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2-Amino-5-methyl-1,2,4-triazolo[1,5-*a*]pyrimidin-7(4*H*)-one

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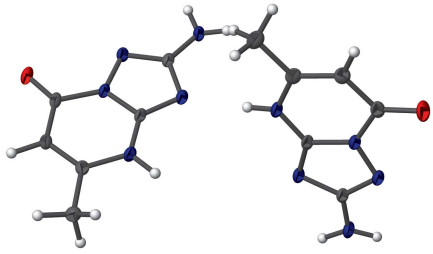
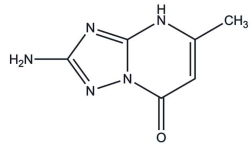
The asymmetric unit of the title compound, $C_6H_7N_5O$, consists of two molecules with almost identical conformations. In the crystal, inversion dimers linked by pairs of N—H···N hydrogen bonds occur for both molecules; further N—H···N and N—H···O hydrogen bonds connect the dimers into a three-dimensional network.

3D view



Chemical scheme



Structure description

As a continuation of our studies of triazolopyrimidine derivatives (Lahmidi *et al.*, 2016; El Hafi *et al.*, 2017), we now report the synthesis and crystal structure of the title compound (Fig. 1).

The asymmetric unit consists of two independent molecules with almost identical conformations; as expected, the molecules are almost planar with r.m.s. deviations for the N1 and N6 molecules of 0.011 and 0.0052 Å, respectively. The dihedral angle between the mean planes of the independent molecules in the asymmetric unit, which are linked by an N1—H1···N7 hydrogen bond, is 78.27 (3)°. In the extended structure, inversion dimers linked by pairs of N—H···N hydrogen bonds generate $R_2^2(8)$ loops for both molecules (Table 1). Further N—H···N and N—H···O hydrogen bonds connect the dimers into a three-dimensional network (Table 1 and Figs. 2 and 3).

Synthesis and crystallization

A mixture of 3,5-diamino-1,2,4-triazole (0.5 g, 5 mmol) and ethyl acetoacetate (0.64 ml, 5 mmol) and 15 ml of acetic acid was refluxed for 6 h. The solution was cooled and

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N7	0.85 (2)	2.00 (2)	2.8520 (18)	176 (2)
N5—H5A···N2^{i}	0.93 (2)	2.20 (2)	3.1240 (18)	173.3 (17)
N5—H5B···O2^{ii}	0.881 (18)	2.097 (19)	2.9733 (18)	172.7 (16)
N6—H6···N3^{iii}	0.944 (19)	1.94 (2)	2.8724 (17)	168.6 (17)
N10—H10A···O1^{iv}	0.863 (18)	2.069 (18)	2.8935 (17)	159.5 (16)
N10—H10B···N8^{v}	0.845 (18)	2.220 (19)	3.0330 (19)	161.2 (16)

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

evaporated to dryness under reduced pressure and ethanol (7 ml) was added. After four days, colourless columnar crystals were recovered in 75% yield.

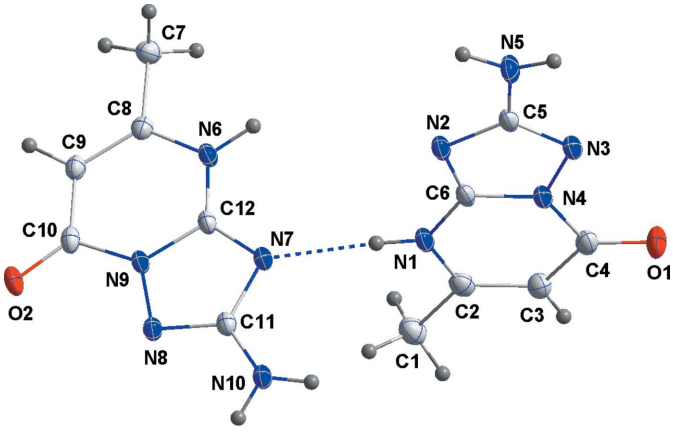


Figure 1
The asymmetric unit with labelling scheme and 50% probability ellipsoids. The N—H···N hydrogen bond is shown by a dashed line.

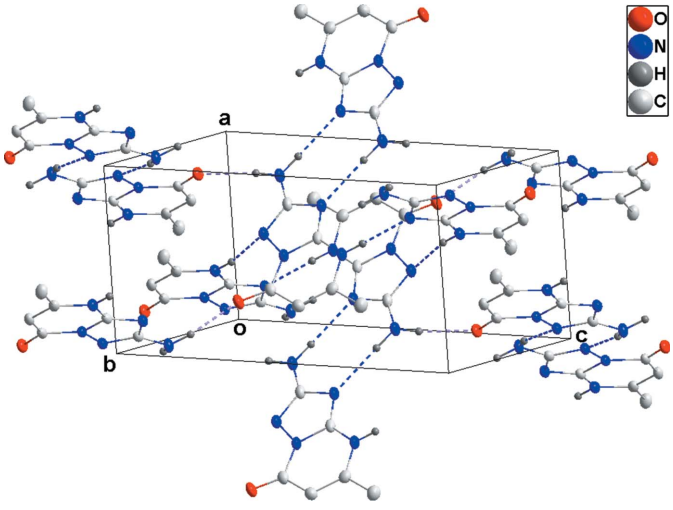


Figure 2
Packing showing the hydrogen-bonding network with the N—H···O and N—H···N hydrogen bonds shown, respectively, as purple and blue dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_7N_5O$
M_r	165.17
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	6.5921 (14), 8.3935 (18), 13.185 (3)
α, β, γ (°)	92.023 (3), 98.309 (3), 99.741 (3)
V (Å^3)	710.1 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.12
Crystal size (mm)	0.39 × 0.16 × 0.09
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.96, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6817, 3503, 2743
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.689
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.138, 1.13
No. of reflections	3503
No. of parameters	251
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.26

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *Mercury* (Macrae, *et al.*, 2008) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x181500 [https://doi.org/10.1107/S2414314618015006]

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Crystal data

$C_6H_7N_5O$
M_r = 165.17
Triclinic, $P\overline{1}$
a = 6.5921 (14) Å
b = 8.3935 (18) Å
c = 13.185 (3) Å
α = 92.023 (3)°
β = 98.309 (3)°
γ = 99.741 (3)°
V = 710.1 (3) Å^3
Z = 4
$F(000)$ = 344
D_x = 1.545 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3414 reflections
θ = 2.5–29.0°
μ = 0.12 mm^{-1}
T = 100 K
Column, colourless
0.39 × 0.16 × 0.09 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.96, T_{max} = 0.99
6817 measured reflections
3503 independent reflections
2743 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 29.3°, θ_{min} = 1.6°
h = −9→8
k = −11→11
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.138
S = 1.13
3503 reflections
251 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0848P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Experimental. The diffraction data were collected in three sets of 363 frames (0.5° width in ω) at φ = 0, 120 and 240°. A scan time of 40 sec/frame was used.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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. The hydrogens attached to C1 and C7 did not refine well as independent atoms and so were included as riding contributions in idealized positions.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.71873 (17)	0.15324 (13)	0.67848 (8)	0.0266 (3)
N1	0.45726 (19)	0.26128 (14)	0.39710 (9)	0.0185 (3)
H1	0.396 (4)	0.275 (2)	0.3374 (17)	0.047 (6)*
N2	0.22945 (19)	0.38112 (14)	0.49382 (9)	0.0185 (3)
N3	0.38526 (19)	0.32482 (14)	0.65319 (9)	0.0185 (3)
H3	0.833 (3)	0.097 (2)	0.5008 (14)	0.038 (5)*
N4	0.48312 (19)	0.26943 (14)	0.57606 (9)	0.0172 (3)
N5	0.0991 (2)	0.46038 (16)	0.64373 (10)	0.0222 (3)
H5A	0.000 (3)	0.501 (2)	0.5988 (15)	0.037 (5)*
H5B	0.090 (3)	0.444 (2)	0.7087 (15)	0.027 (5)*
C1	0.6963 (3)	0.1426 (2)	0.30516 (12)	0.0264 (4)
H1A	0.781469	0.238609	0.283004	0.040*
H1B	0.574460	0.105785	0.252660	0.040*
H1C	0.779082	0.056198	0.314946	0.040*
C2	0.6262 (2)	0.18420 (17)	0.40412 (11)	0.0201 (3)
C3	0.7210 (2)	0.14891 (18)	0.49694 (12)	0.0210 (3)
C4	0.6514 (2)	0.18617 (17)	0.59172 (11)	0.0200 (3)
C5	0.2336 (2)	0.38926 (17)	0.59923 (10)	0.0180 (3)
C6	0.3869 (2)	0.30546 (17)	0.48365 (10)	0.0170 (3)
O2	0.09921 (16)	0.38683 (13)	−0.13731 (7)	0.0218 (3)
N6	0.37698 (19)	0.56222 (14)	0.14978 (9)	0.0173 (3)
H6	0.438 (3)	0.602 (2)	0.2170 (15)	0.035 (5)*
N7	0.24807 (18)	0.29027 (14)	0.19538 (9)	0.0172 (3)
N8	0.09267 (18)	0.19333 (14)	0.03227 (9)	0.0166 (3)
N9	0.18460 (18)	0.35493 (14)	0.03384 (8)	0.0153 (3)
N10	0.0637 (2)	0.01587 (16)	0.16497 (10)	0.0197 (3)
H10A	0.123 (3)	−0.015 (2)	0.2218 (14)	0.023 (4)*
H10B	0.013 (3)	−0.060 (2)	0.1197 (14)	0.022 (4)*
C7	0.4936 (3)	0.83306 (18)	0.09981 (12)	0.0231 (3)
H7A	0.530492	0.885495	0.038129	0.035*
H7B	0.620513	0.831601	0.148471	0.035*
H7C	0.402030	0.893396	0.131765	0.035*

C8	0.3836 (2)	0.66345 (17)	0.07097 (11)	0.0173 (3)
C9	0.2924 (2)	0.61062 (18)	−0.02650 (11)	0.0180 (3)
H9	0.301 (3)	0.6893 (19)	−0.0810 (13)	0.019 (4)*
C10	0.1855 (2)	0.44763 (18)	−0.05244 (11)	0.0175 (3)
C11	0.1343 (2)	0.16154 (17)	0.13023 (10)	0.0161 (3)
C12	0.2755 (2)	0.40717 (17)	0.13117 (10)	0.0155 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0288 (6)	0.0339 (6)	0.0171 (5)	0.0087 (5)	−0.0021 (4)	0.0072 (5)
N1	0.0235 (7)	0.0199 (6)	0.0107 (6)	0.0020 (5)	0.0003 (5)	0.0009 (5)
N2	0.0223 (6)	0.0202 (6)	0.0115 (6)	0.0019 (5)	0.0001 (5)	0.0015 (5)
N3	0.0234 (6)	0.0201 (6)	0.0116 (6)	0.0033 (5)	0.0013 (5)	0.0012 (5)
N4	0.0217 (6)	0.0174 (6)	0.0116 (6)	0.0024 (5)	0.0011 (5)	0.0012 (4)
N5	0.0278 (7)	0.0288 (7)	0.0113 (6)	0.0090 (6)	0.0023 (5)	0.0031 (5)
C1	0.0305 (9)	0.0275 (8)	0.0208 (8)	0.0034 (7)	0.0054 (6)	−0.0010 (6)
C2	0.0211 (7)	0.0179 (7)	0.0196 (7)	−0.0017 (6)	0.0034 (6)	−0.0006 (5)
C3	0.0209 (7)	0.0214 (7)	0.0200 (7)	0.0039 (6)	0.0009 (6)	0.0004 (6)
C4	0.0221 (7)	0.0182 (7)	0.0175 (7)	0.0003 (6)	−0.0007 (6)	0.0020 (5)
C5	0.0234 (7)	0.0157 (7)	0.0125 (7)	−0.0006 (6)	−0.0003 (5)	0.0009 (5)
C6	0.0207 (7)	0.0159 (7)	0.0116 (6)	−0.0019 (5)	−0.0010 (5)	0.0004 (5)
O2	0.0242 (5)	0.0295 (6)	0.0108 (5)	0.0044 (4)	−0.0005 (4)	0.0005 (4)
N6	0.0194 (6)	0.0203 (6)	0.0113 (6)	0.0036 (5)	0.0001 (5)	−0.0006 (5)
N7	0.0197 (6)	0.0193 (6)	0.0117 (6)	0.0032 (5)	0.0002 (5)	0.0005 (4)
N8	0.0180 (6)	0.0182 (6)	0.0130 (6)	0.0029 (5)	0.0004 (5)	0.0018 (4)
N9	0.0168 (6)	0.0190 (6)	0.0098 (6)	0.0037 (5)	0.0008 (4)	0.0003 (4)
N10	0.0268 (7)	0.0184 (6)	0.0122 (6)	0.0019 (5)	−0.0008 (5)	0.0023 (5)
C7	0.0312 (8)	0.0185 (7)	0.0195 (7)	0.0033 (6)	0.0052 (6)	0.0001 (6)
C8	0.0183 (7)	0.0197 (7)	0.0158 (7)	0.0069 (5)	0.0044 (5)	0.0025 (5)
C9	0.0208 (7)	0.0216 (7)	0.0135 (7)	0.0075 (6)	0.0034 (5)	0.0033 (5)
C10	0.0166 (7)	0.0257 (8)	0.0121 (6)	0.0082 (6)	0.0029 (5)	0.0029 (5)
C11	0.0157 (6)	0.0205 (7)	0.0126 (6)	0.0051 (5)	0.0017 (5)	0.0007 (5)
C12	0.0157 (6)	0.0205 (7)	0.0105 (6)	0.0054 (5)	0.0003 (5)	−0.0001 (5)

Geometric parameters (Å, º)

O1—C4	1.2244 (17)	O2—C10	1.2301 (17)
N1—C6	1.3549 (18)	N6—C12	1.3553 (18)
N1—C2	1.373 (2)	N6—C8	1.3662 (18)
N1—H1	0.85 (2)	N6—H6	0.944 (19)
N2—C6	1.3252 (19)	N7—C12	1.3247 (18)
N2—C5	1.3850 (18)	N7—C11	1.3934 (18)
N3—C5	1.3425 (18)	N8—C11	1.3272 (17)
N3—N4	1.3871 (16)	N8—N9	1.3869 (16)
N4—C6	1.3586 (18)	N9—C12	1.3592 (17)
N4—C4	1.4028 (19)	N9—C10	1.4009 (18)
N5—C5	1.339 (2)	N10—C11	1.3528 (19)

N5—H5A	0.93 (2)	N10—H10A	0.863 (18)
N5—H5B	0.881 (18)	N10—H10B	0.845 (18)
C1—C2	1.495 (2)	C7—C8	1.493 (2)
C1—H1A	0.9800	C7—H7A	0.9800
C1—H1B	0.9800	C7—H7B	0.9800
C1—H1C	0.9800	C7—H7C	0.9800
C2—C3	1.358 (2)	C8—C9	1.362 (2)
C3—C4	1.434 (2)	C9—C10	1.434 (2)
C3—H3	0.92 (2)	C9—H9	0.994 (16)

C6—N1—C2	119.78 (12)	C12—N6—C8	119.56 (12)
C6—N1—H1	122.1 (14)	C12—N6—H6	120.7 (11)
C2—N1—H1	118.0 (14)	C8—N6—H6	119.7 (11)
C6—N2—C5	102.16 (12)	C12—N7—C11	101.97 (11)
C5—N3—N4	101.88 (11)	C11—N8—N9	101.91 (11)
C6—N4—N3	109.13 (11)	C12—N9—N8	109.40 (11)
C6—N4—C4	125.85 (12)	C12—N9—C10	125.84 (13)
N3—N4—C4	125.00 (11)	N8—N9—C10	124.76 (11)
C5—N5—H5A	115.3 (12)	C11—N10—H10A	121.1 (11)
C5—N5—H5B	118.1 (12)	C11—N10—H10B	116.2 (12)
H5A—N5—H5B	124.6 (16)	H10A—N10—H10B	114.5 (16)
C2—C1—H1A	109.5	C8—C7—H7A	109.5
C2—C1—H1B	109.5	C8—C7—H7B	109.5
H1A—C1—H1B	109.5	H7A—C7—H7B	109.5
C2—C1—H1C	109.5	C8—C7—H7C	109.5
H1A—C1—H1C	109.5	H7A—C7—H7C	109.5
H1B—C1—H1C	109.5	H7B—C7—H7C	109.5
C3—C2—N1	120.58 (14)	C9—C8—N6	121.13 (13)
C3—C2—C1	123.06 (14)	C9—C8—C7	123.36 (13)
N1—C2—C1	116.36 (13)	N6—C8—C7	115.51 (12)
C2—C3—C4	123.05 (14)	C8—C9—C10	122.51 (13)
C2—C3—H3	119.9 (12)	C8—C9—H9	118.0 (9)
C4—C3—H3	117.0 (12)	C10—C9—H9	119.5 (9)
O1—C4—N4	120.04 (14)	O2—C10—N9	120.15 (14)
O1—C4—C3	128.36 (15)	O2—C10—C9	128.04 (14)
N4—C4—C3	111.60 (12)	N9—C10—C9	111.81 (12)
N5—C5—N3	122.72 (13)	N8—C11—N10	122.11 (13)
N5—C5—N2	122.06 (13)	N8—C11—N7	115.47 (12)
N3—C5—N2	115.20 (13)	N10—C11—N7	122.36 (13)
N2—C6—N1	129.32 (13)	N7—C12—N6	129.63 (12)
N2—C6—N4	111.63 (12)	N7—C12—N9	111.24 (12)
N1—C6—N4	119.05 (13)	N6—C12—N9	119.13 (12)

C5—N3—N4—C6	0.68 (14)	C11—N8—N9—C12	0.65 (14)
C5—N3—N4—C4	−177.92 (13)	C11—N8—N9—C10	179.64 (12)
C6—N1—C2—C3	1.3 (2)	C12—N6—C8—C9	−0.9 (2)
C6—N1—C2—C1	−178.81 (13)	C12—N6—C8—C7	178.26 (12)
N1—C2—C3—C4	1.0 (2)	N6—C8—C9—C10	−0.2 (2)

C1—C2—C3—C4	−178.83 (13)	C7—C8—C9—C10	−179.29 (13)
C6—N4—C4—O1	−176.24 (13)	C12—N9—C10—O2	179.35 (13)
N3—N4—C4—O1	2.1 (2)	N8—N9—C10—O2	0.5 (2)
C6—N4—C4—C3	3.1 (2)	C12—N9—C10—C9	−1.25 (19)
N3—N4—C4—C3	−178.51 (12)	N8—N9—C10—C9	179.92 (11)
C2—C3—C4—O1	176.27 (15)	C8—C9—C10—O2	−179.49 (14)
C2—C3—C4—N4	−3.0 (2)	C8—C9—C10—N9	1.17 (19)
N4—N3—C5—N5	−179.14 (13)	N9—N8—C11—N10	176.94 (12)
N4—N3—C5—N2	−0.87 (15)	N9—N8—C11—N7	−0.47 (15)
C6—N2—C5—N5	178.99 (13)	C12—N7—C11—N8	0.11 (16)
C6—N2—C5—N3	0.71 (16)	C12—N7—C11—N10	−177.30 (13)
C5—N2—C6—N1	179.09 (14)	C11—N7—C12—N6	−179.56 (13)
C5—N2—C6—N4	−0.21 (15)	C11—N7—C12—N9	0.33 (15)
C2—N1—C6—N2	179.42 (13)	C8—N6—C12—N7	−179.24 (14)
C2—N1—C6—N4	−1.3 (2)	C8—N6—C12—N9	0.89 (19)
N3—N4—C6—N2	−0.30 (16)	N8—N9—C12—N7	−0.64 (15)
C4—N4—C6—N2	178.28 (12)	C10—N9—C12—N7	−179.62 (12)
N3—N4—C6—N1	−179.69 (11)	N8—N9—C12—N6	179.26 (11)
C4—N4—C6—N1	−1.1 (2)	C10—N9—C12—N6	0.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N7	0.85 (2)	2.00 (2)	2.8520 (18)	176 (2)
N5—H5*A*···N2^{i}	0.93 (2)	2.20 (2)	3.1240 (18)	173.3 (17)
N5—H5*B*···O2^{ii}	0.881 (18)	2.097 (19)	2.9733 (18)	172.7 (16)
N6—H6···N3^{iii}	0.944 (19)	1.94 (2)	2.8724 (17)	168.6 (17)
N10—H10*A*···O1^{iv}	0.863 (18)	2.069 (18)	2.8935 (17)	159.5 (16)
N10—H10*B*···N8^{v}	0.845 (18)	2.220 (19)	3.0330 (19)	161.2 (16)

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