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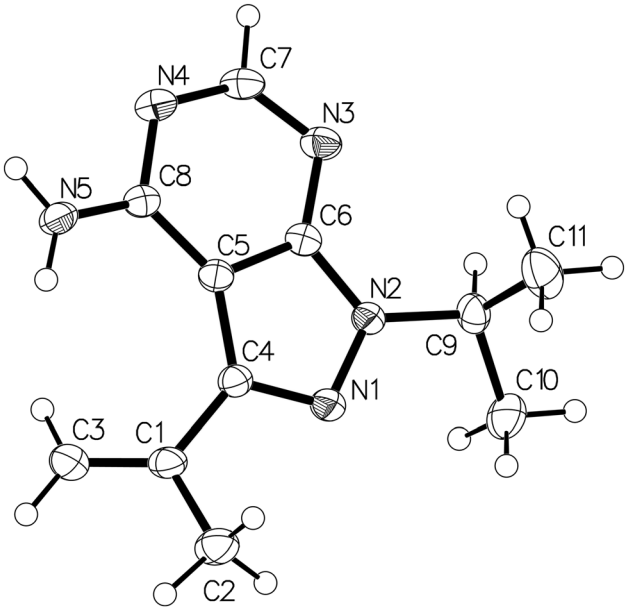
# Crystal structure of 1-isopropyl-3-(prop-1-en-2-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-4-amine, $C_{11}H_{15}N_5$

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**Abstract**

$C_{11}H_{15}N_5$, monoclinic, $P2_1/c$ (no. 14), $a$ = 9.5677(16) Å, $b$ = 8.1755(15) Å, $c$ = 14.846(3) Å, $\beta$ = 93.783(4)°, $V$ = 1158.7(4) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0473, $wR_{ref}(F^2)$ = 0.1425, T = 173 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colorless block |
| Size: | 0.28 × 0.15 × 0.12 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.08 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 27.5°, 99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 7761, 2634, 0.033 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2078 |
| $N(param)_{refined}$: | 148 |
| Programs: | Bruker [1], Olex2 [2], SHELX [3, 4] |

## Source of material

A mixture of 3-iodo-1-isopropyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-4-amine (152 mg, 0.5 mmol), 4,4,5,5-tetramethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborolane (42 mg, 2.5 mmol), DMF (15 mL), Pd(dppf)$Cl_2$ (20 mg, 0.03 mmol), $Na_2CO_3$ (159 mg, 1.5 mmol), and $H_2O$ (0.5 mL) were added and seald in a tube. The reaction system was heated to 100 °C for 2 h and monitored by thin-layer chromatography. After the reaction completed, saturated sodium chloride solution (20 mL) was added. The mixture was extracted with DCM (20 mL) three times. The organic phases were combined, then dried over anhydrous sodium sulfate, and evaporated under reduced pressure. The product was separated by silica gel column chromatography with methanol and dichloromethane ($v/v$ = 5/95) as the eluent to obtain the title compound (yellow solid, 85.8 mg, yield 79%).

## Experimental details

All hydrogen atoms were placed in theoretical positions and refined in riding model with the $U_{iso}$ values set to 1.2 times those of the attached atoms.

## Comment

Purine is a heterocyclic aromatic organic compound produced during metabolism in organisms with a crucial role in human health [5]. The purine derivatives have well antitumor and/or antiviral potential in drug field [6], and many researchers have developed new synthetic methods

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.29269 (16) | 0.38109 (19) | 0.81505 (10) | 0.0255 (4) |
| C2 | 0.39312 (17) | 0.4526 (2) | 0.88640 (11) | 0.0342 (4) |
| H2A | 0.4650 | 0.3714 | 0.9044 | 0.051* |
| H2B | 0.3422 | 0.4833 | 0.9390 | 0.051* |
| H2C | 0.4378 | 0.5497 | 0.8624 | 0.051* |
| C3 | 0.15865 (17) | 0.3502 (2) | 0.82834 (12) | 0.0349 (4) |
| H3A | 0.1007 | 0.2980 | 0.7825 | 0.042* |
| H3B | 0.1212 | 0.3804 | 0.8836 | 0.042* |
| C4 | 0.35130 (15) | 0.33392 (18) | 0.72866 (10) | 0.0212 (3) |
| C5 | 0.28863 (15) | 0.33403 (17) | 0.63892 (10) | 0.0205 (3) |
| C6 | 0.38771 (15) | 0.25893 (17) | 0.58742 (10) | 0.0212 (3) |
| C7 | 0.25267 (17) | 0.27983 (18) | 0.46146 (11) | 0.0269 (4) |
| H7 | 0.2349 | 0.2569 | 0.3990 | 0.032* |
| C8 | 0.16693 (14) | 0.39434 (17) | 0.58947 (10) | 0.0207 (3) |
| C9 | 0.63453 (15) | 0.15545 (19) | 0.61750 (11) | 0.0254 (4) |
| H9 | 0.6144 | 0.0745 | 0.5678 | 0.031* |
| C10 | 0.70884 (18) | 0.0665 (2) | 0.69639 (13) | 0.0388 (4) |
| H10A | 0.7315 | 0.1442 | 0.7455 | 0.058* |
| H10B | 0.7954 | 0.0174 | 0.6771 | 0.058* |
| H10C | 0.6477 | −0.0195 | 0.7176 | 0.058* |
| C11 | 0.72209 (19) | 0.2932 (2) | 0.58098 (14) | 0.0407 (5) |
| H11A | 0.6701 | 0.3448 | 0.5295 | 0.061* |
| H11B | 0.8103 | 0.2485 | 0.5615 | 0.061* |
| H11C | 0.7422 | 0.3747 | 0.6285 | 0.061* |
| N1 | 0.47968 (13) | 0.26930 (15) | 0.73023 (9) | 0.0233 (3) |
| N2 | 0.50004 (12) | 0.22216 (15) | 0.64367 (8) | 0.0215 (3) |
| N3 | 0.37534 (14) | 0.22748 (16) | 0.49757 (9) | 0.0257 (3) |
| N4 | 0.15002 (13) | 0.36040 (15) | 0.50025 (9) | 0.0247 (3) |
| N5 | 0.06744 (13) | 0.48352 (16) | 0.62477 (9) | 0.0266 (3) |
| H5A | −0.0051 | 0.5175 | 0.5903 | 0.032* |
| H5B | 0.0743 | 0.5084 | 0.6826 | 0.032* |

and effective drugs based on purine backbones [7–9]. For instance, ganciclovir [10] and abacavir [11] have been applied as antivirals, and 6-benzylaminopurine and isopentenyladenine have been developed for plant-growth-regulating pesticides [12]. The title compound contain an isomer of the aforementioned purine core, namely the 1*H*-pyrazolo[3,4-*d*]pyrimidine. Based on the above reasons, many 1*H*-pyrazolo[3,4-*d*]pyrimidine derivatives and their crystal structures have been reported [13–18].

The figure shows the title compound. There are one isopropyl group, one prop-1-en-2-yl group and one amino group on the backbone, and the bond lengths of C4–C1, N2–C9, and C8–N5 bonds are 1.484(3) Å, 1.473(2) Å, and 1.333(2) Å, respectively. The pyrimidine group and pyrazole group in the structure are almost in the same plane. The amino substituent on the pyrimidine ring is in the same plane as the core system, and the dihedral angle between the plane formed by the amino group and the core system plane is 179.7. For the title molecule, all bond distances and angles are consistent with the expectation [13, 16, 17].

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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