

Acetone (2,6-dichlorobenzoyl)hydrazone:
chains of π -stacked hydrogen-bonded dimersSolange M. S. V. Wardell,^a
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Key indicators

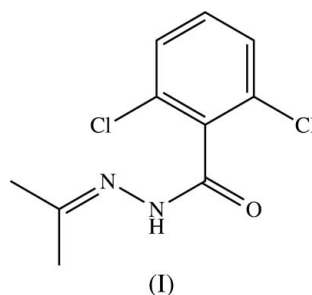
Single-crystal X-ray study
 $T = 120$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.038
 wR factor = 0.096
Data-to-parameter ratio = 18.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $\text{C}_{10}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}$, the aryl ring is almost orthogonal to the rest of the molecule. Molecules are linked into centrosymmetric dimers by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, and these dimers are linked into chains by a single $\pi-\pi$ stacking interaction.

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Comment

We report here the molecular and supramolecular structure of the title compound, (I) (Fig. 1). Apart from the dichlorophenyl ring, the non-H atoms are nearly coplanar, as shown by the leading torsion angles (Table 1). The aryl ring is almost orthogonal to the rest of the molecule, with a dihedral angle of $82.5(2)^\circ$ between the aryl ring and the mean plane through the rest of the non-H atoms. This is a consequence of the repulsive interactions between the lone pairs of electrons on the two Cl atoms and those on atoms N2 and O7.



The molecules are linked by paired $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) into cyclic centrosymmetric $R_2^2(8)$ (Bernstein *et al.*, 1995) dimers (Fig. 2), and these dimers are linked into chains by a single aromatic $\pi-\pi$ stacking interaction. The aryl rings of the molecules at (x, y, z) and $(1-x, 2-y, -z)$ are strictly parallel, with an interplanar spacing of $3.593(2)$ Å. The ring-centroid separation is $3.695(2)$ Å, corresponding to a ring offset of $0.862(2)$ Å. Propagation by inversion of this interaction then links the hydrogen-bonded dimers into a π -stacked chain running parallel to the $[01\bar{1}]$ direction (Fig. 3), but there are no direction-specific interactions between adjacent chains.

Experimental

2,6-Dichlorobenzoylhydrazine (3 mmol) was dissolved in acetone (30 ml) and the solution was heated under reflux for 1 h. The solution was then cooled and the excess solvent was removed under reduced pressure. The resulting solid product, (I), was crystallized from ethanol.

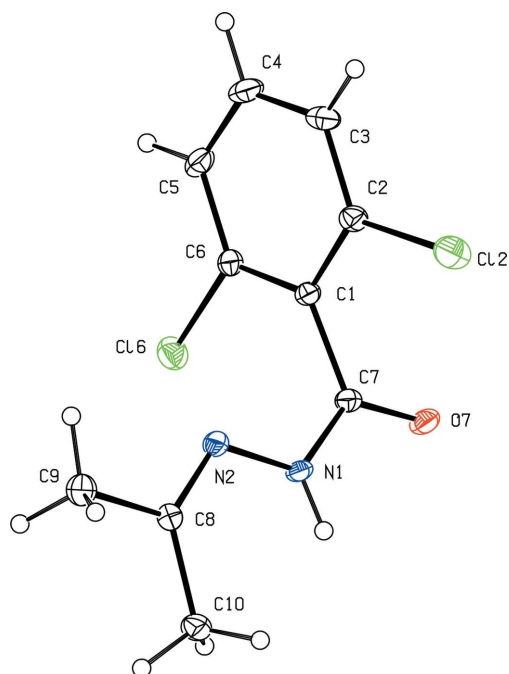


Figure 1
A molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

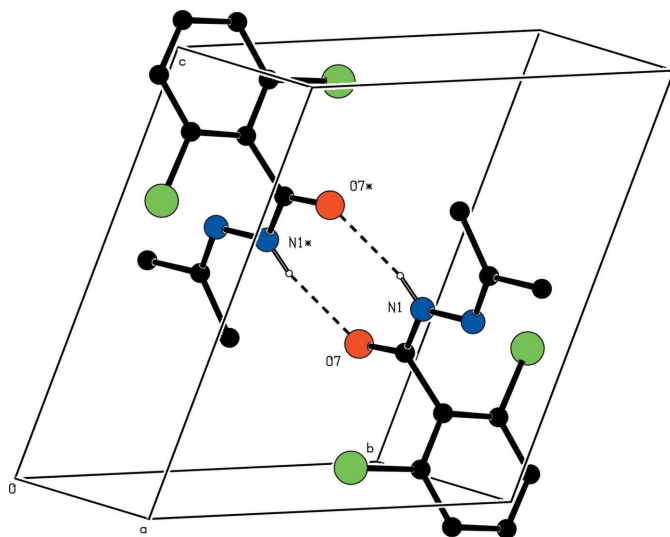


Figure 2
The molecular structure of compound (I), showing the formation of a hydrogen-bonded (dashed lines) $R_2^2(8)$ dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(1-x, 1-y, 1-z)$.

Crystal data

$C_{10}H_{10}Cl_2N_2O$
 $M_r = 245.10$
 Triclinic, $P\bar{1}$
 $a = 7.4980$ (3) Å
 $b = 8.1320$ (2) Å
 $c = 9.7759$ (3) Å
 $\alpha = 71.609$ (2)°
 $\beta = 80.822$ (2)°
 $\gamma = 89.033$ (2)°

$V = 558.03$ (3) Å³
 $Z = 2$
 $D_x = 1.459$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.56$ mm⁻¹
 $T = 120$ (2) K
 Lath, colourless
 $0.42 \times 0.10 \times 0.08$ mm

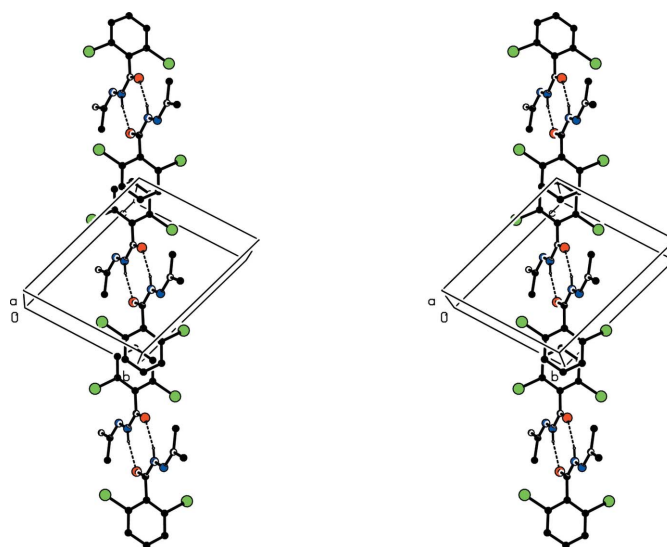


Figure 3
A stereoscopic view of part of the crystal structure of compound (I), showing the formation of a π -stacked chain of hydrogen-bonded (dashed lines) dimers along $[01\bar{1}]$. For the sake of clarity, H atoms bonded to C atoms have been omitted.

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.822$, $T_{\max} = 0.957$

13458 measured reflections
 2568 independent reflections
 1970 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$
 $\theta_{\max} = 27.6^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.096$
 $S = 1.03$
 2568 reflections
 138 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.2175P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.29$ e Å⁻³
 $\Delta\rho_{\min} = -0.34$ e Å⁻³

Table 1

Selected torsion angles (°).

C2–C1–C7–N1	101.4 (2)	C7–N1–N2–C8	175.32 (16)
C1–C7–N1–N2	–2.8 (2)	N1–N2–C8–C9	178.37 (15)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O7^i$	0.85	2.09	2.9232 (18)	169

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

All atoms were located in difference maps and then treated as riding atoms, with C–H = 0.95 (aromatic) or 0.98 Å (methyl) and N–H = 0.85 Å, and with $U_{\text{iso}}(\text{H}) = kU_{\text{eq}}(\text{C,N})$, where $k = 1.5$ for the methyl groups and $k = 1.2$ for all other H atoms.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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