Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 3-Pyridin-2-yl-1*H*-1,2,4-triazol-5-amine

**Anton V. Dolzhenko,[a]* Geok Kheng Tan,[b] Lip Lin Koh,[b] Anna V. Dolzhenko[a] and Wai Keung Chui[a]**

[a]Department of Pharmacy, Faculty of Science, National University of Singapore, 18 Science Drive 4, Singapore 117543, Singapore, and [b]Department of Chemistry, Faculty of Science, National University of Singapore, 3 Science Drive 3, Singapore 117543, Singapore
Correspondence e-mail: phada@nus.edu.sg

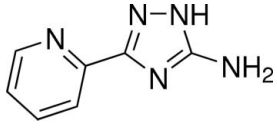
Received 13 November 2008; accepted 11 December 2008

Key indicators: single-crystal X-ray study; $T$ = 223 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.042; $wR$ factor = 0.110; data-to-parameter ratio = 14.6.

In the title compound, $C_7H_7N_5$, the non-H atoms are almost coplanar (r.m.s. deviation = 0.050 Å), with the N atom of pyridine ring oriented to the N—N(H) side of the 1,2,4-triazole ring. The mean planes of the pyridine and 1,2,4-triazole rings form a dihedral angle of 5.58 (7)°. The N atom of the amino group adopts a pyramidal configuration. The molecules are linked into a two-dimensional network parallel to (10$\bar{1}$) by N—H···N hydrogen bonds.

## Related literature

For 1,2,4-triazol-5-amines as building blocks in the synthesis of fused heterocyclic systems, see: Dolzhenko *et al.* (2006, 2007*a*,*b*); Fischer, (2007). For a summary of structural data for 1,2,4-triazoles, see: Buzykin *et al.* (2006). For crystal structures of Cu$^{II}$ complexes with 3-pyridin-2-yl-1,2,4-triazol-5-amine, see: Ferrer *et al.* (2004).




## Experimental

### Crystal data

$C_7H_7N_5$
$M_r$ = 161.18
Monoclinic, $P2_1/n$
$a$ = 7.3863 (6) Å
$b$ = 7.9096 (6) Å
$c$ = 13.2157 (11) Å
$\beta$ = 91.832 (2)°
$V$ = 771.70 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 223 (2) K
0.36 × 0.16 × 0.12 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min}$ = 0.967, $T_{max}$ = 0.989
5336 measured reflections
1772 independent reflections
1519 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.110
$S$ = 1.05
1772 reflections
121 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2*N*···N5$^{i}$ | 0.90 (2) | 2.01 (2) | 2.9010 (16) | 171 (1) |
| N4—H4*A*···N3$^{ii}$ | 0.90 (2) | 2.11 (2) | 2.9971 (16) | 172 (1) |
| N4—H4*B*···N1$^{i}$ | 0.93 (2) | 2.19 (2) | 3.0264 (16) | 151 (1) |

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Medical Research Council, Singapore (grant Nos. NMRC/NIG/0019/2008 and NMRC/NIG/0020/2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2719).

## References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS GmbH, Karlsruhe, Germany.
Buzykin, B. I., Mironova, E. V., Nabiullin, V. N., Gubaidullin, A. T. & Litvinov, I. A. (2006). *Russ. J. Gen. Chem.* **76**, 1471–1486.
Dolzhenko, A. V., Dolzhenko, A. V. & Chui, W. K. (2006). *Heterocycles*, **68**, 1723–1759.
Dolzhenko, A. V., Dolzhenko, A. V. & Chui, W. K. (2007*a*). *Heterocycles*, **71**, 429–436.
Dolzhenko, A. V., Dolzhenko, A. V. & Chui, W. K. (2007*b*). *Tetrahedron*, **63**, 12888–12895.
Ferrer, S., Ballesteros, R., Sambartolome, A., Gonzalez, M., Alzuet, G., Borras, J. & Liu, M. (2004). *J. Inorg. Biochem.* **98**, 1436–1446.
Fischer, G. (2007). *Adv. Heterocycl. Chem.* **95**, 143–219.
Sheldrick, G. M. (2001). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2009). E**65**, o125 [doi:10.1107/S1600536808042177]

## 3-Pyridin-2-yl-1*H*-1,2,4-triazol-5-amine

**Anton V. Dolzhenko, Geok Kheng Tan, Lip Lin Koh, Anna V. Dolzhenko and Wai Keung Chui**

### S1. Comment

1,2,4-Triazol-5-amines have been recognized as valuable synthons for the construction of fused heterocyclic systems, *e.g.* 1,2,4-triazolo[1,5-*a*]pyrimidines (Fischer, 2007) and 1,2,4-triazolo[1,5-*a*][1,3,5]triazines (Dolzhenko *et al.*, 2006). It also should be mentioned that 1,2,4-triazol-5-amines are widely used as ligands and crystallographic data on three different mononuclear complexes of 3-pyridin-2-yl-1,2,4-triazol-5-amine with $Cu^{II}$ have been reported by Ferrer *et al.* (2004). However, no crystallographic study has been performed on the ligand.

In continuation of our investigations on using 1,2,4-triazol-5-amines in the synthesis of fused heterocyclic systems (Dolzhenko *et al.*, 2007*a*,b), we report herein the crystal structure of a synthetically important building block *viz.* 3-pyridin-2-yl-1,2,4-triazol-5-amine.

Due to annular tautomerism, 3-pyridin-2-yl-1,2,4-triazol-5-amine may theoretically exist in three tautomeric forms (**A**, **B** and **C**) and for each of them, rotameric structures **A′**, **B′** and **C′** are possible (Fig.1). As observed in reported $Cu^{II}$ complexes (Ferrer *et al.*, 2004), 3-pyridin-2-yl-1,2,4-triazol-5-amine was the only tautomeric form found in the crystal (Fig. 2). However, the molecule exists in the crystal as rotamer **A** in contrast to rotamer **A′** found in $Cu^{II}$ complexes.

Bond lengths and angles in the molecule of 3-pyridin-2-yl-1,2,4-triazol-5-amine are within normal ranges, and comparable with values summarized for 1,2,4-triazoles by Buzykin *et al.* (2006). 3-Pyridin-2-yl-1,2,4-triazol-5-amine has practically planar geometry with slight deviation of the pyridyl moiety, which makes a dihedral angle of 5.58 (7)° with mean plane of the 1,2,4-triazole ring. The nitrogen atom (N4) of the amino group adopts a pyramidal configuration with 0.26 (2) Å deviation of the nitrogen atom from the C2/H4A/H4B plane.

The molecules are linked into a two-dimensional network parallel to the $(10\bar{1})$ by N—H···N hydrogen bonds (Table 1 and Fig.3).

### S2. Experimental

3-Pyridin-2-yl-1,2,4-triazol-5-amine was prepared according to general method reported by Dolzhenko *et al.* (2007*a*,b). Single crystals suitable for crystallographic analysis were grown by recrystallization from ethanol.

### S3. Refinement

N-bound H-atoms were located in a difference map and refined freely [N—H = 0.90 (2)–0.92 (2) Å]. C-bound H atoms were positioned geometrically (C—H = 0.94 Å) and were constrained in a riding motion approximation with $U_{iso}$(H) = 1.2$U_{eq}$(C).

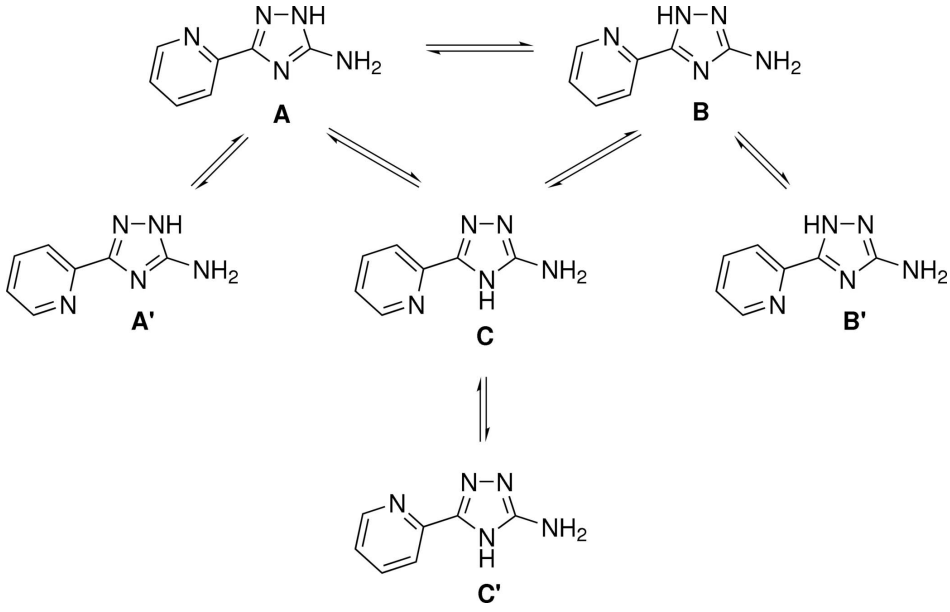



**Figure 1**

Possible tautomers and rotamers of 3-pyridin-2-yl-1,2,4-triazol-5-amine.

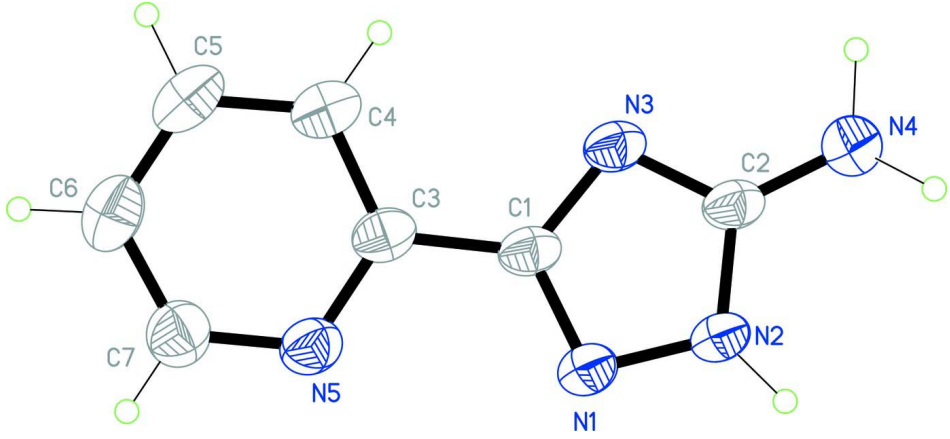



**Figure 2**

The molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

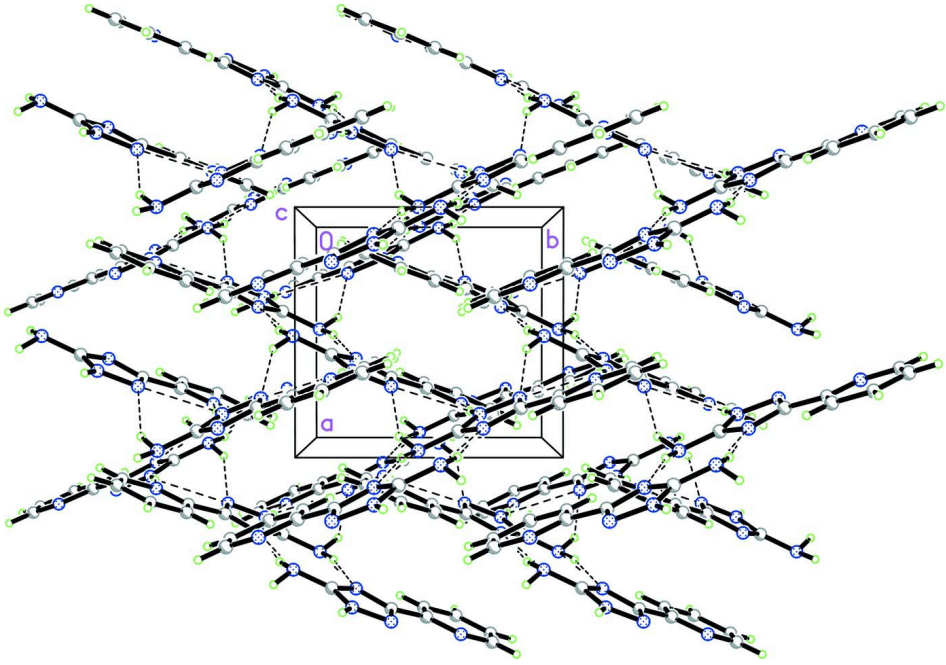



**Figure 3**

Molecular packing of the title compound, viewed along the *c* axis.

### 3-Pyridin-2-yl-1*H*-1,2,4-triazol-5-amine

*Crystal data*

$C_7H_7N_5$
$M_r = 161.18$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.3863$ (6) Å
$b = 7.9096$ (6) Å
$c = 13.2157$ (11) Å
$\beta = 91.832$ (2)°
$V = 771.70$ (11) Å$^3$
$Z = 4$

$F(000) = 336$
$D_x = 1.387$ Mg m$^{-3}$
Melting point: 493 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1841 reflections
$\theta = 3.0$–26.6°
$\mu = 0.10$ mm$^{-1}$
$T = 223$ K
Block, colourless
0.36 × 0.16 × 0.12 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.967$, $T_{max} = 0.989$

5336 measured reflections
1772 independent reflections
1519 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -9 \rightarrow 9$
$k = -8 \rightarrow 10$
$l = -14 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.110$

$S = 1.05$
1772 reflections
121 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.1487P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.72741 (16) | 0.34999 (14) | 0.68693 (8) | 0.0383 (3) |
| N2 | 0.66107 (16) | 0.19639 (15) | 0.71630 (8) | 0.0393 (3) |
| H2N | 0.669 (2) | 0.164 (2) | 0.7817 (14) | 0.052 (5)* |
| N3 | 0.61324 (14) | 0.20352 (14) | 0.55193 (8) | 0.0345 (3) |
| N4 | 0.51489 (16) | −0.04181 (15) | 0.64256 (9) | 0.0398 (3) |
| H4A | 0.488 (2) | −0.095 (2) | 0.5842 (13) | 0.049 (4)* |
| H4B | 0.564 (2) | −0.106 (2) | 0.6948 (13) | 0.050 (4)* |
| N5 | 0.80901 (15) | 0.62905 (15) | 0.56803 (8) | 0.0388 (3) |
| C1 | 0.69411 (16) | 0.34759 (16) | 0.58805 (9) | 0.0331 (3) |
| C2 | 0.59494 (16) | 0.11150 (17) | 0.63532 (9) | 0.0343 (3) |
| C3 | 0.74353 (16) | 0.48955 (17) | 0.52229 (9) | 0.0343 (3) |
| C4 | 0.72299 (19) | 0.47748 (19) | 0.41755 (10) | 0.0425 (3) |
| H4 | 0.6758 | 0.3786 | 0.3873 | 0.051* |
| C5 | 0.77288 (19) | 0.6128 (2) | 0.35870 (11) | 0.0491 (4) |
| H5 | 0.7598 | 0.6076 | 0.2878 | 0.059* |
| C6 | 0.8419 (2) | 0.7554 (2) | 0.40516 (12) | 0.0486 (4) |
| H6 | 0.8781 | 0.8489 | 0.3668 | 0.058* |
| C7 | 0.85663 (19) | 0.75796 (19) | 0.50930 (12) | 0.0455 (4) |
| H7 | 0.9029 | 0.8561 | 0.5408 | 0.055* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0476 (6) | 0.0387 (6) | 0.0282 (5) | −0.0007 (5) | −0.0076 (4) | 0.0006 (4) |
| N2 | 0.0518 (7) | 0.0392 (6) | 0.0261 (6) | −0.0013 (5) | −0.0092 (5) | 0.0000 (5) |
| N3 | 0.0362 (5) | 0.0396 (6) | 0.0273 (5) | 0.0042 (4) | −0.0059 (4) | −0.0028 (4) |
| N4 | 0.0498 (7) | 0.0397 (6) | 0.0291 (6) | −0.0021 (5) | −0.0110 (5) | −0.0001 (5) |
| N5 | 0.0420 (6) | 0.0409 (6) | 0.0332 (6) | 0.0030 (5) | −0.0043 (5) | 0.0012 (5) |
| C1 | 0.0330 (6) | 0.0385 (7) | 0.0273 (6) | 0.0057 (5) | −0.0056 (5) | −0.0035 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0357 (6) | 0.0391 (7) | 0.0274 (6) | 0.0053 (5) | −0.0068 (5) | −0.0030 (5) |
| C3 | 0.0305 (6) | 0.0419 (7) | 0.0301 (6) | 0.0076 (5) | −0.0028 (5) | −0.0010 (5) |
| C4 | 0.0442 (7) | 0.0522 (8) | 0.0310 (7) | 0.0046 (6) | −0.0016 (5) | −0.0025 (6) |
| C5 | 0.0488 (8) | 0.0683 (10) | 0.0304 (7) | 0.0080 (7) | 0.0032 (6) | 0.0071 (7) |
| C6 | 0.0444 (8) | 0.0558 (9) | 0.0457 (8) | 0.0057 (7) | 0.0046 (6) | 0.0150 (7) |
| C7 | 0.0454 (8) | 0.0447 (8) | 0.0460 (8) | 0.0013 (6) | −0.0035 (6) | 0.0050 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.3221 (16) | N5—C3 | 1.3410 (17) |
| N1—N2 | 1.3708 (16) | C1—C3 | 1.4729 (18) |
| N2—C2 | 1.3422 (16) | C3—C4 | 1.3909 (18) |
| N2—H2N | 0.902 (19) | C4—C5 | 1.380 (2) |
| N3—C2 | 1.3312 (17) | C4—H4 | 0.94 |
| N3—C1 | 1.3656 (16) | C5—C6 | 1.374 (2) |
| N4—C2 | 1.3538 (18) | C5—H5 | 0.94 |
| N4—H4A | 0.896 (18) | C6—C7 | 1.377 (2) |
| N4—H4B | 0.925 (17) | C6—H6 | 0.94 |
| N5—C7 | 1.3354 (18) | C7—H7 | 0.94 |
| | | | |
| C1—N1—N2 | 102.14 (10) | N5—C3—C4 | 122.10 (13) |
| C2—N2—N1 | 109.99 (11) | N5—C3—C1 | 116.99 (11) |
| C2—N2—H2N | 129.2 (11) | C4—C3—C1 | 120.91 (12) |
| N1—N2—H2N | 120.8 (11) | C5—C4—C3 | 119.01 (14) |
| C2—N3—C1 | 102.81 (10) | C5—C4—H4 | 120.5 |
| C2—N4—H4A | 116.4 (10) | C3—C4—H4 | 120.5 |
| C2—N4—H4B | 112.7 (10) | C6—C5—C4 | 119.12 (14) |
| H4A—N4—H4B | 117.2 (14) | C6—C5—H5 | 120.4 |
| C7—N5—C3 | 117.65 (12) | C4—C5—H5 | 120.4 |
| N1—C1—N3 | 115.02 (12) | C5—C6—C7 | 118.36 (14) |
| N1—C1—C3 | 122.04 (12) | C5—C6—H6 | 120.8 |
| N3—C1—C3 | 122.94 (11) | C7—C6—H6 | 120.8 |
| N3—C2—N2 | 110.03 (12) | N5—C7—C6 | 123.76 (15) |
| N3—C2—N4 | 127.19 (11) | N5—C7—H7 | 118.1 |
| N2—C2—N4 | 122.71 (12) | C6—C7—H7 | 118.1 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*N*···N5$^{i}$ | 0.90 (2) | 2.01 (2) | 2.9010 (16) | 171 (1) |
| N4—H4*A*···N3$^{ii}$ | 0.90 (2) | 2.11 (2) | 2.9971 (16) | 172 (1) |
| N4—H4*B*···N1$^{i}$ | 0.93 (2) | 2.19 (2) | 3.0264 (16) | 151 (1) |

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1, −*y*, −*z*+1.