IUCrData

(5Z,7Z)-N^5,N^7-Bis(pyridin-2-yl)-5H-6,7-dihydro-pyrrolo[3,4-b]pyrazine-5,7-diimine

Maciej Posel[a] and Helen Stoeckli-Evans[b]*

[a]Institute of Chemistry, University of Neuchâtel, Av de Bellevaux 51, CH-2000 Neuchâtel, Switzerland, and [b]Institute of Physics, University of Neuchâtel, rue Emile-Argand 11, CH-2000 Neuchâtel, Switzerland. *Correspondence e-mail: helen.stoeckli-evans@unine.ch

The whole molecule of the title compound, $C_{16}H_{11}N_7$, is relatively planar, with an r.m.s. deviation of 0.061 Å for all 23 heteroatoms. It exhibits symmetric three-centre (bifurcated) intramolecular hydrogen bonds. In the crystal, molecules are linked by C—H···N hydrogen bonds, forming 3_1 helices propagating along the c-axis direction. Within the helices, there is evidence of offset π–π stacking being present [intercentroid distances = 3.648 (6) and 3.832 (6) Å].

3D view

Chemical scheme
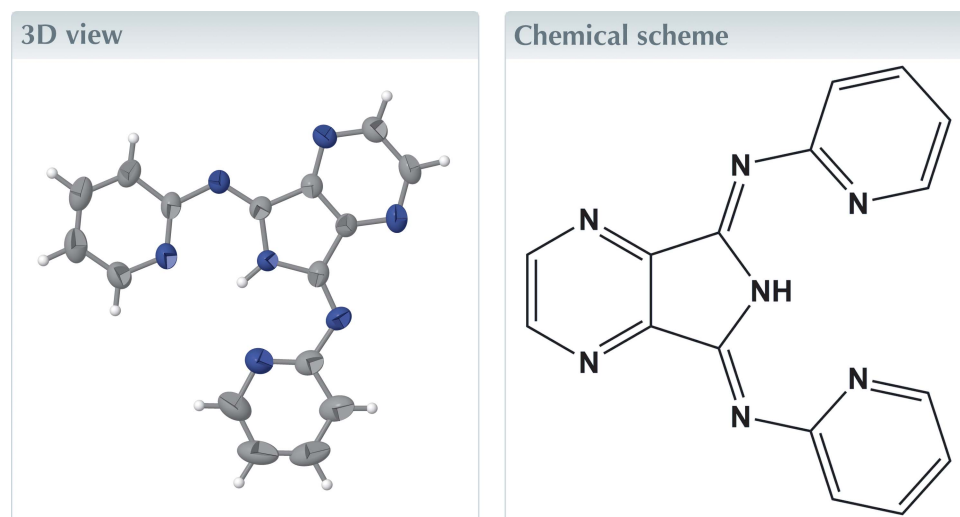
Structure description

Symmetrical isoindolines have been synthesized to study a number of properties, such as their birefringence (Wong et al., 2012). The isoindoline 1,3-bis(2-pyridylimino)isoindoline [systematic name: (1Z,3Z)-N^1,N^3-bis(pyridin-2-yl)isoindoline-1,3-diimine], possesses mirror symmetry and exhibits symmetric three-centre (bifurcated) intramolecular hydrogen bonds (Schilf, 2004). Such compounds are ideal tridentate ligands; for example, a series of six bis(pyridylimino)isoindolines with different substituents in the 4-position on the pyridine rings have been used to form homoleptic iron complexes for the study of their temperature-dependent spin and redox states (Scheja et al., 2015). The title compound, the pyrazine analogue of 1,3-bis(2-pyridylimino)isoindoline, was synthesized to study its coordination behaviour with transition metals (Posel, 1998).

The molecular structure of the title compound is illustrated in Fig. 1. The molecule is relatively planar (r.m.s. deviation of 0.061 Å for all 23 heteroatoms), with the two pyridine rings (N4/C6–C10) and (N7/C12–C16) being inclined to each other by 2.7 (5)° and to the central pyrrolopyrazine unit (N1/N2/N5/C1–C5/C11) by 4.0 (4) and 4.6 (4)°, respectively. As in 1,3-bis(2-pyridylimino)isoindoline (Schilf, 2004), the title compound exhibits three-centre (bifurcated) intramolecular hydrogen bonds (Fig. 1 and Table 1), and the configuration about the C=N bonds (C5=N3 and C11=N6) is Z.

In the crystal, molecules are linked by C—H···N hydrogen bonds, forming 3_1 helices propagating along the c-axis direction (Fig. 2 and Table 1). Within the helices there is
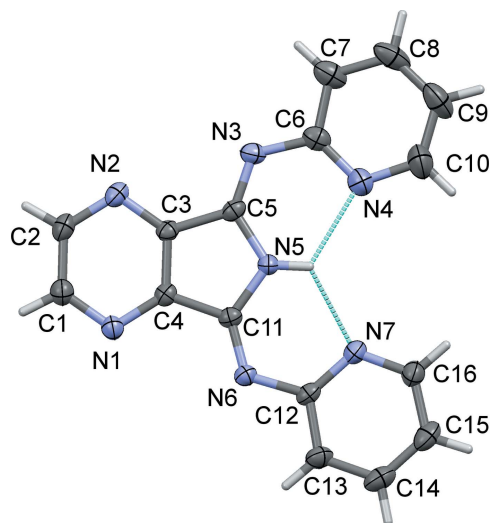
Figure 1
The molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 50% probability level. The intramolecular three-centre (bifurcated) N—H···N hydrogen bonds are shown as dashed lines (see Table 1).

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—H5N···N4	0.88 (6)	2.12 (7)	2.653 (11)	119 (5)
N5—H5N···N7	0.88 (6)	2.12 (6)	2.670 (8)	120 (5)
C2—H2···N2^i	0.93	2.62	3.395 (11)	141

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

Fig. 3. There is no evidence of any residual electron density being present in these cavities on examination of the final difference Fourier map (see Table 2).

Synthesis and crystallization

The title compound was synthesized by the reaction of pyrazine-2,3-dicarbonitrile with 2-aminopyridine.

Synthesis of pyrazine-2,3-dicarbonitrile (L). 12.5 ml of deionized water in a round-bottomed flask fitted with a reflux condenser was acidified with H_2SO_4 (tech.) to pH = 1, then with vigorous stirring 2.7 g (0.025 mol) of 2,3-diaminomaleo-nitrile were added. After it had dissolved (temp = 323 K), a suspension of 5.8 g (0.0 3 mol) of a 30% aqueous solution of glyoxal was added slowly dropwise. An orange precipitate was obtained and the suspension was warmed to 370 K and stirred at this temperature for 1.3 h. The suspension was then cooled to room temperature, and the orange product filtered off and washed several times with small amounts of deionized water. Immediately after, the product was purified by dissolving in a mixture of diluted oxalic acid (2–3% aqueous solution) and ethanol and heating it almost to boiling point, with the addition of active carbon; the mixture was then heated to reflux for 10 min and filtered immediately. The pale-yellow solution was left overnight in a refrigerator and the next day a white crystalline product was filtered off and washed several times with ethanol. The product was dried under vacuum in a

evidence of offset π–π stacking involving the pyrazine ring (N1/N2/C1–C4; centroid $Cg2$) and pyridine ring (N7/C12–C16; centroid $Cg4$), and the two pyridine rings (N4/C6–C10; centroid $Cg3$, and N7/C12–C16; centroid $Cg4$): $Cg2\cdots Cg4^{ii}$ = 3.648 (6) Å, interplanar distance = 3.264 (4) Å, slippage = 1.63 Å, and $Cg3\cdots Cg4^{iii}$ = 3.832 (6) Å, interplanar distance = 3.338 (4) Å, slippage = 1.884 Å; symmetry codes: (ii) $x, x - y, z + \frac{1}{2}$, (iii) $x, x - y, z - \frac{1}{2}$.

There are small channel-like cavities in the crystal, with a total potential solvent area volume of *ca* 72 Å^3 (*ca* 1.1% of the unit-cell volume). They are represented in brown/yellow in
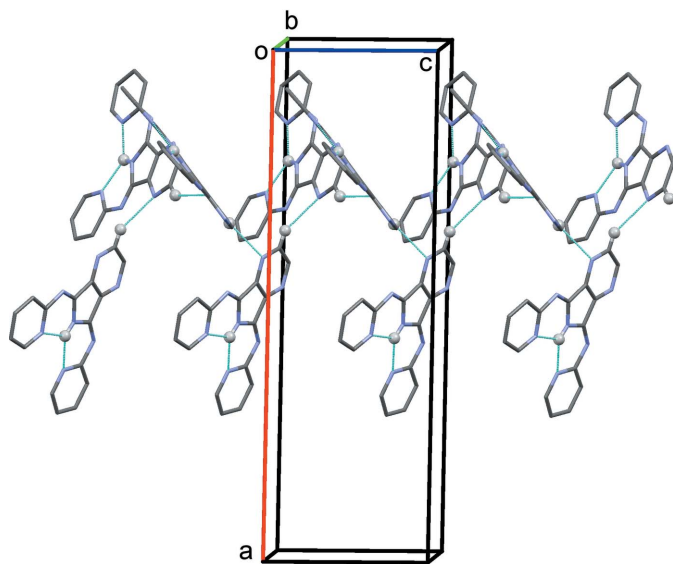

Figure 2
A partial view along the *b* axis of the crystal packing of the title compound. The intra- and intermolecular hydrogen bonds are shown as dashed lines (see Table 1; atoms H5N and H2 are shown as grey balls).
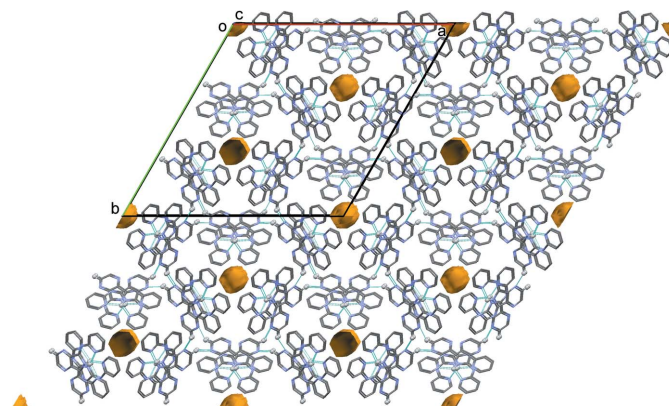

Figure 3
A view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1) and only H atoms H5N and H2 have been included (grey balls). The small cavities (*ca* 1.1% of the unit-cell volume) are represented in brown/yellow (*Mercury*; Macrae *et al.*, 2008).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{11}N_7$
M_r	301.32
Crystal system, space group	Trigonal, $R3c$:H
Temperature (K)	293
a, c (Å)	29.781 (4), 8.3901 (14)
V (Å^3)	6444.3 (19)
Z	18
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	$0.68 \times 0.19 \times 0.19$
Data collection	
Diffractometer	Stoe Siemens AED2 four-circle
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7762, 2629, 1606
R_{int}	0.115
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.147, 1.10
No. of reflections	2629
No. of parameters	213
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.18

Computer programs: *STADI4* and *X-RED* (Stoe & Cie, 1997), *SHELXS97* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

desiccator over silica (yield 2.8 g, 86%; m.p. 404–405 K). IR (KBr pellet, cm^{-1}): 3425, 3105, 3075, 3056, 2929, 2818, 2708, 2359, 2296, 2245, 2103, 1977, 1862, 1748, 1645, 1564, 1551, 1525, 1413, 1387, 1270, 1224, 1178, 1143, 1121, 1082, 1053, 990, 972, 876, 865, 695, 613, 574, 537, 470, 446. This compound (CAS-number 13481–25-9) is also available commercially.

Synthesis of the title compound. A round-bottomed flask was charged with 0.65 g (5 mmol) of **L**, 0.06 g (0.054 mmol) of anhydrous $CaCl_2$ and 0.99 g (10.5 mmol) of 2-aminopyridine and 25 ml of dry 1-butanol. The mixture was heated for 48 h at 333 K to give a green product. The resulting solution was evaporated to dryness under reduced pressure, and the residue was dissolved in 40 ml of deionized water. The product was extracted several times with chloroform (4 × 100 ml), then the solution was again evaporated to dryness under

reduced pressure and dried in a vacuum desiccator over silica (yield: 1.35 g, 89.6%). The pale-green–brown product was chromatographed over silica (Kieselgel 60 particle size 0.063–0.200, 70–230 Mesh ASTM, Merck) with chloroform as eluent; the yellow fraction was collected. After evaporated to dryness under reduced pressure, the yellow product obtained was dried in a vacuum desiccator over silica (yield 0.5 g, 37%; m.p. 547–548 K). Calculated for $C_{16}H_{11}N_7$ (%): C 63.78, H 3.68, N 32.54; found: C 63.69, H 3.89, N 32.40%. IR (KBr pellet, cm^{-1}): 3443, 3057, 1706, 1641, 1607, 1581, 1554, 1477, 1458, 1435, 1378, 1354, 1296, 1261, 1249, 1203, 1166, 1139, 1091, 1053, 998, 870, 790, 736, 725, 705, 538, 484, 431, 413.

Note: Despite many crystallization attempts, it was not possible to obtain suitable crystals of the yellow product. The only crystals of the title compound, suitable for crystal structure analysis, were obtained from reactions of the title compound with metal salts.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NH hydrogen was located in a difference Fourier map and freely refined.

References

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Posel, M. (1998). PhD thesis, University of Neuchâtel, Switzerland.
Scheja, A., Baade, D., Menzel, D., Pietzonka, C., Schweyen, P. & Bröring, M. (2015). *Chem. Eur. J.* **21**, 14196–14204.
Schilf, W. (2004). *J. Mol. Struct.* **691**, 141–148.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stoe & Cie (1997). *STADI4* and *X-RED*. Stoe & Cie GmbH, Damstadt, Germany.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Wong, E. W. Y., Ovens, J. S. & Leznoff, D. B. (2012). *Chem. Eur. J.* **18**, 6781–6787.

full crystallographic data

(5*Z*,7*Z*)-*N*⁵,*N*⁷-Bis(pyridin-2-yl)-5*H*-6,7-dihydropyrrolo[3,4-*b*]pyrazine-5,7-di-imine

Maciej Posel and Helen Stoeckli-Evans

(5*Z*,7*Z*)-*N*⁵,*N*⁷-Bis(pyridin-2-yl)-5*H*-6,7-dihydropyrrolo[3,4-*b*]pyrazine-5,7-diimine

Crystal data

$C_{16}H_{11}N_7$	$D_x = 1.398$ Mg m^{-3}
$M_r = 301.32$	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Trigonal, $R3c$:H	Cell parameters from 17 reflections
$a = 29.781$ (4) Å	$\theta = 12.8$–$19.2°$
$c = 8.3901$ (14) Å	$\mu = 0.09$ mm^{-1}
$V = 6444.3$ (19) Å^3	$T = 293$ K
$Z = 18$	Rod, brown
$F(000) = 2808$	$0.68 \times 0.19 \times 0.19$ mm

Data collection

Stoe Siemens AED2 four-circle diffractometer	$R_{int} = 0.115$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.5°$, $\theta_{min} = 2.4°$
Plane graphite monochromator	$h = -35 \rightarrow 36$
$\omega/2\theta$ scans	$k = -18 \rightarrow 36$
7762 measured reflections	$l = -10 \rightarrow 9$
2629 independent reflections	3 standard reflections every 60 min
1606 reflections with $I > 2\sigma(I)$	intensity decay: 2%

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.066$	
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2 + 9.7595P]$
$S = 1.10$	where $P = (F_o^2 + 2F_c^2)/3$
2629 reflections	$(\Delta/\sigma)_{max} < 0.001$
213 parameters	$\Delta\rho_{max} = 0.19$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0017 (2)

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.

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

	x	y	z	U_{iso}*/U_{eq}
N1	0.3344 (2)	0.1923 (2)	0.7094 (7)	0.0466 (16)
N2	0.2900 (2)	0.2525 (2)	0.5971 (7)	0.0469 (17)
N3	0.1969 (3)	0.1841 (2)	0.3886 (7)	0.0461 (17)
N4	0.1451 (3)	0.1023 (3)	0.2631 (9)	0.066 (2)
N5	0.2247 (2)	0.1224 (2)	0.4508 (7)	0.0387 (15)
H5N	0.201 (2)	0.095 (2)	0.399 (8)	0.07 (3)*
N6	0.2733 (2)	0.0847 (2)	0.5673 (7)	0.0405 (15)
N7	0.2067 (3)	0.0269 (2)	0.3879 (8)	0.0466 (17)
C1	0.3524 (3)	0.2415 (3)	0.7485 (10)	0.051 (2)
H1	0.3811	0.2573	0.8156	0.061*
C2	0.3310 (3)	0.2710 (3)	0.6946 (10)	0.051 (2)
H2	0.3459	0.3053	0.7283	0.062*
C3	0.2718 (3)	0.2029 (3)	0.5587 (8)	0.0383 (18)
C4	0.2929 (3)	0.1738 (3)	0.6132 (8)	0.0369 (18)
C5	0.2269 (3)	0.1699 (3)	0.4560 (9)	0.0412 (18)
C6	0.1564 (3)	0.1507 (4)	0.2875 (9)	0.050 (2)
C7	0.1303 (4)	0.1729 (4)	0.2118 (11)	0.064 (3)
H7	0.1391	0.2071	0.2320	0.077*
C8	0.0912 (4)	0.1426 (5)	0.1063 (12)	0.078 (3)
H8	0.0734	0.1563	0.0530	0.093*
C9	0.0785 (4)	0.0923 (5)	0.0803 (12)	0.087 (4)
H9	0.0519	0.0711	0.0106	0.105*
C10	0.1060 (4)	0.0741 (4)	0.1597 (14)	0.090 (3)
H10	0.0975	0.0399	0.1417	0.108*
C11	0.2634 (3)	0.1217 (3)	0.5432 (8)	0.0365 (17)
C12	0.2447 (3)	0.0363 (3)	0.4909 (9)	0.0401 (17)
C13	0.2587 (3)	−0.0006 (3)	0.5267 (11)	0.054 (2)
H13	0.2854	0.0070	0.5984	0.065*
C14	0.2327 (4)	−0.0486 (3)	0.4549 (11)	0.065 (3)
H14	0.2411	−0.0741	0.4785	0.078*
C15	0.1944 (4)	−0.0579 (3)	0.3483 (11)	0.063 (3)
H15	0.1767	−0.0897	0.2962	0.075*
C16	0.1822 (3)	−0.0197 (3)	0.3189 (11)	0.054 (2)
H16	0.1557	−0.0267	0.2473	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.043 (4)	0.045 (4)	0.050 (4)	0.021 (3)	−0.007 (3)	−0.007 (3)

N2	0.057 (4)	0.035 (4)	0.046 (4)	0.021 (3)	0.005 (4)	0.000 (3)
N3	0.054 (4)	0.054 (4)	0.041 (4)	0.035 (4)	−0.002 (3)	0.002 (3)
N4	0.058 (5)	0.059 (5)	0.079 (6)	0.027 (4)	−0.018 (4)	−0.007 (4)
N5	0.040 (4)	0.033 (4)	0.042 (4)	0.018 (3)	−0.008 (3)	−0.001 (3)
N6	0.042 (4)	0.037 (4)	0.045 (4)	0.021 (3)	−0.002 (3)	−0.003 (3)
N7	0.050 (4)	0.034 (4)	0.052 (4)	0.019 (3)	−0.003 (3)	−0.002 (3)
C1	0.047 (5)	0.049 (5)	0.052 (5)	0.021 (4)	−0.003 (4)	−0.006 (4)
C2	0.057 (5)	0.037 (5)	0.052 (5)	0.016 (4)	0.001 (4)	−0.007 (4)
C3	0.046 (5)	0.036 (4)	0.033 (4)	0.021 (4)	0.002 (3)	0.004 (3)
C4	0.037 (4)	0.035 (4)	0.036 (4)	0.016 (4)	0.007 (3)	0.002 (3)
C5	0.046 (5)	0.037 (4)	0.043 (5)	0.023 (4)	0.008 (4)	0.002 (4)
C6	0.048 (5)	0.065 (6)	0.044 (5)	0.034 (5)	0.006 (4)	0.004 (4)
C7	0.068 (6)	0.103 (8)	0.043 (5)	0.059 (6)	0.003 (5)	0.000 (5)
C8	0.075 (7)	0.138 (10)	0.054 (6)	0.079 (8)	−0.001 (5)	0.003 (7)
C9	0.061 (7)	0.136 (10)	0.072 (7)	0.055 (7)	−0.022 (5)	−0.023 (7)
C10	0.074 (7)	0.083 (8)	0.100 (8)	0.030 (6)	−0.034 (7)	−0.027 (7)
C11	0.037 (4)	0.038 (4)	0.038 (4)	0.021 (4)	0.006 (3)	0.003 (3)
C12	0.045 (4)	0.031 (4)	0.044 (4)	0.019 (4)	0.010 (4)	0.004 (3)
C13	0.062 (5)	0.050 (5)	0.062 (5)	0.038 (5)	0.001 (4)	−0.001 (4)
C14	0.087 (7)	0.049 (6)	0.071 (6)	0.043 (6)	0.012 (6)	0.005 (5)
C15	0.079 (7)	0.038 (5)	0.062 (6)	0.023 (5)	0.012 (5)	0.003 (4)
C16	0.056 (5)	0.043 (5)	0.055 (5)	0.019 (4)	−0.006 (4)	−0.004 (4)

Geometric parameters (Å, º)

N1—C1	1.324 (9)	C3—C5	1.477 (10)
N1—C4	1.341 (9)	C4—C11	1.472 (9)
N2—C3	1.335 (9)	C6—C7	1.400 (11)
N2—C2	1.338 (10)	C7—C8	1.380 (13)
N3—C5	1.293 (9)	C7—H7	0.9300
N3—C6	1.402 (10)	C8—C9	1.367 (14)
N4—C6	1.319 (11)	C8—H8	0.9300
N4—C10	1.354 (11)	C9—C10	1.362 (14)
N5—C5	1.384 (8)	C9—H9	0.9300
N5—C11	1.397 (9)	C10—H10	0.9300
N5—H5N	0.88 (3)	C12—C13	1.389 (10)
N6—C11	1.288 (9)	C13—C14	1.378 (11)
N6—C12	1.410 (9)	C13—H13	0.9300
N7—C16	1.335 (9)	C14—C15	1.364 (12)
N7—C12	1.340 (9)	C14—H14	0.9300
C1—C2	1.396 (11)	C15—C16	1.379 (11)
C1—H1	0.9300	C15—H15	0.9300
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.377 (10)		
C1—N1—C4	112.6 (7)	C6—C7—H7	121.1
C3—N2—C2	112.6 (7)	C9—C8—C7	120.0 (9)
C5—N3—C6	121.5 (7)	C9—C8—H8	120.0

C6—N4—C10	116.7 (8)	C7—C8—H8	120.0
C5—N5—C11	112.3 (6)	C10—C9—C8	117.8 (10)
C5—N5—H5N	123 (6)	C10—C9—H9	121.1
C11—N5—H5N	124 (6)	C8—C9—H9	121.1
C11—N6—C12	121.6 (6)	N4—C10—C9	124.5 (10)
C16—N7—C12	117.4 (7)	N4—C10—H10	117.7
N1—C1—C2	123.8 (8)	C9—C10—H10	117.7
N1—C1—H1	118.1	N6—C11—N5	129.9 (6)
C2—C1—H1	118.1	N6—C11—C4	124.6 (6)
N2—C2—C1	123.3 (7)	N5—C11—C4	105.5 (6)
N2—C2—H2	118.3	N7—C12—C13	122.2 (7)
C1—C2—H2	118.3	N7—C12—N6	121.4 (6)
N2—C3—C4	123.8 (7)	C13—C12—N6	116.5 (7)
N2—C3—C5	127.4 (7)	C14—C13—C12	119.4 (8)
C4—C3—C5	108.7 (6)	C14—C13—H13	120.3
N1—C4—C3	123.9 (7)	C12—C13—H13	120.3
N1—C4—C11	127.9 (7)	C15—C14—C13	118.5 (8)
C3—C4—C11	108.2 (6)	C15—C14—H14	120.8
N3—C5—N5	129.2 (7)	C13—C14—H14	120.8
N3—C5—C3	125.5 (7)	C14—C15—C16	119.2 (9)
N5—C5—C3	105.2 (6)	C14—C15—H15	120.4
N4—C6—C7	123.1 (9)	C16—C15—H15	120.4
N4—C6—N3	121.9 (7)	N7—C16—C15	123.4 (8)
C7—C6—N3	115.0 (8)	N7—C16—H16	118.3
C8—C7—C6	117.9 (10)	C15—C16—H16	118.3
C8—C7—H7	121.1		
C4—N1—C1—C2	−0.4 (11)	N3—C6—C7—C8	177.8 (7)
C3—N2—C2—C1	0.6 (11)	C6—C7—C8—C9	0.9 (13)
N1—C1—C2—N2	−0.4 (13)	C7—C8—C9—C10	−0.8 (16)
C2—N2—C3—C4	−0.1 (10)	C6—N4—C10—C9	0.3 (17)
C2—N2—C3—C5	179.1 (7)	C8—C9—C10—N4	0.2 (19)
C1—N1—C4—C3	0.9 (10)	C12—N6—C11—N5	2.8 (11)
C1—N1—C4—C11	178.6 (7)	C12—N6—C11—C4	−177.3 (6)
N2—C3—C4—N1	−0.8 (11)	C5—N5—C11—N6	179.8 (7)
C5—C3—C4—N1	179.9 (7)	C5—N5—C11—C4	−0.1 (8)
N2—C3—C4—C11	−178.8 (6)	N1—C4—C11—N6	1.0 (11)
C5—C3—C4—C11	1.8 (7)	C3—C4—C11—N6	179.0 (7)
C6—N3—C5—N5	−3.1 (12)	N1—C4—C11—N5	−179.1 (7)
C6—N3—C5—C3	177.3 (6)	C3—C4—C11—N5	−1.1 (7)
C11—N5—C5—N3	−178.4 (7)	C16—N7—C12—C13	−0.2 (11)
C11—N5—C5—C3	1.2 (8)	C16—N7—C12—N6	178.8 (7)
N2—C3—C5—N3	−1.5 (12)	C11—N6—C12—N7	1.2 (10)
C4—C3—C5—N3	177.8 (7)	C11—N6—C12—C13	−179.7 (7)
N2—C3—C5—N5	178.8 (7)	N7—C12—C13—C14	−0.2 (12)
C4—C3—C5—N5	−1.9 (8)	N6—C12—C13—C14	−179.3 (7)
C10—N4—C6—C7	−0.2 (13)	C12—C13—C14—C15	1.1 (13)
C10—N4—C6—N3	−178.2 (8)	C13—C14—C15—C16	−1.4 (13)

C5—N3—C6—N4	3.7 (11)	C12—N7—C16—C15	−0.2 (12)
C5—N3—C6—C7	−174.4 (7)	C14—C15—C16—N7	1.0 (13)
N4—C6—C7—C8	−0.4 (13)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N5—H5*N*⋯N4	0.88 (6)	2.12 (7)	2.653 (11)	119 (5)
N5—H5*N*⋯N7	0.88 (6)	2.12 (6)	2.670 (8)	120 (5)
C2—H2⋯N2[i]	0.93	2.62	3.395 (11)	141

Symmetry code: (i) $-y+2/3$, $x-y+1/3$, $z+1/3$.