Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,6-Bis(2-methyl-1,3-diazinan-2-yl)-pyridine

Quoc-Cuong Ton[a] and Michael Bolte[b]*

[a]Institut für Organische Chemie und Chemische Biologie, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany, and [b]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

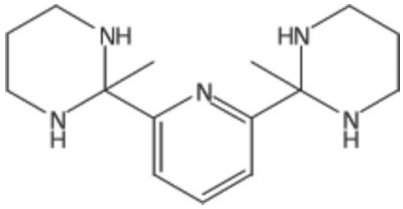
Received 29 November 2010; accepted 30 November 2010

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.098; data-to-parameter ratio = 14.6.

The title compound, $C_{15}H_{25}N_5$, is an aminalization product between 2,6-diacetylpyridine and 1,3-diaminopropane. It crystallizes with two independent molecules in the asymmetric unit with different conformations. In the first molecule, the methyl groups are *cis* oriented with respect to the pyridine ring [N—C—C—C torsion angles = 72.5 (1) and 80.3 (1)°], while they are *trans* oriented in the second molecule [N—C—C—C torsion angles = 82.6 (1) and −90.8 (1)°]. Each of the two molecules forms centrosymmetric dimers held together by N—H···N hydrogen bonds, thus forming $R_2^2(16)$ rings. The two dimers are interlinked by additional N—H···N bonds into $R_4^4(14)$ rings, building chains along the *a* axis. These patterns influence the orientation (either equatorial or axial) of the N—H bonds.

Related literature

For 2,6-diacetylpyridine, see: Burnet *et al.* (2003) and for 1,3-diaminopropane, see: Thalladi *et al.* (2000).



Experimental

Crystal data

$C_{15}H_{25}N_5$
M_r = 275.40
Monoclinic, $P2_1/c$
a = 18.715 (4) Å
b = 7.512 (2) Å
c = 22.730 (5) Å
β = 102.07 (3)°
V = 3124.9 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 173 K
0.40 × 0.32 × 0.30 mm

Data collection

Stoe IPDS II two-circle diffractometer
41522 measured reflections
5758 independent reflections
4924 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.098
S = 1.35
5758 reflections
394 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···N5^{i}	0.893 (16)	2.596 (15)	3.3984 (16)	149.9 (12)
N4—H4N···N4′^{ii}	0.908 (16)	2.623 (16)	3.4716 (16)	155.8 (13)
N3′—H3′N···N5′^{iii}	0.873 (15)	2.418 (15)	3.2662 (17)	164.2 (12)

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We gratefully thank Professor Dr Ernst Egert for his support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5081).

References

Burnet, S., Hall, A. K., Hall, J. M., Harrowfield, J. M., Koutsantonis, G. A., Sanford, V., Sauter, D., Skelton, B. W. & White, A. H. (2003). *Supramol. Chem.* **15**, 291–312.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Thalladi, V. R., Boese, R. & Weiss, C.-H. (2000). *Angew. Chem. Int. Ed.* **39**, 918–922.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, o41 [https://doi.org/10.1107/S1600536810050063]

2,6-Bis(2-methyl-1,3-diazinan-2-yl)pyridine

Quoc-Cuong Ton and Michael Bolte

S1. Comment

The aim of this investigation was to cocrystallize 2,6-diacetylpyridine (Burnet *et al.*, 2003) with 1,3-diaminopropane (Thalladi *et al.*, 2000). Unfortunately crystals of the title compound were obtained due to an aminalization reaction between the starting compounds (Fig. 2).

S2. Experimental

The starting compounds were purchased from Aldrich and Lancaster and utilized for a cocrystallization experiment without purification. 2,6-diacetylpyridine (10 mg) was added to an excess of 1,3-diaminopropane (0.8 ml). The mixture in a flask was set aside at room temperature. After several months colourless crystals were obtained.

S3. Refinement

H atoms bonded to C were refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C)] using a riding model with $C_{aromatic}$—H = 0.95 Å, $C_{methylene}$—H = 0.99 Å, or $C_{tertiary}$—H = 0.98 Å, respectively. H atoms bonded to N were freely refined.

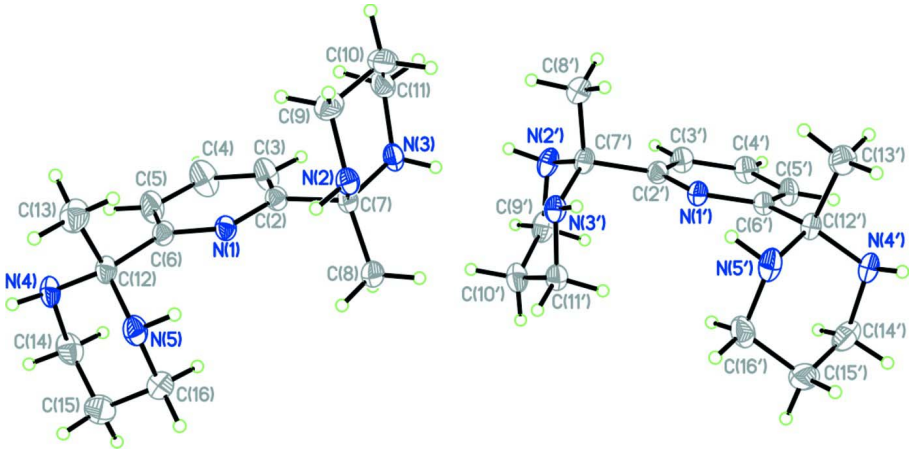


Figure 1

A perspective view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

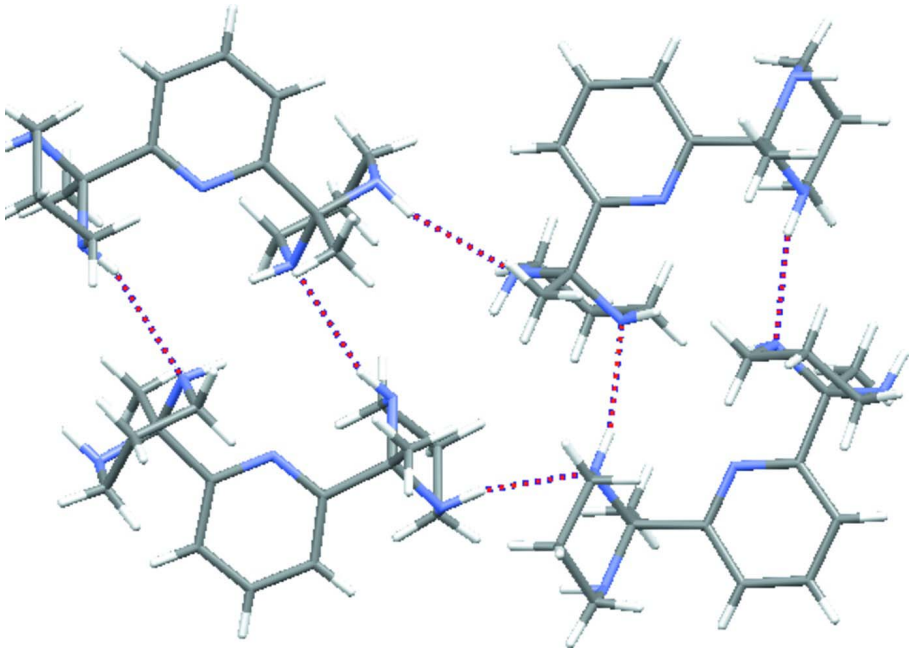


Figure 2

A partial packing diagram for (I). N—H···N hydrogen bonds are shown as dashed lines.

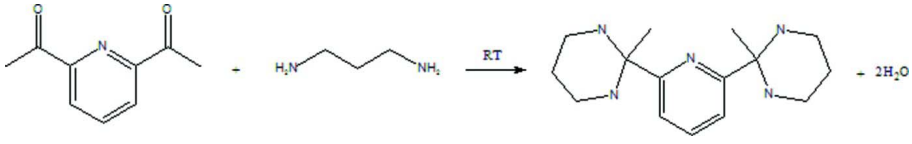


Figure 3

Reaction scheme between 2,6-diacetylpyridine and 1,3-diaminopropane.

2,6-Bis(2-methyl-1,3-diazinan-2-yl)pyridine

Crystal data

$C_{15}H_{25}N_5$
$M_r = 275.40$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 18.715$ (4) Å
$b = 7.512$ (2) Å
$c = 22.730$ (5) Å
$\beta = 102.07$ (3)°
$V = 3124.9$ (13) Å^3
$Z = 8$
$F(000) = 1200$
$D_x = 1.171$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 38746 reflections
$\theta = 3.3$–$25.7°$
$\mu = 0.07$ mm^{-1}
$T = 173$ K
Block, colourless
0.40 × 0.32 × 0.30 mm

Data collection

Stoe IPDS II two-circle diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
41522 measured reflections
5758 independent reflections
4924 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.3°$
$h = -22 \rightarrow 22$
$k = -9 \rightarrow 9$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.098$
$S = 1.35$
5758 reflections
394 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0182 (13)

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}
N1	0.01315 (5)	0.64048 (12)	0.38741 (4)	0.0208 (2)
C2	0.06102 (6)	0.70659 (15)	0.35629 (5)	0.0219 (2)
C3	0.03859 (7)	0.78073 (19)	0.29935 (6)	0.0337 (3)
H3	0.0733	0.8227	0.2775	0.040*
C4	−0.03613 (7)	0.7920 (2)	0.27508 (6)	0.0419 (4)
H4	−0.0530	0.8449	0.2367	0.050*
C5	−0.08588 (6)	0.72571 (18)	0.30721 (6)	0.0336 (3)
H5	−0.1370	0.7337	0.2915	0.040*
C6	−0.05903 (6)	0.64714 (15)	0.36306 (5)	0.0222 (2)
C7	0.14237 (5)	0.67781 (15)	0.38678 (5)	0.0205 (2)
C8	0.15860 (6)	0.47996 (15)	0.38048 (5)	0.0262 (3)
H8A	0.1275	0.4091	0.4013	0.039*
H8B	0.2101	0.4565	0.3984	0.039*
H8C	0.1486	0.4476	0.3378	0.039*
N2	0.15809 (5)	0.71862 (13)	0.45185 (4)	0.0226 (2)
H2N	0.1276 (8)	0.658 (2)	0.4698 (6)	0.034 (4)*
C9	0.15049 (7)	0.90860 (17)	0.46430 (6)	0.0319 (3)
H9A	0.1608	0.9292	0.5083	0.038*
H9B	0.0999	0.9482	0.4473	0.038*
C10	0.20407 (7)	1.01382 (17)	0.43596 (6)	0.0363 (3)
H10A	0.2548	0.9798	0.4548	0.044*
H10B	0.1982	1.1428	0.4426	0.044*
C11	0.18907 (7)	0.97400 (16)	0.36861 (6)	0.0325 (3)

H11A	0.1409	1.0243	0.3495	0.039*
H11B	0.2266	1.0338	0.3507	0.039*
N3	0.18942 (5)	0.78179 (13)	0.35523 (4)	0.0255 (2)
H3N	0.2350 (8)	0.7418 (18)	0.3682 (6)	0.028 (3)*
C12	−0.10820 (6)	0.56698 (15)	0.40310 (5)	0.0228 (2)
C13	−0.11675 (7)	0.70647 (19)	0.45014 (6)	0.0357 (3)
H13A	−0.0687	0.7351	0.4749	0.054*
H13B	−0.1483	0.6593	0.4758	0.054*
H13C	−0.1388	0.8144	0.4299	0.054*
N4	−0.18088 (5)	0.52752 (14)	0.36689 (5)	0.0267 (2)
H4N	−0.2100 (9)	0.506 (2)	0.3935 (7)	0.041 (4)*
C14	−0.18228 (7)	0.37221 (18)	0.32745 (6)	0.0339 (3)
H14A	−0.1575	0.4035	0.2944	0.041*
H14B	−0.2337	0.3429	0.3093	0.041*
C15	−0.14553 (7)	0.20842 (19)	0.35991 (7)	0.0405 (3)
H15A	−0.1422	0.1137	0.3303	0.049*
H15B	−0.1750	0.1627	0.3881	0.049*
C16	−0.06904 (7)	0.25698 (17)	0.39462 (7)	0.0353 (3)
H16A	−0.0463	0.1529	0.4180	0.042*
H16B	−0.0380	0.2916	0.3662	0.042*
N5	−0.07435 (5)	0.40640 (14)	0.43568 (4)	0.0270 (2)
H5N	−0.0281 (8)	0.4360 (19)	0.4533 (6)	0.033 (4)*
N1′	0.51250 (5)	0.59589 (12)	0.38384 (4)	0.0199 (2)
C2′	0.47119 (6)	0.66760 (14)	0.33387 (5)	0.0204 (2)
C3′	0.49877 (6)	0.70014 (16)	0.28223 (5)	0.0250 (3)
H3′	0.4691	0.7533	0.2477	0.030*
C4′	0.57073 (6)	0.65272 (16)	0.28268 (5)	0.0264 (3)
H4′	0.5907	0.6729	0.2481	0.032*
C5′	0.61335 (6)	0.57584 (16)	0.33375 (5)	0.0249 (2)
H5′	0.6624	0.5416	0.3346	0.030*
C6′	0.58237 (5)	0.55030 (14)	0.38369 (5)	0.0200 (2)
C7′	0.39231 (6)	0.71995 (15)	0.33837 (5)	0.0220 (2)
C8′	0.39689 (6)	0.90350 (16)	0.36847 (6)	0.0302 (3)
H8′1	0.4269	0.8954	0.4092	0.045*
H8′2	0.3477	0.9438	0.3705	0.045*
H8′3	0.4190	0.9886	0.3449	0.045*
N2′	0.34706 (5)	0.73352 (14)	0.27711 (4)	0.0272 (2)
H2′N	0.3052 (8)	0.7831 (19)	0.2808 (6)	0.033 (4)*
C9′	0.33042 (6)	0.55788 (17)	0.24825 (5)	0.0288 (3)
H9′1	0.3758	0.5078	0.2390	0.035*
H9′2	0.2950	0.5741	0.2097	0.035*
C10′	0.29904 (6)	0.42461 (17)	0.28693 (5)	0.0291 (3)
H10C	0.2955	0.3055	0.2679	0.035*
H10D	0.2494	0.4621	0.2904	0.035*
C11′	0.34896 (6)	0.41589 (15)	0.34943 (5)	0.0248 (2)
H11C	0.3271	0.3373	0.3759	0.030*
H11D	0.3971	0.3664	0.3465	0.030*
N3′	0.35806 (5)	0.59662 (13)	0.37478 (4)	0.0221 (2)

H3′N	0.3836 (8)	0.5952 (18)	0.4116 (7)	0.030 (3)*
C12′	0.62660 (6)	0.47668 (15)	0.44412 (5)	0.0208 (2)
C13′	0.66464 (7)	0.63378 (17)	0.48080 (6)	0.0335 (3)
H13D	0.6278	0.7182	0.4887	0.050*
H13E	0.6969	0.6935	0.4581	0.050*
H13F	0.6936	0.5902	0.5191	0.050*
N4′	0.68328 (5)	0.35340 (13)	0.43324 (5)	0.0256 (2)
H4′N	0.7143 (7)	0.3368 (18)	0.4685 (6)	0.029 (3)*
C14′	0.65331 (7)	0.18110 (18)	0.40894 (6)	0.0360 (3)
H14C	0.6943	0.0982	0.4084	0.043*
H14D	0.6268	0.1983	0.3668	0.043*
C15′	0.60164 (7)	0.09624 (18)	0.44454 (7)	0.0407 (3)
H15C	0.5785	−0.0105	0.4231	0.049*
H15D	0.6295	0.0584	0.4845	0.049*
C16′	0.54299 (7)	0.22950 (18)	0.45217 (6)	0.0364 (3)
H16C	0.5118	0.2578	0.4125	0.044*
H16D	0.5117	0.1777	0.4779	0.044*
N5′	0.57811 (5)	0.39283 (15)	0.48008 (4)	0.0281 (2)
H5′N	0.5420 (9)	0.474 (2)	0.4791 (7)	0.045 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0161 (4)	0.0239 (5)	0.0212 (5)	−0.0001 (3)	0.0011 (3)	−0.0006 (4)
C2	0.0188 (5)	0.0242 (6)	0.0218 (6)	−0.0005 (4)	0.0018 (4)	0.0006 (4)
C3	0.0234 (6)	0.0486 (8)	0.0277 (6)	−0.0040 (5)	0.0017 (5)	0.0137 (6)
C4	0.0289 (7)	0.0595 (9)	0.0320 (7)	−0.0031 (6)	−0.0056 (5)	0.0224 (6)
C5	0.0178 (6)	0.0443 (7)	0.0342 (7)	0.0009 (5)	−0.0045 (5)	0.0100 (6)
C6	0.0173 (5)	0.0243 (6)	0.0236 (6)	0.0012 (4)	0.0009 (4)	−0.0018 (4)
C7	0.0159 (5)	0.0249 (6)	0.0201 (5)	−0.0005 (4)	0.0023 (4)	0.0017 (4)
C8	0.0202 (5)	0.0270 (6)	0.0303 (6)	0.0006 (4)	0.0028 (5)	−0.0012 (5)
N2	0.0191 (5)	0.0267 (5)	0.0213 (5)	−0.0009 (4)	0.0023 (4)	0.0007 (4)
C9	0.0309 (6)	0.0304 (6)	0.0322 (6)	0.0033 (5)	0.0013 (5)	−0.0073 (5)
C10	0.0323 (7)	0.0230 (6)	0.0488 (8)	−0.0019 (5)	−0.0025 (6)	−0.0020 (5)
C11	0.0230 (6)	0.0291 (6)	0.0439 (7)	−0.0021 (5)	0.0036 (5)	0.0120 (6)
N3	0.0168 (5)	0.0310 (5)	0.0289 (5)	−0.0009 (4)	0.0052 (4)	0.0061 (4)
C12	0.0157 (5)	0.0292 (6)	0.0226 (5)	0.0007 (4)	0.0018 (4)	−0.0027 (5)
C13	0.0329 (7)	0.0418 (7)	0.0331 (7)	0.0005 (6)	0.0084 (5)	−0.0108 (6)
N4	0.0139 (4)	0.0379 (6)	0.0275 (5)	−0.0007 (4)	0.0030 (4)	−0.0043 (4)
C14	0.0268 (6)	0.0429 (8)	0.0298 (6)	−0.0083 (5)	0.0009 (5)	−0.0097 (5)
C15	0.0377 (7)	0.0336 (7)	0.0498 (8)	−0.0065 (6)	0.0080 (6)	−0.0106 (6)
C16	0.0289 (6)	0.0289 (7)	0.0483 (8)	0.0030 (5)	0.0089 (6)	0.0010 (6)
N5	0.0191 (5)	0.0340 (6)	0.0264 (5)	−0.0008 (4)	0.0012 (4)	0.0034 (4)
N1′	0.0170 (4)	0.0236 (5)	0.0187 (4)	0.0017 (3)	0.0028 (3)	0.0017 (4)
C2′	0.0189 (5)	0.0215 (5)	0.0202 (5)	0.0008 (4)	0.0023 (4)	0.0024 (4)
C3′	0.0245 (6)	0.0293 (6)	0.0207 (6)	0.0008 (5)	0.0036 (4)	0.0076 (5)
C4′	0.0267 (6)	0.0338 (6)	0.0208 (6)	−0.0018 (5)	0.0093 (4)	0.0047 (5)
C5′	0.0180 (5)	0.0328 (6)	0.0247 (6)	0.0012 (4)	0.0066 (4)	0.0021 (5)

C6′	0.0173 (5)	0.0216 (5)	0.0208 (5)	0.0003 (4)	0.0033 (4)	0.0003 (4)
C7′	0.0189 (5)	0.0275 (6)	0.0189 (5)	0.0041 (4)	0.0025 (4)	0.0033 (4)
C8′	0.0259 (6)	0.0290 (6)	0.0351 (7)	0.0041 (5)	0.0054 (5)	0.0001 (5)
N2′	0.0222 (5)	0.0360 (6)	0.0212 (5)	0.0102 (4)	−0.0005 (4)	0.0057 (4)
C9′	0.0226 (6)	0.0433 (7)	0.0183 (5)	0.0057 (5)	−0.0005 (4)	−0.0012 (5)
C10′	0.0198 (5)	0.0392 (7)	0.0276 (6)	−0.0005 (5)	0.0032 (5)	−0.0072 (5)
C11′	0.0210 (5)	0.0284 (6)	0.0254 (6)	0.0007 (4)	0.0057 (4)	0.0016 (5)
N3′	0.0188 (4)	0.0295 (5)	0.0173 (5)	0.0020 (4)	0.0023 (4)	0.0013 (4)
C12′	0.0168 (5)	0.0264 (6)	0.0192 (5)	0.0033 (4)	0.0035 (4)	0.0016 (4)
C13′	0.0319 (6)	0.0324 (7)	0.0306 (6)	0.0023 (5)	−0.0060 (5)	−0.0019 (5)
N4′	0.0179 (5)	0.0331 (5)	0.0249 (5)	0.0073 (4)	0.0026 (4)	0.0025 (4)
C14′	0.0372 (7)	0.0330 (7)	0.0345 (7)	0.0135 (5)	0.0000 (6)	−0.0044 (5)
C15′	0.0383 (7)	0.0274 (7)	0.0484 (8)	−0.0012 (5)	−0.0094 (6)	0.0076 (6)
C16′	0.0224 (6)	0.0410 (7)	0.0421 (8)	−0.0046 (5)	−0.0018 (5)	0.0194 (6)
N5′	0.0213 (5)	0.0400 (6)	0.0242 (5)	0.0072 (4)	0.0074 (4)	0.0091 (4)

Geometric parameters (Å, º)

N1—C2	1.3471 (15)	N1′—C2′	1.3456 (14)
N1—C6	1.3494 (14)	N1′—C6′	1.3523 (14)
C2—C3	1.3908 (17)	C2′—C3′	1.3992 (16)
C2—C7	1.5504 (15)	C2′—C7′	1.5515 (15)
C3—C4	1.3943 (18)	C3′—C4′	1.3909 (16)
C3—H3	0.9500	C3′—H3′	0.9500
C4—C5	1.3903 (19)	C4′—C5′	1.3892 (17)
C4—H4	0.9500	C4′—H4′	0.9500
C5—C6	1.3949 (17)	C5′—C6′	1.3916 (16)
C5—H5	0.9500	C5′—H5′	0.9500
C6—C12	1.5453 (16)	C6′—C12′	1.5499 (15)
C7—N3	1.4709 (14)	C7′—N2′	1.4742 (15)
C7—N2	1.4786 (15)	C7′—N3′	1.4752 (15)
C7—C8	1.5297 (16)	C7′—C8′	1.5337 (17)
C8—H8A	0.9800	C8′—H8′1	0.9800
C8—H8B	0.9800	C8′—H8′2	0.9800
C8—H8C	0.9800	C8′—H8′3	0.9800
N2—C9	1.4676 (16)	N2′—C9′	1.4774 (17)
N2—H2N	0.893 (16)	N2′—H2′N	0.887 (15)
C9—C10	1.5217 (19)	C9′—C10′	1.5284 (18)
C9—H9A	0.9900	C9′—H9′1	0.9900
C9—H9B	0.9900	C9′—H9′2	0.9900
C10—C11	1.527 (2)	C10′—C11′	1.5297 (17)
C10—H10A	0.9900	C10′—H10C	0.9900
C10—H10B	0.9900	C10′—H10D	0.9900
C11—N3	1.4758 (17)	C11′—N3′	1.4707 (15)
C11—H11A	0.9900	C11′—H11C	0.9900
C11—H11B	0.9900	C11′—H11D	0.9900
N3—H3N	0.894 (14)	N3′—H3′N	0.873 (15)
C12—N4	1.4653 (14)	C12′—N4′	1.4676 (14)

C12—N5	1.4862 (15)	C12′—N5′	1.4830 (15)
C12—C13	1.5293 (17)	C12′—C13′	1.5318 (16)
C13—H13A	0.9800	C13′—H13D	0.9800
C13—H13B	0.9800	C13′—H13E	0.9800
C13—H13C	0.9800	C13′—H13F	0.9800
N4—C14	1.4683 (16)	N4′—C14′	1.4715 (17)
N4—H4N	0.908 (16)	N4′—H4′N	0.894 (14)
C14—C15	1.523 (2)	C14′—C15′	1.524 (2)
C14—H14A	0.9900	C14′—H14C	0.9900
C14—H14B	0.9900	C14′—H14D	0.9900
C15—C16	1.5271 (19)	C15′—C16′	1.522 (2)
C15—H15A	0.9900	C15′—H15C	0.9900
C15—H15B	0.9900	C15′—H15D	0.9900
C16—N5	1.4764 (17)	C16′—N5′	1.4715 (18)
C16—H16A	0.9900	C16′—H16C	0.9900
C16—H16B	0.9900	C16′—H16D	0.9900
N5—H5N	0.901 (15)	N5′—H5′N	0.905 (17)
C2—N1—C6	119.31 (9)	C2′—N1′—C6′	118.98 (9)
N1—C2—C3	122.14 (10)	N1′—C2′—C3′	122.03 (10)
N1—C2—C7	114.37 (9)	N1′—C2′—C7′	115.63 (9)
C3—C2—C7	123.29 (10)	C3′—C2′—C7′	122.28 (10)
C2—C3—C4	118.36 (12)	C4′—C3′—C2′	118.40 (10)
C2—C3—H3	120.8	C4′—C3′—H3′	120.8
C4—C3—H3	120.8	C2′—C3′—H3′	120.8
C5—C4—C3	119.79 (11)	C5′—C4′—C3′	119.90 (11)
C5—C4—H4	120.1	C5′—C4′—H4′	120.1
C3—C4—H4	120.1	C3′—C4′—H4′	120.1
C4—C5—C6	118.44 (11)	C4′—C5′—C6′	118.32 (10)
C4—C5—H5	120.8	C4′—C5′—H5′	120.8
C6—C5—H5	120.8	C6′—C5′—H5′	120.8
N1—C6—C5	121.89 (11)	N1′—C6′—C5′	122.36 (10)
N1—C6—C12	114.35 (9)	N1′—C6′—C12′	115.19 (9)
C5—C6—C12	123.73 (10)	C5′—C6′—C12′	122.38 (9)
N3—C7—N2	111.31 (9)	N2′—C7′—N3′	110.01 (9)
N3—C7—C8	108.63 (9)	N2′—C7′—C8′	109.07 (9)
N2—C7—C8	107.05 (9)	N3′—C7′—C8′	107.73 (9)
N3—C7—C2	109.88 (9)	N2′—C7′—C2′	108.77 (9)
N2—C7—C2	112.93 (9)	N3′—C7′—C2′	114.13 (9)
C8—C7—C2	106.82 (9)	C8′—C7′—C2′	106.99 (9)
C7—C8—H8A	109.5	C7′—C8′—H8′1	109.5
C7—C8—H8B	109.5	C7′—C8′—H8′2	109.5
H8A—C8—H8B	109.5	H8′1—C8′—H8′2	109.5
C7—C8—H8C	109.5	C7′—C8′—H8′3	109.5
H8A—C8—H8C	109.5	H8′1—C8′—H8′3	109.5
H8B—C8—H8C	109.5	H8′2—C8′—H8′3	109.5
C9—N2—C7	112.79 (9)	C7′—N2′—C9′	112.56 (9)
C9—N2—H2N	108.2 (9)	C7′—N2′—H2′N	106.5 (9)

C7—N2—H2N	109.7 (9)	C9′—N2′—H2′N	108.0 (9)
N2—C9—C10	108.94 (10)	N2′—C9′—C10′	113.59 (10)
N2—C9—H9A	109.9	N2′—C9′—H9′1	108.8
C10—C9—H9A	109.9	C10′—C9′—H9′1	108.8
N2—C9—H9B	109.9	N2′—C9′—H9′2	108.8
C10—C9—H9B	109.9	C10′—C9′—H9′2	108.8
H9A—C9—H9B	108.3	H9′1—C9′—H9′2	107.7
C9—C10—C11	108.86 (10)	C9′—C10′—C11′	109.20 (9)
C9—C10—H10A	109.9	C9′—C10′—H10C	109.8
C11—C10—H10A	109.9	C11′—C10′—H10C	109.8
C9—C10—H10B	109.9	C9′—C10′—H10D	109.8
C11—C10—H10B	109.9	C11′—C10′—H10D	109.8
H10A—C10—H10B	108.3	H10C—C10′—H10D	108.3
N3—C11—C10	112.98 (10)	N3′—C11′—C10′	108.81 (9)
N3—C11—H11A	109.0	N3′—C11′—H11C	109.9
C10—C11—H11A	109.0	C10′—C11′—H11C	109.9
N3—C11—H11B	109.0	N3′—C11′—H11D	109.9
C10—C11—H11B	109.0	C10′—C11′—H11D	109.9
H11A—C11—H11B	107.8	H11C—C11′—H11D	108.3
C7—N3—C11	112.97 (10)	C11′—N3′—C7′	112.85 (9)
C7—N3—H3N	106.7 (9)	C11′—N3′—H3′N	111.1 (9)
C11—N3—H3N	107.8 (9)	C7′—N3′—H3′N	109.3 (9)
N4—C12—N5	111.38 (9)	N4′—C12′—N5′	111.85 (9)
N4—C12—C13	108.09 (9)	N4′—C12′—C13′	107.93 (9)
N5—C12—C13	107.68 (10)	N5′—C12′—C13′	107.19 (9)
N4—C12—C6	110.20 (9)	N4′—C12′—C6′	110.29 (9)
N5—C12—C6	111.44 (9)	N5′—C12′—C6′	111.41 (8)
C13—C12—C6	107.89 (10)	C13′—C12′—C6′	107.99 (9)
C12—C13—H13A	109.5	C12′—C13′—H13D	109.5
C12—C13—H13B	109.5	C12′—C13′—H13E	109.5
H13A—C13—H13B	109.5	H13D—C13′—H13E	109.5
C12—C13—H13C	109.5	C12′—C13′—H13F	109.5
H13A—C13—H13C	109.5	H13D—C13′—H13F	109.5
H13B—C13—H13C	109.5	H13E—C13′—H13F	109.5
C12—N4—C14	113.55 (9)	C12′—N4′—C14′	112.71 (9)
C12—N4—H4N	106.1 (10)	C12′—N4′—H4′N	107.1 (9)
C14—N4—H4N	109.3 (10)	C14′—N4′—H4′N	109.8 (9)
N4—C14—C15	113.43 (11)	N4′—C14′—C15′	113.76 (11)
N4—C14—H14A	108.9	N4′—C14′—H14C	108.8
C15—C14—H14A	108.9	C15′—C14′—H14C	108.8
N4—C14—H14B	108.9	N4′—C14′—H14D	108.8
C15—C14—H14B	108.9	C15′—C14′—H14D	108.8
H14A—C14—H14B	107.7	H14C—C14′—H14D	107.7
C14—C15—C16	109.68 (11)	C16′—C15′—C14′	109.76 (11)
C14—C15—H15A	109.7	C16′—C15′—H15C	109.7
C16—C15—H15A	109.7	C14′—C15′—H15C	109.7
C14—C15—H15B	109.7	C16′—C15′—H15D	109.7
C16—C15—H15B	109.7	C14′—C15′—H15D	109.7

H15A—C15—H15B	108.2	H15C—C15′—H15D	108.2
N5—C16—C15	109.18 (10)	N5′—C16′—C15′	109.26 (10)
N5—C16—H16A	109.8	N5′—C16′—H16C	109.8
C15—C16—H16A	109.8	C15′—C16′—H16C	109.8
N5—C16—H16B	109.8	N5′—C16′—H16D	109.8
C15—C16—H16B	109.8	C15′—C16′—H16D	109.8
H16A—C16—H16B	108.3	H16C—C16′—H16D	108.3
C16—N5—C12	112.33 (9)	C16′—N5′—C12′	112.71 (10)
C16—N5—H5N	106.5 (9)	C16′—N5′—H5′N	106.6 (10)
C12—N5—H5N	106.9 (9)	C12′—N5′—H5′N	103.9 (10)
C6—N1—C2—C3	−0.52 (17)	C6′—N1′—C2′—C3′	−1.46 (16)
C6—N1—C2—C7	−175.43 (9)	C6′—N1′—C2′—C7′	−178.67 (9)
N1—C2—C3—C4	2.3 (2)	N1′—C2′—C3′—C4′	1.42 (17)
C7—C2—C3—C4	176.79 (12)	C7′—C2′—C3′—C4′	178.44 (10)
C2—C3—C4—C5	−1.6 (2)	C2′—C3′—C4′—C5′	−0.30 (18)
C3—C4—C5—C6	−0.8 (2)	C3′—C4′—C5′—C6′	−0.70 (18)
C2—N1—C6—C5	−2.05 (17)	C2′—N1′—C6′—C5′	0.39 (16)
C2—N1—C6—C12	179.94 (9)	C2′—N1′—C6′—C12′	177.37 (9)
C4—C5—C6—N1	2.68 (19)	C4′—C5′—C6′—N1′	0.68 (17)
C4—C5—C6—C12	−179.50 (12)	C4′—C5′—C6′—C12′	−176.09 (10)
N1—C2—C7—N3	−169.79 (9)	N1′—C2′—C7′—N2′	−159.75 (9)
C3—C2—C7—N3	15.36 (15)	C3′—C2′—C7′—N2′	23.05 (14)
N1—C2—C7—N2	−44.86 (13)	N1′—C2′—C7′—N3′	−36.50 (13)
C3—C2—C7—N2	140.29 (12)	C3′—C2′—C7′—N3′	146.30 (11)
N1—C2—C7—C8	72.55 (12)	N1′—C2′—C7′—C8′	82.56 (12)
C3—C2—C7—C8	−102.30 (13)	C3′—C2′—C7′—C8′	−94.63 (12)
N3—C7—N2—C9	56.72 (12)	N3′—C7′—N2′—C9′	−53.26 (12)
C8—C7—N2—C9	175.30 (9)	C8′—C7′—N2′—C9′	−171.21 (10)
C2—C7—N2—C9	−67.42 (12)	C2′—C7′—N2′—C9′	72.43 (12)
C7—N2—C9—C10	−60.40 (12)	C7′—N2′—C9′—C10′	51.37 (13)
N2—C9—C10—C11	57.28 (13)	N2′—C9′—C10′—C11′	−51.67 (13)
C9—C10—C11—N3	−53.72 (13)	C9′—C10′—C11′—N3′	55.04 (12)
N2—C7—N3—C11	−50.79 (12)	C10′—C11′—N3′—C7′	−61.18 (11)
C8—C7—N3—C11	−168.41 (9)	N2′—C7′—N3′—C11′	59.80 (11)
C2—C7—N3—C11	75.06 (11)	C8′—C7′—N3′—C11′	178.57 (9)
C10—C11—N3—C7	50.98 (13)	C2′—C7′—N3′—C11′	−62.78 (12)
N1—C6—C12—N4	−161.87 (9)	N1′—C6′—C12′—N4′	151.51 (9)
C5—C6—C12—N4	20.16 (16)	C5′—C6′—C12′—N4′	−31.51 (15)
N1—C6—C12—N5	−37.69 (13)	N1′—C6′—C12′—N5′	26.68 (13)
C5—C6—C12—N5	144.34 (12)	C5′—C6′—C12′—N5′	−156.34 (10)
N1—C6—C12—C13	80.32 (12)	N1′—C6′—C12′—C13′	−90.77 (11)
C5—C6—C12—C13	−97.65 (13)	C5′—C6′—C12′—C13′	86.21 (13)
N5—C12—N4—C14	−51.19 (13)	N5′—C12′—N4′—C14′	50.94 (13)
C13—C12—N4—C14	−169.29 (11)	C13′—C12′—N4′—C14′	168.61 (10)
C6—C12—N4—C14	73.03 (13)	C6′—C12′—N4′—C14′	−73.64 (12)
C12—N4—C14—C15	50.09 (15)	C12′—N4′—C14′—C15′	−50.04 (13)
N4—C14—C15—C16	−51.80 (15)	N4′—C14′—C15′—C16′	52.01 (14)

C14—C15—C16—N5	55.64 (15)	C14′—C15′—C16′—N5′	−55.21 (14)
C15—C16—N5—C12	−59.44 (14)	C15′—C16′—N5′—C12′	58.90 (13)
N4—C12—N5—C16	56.92 (12)	N4′—C12′—N5′—C16′	−56.78 (12)
C13—C12—N5—C16	175.27 (9)	C13′—C12′—N5′—C16′	−174.89 (9)
C6—C12—N5—C16	−66.59 (12)	C6′—C12′—N5′—C16′	67.17 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···N5^{i}	0.893 (16)	2.596 (15)	3.3984 (16)	149.9 (12)
N4—H4*N*···N4′^{ii}	0.908 (16)	2.623 (16)	3.4716 (16)	155.8 (13)
N3′—H3′*N*···N5′^{iii}	0.873 (15)	2.418 (15)	3.2662 (17)	164.2 (12)

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