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Methyl (*E*)-3-acetamido-2-butenoate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.148
Data-to-parameter ratio = 18.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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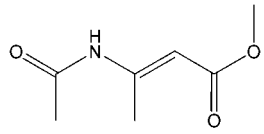
The crystal structure determination of the title compound, $C_7H_{11}NO_3$, shows that it is the *E* isomer. An N—H···O intermolecular hydrogen bond is observed. The molecules are linked along [101] through this intermolecular hydrogen bond.

Comment

The title compound, (I), is one of the isomers of methyl 3-acetamido-2-butenoate, a prochiral olefinic substrate for producing β-amino acids and derivatives by asymmetric hydrogenation (Hackler & Wickiser, 1985; Lubell *et al.*, 1991). The *E* isomer gives a much higher enantiomeric excess than the *Z* isomer in the asymmetric hydrogenation reaction (Burk *et al.*, 1996). The structure determination of (I) was conducted in order to obtain more knowledge about β-amino acids and their derivatives.



(I)

Fig. 1 shows a perspective view of the molecule. The deviations of the angles C4—C3—C7 [126.40 (17)°], C3—C4—C5 [124.88 (17)°] and N1—C3—C7 [110.64 (15)°] from the value of 120° results in a close approach between the methyl group on C3 and the carbonyl group on C4. The molecules are connected by intermolecular N—H···O hydrogen bonds (Table 1), to give chains along [101], as shown in Fig. 2.

Experimental

The title compound was synthesized according to the literature method (Zhu *et al.*, 1999). A crystal suitable for X-ray analysis was slowly grown in a mixed solvent of ethyl acetate and hexane (EA/nexane 1:6) at room temperature. ^{1}H NMR (400 MHz, acetone-d_6, p.p.m.): δ 2.03 (*s*, 3H), 2.29 (*s*, 3H), 3.58 (*s*, 3H), 6.85 (*d*, *J* = 1 Hz, 1H), 8.79 (*br*, 1H).

Crystal data

$C_7H_{11}NO_3$
M_r = 157.17
Monoclinic, $P2_1/n$
a = 8.099 (2) Å
b = 12.761 (2) Å
c = 8.750 (2) Å
β = 110.268 (4)°
V = 848.4 (2) Å^3
Z = 4
D_x = 1.231 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1994 reflections
θ = 1–27.5°
μ = 0.10 mm^{-1}
T = 294 (2) K
Prism, colourless
0.36 × 0.32 × 0.30 mm

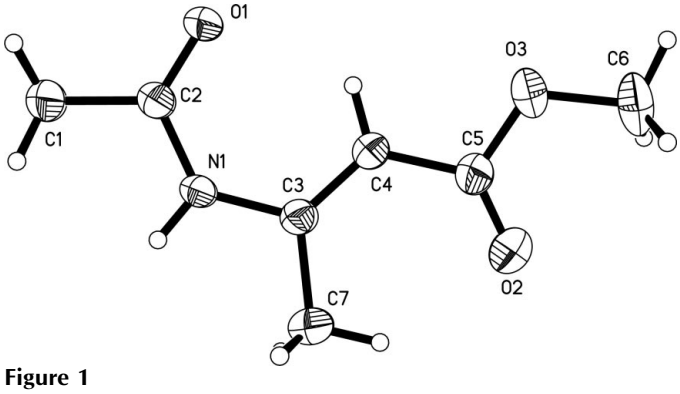


Figure 1
The molecular structure of (I), showing ellipsoids at the 30% probability level (Siemens, 1995).

Data collection

Siemens SMART CCD area-detector diffractometer	1945 independent reflections
φ and ω scans	994 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.038$
$T_{min} = 0.966$, $T_{max} = 0.972$	$\theta_{max} = 27.5^\circ$
5609 measured reflections	$h = -10 \rightarrow 9$
	$k = -14 \rightarrow 16$
	$l = -7 \rightarrow 11$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.148$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
1945 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
103 parameters	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.07	2.9188 (19)	169

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

H atoms were included in the riding-model approximation with U_{iso} values equal to U_{eq} of the atom to which they are bound.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995) and *SHELXTL-NT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

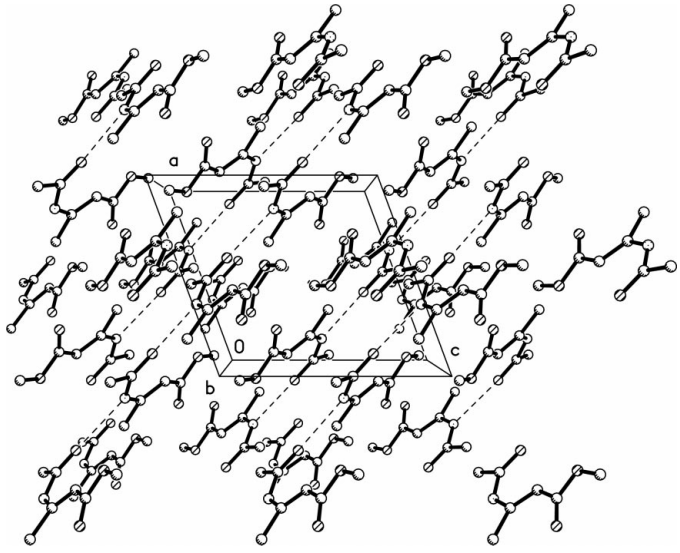


Figure 2
Packing diagram for the title compound. Hydrogen bonds are shown as dashed lines.

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