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3-(1*H*-Indol-3-yl)-2-(2-methylacryloyl)propanoic acid

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.008 Å
R factor = 0.069
wR factor = 0.200
Data-to-parameter ratio = 9.2

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

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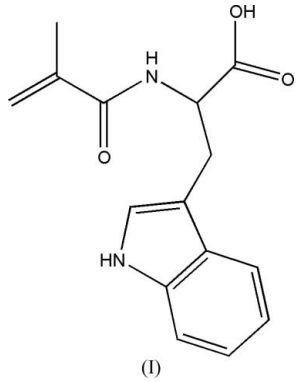
In the crystal structure of the title compound, $C_{15}H_{16}N_2O_3$, N—H···O and O—H···O hydrogen bonds link the molecules into a three-dimensional network, in which they may be effective in the stabilization of the crystal structure.

Comment

The crystal structrure determination of (I) has been carried out in order to elucidate the molecular conformation. We here report its synthesis and crystal structure.



(I)

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

As can be seen from the packing diagram (Fig. 2), intermolecular N—H···O and O—H···O hydrogen bonds

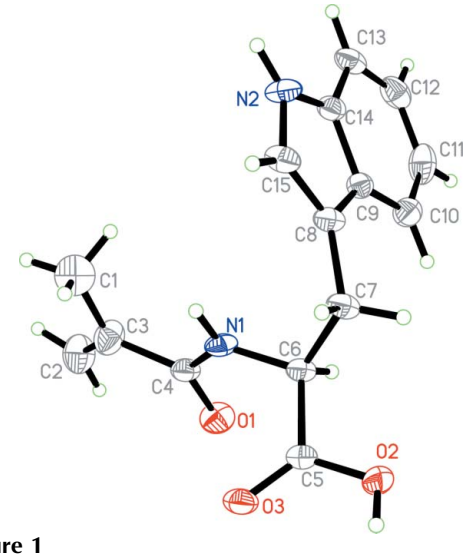


Figure 1
The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

(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

To a well stirred aqueous solution of tryptophan (2.5 g in 50 ml H_2O) and sodium hydroxide (0.54 g in 5 ml of H_2O), acryloyl chloride (1.3 ml) containing diphenylpicrylhydrazyl (0.01%) polymerization inhibitor and sodium hydroxide solution (0.54 g in 5 ml of H_2O) were added dropwise simultaneously over a 30 min period and the stirring was continued for 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 the resulting solid was filtered off and crystallized from ethyl acetate (yield 45%, m.p. 415–416 K).

Crystal data

$C_{15}H_{16}N_2O_3$
M_r = 272.30
Orthorhombic, $P2_12_12_1$
a = 9.4220 (19) Å
b = 10.587 (2) Å
c = 14.328 (3) Å
V = 1429.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.974, T_{max} = 0.982
1634 measured reflections
1612 independent reflections
1211 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.200
S = 1.06
1612 reflections
175 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*A*···O1^{i}	0.82	1.76	2.580 (5)	176
N2—H2*D*···O3^{ii}	0.86	2.14	2.946 (6)	157

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x-1, y, z$.

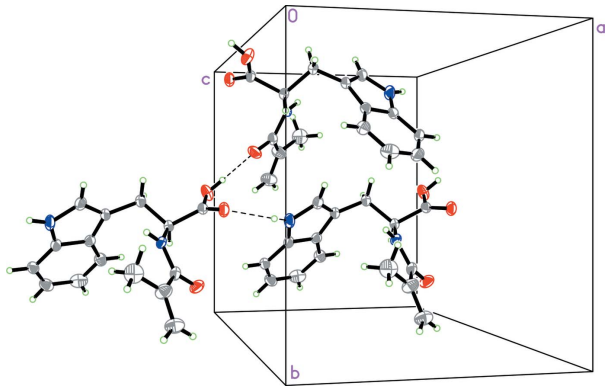


Figure 2
A partial packing diagram for (I). O—H···O hydrogen bonds are shown as dashed lines.

H atoms were positioned geometrically, with O—H = 0.82 Å, N—H = 0.86 Å, and C—H = 0.93 and 0.98 Å (for aromatic and methine, respectively), 0.93 and 0.97 Å (for methylene), and 0.96 Å (for methyl), and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,N,O), where x = 1.5 for hydroxy and methyl H, and x = 1.2 for all other H atoms.

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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