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## Key indicators

Single-crystal X-ray study  
 $T = 292\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$   
 $R$  factor = 0.053  
 $wR$  factor = 0.118  
Data-to-parameter ratio = 7.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Two tautomers in one crystal structure:  
ethyl 6(4)-oxo-1,6(1,4)-dihydropyrimidine-  
5-carboxylateThe crystal structure of the title compound,  $\text{C}_7\text{H}_8\text{N}_2\text{O}_3$ , contains a 1:1 mixture of two tautomers, *viz.* ethyl 6-oxo-1,6-dihydropyrimidine-5-carboxylate and ethyl 4-oxo-1,4-dihydropyrimidine-5-carboxylate. The molecules are linked into a three-dimensional network by  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds.Received 26 September 2006  
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## Comment

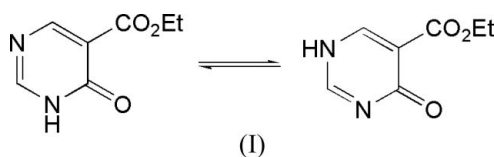
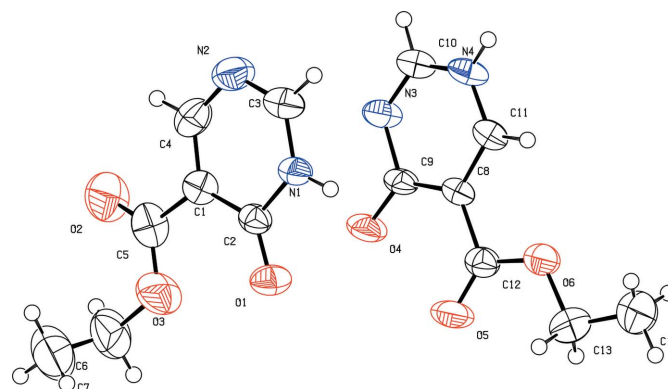
Pyrimidine-containing compounds have been intensively studied because of the biological activity which they usually exhibit (Rosowsky *et al.*, 2003). The title compound, (I), which may be a novel precursor of bioactive heterocyclic compounds, was designed and synthesized in our laboratory.Interestingly, the crystal structure (Fig. 1) consists of a 1:1 mixture of two tautomers, involving the exchange of a H atom between the two ring N atoms. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR data for (I) suggested that only one tautomer is present in solution. A similar case of prototropic annular tautomerism has been studied in an imidazole derivative (Kubicki, 2004).All bond lengths and angles are within normal ranges. The crystal packing (Fig. 2) of (I) is stabilized by strong  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and weak  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds between different tautomers.

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are depicted as spheres with arbitrary radii.

## Experimental

A solution containing diethyl 2-(ethoxymethylene)malonate (1.08 g, 1 mmol) and formamidine (0.264 g, 6 mmol) in anhydrous ethanol (30 ml) was refluxed for 24 h; the solvent was then removed under reduced pressure. Crystals suitable for an X-ray investigation were obtained by recrystallization from methanol and chloroform (1:2 v/v).

### Crystal data

$C_7H_8N_2O_3$	$Z = 8$
$M_r = 168.15$	$D_x = 1.441 \text{ Mg m}^{-3}$
Monoclinic, $C_c$	Mo $K\alpha$ radiation
$a = 4.768 (3) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$b = 25.590 (16) \text{ \AA}$	$T = 292 (2) \text{ K}$
$c = 12.821 (8) \text{ \AA}$	Plate, colorless
$\beta = 97.687 (10)^\circ$	$0.40 \times 0.10 \times 0.03 \text{ mm}$
$V = 1550.4 (17) \text{ \AA}^3$	

### Data collection

Bruker SMART APEX CCD diffractometer	1526 independent reflections
$\varphi$ and $\omega$ scans	1121 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.053$
4986 measured reflections	$\theta_{\text{max}} = 26.0^\circ$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2]$
$wR(F^2) = 0.118$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1526 reflections	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
219 parameters	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

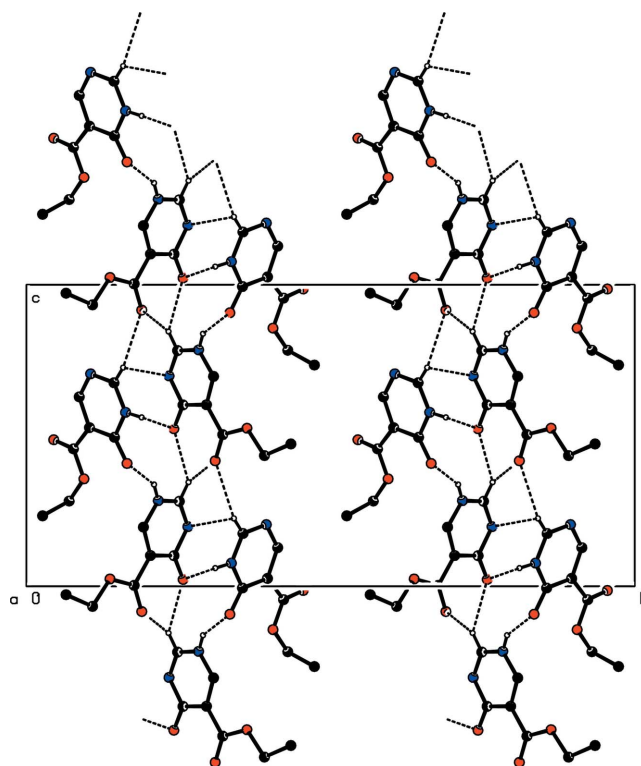
**Table 1**

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O4^i$	0.86	2.00	2.847 (5)	170
$C3-H3\cdots N3^i$	0.93	2.54	3.188 (7)	127
$N4-H4A\cdots O1^{ii}$	0.86	2.01	2.789 (5)	151
$C3-H3\cdots O5^{ii}$	0.93	2.55	3.307 (6)	139
$C10-H10\cdots O4^{ii}$	0.93	2.50	3.135 (6)	125
$C10-H10\cdots O5^{iii}$	0.93	2.55	3.281 (7)	136

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

All carbon-bound H atoms were positioned geometrically and then treated as riding, with  $C_{sp^2}-H = 0.93 \text{ \AA}$ , methyl  $C-H = 0.96 \text{ \AA}$  and methylene  $C-H = 0.97 \text{ \AA}$ , and with  $U_{\text{iso}}(H) = xU_{\text{eq}}(C)$ , where  $x = 1.5$  for methyl and 1.2 for other H atoms. Atoms H1 and H4A, attached to N1 and N4, respectively, were located in a difference map and refined as riding in their as-found positions, with  $N-H = 0.86 \text{ \AA}$  and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(N)$ . In the absence of significant anomalous scattering effects, 1391 Friedel pairs were merged.



**Figure 2**

A view of the packing in the crystal structure. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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