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(*E*)-Ethyl 3-acetamido-2-hexenoate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.166
Data-to-parameter ratio = 20.8

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

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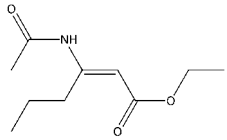
The crystal structure of the (*E*)-isomer of the title compound, $C_{10}H_{17}NO_3$, is reported. The molecules are linked along the *c* axis by intermolecular N—H···O hydrogen bonds.

Comment

The title compound (*E*)-ethyl 3-acetamido-2-hexenoate, (I), is one of the isomers of ethyl 3-acetamido-2-hexenoate, a prochiral olefinic substrate for producing β-amino acids and derivatives by asymmetric hydrogenation (Lubell *et al.*, 1991; Yasutake *et al.*, 2001). The enantiomeric excess of the hydrogenation product of the (*Z*) and (*E*) isomers is significantly different. The crystal structure of (I) (Fig. 1) exhibits bond lengths and angles within normal ranges (Table 1). In the packing, the molecules are interconnected by N—H···O hydrogen bonding (Table 2). The hydrogen bonds link the molecules along the *c* axis (Fig. 2).



(I)

Experimental

(*E*)-Ethyl 3-acetamido-2-hexenoate was synthesized according to literature methods (Zhu *et al.* 1999) A crystal suitable for X-ray analysis was grown slowly in a mixed solvent (ethyl acetate and hexane) at room temperature. ^{1}H NMR (500 MHz, acetone-d_6, Varian): δ 0.92 (*t*, *J* = 7.36 Hz, 3H), 1.21 (*t*, *J* = 7.11 Hz, 3H), 1.56 (*m*, 2H), 2.04 (*s*, 3H), 2.72 (*m*, 2H), 4.06 (*q*, *J* = 7.11 Hz, 2H), 6.91 (*s*, 1H), 8.72 (*br*, 1H).

Crystal data

$C_{10}H_{17}NO_3$
M_r = 199.25
Monoclinic, $P2_1/c$
a = 11.036 (2) Å
b = 12.260 (2) Å
c = 9.5764 (18) Å
β = 113.851 (4)°
V = 1185.0 (4) Å^3
Z = 4
D_x = 1.117 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2265 reflections
θ = 1–27.5°
μ = 0.08 mm^{-1}
T = 294 (2) K
Block, colorless
0.40 × 0.32 × 0.30 mm

Data collection

Siemens CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.976
7877 measured reflections
2709 independent reflections
1073 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.5°
h = −14 → 14
k = −15 → 13
l = −12 → 12

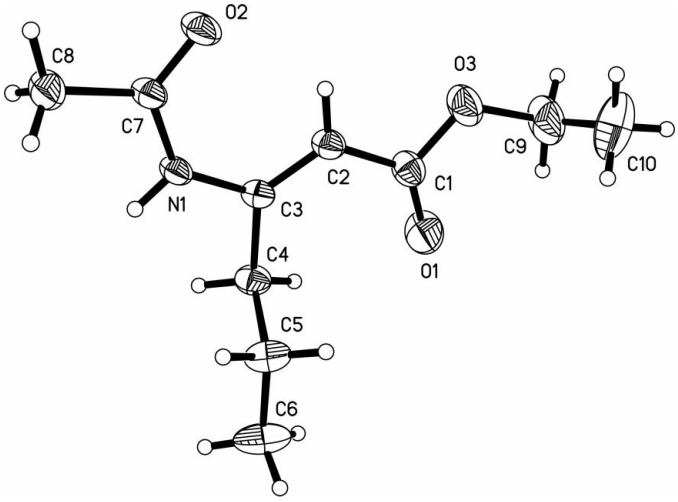


Figure 1
Molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level.

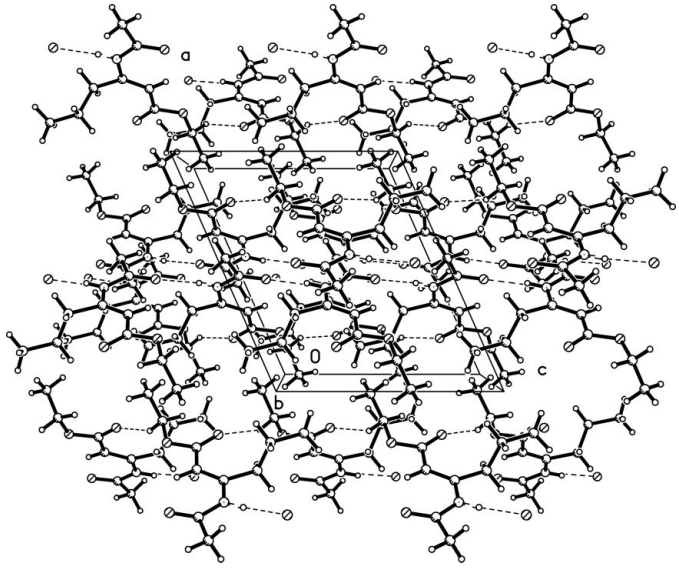


Figure 2
Packing diagram for (I). The hydrogen bonds are indicated by dashed lines.

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.166$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.09$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
2709 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
130 parameters	

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.195 (3)	N1—C7	1.357 (3)
O2—C7	1.223 (2)	C2—C3	1.336 (3)
C1—O3—C9	117.8 (2)	O1—C1—C2	128.3 (2)
C7—N1—C3	130.14 (17)		
O1—C1—C2—C3	−2.7 (4)	C1—C2—C3—C4	0.1 (4)
C1—C2—C3—N1	178.6 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	2.07	2.920 (2)	167

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

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

Data collection: *SMART* (Bruker, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000) and *SHELXTL-NT* (Bruker, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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