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N-Acryloylglycine

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.102
Data-to-parameter ratio = 7.7

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

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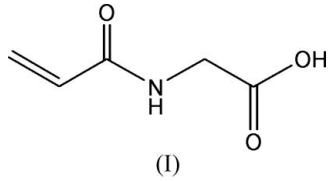
In the crystal structure of the title compound, $C_5H_7NO_3$, intermolecular hydrogen bonds, link the molecules into a three-dimensional network.

Comment

N-Acryloyl amino acids are useful as synthetic intermediates and as free radical addition monomers, and have been utilized to prepare radiation-sensitive (Heilmann & Palensky, 1981), pressure-sensitive, hydrophilic and hydrophobic (Heilmann & Rasmussen, 1984) polymers. We report here the crystal structure of the title compound, (I).



(I)

In the molecule of (I) (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

The O1/O2/C1/C2/N1 and N1/O3/C3/C4/C5 units are nearly planar, with maximum deviations from the least-squares planes of 0.0240 (3) Å (for C2) and 0.0458 (3) Å (for C5); the dihedral angle between the planes is 12.64 (2)°.

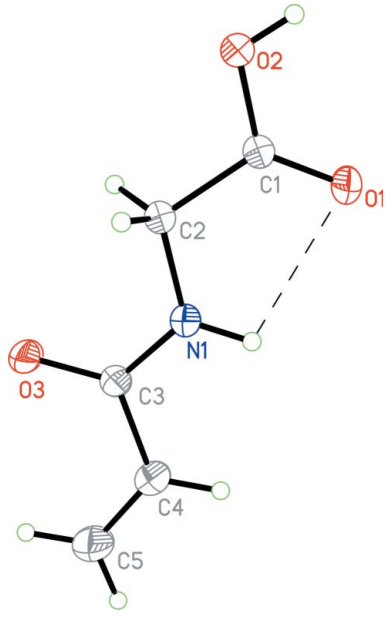


Figure 1
The molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

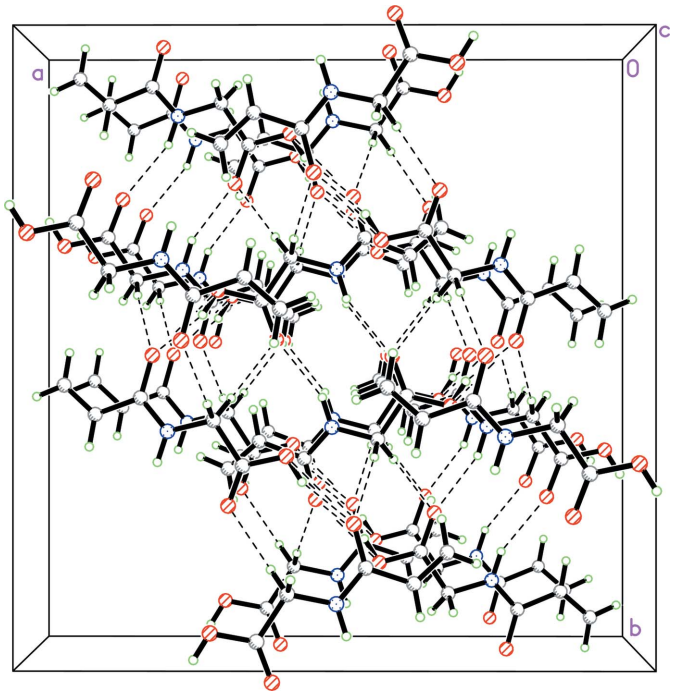


Figure 2
A packing diagram of (I). The intermolecular hydrogen bonds are shown as dashed lines.

As can be seen from the packing diagram (Fig. 2), intermolecular hydrogen bonds (Table 1) link the molecules into a three dimensional network, in which they may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

Acryloyl chloride (5 ml, 0.11 mol) containing diphenylpicrylhydrazyl polymerization inhibitor (0.01%) and sodium hydroxide (4.0 g, 0.1 mol) in aqueous solution (40 ml water) were simultaneously added dropwise over a 30 min period to a well stirred aqueous solution (100 ml water) of glycine (7.5 g, 0.1 mol) and sodium hydroxide (4.4 g, 0.2 mol), and stirred for a futher 1 h. The reaction mixture was kept at 273 K in an ice–water bath. The solution was acidified to pH = 2 with 6 *N* HCl and extracted with five portions of ethyl acetate (50 ml). The ethyl acetate solution was dried with anhydrous magnesium sulfate, and the product was purified by repeated crystallization.

Crystal data

$C_5H_7NO_3$
M_r = 129.12
Orthorhombic, *Fdd*2
a = 18.212 (4) Å
b = 18.318 (4) Å
c = 7.5330 (15) Å
V = 2513.0 (9) Å^3
Z = 16
D_x = 1.365 Mg m^{-3}
Mo *K*α radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
1307 measured reflections
666 independent reflections
614 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.102
S = 1.04
666 reflections
87 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.5439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.90 (3)	2.35 (3)	2.712 (3)	104 (2)
N1—H1···O1^{i}	0.90 (3)	2.14 (3)	3.001 (3)	159.00
C2—H2*A*···O3^{ii}	0.97	2.54	3.481 (4)	163

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

The N-bound H atom was located in a difference map and refined freely [N—H = 0.90 (3) Å]. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å (for methine and terminal alkene), O—H = 0.82 Å (for OH) and C—H = 0.97 Å (for methylene), and constrained to ride on their parent atoms with U_{iso}(H) = xU_{eq}(C/O), where *x* = 1.5 for hydroxyl H and *x* = 1.2 for all other H. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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