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# 1-[5-(3,6-Dichloropyridin-2-yl)-2,2-dimethyl-1,3,4-oxadiazol-3-yl]ethanone

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**Key indicators**

Single-crystal X-ray study
*T* = 173 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.040
*wR* factor = 0.135
Data-to-parameter ratio = 17.8

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



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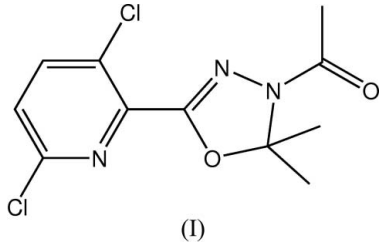
The title compound, $C_{11}H_{11}Cl_2N_3O_2$, shows an approximately planar oxadiazoline ring and a small twist between its two ring systems. In the crystal structure, molecules are linked into chains *via* C—H···O interactions and centrosymmetrically related chains are connected into double chains *via* weaker C—H···N interactions.

## Comment

1,3,4-Oxadiazolines are reported to possess a wide range of pharmaceutical activity, such as anticonvulsant (Dogan *et al.*, 1998), antifungal (Singh & Hasan, 2002), anti-HIV (Chimirri *et al.*, 1994), anti-inflammatory (Tinperciuc *et al.*, 1999) and antitumor (Chimirri *et al.*, 1996) properties. 3-Acetyl-2,5-disubstituted-1,3,4-oxadiazolines are also known to exhibit antimicrobial activity (Hassan *et al.*, 1983; Khalil *et al.*, 1993). The title compound, (I), was investigated as a continuation of our interest in this area (Song *et al.*, 2006).




(I)

The five-membered oxadiazoline ring in (I) (Fig. 1) is approximately planar, with maximum deviations from the

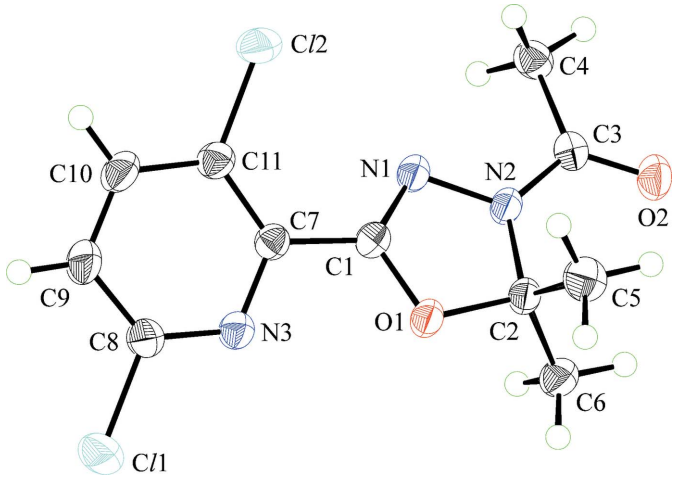



**Figure 1**
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

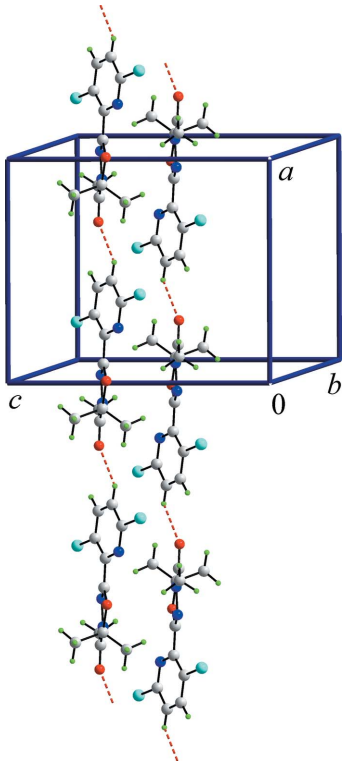



**Figure 2**
Double-chain formation in (I) aligned along the *a* axis. Color code: Cl (cyan), O (red), N (blue), C (gray) and H (green). Red dashed lines indicate C—H···O interactions.

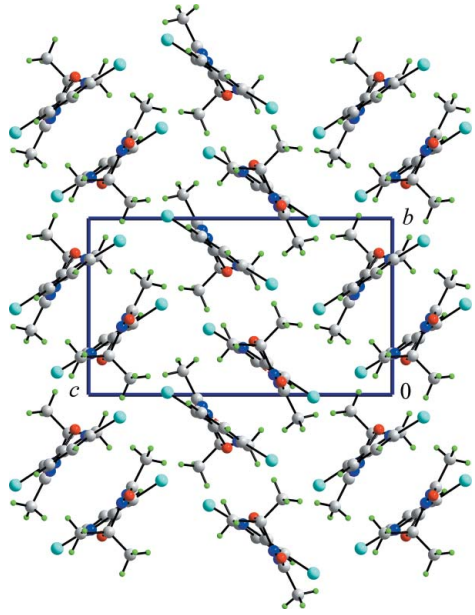



**Figure 3**
Herring-bone packing in (I), viewed down the *a* axis. The color code is as for Fig. 2.

least-squares plane (O1/N1/N2/C1/C2) of 0.057 (1) and −0.064 (2) Å for atoms N2 and C2, respectively. Within this ring, there is a formal C1═N1 double bond, although the bond distance for C1—O1 suggests some delocalization of π-electron density over the O1/C1/N1 chromophore (Table 1). The N1—C1—C7—N3 torsion angle of 153.72 (16)° indicates a relatively small twist between the two ring systems [dihedral angle = 25.90 (9)°], and the acyl group is coplanar with the oxadiazoline ring [N1—N2—C3—O2 = 174.51 (15)° and dihedral angle = 1.8 (2)°].

The crystal structure of (I) is stabilized by a combination of C—H···O, C—H···N and C—H···Cl interactions. As illustrated in Fig. 2, molecules are linked into chains parallel to the *a* axis *via* C—H···O interactions (Table 2). Antiparallel chains face each other, allowing for the formation of weak C—H···N interactions (Table 2) between centrosymmetric pairs. Double-chains are packed in a herringbone manner (Fig. 3) with C—H···Cl interactions between them, the shortest of which involves Cl1 (Table 2).

## Experimental

Compound (I) was prepared according to the literature procedure (Yale *et al.*, 1953). A solution of 3,6-dichloropyridine-2-carboxylic acid isopropylidenehydrazide (0.5 g, 2.03 mmol) in acetic anhydride (10 ml) was refluxed for 0.5 h. The acetic anhydride was then distilled under vacuum and the residue was recrystallized from ethyl acetate (10 ml) to yield colorless crystals (yield 0.42 g, 71.4%; m.p. 433 K) by slow evaporation over two days at room temperature.

*Crystal data*

$C_{11}H_{11}Cl_2N_3O_2$
$M_r$ = 288.13
Monoclinic, $P2_1/n$
$a$ = 11.1149 (19) Å
$b$ = 8.1943 (13) Å
$c$ = 14.122 (2) Å
$\beta$ = 93.554 (3)°
$V$ = 1283.8 (4) Å$^3$
$Z$ = 4
$D_x$ = 1.491 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.50 mm$^{-1}$
$T$ = 173 (2) K
Plate, colorless
0.55 × 0.35 × 0.03 mm

*Data collection*

Rigaku AFC12$\kappa$/SATURN724 CCD diffractometer
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.668, $T_{max}$ = 1.000
32711 measured reflections
2924 independent reflections
2887 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 27.5°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.135
$S$ = 1.18
2924 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.4744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C1 | 1.3587 (19) | N2—C2 | 1.486 (2) |
| O1—C2 | 1.4630 (18) | N2—C3 | 1.363 (2) |
| O2—C3 | 1.225 (2) | N3—C7 | 1.347 (2) |
| N1—C1 | 1.277 (2) | N3—C8 | 1.316 (2) |
| N1—N2 | 1.3938 (18) | | |
| C1—O1—C2 | 106.74 (12) | N1—N2—C3 | 121.08 (14) |
| N2—N1—C1 | 105.01 (13) | C2—N2—C3 | 127.35 (13) |
| N1—N2—C2 | 110.86 (12) | C8—N3—C7 | 117.74 (15) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9···O2$^{i}$ | 0.95 | 2.43 | 3.092 (2) | 127 |
| C6—H6$B$···N1$^{ii}$ | 0.98 | 2.59 | 3.526 (2) | 161 |
| C4—H4$B$···Cl1$^{iii}$ | 0.98 | 2.89 | 3.672 (2) | 138 |

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

H atoms were placed in calculated positions and allowed to ride on their parent atoms, with C—H = 0.95–0.98 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C). Methyl group C4 was allowed to rotate about its local threefold axis.

Data collection: *CrystalClear* (Rigaku Americas Corporation, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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