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N′-[(*E*)-5-Oxopyrrolidin-2-ylidene]pyridine-2-carbohydrazide

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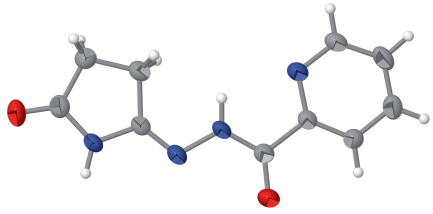
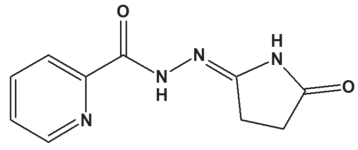
In the title compound, $C_{10}H_{10}N_4O_2$, the dihedral angle between the planes of the pyridine and oxopyrrolidine rings is 6.9 (2)°. In the crystal, inversion dimers linked by pairwise N—H···O hydrogen bonds generate $R_2^2(14)$ loops.

3D view



Chemical scheme



Structure description

Pyridine-2-carbohydrazides are organic compounds containing a pyridine ring substituted with a carbohydrazide (–CONHNH$_2$–) group at the 2-position. These compounds are valuable in organic and medicinal chemistry due to their diverse biological activities and reactivity. They have been studied extensively for their medicinal properties (*e.g.* Khan *et al.*, 2022; Pitucha *et al.*, 2020; Marinescu & Popa, 2022). As part of our work in this area, we now report the synthesis and structure of *N*′-[(*E*)-5-oxopyrrolidin-2-ylidene] pyridine-2-carbohydrazide.

The title compound crystallizes in the triclinic space group $P\overline{1}$ with one molecule in the asymmetric unit (Fig. 1). The molecule is not exactly planar, but can be divided into three almost planar fragments, *viz.* a pyridine ring, a carbohydrazide unit (O1/C6/N2/N3) and an oxopyrrolidine ring. The carbohydrazide unit forms dihedral angles of 3.9 (2) and 5.2 (2)° with the N1/C1–C5 pyridine and N4/C7–C10 oxopyrrolidine rings, respectively. The dihedral angle between the planes of the pyridine and oxopyrrolidine rings is 6.9 (2)°. Pyridine atom N1 and carbohydrazide atom N2 are *cis* with respect to each other [torsion angles N1—C5—C6—N2 and N1—C5—C6—O1 = −0.9 (3) and 177.6 (2)°, respectively]. Hydrazide atom H2 and oxopyrrolidine atom H4 are *trans* with respect to each other [torsion angle N2—N3—C7—N4 = 179.33 (18)°]. In addition, the C6—N2 bond length of 1.322 (3) Å agrees well with equivalent bonds in similar structures, being intermediate between a typical C—N single bond (∼1.47 Å) and a C=N double bond

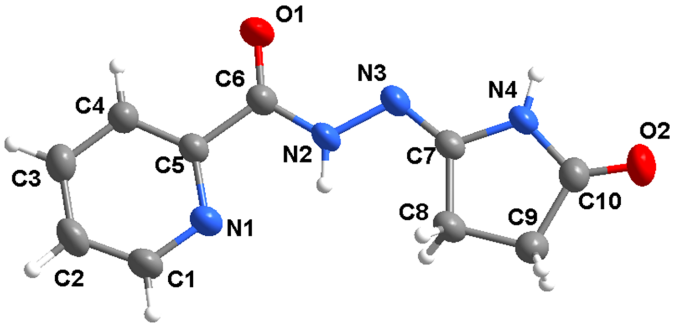


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

(∼1.29 Å). The N2—N3 bond length of 1.396 (2) Å also shows partial double-bond character, suggesting extensive delocalization in the compound (Singh *et al.*, 2006).

In the extended structure, the molecules forms dimers through pairwise N—H···O hydrogen bonds (Table 1 and Fig. 2), which generate $R_2^2(14)$ loops. These dimers are further connected into a two-dimensional framework *via* short C···C contacts (3.23–3.39 Å), which are likely of van der Waals nature and occur between symmetry-related C atoms of adjacent molecules (Fig. 3).

Synthesis and crystallization

A solution of pyridine-2-carbohydrazide in ethanol (2.05 g, 1.5 mmol in 125 ml) was added to a mixture of ethyl 4-ethoxy-4-iminobutanoate hydrochloride (3.46 g, 1.65 mmol) and DIPEA (*N*,*N*-diisopropylethylamine) (2.85 ml, 1.72 mmol) in ethanol (125 ml) (Fig. 4). The reaction mixture was then refluxed for 8 h. After cooling to room temperature, the solvent was removed under reduced pressure. The resulting suspension was diluted with water (250 ml) and stirred to yield a white solid. The solid was collected by filtration, dried and recrystallized from acetonitrile solution. Crystals suitable for X-ray analysis were obtained by recrystallization from dimethylformamide (DMF) solution (yield: 8%, 0.3 g). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.31 (*s*, 0.5H), 10.96 (*s*, 0.5H), 10.74 (*s*, 0.5H), 10.61 (*s*, 0.5H), 8.66 (*d*, J = 4.6 Hz, 1H), 8.06–7.98 (*m*, 2H), 7.61 (*dd*, J = 3.8, 1.9 Hz, 1H), 2.92 (*t*, J = 7.2 Hz, 1H), 2.78 (*t*, J = 7.6 Hz, 1H). IR (KBr, ν, cm^{-1}): 3443, 3315, 3112, 1759, 1681, 1655, 1592, 1538, 1432, 1227, 900, 818, 579, 428. LC/MS (ESI): m/z 219 $[MH]^+$. Elemental analysis calculated (%) for $C_{10}H_{10}N_4O_2$: C 55.04, H 3.62, N 14.66; found: C 55.02, H 3.59, N 14.63.

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O1^{i}	0.86	2.02	2.822 (2)	154

Symmetry code: (i) $-x, -y+1, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{10}N_4O_2$
M_r	218.22
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	5.6332 (5), 7.6439 (7), 11.7293 (11)
α, β, γ (°)	95.859 (8), 96.353 (8), 99.682 (8)
V (Å^3)	491.04 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.18 × 0.12 × 0.04
Data collection	
Diffractometer	Rigaku Xcalibur Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.716, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4130, 1734, 1120
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.121, 1.01
No. of reflections	1734
No. of parameters	146
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.17

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

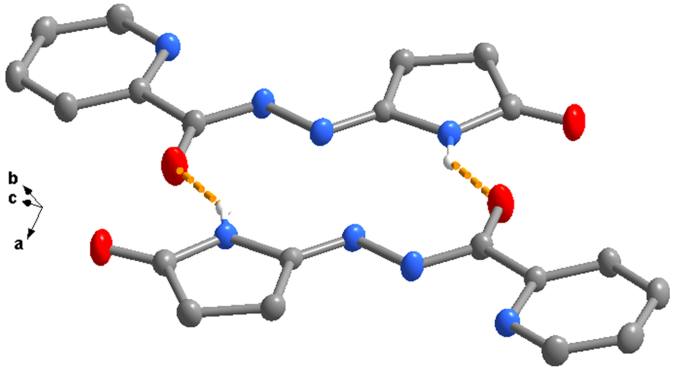


Figure 2
A dimer formed through pairwise N—H···O hydrogen bonds.

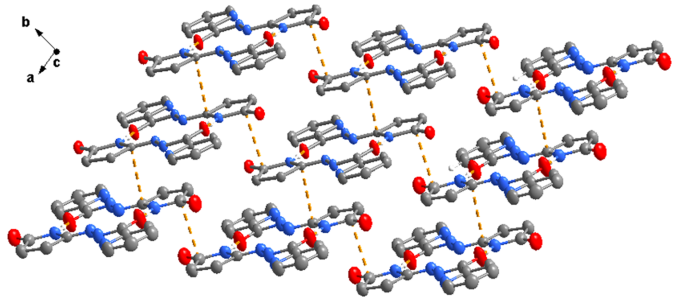


Figure 3
A view normal to the *ab* plane of the crystal structure of the title compound, showing the two-dimensional supramolecular network.

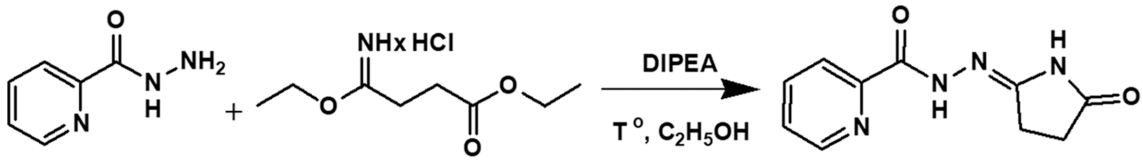


Figure 4
Synthesis scheme for the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Khan, F., Yaqoob, S., Ali, S., Tanveer, N., Wang, Y., Ashraf, S., Hasan, K. A., Khalifa, S. A. M., Shou, Q., Ul-Haq, Z., Jiang, Z. H. & El-Seedi, H. R. (2022). *Molecules* **28**, 212.

Marinescu, M. & Popa, C. (2022). *Int. J. Mol. Sci.* **23**, 5659.

Pitucha, M., Karczmarzyk, Z., Swatko-Ossor, M., Drozd, M., Wysocki, W., Ginalska, G., Urbanczyk-Lipkowska, Z., Kowalczuk, D. & Morawiak, M. (2020). *J. Mol. Struct.* **1219**, 128552.

Rigaku OD (2021). *CrysAlis PRO*. Rigaku Oxford Diffraction Ltd, Yarnton, Oxfordshire, England.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Singh, N. K., Butcher, R. J. & Tripathi, P. (2006). *Acta Cryst.* E**62**, o1405–o1407.

full crystallographic data

IUCrData (2025). **10**, x250896 [https://doi.org/10.1107/S241431462500896X]

N′-[(*E*)-5-Oxopyrrolidin-2-ylidene]pyridine-2-carbohydrazide

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Crystal data

$C_{10}H_{10}N_4O_2$
M_r = 218.22
Triclinic, $P\overline{1}$
a = 5.6332 (5) Å
b = 7.6439 (7) Å
c = 11.7293 (11) Å
α = 95.859 (8)°
β = 96.353 (8)°
γ = 99.682 (8)°
V = 491.04 (8) Å^3
Z = 2
$F(000)$ = 228
D_x = 1.476 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 990 reflections
θ = 2.7–24.0°
μ = 0.11 mm^{-1}
T = 293 K
Plate, colourless
0.18 × 0.12 × 0.04 mm

Data collection

Rigaku Xcalibur Eos diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1593 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2021)
T_{min} = 0.716, T_{max} = 1.000
4130 measured reflections
1734 independent reflections
1120 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°, θ_{min} = 2.7°
h = −6→6
k = −9→8
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.121
S = 1.01
1734 reflections
146 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.019 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All H atoms were placed geometrically (C—H = 0.93–0.97 Å and N—H = 0.86 Å) and refined as riding atoms, with U_{iso}(H) = 1.2U_{eq}(carrier).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.2261 (3)	0.2881 (3)	0.25651 (14)	0.0656 (6)
O2	0.6944 (3)	0.9414 (2)	0.63831 (14)	0.0578 (6)
N1	0.1853 (4)	0.3516 (3)	0.05028 (15)	0.0402 (5)
N2	0.1546 (4)	0.4460 (3)	0.26871 (15)	0.0416 (6)
H2	0.278937	0.471361	0.233005	0.050*
N3	0.1655 (4)	0.5201 (3)	0.38345 (15)	0.0392 (5)
N4	0.4061 (3)	0.7230 (2)	0.52866 (14)	0.0372 (5)
H4	0.308537	0.706286	0.579587	0.045*
C1	0.2008 (5)	0.3059 (3)	−0.0616 (2)	0.0467 (7)
H1	0.341810	0.352645	−0.090781	0.056*
C2	0.0195 (5)	0.1935 (3)	−0.1359 (2)	0.0482 (7)
H2A	0.039786	0.164612	−0.212720	0.058*
C3	−0.1905 (5)	0.1248 (3)	−0.0955 (2)	0.0470 (7)
H3	−0.315240	0.048043	−0.143784	0.056*
C4	−0.2127 (5)	0.1729 (3)	0.01988 (19)	0.0422 (6)
H4A	−0.354490	0.130957	0.049950	0.051*
C5	−0.0224 (4)	0.2831 (3)	0.08845 (18)	0.0341 (6)
C6	−0.0415 (4)	0.3380 (3)	0.21342 (19)	0.0380 (6)
C7	0.3606 (4)	0.6329 (3)	0.41794 (18)	0.0320 (6)
C8	0.5706 (4)	0.6949 (3)	0.35502 (19)	0.0410 (6)
H8A	0.518851	0.753902	0.289671	0.049*
H8B	0.643339	0.595005	0.327358	0.049*
C9	0.7488 (4)	0.8250 (3)	0.44387 (19)	0.0456 (7)
H9A	0.897665	0.779229	0.460945	0.055*
H9B	0.788117	0.940108	0.415897	0.055*
C10	0.6218 (4)	0.8415 (3)	0.5493 (2)	0.0401 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0498 (12)	0.0928 (15)	0.0417 (11)	−0.0198 (11)	0.0219 (10)	−0.0139 (10)
O2	0.0616 (13)	0.0639 (13)	0.0365 (10)	−0.0063 (10)	0.0007 (9)	−0.0121 (9)
N1	0.0406 (13)	0.0460 (13)	0.0325 (11)	0.0000 (10)	0.0127 (10)	0.0017 (9)
N2	0.0420 (13)	0.0517 (13)	0.0267 (11)	−0.0043 (10)	0.0146 (10)	−0.0063 (9)
N3	0.0419 (13)	0.0470 (13)	0.0267 (11)	0.0031 (11)	0.0104 (10)	−0.0025 (9)
N4	0.0370 (12)	0.0481 (12)	0.0249 (10)	0.0038 (10)	0.0097 (9)	−0.0022 (9)
C1	0.0459 (16)	0.0586 (17)	0.0343 (15)	−0.0001 (14)	0.0166 (13)	0.0024 (12)

C2	0.0614 (19)	0.0546 (17)	0.0277 (13)	0.0075 (15)	0.0103 (13)	0.0003 (12)
C3	0.0514 (17)	0.0502 (16)	0.0336 (14)	0.0000 (13)	0.0004 (13)	−0.0014 (12)
C4	0.0383 (15)	0.0499 (15)	0.0340 (14)	−0.0036 (12)	0.0080 (11)	−0.0005 (11)
C5	0.0362 (14)	0.0373 (14)	0.0274 (12)	0.0026 (11)	0.0070 (11)	0.0018 (10)
C6	0.0393 (15)	0.0387 (14)	0.0336 (14)	−0.0013 (12)	0.0106 (12)	0.0003 (11)
C7	0.0353 (14)	0.0339 (13)	0.0279 (12)	0.0081 (11)	0.0073 (11)	0.0021 (10)
C8	0.0437 (15)	0.0448 (15)	0.0342 (14)	0.0054 (12)	0.0123 (12)	−0.0001 (11)
C9	0.0374 (15)	0.0535 (16)	0.0424 (15)	0.0006 (13)	0.0081 (12)	−0.0014 (12)
C10	0.0407 (16)	0.0423 (15)	0.0354 (14)	0.0064 (13)	0.0019 (12)	0.0005 (12)

Geometric parameters (Å, º)

O1—C6	1.226 (2)	C2—C3	1.366 (3)
O2—C10	1.216 (3)	C3—H3	0.9300
N1—C1	1.340 (3)	C3—C4	1.390 (3)
N1—C5	1.342 (3)	C4—H4A	0.9300
N2—H2	0.8600	C4—C5	1.368 (3)
N2—N3	1.396 (2)	C5—C6	1.504 (3)
N2—C6	1.322 (3)	C7—C8	1.498 (3)
N3—C7	1.276 (3)	C8—H8A	0.9700
N4—H4	0.8600	C8—H8B	0.9700
N4—C7	1.382 (3)	C8—C9	1.518 (3)
N4—C10	1.370 (3)	C9—H9A	0.9700
C1—H1	0.9300	C9—H9B	0.9700
C1—C2	1.376 (3)	C9—C10	1.500 (3)
C2—H2A	0.9300		

C1—N1—C5	116.3 (2)	C4—C5—C6	120.1 (2)
N3—N2—H2	119.1	O1—C6—N2	124.8 (2)
C6—N2—H2	119.1	O1—C6—C5	121.7 (2)
C6—N2—N3	121.87 (19)	N2—C6—C5	113.48 (19)
C7—N3—N2	112.39 (18)	N3—C7—N4	121.6 (2)
C7—N4—H4	123.3	N3—C7—C8	130.20 (19)
C10—N4—H4	123.3	N4—C7—C8	108.2 (2)
C10—N4—C7	113.35 (19)	C7—C8—H8A	110.8
N1—C1—H1	118.2	C7—C8—H8B	110.8
N1—C1—C2	123.6 (2)	C7—C8—C9	104.83 (17)
C2—C1—H1	118.2	H8A—C8—H8B	108.9
C1—C2—H2A	120.4	C9—C8—H8A	110.8
C3—C2—C1	119.3 (2)	C9—C8—H8B	110.8
C3—C2—H2A	120.4	C8—C9—H9A	110.7
C2—C3—H3	120.9	C8—C9—H9B	110.7
C2—C3—C4	118.2 (2)	H9A—C9—H9B	108.8
C4—C3—H3	120.9	C10—C9—C8	105.28 (18)
C3—C4—H4A	120.5	C10—C9—H9A	110.7
C5—C4—C3	118.9 (2)	C10—C9—H9B	110.7
C5—C4—H4A	120.5	O2—C10—N4	125.0 (2)
N1—C5—C4	123.7 (2)	O2—C10—C9	126.9 (2)

N1—C5—C6	116.2 (2)	N4—C10—C9	108.08 (19)
N1—C1—C2—C3	0.8 (4)	C3—C4—C5—N1	1.5 (4)
N1—C5—C6—O1	177.6 (2)	C3—C4—C5—C6	179.7 (2)
N1—C5—C6—N2	−0.9 (3)	C4—C5—C6—O1	−0.8 (4)
N2—N3—C7—N4	179.33 (18)	C4—C5—C6—N2	−179.3 (2)
N2—N3—C7—C8	0.2 (3)	C5—N1—C1—C2	−0.8 (4)
N3—N2—C6—O1	−2.4 (4)	C6—N2—N3—C7	−174.0 (2)
N3—N2—C6—C5	176.01 (18)	C7—N4—C10—O2	176.4 (2)
N3—C7—C8—C9	−178.2 (2)	C7—N4—C10—C9	−3.8 (3)
N4—C7—C8—C9	2.6 (2)	C7—C8—C9—C10	−4.6 (2)
C1—N1—C5—C4	−0.3 (3)	C8—C9—C10—O2	−175.0 (2)
C1—N1—C5—C6	−178.6 (2)	C8—C9—C10—N4	5.2 (3)
C1—C2—C3—C4	0.4 (4)	C10—N4—C7—N3	−178.6 (2)
C2—C3—C4—C5	−1.5 (4)	C10—N4—C7—C8	0.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1^{i}	0.86	2.02	2.822 (2)	154

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.