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The crystal structure of 5-bromo-2-(2-methyl-2H-tetrazol-5-yl)pyridine, $C_7H_6BrN_5$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.24 × 0.21 × 0.17 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	4.57 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	29.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7994, 4190, 0.028
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2696
$N(\text{param})_{\text{refined}}$:	237
Programs:	CrysAlis ^{PRO} [1], SHELX [2], SUPERFLIP [3], Olex2 [4]

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Abstract

$C_7H_6BrN_5$, triclinic, $P\bar{1}$ (no. 2), $a = 8.3319(4)$ Å, $b = 10.0666(5)$ Å, $c = 11.4042(6)$ Å, $\alpha = 107.213(5)^\circ$, $\beta = 99.394(4)^\circ$, $\gamma = 95.540(4)^\circ$, $V = 890.71(8)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0452$, $wR_{\text{ref}}(F^2) = 0.0972$, $T = 293(2)$ K.

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The asymmetric unit of the title 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.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.44510(5)	0.72468(3)	0.04301(4)	0.05319(15)
Br2	−0.28943(5)	−0.00876(4)	0.28107(4)	0.06311(17)
C1	0.2354(4)	0.4913(3)	0.0550(3)	0.0401(8)
H1	0.2733	0.5332	0.1409	0.048*
C2	0.2927(4)	0.5550(3)	−0.0250(3)	0.0359(8)
C3	0.2416(4)	0.4947(3)	−0.1518(3)	0.0410(8)
H3	0.2811	0.5351	−0.2072	0.049*
C4	0.1303(4)	0.3729(3)	−0.1947(3)	0.0409(8)
H4	0.0914	0.3296	−0.2803	0.049*
C5	0.0764(4)	0.3150(3)	−0.1091(3)	0.0336(8)
C6	−0.0449(4)	0.1867(3)	−0.1516(3)	0.0344(8)
C7	−0.2890(5)	−0.0990(3)	−0.1233(4)	0.0530(10)
H7A	−0.2119	−0.1495	−0.0892	0.079*
H7B	−0.3637	−0.1630	−0.1955	0.079*
H7C	−0.3499	−0.0561	−0.0613	0.079*
C8	−0.0390(5)	0.2006(3)	0.4522(3)	0.0465(9)
H8	−0.0665	0.1557	0.5083	0.056*
C9	−0.1221(4)	0.1491(3)	0.3300(3)	0.0385(8)
C10	−0.0824(4)	0.2125(3)	0.2452(3)	0.0450(9)
H10	−0.1361	0.1784	0.1616	0.054*
C11	0.0385(5)	0.3275(3)	0.2870(3)	0.0429(9)
H11	0.0682	0.3726	0.2317	0.051*
C12	0.1164(4)	0.3763(3)	0.4122(3)	0.0337(7)
C13	0.2456(4)	0.4988(3)	0.4608(3)	0.0345(8)
C14	0.5067(5)	0.7776(4)	0.4374(4)	0.0600(11)
H14A	0.5730	0.8449	0.5121	0.090*
H14B	0.4344	0.8247	0.3947	0.090*
H14C	0.5767	0.7334	0.3835	0.090*
N1	0.1292(3)	0.3736(3)	0.0155(2)	0.0387(7)
N2	−0.0878(3)	0.1123(3)	−0.0788(2)	0.0367(7)

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
N3	−0.1997(3)	0.0108(3)	−0.1599(3)	0.0385(7)
N4	−0.2280(4)	0.0181(3)	−0.2734(3)	0.0506(8)
N5	−0.1306(4)	0.1302(3)	−0.2713(3)	0.0497(8)
N6	0.0791(4)	0.3119(3)	0.4943(3)	0.0456(8)
N7	0.3303(4)	0.5504(3)	0.5798(3)	0.0437(7)
N8	0.4346(4)	0.6601(3)	0.5844(3)	0.0460(8)
N9	0.4088(3)	0.6704(3)	0.4711(3)	0.0408(7)
N10	0.2922(3)	0.5733(3)	0.3897(3)	0.0402(7)

Source of material

The title compound was synthesized according to a reported procedure [5]. Crystals were obtained by slow evaporation of mixed solution of petroleum ether and ethyl acetate (5:1, v/v) at room temperature after a week.

Experimental details

All H atoms were included in calculated positions and refined as riding atoms, with N–H = 0.86 Å, C–H = 0.93–0.98 Å, with *U*_{iso} (H) = 1.5*U*_{eq} (methyl C) or 1.2*U*_{eq} (C, N) for other H atoms.

Comment

The title compound is an important intermediate in the synthesis of Tedizolid. It has been reported that Tedizolid shows antibacterial activity and antioxidant activity [6, 7]. Tedizolid has an effective antibacterial effect on most clinically relevant gram-positive pathogens [8]. It has good therapeutic effect on pulmonary tuberculosis [9]. The title compound consist one tetrazole ring and pyridine ring, one methyl group bound to the tetrazole ring and one bromine atom bound to the pyridine ring. The structure of this compound is similar to the compounds which contain tetrazole rings [10, 11]. This contribution is part of our continuing interest in the synthesis organic pharmaceuticals.

Single-crystal structure analysis reveals that there are two molecules in the asymmetric unit of the title crystal structure. Bond lengths and angles are all in the expected ranges. For example, the N–C bond distance (N1–C1) is 1.319(4) Å, and distance (N2–C6) is 1.339(4) Å. In title compound, there are 1,2,3,4-tetrazole rings. In one molecule, the N–N bond distance (N2–N3, N3–N4 and N5–N4) is 1.321(3) Å, 1.303(4) Å, and 1.316(4) Å, respectively. In another molecule, the N–N bond distance (N8–N7, N9–N8 and N9–N10) is 1.320(4) Å, 1.311(4) Å, and 1.322(4) Å, respectively. Interestingly, the two crystallographically independent molecules are conformers (180° rotation about the central C–C bond (see the figure). Each molecule is almost coplanar. In addition, the dihedral angles between 2-pyridine substituents and 1,2,3,4-tetrazole ring are 11.29(3) Å, and 1.62(3) Å.

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