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1-(Carbamoylmethyl)-5-oxopyrrolidin-3-yl propionate

Chen Xin, Lin Jie, Yu Ming and Zuo-Liang Jing*

College of Sciences, Tianjin University of Science and Technology, Tianjin 300222, People's Republic of China

Correspondence e-mail: jzl74@tust.edu.cn

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Key indicators

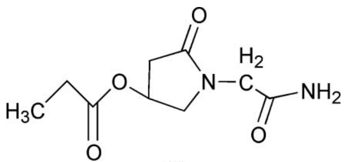
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.152
Data-to-parameter ratio = 12.4

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

The title compound, $C_9H_{14}N_2O_4$, was prepared from 2-(4-hydroxy-2-oxocyclopentyl)acetamide and propionic acid anhydride. In the crystal structure, molecules are linked through N—H⋯O hydrogen bonds, forming an extended supramolecular assembly which contributes to the stability of the structure in the solid state.

Comment

The synthesis of new intentionally designed crystal structures is part of a major strand of modern chemistry (Belloni *et al.*, 2005; Tynan *et al.*, 2005). One of the aims of crystal engineering is to establish control over the preparation of crystalline solid materials so that their subsequent architecture and properties are predictable. As part of an investigation of crystal structures with strong intermolecular bonding that might provide useful information in the field of crystal engineering, we report here the synthesis and crystal structure of the title compound, (I).



(I)

A view of the molecular structure of (I) is shown in Fig. 1 and selected bond lengths and angles in (I) are given in Table 1. They are all within normal ranges. Molecules are linked through N—H⋯O hydrogen bonds (Table 2), forming a supramolecular assembly that extends throughout the crystal structure, leading to enhanced stability. Fig. 2 shows a portion of this extensively hydrogen-bonded supramolecular assembly.

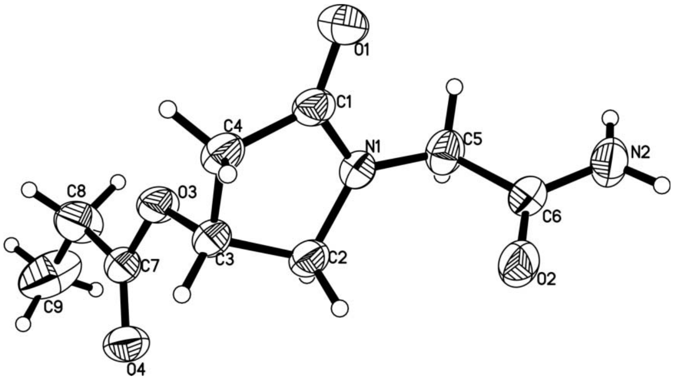


Figure 1
A view of the title compound, shown with 30% probability displacement ellipsoids.

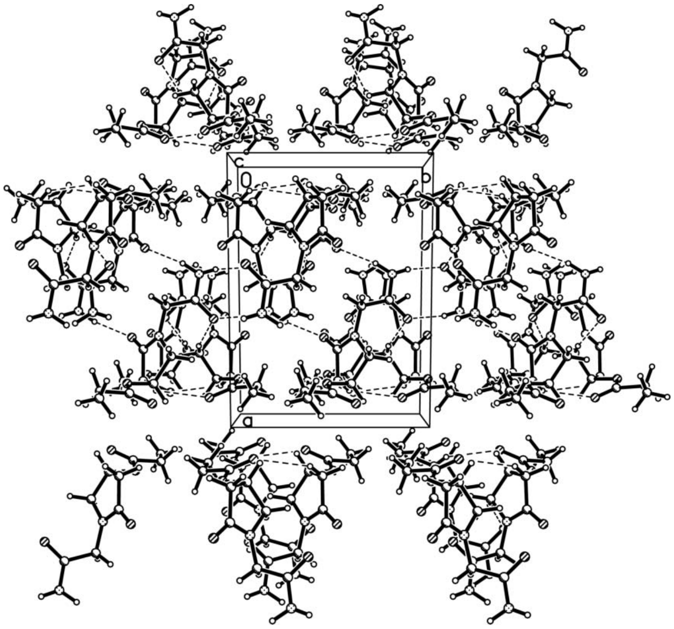


Figure 2
A view down the *c* axis of a portion of the crystal structure, showing the extensive intermolecular hydrogen-bonding interactions (dashed lines).

Experimental

An anhydrous pyridine solution of 2-(4-hydroxy-2-oxocyclopentyl)-acetamide (1.54 g, 10 mmol) was added to propionic acid anhydride (1.30 g, 10 mmol). The mixture was stirred at 298 K for 20 h under nitrogen, and a white precipitate formed. This product was isolated and recrystallized from pyridine, and then dried *in vacuo* to give the pure compound in 98% yield. White single crystals of (I) suitable for X-ray analysis were obtained by the slow evaporation of a pyridine solution of (I).

Crystal data

$C_9H_{14}N_2O_4$
$M_r = 214.22$
Monoclinic, $P2_1/c$
$a = 12.6981\ (17)$ Å
$b = 9.0630\ (13)$ Å
$c = 9.5362\ (13)$ Å
$\beta = 104.592\ (2)^\circ$
$V = 1062.1\ (3)$ Å^3
$Z = 4$

$D_x = 1.340$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1021 reflections
$\theta = 2.8$–21.3°
$\mu = 0.11$ mm^{-1}
$T = 294\ (2)$ K
Block, white
0.32 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{\min} = 0.901$, $T_{\max} = 0.983$
5641 measured reflections

1811 independent reflections
993 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\max} = 25.0^\circ$
$h = -8 \rightarrow 15$
$k = -10 \rightarrow 10$
$l = -8 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.152$
$S = 0.97$
1811 reflections
146 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0912P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.025 (6)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.230 (3)	N1—C1	1.340 (3)
O2—C6	1.231 (3)	N1—C5	1.435 (3)
O3—C7	1.334 (3)	N1—C2	1.462 (3)
O3—C3	1.452 (3)	N2—C6	1.312 (4)
O4—C7	1.196 (3)		
C7—O3—C3	117.66 (18)	C1—N1—C2	113.1 (2)
C1—N1—C5	122.7 (2)	C5—N1—C2	123.8 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2$^{\rm i}$	0.85 (3)	2.14 (3)	2.974 (3)	166 (3)
N2—H2B···O1$^{\rm ii}$	0.94 (4)	2.04 (4)	2.964 (4)	168 (3)

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$.

C-bound H atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.96–0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). H atoms attached to N atoms were located in a difference Fourier map and refined freely.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2006). E**62**, o678–o679 Xin *et al.* • $C_9H_{14}N_2O_4$ **o679**