

2-Amino-4,6-dimethylpyrimidine–4-hydroxybenzoic acid (1/1)

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Key indicators

Single-crystal X-ray study
 $T = 120$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.058
 wR factor = 0.130
Data-to-parameter ratio = 8.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

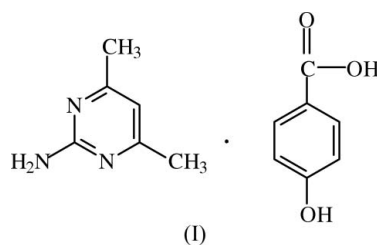
In the title compound, $\text{C}_6\text{H}_9\text{N}_3 \cdot \text{C}_7\text{H}_6\text{O}_3$, the 2-amino-4,6-dimethylpyrimidine and 4-hydroxybenzoic acid molecules link together *via* $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds to form an eight-membered $R_2^2(8)$ ring. Further hydrogen bonds and $\text{C}-\text{H} \cdots \text{O}$ interactions result in the formation of a three-dimensional network.

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Comment

The crystal structures of various aminopyrimidine carboxylates (Hu *et al.*, 2002) and cocrystals (Chinnakali *et al.*, 1999) have been described. From our laboratory, the crystal structures of 2-amino-4,6-dimethylpyrimidinium bromide 2-amino-4,6-dimethylpyrimidine monohydrate (Panneerselvam *et al.*, 2004) and 2-amino-4,6-dimethylpyrimidine cinnamic acid (1/2) (Balasubramani *et al.*, 2005) have been reported. In this paper, the hydrogen-bonding patterns in the title compound, (I), are described.



The asymmetric unit of (I) contains a 2-amino-4,6-dimethylpyrimidine (AMPY) molecule and a 4-hydroxybenzoic (4-HBZ) acid molecule (Fig. 1). Both species are neutral, thus (I) is an adduct rather than a molecular salt. Atoms O2 and the $-\text{N}2\text{H}_2$ group act as hydrogen-bond donors to atoms N1 and O3, respectively, to form an eight-membered ring, which has the graph-set notation $R_2^2(8)$ (Etter, 1990; Bernstein *et al.*, 1995). This type of interaction has been observed in the crystal structures of other 2-aminopyrimidine–carboxylic acid adducts (Lynch & Jones, 2004).

The second H atom of the 2-amino group links to an O2 atom in an adjacent molecule *via* an $\text{N}-\text{H} \cdots \text{O}$ bond, and one of the C atoms (C11) of 4-HBZ is hydrogen bonded to O3 *via* a $\text{C}-\text{H} \cdots \text{O}$ interaction to form a ring having graph-set notation $R_2^3(8)$, leading to the supramolecular chain shown in Fig. 2. Hence, O3 acts as a bifurcated acceptor. The 4-HBZ hydroxy (O1) group is hydrogen bonded to pyrimidine atom N3 *via* an $\text{O}-\text{H} \cdots \text{N}$ interaction, to form a chain as shown in Fig. 3.

Aromatic $\pi-\pi$ interactions between the pyrimidine ring of AMPY and the benzene ring of 4-HBZ are also observed in

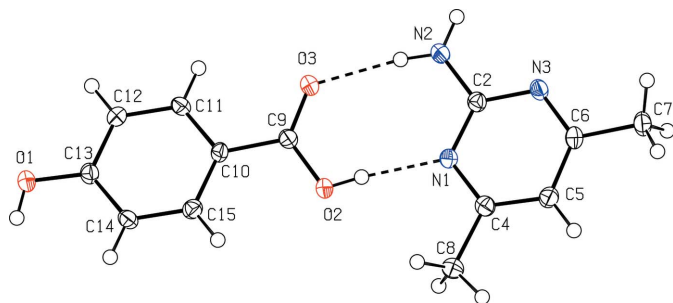


Figure 1
ORTEP (Johnson, 1976) view of the asymmetric unit of (I), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

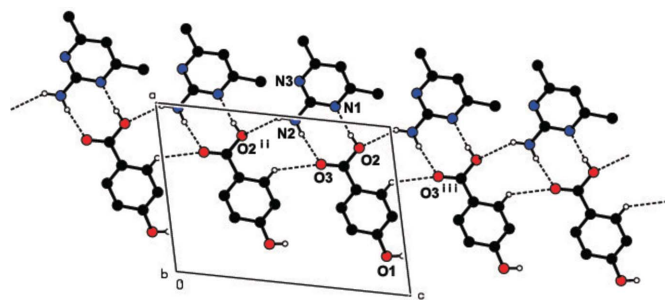


Figure 2
A view of the supramolecular chain in (I). Dashed lines indicate hydrogen bonds and H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (ii) $x, -y, \frac{1}{2} + z$; (iii) $x, -y, z - \frac{1}{2}$]

(I). The perpendicular separation is 3.552 Å, and the centroid-to-centroid distance is 3.660 (9) Å. The slip angle (the angle between the centroid-to-centroid vector and the normal to the plane) is 19.86°. These values are typical for aromatic π - π stacking interactions (Hunter, 1994).

Experimental

Hot methanol solutions (20 ml) of 2-amino-4,6-dimethylpyrimidine (30 mg, Aldrich) and 4-hydroxybenzoic acid (32 mg, LOBA Chemie, India) were mixed and warmed over a water bath for a few minutes. The resulting solution was allowed to cool slowly at room temperature. Crystals of (I) appeared from the mother liquor after a few days.

Crystal data

$C_6H_9N_3 \cdot C_7H_6O_3$	$Z = 4$
$M_r = 261.28$	$D_x = 1.401 \text{ Mg m}^{-3}$
Monoclinic, Cc	Mo $K\alpha$ radiation
$a = 9.0693 (3) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 11.1141 (4) \text{ \AA}$	$T = 120 (2) \text{ K}$
$c = 12.6080 (5) \text{ \AA}$	Cube, colourless
$\beta = 102.916 (2)^\circ$	$0.20 \times 0.20 \times 0.20 \text{ mm}$
$V = 1238.70 (8) \text{ \AA}^3$	

Data collection

Bruker–Nonius KappaCCD diffractometer	4983 measured reflections
φ and ω scans	1419 independent reflections
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	1360 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.980, T_{\max} = 0.980$	$R_{\text{int}} = 0.023$
	$\theta_{\text{max}} = 27.5^\circ$

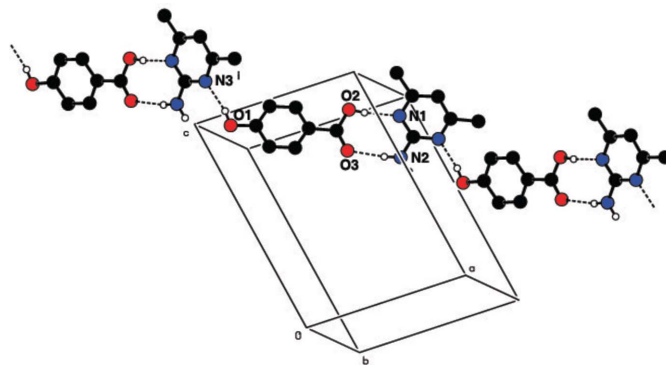


Figure 3
A view of the hydrogen-bonding patterns in (I). Dashed lines indicate hydrogen bonds and H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (i) $1 + x, -y, z - \frac{1}{2}$]

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.058$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.130$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.34$	$\Delta\rho_{\text{max}} = 0.97 \text{ e \AA}^{-3}$
1419 reflections	$\Delta\rho_{\text{min}} = -0.93 \text{ e \AA}^{-3}$
177 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.171 (13)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1 \cdots N3^i$	0.82	1.94	2.742 (3)	167
$O2-H2 \cdots N1$	0.82	1.90	2.711 (3)	173
$N2-H2A \cdots O3$	0.86	2.00	2.843 (3)	168
$N2-H2B \cdots O2^{ii}$	0.86	2.56	3.229 (3)	135
$C15-H15 \cdots O3^{iii}$	0.93	2.55	3.181 (3)	126

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

In the absence of significant anomalous scattering effects, Friedel pairs were averaged. All the H atoms were positioned geometrically ($C-H = 0.93-0.96 \text{ \AA}$, $N-H = 0.86 \text{ \AA}$ and $O-H = 0.82 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(\text{carrier})$.

Data collection: DENZO (Otwinowski & Minor, 1997) and COLLECT (Hooft, 1998); cell refinement: DENZO and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003) and ORTEP (Johnson, 1976); software used to prepare material for publication: PLATON.

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