 (6)	0.63392 (8)	0.0716 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0448 (11)	0.0354 (10)	0.0335 (10)	-0.0010 (9)	0.0157 (9)	-0.0022 (8)
C2	0.0456 (12)	0.0359 (11)	0.0347 (10)	0.0036 (9)	0.0103 (9)	0.0004 (9)
C3	0.0435 (12)	0.0443 (12)	0.0335 (10)	0.0036 (9)	0.0071 (9)	-0.0037 (9)
C4	0.0516 (13)	0.0381 (12)	0.0453 (12)	-0.0011 (10)	0.0129 (10)	-0.0066 (10)
C5	0.0552 (13)	0.0331 (11)	0.0468 (12)	0.0031 (10)	0.0163 (10)	0.0038 (9)

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C6	0.0512 (13)	0.0432 (12)	0.0325 (10)	0.0001 (10)	0.0090 (9)	0.0027 (9)
C7	0.0421 (11)	0.0355 (10)	0.0295 (9)	0.0026 (9)	0.0103 (8)	0.0006 (8)
C8	0.0390 (11)	0.0354 (11)	0.0329 (10)	0.0029 (8)	0.0098 (8)	0.0016 (8)
C9	0.0641 (16)	0.0570 (15)	0.0413 (12)	-0.0134 (12)	0.0226 (11)	-0.0022 (11)
C10	0.0679 (17)	0.0681 (18)	0.0550 (15)	-0.0263 (14)	0.0213 (13)	0.0010 (13)
C11	0.0656 (16)	0.0569 (16)	0.0548 (15)	-0.0226 (13)	0.0120 (12)	-0.0103 (12)
C12	0.0697 (17)	0.0625 (16)	0.0418 (13)	-0.0181 (13)	0.0195 (12)	-0.0142 (12)
C13	0.0530 (13)	0.0470 (13)	0.0383 (11)	-0.0120 (11)	0.0181 (10)	-0.0051 (10)
N1	0.0544 (11)	0.0387 (10)	0.0257 (8)	-0.0073 (8)	0.0120 (8)	-0.0025 (7)
O1	0.0769 (11)	0.0517 (10)	0.0306 (8)	-0.0128 (8)	0.0215 (7)	-0.0043 (7)
Cl1	0.0752 (5)	0.0601 (4)	0.0419 (3)	0.0005 (3)	-0.0076 (3)	-0.0028 (3)
Cl2	0.0945 (6)	0.0372 (3)	0.0729 (5)	0.0021 (3)	0.0066 (4)	0.0131 (3)

Geometric parameters (Å, °)

C1—C2	1.389 (3)	C7—C8	1.491 (3)
C1—C6	1.392 (3)	C8—C13	1.385 (3)
C1—N1	1.419 (3)	C8—C9	1.387 (3)
C2—C3	1.383 (3)	C9—C10	1.375 (4)
C2—H2	1.01 (2)	C9—H9	0.91 (3)
C3—C4	1.384 (3)	C10—C11	1.375 (4)
C3—Cl1	1.736 (2)	C10—H10	0.91 (3)
C4—C5	1.377 (3)	C11—C12	1.369 (4)
C4—H4	1.09 (3)	C11—H11	0.92 (3)
C5—C6	1.382 (3)	C12—C13	1.381 (3)
C5—Cl2	1.734 (2)	C12—H12	0.95 (3)
C6—H6	0.95 (3)	C13—H13	0.87 (3)
C7—O1	1.226 (2)	N1—H1N	0.83 (3)
C7—N1	1.358 (3)		
C2—C1—C6	120.66 (19)	C13—C8—C9	118.3 (2)
C2—C1—N1	120.79 (19)	C13—C8—C7	123.98 (19)
C6—C1—N1	118.54 (19)	C9—C8—C7	117.74 (18)
C3—C2—C1	118.4 (2)	C10—C9—C8	120.9 (2)
C3—C2—H2	121.4 (14)	C10—C9—H9	119.7 (19)
C1—C2—H2	120.0 (14)	C8—C9—H9	119.5 (19)
C2—C3—C4	122.5 (2)	C11—C10—C9	120.1 (2)
C2—C3—Cl1	119.37 (17)	C11—C10—H10	123 (2)
C4—C3—Cl1	118.13 (17)	C9—C10—H10	116 (2)
C5—C4—C3	117.3 (2)	C12—C11—C10	120.0 (2)
C5—C4—H4	120.5 (14)	C12—C11—H11	121.7 (19)
C3—C4—H4	122.3 (14)	C10—C11—H11	118 (2)
C4—C5—C6	122.7 (2)	C11—C12—C13	120.1 (2)
C4—C5—Cl2	118.68 (18)	C11—C12—H12	122.4 (19)
C6—C5—Cl2	118.63 (18)	C13—C12—H12	117.3 (19)
C5—C6—C1	118.4 (2)	C12—C13—C8	120.7 (2)
C5—C6—H6	118.9 (17)	C12—C13—H13	118.0 (18)
C1—C6—H6	122.7 (17)	C8—C13—H13	121.0 (18)
O1—C7—N1	122.05 (19)	C7—N1—C1	123.09 (16)
O1—C7—C8	120.68 (18)	C7—N1—H1N	119.4 (17)

N1—C7—C8	117.25 (17)	C1—N1—H1N	115.4 (17)
C6—C1—C2—C3	-2.5 (3)	O1—C7—C8—C9	-9.3 (3)
N1—C1—C2—C3	176.84 (19)	N1—C7—C8—C9	169.2 (2)
C1—C2—C3—C4	1.9 (3)	C13—C8—C9—C10	1.3 (4)
C1—C2—C3—C11	-176.86 (16)	C7—C8—C9—C10	180.0 (2)
C2—C3—C4—C5	0.1 (3)	C8—C9—C10—C11	-1.4 (4)
C11—C3—C4—C5	178.90 (17)	C9—C10—C11—C12	0.2 (5)
C3—C4—C5—C6	-1.6 (4)	C10—C11—C12—C13	0.8 (5)
C3—C4—C5—C12	-179.98 (17)	C11—C12—C13—C8	-0.8 (4)
C4—C5—C6—C1	1.0 (3)	C9—C8—C13—C12	-0.2 (4)
C12—C5—C6—C1	179.39 (17)	C7—C8—C13—C12	-178.8 (2)
C2—C1—C6—C5	1.1 (3)	O1—C7—N1—C1	1.4 (3)
N1—C1—C6—C5	-178.3 (2)	C8—C7—N1—C1	-177.06 (19)
O1—C7—C8—C13	169.3 (2)	C2—C1—N1—C7	-47.9 (3)
N1—C7—C8—C13	-12.2 (3)	C6—C1—N1—C7	131.4 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1N...O1 ⁱ	0.83 (3)	2.18 (3)	2.964 (2)	157 (2)

Symmetry codes: (i) *x*, -*y*+3/2, *z*+1/2.

Fig. 1

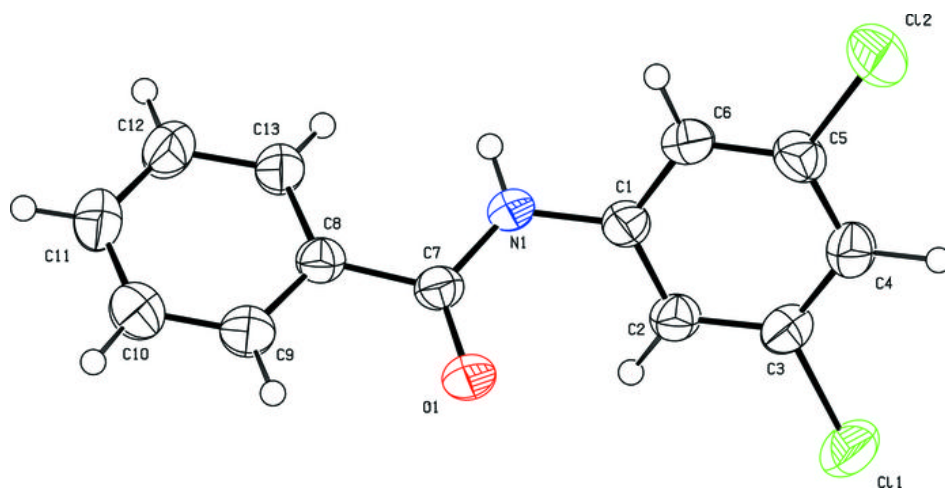


Fig. 2

