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## Key indicators

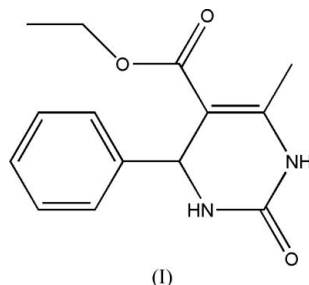
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$   
 $R$  factor = 0.062  
 $wR$  factor = 0.180  
Data-to-parameter ratio = 7.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydro-  
pyrimidine-5-carboxylate

The title compound,  $\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}_3$ , is chiral. There are two molecules in the asymmetric unit, which are related by an approximate non-crystallographic twofold screw axis. Molecules of the title compound are linked by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen-bond interactions involving the H atoms of the amino groups and O atoms of the keto groups, thus forming a zigzag structure.

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## Comment

3,4-Dihydropyrimidin-2-(1*H*)-one derivatives have attracted considerable attention because of their pharmacological function and importance as calcium antagonists (Kappe *et al.*, 1999; Grover *et al.*, 1995). As part of our investigation of 3,4-dihydropyrimidin-2-(1*H*)-one derivatives, we report here the structure of the title compound, (I), a representative of this class.



The molecular structure of compound (I) is shown in Fig. 1. The H atom of the amino group links to an O atom of the keto group in an adjacent molecule *via* an  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond (Table 1), resulting in the formation of an eight-membered ring, which is connected to neighbouring eight-membered rings through shared  $\text{C}=\text{O}$  groups, thus forming a zigzag structure. Furthermore, a C atom of the methyl group is hydrogen-bonded to an O atom of the acetate group *via* a  $\text{C}-\text{H}\cdots\text{O}$  intramolecular hydrogen-bond to form a six-membered ring. These are shown in Fig. 2. Bond lengths and angles agree with accepted values (Portilla *et al.*, 2006); full details are given in the archived CIF.

## Experimental

A mixture of urea (51 mmol), ethyl acetoacetate (78 mmol) and benzaldehyde (49 mmol) in absolute ethanol (30 ml) and concentrated hydrochloric acid (10 drops) was heated to reflux for 4.5 h. Upon cooling to room temperature, a crude product crystallized. The precipitate was filtered off, washed with propan-2-ol and recrystallized from propan-2-ol to afford the desired product as a colourless

solid (m.p. 475 K). Colourless single crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of an aqueous ethanol (95%) solution at ambient temperature after 12 d Elemental analysis, calculated for  $C_{14}H_{16}N_2O_3$ : C 64.60, H 6.19, N 10.76%; found: C 64.25, H 6.21, N 10.68%.

#### Crystal data

$C_{14}H_{16}N_2O_3$	$Z = 4$
$M_r = 260.29$	$D_x = 1.299 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 11.516 (3) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 7.429 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 16.101 (3) \text{ \AA}$	Needle, colourless
$\beta = 104.878 (3)^\circ$	$0.52 \times 0.11 \times 0.08 \text{ mm}$
$V = 1331.3 (6) \text{ \AA}^3$	

#### Data collection

Bruker SMART CCD area-detector diffractometer	6562 measured reflections
$\varphi$ and $\omega$ scans	2505 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1614 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.954$ , $T_{\max} = 0.993$	$R_{\text{int}} = 0.056$
	$\theta_{\text{max}} = 25.0^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.0608P]$
$R[F^2 > 2\sigma(F^2)] = 0.062$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.180$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
2505 reflections	$\Delta\rho_{\text{min}} = -0.46 \text{ e \AA}^{-3}$
331 parameters	
H-atom parameters constrained	

**Table 1**

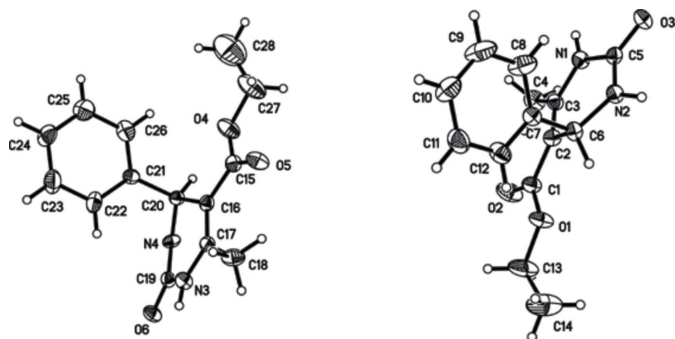
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O6^i$	0.86	2.17	2.993 (7)	161
$N2-H2\cdots O6^ii$	0.86	2.07	2.907 (7)	166
$N3-H3\cdots O3^{iii}$	0.86	2.07	2.927 (7)	172
$N4-H4\cdots O3^{iv}$	0.86	2.15	2.947 (7)	154
$C18-H18A\cdots O5$	0.96	2.25	2.844 (8)	119

Symmetry codes: (i)  $x, y, z - 1$ ; (ii)  $x, y + 1, z - 1$ ; (iii)  $x, y, z + 1$ ; (iv)  $x, y - 1, z + 1$ .

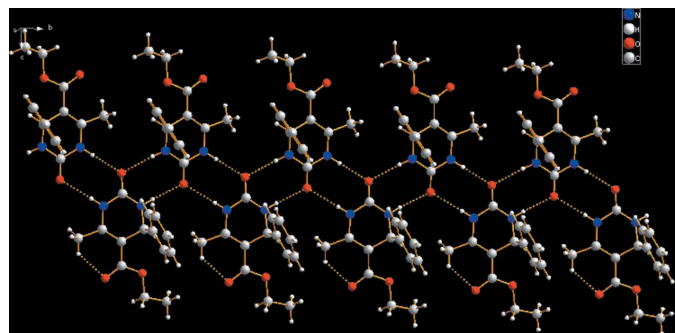
All H atoms were geometrically fixed in calculated positions and allowed to ride on their parent atoms, with  $C-H = 0.93-0.97 \text{ \AA}$  and  $N-H = 0.86 \text{ \AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ . In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000) and DIAMOND (Brandenburg, 2004); software used to prepare material for publication: SHELXTL.



**Figure 1**

The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.



**Figure 2**

Part of the crystal structure of (I), showing the eight-membered rings formed by  $N-H\cdots O$  intermolecular hydrogen-bonds and the six-membered rings formed by  $C-H\cdots O$  intramolecular hydrogen-bonds (indicated by dashed lines).

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