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## Key indicators

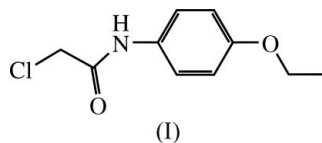
Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.101  
Data-to-parameter ratio = 16.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2-Chloro-*N*-(4-ethoxyphenyl)acetamide

In the molecule of the title compound,  $\text{C}_{10}\text{H}_{12}\text{ClNO}_2$ , an intramolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bond forms a non-planar six-membered ring. In the crystal structure, the molecules are linked by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming infinite chains along the  $c$  axis. The packing is further stabilized by  $\text{C}-\text{H}\cdots\pi$  interactions.

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## Comment

*N*-Phenyl-2-chloroacetamide is an important intermediate in organic synthesis. It can be used in the synthesis of many derivatives such as quinolin-8-yloxyacetamide (Zhang *et al.*, 2006), 2,5-piperazinedione (Wen *et al.*, 2006) and 2,2-(1,3,4-thiadiazolyl-2,5-dithio)diacetamide (Wen *et al.*, 2005). We present here the crystal structure of the title compound, (I).



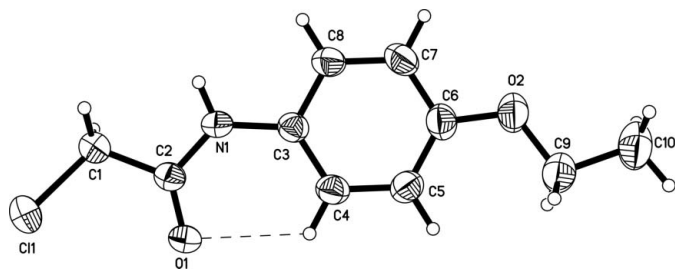
In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The  $\text{C1}-\text{C2}$  [1.517 (2) Å] bond is longer than  $\text{C9}-\text{C10}$  [1.507 (3) Å], owing to the presence of the Cl atom.

Ring *A* (C3–C8) and the C1–C3/O1/N1 group are, of course, planar and the dihedral angle between them is  $6.44$  (4)°. An intramolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bond (Table 1) forms a six-membered ring *B* (O1/N1/H4A/C2–C4), which is not planar, having a total puckering amplitude,  $Q_T$ , of 1.1162 (3) Å (Cremer & Pople, 1975).

As can be seen from the packing diagram (Fig. 2), intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 1) link the molecules into infinite chains along the  $c$  axis, stabilizing the crystal structure. The packing is further stabilized by  $\text{C}-\text{H}\cdots\pi$  interactions (Table 1). Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

## Experimental

For the preparation of the title compound, chloroacetyl chloride (5.65 g, 0.05 mol) was added to a solution of 4-ethoxyaniline (6.85 g, 0.05 mol) and triethylamine (5.1 g, 0.05 mol) in benzene (50 ml) within 30 min with cooling in an ice bath, and then the resulting mixture was stirred at room temperature for 4 h. After separation of the triethylamine hydrochloride by filtration, the organic phase was washed three times with water. The benzene layer was removed and the solvent evaporated. The title compound was obtained after drying the colorless powder at room temperature for 48 h. Colorless single



**Figure 1**

The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular hydrogen bond is shown as a dashed line.

crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution over a period of 10 d.

#### Crystal data

$C_{10}H_{12}ClNO_2$   
 $M_r = 213.66$   
 Monoclinic,  $P2_1/c$   
 $a = 11.3149$  (13) Å  
 $b = 10.0120$  (12) Å  
 $c = 9.1966$  (11) Å  
 $\beta = 97.155$  (2)°  
 $V = 1033.7$  (2) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.373$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.34$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 Block, colorless  
 $0.31 \times 0.25 \times 0.10$  mm

#### Data collection

Siemens SMART 1000 CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.901$ ,  $T_{\max} = 0.967$

5631 measured reflections  
 2027 independent reflections  
 1715 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.022$   
 $\theta_{\text{max}} = 26.0^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.102$   
 $S = 1.02$   
 2027 reflections  
 127 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.351P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), with 1308 Friedel pairs  
 Flack parameter: 0.09 (11)

**Table 1**

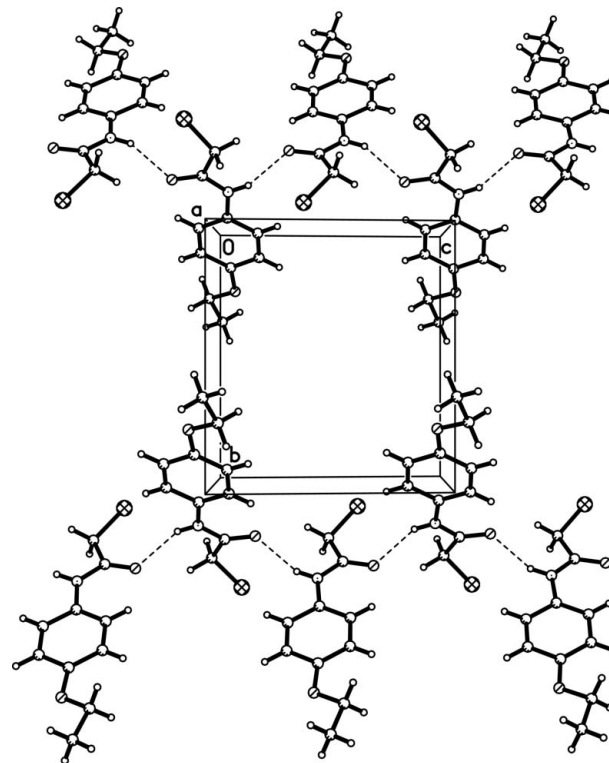
Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C3–C8 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots O1^i$	0.86	2.14	2.898 (2)	147
$C4-H4A\cdots O1$	0.93	2.36	2.945 (2)	120
$C1-H1B\cdots Cg1^{ii}$	0.97	2.69	3.551	148
$C9-H9B\cdots Cg1^{iii}$	0.97	2.77	3.650	152

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

H atoms were positioned geometrically, with  $N-H = 0.86$  Å (for NH) and  $C-H = 0.93, 0.97$  and  $0.96$  Å for aromatic, methine and methyl H atoms, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(H) = xU_{\text{eq}}(C,N)$ , where  $x = 1.5$  for methyl H and  $x = 1.2$  for all other H atoms.



**Figure 2**

A partial packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT; data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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