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N-Formylglycine

Carl Henrik Görbitz[a]* and Einar Sagstuen[b]

[a]Department of Chemistry, University of Oslo, PO Box 1033 Blindern, N-0315 Oslo, Norway, and [b]Department of Physics, University of Oslo, PO Box 1048 Blindern, N-0316 Oslo, Norway

Correspondence e-mail: c.h.gorbitz@kjemi.uio.no

Key indicators

Single-crystal X-ray study
T = 105 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.122
Data-to-parameter ratio = 12.0

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

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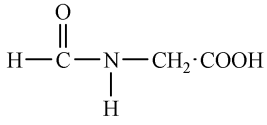
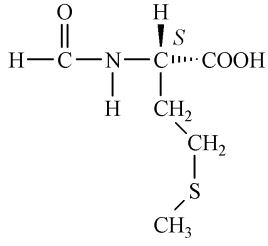
The title compound, $C_3H_5NO_3$, is used as a model system for studies of radiation damage in more complex polypeptides. The crystal structure is only the third of an isolated *N*-formyl amino acid. Essentially planar molecules form hydrogen-bonded sheets with three types of intermolecular interactions, including a very rare >N—H···O hydrogen bond with the OH group of the carboxylic acid function as the acceptor.

Comment

The radiation chemistry of amino acids has been studied for many years to learn about the responses to radiation of more complex polypeptides (Sagstuen *et al.*, 2004). However, it is clear that the peptide bond modifies the radiation behavior, and investigating model systems exhibiting this important function is thus useful. *N*-Formylglycine, (I), is the simplest peptide derived from a natural amino acid, and it also forms a 1:1 crystalline complex with the nucleic acid base cytosine (Ohki *et al.*, 1975). Protein–DNA interactions are of interest with regard to the possibility of intermolecular charge transfer resulting from radiation-induced charge injection in the systems. For electron paramagnetic resonance (EPR) studies of the radiation action on compounds modeling such interactions (Vågane, 2002), the crystal structure of (I) is a prerequisite.



(I)



(II)

The molecular structure of (I) is shown in Fig. 1; bond lengths and angles are normal. Apart from the cytosine complex of (I) (Ohki *et al.*, 1975), in which the peptide molecule is present as an anion, only two structures of *N*-formyl amino acids have been reported in the past, *viz* *N*-formyl-L-methionine, (II) (Chen & Parthasarathy, 1977), and *N*-formyl-2,2-diethylglycine (Valle *et al.*, 1992). Both compounds share the planar backbone geometry of (I), as defined by the torsion angles listed in Table 1. In contrast, *N*-formylglycine in the cytosine complex has C1—C2—N1—C3 = −81.1°, giving the peptide molecule a twisted conformation.

The crystal packing of (I) is depicted in Fig. 2. Peptide molecules are connected by hydrogen bonds and form two-

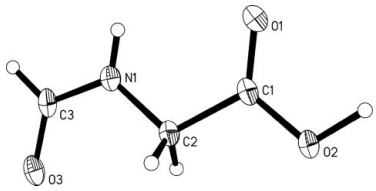


Figure 1
The molecular structure of *N*-formylglycine. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary size.

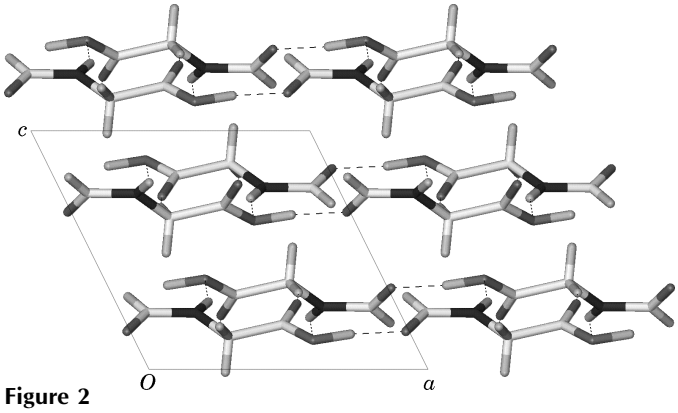


Figure 2
The molecular packing and unit cell, viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

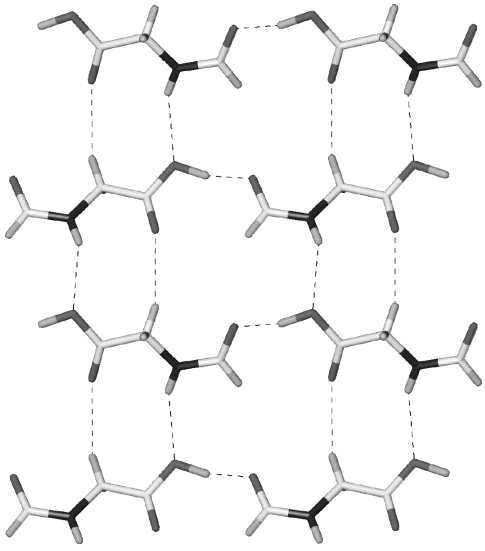


Figure 3
A hydrogen-bonded layer in the structure of *N*-formylglycine. The view is perpendicular to the *ab* plane. Dashed lines indicate hydrogen bonds.

dimensional sheets perpendicular to the *ab* plane. Individual sheets contain three types of hydrogen bonds (Fig. 3 and Table 2). The COOH···O=C(amide) interaction is highly abundant in *N*-acyl amino acid structures, but the >N—H···OH—C=O contact is very rare indeed, since the O=C(carboxyl) is usually the preferred acceptor. This special hydrogen bond was found only for (*S*)-*N*-acetyl-α-phenylglycine (Salas-Coronado *et al.*, 2001) among 28 reasonably simple *N*-acetyl amino acids in the Cambridge Structural Database (Version 5.25, November 2003; Allen, 2002), but also for (II) (Chen & Parthasarathy, 1977). The structures of (I) and (II) are very similar, with the same overall crystal packing arrangement and intermolecular interactions, including the third type of hydrogen bond in Table 2, a C^{α}—H···O=C—OH motif.

Experimental

N-Formylglycine was obtained from Sigma–Aldrich and Fluka. Prismatic crystals were prepared by recrystallization from aqueous solution at room temperature. Twinning was common for larger crystals.

Crystal data

$C_3H_5NO_3$
M_r = 103.08
Monoclinic, $P2_1/c$
a = 7.4378 (15) Å
b = 9.1650 (19) Å
c = 7.1002 (14) Å
β = 116.348 (3)°
V = 433.72 (15) Å^3
Z = 4
D_x = 1.579 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1914 reflections
θ = 3.1–27.1°
μ = 0.14 mm^{-1}
T = 105 (2) K
Block, colourless
1.10 × 0.85 × 0.50 mm

Data collection

Bruker SMART CCD diffractometer
ω rotation scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.773, T_{max} = 0.930
2491 measured reflections
948 independent reflections
877 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.1°
$h = -8 \rightarrow 9$
$k = -9 \rightarrow 11$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.06
948 reflections
79 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0670P)^2 + 0.3254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.024
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected torsion angles (°).

O1—C1—C2—N1	10.2 (2)	C2—N1—C3—O3	−1.2 (2)
C1—C2—N1—C3	169.77 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.85 (2)	2.31 (2)	3.100 (2)	154 (2)
O2—H2···O3^{ii}	1.06 (2)	1.48 (2)	2.5229 (16)	165 (2)
C2—H21···O1^{iii}	0.93 (2)	2.43 (2)	3.327 (2)	160.9 (17)

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

Positional parameters were refined for all H atoms. U_{iso} values were $1.2U_{eq}$ or $1.5U_{eq}$ (carboxylate) of the carrier atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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