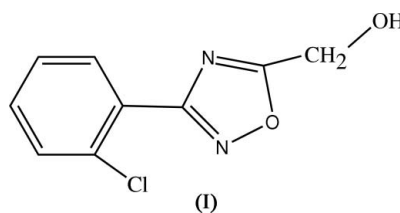
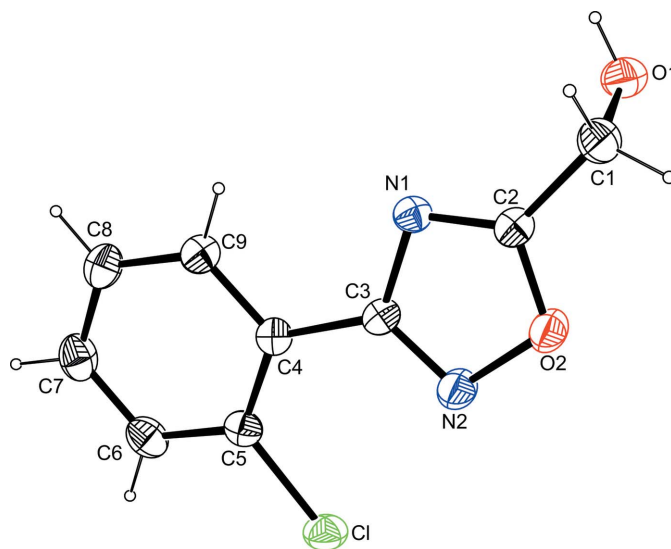


**[3-(2-Chlorophenyl)-1,2,4-oxadiazol-5-yl]methanol****Xiao-Chen Yan,\* Hai-Bo Wang  
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wanghaibo@njut.edu.cn**Key indicators**Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.049  
 $wR$  factor = 0.132  
Data-to-parameter ratio = 13.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.In the title compound,  $\text{C}_9\text{H}_7\text{ClN}_2\text{O}_2$ , the occurrence of  $\text{O}-\text{H}\cdots\text{N}$  hydrogen-bond interactions results in the formation of a pseudo-dimer arranged around an inversion center.Received 17 May 2006  
Accepted 22 May 2006**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 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 a 2-chloro group.The molecular structure of (I), shown in Fig. 1, is roughly planar, the dihedral angle between the benzene ring and the oxadiazole ring being only  $6.2(1)^\circ$ . There are  $\text{O}-\text{H}\cdots\text{N}$ **Figure 1**

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms are shown as small spheres of arbitrary radii.

intermolecular hydrogen bonds, resulting in the formation of a pseudo-dimer arranged around an inversion center (Table 1 and Fig. 2).

### Experimental

Hexamethylenetetramine (90 mmol) was dissolved in acetic acid (70 ml) and water (70 mmol). 3-(2-Chlorophenyl)-5-chloromethyl-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. It was crystallized 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

$C_9H_7ClN_2O_2$	$Z = 4$
$M_r = 210.62$	$D_x = 1.573 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 7.4280 (15) \text{ \AA}$	$\mu = 0.40 \text{ mm}^{-1}$
$b = 14.202 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 8.8050 (18) \text{ \AA}$	Block, colourless
$\beta = 106.76 (3)^\circ$	$0.40 \times 0.30 \times 0.30 \text{ mm}$
$V = 889.4 (3) \text{ \AA}^3$	

#### Data collection

Enraf–Nonius CAD-4 diffractometer	1739 independent reflections
$\omega/2\theta$ scans	1399 reflections with $I > 2\sigma(I)$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$R_{\text{int}} = 0.017$
$T_{\text{min}} = 0.856$ , $T_{\text{max}} = 0.889$	$\theta_{\text{max}} = 26.0^\circ$
1874 measured reflections	3 standard reflections every 200 reflections
	intensity decay: none

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.2802P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.132$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
1739 reflections	$\Delta\rho_{\text{min}} = -0.44 \text{ e \AA}^{-3}$
128 parameters	
H-atom parameters constrained	

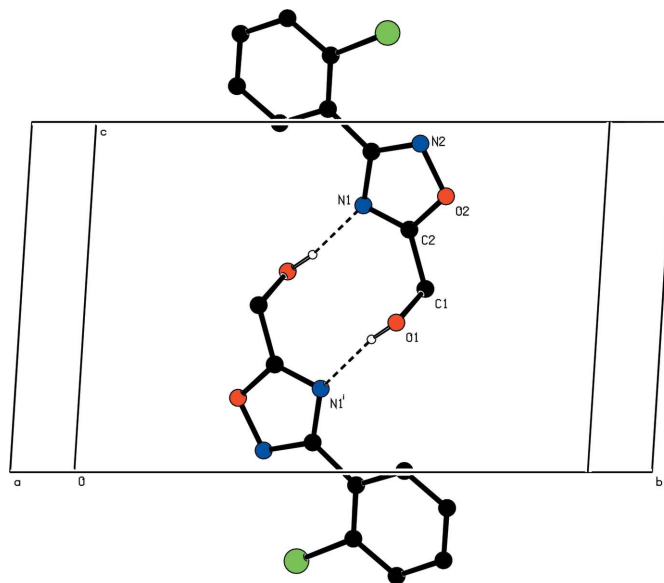
**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1\cdots N1^i$	0.82	2.04	2.849 (3)	170

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with  $C-H = 0.95$



**Figure 2**

Partial packing view, showing the formation of a pseudo-dimer through intermolecular  $O-H\cdots N$  hydrogen bonds (dashed lines). [Symmetry codes: (i)  $-x + 1, -y + 1, -z + 1$ .]

(aromatic) or  $0.99 \text{ \AA}$  (methylene) and  $O-H = 0.82 \text{ \AA}$ , with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C,O)$

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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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