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N,*N*-Dimethyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-4-amine monohydrate

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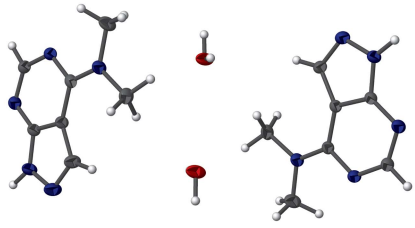
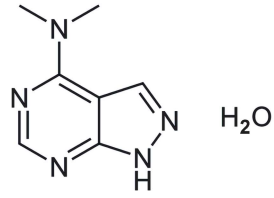
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_7H_9N_5\cdot H_2O$, consists of two formula units differing slightly in the orientation of the dimethylamino groups. In the crystal, a combination of O—H···N and N—H···O hydrogen bonds involving the water molecules of crystallization, as well as slipped π-stacking interactions between pyrazolopyrimidine units form layers parallel to the *bc* plane.

3D view



Chemical scheme



Structure description

Pyrazolo[3,4-*d*]pyrimidines display a broad spectrum of biological activity including antiviral, antitubercular (Trivedi *et al.*, 2012) and antibacterial agents (Bondock *et al.*, 2008). The present work is a continuation of the investigation of pyrazolo[3,4-*d*]pyri-]pyrimidine derivatives reported by our team (El Hafi *et al.*, 2017).

The asymmetric unit consists of two independent molecules and two water molecules of crystallization (Fig. 1). The main molecules differ primarily in the orientation of the dimethylamino substituent. Thus, the C2—C1—N5—C6 torsion angle is −6.3 (2)° while the C9—C8—N10—C14 torsion angle is 5.4 (2)°. The bicyclic moieties are slightly twisted, as seen from the dihedral angles of 1.99 (9) and 1.56 (9)° between the five- and six-membered rings.

In the crystal, head-to-tail, slipped π-stacking interactions between the five- and six-membered rings of the N1-containing molecule with those in the N5-containing molecule form dimers with a centroid–centroid distance of 3.543 (1) Å for the N1/N2/C4/C2/C3 ring and the N8/C11/C9/C8/N9/C12 ring at $x, y-1, z$, while for the N3/C4/C2/C1/N4/C5

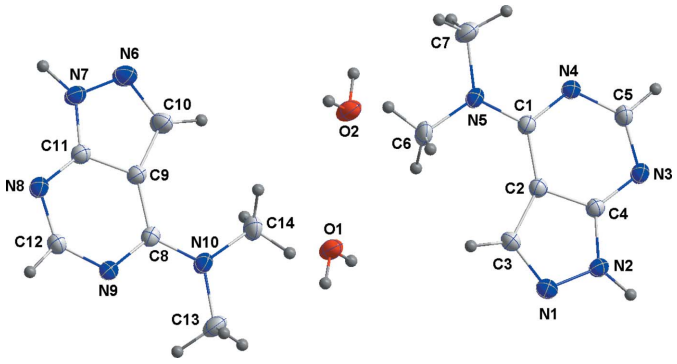


Figure 1
The asymmetric unit with labeling scheme and 50% probability displacement ellipsoids.

and N6/N7/C11/C9/C10 rings the corresponding distance is 3.750 (1) Å. The dimers are connected into chains parallel to the *b*-axis direction by N2—H2···O1 and O1—H1*A*—N8 hydrogen bonds (Table 1). In the center of Fig. 2 are two dimers connected by hydrogen bonding to the water molecules of crystallization and representing a portion of one chain. The chains are elaborated into layers parallel to the bc plane by O2—H2*A*—N9 and O1—H1*B*—N4 hydrogen bonds (Table 1 and Figs. 2 and 3). In the layers, the mean planes of the bicyclic moieties in adjacent chains are inclined to one another by 30.1 (1)°.

Synthesis and crystallization

To a solution of 1*H*-pyrazolo[3,4-*d*]pyrimidine-4-thione (0.5 g, 3.3 mmol) in DMF (15 ml) was added a catalytic amount of tetra-*n*-butylammonium bromide and potassium carbonate (0.54 g, 3.96 mmol). The mixture was heated to reflux for 12 h.

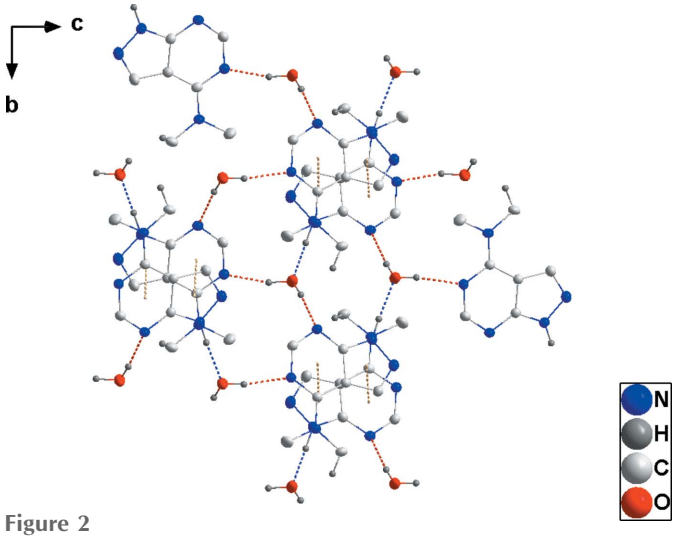


Figure 2
Plan view of a portion of one layer showing the O—H···N and N—H···O hydrogen bonds (red and blue dashed lines, respectively) and the π-stacking interactions (tan dashed lines) projected along the *a*-axis direction.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.94 (2)	1.82 (2)	2.7546 (18)	173 (2)
N7—H7···O2^{ii}	0.99 (2)	1.74 (2)	2.7256 (19)	179 (3)
O1—H1*A*···N8^{i}	0.93 (3)	1.94 (3)	2.8607 (19)	172 (2)
O1—H1*B*···N4^{iii}	0.88 (3)	1.95 (3)	2.8158 (18)	170 (2)
O2—H2*A*···N9^{iv}	0.97 (3)	1.86 (3)	2.8042 (18)	166 (2)
O2—H2*B*···N3^{ii}	0.89 (3)	1.98 (3)	2.865 (2)	173 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_7H_9N_5\cdot H_2O$
M_r	181.21
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	14.5177 (5), 8.3622 (3), 14.9892 (6)
β (°)	110.724 (2)
V (Å^3)	1701.95 (11)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.85
Crystal size (mm)	0.13 × 0.12 × 0.09
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.75, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12386, 3309, 2718
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.122, 1.04
No. of reflections	3309
No. of parameters	312
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.25

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

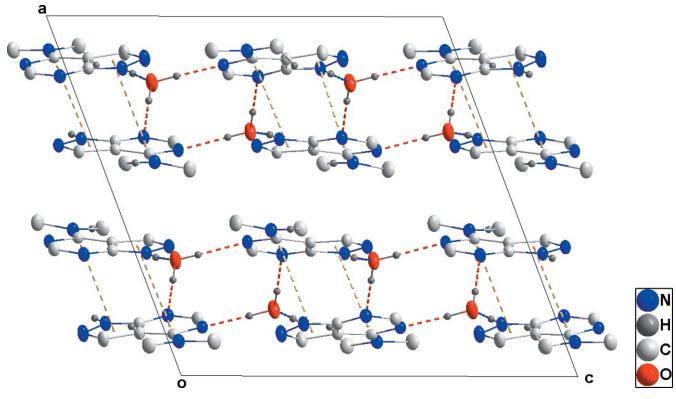


Figure 3
View of the layer structure projected along the *b*-axis direction. Intermolecular interactions are depicted as in Fig. 2.

The solution was filtered and the solvent removed under reduced pressure. The resulting residue was purified by column chromatography (EtOAc/hexane 8/2). The title compound was recrystallized from ethanol solution, at room temperature, giving colorless crystals (yield: 40%; m.p. 371–373 K).

Refinement

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

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180243 [https://doi.org/10.1107/S2414314618002432]

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Crystal data

$C_7H_9N_5·H_2O$
M_r = 181.21
Monoclinic, $P2_1/c$
a = 14.5177 (5) Å
b = 8.3622 (3) Å
c = 14.9892 (6) Å
β = 110.724 (2)°
V = 1701.95 (11) Å^3
Z = 8
$F(000)$ = 768
D_x = 1.414 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8628 reflections
θ = 6.0–72.4°
μ = 0.85 mm^{-1}
T = 150 K
Plate, colourless
0.13 × 0.12 × 0.09 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.75, T_{max} = 0.93
12386 measured reflections
3309 independent reflections
2718 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 72.4°, θ_{min} = 3.3°
h = −17→16
k = −10→10
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.04
3309 reflections
312 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
$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 0.6351P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Special details

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. Independent refinement of the H-atoms of the C13 methyl group gave an unacceptible geometry so these were included as riding contributions in calculated positions.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.35991 (10)	−0.08305 (16)	0.59163 (10)	0.0250 (3)
N2	0.34162 (10)	−0.20751 (15)	0.52829 (9)	0.0221 (3)
H2	0.3287 (17)	−0.309 (3)	0.5484 (16)	0.045 (6)*
N3	0.33702 (10)	−0.25750 (15)	0.36887 (9)	0.0236 (3)
N4	0.37264 (10)	−0.02269 (15)	0.29363 (9)	0.0220 (3)
N5	0.40567 (10)	0.22662 (15)	0.36469 (9)	0.0232 (3)
C1	0.38315 (11)	0.07230 (17)	0.36999 (11)	0.0191 (3)
C2	0.37115 (11)	0.00241 (17)	0.45202 (11)	0.0190 (3)
C3	0.37741 (12)	0.04219 (18)	0.54641 (11)	0.0223 (3)
H3	0.3931 (14)	0.145 (2)	0.5792 (14)	0.029 (5)*
C4	0.34815 (11)	−0.16102 (17)	0.44479 (11)	0.0194 (3)
C5	0.35117 (12)	−0.17807 (17)	0.29836 (11)	0.0231 (3)
H5	0.3459 (14)	−0.246 (2)	0.2426 (14)	0.028 (5)*
N6	0.11735 (12)	1.09738 (17)	0.29206 (10)	0.0315 (3)
C6	0.40961 (14)	0.33787 (18)	0.44047 (13)	0.0270 (4)
H6A	0.4672 (17)	0.321 (3)	0.4968 (16)	0.040 (6)*
H6B	0.3490 (16)	0.327 (2)	0.4575 (15)	0.034 (5)*
H6C	0.4086 (16)	0.446 (3)	0.4144 (15)	0.041 (6)*
C7	0.42515 (15)	0.2901 (2)	0.28240 (13)	0.0313 (4)
H7A	0.364 (2)	0.329 (3)	0.233 (2)	0.067 (8)*
H7B	0.4553 (16)	0.205 (3)	0.2542 (15)	0.045 (6)*
H7C	0.470 (2)	0.378 (3)	0.3036 (19)	0.063 (7)*
N7	0.14486 (10)	1.21815 (16)	0.35787 (10)	0.0257 (3)
H7	0.1599 (15)	1.323 (3)	0.3362 (15)	0.037 (5)*
N8	0.16768 (10)	1.26041 (15)	0.52296 (10)	0.0237 (3)
N9	0.13523 (9)	1.02412 (15)	0.59898 (9)	0.0214 (3)
N10	0.09608 (10)	0.77770 (15)	0.52618 (10)	0.0239 (3)
C8	0.11589 (11)	0.93300 (17)	0.51981 (11)	0.0195 (3)
C9	0.11820 (11)	1.00684 (17)	0.43506 (11)	0.0213 (3)
C10	0.10148 (13)	0.9713 (2)	0.33780 (12)	0.0285 (4)
H10	0.0784 (16)	0.867 (3)	0.3032 (16)	0.041 (6)*
C11	0.14572 (11)	1.16857 (17)	0.44357 (11)	0.0208 (3)
C13	0.09545 (14)	0.7092 (2)	0.61547 (12)	0.0305 (4)
H13A	0.163244	0.687890	0.657711	0.046*
H13B	0.058005	0.609046	0.602261	0.046*
H13C	0.064677	0.784759	0.646418	0.046*
C14	0.08358 (14)	0.66887 (19)	0.44671 (13)	0.0288 (4)
H14A	0.0172 (17)	0.687 (3)	0.3924 (16)	0.043 (6)*

H14B	0.0928 (19)	0.560 (3)	0.4751 (18)	0.057 (7)*
H14C	0.1366 (17)	0.686 (3)	0.4205 (16)	0.046 (6)*
C12	0.15937 (12)	1.17870 (18)	0.59506 (11)	0.0223 (3)
H12	0.1724 (14)	1.233 (2)	0.6551 (14)	0.029 (5)*
O1	0.32101 (10)	0.49247 (14)	0.59478 (9)	0.0319 (3)
H1A	0.267 (2)	0.425 (3)	0.5696 (19)	0.063 (8)*
H1B	0.338 (2)	0.489 (3)	0.657 (2)	0.062 (8)*
O2	0.18478 (11)	0.50803 (14)	0.29669 (9)	0.0338 (3)
H2A	0.1662 (19)	0.516 (3)	0.228 (2)	0.059 (7)*
H2B	0.236 (2)	0.574 (3)	0.3215 (18)	0.057 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0310 (7)	0.0254 (7)	0.0194 (7)	0.0000 (5)	0.0098 (6)	−0.0008 (5)
N2	0.0284 (7)	0.0194 (6)	0.0187 (7)	−0.0009 (5)	0.0088 (6)	0.0015 (5)
N3	0.0334 (7)	0.0168 (6)	0.0204 (7)	−0.0023 (5)	0.0093 (6)	−0.0006 (5)
N4	0.0296 (7)	0.0188 (6)	0.0186 (6)	−0.0012 (5)	0.0097 (6)	−0.0003 (5)
N5	0.0310 (7)	0.0161 (6)	0.0233 (7)	−0.0029 (5)	0.0108 (6)	0.0002 (5)
C1	0.0207 (7)	0.0168 (7)	0.0195 (7)	−0.0003 (5)	0.0067 (6)	0.0003 (5)
C2	0.0208 (7)	0.0173 (7)	0.0184 (7)	0.0007 (5)	0.0062 (6)	0.0004 (5)
C3	0.0273 (8)	0.0213 (7)	0.0194 (8)	−0.0005 (6)	0.0095 (7)	−0.0018 (6)
C4	0.0219 (7)	0.0181 (7)	0.0175 (7)	0.0010 (5)	0.0062 (6)	0.0010 (5)
C5	0.0309 (8)	0.0175 (7)	0.0205 (8)	0.0000 (6)	0.0087 (7)	−0.0015 (6)
N6	0.0455 (9)	0.0294 (7)	0.0202 (7)	−0.0070 (6)	0.0122 (7)	−0.0020 (6)
C6	0.0364 (9)	0.0154 (7)	0.0269 (9)	−0.0009 (6)	0.0083 (8)	−0.0027 (6)
C7	0.0436 (10)	0.0242 (8)	0.0286 (9)	−0.0067 (7)	0.0159 (8)	0.0041 (7)
N7	0.0354 (8)	0.0226 (7)	0.0191 (7)	−0.0040 (5)	0.0095 (6)	0.0016 (5)
N8	0.0300 (7)	0.0181 (6)	0.0229 (7)	−0.0015 (5)	0.0094 (6)	−0.0006 (5)
N9	0.0249 (7)	0.0196 (6)	0.0202 (7)	0.0000 (5)	0.0087 (5)	0.0004 (5)
N10	0.0318 (7)	0.0168 (6)	0.0225 (7)	−0.0037 (5)	0.0090 (6)	0.0000 (5)
C8	0.0187 (7)	0.0172 (7)	0.0223 (8)	0.0004 (5)	0.0068 (6)	0.0011 (6)
C9	0.0250 (8)	0.0195 (7)	0.0199 (8)	−0.0016 (6)	0.0088 (6)	0.0006 (6)
C10	0.0390 (9)	0.0266 (8)	0.0205 (8)	−0.0062 (7)	0.0114 (7)	−0.0033 (6)
C11	0.0230 (8)	0.0201 (7)	0.0194 (8)	−0.0003 (6)	0.0075 (6)	0.0014 (6)
C13	0.0404 (10)	0.0238 (8)	0.0270 (9)	−0.0053 (7)	0.0114 (8)	0.0058 (6)
C14	0.0386 (10)	0.0184 (8)	0.0290 (9)	−0.0030 (6)	0.0114 (8)	−0.0042 (6)
C12	0.0271 (8)	0.0198 (7)	0.0203 (8)	0.0001 (6)	0.0085 (7)	−0.0024 (6)
O1	0.0510 (8)	0.0243 (6)	0.0212 (6)	−0.0113 (5)	0.0138 (6)	−0.0012 (5)
O2	0.0526 (8)	0.0265 (6)	0.0217 (6)	−0.0145 (5)	0.0124 (6)	−0.0012 (5)

Geometric parameters (Å, º)

N1—C3	1.320 (2)	N7—C11	1.3456 (19)
N1—N2	1.3699 (18)	N7—H7	0.98 (2)
N2—C4	1.3456 (19)	N8—C12	1.320 (2)
N2—H2	0.94 (2)	N8—C11	1.3561 (19)
N3—C5	1.325 (2)	N9—C12	1.3460 (19)

N3—C4	1.3572 (19)	N9—C8	1.3534 (19)
N4—C5	1.3439 (19)	N10—C8	1.3408 (19)
N4—C1	1.3567 (19)	N10—C14	1.458 (2)
N5—C1	1.3404 (19)	N10—C13	1.459 (2)
N5—C6	1.454 (2)	C8—C9	1.424 (2)
N5—C7	1.459 (2)	C9—C11	1.403 (2)
C1—C2	1.427 (2)	C9—C10	1.422 (2)
C2—C4	1.402 (2)	C10—H10	1.01 (2)
C2—C3	1.425 (2)	C13—H13A	0.9800
C3—H3	0.98 (2)	C13—H13B	0.9800
C5—H5	0.99 (2)	C13—H13C	0.9800
N6—C10	1.321 (2)	C14—H14A	1.03 (2)
N6—N7	1.3687 (19)	C14—H14B	0.99 (3)
C6—H6A	0.97 (2)	C14—H14C	0.99 (2)
C6—H6B	1.00 (2)	C12—H12	0.97 (2)
C6—H6C	0.98 (2)	O1—H1A	0.93 (3)
C7—H7A	0.99 (3)	O1—H1B	0.88 (3)
C7—H7B	1.00 (2)	O2—H2A	0.97 (3)
C7—H7C	0.96 (3)	O2—H2B	0.89 (3)

C3—N1—N2	105.79 (13)	C11—N7—N6	111.25 (13)
C4—N2—N1	111.41 (12)	C11—N7—H7	131.4 (12)
C4—N2—H2	130.3 (14)	N6—N7—H7	117.4 (12)
N1—N2—H2	118.2 (14)	C12—N8—C11	111.35 (13)
C5—N3—C4	111.41 (12)	C12—N9—C8	118.61 (13)
C5—N4—C1	118.72 (13)	C8—N10—C14	120.94 (14)
C1—N5—C6	120.85 (13)	C8—N10—C13	121.10 (13)
C1—N5—C7	121.62 (13)	C14—N10—C13	117.72 (13)
C6—N5—C7	117.52 (13)	N10—C8—N9	117.78 (14)
N5—C1—N4	118.07 (13)	N10—C8—C9	123.85 (14)
N5—C1—C2	123.52 (14)	N9—C8—C9	118.37 (13)
N4—C1—C2	118.40 (13)	C11—C9—C10	103.55 (13)
C4—C2—C3	103.54 (13)	C11—C9—C8	115.65 (13)
C4—C2—C1	115.54 (13)	C10—C9—C8	140.79 (14)
C3—C2—C1	140.89 (14)	N6—C10—C9	111.55 (14)
N1—C3—C2	111.62 (13)	N6—C10—H10	120.8 (13)
N1—C3—H3	119.6 (11)	C9—C10—H10	127.7 (13)
C2—C3—H3	128.8 (11)	N7—C11—N8	125.67 (14)
N2—C4—N3	125.56 (13)	N7—C11—C9	107.70 (13)
N2—C4—C2	107.64 (13)	N8—C11—C9	126.62 (14)
N3—C4—C2	126.78 (14)	N10—C13—H13A	109.5
N3—C5—N4	129.15 (14)	N10—C13—H13B	109.5
N3—C5—H5	113.6 (11)	H13A—C13—H13B	109.5
N4—C5—H5	117.3 (11)	N10—C13—H13C	109.5
C10—N6—N7	105.95 (13)	H13A—C13—H13C	109.5
N5—C6—H6A	112.0 (13)	H13B—C13—H13C	109.5
N5—C6—H6B	110.4 (12)	N10—C14—H14A	111.6 (13)
H6A—C6—H6B	109.4 (17)	N10—C14—H14B	105.2 (14)

N5—C6—H6C	106.6 (13)	H14A—C14—H14B	114.7 (19)
H6A—C6—H6C	111.5 (18)	N10—C14—H14C	110.0 (13)
H6B—C6—H6C	106.9 (17)	H14A—C14—H14C	107.8 (18)
N5—C7—H7A	111.4 (16)	H14B—C14—H14C	107.3 (19)
N5—C7—H7B	110.2 (13)	N8—C12—N9	129.32 (14)
H7A—C7—H7B	109 (2)	N8—C12—H12	118.4 (11)
N5—C7—H7C	108.1 (16)	N9—C12—H12	112.3 (11)
H7A—C7—H7C	108 (2)	H1A—O1—H1B	107 (2)
H7B—C7—H7C	110 (2)	H2A—O2—H2B	106 (2)

C3—N1—N2—C4	0.35 (17)	C10—N6—N7—C11	−0.31 (19)
C6—N5—C1—N4	174.64 (14)	C14—N10—C8—N9	−174.25 (14)
C7—N5—C1—N4	−4.1 (2)	C13—N10—C8—N9	0.0 (2)
C6—N5—C1—C2	−6.3 (2)	C14—N10—C8—C9	5.4 (2)
C7—N5—C1—C2	174.90 (15)	C13—N10—C8—C9	179.64 (15)
C5—N4—C1—N5	179.26 (14)	C12—N9—C8—N10	177.22 (14)
C5—N4—C1—C2	0.2 (2)	C12—N9—C8—C9	−2.5 (2)
N5—C1—C2—C4	−179.67 (14)	N10—C8—C9—C11	−176.56 (14)
N4—C1—C2—C4	−0.6 (2)	N9—C8—C9—C11	3.1 (2)
N5—C1—C2—C3	−2.2 (3)	N10—C8—C9—C10	3.1 (3)
N4—C1—C2—C3	176.83 (18)	N9—C8—C9—C10	−177.20 (19)
N2—N1—C3—C2	−0.11 (18)	N7—N6—C10—C9	0.1 (2)
C4—C2—C3—N1	−0.15 (17)	C11—C9—C10—N6	0.2 (2)
C1—C2—C3—N1	−177.81 (18)	C8—C9—C10—N6	−179.54 (19)
N1—N2—C4—N3	177.86 (14)	N6—N7—C11—N8	−178.51 (15)
N1—N2—C4—C2	−0.45 (17)	N6—N7—C11—C9	0.43 (18)
C5—N3—C4—N2	−177.72 (15)	C12—N8—C11—N7	178.17 (15)
C5—N3—C4—C2	0.3 (2)	C12—N8—C11—C9	−0.6 (2)
C3—C2—C4—N2	0.35 (16)	C10—C9—C11—N7	−0.35 (17)
C1—C2—C4—N2	178.72 (13)	C8—C9—C11—N7	179.44 (13)
C3—C2—C4—N3	−177.93 (15)	C10—C9—C11—N8	178.57 (15)
C1—C2—C4—N3	0.4 (2)	C8—C9—C11—N8	−1.6 (2)
C4—N3—C5—N4	−0.9 (2)	C11—N8—C12—N9	1.5 (2)
C1—N4—C5—N3	0.7 (3)	C8—N9—C12—N8	0.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.94 (2)	1.82 (2)	2.7546 (18)	173 (2)
N7—H7···O2^{ii}	0.99 (2)	1.74 (2)	2.7256 (19)	179 (3)
O1—H1*A*···N8^{i}	0.93 (3)	1.94 (3)	2.8607 (19)	172 (2)
O1—H1*B*···N4^{iii}	0.88 (3)	1.95 (3)	2.8158 (18)	170 (2)
O2—H2*A*···N9^{iv}	0.97 (3)	1.86 (3)	2.8042 (18)	166 (2)
O2—H2*B*···N3^{ii}	0.89 (3)	1.98 (3)	2.865 (2)	173 (2)

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