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N-[3-Acetamido-1,3-bis(4-ethylphenyl)butenyl]-acetamide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.082
Data-to-parameter ratio = 19.9

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

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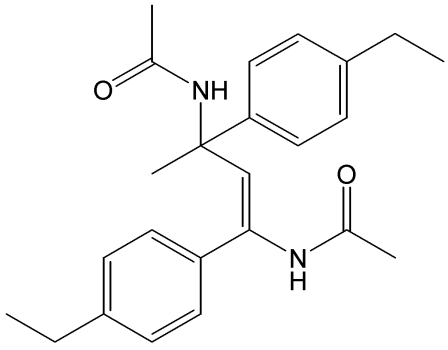
Both intra- and intermolecular N—H···O hydrogen bonds are found in the structure of the title compound, $C_{24}H_{30}N_2O_2$. Molecules are assembled into chains, along the *b* axis, *via* intermolecular interactions.

Comment

The title compound, *N*-[3-acetamido-1,3-bis(4-ethylphenyl)-butenyl]acetamide, (I), is one of the by-products obtained during the synthesis of *N*-[1-(4-ethylphenyl)ethenyl]acetamide (Burk *et al.*, 1998). In this study, the structure determination of (I) was conducted in order to obtain more knowledge about enamide compounds.



(I)

In the crystal structure (Fig. 1), the C13—C14 bond distance of 1.336 (3) Å is indicative of double-bond character. The C13—C14—C17—C22, C15—N2—C14—C17 and C15—N2—C14—C13 torsion angles are 23.8 (4), 63.2 (3) and −124.7 (3)°, suggesting little conjugation in this residue, although the C3—C13—C14—C17 torsion angle is 177.0 (2)°. Atom H2*A* of amine-N2 forms an intramolecular hydrogen bond with O1 (Table 1). Atom H1*A* of amine-N1 forms an intermolecular hydrogen bond with O2*A* of another molecule (x, $1/2-y$, $z-1/2$). As illustrated in Fig. 2, these interactions link the molecules in chains along the *b* axis.

Experimental

The title compound was synthesized according to the literature method of Burk *et al.* (1998). A crystal suitable for X-ray analysis was slowly grown from a mixed solvent (ethyl acetate/hexane = 1:5) at room temperature. ^{1}H NMR (500 MHz, $CDCl_3$, Varian): δ 1.18–1.22 (*m*, 6H), 1.35 (*s*, 3H), 1.63 (*s*, 3H), 2.09 (*s*, 3H), 2.59–2.63 (*m*, 4H), 5.37 (*s*, 1H), 6.02 (*s*, 1H), 7.12–7.20 (*m*, 6H), 7.35 (*d*, *J* = 8.5 Hz, 2H), 8.97 (*s*, 1H).

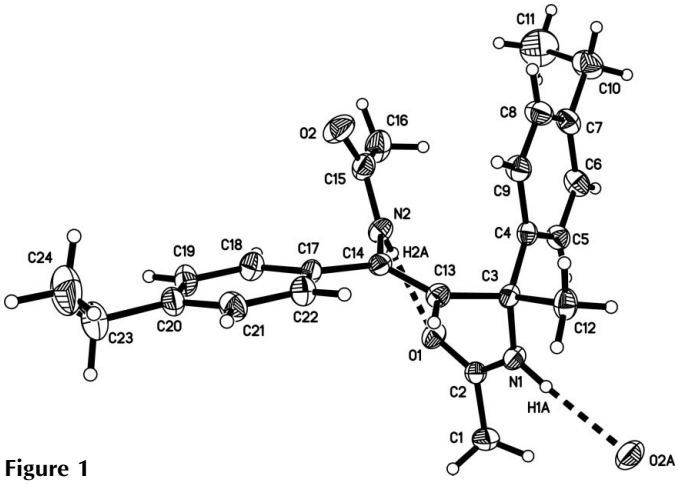


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level (Siemens, 1995).

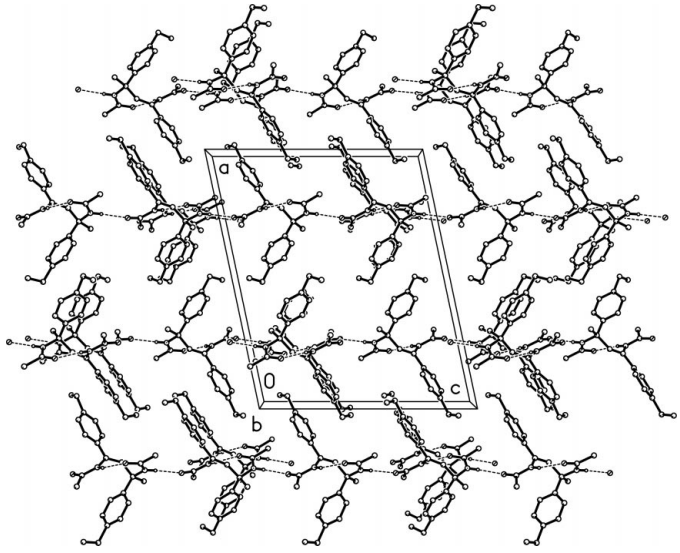


Figure 2
Packing diagram for (I). Hydrogen bonds are indicated by dashed lines.

Crystal data

$C_{24}H_{30}N_2O_2$	D_x = 1.113 Mg m^{-3}
M_r = 378.50	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1867 reflections
a = 20.773 (4) Å	θ = 1–27.5°
b = 6.5109 (10) Å	μ = 0.07 mm^{-1}
c = 17.063 (3) Å	T = 294 (2) K
β = 101.918 (4)°	Prism, colorless
V = 2258.0 (6) Å^3	0.28 × 0.23 × 0.20 mm
Z = 4	

Data collection

Bruker CCD area-detector diffractometer	5141 independent reflections
φ and ω scans	1539 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.083
T_{min} = 0.981, T_{max} = 0.986	θ_{max} = 27.5°
11299 measured reflections	$h = -20 \rightarrow 26$
	$k = -7 \rightarrow 8$
	$l = -22 \rightarrow 16$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.005P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.082	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.91	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
5141 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
258 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	2.11	2.964 (3)	175
N2—H2A···O1	0.86	2.01	2.753 (3)	144

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

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* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SHELXTL-NT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); 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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