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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.010$ Å
 R factor = 0.066
 wR factor = 0.149
Data-to-parameter ratio = 13.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

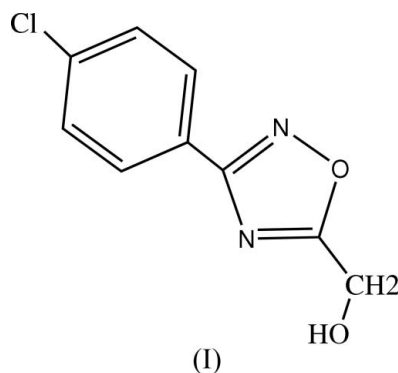
[3-(4-Chlorophenyl)-1,2,4-oxadiazol-5-yl]methanol

The molecule of the title compound, $\text{C}_9\text{H}_7\text{ClN}_2\text{O}_2$, is essentially planar except for H atoms, and the occurrence of $\text{O}-\text{H}\cdots\text{N}$ hydrogen-bonding interactions results in the formation of a dimer.

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Comment

1,2,4-Oxadiazoles represent an important class of five-membered heterocycles. Some derivatives of 1,2,4-oxadiazoles have anti-inflammatory (Nicolaidis *et al.*, 1998) and anti-picornaviral (Romero, 2001) properties. We are focusing our synthetic and structural studies on new oxadiazole derivatives and we have recently published the synthesis and structure of [3-(2-methylphenyl)-1,2,4-oxadiazol-5-yl]methanol (Yan *et al.*, 2006). We report here the structure of its close analogue, (I), in which 2-methylphenyl is replaced by 4-chlorophenyl.



The molecule is essentially planar, except for H atoms, the benzene and the oxadiazole ring making a dihedral angle of $5.9(4)^\circ$ (Fig. 1). The occurrence of $\text{O}-\text{H}\cdots\text{N}$ hydrogen-bonding interactions results in the formation of a dimer of topology $R_2^2(10)$, according to graph-set theory (Etter, 1990) (Fig. 2). The dimers are further connected to each other through $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1 and Fig. 2), forming a sheet.

Experimental

Hexamethylenetetramine (90 mmol) was dissolved in acetic acid (70 ml) and water (70 mmol). 5-Chloromethyl-3-(4-chlorophenyl)-1,2,4-oxadiazole (30 mmol) was added to this mixture. The resulting mixture was refluxed for 3 h. After cooling and filtering, crude compound (I) was obtained. Pure compound (I) was obtained by crystallizing from a mixture of ethyl acetate (6 ml) and petroleum ether (6 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

C₉H₇ClN₂O₂
M_r = 210.62
 Monoclinic, *C2/c*
a = 27.789 (2) Å
b = 4.0141 (5) Å
c = 21.4570 (15) Å
 β = 127.56 (3)°
V = 1897.4 (8) Å³

Z = 8
D_x = 1.475 Mg m⁻³
 Mo *K*α radiation
 μ = 0.38 mm⁻¹
T = 293 (2) K
 Block, colourless
 0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4
 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
T_{min} = 0.929, *T_{max}* = 0.963
 1746 measured reflections

1746 independent reflections
 698 reflections with *I* > 2σ(*I*)
 θ_{\max} = 26.0°
 3 standard reflections
 every 200 reflections
 intensity decay: none

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.066
wR(*F*²) = 0.149
S = 0.99
 1746 reflections
 130 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 2P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.14 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.14 \text{ e \AA}^{-3}$

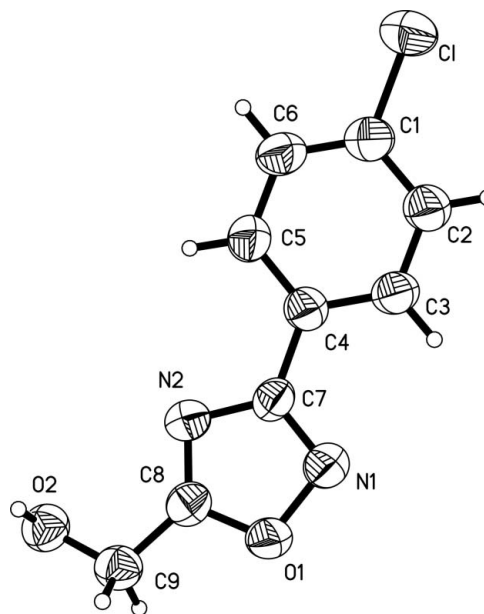


Figure 1

The molecular structure of compound (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as spheres of arbitrary radii.

Table 1

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>
O2—H···N2 ⁱ	0.83 (8)	2.05 (9)	2.880 (9)	175 (8)
C9—H9B···O2 ⁱⁱ	0.97	2.53	3.209 (8)	127

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

The hydroxy H atom was refined freely with a fixed isotropic displacement parameter of 0.109 Å². All other H atoms were treated as riding on their parent atoms, with C—H = 0.93 (aromatic) and 0.97 Å (CH₂), with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXS97*.

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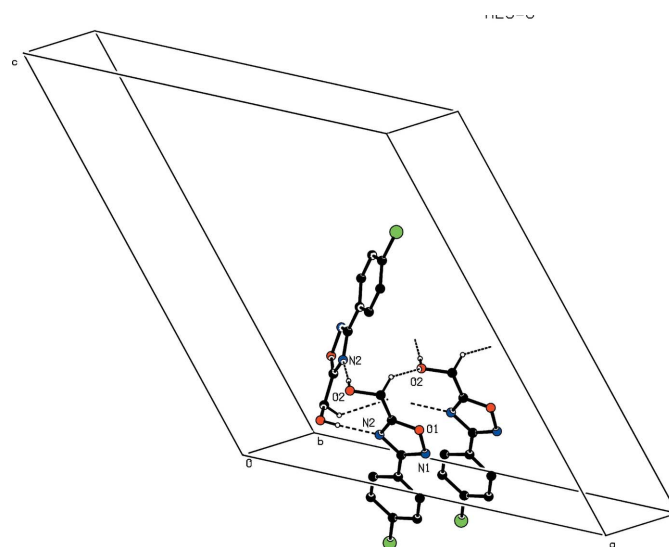


Figure 2

Partial packing view showing the O—H···N and C—H···O hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) $1 - x, y, \frac{1}{2} - z$; (ii) $x, 1 + y, z$]

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