5-Fluorouracil–1,4-dioxane (4/1)
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A solvate of 5-fluorouracil with 1,4-dioxane, \(4\text{C}_4\text{H}_5\text{FN}_2\text{O}_2\cdot\text{C}_4\text{H}_8\text{O}_2\), is reported. It crystallizes in the triclinic space group \(\text{P}\overline{1}\). Two molecules of 5-fluorouracil are present in the asymmetric unit, together with one-half molecule of 1,4-dioxane, which lies on a centre of symmetry. In the crystal structure, ribbons of 5-fluorouracil molecules are joined by 1,4-dioxane-mediated interactions, forming sheets parallel to the \((211)\) planes.

**Comment**

In the course of a polymorph screen performed on 5-fluorouracil, three solvates were discovered; the crystal structure of one of these solvates is reported here.

The title compound, (I), crystallizes in the space group \(\text{P}\overline{1}\) with two molecules of 5-fluorouracil and one-half molecule of 1,4-dioxane in the asymmetric unit (Fig. 1). The 1,4-dioxane molecule is located on a crystallographic centre of symmetry. Four distinct \(\text{N} \cdots \text{H} \cdots \text{O}\) hydrogen bonds occur in the crystal structure (Table 1). Both the crystallographically independent 5-fluorouracil molecules are present as centrosymmetric hydrogen-bonded dimers. One dimer contains the hydrogen bond \(\text{N}3 \cdots \text{H}3\cdots\text{O}7\cdots\) (symmetry codes are given in Table 1), with a donor–acceptor distance of 2.857 (2) Å, while the other dimer contains the hydrogen bond \(\text{N}13 \cdots \text{H}13\cdots\text{O}18\cdots\) [2.824 (2) Å]. These dimers are linked, forming ribbon-like structures, by \(\text{N}1 \cdots \text{H}1 \cdots \text{O}17\) hydrogen bonds. Adjacent
ribbons of 5-fluorouracil molecules are linked, forming sheets parallel to the (211) planes via 1,4-dioxane molecules which act as N1—H1···O21 [N···O = 2.746 (2) Å] hydrogen-bond bridges (Fig. 2).

Experimental

5-Fluorouracil was obtained from the Aldrich Chemical Company Inc. The crystals were grown by solvent evaporation of a saturated solution of 5-fluorouracil in 1,4-dioxane.

Crystal data

4C₄H₃FN₂O₂·C₄H₈O₂
Mᵣ = 608.44
Triclinic, P₁
a = 7.0847 (11) Å
b = 8.4733 (13) Å
c = 10.2291 (15) Å
α = 98.128 (3)°
β = 96.913 (3)°
γ = 99.785 (3)°
V = 592.45 (16) Å³
Z = 1
Dᵣ = 1.705 Mg m⁻³
Mo Kα radiation
θ = 2.5–26.7°
μ = 0.16 mm⁻¹
T = 150 (2) K
Plate, colourless
h = −9 to 9
k = −11 to 11
l = −13 to 13

Crystallographic data

Data collection

Bruker SMART APEX diffractometer
Narrow-frameω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_max = 0.995
T_min = 0.947
2741 independent reflections
2131 reflections with I > 2σ(I)
5320 measured reflections

Data reduction

Rint = 0.029
wR(F²) = 0.114
S = 1.08

Refinement

Refinement on F²
wR(F²) = 0.052
S = 1.08
2741 reflections
230 parameters
All H-atom parameters refined

Table 1

Hydrogen-bonding geometry (Å, °).

<table>
<thead>
<tr>
<th>D—H···A</th>
<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
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<tbody>
<tr>
<td>N1—H1···O17i</td>
<td>0.83 (3)</td>
<td>1.98 (3)</td>
<td>2.798 (2)</td>
<td>167 (2)</td>
</tr>
<tr>
<td>N3—H3···O10iii</td>
<td>0.91 (2)</td>
<td>1.95 (2)</td>
<td>2.857 (2)</td>
<td>176 (2)</td>
</tr>
<tr>
<td>N11—H11···O21</td>
<td>0.91 (2)</td>
<td>1.84 (2)</td>
<td>2.746 (2)</td>
<td>171 (2)</td>
</tr>
<tr>
<td>N13—H13···O18iv</td>
<td>0.85 (2)</td>
<td>1.98 (2)</td>
<td>2.824 (2)</td>
<td>175 (2)</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) x, 1 + y, z; (ii) −x, 1 − y, 1 − z; (iii) 1 − x, 1 − y, 1 − z.

All H atoms were located in a difference map and were refined isotropically. C—H distances were in the range 0.93 (2)–1.00 (2) Å and N—H distances were in the range 0.83 (3)–0.91 (2) Å.

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References