Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Ethoxypyridin-2-amine

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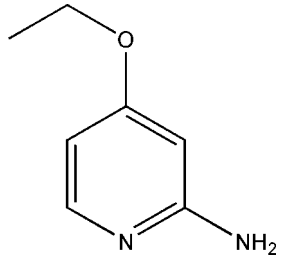
Received 1 August 2008; accepted 2 August 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.124; data-to-parameter ratio = 14.2.

The title compound, $C_7H_{10}N_2O$, crystallizes with two independent molecules in the asymmetric unit. The bond lengths and angles in the molecules are within normal ranges. The crystal structure is stabilized by intermolecular N—H···N hydrogen bonds, linking the two independent molecules into hydrogen-bonded dimers.

Related literature

For related literatures, see: Cai *et al.* (2006); Yale (1976). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_7H_{10}N_2O$
M_r = 138.17
Triclinic, $P\overline{1}$
a = 9.167 (2) Å
b = 9.470 (2) Å
c = 9.541 (3) Å
α = 87.716 (3)°
β = 87.714 (4)°
γ = 64.189 (3)°
V = 744.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.60 × 0.38 × 0.31 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.901, T_{max} = 0.974
3749 measured reflections
2582 independent reflections
2110 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.123
S = 1.02
2582 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N1^{i}	0.86	2.19	3.029 (2)	164
N4—H4B···N3^{ii}	0.86	2.16	3.013 (2)	173

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+2, -z+1$.

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2167).

References

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Yale, H. L. (1976). US patent 3 965 100.

supporting information

Acta Cryst. (2008). E**64**, o1749 [doi:10.1107/S1600536808024847]

4-Ethoxypyridin-2-amine

Lihua Mao and Yan Chen

S1. Comment

2-Amino-4-ethoxypyridine is a useful intermediate for the synthesis of various heterocyclic compounds (Cai *et al.*, 2006; Yale, 1976). In this paper, we report the crystal structure of the title compound (I). The title compound crystallizes with two independent molecules in the asymmetric unit. All bond lengths are normal (Allen *et al.*, 1987). Intermolecular N—H···N hydrogen bonds link the two independent molecules into hydrogen-bonded dimers. The crystal packing is further stabilized by van der Waals forces.

S2. Experimental

2-amino-4-chloropyridine (12.9 g, 0.1 mol) and sodium ethoxide (12.8 g, 0.2 mol) were reacted in 100 ml ethanol in a stainless steel bomb at 150°C for 3 h. The desired compound was obtained as a slightly yellow solid in 50% yield (1.9 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a solution in a hexane/dichloromethane mixture (1:4 *v*/*v*) at room temperature over a period of one week.

S3. Refinement

H atoms bonded to N atoms were located in a difference map and refined with distance restraints of N—H = 0.86Å, and with U_{iso}(H) = 1.2U_{eq}(N). Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

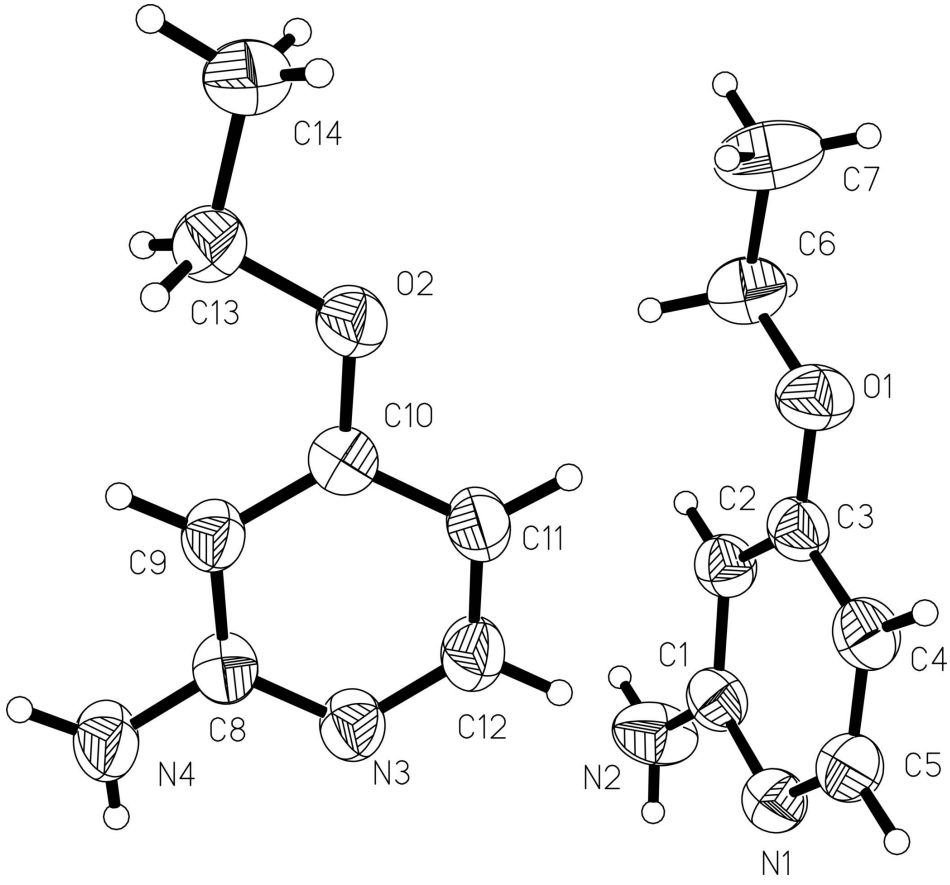

Figure 1

View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level.

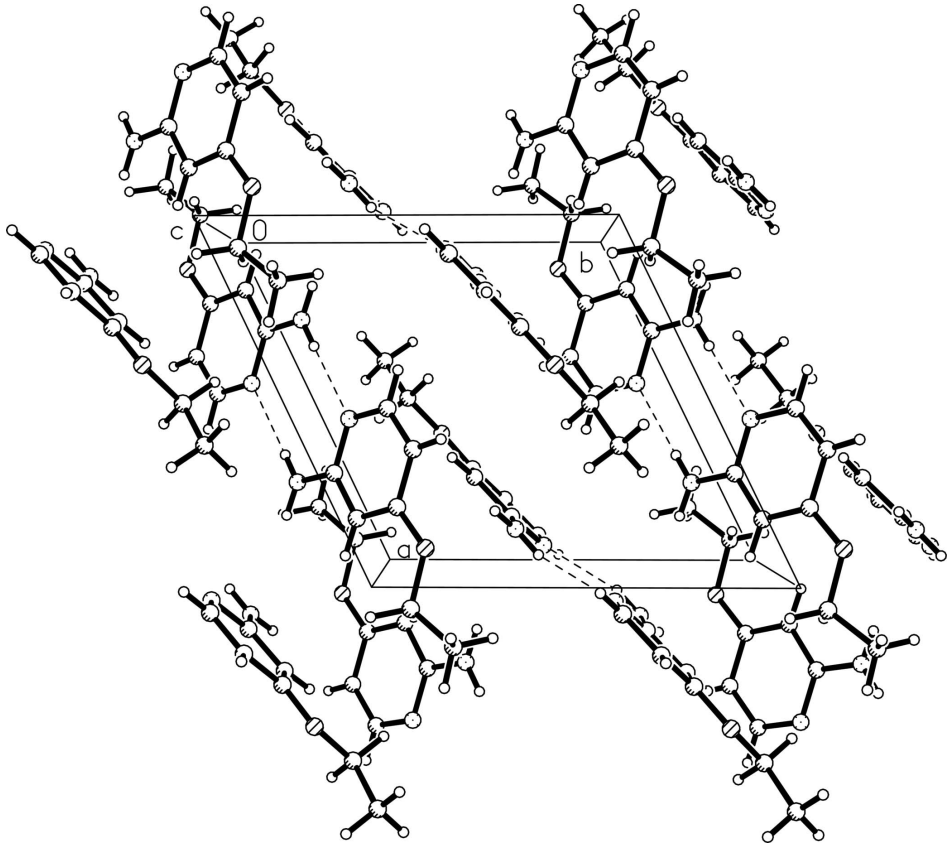

Figure 2

Packing diagram of structure of (I), view along the *c* axis. Hydrogen bonds are shown as dashed lines.

4-Ethoxypyridin-2-amine

Crystal data

$C_7H_{10}N_2O$
$M_r = 138.17$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.167$ (2) Å
$b = 9.470$ (2) Å
$c = 9.541$ (3) Å
$\alpha = 87.716$ (3)°
$\beta = 87.714$ (4)°
$\gamma = 64.189$ (3)°
$V = 744.8$ (3) Å^3
$Z = 4$
$F(000) = 296$
$D_x = 1.232$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1699 reflections
$\theta = 2.8$–$23.1°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, yellow
0.60 × 0.38 × 0.31 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.901$, $T_{max} = 0.974$
3749 measured reflections
2582 independent reflections
2110 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 11$
$l = -11 \rightarrow 7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.123$
$S = 1.02$
2582 reflections
182 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 0.1056P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.040 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.59961 (14)	0.31435 (14)	0.17306 (12)	0.0647 (3)
O2	0.09387 (12)	0.83919 (12)	0.15720 (11)	0.0568 (3)
N1	0.93140 (16)	0.44443 (15)	0.33834 (14)	0.0559 (4)
N2	0.8694 (2)	0.3953 (2)	0.56360 (15)	0.0763 (5)
H2B	0.9418	0.4221	0.5910	0.092*
H2C	0.8150	0.3666	0.6242	0.092*
N3	0.44815 (15)	0.88727 (15)	0.37838 (14)	0.0557 (4)
N4	0.26244 (17)	1.10399 (17)	0.49027 (15)	0.0703 (5)
H4B	0.3410	1.1061	0.5350	0.084*
H4C	0.1649	1.1736	0.5056	0.084*
C1	0.84095 (18)	0.39828 (17)	0.42438 (16)	0.0516 (4)
C2	0.72722 (18)	0.35088 (17)	0.37698 (16)	0.0521 (4)
H2A	0.6669	0.3189	0.4401	0.063*
C3	0.70648 (18)	0.35259 (17)	0.23495 (16)	0.0508 (4)
C4	0.8027 (2)	0.39719 (19)	0.14405 (17)	0.0576 (4)
H4A	0.7938	0.3970	0.0473	0.069*
C5	0.9098 (2)	0.44086 (19)	0.20049 (17)	0.0586 (4)
H5A	0.9731	0.4707	0.1389	0.070*
C6	0.4922 (2)	0.2715 (2)	0.25818 (19)	0.0682 (5)
H6A	0.4340	0.3519	0.3260	0.082*
H6B	0.5528	0.1732	0.3085	0.082*
C7	0.3764 (3)	0.2550 (3)	0.1622 (2)	0.0951 (7)
H7A	0.3023	0.2263	0.2159	0.143*

H7B	0.4354	0.1752	0.0957	0.143*
H7C	0.3171	0.3530	0.1132	0.143*
C8	0.29236 (18)	0.99108 (18)	0.39569 (15)	0.0506 (4)
C9	0.16603 (18)	0.98351 (18)	0.32351 (16)	0.0511 (4)
H9A	0.0594	1.0573	0.3380	0.061*
C10	0.20318 (18)	0.86432 (17)	0.23054 (15)	0.0480 (4)
C11	0.36506 (19)	0.75665 (18)	0.21075 (17)	0.0568 (4)
H11A	0.3941	0.6753	0.1483	0.068*
C12	0.47882 (19)	0.77452 (19)	0.28565 (18)	0.0596 (4)
H12A	0.5864	0.7029	0.2714	0.072*
C13	−0.07465 (19)	0.9457 (2)	0.17306 (18)	0.0605 (4)
H13A	−0.0939	1.0486	0.1348	0.073*
H13B	−0.1069	0.9557	0.2716	0.073*
C14	−0.1699 (2)	0.8813 (2)	0.0962 (2)	0.0806 (6)
H14A	−0.2832	0.9508	0.1049	0.121*
H14B	−0.1507	0.7799	0.1352	0.121*
H14C	−0.1371	0.8718	−0.0012	0.121*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0665 (7)	0.0772 (8)	0.0598 (7)	−0.0395 (7)	−0.0091 (6)	−0.0017 (6)
O2	0.0522 (6)	0.0562 (7)	0.0601 (7)	−0.0206 (5)	−0.0068 (5)	−0.0106 (5)
N1	0.0577 (8)	0.0564 (8)	0.0557 (8)	−0.0264 (7)	−0.0021 (6)	−0.0038 (6)
N2	0.1046 (12)	0.0994 (12)	0.0514 (8)	−0.0687 (11)	−0.0128 (8)	0.0064 (8)
N3	0.0489 (7)	0.0531 (8)	0.0580 (8)	−0.0148 (6)	−0.0073 (6)	−0.0054 (6)
N4	0.0526 (8)	0.0734 (10)	0.0741 (10)	−0.0143 (7)	−0.0102 (7)	−0.0284 (8)
C1	0.0562 (9)	0.0425 (8)	0.0532 (9)	−0.0186 (7)	−0.0054 (7)	−0.0003 (6)
C2	0.0557 (9)	0.0466 (9)	0.0535 (9)	−0.0219 (7)	−0.0009 (7)	0.0002 (7)
C3	0.0501 (8)	0.0418 (8)	0.0572 (9)	−0.0164 (7)	−0.0049 (7)	−0.0040 (7)
C4	0.0648 (10)	0.0591 (10)	0.0486 (9)	−0.0263 (8)	−0.0019 (7)	−0.0045 (7)
C5	0.0624 (10)	0.0625 (10)	0.0538 (9)	−0.0303 (8)	0.0052 (7)	−0.0040 (7)
C6	0.0628 (10)	0.0736 (12)	0.0730 (11)	−0.0342 (9)	−0.0093 (9)	0.0062 (9)
C7	0.0799 (14)	0.1224 (19)	0.1023 (16)	−0.0620 (14)	−0.0346 (12)	0.0319 (14)
C8	0.0507 (9)	0.0497 (9)	0.0464 (8)	−0.0167 (7)	−0.0048 (6)	−0.0018 (7)
C9	0.0450 (8)	0.0487 (9)	0.0523 (8)	−0.0130 (7)	−0.0030 (6)	−0.0040 (7)
C10	0.0515 (8)	0.0476 (8)	0.0451 (8)	−0.0216 (7)	−0.0043 (6)	0.0023 (6)
C11	0.0557 (9)	0.0493 (9)	0.0603 (9)	−0.0172 (8)	0.0001 (7)	−0.0118 (7)
C12	0.0481 (9)	0.0513 (9)	0.0693 (10)	−0.0116 (7)	−0.0018 (8)	−0.0083 (8)
C13	0.0528 (9)	0.0603 (10)	0.0650 (10)	−0.0207 (8)	−0.0045 (8)	−0.0074 (8)
C14	0.0627 (11)	0.0813 (13)	0.1024 (15)	−0.0335 (10)	−0.0108 (10)	−0.0174 (11)

Geometric parameters (Å, º)

O1—C3	1.3460 (19)	C5—H5A	0.9300
O1—C6	1.433 (2)	C6—C7	1.490 (3)
O2—C10	1.3518 (18)	C6—H6A	0.9700
O2—C13	1.4364 (19)	C6—H6B	0.9700

N1—C1	1.336 (2)	C7—H7A	0.9600
N1—C5	1.342 (2)	C7—H7B	0.9600
N2—C1	1.361 (2)	C7—H7C	0.9600
N2—H2B	0.8600	C8—C9	1.400 (2)
N2—H2C	0.8600	C9—C10	1.378 (2)
N3—C12	1.340 (2)	C9—H9A	0.9300
N3—C8	1.3434 (19)	C10—C11	1.397 (2)
N4—C8	1.3545 (19)	C11—C12	1.360 (2)
N4—H4B	0.8600	C11—H11A	0.9300
N4—H4C	0.8600	C12—H12A	0.9300
C1—C2	1.398 (2)	C13—C14	1.491 (2)
C2—C3	1.374 (2)	C13—H13A	0.9700
C2—H2A	0.9300	C13—H13B	0.9700
C3—C4	1.394 (2)	C14—H14A	0.9600
C4—C5	1.355 (2)	C14—H14B	0.9600
C4—H4A	0.9300	C14—H14C	0.9600

C3—O1—C6	119.52 (13)	C6—C7—H7B	109.5
C10—O2—C13	118.61 (11)	H7A—C7—H7B	109.5
C1—N1—C5	116.21 (13)	C6—C7—H7C	109.5
C1—N2—H2B	120.0	H7A—C7—H7C	109.5
C1—N2—H2C	120.0	H7B—C7—H7C	109.5
H2B—N2—H2C	120.0	N3—C8—N4	116.04 (14)
C12—N3—C8	116.47 (13)	N3—C8—C9	122.94 (14)
C8—N4—H4B	120.0	N4—C8—C9	121.01 (14)
C8—N4—H4C	120.0	C10—C9—C8	118.52 (14)
H4B—N4—H4C	120.0	C10—C9—H9A	120.7
N1—C1—N2	115.68 (14)	C8—C9—H9A	120.7
N1—C1—C2	123.24 (14)	O2—C10—C9	125.11 (14)
N2—C1—C2	121.06 (15)	O2—C10—C11	115.89 (13)
C3—C2—C1	118.51 (14)	C9—C10—C11	118.98 (14)
C3—C2—H2A	120.7	C12—C11—C10	117.94 (14)
C1—C2—H2A	120.7	C12—C11—H11A	121.0
O1—C3—C2	125.72 (14)	C10—C11—H11A	121.0
O1—C3—C4	115.54 (14)	N3—C12—C11	125.14 (15)
C2—C3—C4	118.74 (14)	N3—C12—H12A	117.4
C5—C4—C3	118.19 (15)	C11—C12—H12A	117.4
C5—C4—H4A	120.9	O2—C13—C14	107.85 (14)
C3—C4—H4A	120.9	O2—C13—H13A	110.1
N1—C5—C4	125.08 (15)	C14—C13—H13A	110.1
N1—C5—H5A	117.5	O2—C13—H13B	110.1
C4—C5—H5A	117.5	C14—C13—H13B	110.1
O1—C6—C7	107.17 (15)	H13A—C13—H13B	108.4
O1—C6—H6A	110.3	C13—C14—H14A	109.5
C7—C6—H6A	110.3	C13—C14—H14B	109.5
O1—C6—H6B	110.3	H14A—C14—H14B	109.5
C7—C6—H6B	110.3	C13—C14—H14C	109.5
H6A—C6—H6B	108.5	H14A—C14—H14C	109.5

C6—C7—H7A	109.5	H14B—C14—H14C	109.5
C5—N1—C1—N2	177.01 (15)	C12—N3—C8—N4	179.60 (15)
C5—N1—C1—C2	−1.1 (2)	C12—N3—C8—C9	0.8 (2)
N1—C1—C2—C3	−0.4 (2)	N3—C8—C9—C10	0.0 (2)
N2—C1—C2—C3	−178.37 (15)	N4—C8—C9—C10	−178.74 (15)
C6—O1—C3—C2	1.9 (2)	C13—O2—C10—C9	1.6 (2)
C6—O1—C3—C4	−178.15 (14)	C13—O2—C10—C11	179.93 (13)
C1—C2—C3—O1	−178.26 (14)	C8—C9—C10—O2	177.69 (14)
C1—C2—C3—C4	1.8 (2)	C8—C9—C10—C11	−0.6 (2)
O1—C3—C4—C5	178.35 (14)	O2—C10—C11—C12	−178.04 (14)
C2—C3—C4—C5	−1.7 (2)	C9—C10—C11—C12	0.4 (2)
C1—N1—C5—C4	1.2 (2)	C8—N3—C12—C11	−1.1 (3)
C3—C4—C5—N1	0.2 (3)	C10—C11—C12—N3	0.5 (3)
C3—O1—C6—C7	173.22 (16)	C10—O2—C13—C14	−173.07 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···N1^{i}	0.86	2.19	3.029 (2)	164
N4—H4*B*···N3^{ii}	0.86	2.16	3.013 (2)	173

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