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Key indicators

Single-crystal X-ray study
 T = 120 K
 Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
 R factor = 0.038
 wR factor = 0.096
 Data-to-parameter ratio = 18.6

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Acetone (2,6-dichlorobenzoyl)hydrazone: chains of π -stacked hydrogen-bonded dimers

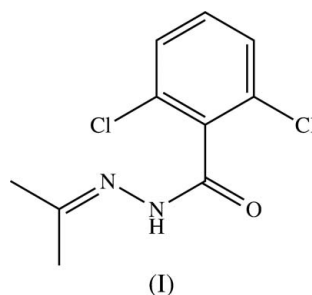
In the title compound, $\text{C}_{10}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}$, the aryl ring is almost orthogonal to the rest of the molecule. Molecules are linked into centrosymmetric dimers by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, and these dimers are linked into chains by a single π - π 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 π - π 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 $3.593(2) \text{ \AA}$. The ring-centroid separation is $3.695(2) \text{ \AA}$, corresponding to a ring offset of $0.862(2) \text{ \AA}$. 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.

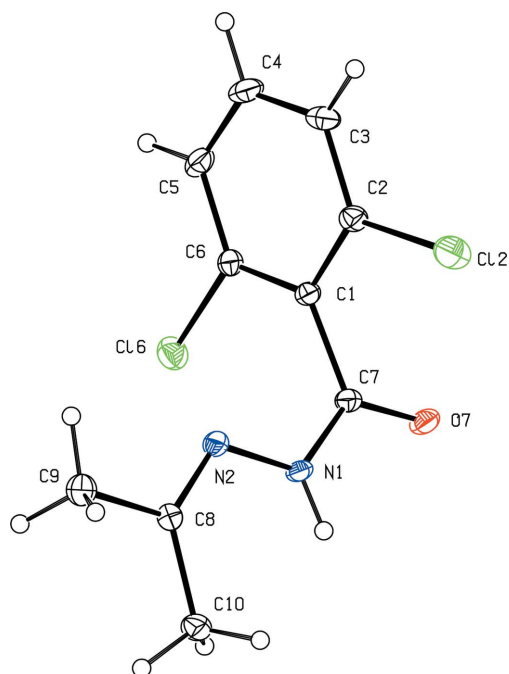


Figure 1
A molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

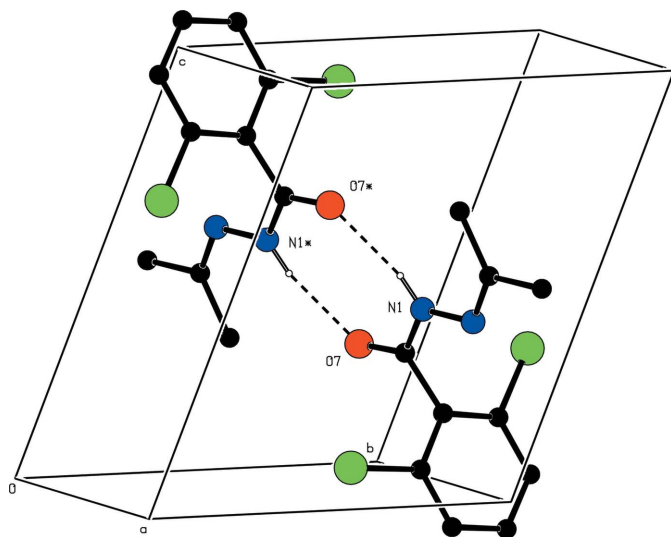


Figure 2
The molecular structure of compound (I), showing the formation of a hydrogen-bonded (dashed lines) $R_2^2(8)$ dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(1-x, 1-y, 1-z)$.

Crystal data

| | |
|------------------------------|---|
| $C_{10}H_{10}Cl_2N_2O$ | $V = 558.03 (3) \text{ \AA}^3$ |
| $M_r = 245.10$ | $Z = 2$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.459 \text{ Mg m}^{-3}$ |
| $a = 7.4980 (3) \text{ \AA}$ | Mo $K\alpha$ radiation |
| $b = 8.1320 (2) \text{ \AA}$ | $\mu = 0.56 \text{ mm}^{-1}$ |
| $c = 9.7759 (3) \text{ \AA}$ | $T = 120 (2) \text{ K}$ |
| $\alpha = 71.609 (2)^\circ$ | Lath, colourless |
| $\beta = 80.822 (2)^\circ$ | $0.42 \times 0.10 \times 0.08 \text{ mm}$ |
| $\gamma = 89.033 (2)^\circ$ | |

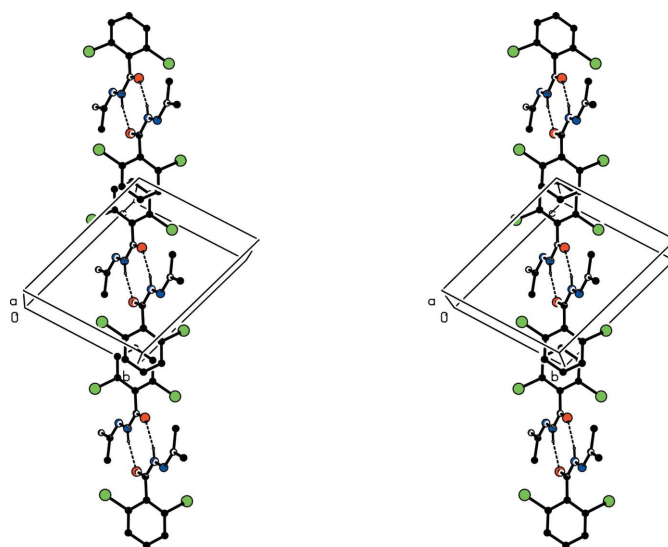


Figure 3
A stereoscopic view of part of the crystal structure of compound (I), showing the formation of a π -stacked chain of hydrogen-bonded (dashed lines) dimers along $[01\bar{1}]$. For the sake of clarity, H atoms bonded to C atoms have been omitted.

Data collection

| | |
|---|--|
| Bruker Nonius KappaCCD area-detector diffractometer | 13458 measured reflections |
| φ and ω scans | 2568 independent reflections |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2003) | 1970 reflections with $I > 2\sigma(I)$ |
| $T_{\min} = 0.822$, $T_{\max} = 0.957$ | $R_{\text{int}} = 0.045$ |
| | $\theta_{\max} = 27.6^\circ$ |

Refinement

| | |
|---------------------------------|---|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.2175P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.096$ | $(\Delta/\sigma)_{\max} = 0.001$ |
| $S = 1.03$ | $\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$ |
| 2568 reflections | $\Delta\rho_{\min} = -0.34 \text{ e \AA}^{-3}$ |
| 138 parameters | |
| H-atom parameters constrained | |

Table 1

Selected torsion angles ($^\circ$).

| | | | |
|-------------|-----------|-------------|-------------|
| 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 (\AA , $^\circ$).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------|-------|-------------|-------------|---------------|
| $N1-H1\cdots O7^i$ | 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 \AA (methyl) and $N-H = 0.85 \text{ \AA}$, and with $U_{\text{iso}}(H) = kU_{\text{eq}}(C,N)$, 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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