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2,6-Bis(4*H*-1,2,4-triazol-4-yl)pyridine dihydrate

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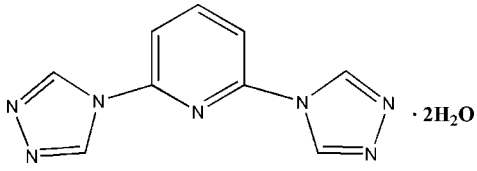
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.094; data-to-parameter ratio = 6.4.

In the asymmetric unit of the title compound, $C_9H_7N_7\cdot 2H_2O$, there are two formula units in which the two triazole rings of each of the organic component molecules form dihedral angles of 7.0 (4)/6.9 (4) and 2.7 (4)/3.6 (4)° with the respective central pyridine rings. The four water molecules of solvation form O—H···O hydrogen bonds among themselves and O—H···N bonds with the N-atom acceptors of the triazine rings, giving a three-dimensional framework structure.

Related literature

For the synthesis of the title compound, see: Wiley & Hart (1953). For properties of related compounds, see: Haasnoot (2000).



Experimental

Crystal data

$C_9H_7N_7\cdot 2H_2O$
M_r = 249.25
Monoclinic, $P2_1$
a = 7.052 (8) Å
b = 17.862 (16) Å
c = 9.715 (8) Å
β = 111.158 (9)°
V = 1141.2 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.30 × 0.29 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.635, T_{max} = 1.000
6610 measured reflections
2096 independent reflections
1789 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.19
2096 reflections
325 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1^{i}	0.85	1.98	2.814 (5)	165
O1—H1B···N7^{ii}	0.85	2.07	2.904 (5)	168
O2—H2A···O4	0.85	1.87	2.709 (5)	169
O2—H2B···O1	0.85	2.00	2.850 (6)	174
O3—H3A···O1^{iii}	0.85	2.05	2.888 (5)	169
O3—H3B···O2	0.85	2.07	2.916 (6)	170
O4—H4A···N13^{iv}	0.85	1.98	2.822 (5)	170
O4—H4B···N8^{v}	0.85	2.06	2.873 (5)	159

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2114).

References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wiley, R. H. & Hart, A. J. (1953). *J. Org. Chem.* **18**, 1368–1371.

supporting information

Acta Cryst. (2011). E**67**, o1631 [doi:10.1107/S1600536811022215]

2,6-Bis(4*H*-1,2,4-triazol-4-yl)pyridine dihydrate

Shang Yuan Liu and Ying Wang

S1. Comment

The field of molecular materials has known rapid development in recent years, with molecular-based compounds which exhibit interesting magnetic and luminescent properties having been described (Haasnoot, 2000). One of the requirements for producing such macroscopic properties is to create interactions between the molecular units and the active sites within the crystal lattices. 1,2,4-Triazole and in particular its derivatives are very interesting as bridging ligands. Here we report the synthesis and the crystal structure of the title compound, the dihydrate of 2,6-di(4*H*-1,2,4-triazol-4-yl)pyridine, $C_9H_7N_7$. $2(H_2O)$ (I).

In the asymmetric unit of (I) there are two molecular units (Fig. 1) in which the two triazole rings of each of the organic component molecules form dihedral angles of 7.0, 6.9 (4)° and 2.7, 3.6 (4)° with the respective pyridine rings. The four water molecules of solvation form hydrogen bonds with the N atom acceptors only of the triazine rings (Table 1) giving a three-dimensional framework structure (Fig. 2).

S2. Experimental

A mixture of 1.3 g (0.012 mol) of 2,6-diaminopyridine and 2.0 g (0.023 mol) of diformylhydrazine was heated slowly to 160°C and held at 160-170°C for 30 min. The crystals, which separated on cooling, were collected and recrystallized from water to give 0.70 g of (I) (yield 13%). After several recrystallizations from water and from alcohol, the air-dried product was obtained as white needles, m.p. 325-327 K (placed in hot block at 320 K). The analysis was obtained on the air-dried sample. Anal. Calcd for $C_9H11_{11}N_7O_2$: C, 46.75; H, 3.92%. Found: C, 46.55; H, 3.96%.

S3. Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C or O atoms with C—H = 0.93 Å and O—H = 0.85 Å and U_{iso}H = 1.2 or 1.5U_{eq}(C or O). Friedel pairs were averaged for the data used in the final cycles of the refinement.

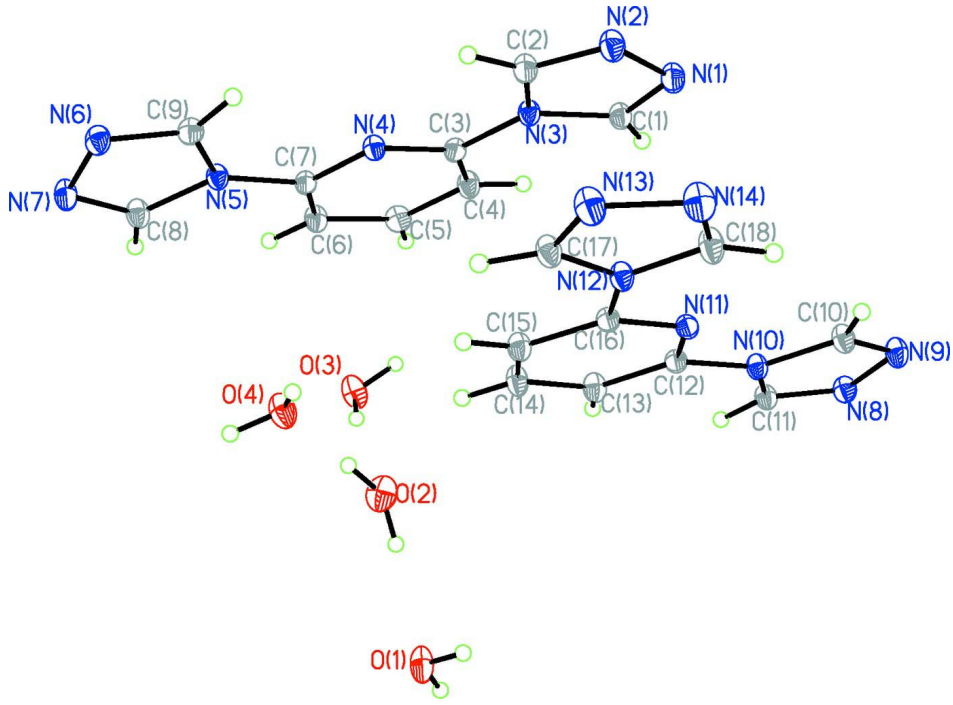

Figure 1

Molecular conformation and atom numbering scheme for the two independent molecules of $C_9H_7N_7$ and the four water molecules of solvation in the asymmetric unit of (I). Probability spheres are drawn at the 15% level.

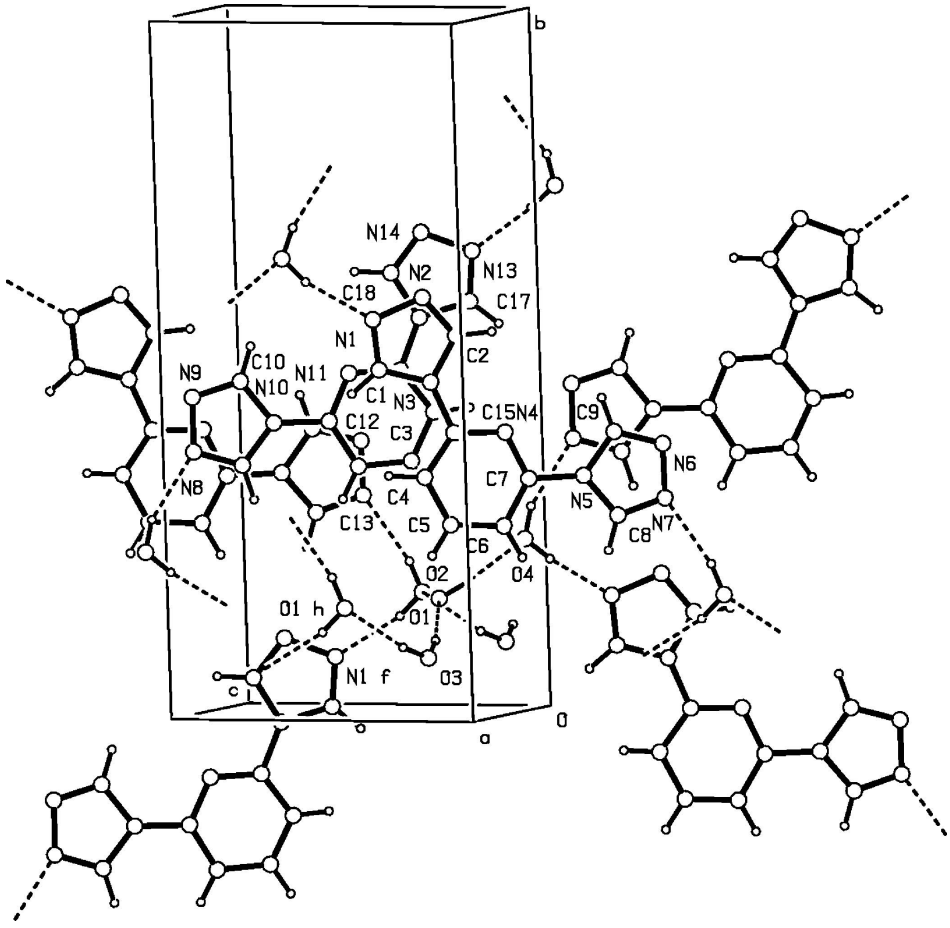

Figure 2

The packing of (I) in the unit cell showing hydrogen-bonding interactions.

2,6-Bis(4*H*-1,2,4-triazol-4-yl)pyridine dihydrate

Crystal data

$C_9H_7N_7·2H_2O$
M_r = 249.25
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 7.052 (8) Å
b = 17.862 (16) Å
c = 9.715 (8) Å
β = 111.158 (9)°
V = 1141.2 (19) Å^3
Z = 4
$F(000)$ = 520
D_x = 1.451 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1604 reflections
θ = 2.3–23.1°
μ = 0.11 mm^{-1}
T = 293 K
Block, colorless
0.30 × 0.29 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.635, T_{max} = 1.000
6610 measured reflections
2096 independent reflections
1789 reflections with $I > 2\sigma(I)$

R_{int} = 0.028
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −7→8
k = −20→21
l = −11→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.19
2096 reflections
325 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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	0.8333 (4)	0.57130 (16)	0.3342 (3)	0.0478 (9)
N2	0.7010 (5)	0.60054 (15)	0.2019 (3)	0.0486 (9)
N3	0.7201 (4)	0.47959 (13)	0.1779 (2)	0.0362 (8)
N4	0.5316 (4)	0.40426 (13)	−0.0145 (2)	0.0346 (8)
N5	0.3281 (4)	0.33831 (14)	−0.2179 (2)	0.0361 (7)
N6	0.1060 (4)	0.37967 (15)	−0.4259 (3)	0.0441 (9)
N7	0.0990 (4)	0.30183 (16)	−0.4263 (3)	0.0481 (9)
C1	0.8413 (5)	0.49967 (18)	0.3165 (3)	0.0397 (10)
C2	0.6375 (5)	0.54465 (17)	0.1118 (3)	0.0438 (10)
C3	0.6778 (4)	0.40638 (17)	0.1168 (3)	0.0349 (9)
C4	0.7786 (5)	0.34433 (19)	0.1922 (3)	0.0439 (10)
C5	0.7209 (5)	0.27547 (18)	0.1262 (3)	0.0454 (11)
C6	0.5697 (5)	0.27085 (18)	−0.0111 (3)	0.0426 (10)
C7	0.4817 (4)	0.33686 (17)	−0.0757 (3)	0.0342 (9)
C8	0.2312 (5)	0.27945 (18)	−0.3025 (3)	0.0448 (11)
C9	0.2422 (5)	0.39963 (17)	−0.3011 (3)	0.0400 (10)
N8	0.9611 (4)	0.38269 (15)	0.9078 (3)	0.0438 (9)
N9	0.9503 (4)	0.46049 (16)	0.9104 (3)	0.0476 (10)
N10	0.7369 (4)	0.41986 (14)	0.6977 (2)	0.0359 (7)
N11	0.5207 (4)	0.48637 (13)	0.5001 (3)	0.0349 (8)
N12	0.3162 (4)	0.56230 (14)	0.3130 (2)	0.0373 (8)
N13	0.1657 (5)	0.65496 (17)	0.1704 (3)	0.0554 (10)

N14	0.2856 (5)	0.68389 (16)	0.3071 (3)	0.0569 (10)
C10	0.8165 (5)	0.48092 (18)	0.7842 (3)	0.0451 (11)
C11	0.8331 (5)	0.36112 (17)	0.7816 (3)	0.0399 (10)
C12	0.5915 (4)	0.41913 (18)	0.5521 (3)	0.0343 (9)
C13	0.5325 (5)	0.35351 (17)	0.4748 (3)	0.0436 (11)
C14	0.3899 (5)	0.35832 (18)	0.3354 (3)	0.0477 (11)
C15	0.3103 (5)	0.42704 (18)	0.2768 (3)	0.0426 (10)
C16	0.3835 (4)	0.48866 (17)	0.3647 (3)	0.0339 (9)
C17	0.1877 (5)	0.58319 (18)	0.1776 (3)	0.0450 (11)
C18	0.3716 (5)	0.62737 (18)	0.3880 (3)	0.0507 (11)
O1	0.0057 (4)	0.16140 (14)	0.4125 (2)	0.0636 (9)
O2	0.3057 (5)	0.15947 (15)	0.2795 (3)	0.0725 (10)
O3	0.6429 (5)	0.08242 (16)	0.2340 (3)	0.0749 (10)
O4	0.1440 (4)	0.24252 (14)	0.0311 (2)	0.0625 (8)
H1	0.91930	0.46660	0.38870	0.0480*
H2	0.54740	0.54870	0.01480	0.0530*
H4	0.88170	0.34870	0.28420	0.0530*
H5	0.78400	0.23220	0.17450	0.0540*
H6	0.52900	0.22510	−0.05800	0.0510*
H8	0.25680	0.22950	−0.27490	0.0530*
H9	0.27680	0.44890	−0.27220	0.0480*
H10	0.78000	0.53030	0.75650	0.0540*
H11	0.81000	0.31140	0.75220	0.0480*
H13	0.58720	0.30770	0.51560	0.0520*
H14	0.34610	0.31510	0.27950	0.0570*
H15	0.21210	0.43130	0.18270	0.0510*
H17	0.12400	0.55040	0.10040	0.0540*
H18	0.46030	0.63090	0.48550	0.0610*
H1A	0.04450	0.12750	0.47830	0.0760*
H1B	0.02170	0.20560	0.44750	0.0760*
H2A	0.26290	0.18190	0.19670	0.0870*
H2B	0.22270	0.15830	0.32480	0.0870*
H3A	0.75790	0.10000	0.28750	0.0900*
H3B	0.53790	0.10490	0.23620	0.0900*
H4A	0.06240	0.21210	−0.02880	0.0750*
H4B	0.11000	0.28830	0.01600	0.0750*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0556 (17)	0.0435 (18)	0.0387 (14)	−0.0044 (14)	0.0102 (13)	−0.0062 (12)
N2	0.0578 (18)	0.0382 (16)	0.0420 (15)	−0.0014 (13)	0.0087 (13)	−0.0034 (12)
N3	0.0405 (14)	0.0313 (14)	0.0313 (12)	0.0007 (11)	0.0065 (11)	0.0000 (10)
N4	0.0365 (13)	0.0302 (15)	0.0320 (13)	0.0022 (10)	0.0061 (10)	0.0011 (10)
N5	0.0399 (13)	0.0300 (13)	0.0325 (12)	0.0003 (12)	0.0058 (10)	−0.0001 (11)
N6	0.0450 (15)	0.0418 (18)	0.0363 (15)	0.0030 (13)	0.0037 (13)	0.0064 (11)
N7	0.0549 (17)	0.0401 (18)	0.0361 (14)	−0.0026 (13)	0.0007 (13)	−0.0027 (11)
C1	0.0438 (17)	0.0359 (19)	0.0329 (16)	−0.0033 (15)	0.0060 (14)	−0.0015 (13)

C2	0.0513 (18)	0.0361 (19)	0.0365 (16)	−0.0009 (16)	0.0069 (14)	−0.0024 (14)
C3	0.0423 (17)	0.0285 (17)	0.0321 (15)	0.0009 (13)	0.0113 (13)	0.0007 (12)
C4	0.0451 (18)	0.0398 (18)	0.0367 (16)	0.0028 (15)	0.0026 (14)	0.0019 (14)
C5	0.0510 (19)	0.0327 (18)	0.0453 (18)	0.0074 (14)	0.0088 (15)	0.0118 (13)
C6	0.0530 (19)	0.0283 (17)	0.0399 (17)	0.0025 (14)	0.0090 (15)	0.0006 (12)
C7	0.0378 (16)	0.0309 (16)	0.0306 (14)	−0.0009 (14)	0.0085 (12)	0.0004 (13)
C8	0.053 (2)	0.0309 (18)	0.0411 (19)	−0.0016 (14)	0.0058 (16)	−0.0023 (13)
C9	0.0444 (17)	0.0328 (18)	0.0389 (17)	0.0037 (13)	0.0105 (14)	0.0047 (13)
N8	0.0491 (16)	0.0393 (17)	0.0369 (15)	0.0010 (12)	0.0082 (13)	0.0032 (11)
N9	0.0524 (17)	0.0416 (18)	0.0373 (15)	0.0004 (13)	0.0022 (13)	−0.0022 (12)
N10	0.0393 (13)	0.0306 (13)	0.0305 (12)	0.0007 (12)	0.0038 (10)	−0.0002 (11)
N11	0.0371 (14)	0.0328 (15)	0.0318 (12)	−0.0036 (11)	0.0088 (11)	−0.0003 (10)
N12	0.0427 (14)	0.0308 (15)	0.0307 (13)	0.0007 (11)	0.0039 (11)	0.0011 (10)
N13	0.0616 (18)	0.0407 (18)	0.0473 (16)	0.0017 (14)	−0.0004 (14)	0.0062 (12)
N14	0.070 (2)	0.0359 (16)	0.0506 (17)	0.0075 (14)	0.0045 (15)	0.0061 (13)
C10	0.051 (2)	0.0343 (19)	0.0425 (17)	−0.0004 (15)	0.0077 (16)	−0.0026 (14)
C11	0.0459 (17)	0.0308 (17)	0.0377 (16)	−0.0008 (13)	0.0087 (14)	0.0012 (12)
C12	0.0378 (15)	0.0316 (16)	0.0316 (14)	−0.0007 (13)	0.0102 (12)	0.0014 (13)
C13	0.054 (2)	0.0283 (18)	0.0412 (17)	0.0043 (14)	0.0083 (15)	−0.0008 (13)
C14	0.058 (2)	0.035 (2)	0.0407 (17)	−0.0034 (15)	0.0066 (16)	−0.0083 (14)
C15	0.0457 (18)	0.0387 (18)	0.0355 (15)	−0.0011 (15)	0.0050 (14)	−0.0013 (14)
C16	0.0363 (16)	0.0315 (17)	0.0316 (14)	−0.0002 (13)	0.0096 (13)	0.0021 (12)
C17	0.050 (2)	0.0362 (19)	0.0370 (17)	−0.0035 (15)	0.0014 (14)	0.0027 (14)
C18	0.064 (2)	0.0342 (19)	0.0401 (16)	0.0020 (17)	0.0021 (15)	−0.0022 (14)
O1	0.0880 (18)	0.0428 (14)	0.0407 (12)	−0.0062 (13)	0.0001 (12)	−0.0008 (10)
O2	0.0855 (19)	0.0621 (18)	0.0589 (15)	0.0193 (15)	0.0128 (14)	0.0157 (13)
O3	0.0718 (18)	0.0639 (17)	0.0754 (18)	−0.0105 (14)	0.0103 (14)	−0.0183 (14)
O4	0.0628 (15)	0.0468 (15)	0.0571 (13)	−0.0005 (12)	−0.0034 (12)	0.0059 (11)

Geometric parameters (Å, º)

O1—H1A	0.8500	N11—C12	1.329 (4)
O1—H1B	0.8500	N12—C18	1.352 (4)
O2—H2B	0.8500	N12—C16	1.427 (4)
O2—H2A	0.8500	N12—C17	1.353 (4)
O3—H3A	0.8500	N13—C17	1.290 (5)
O3—H3B	0.8500	N13—N14	1.391 (4)
N1—N2	1.389 (4)	N14—C18	1.289 (4)
N1—C1	1.295 (5)	C3—C4	1.376 (5)
N2—C2	1.296 (4)	C4—C5	1.379 (5)
N3—C1	1.357 (4)	C5—C6	1.377 (4)
N3—C3	1.423 (4)	C6—C7	1.374 (5)
N3—C2	1.354 (4)	C1—H1	0.9300
N4—C3	1.320 (4)	C2—H2	0.9300
N4—C7	1.333 (4)	C4—H4	0.9300
N5—C9	1.366 (4)	C5—H5	0.9300
N5—C8	1.357 (4)	C6—H6	0.9300
N5—C7	1.415 (4)	C8—H8	0.9300

N6—N7	1.391 (4)	C9—H9	0.9300
N6—C9	1.296 (4)	C12—C13	1.373 (5)
N7—C8	1.291 (4)	C13—C14	1.367 (4)
O4—H4A	0.8500	C14—C15	1.384 (5)
O4—H4B	0.8500	C15—C16	1.374 (5)
N8—C11	1.291 (4)	C10—H10	0.9300
N8—N9	1.393 (4)	C11—H11	0.9300
N9—C10	1.301 (4)	C13—H13	0.9300
N10—C12	1.416 (4)	C14—H14	0.9300
N10—C10	1.368 (4)	C15—H15	0.9300
N10—C11	1.351 (4)	C17—H17	0.9300
N11—C16	1.323 (4)	C18—H18	0.9300

H1A—O1—H1B	114.00	N3—C1—H1	125.00
H2A—O2—H2B	115.00	N2—C2—H2	125.00
H3A—O3—H3B	117.00	N3—C2—H2	125.00
N2—N1—C1	107.2 (3)	C3—C4—H4	121.00
N1—N2—C2	106.8 (3)	C5—C4—H4	121.00
C1—N3—C2	104.7 (2)	C4—C5—H5	120.00
C1—N3—C3	128.3 (2)	C6—C5—H5	120.00
C2—N3—C3	127.0 (2)	C5—C6—H6	121.00
C3—N4—C7	116.5 (2)	C7—C6—H6	121.00
C8—N5—C9	104.1 (2)	N5—C8—H8	124.00
C7—N5—C8	128.2 (3)	N7—C8—H8	124.00
C7—N5—C9	127.7 (3)	N6—C9—H9	125.00
N7—N6—C9	106.9 (3)	N5—C9—H9	125.00
N6—N7—C8	107.1 (3)	N9—C10—N10	110.7 (3)
H4A—O4—H4B	115.00	N8—C11—N10	111.6 (3)
N9—N8—C11	106.9 (3)	N10—C12—C13	121.4 (3)
N8—N9—C10	106.8 (3)	N11—C12—C13	124.5 (3)
C10—N10—C12	127.6 (3)	N10—C12—N11	114.1 (3)
C10—N10—C11	104.1 (2)	C12—C13—C14	117.2 (3)
C11—N10—C12	128.3 (3)	C13—C14—C15	120.5 (3)
C12—N11—C16	116.5 (3)	C14—C15—C16	116.7 (3)
C17—N12—C18	104.4 (2)	N11—C16—C15	124.7 (3)
C16—N12—C17	128.1 (2)	N12—C16—C15	121.1 (2)
C16—N12—C18	127.4 (2)	N11—C16—N12	114.2 (2)
N14—N13—C17	107.3 (3)	N12—C17—N13	110.6 (3)
N13—N14—C18	106.3 (3)	N12—C18—N14	111.3 (3)
N1—C1—N3	110.5 (3)	N10—C10—H10	125.00
N2—C2—N3	110.9 (3)	N9—C10—H10	125.00
N3—C3—C4	121.9 (3)	N10—C11—H11	124.00
N4—C3—C4	124.4 (3)	N8—C11—H11	124.00
N3—C3—N4	113.7 (2)	C14—C13—H13	121.00
C3—C4—C5	117.5 (3)	C12—C13—H13	121.00
C4—C5—C6	120.0 (3)	C13—C14—H14	120.00
C5—C6—C7	117.1 (3)	C15—C14—H14	120.00
N4—C7—N5	113.9 (2)	C14—C15—H15	122.00

N5—C7—C6	121.5 (3)	C16—C15—H15	122.00
N4—C7—C6	124.6 (3)	N13—C17—H17	125.00
N5—C8—N7	111.2 (3)	N12—C17—H17	125.00
N5—C9—N6	110.7 (3)	N12—C18—H18	124.00
N1—C1—H1	125.00	N14—C18—H18	124.00
C1—N1—N2—C2	−0.3 (4)	C12—N10—C10—N9	−178.3 (3)
N2—N1—C1—N3	0.0 (4)	C11—N10—C12—N11	178.5 (3)
N1—N2—C2—N3	0.4 (4)	C11—N10—C12—C13	−1.4 (5)
C2—N3—C1—N1	0.2 (4)	C10—N10—C12—N11	−3.5 (5)
C3—N3—C1—N1	−176.3 (3)	C10—N10—C12—C13	176.5 (3)
C1—N3—C2—N2	−0.3 (4)	C16—N11—C12—N10	−179.6 (3)
C3—N3—C2—N2	176.2 (3)	C12—N11—C16—C15	0.5 (5)
C1—N3—C3—N4	170.9 (3)	C16—N11—C12—C13	0.4 (5)
C1—N3—C3—C4	−7.3 (5)	C12—N11—C16—N12	−178.6 (3)
C2—N3—C3—N4	−4.9 (5)	C17—N12—C16—C15	−3.5 (5)
C2—N3—C3—C4	176.9 (3)	C18—N12—C16—N11	−2.4 (5)
C7—N4—C3—N3	−178.4 (3)	C18—N12—C16—C15	178.5 (3)
C7—N4—C3—C4	−0.2 (5)	C16—N12—C17—N13	−178.6 (3)
C3—N4—C7—N5	−178.4 (3)	C18—N12—C17—N13	−0.2 (4)
C3—N4—C7—C6	0.8 (5)	C16—N12—C18—N14	178.5 (3)
C8—N5—C7—N4	−173.2 (3)	C17—N12—C16—N11	175.6 (3)
C8—N5—C7—C6	7.6 (5)	C17—N12—C18—N14	0.1 (4)
C9—N5—C7—N4	6.3 (5)	C17—N13—N14—C18	−0.2 (4)
C9—N5—C7—C6	−172.9 (3)	N14—N13—C17—N12	0.3 (4)
C7—N5—C8—N7	179.9 (3)	N13—N14—C18—N12	0.1 (4)
C9—N5—C8—N7	0.3 (4)	N3—C3—C4—C5	177.4 (3)
C7—N5—C9—N6	−180.0 (3)	N4—C3—C4—C5	−0.7 (5)
C8—N5—C9—N6	−0.5 (4)	C3—C4—C5—C6	1.0 (5)
C9—N6—N7—C8	−0.2 (4)	C4—C5—C6—C7	−0.5 (5)
N7—N6—C9—N5	0.4 (4)	C5—C6—C7—N4	−0.4 (5)
N6—N7—C8—N5	−0.1 (4)	C5—C6—C7—N5	178.6 (3)
N9—N8—C11—N10	0.5 (4)	N10—C12—C13—C14	179.4 (3)
C11—N8—N9—C10	−0.5 (4)	N11—C12—C13—C14	−0.6 (5)
N8—N9—C10—N10	0.3 (4)	C12—C13—C14—C15	0.0 (5)
C11—N10—C10—N9	0.0 (4)	C13—C14—C15—C16	0.7 (5)
C10—N10—C11—N8	−0.3 (4)	C14—C15—C16—N11	−1.0 (5)
C12—N10—C11—N8	178.0 (3)	C14—C15—C16—N12	178.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N1^{i}	0.85	1.98	2.814 (5)	165
O1—H1*B*···N7^{ii}	0.85	2.07	2.904 (5)	168
O2—H2*A*···O4	0.85	1.87	2.709 (5)	169
O2—H2*B*···O1	0.85	2.00	2.850 (6)	174
O3—H3*A*···O1^{iii}	0.85	2.05	2.888 (5)	169
O3—H3*B*···O2	0.85	2.07	2.916 (6)	170

O4—H4*A*···N13^{iv}	0.85	1.98	2.822 (5)	170
O4—H4*B*···N8^{v}	0.85	2.06	2.873 (5)	159

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