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Ethyl (*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 = 0.053
wR factor = 0.153
Data-to-parameter ratio = 19.3

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

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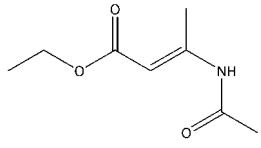
The crystal structure determination of the title compound, $C_8H_{13}NO_3$, shows that it is the *E* isomer. An N—H···O intermolecular hydrogen bond is observed and is responsible for the formation of infinite chains stretching along the *b* axis of the crystal.

Comment

The title compound, (I), is one of the products obtained from ethyl 3-amine-2-butenoate on reflux with acetic anhydride for a period of 24 h. This prochiral olefin is a model substrate studied in the asymmetric hydrogenation reaction (Hackler & Wickiser, 1985; Lubell *et al.*, 1991). The structure determination of (I) was conducted in order to obtain more stereochemical information about the behaviour of these kinds of substrates in hydrogenation reactions.



(I)

The crystal structure of (I) (Fig. 1) shows that the molecule is nearly planar. The angles C3—C4—C5 [124.71 (19)°] and C4—C3—C8 [125.27 (18)°] are wider and N1—C3—C8 [112.12 (16)°] narrower than the value of 120°. This results in a close mutual repulsion between the methyl group on C3 and the carbonyl group on C4 (Table 1). The molecules in the crystal structure are interconnected by N—H···O hydrogen bonding (Table 2). As shown in the packing diagram (Fig. 2), the N—H···O hydrogen bonds link the molecules along the *b* axis.

Experimental

The title compound was synthesized according the literature method (Zhu *et al.*, 1999) A crystal suitable for X-ray analysis was grown slowly from a mixture of ethyl acetate and hexane at room temperature. ^{1}H NMR (400 MHz, acetone-d_6, p.p.m.): δ 1.24 (*t*, *J* = 7.1 Hz, 3H), 2.06 (*s*, 3H), 2.33 (*s*, 3H), 4.09 (*q*, *J* = 7.1 Hz, 2H), 6.89 (*d*, *J* = 1 Hz, 1H), 8.79 (*br*, 1H).

Crystal data

$C_8H_{13}NO_3$
M_r = 171.19
Monoclinic, *C*2/*c*
a = 20.006 (4) Å
b = 9.545 (2) Å
c = 11.922 (2) Å
β = 124.479 (4)°
V = 1876.7 (6) Å^3
Z = 8
D_x = 1.212 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2174 reflections
θ = 1–27.5°
μ = 0.09 mm^{-1}
T = 294 (2) K
Plate, colourless
0.34 × 0.28 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.969, T_{max} = 0.991
6283 measured reflections
2162 independent reflections
1053 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.6°
$h = -22 \rightarrow 25$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.153
S = 1.05
2162 reflections
112 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.220 (2)	C3—C4	1.333 (3)
O2—C5	1.200 (2)	C3—C8	1.495 (3)
N1—C2	1.358 (2)	C4—C5	1.463 (3)
N1—C3	1.398 (2)		
O1—C2—N1	122.88 (17)	C3—C4—C5	124.71 (19)
O1—C2—C1	121.88 (17)	O2—C5—C4	128.1 (2)
C4—C3—C8	125.27 (18)	O3—C5—C4	109.46 (17)
N1—C3—C8	112.12 (16)		
C3—N1—C2—O1	2.3 (3)	C6—O3—C5—C4	178.83 (17)
C8—C3—C4—C5	0.2 (3)	C3—C4—C5—O3	−171.69 (19)
C6—O3—C5—O2	−1.5 (3)	C5—O3—C6—C7	−178.91 (19)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.10	2.943 (2)	165

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

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*.

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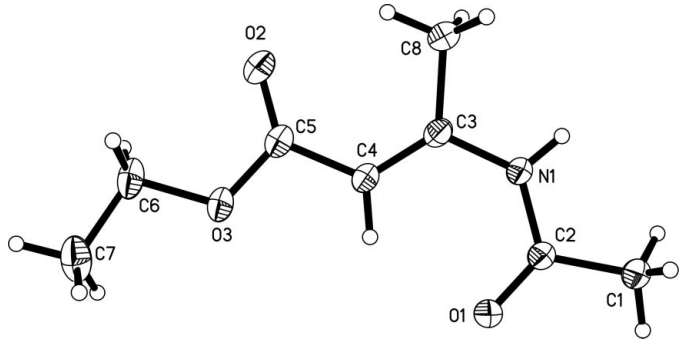

Figure 1
The molecular structure of (I), showing ellipsoids at the 30% probability level (Siemens, 1995).

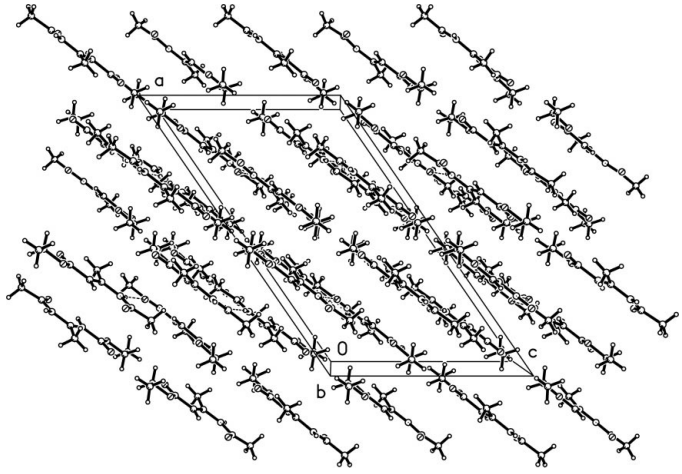

Figure 2
Packing diagram for (I). The hydrogen bonds are indicated by dashed lines.

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