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2-Amino-6-(piperidin-1-yl)-4-*p*-tolylpyridine-3,5-dicarbonitrile

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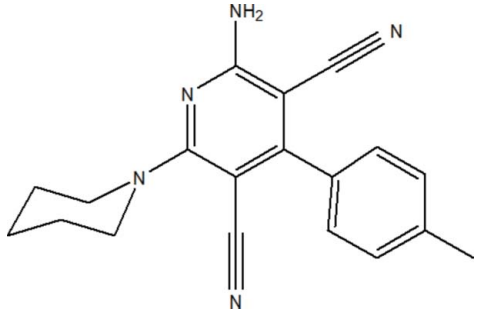
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.148; data-to-parameter ratio = 17.0.

In the title compound, $C_{19}H_{19}N_5$, the piperidine ring adopts a chair conformation. The pyridine ring is essentially planar, with a maximum deviation of 0.039 (2) Å for a C atom substituted with a carbonitrile group. The mean plane of the central pyridine ring makes the dihedral angles of 37.90 (14) and 56.10 (12)° with the piperidine and benzene rings, respectively. In the crystal, molecules are linked *via* N—H···N and C—H···N hydrogen bonds, forming chains along [101], and enclosing $R_2^2(17)$ ring motifs. The chains are linked by further C—H···N hydrogen bonds, forming two-dimensional networks lying parallel to $(10\bar{1})$, and enclosing inversion dimers with $R_2^2(20)$ ring motifs.

Related literature

For background to pyridine derivatives and their biological activity, see: Chaubey & Pandeya (2011). For puckering parameters, see: Cremer & Pople (1975). For graph-set notation, see: Bernstein *et al.* (1995). For a related structure, see: Inglebert *et al.* (2011).



Experimental

Crystal data

$C_{19}H_{19}N_5$
M_r = 317.39
Monoclinic, $P2_1/n$
a = 14.8695 (12) Å
b = 7.7350 (6) Å
c = 15.2791 (13) Å
β = 107.196 (8)°
V = 1678.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 K
0.37 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.972, T_{max} = 0.981
7726 measured reflections
3705 independent reflections
1346 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.148
S = 0.77
3705 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*C*···N3^{i}	0.86	2.18	2.999 (4)	160
C2—H2*B*···N4^{ii}	0.97	2.62	3.509 (4)	153
C19—H19*A*···N4^{iii}	0.96	2.61	3.509 (4)	156

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

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: *ORTEP-3* for Windows (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors gratefully acknowledge Dr Babu Varghese, SAIF, IIT, Chennai, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2416).

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supporting information

Acta Cryst. (2013). E**69**, o1807 [doi:10.1107/S1600536813030845]

2-Amino-6-(piperidin-1-yl)-4-*p*-tolylpyridine-3,5-dicarbonitrile

S. Antony Inglebert, Jayabal Kamalraja, K. Sethusankar and Gnanasambandam Vasuki

S1. Comment

Pyridine ring system is widely distributed in nature, especially in plant kingdom. Many important alkaloids atropine from Deadly nightshade (*Atropa belladonna*) contains saturated pyridine nucleus. The pyridine is found to have a large number of biological activities those including antiviral, anticancer, antimicrobial, antidiabetic and antitubercular. Pyridine is also a very active neutraceutical found in the form of vitamin B3 (Chaubey & Pandeya, 2011).

The cyano groups are flipped to different sides of the pyridine plane with atoms C12 & N3 showing deviations of 0.3416 (1)Å and 0.6489 (1)Å, while atoms C11 & N4 are bent out of the pyridine plane by -0.0866 (1)Å and -0.1408 (1)Å, respectively. The pyridine ring (N1/C6–C10) forms dihedral angles of 37.90 (14)° and 56.10 (12)° with piperidine (N2/C1–C5) and phenyl ring (C13–C18).

The pyridine ring is essentially planar with a maximum deviation of -0.039 (2) Å for C7 atom. The piperidine ring adopts a *chair* conformation [puckering parameters (Cremer & Pople, 1975): Q = 0.579 (3)Å, θ = 172.5 (4)° and φ = 152 (3)°]. The amino group lies in the pyridine ring. The title compound exhibits the structural similarities with the reported related structure (Inglebert *et al.*, 2011).

In the crystal, molecules are connected through the intermolecular C—H···N and N—H···N hydrogen bonds, generating a $R_2^2(17)$ (Bernstein *et al.*, 1995) motif and also chain along *a* axis. In addition, another pair of intermolecular, C—H···N hydrogen bond link neighbouring molecules, forming an inversion dimer and generate a $R_2^2(20)$ ring motif (Table 1).

S2. Experimental

Initially a mixture of 4–methylbenzaldehyde (2 mmol, 0.24 g), malononitrile (3 mmol, 0.198 g), piperidine (1.5 mmol, 0.128 g) and was stirred without any solvent at room temperature. A solid appeared immediately which was dissolved in a minimum amount (3 ml) of ethanol and the solution was refluxed until completion of the reaction (monitered by *TLC*). The reaction mixture was cooled. Ethanol was evaporated under reduced pressure and the residue was extracted with dichloromethane (3×10ml). Evaporation of solvent left the crude solid which was subjected to silica gel column chromatography [25 : 75 / ethyl acetate : hexane] and the product was recrystallized from dichloromethane.

S3. Refinement

H atoms were placed in idealized positions and allowed to ride on the parent atoms,with C—H bond lengths fixed to 0.93Å (aromatic H), 0.96Å (methyl H),0.97Å (methylene H), 0.86Å (N—H) and U_{iso}(H) = 1.2–1.5U_{eq}(C,N).

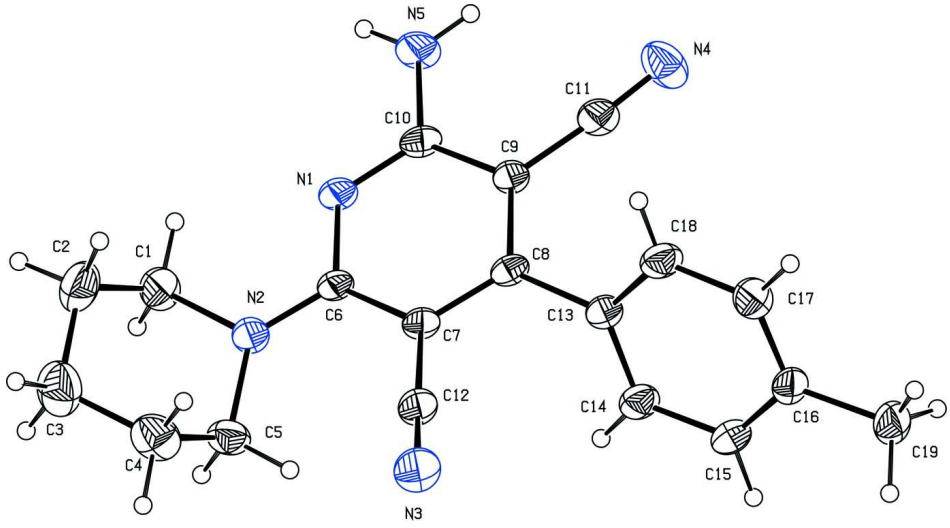

Figure 1

A view of the molecular structure, showing the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

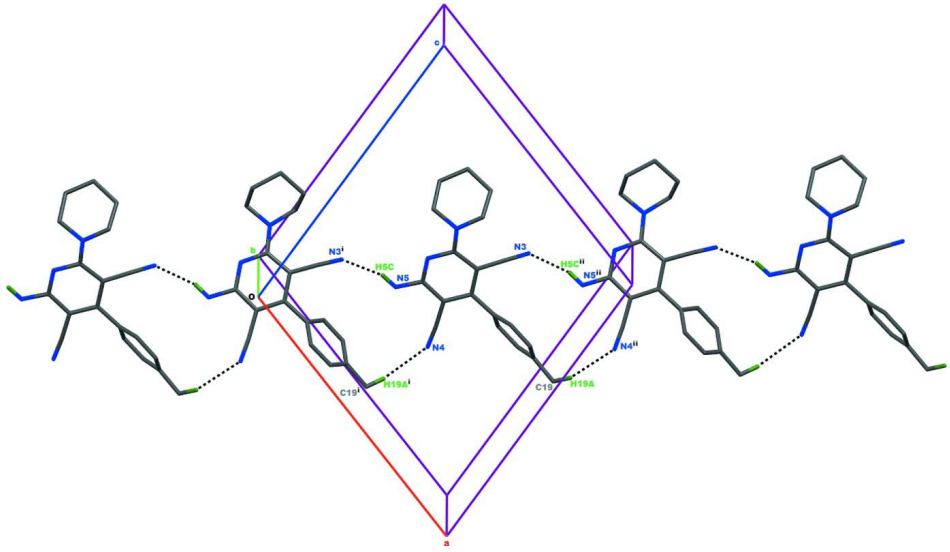

Figure 2

The packing structure of the title compound shows two intermolecular C—H···N and N—H···N hydrogen bond to generate $R_2^2(17)$ motif. H atoms have been omited for clarity.

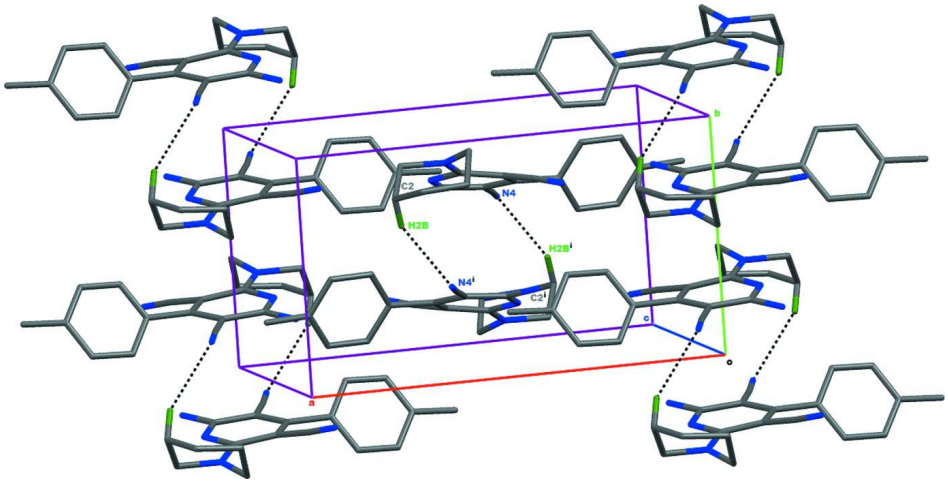

Figure 3

The packing structure of the title compound shows another pair of intermolecular C—H···N hydrogen bonds to form inversion dimer. H atoms have been omited for clarity.

2-Amino-6-(piperidin-1-yl)-4-*p*-tolylpyridine-3,5-dicarbonitrile

Crystal data

$C_{19}H_{19}N_5$
$M_r = 317.39$
Monoclinic, $P2_1/n$
Hall symbol: -p 2yn
$a = 14.8695$ (12) Å
$b = 7.7350$ (6) Å
$c = 15.2791$ (13) Å
$\beta = 107.196$ (8)°
$V = 1678.8$ (2) Å^3
$Z = 4$
$F(000) = 672$
$D_x = 1.256$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3705 reflections
$\theta = 2.8$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Block, colourless
0.37 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine–focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.972$, $T_{max} = 0.981$
7726 measured reflections
3705 independent reflections
1346 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
$h = -19\rightarrow8$
$k = -10\rightarrow9$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.148$
$S = 0.77$
3705 reflections
218 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.0452P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*–factor w*R* 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 $F^2 > 2\sigma(F^2)$ 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}
C1	0.18652 (19)	0.6347 (4)	−0.1252 (2)	0.0608 (9)
H1A	0.2077	0.5189	−0.1334	0.073*
H1B	0.2152	0.6684	−0.0619	0.073*
C2	0.2160 (2)	0.7592 (4)	−0.1883 (3)	0.0738 (10)
H2A	0.2834	0.7499	−0.1776	0.089*
H2B	0.2025	0.8763	−0.1733	0.089*
C3	0.1661 (3)	0.7255 (4)	−0.2895 (3)	0.0804 (11)
H3A	0.1796	0.8190	−0.3261	0.097*
H3B	0.1895	0.6189	−0.3083	0.097*
C4	0.0606 (2)	0.7120 (4)	−0.3062 (2)	0.0694 (9)
H4A	0.0355	0.8241	−0.2971	0.083*
H4B	0.0305	0.6762	−0.3689	0.083*
C5	0.0396 (2)	0.5832 (4)	−0.24158 (19)	0.0541 (8)
H5A	−0.0280	0.5735	−0.2534	0.065*
H5B	0.0636	0.4707	−0.2516	0.065*
C6	0.03918 (17)	0.6941 (3)	−0.08729 (18)	0.0377 (6)
C7	−0.06080 (18)	0.7199 (3)	−0.10909 (17)	0.0393 (7)
C8	−0.09990 (17)	0.7577 (3)	−0.03913 (17)	0.0371 (6)
C9	−0.04006 (17)	0.7845 (3)	0.04943 (17)	0.0390 (6)
C10	0.05840 (18)	0.7707 (3)	0.06310 (18)	0.0423 (7)
C11	−0.07316 (18)	0.8218 (4)	0.1260 (2)	0.0469 (7)
C12	−0.1223 (2)	0.7317 (4)	−0.2007 (2)	0.0501 (7)
C13	−0.20408 (17)	0.7636 (3)	−0.05558 (17)	0.0389 (7)
C14	−0.25728 (18)	0.6183 (3)	−0.09053 (18)	0.0480 (7)
H14	−0.2291	0.5234	−0.1090	0.058*
C15	−0.35192 (19)	0.6144 (4)	−0.09781 (19)	0.0503 (8)
H15	−0.3865	0.5158	−0.1212	0.060*
C16	−0.39660 (18)	0.7517 (4)	−0.07161 (18)	0.0457 (7)
C17	−0.34374 (19)	0.8981 (4)	−0.04005 (19)	0.0530 (8)
H17	−0.3729	0.9948	−0.0245	0.064*
C18	−0.24811 (19)	0.9038 (4)	−0.03101 (19)	0.0510 (8)
H18	−0.2137	1.0029	−0.0082	0.061*
C19	−0.49842 (18)	0.7409 (4)	−0.0753 (2)	0.0621 (9)
H19A	−0.5336	0.6874	−0.1317	0.093*
H19B	−0.5224	0.8552	−0.0719	0.093*

H19C	−0.5044	0.6734	−0.0246	0.093*
N1	0.09533 (14)	0.7257 (3)	−0.00185 (15)	0.0435 (6)
N2	0.08305 (15)	0.6368 (3)	−0.14634 (15)	0.0494 (6)
N3	−0.17316 (17)	0.7510 (3)	−0.27279 (18)	0.0718 (8)
N4	−0.09375 (18)	0.8519 (3)	0.19069 (18)	0.0690 (8)
N5	0.11881 (16)	0.8013 (3)	0.14709 (15)	0.0639 (7)
H5C	0.1785	0.7910	0.1561	0.077*
H5D	0.0976	0.8310	0.1915	0.077*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0354 (18)	0.091 (2)	0.051 (2)	0.0125 (16)	0.0047 (15)	−0.0054 (17)
C2	0.0436 (19)	0.088 (2)	0.091 (3)	−0.0040 (17)	0.0231 (19)	−0.004 (2)
C3	0.081 (3)	0.096 (3)	0.072 (3)	0.000 (2)	0.034 (2)	0.015 (2)
C4	0.073 (2)	0.084 (2)	0.045 (2)	0.0123 (18)	0.0078 (18)	0.0084 (17)
C5	0.0489 (18)	0.0681 (19)	0.0394 (18)	0.0019 (15)	0.0037 (14)	−0.0112 (15)
C6	0.0289 (15)	0.0466 (15)	0.0312 (16)	−0.0013 (12)	−0.0008 (12)	−0.0032 (13)
C7	0.0308 (14)	0.0550 (17)	0.0243 (15)	−0.0002 (13)	−0.0041 (12)	0.0013 (12)
C8	0.0289 (14)	0.0418 (15)	0.0321 (15)	−0.0006 (12)	−0.0043 (12)	0.0029 (12)
C9	0.0305 (14)	0.0521 (16)	0.0287 (16)	0.0030 (13)	0.0001 (12)	0.0008 (13)
C10	0.0328 (15)	0.0516 (16)	0.0308 (16)	0.0012 (13)	−0.0086 (13)	0.0005 (13)
C11	0.0366 (17)	0.0588 (17)	0.0363 (18)	0.0075 (14)	−0.0032 (14)	0.0022 (15)
C12	0.0346 (16)	0.073 (2)	0.0365 (17)	−0.0008 (15)	0.0006 (13)	−0.0015 (15)
C13	0.0291 (14)	0.0505 (16)	0.0302 (15)	0.0044 (13)	−0.0018 (11)	0.0026 (13)
C14	0.0348 (17)	0.0562 (18)	0.0464 (19)	−0.0003 (15)	0.0018 (14)	−0.0069 (14)
C15	0.0346 (17)	0.0627 (19)	0.0467 (19)	−0.0072 (15)	0.0013 (14)	−0.0071 (15)
C16	0.0298 (15)	0.0728 (19)	0.0286 (16)	−0.0015 (16)	−0.0005 (12)	0.0051 (15)
C17	0.0378 (18)	0.069 (2)	0.048 (2)	0.0125 (16)	0.0066 (14)	−0.0023 (15)
C18	0.0380 (17)	0.0588 (18)	0.0479 (19)	−0.0024 (15)	−0.0002 (14)	−0.0071 (15)
C19	0.0348 (16)	0.103 (2)	0.045 (2)	−0.0013 (16)	0.0072 (14)	−0.0007 (17)
N1	0.0292 (12)	0.0603 (14)	0.0322 (14)	0.0019 (11)	−0.0043 (10)	−0.0048 (11)
N2	0.0321 (13)	0.0779 (16)	0.0332 (14)	0.0014 (12)	0.0019 (11)	−0.0058 (12)
N3	0.0418 (15)	0.122 (2)	0.0382 (16)	0.0048 (15)	−0.0092 (12)	0.0035 (15)
N4	0.069 (2)	0.095 (2)	0.0407 (17)	0.0215 (15)	0.0134 (15)	0.0021 (15)
N5	0.0350 (13)	0.1071 (19)	0.0366 (15)	0.0111 (13)	−0.0094 (11)	−0.0156 (14)

Geometric parameters (Å, º)

C1—N2	1.476 (3)	C9—C10	1.420 (3)
C1—C2	1.516 (4)	C9—C11	1.426 (4)
C1—H1A	0.9700	C10—N1	1.315 (3)
C1—H1B	0.9700	C10—N5	1.352 (3)
C2—C3	1.528 (4)	C11—N4	1.142 (3)
C2—H2A	0.9700	C12—N3	1.147 (3)
C2—H2B	0.9700	C13—C18	1.375 (3)
C3—C4	1.517 (4)	C13—C14	1.388 (3)
C3—H3A	0.9700	C14—C15	1.379 (3)

C3—H3B	0.9700	C14—H14	0.9300
C4—C5	1.498 (4)	C15—C16	1.374 (4)
C4—H4A	0.9700	C15—H15	0.9300
C4—H4B	0.9700	C16—C17	1.381 (4)
C5—N2	1.467 (3)	C16—C19	1.501 (4)
C5—H5A	0.9700	C17—C18	1.388 (4)
C5—H5B	0.9700	C17—H17	0.9300
C6—N2	1.336 (3)	C18—H18	0.9300
C6—N1	1.348 (3)	C19—H19A	0.9600
C6—C7	1.438 (3)	C19—H19B	0.9600
C7—C8	1.390 (3)	C19—H19C	0.9600
C7—C12	1.431 (4)	N5—H5C	0.8600
C8—C9	1.398 (3)	N5—H5D	0.8600
C8—C13	1.495 (3)		

N2—C1—C2	109.4 (2)	C8—C9—C10	117.7 (2)
N2—C1—H1A	109.8	C8—C9—C11	123.3 (2)
C2—C1—H1A	109.8	C10—C9—C11	119.0 (2)
N2—C1—H1B	109.8	N1—C10—N5	117.0 (2)
C2—C1—H1B	109.8	N1—C10—C9	123.4 (2)
H1A—C1—H1B	108.2	N5—C10—C9	119.5 (3)
C1—C2—C3	113.0 (3)	N4—C11—C9	175.6 (3)
C1—C2—H2A	109.0	N3—C12—C7	175.8 (3)
C3—C2—H2A	109.0	C18—C13—C14	118.7 (2)
C1—C2—H2B	109.0	C18—C13—C8	122.1 (2)
C3—C2—H2B	109.0	C14—C13—C8	119.0 (2)
H2A—C2—H2B	107.8	C15—C14—C13	120.1 (3)
C4—C3—C2	110.4 (3)	C15—C14—H14	120.0
C4—C3—H3A	109.6	C13—C14—H14	120.0
C2—C3—H3A	109.6	C16—C15—C14	122.0 (3)
C4—C3—H3B	109.6	C16—C15—H15	119.0
C2—C3—H3B	109.6	C14—C15—H15	119.0
H3A—C3—H3B	108.1	C15—C16—C17	117.5 (2)
C5—C4—C3	110.0 (3)	C15—C16—C19	121.0 (3)
C5—C4—H4A	109.7	C17—C16—C19	121.5 (3)
C3—C4—H4A	109.7	C16—C17—C18	121.4 (3)
C5—C4—H4B	109.7	C16—C17—H17	119.3
C3—C4—H4B	109.7	C18—C17—H17	119.3
H4A—C4—H4B	108.2	C13—C18—C17	120.3 (3)
N2—C5—C4	110.5 (2)	C13—C18—H18	119.9
N2—C5—H5A	109.6	C17—C18—H18	119.9
C4—C5—H5A	109.6	C16—C19—H19A	109.5
N2—C5—H5B	109.6	C16—C19—H19B	109.5
C4—C5—H5B	109.6	H19A—C19—H19B	109.5
H5A—C5—H5B	108.1	C16—C19—H19C	109.5
N2—C6—N1	115.3 (2)	H19A—C19—H19C	109.5
N2—C6—C7	124.6 (2)	H19B—C19—H19C	109.5
N1—C6—C7	120.1 (2)	C10—N1—C6	120.1 (2)

C8—C7—C12	116.6 (2)	C6—N2—C5	127.2 (2)
C8—C7—C6	119.3 (2)	C6—N2—C1	122.8 (2)
C12—C7—C6	123.6 (3)	C5—N2—C1	109.8 (2)
C7—C8—C9	119.0 (2)	C10—N5—H5C	120.0
C7—C8—C13	121.7 (2)	C10—N5—H5D	120.0
C9—C8—C13	119.3 (2)	H5C—N5—H5D	120.0
N2—C1—C2—C3	−53.8 (3)	C9—C8—C13—C14	−120.1 (3)
C1—C2—C3—C4	50.1 (4)	C18—C13—C14—C15	−1.7 (4)
C2—C3—C4—C5	−52.2 (4)	C8—C13—C14—C15	173.6 (2)
C3—C4—C5—N2	60.4 (3)	C13—C14—C15—C16	0.2 (4)
N2—C6—C7—C8	171.4 (2)	C14—C15—C16—C17	2.1 (4)
N1—C6—C7—C8	−7.6 (4)	C14—C15—C16—C19	−176.6 (3)
N2—C6—C7—C12	−17.2 (4)	C15—C16—C17—C18	−2.9 (4)
N1—C6—C7—C12	163.8 (2)	C19—C16—C17—C18	175.7 (3)
C12—C7—C8—C9	−166.5 (2)	C14—C13—C18—C17	0.8 (4)
C6—C7—C8—C9	5.6 (4)	C8—C13—C18—C17	−174.3 (3)
C12—C7—C8—C13	15.9 (4)	C16—C17—C18—C13	1.5 (4)
C6—C7—C8—C13	−172.1 (2)	N5—C10—N1—C6	−179.7 (2)
C7—C8—C9—C10	−0.3 (3)	C9—C10—N1—C6	1.7 (4)
C13—C8—C9—C10	177.4 (2)	N2—C6—N1—C10	−175.2 (2)
C7—C8—C9—C11	−179.2 (2)	C7—C6—N1—C10	3.9 (4)
C13—C8—C9—C11	−1.5 (4)	N1—C6—N2—C5	176.4 (2)
C8—C9—C10—N1	−3.6 (4)	C7—C6—N2—C5	−2.6 (4)
C11—C9—C10—N1	175.4 (2)	N1—C6—N2—C1	−9.6 (4)
C8—C9—C10—N5	177.9 (2)	C7—C6—N2—C1	171.4 (2)
C11—C9—C10—N5	−3.1 (4)	C4—C5—N2—C6	109.7 (3)
C7—C8—C13—C18	−127.4 (3)	C4—C5—N2—C1	−64.9 (3)
C9—C8—C13—C18	55.0 (3)	C2—C1—N2—C6	−114.6 (3)
C7—C8—C13—C14	57.5 (3)	C2—C1—N2—C5	60.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*C*···N3^{i}	0.86	2.18	2.999 (4)	160
C2—H2*B*···N4^{ii}	0.97	2.62	3.509 (4)	153
C19—H19*A*···N4^{iii}	0.96	2.61	3.509 (4)	156

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