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2,6-Dichloro-*N*-(4-chlorophenyl)-benzamide

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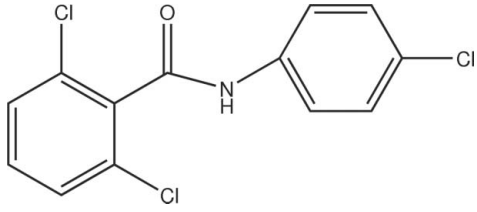
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.057; wR factor = 0.181; data-to-parameter ratio = 15.1.

In the title compound, $C_{13}H_8Cl_3NO$, the dihedral angle between the benzene rings is 63.2 (2)°. In the crystal, N—H···O hydrogen bonds link the molecules into $C(4)$ chains propagating in [001]. Weak aromatic π–π stacking also occurs [centroid–centroid separations = 3.759 (3) and 3.776 (3) Å].

Related literature

For further synthetic details, see: Lai & Huang (2005).



Experimental

Crystal data

$C_{13}H_8Cl_3NO$
M_r = 300.55
Monoclinic, $P2_1/c$
a = 11.241 (2) Å
b = 12.590 (3) Å
c = 9.6450 (19) Å
β = 100.60 (3)°
V = 1341.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.825, T_{max} = 0.936
2587 measured reflections
2459 independent reflections
1481 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.181
S = 1.00
2459 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···O^{i}	0.86	1.97	2.828 (4)	176

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1989); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXL97*; software used to prepare material for publication: *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6644).

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supporting information

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2,6-Dichloro-*N*-(4-chlorophenyl)benzamide

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S1. Experimental

2,6-Dichlorobenzoyl chloride (0.02 mol, 4.20 g)and 4-chloroaniline (0.02 mol, 2.55 g) were refluxed in triethylamine (6 ml) and tetrahydrofuran (50 ml) for 8h, then the solvents were evaporated to give raw product, which was finally washed by water and collected by filtration. Colourless blocks were obtained by slow evaporation of an ethyl acetate solution.

S2. Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å and C-H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N).

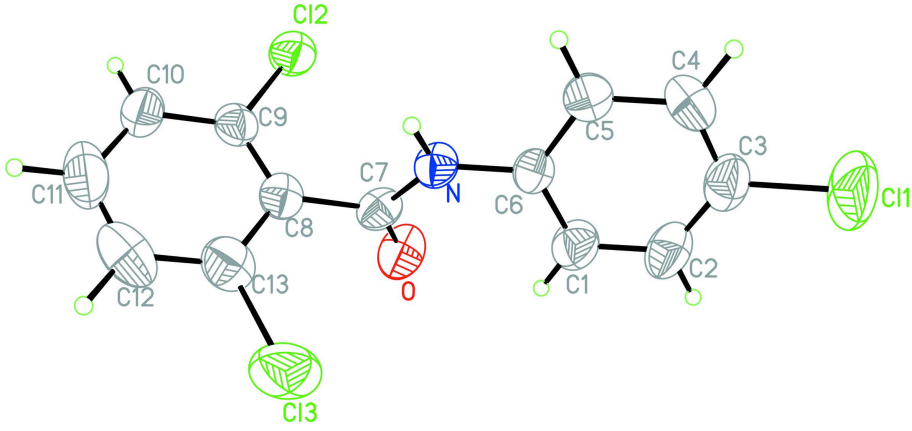

Figure 1

The molecular structure of the title molecule, with displacement ellipsoids drawn at the 50% probability level.

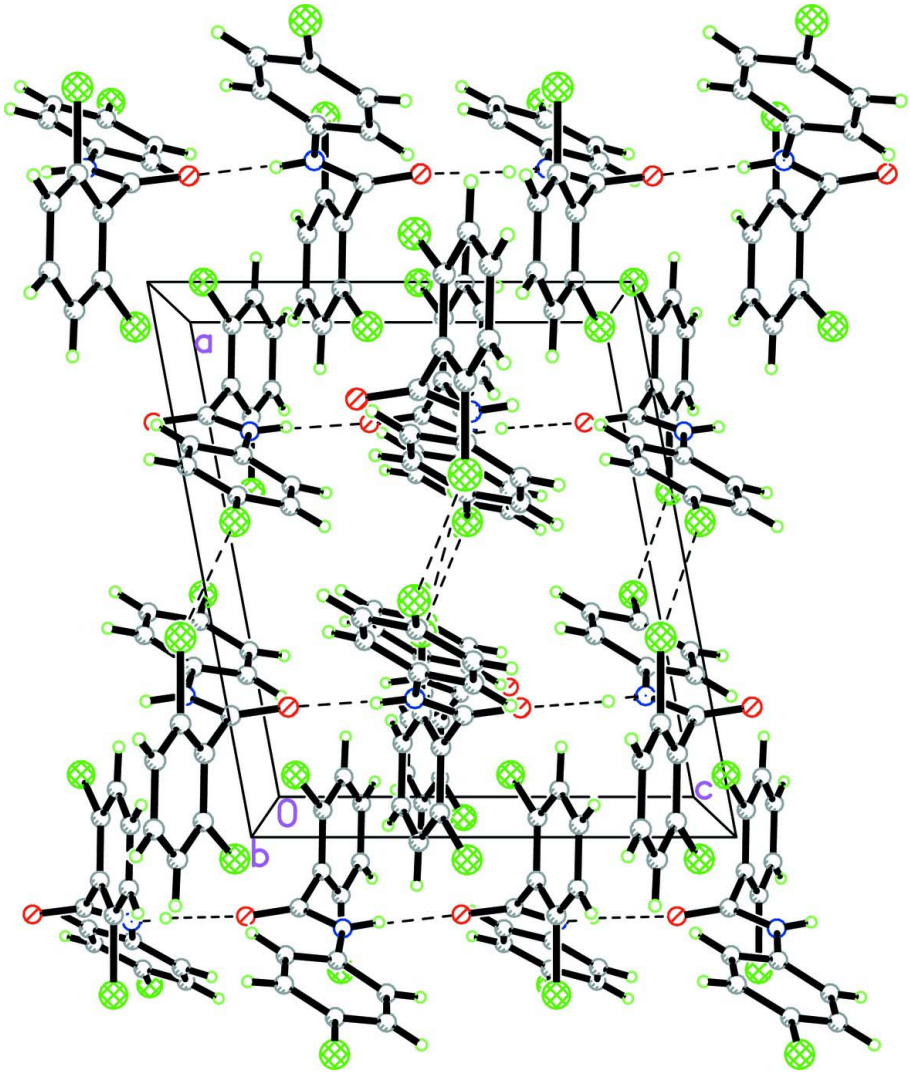

Figure 2

A packing diagram of (I) viewed down the *b* axis. Hydrogen bonds are drawn as dashed lines.

2,6-Dichloro-*N*-(4-chlorophenyl)benzamide

Crystal data

$C_{13}H_8Cl_3NO$
$M_r = 300.55$
Monoclinic, $P2_1/c$
$a = 11.241$ (2) Å
$b = 12.590$ (3) Å
$c = 9.6450$ (19) Å
$\beta = 100.60$ (3)°
$V = 1341.7$ (5) Å^3
$Z = 4$
$F(000) = 608$

$D_x = 1.488$ Mg m^{-3}
Melting point: 397 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–13°
$\mu = 0.67$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.825, T_{max} = 0.936
2587 measured reflections
2459 independent reflections
1481 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.4°, θ_{min} = 1.8°
$h = -13\rightarrow0$
$k = 0\rightarrow15$
$l = -11\rightarrow11$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.181
S = 1.00
2459 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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}
N	0.7580 (3)	0.3117 (2)	0.1127 (3)	0.0423 (8)
H0A	0.7677	0.2870	0.1972	0.051*
O	0.7776 (3)	0.2668 (2)	−0.1093 (3)	0.0660 (9)
Cl1	0.57123 (16)	0.75067 (10)	0.0703 (2)	0.1055 (6)
C1	0.7243 (4)	0.4801 (4)	−0.0171 (5)	0.0593 (12)
H1A	0.7651	0.4547	−0.0859	0.071*
Cl2	0.64198 (10)	0.05573 (10)	0.07481 (12)	0.0617 (4)
C2	0.6810 (5)	0.5830 (4)	−0.0246 (5)	0.0668 (13)
H2A	0.6917	0.6268	−0.0990	0.080*
Cl3	1.06285 (13)	0.25773 (11)	0.06642 (19)	0.0927 (6)
C3	0.6224 (4)	0.6202 (4)	0.0774 (6)	0.0594 (12)
C4	0.6040 (4)	0.5568 (4)	0.1854 (6)	0.0660 (13)
H4A	0.5638	0.5829	0.2543	0.079*
C5	0.6460 (4)	0.4524 (4)	0.1924 (5)	0.0544 (11)
H5A	0.6323	0.4082	0.2652	0.065*

C6	0.7070 (3)	0.4148 (3)	0.0926 (4)	0.0394 (9)
C7	0.7928 (4)	0.2481 (3)	0.0165 (4)	0.0443 (10)
C8	0.8579 (4)	0.1497 (3)	0.0788 (4)	0.0434 (10)
C9	0.7988 (4)	0.0590 (3)	0.1085 (4)	0.0465 (10)
C10	0.8603 (5)	−0.0302 (4)	0.1654 (5)	0.0595 (12)
H10A	0.8188	−0.0911	0.1831	0.071*
C11	0.9838 (5)	−0.0267 (5)	0.1951 (6)	0.0765 (15)
H11A	1.0264	−0.0859	0.2346	0.092*
C12	1.0461 (5)	0.0615 (5)	0.1683 (6)	0.0753 (15)
H12A	1.1302	0.0628	0.1906	0.090*
C13	0.9836 (4)	0.1479 (4)	0.1082 (5)	0.0593 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N	0.055 (2)	0.0430 (19)	0.0289 (16)	0.0040 (16)	0.0070 (14)	0.0032 (15)
O	0.109 (3)	0.0540 (19)	0.0365 (17)	0.0039 (17)	0.0164 (17)	−0.0042 (14)
Cl1	0.1079 (13)	0.0498 (8)	0.1576 (16)	0.0283 (8)	0.0215 (11)	0.0106 (9)
C1	0.077 (3)	0.052 (3)	0.051 (3)	0.006 (2)	0.018 (2)	0.010 (2)
Cl2	0.0515 (7)	0.0637 (7)	0.0707 (8)	−0.0022 (5)	0.0132 (5)	0.0087 (6)
C2	0.085 (4)	0.046 (3)	0.068 (3)	0.004 (3)	0.011 (3)	0.016 (2)
Cl3	0.0706 (9)	0.0743 (10)	0.1392 (14)	−0.0252 (7)	0.0347 (9)	−0.0239 (9)
C3	0.048 (3)	0.043 (3)	0.084 (4)	0.003 (2)	0.002 (2)	0.003 (2)
C4	0.063 (3)	0.063 (3)	0.078 (3)	0.013 (2)	0.028 (3)	−0.007 (3)
C5	0.062 (3)	0.052 (3)	0.053 (3)	0.004 (2)	0.019 (2)	0.006 (2)
C6	0.042 (2)	0.036 (2)	0.039 (2)	−0.0007 (17)	0.0032 (17)	−0.0009 (17)
C7	0.058 (3)	0.044 (2)	0.031 (2)	−0.0057 (19)	0.0088 (18)	−0.0004 (18)
C8	0.052 (2)	0.043 (2)	0.036 (2)	0.0019 (19)	0.0082 (18)	−0.0073 (18)
C9	0.049 (2)	0.052 (2)	0.040 (2)	0.006 (2)	0.0127 (18)	−0.001 (2)
C10	0.071 (3)	0.049 (3)	0.061 (3)	0.013 (2)	0.021 (2)	0.011 (2)
C11	0.076 (4)	0.076 (4)	0.076 (4)	0.032 (3)	0.008 (3)	0.011 (3)
C12	0.046 (3)	0.095 (4)	0.082 (4)	0.013 (3)	0.003 (3)	−0.013 (3)
C13	0.055 (3)	0.052 (3)	0.071 (3)	−0.003 (2)	0.013 (2)	−0.015 (2)

Geometric parameters (Å, º)

N—C7	1.338 (5)	C4—H4A	0.9300
N—C6	1.417 (5)	C5—C6	1.366 (5)
N—H0A	0.8600	C5—H5A	0.9300
O—C7	1.216 (4)	C7—C8	1.506 (5)
Cl1—C3	1.737 (5)	C8—C9	1.378 (6)
C1—C6	1.381 (5)	C8—C13	1.389 (6)
C1—C2	1.382 (6)	C9—C10	1.379 (6)
C1—H1A	0.9300	C10—C11	1.365 (7)
Cl2—C9	1.733 (4)	C10—H10A	0.9300
C2—C3	1.365 (7)	C11—C12	1.363 (7)
C2—H2A	0.9300	C11—H11A	0.9300
Cl3—C13	1.732 (5)	C12—C13	1.365 (7)

C3—C4	1.358 (7)	C12—H12A	0.9300
C4—C5	1.394 (6)		
C7—N—C6	128.0 (3)	O—C7—N	124.9 (4)
C7—N—H0A	116.0	O—C7—C8	121.7 (4)
C6—N—H0A	116.0	N—C7—C8	113.4 (3)
C6—C1—C2	120.1 (4)	C9—C8—C13	117.1 (4)
C6—C1—H1A	120.0	C9—C8—C7	123.2 (4)
C2—C1—H1A	120.0	C13—C8—C7	119.7 (4)
C3—C2—C1	119.8 (4)	C8—C9—C10	122.2 (4)
C3—C2—H2A	120.1	C8—C9—Cl2	119.6 (3)
C1—C2—H2A	120.1	C10—C9—Cl2	118.3 (3)
C4—C3—C2	120.9 (4)	C11—C10—C9	118.2 (5)
C4—C3—Cl1	119.4 (4)	C11—C10—H10A	120.9
C2—C3—Cl1	119.7 (4)	C9—C10—H10A	120.9
C3—C4—C5	119.6 (4)	C12—C11—C10	121.7 (5)
C3—C4—H4A	120.2	C12—C11—H11A	119.2
C5—C4—H4A	120.2	C10—C11—H11A	119.2
C6—C5—C4	120.2 (4)	C11—C12—C13	119.1 (5)
C6—C5—H5A	119.9	C11—C12—H12A	120.4
C4—C5—H5A	119.9	C13—C12—H12A	120.4
C5—C6—C1	119.5 (4)	C12—C13—C8	121.7 (5)
C5—C6—N	117.6 (3)	C12—C13—Cl3	119.2 (4)
C1—C6—N	122.7 (4)	C8—C13—Cl3	119.1 (4)
C6—C1—C2—C3	0.8 (7)	O—C7—C8—C13	82.0 (5)
C1—C2—C3—C4	−1.2 (8)	N—C7—C8—C13	−96.3 (5)
C1—C2—C3—Cl1	178.4 (4)	C13—C8—C9—C10	0.3 (6)
C2—C3—C4—C5	0.2 (7)	C7—C8—C9—C10	179.9 (4)
Cl1—C3—C4—C5	−179.4 (4)	C13—C8—C9—Cl2	179.9 (3)
C3—C4—C5—C6	1.2 (7)	C7—C8—C9—Cl2	−0.5 (5)
C4—C5—C6—C1	−1.6 (6)	C8—C9—C10—C11	1.2 (6)
C4—C5—C6—N	173.8 (4)	Cl2—C9—C10—C11	−178.5 (4)
C2—C1—C6—C5	0.6 (7)	C9—C10—C11—C12	−0.8 (8)
C2—C1—C6—N	−174.5 (4)	C10—C11—C12—C13	−1.1 (8)
C7—N—C6—C5	161.0 (4)	C11—C12—C13—C8	2.6 (8)
C7—N—C6—C1	−23.7 (6)	C11—C12—C13—Cl3	−177.0 (4)
C6—N—C7—O	−5.6 (7)	C9—C8—C13—C12	−2.2 (6)
C6—N—C7—C8	172.6 (3)	C7—C8—C13—C12	178.2 (4)
O—C7—C8—C9	−97.7 (5)	C9—C8—C13—Cl3	177.4 (3)
N—C7—C8—C9	84.1 (5)	C7—C8—C13—Cl3	−2.2 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0*A*···O^{i}	0.86	1.97	2.828 (4)	176

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