Data collection: *AED* (Bocelli *et al.*, 1993). Cell refinement: *AED*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Software used to prepare material for publication: *SHELXL*93.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: CF1175). Services for accessing these data are described at the back of the journal.

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2-(*N*-Acetylamino)pent-4-ynamide

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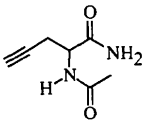
Abstract

The title compound, $C_7H_{10}N_2O_2$, displays extensive hydrogen-bonding interactions which give rise to connected 10- and 11-membered rings throughout the lattice.

Comment

Inter- and intramolecular hydrogen-bonding interactions are essential for the biological activity of proteins and oligopeptides. In order to probe the nature of their hydrogen-bonding potential, peptidomimetics have been developed (Gung & Zhu, 1996; Mrksich & Dervan, 1995; Gante, 1994). A systematic study of the hydrogen-bonding characteristics of alkynylamino acid amidates (Crisp *et al.*, 1997) has been undertaken in order to ascertain the structural motifs important in defining



(I)

the three-dimensional arrays within oligopeptides. As a part of this study, the title compound, (I), has been investigated crystallographically.

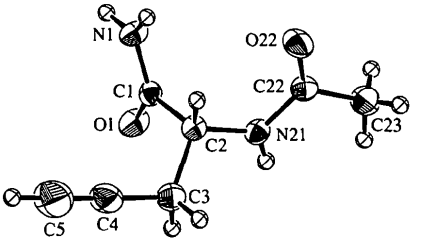


Fig. 1. The title structure drawn with 50% probability ellipsoids.

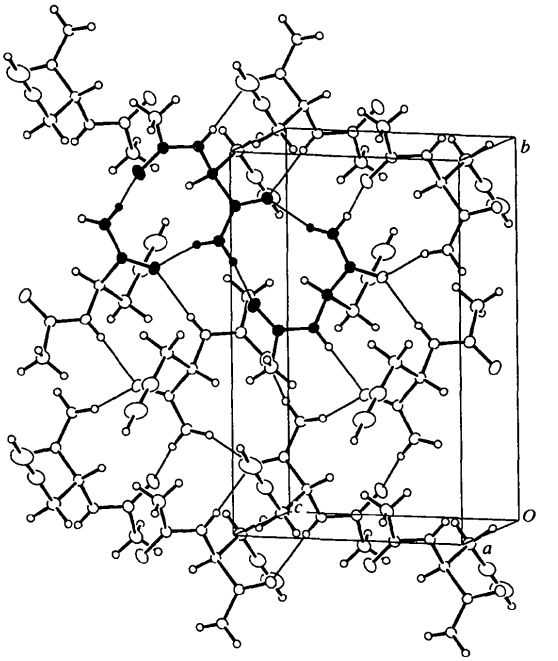


Fig. 2 Unit-cell contents highlighting the different hydrogen-bonding associations.

The molecular structure of (I) is shown in Fig. 1. The amino residue is almost orthogonal to the acetoamide residue, as seen in the O1—C1—C2—N21 torsion angle of 71.6 (2)°. This arrangement precludes intramolecular hydrogen bonding. There are, however, significant intermolecular hydrogen-bonding contacts in the lattice.

The molecules are connected *via* an extensive hydrogen-bonding network; see Table 2 and Fig. 2. Centrosymmetrically related aminocarbonyl residues form 10-membered rings designated $R_2^2(10)$ (Etter, 1990). These rings are linked by sharing each of the two C1—O1 edges with two 11-membered rings formed between the amido group of one molecule and the amido and acetoamido ends of a symmetry-related molecule; *i.e.* $R_2^2(11)$. Significant intermolecular interactions involving acetylene residues have been noted (Desiraju, 1996), however, no such contacts are found in the present structure, with the closest interaction of 2.82 (3) Å occurring between O22 and H5^{i} [symmetry code: (i) $x-1, \frac{1}{2}-y, -\frac{1}{2}+z$].

Experimental

The title compound was produced from the direct amidation of ethyl 2-(*N*-acetyl)pent-4-ynoate with saturated ammonia solution in methanol (Kent *et al.*, 1985). Recrystallization was from methanol at room temperature; m.p. 445–446 K.

Crystal data

$C_7H_{10}N_2O_2$
M_r = 154.17
Monoclinic
$P2_1/c$
a = 7.516 (1) Å
b = 12.962 (2) Å
c = 8.550 (1) Å
β = 97.78 (1)°
V = 825.3 (2) Å^3
Z = 4
D_x = 1.241 Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
λ = 0.7107 Å
Cell parameters from 21 reflections
θ = 25.2–27.2°
μ = 0.093 mm^{-1}
T = 213 K
Block
0.32 × 0.32 × 0.23 mm
Colourless

Data collection

Rigaku AFC-6*R* diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2143 measured reflections
2001 independent reflections
1405 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.6°
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 16$
$l = -11 \rightarrow 11$
3 standard reflections
every 400 reflections
intensity decay: 4.00%

Refinement

Refinement on F
R = 0.044
wR = 0.051
S = 2.151
1405 reflections
140 parameters
All H-atom parameters refined (located from a difference map)
$w = 1/[\sigma^2(F_o) + (0.021F)^2]$
$(\Delta/\sigma)_{max}$ = 0.0055
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. *Selected geometric parameters (Å, °)*

O1—C1	1.238 (2)	C1—C2	1.528 (2)
O22—C22	1.233 (2)	C2—C3	1.534 (2)
N1—C1	1.319 (2)	C3—C4	1.464 (3)
N21—C2	1.456 (2)	C4—C5	1.169 (3)
N21—C22	1.338 (2)	C22—C23	1.500 (3)
C2—N21—C22	124.1 (1)	C1—C2—C3	111.8 (1)
O1—C1—N1	123.1 (2)	C2—C3—C4	112.8 (2)
O1—C1—C2	120.0 (1)	C3—C4—C5	178.1 (3)
N1—C1—C2	116.9 (1)	O22—C22—N21	122.8 (2)
N21—C2—C1	107.5 (1)	O22—C22—C23	122.2 (2)
N21—C2—C3	108.9 (1)	N21—C22—C23	115.0 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*a*···O1^{i}	0.88 (2)	2.01 (2)	2.866 (2)	161 (2)
N1—H1*b*···O22^{ii}	0.95 (2)	1.95 (2)	2.891 (2)	168 (2)
N21—H21···O1^{iii}	0.83 (2)	2.05 (2)	2.867 (2)	166 (2)

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

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1992). Program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994). Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *TEXSAN*.

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