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

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.082
Data-to-parameter ratio = 8.5

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

The title compound, $C_8H_{12}N_2O_4$, was prepared from 2-(4-hydroxy-2-oxopyrrolidin-1-yl)acetamide and acetic anhydride. In the crystal structure, molecules are linked through N—H···O hydrogen bonds to form an extended network, which contributes to the stability of the structure in the solid state.

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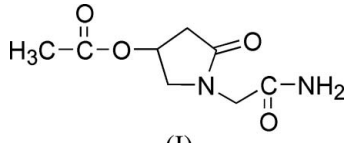
Comment

The syntheses of new intentionally designed crystal structures are 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. In an investigation of a crystal structure with strong intermolecular bonding that might provide useful information to the field of crystal engineering, we report here the synthesis and the crystal structures of the title compound, (I).



(I)

A view of one molecule of (I) is shown in Fig. 1, and selected bond length and bond angle values are shown in Table 1. They are all within the normal ranges for such values. The molecules are linked through hydrogen bonds N—H···O (Table 2) to form a network that extends throughout the crystal structure, which leads to a very stable crystal structure. Fig. 2 shows a

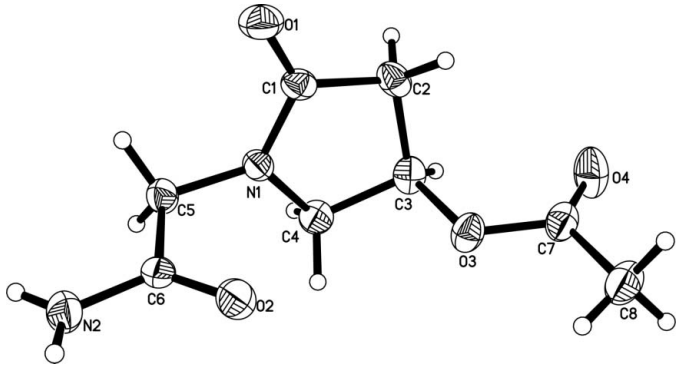


Figure 1
A view of the title compound, with 30% probability displacement ellipsoids.

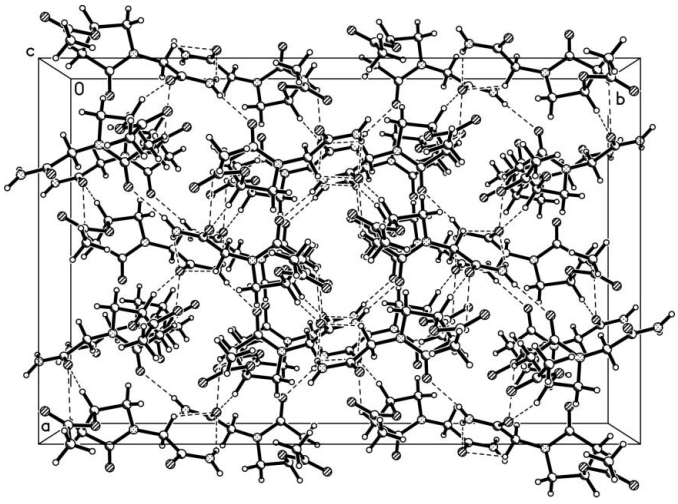


Figure 2
A view down the *c* axis of a portion of the crystal structure, showing extensive intermolecular hydrogen-bonding interactions (dashed lines). The horizontal direction is approximately parallel to the *b* axis of the unit cell.

portion of this extensively hydrogen-bonded supramolecular assembly.

Experimental

An anhydrous pyridine solution of 2-(4-hydroxy-2-oxopyrrolidin-1-yl)acetamide (1.58 g, 10 mmol) was added to acetic anhydride (1.02 g, 10 mmol). The mixture was stirred at 298 K for 25 h under nitrogen, and a white precipitate appeared. This product was isolated and recrystallized from pyridine, and then dried *in vacuo* to give a pure compound in 85% 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

$C_8H_{12}N_2O_4$
M_r = 200.20
Orthorhombic, *Fdd*2
a = 16.838 (9) Å
b = 26.184 (14) Å
c = 8.419 (5) Å
V = 3712 (3) Å^3
Z = 16
D_x = 1.433 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1534 reflections
θ = 2.8–21.8°
μ = 0.12 mm^{-1}
T = 294 (2) K
Block, white
0.56 × 0.34 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.924, T_{max} = 0.975
5984 measured reflections
1157 independent reflections
929 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.7°
h = −21 → 21
k = −19 → 34
l = −10 → 10

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.082
S = 1.04
1157 reflections
136 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.221 (3)	N1—C1	1.341 (2)
O2—C6	1.224 (3)	N1—C5	1.438 (2)
O3—C7	1.349 (3)	N1—C4	1.450 (3)
O3—C3	1.455 (3)	N2—C6	1.335 (3)
O4—C7	1.203 (3)		
C7—O3—C3	115.75 (17)	C5—N1—C4	122.25 (15)
C1—N1—C5	123.84 (17)	C6—N2—H2*C*	119.9 (19)
C1—N1—C4	113.91 (16)	C6—N2—H2*D*	115 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*C*···O2^{i}	0.86 (4)	2.41 (4)	3.189 (4)	152 (3)
N2—H2*D*···O1^{ii}	0.92 (4)	2.20 (4)	3.113 (3)	168 (4)

Symmetry codes: (i) $-x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x-\frac{1}{4}, y-\frac{1}{4}, z+\frac{1}{4}$.

C-bound H atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.96–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). H atoms attached to N atoms were located in a difference Fourier map and then refined freely. In the absence of significant anomalous scattering, Friedel pairs were merged.

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

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