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# 4-(2-Pyridyl)-1*H*,2*H*-pyrido[1,2-*c*]pyrimidine-1,3-dione

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.044
$wR$ factor = 0.127
Data-to-parameter ratio = 14.8

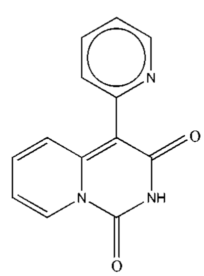
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



The maximum deviation from the mean plane of the pyridopyrimidine skeleton of the title compound, $C_{13}H_9N_3O_2$, indicates a reasonably planar system. The planar pyridyl ring is twisted with respect to the pyrido[1,2-*c*]pyrimidine-1,3-dione fragment. The molecules form centrosymmetric dimers *via* intermolecular N—H···O hydrogen bonds. Short intra- and intermolecular C—H···O and C—H···N contacts are observed.

## Comment

In continuation of our research on the synthesis of condensed heterobicyclic compounds, we have focused our interest on derivatives of 4-(aryl/heteroaryl)pyrido[1,2-*c*]pyrimidine (Herold *et al.*, 1999; Herold, Kleps, Anulewicz-Ostrowska & Szczęsna, 2002; Herold, Kleps, Wolska & Nowak, 2002). The resulting compounds will be further applied as starting materials in the synthesis of new ligands of the 5-$HT_{1A}$ receptor. Due to the increased lipophilicity, the presence of an imide group in their structure, and the elements providing a possibility of interaction with the 5-$HT_{1A}$ receptor, higher affinity and selectivity for this receptor can be expected for 4-(2-pyridyl)-1*H*,2*H*-pyrido[1,2-*c*]pyrimidine-1,3-dione derivatives (Orjales *et al.*, 1995; López-Rodriquez *et al.*, 1999; Herold, Kleps, Wolska & Nowak, 2002).




(I)

The molecular structure of the title compound, (I), showing the labelling scheme, is presented in Fig. 1. The pyridopyrimidine fragment is essentially planar, with no atomic deviation greater than 0.071 (1) Å (for C6) from the least-squares plane. Atoms O10 and O11 are found to be only marginally out of this plane [−0.120 (2) and −0.105 (2) Å for O10 and O11, respectively]. The pyridyl ring is planar, with deviations from the mean plane ranging from −0.001 (1) Å for N6′ to 0.009 (1) Å for C2′, and makes an angle of 56.64 (6)° with the mean plane of the pyridopyrimidine system. The twisting of the heteroaryl substituent at C4 with respect to the pyrido[1,2-*c*]pyrimidine-1,3-dione skeleton can be described by the torsion angle C3—C4—C1′—N6′ of 126.9 (1)°. This twisting is probably due to steric reasons and is stabilized by a

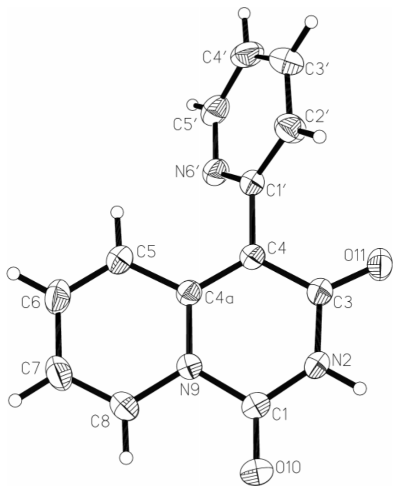



**Figure 1**
A view of the title compound, with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

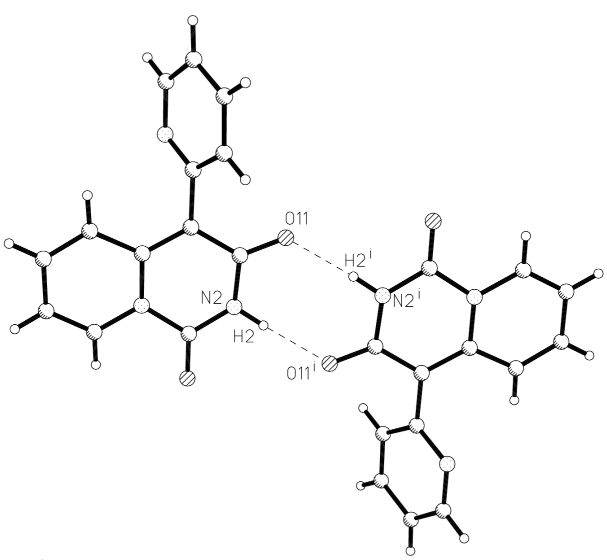



**Figure 2**
The centrosymmetric hydrogen-bonded dimer [symmetry code: (i) $2-x$, $1-y$, $-z$]. Hydrogen bonds are drawn as dashed lines.

short intramolecular C5—H5···N6′ contact (Table 2). A similar arrangement of the substituent at C4 has been confirmed in the 4-arylhexahydropyridopyrimidine derivatives (Herold *et al.*, 1999, 2000; Maciejewska *et al.*, 2000; Wolska & Herold, 1999, 2000, 2002) and for these compounds the most interesting feature is the formation of centrosymmetric dimers by means of intermolecular hydrogen bonds. In (I), the molecules are also connected into centrosymmetric dimers and they are held together by a pair of N—H···O hydrogen bonds (Fig. 2). As a result, the C3═O11 bond length is slightly longer than C1═O10 (Table 1). Atoms O10, O11 and N6′ are also involved in weak intermolecular C—H···O and C—H···N hydrogen bonds (Desiraju, 1996), which result from the crystal packing of the molecules. The geometric parameters of all hydrogen bonds are listed in Table 2. The pattern of bond lengths and angles is quite typical; only the C4—C4a bond length is insignificantly longer than the same distance in the pyridopyrimidine derivatives reported hitherto (Herold *et al.*, 1999, 2000; Maciejewska *et al.*, 2000; Wolska & Herold, 1999, 2000, 2002) and typical C$sp^2$—C$sp^2$ bond lengths (Allen *et al.*, 1987), and this may be a result of delocalization of $\pi$-electrons in this fragment of the molecule.

## Experimental

The title compound was prepared in accordance with Herold (2003). A multi-stage preparation technique were used to obtain 4-(2-pyridyl)-1*H*,2*H*-pyrido[1,2-*c*]pyrimidine-1,3-dione. First the respective $\alpha$,$\alpha$-bis(2-pyridyl)acetonitrile was synthesized. For the next step, this acetonitrile was hydrolyzed using a mixture of sulfuric and acetic acids and $\alpha$,$\alpha$-(2-pyridyl)acetamide was obtained. The final compound was obtained by condensation above acetamide. Crystals were grown from ethanol solution by slow evaporation.

*Crystal data*

| | |
|---|---|
| $C_{13}H_9N_3O_2$ | $D_x = 1.467$ Mg m$^{-3}$ |
| $M_r = 239.23$ | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/c$ | Cell parameters from 5139 reflections |
| $a = 8.631$ (2) Å | $\theta = 2.0$–27.1° |
| $b = 8.041$ (2) Å | $\mu = 0.10$ mm$^{-1}$ |
| $c = 16.054$ (3) Å | $T = 293$ (2) K |
| $\beta = 103.51$ (3)° | Prism, yellow |
| $V = 1083.3$ (4) Å$^3$ | 0.55 × 0.50 × 0.40 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Kuma KM-4 CCD diffractometer | $R_{int} = 0.014$ |
| $\omega/2\theta$ scans | $\theta_{max} = 28.0°$ |
| 6578 measured reflections | $h = -11 \rightarrow 11$ |
| 2608 independent reflections | $k = -10 \rightarrow 10$ |
| 2374 reflections with $I > 2\sigma(I)$ | $l = -21 \rightarrow 14$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 0.2921P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.127$ | $(\Delta/\sigma)_{max} = 0.006$ |
| $S = 1.07$ | $\Delta\rho_{max} = 0.24$ e Å$^{-3}$ |
| 2608 reflections | $\Delta\rho_{min} = -0.23$ e Å$^{-3}$ |
| 176 parameters | Extinction correction: *SHELXL*97 |
| H atoms treated by a mixture of independent and constrained refinement | Extinction coefficient: 0.079 (7) |

**Table 1**
Selected geometric parameters (Å).

| | | | |
|---|---|---|---|
| C1—O10 | 1.2171 (15) | C4—C4a | 1.3873 (15) |
| C3—O11 | 1.2388 (15) | C4a—C5 | 1.4377 (15) |

**Table 2**
Intra- and intermolecular contacts (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5···N6′ | 0.93 | 2.55 | 3.0658 (18) | 115 |
| N2—H2···O11$^{i}$ | 0.892 (17) | 1.950 (17) | 2.8293 (15) | 168.4 (15) |
| C5—H5···O11$^{ii}$ | 0.93 | 2.81 | 3.4095 (18) | 124 |
| C2′—H2′···N6′$^{ii}$ | 0.93 | 2.76 | 3.4097 (18) | 127 |
| C6—H6···O10$^{iii}$ | 0.93 | 2.55 | 3.3539 (17) | 145 |
| C7—H7···N6′$^{iv}$ | 0.93 | 2.55 | 3.4780 (18) | 172 |
| C3′—H3′···O10$^{v}$ | 0.93 | 2.66 | 3.5165 (19) | 154 |

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

For H2, which is involved in an N—H···O hydrogen bond, positional and isotropic displacement parameters were refined. The other H atoms were refined with a riding model and their $U_{iso}$ values were set at 1.2$U_{eq}$ of their carrier atoms.

Data collection: *CrysAlisCCD* (Kuma, 2001); cell refinement: *CrysAlisRED* (Kuma, 2001); data reduction: *CrysAlisRED*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *Stereochemical Workstation* (Siemens, 1989); software used to prepare material for publication: *SHELXL*97.

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