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2-Amino-4-(4-chlorophenyl)-6-(pyrrolidin-1-yl)pyridine-3,5-dicarbonitrile

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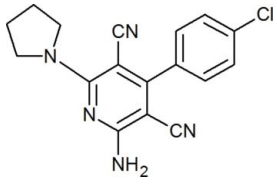
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.042; wR factor = 0.097; data-to-parameter ratio = 15.1.

In the title compound, $C_{17}H_{14}ClN_5$, two C atoms and their attached H atoms of the pyrrolidine ring are disordered over two sets of sites with an occupancy ratio of 0.638 (10): 0.362 (10). The benzene and pyridine rings are inclined to one another by 60.57 (8)°. In the crystal, the amino group forms an N—H···N hydrogen bond with one of the cyano groups, linking the molecules into chains along [010].

Related literature

For a similar compound, see: Inglebert *et al.* (2011). For related structures, see: Chao *et al.* (1975); Kvick *et al.* (1976). For bond-length data, see: Atoji & Lipscomb (1953). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{17}H_{14}ClN_5$
M_r = 323.77
Triclinic, $P\overline{1}$
a = 7.318 (5) Å
b = 9.060 (5) Å
c = 12.011 (5) Å
α = 87.196 (5)°
β = 80.477 (5)°
γ = 83.795 (5)°
V = 780.4 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 295 K
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.916, T_{max} = 0.939
6077 measured reflections
3570 independent reflections
1887 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.097
S = 0.85
3570 reflections
237 parameters
11 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N4^{i}	0.92 (1)	2.12 (1)	2.992 (3)	160 (2)

Symmetry code: (i) $x, y+1, z$.

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* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2335).

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supporting information

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2-Amino-4-(4-chlorophenyl)-6-(pyrrolidin-1-yl)pyridine-3,5-dicarbonitrile

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

S1. Comment

Pyridine and its derivatives play an important role in hetrocyclic chemistry. Pyridine containing compounds are the new class of anti–*HIV* molecules, which particularly inhibit *RNA* dependent *DNA* polymerase or reverse transcriptace and thus act as non–nucleoside reverse transcriptace inhibitors. They also exhibit cytotoxic, anti–cancer, anti–tumour and anti–bacterial activity.

The pyrrolidine ring adopts a twisted conformation in both the major and minor conformers (occupancy factors of 0.638 (10)/0.362 (10) respectively). Puckering parameters (Cremer & Pople, 1975) are q_2 and φ_2, of 0.422 (6)Å and 273.9 (4)° for the major conformer (N5/C15/C16/C17/C18) and 0.469 (10)Å and 86.4 (6)°, respectively, for the minor conformer (N5/C15/C16′/C17′/C18).

The bond lengths of the nitrile groups attached to pyridine ring are typical (N4≡C11 = 1.148 (2)Å and C9≡N3 = 1.142 (2)Å). The nitrile groups form angles with parent C atoms: 177.1 (2)° and 174.5 (2)°. The sum angles around the atom C12 are slightly less 360° (real 358.0 (2)°) - deformed by the amino group, as seen in other aminopyridines (Chao *et al.*, 1975; Kvick *et al.*, 1976). This behaviour characterizes the resonance of the N2 lone pair with the aromatic ring. The effect can also be verified by the shortening of the C12—N2 bond (1.345 (2)Å) relative to a normal single C—N bond (1.483Å for C—N in methaneamine (Atoji & Lipscomb, 1953).

The amino group is planar with the pyridine ring as indicated by the torsion angle N2—C12—N1—C13 = 179.75 (16)°. The chlorine atom attached at C1 deviates by -0.0817 (3)Å from the mean plane of the phenyl ring. The title structure exhibits structural similarities with the previously reported structure (Inglebert *et al.*, 2011).

In the crystal structure, the classical intermolecular N2—H2B···N4^{i} hydrogen bonds link the molecules into chains along the *b* axis. Symmetry code: (i) *x*, *y*+1, *z*.

S2. Experimental

A mixture of 4–chlorobenzaldehyde (2 mmoL, 0.28 g), malononitrile (3 mmoL, 0.198 g), pyrrolidine (1.5 mmoL, 0.1 g) was stirred without any solvent at room temperature. A solid appeared immediately which has 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 dicholoro-methane (3×10 ml). Evaporation of solvent left the crude solid which was subjected to silica gel column chromatography [25:75 ethyl acetate/hexane] and the product was recrysallized from dichloromethane.

S3. Refinement

H atoms attached to C atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.93Å (aromatic H) and C—H = 0.97Å (methylene H) U_{iso}(H) = 1.2U_{eq}(C). H atoms of amino group were located from difference Fourier map and refined freely.

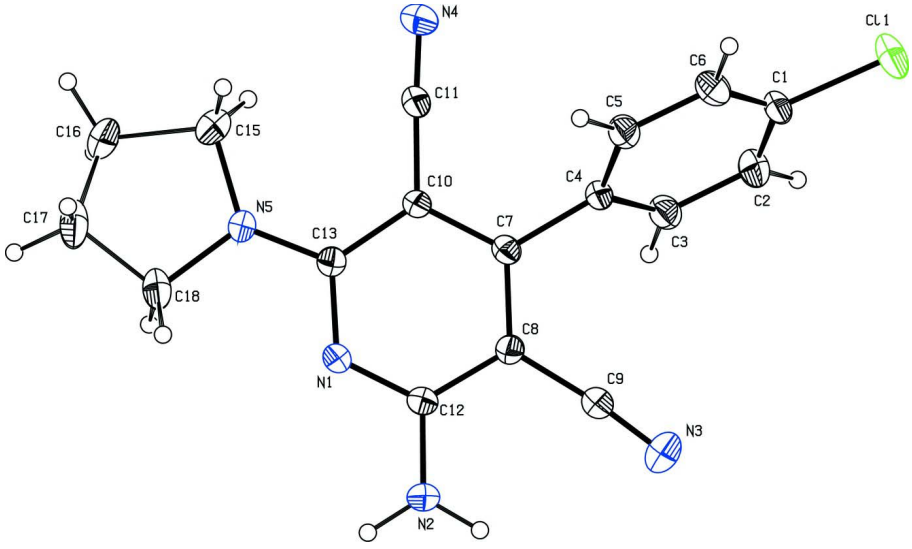

Figure 1

The molecular structure of the title compound, showing the atom numbering scheme. Displacement ellipsoids are drawn at 30% probability level. H atoms are presented as small spheres of arbitary radius. The minor occupancy disordered atoms have been omitted for clarity.

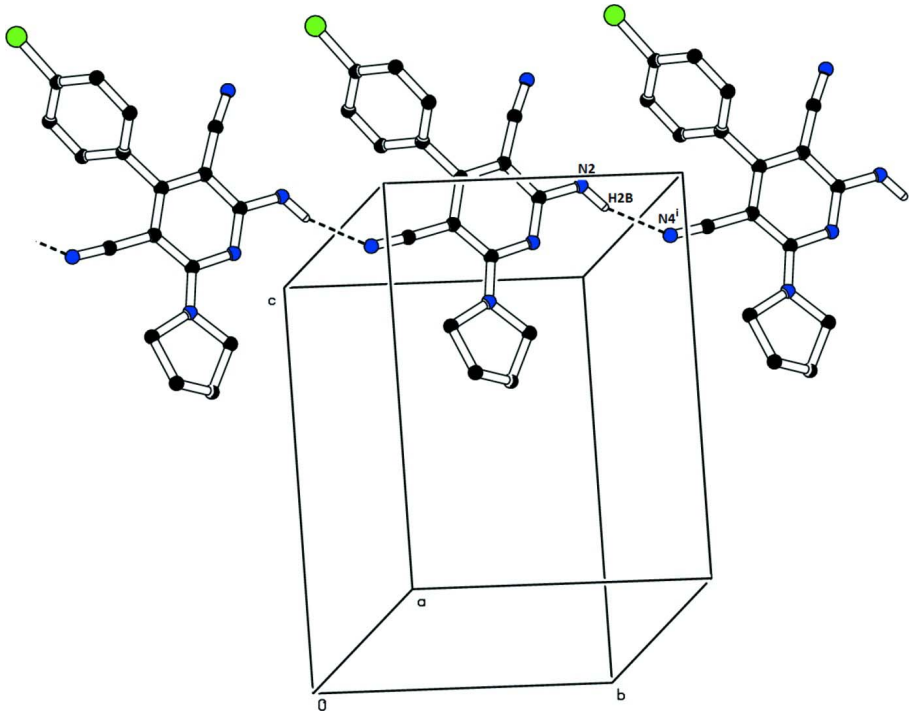

Figure 2

The packing diagram of the title compound, which shows intermolecular N2—H2B···N4^{i} interactions (dashed lines). H atoms not involved in hydrogen bonds have been omitted for clarity.

2-Amino-4-(4-chlorophenyl)-6-(pyrrolidin-1-yl)pyridine-3,5-dicarbonitrile

Crystal data

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$M_r = 323.77$
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Hall symbol: -P 1
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$c = 12.011$ (5) Å
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$\beta = 80.477$ (5)°
$\gamma = 83.795$ (5)°
$V = 780.4$ (8) Å^3
$Z = 2$
$F(000) = 336$
$D_x = 1.378$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3570 reflections
$\theta = 2.8$–$29.3°$
$\mu = 0.25$ mm^{-1}
$T = 295$ K
Block, colourless
0.35 × 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)
$T_{min} = 0.916$, $T_{max} = 0.939$
6077 measured reflections
3570 independent reflections
1887 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 29.3°$, $\theta_{min} = 2.8°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 11$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.097$
$S = 0.85$
3570 reflections
237 parameters
11 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
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.014 (2)

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 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}	Occ. (<1)
C1	0.7572 (3)	0.0214 (2)	1.33801 (16)	0.0432 (5)	
C2	0.9078 (3)	0.1010 (2)	1.30733 (17)	0.0459 (5)	

H2	1.0082	0.0866	1.3465	0.055*	
C3	0.9092 (3)	0.2024 (2)	1.21800 (16)	0.0390 (5)	
H3	1.0107	0.2572	1.1977	0.047*	
C4	0.7624 (2)	0.22397 (19)	1.15801 (14)	0.0311 (4)	
C5	0.6137 (3)	0.1396 (2)	1.18885 (16)	0.0409 (5)	
H5	0.5149	0.1510	1.1484	0.049*	
C6	0.6108 (3)	0.0393 (2)	1.27858 (17)	0.0486 (5)	
H6	0.5101	−0.0163	1.2990	0.058*	
C7	0.7579 (2)	0.34351 (18)	1.06767 (15)	0.0287 (4)	
C8	0.7651 (2)	0.48942 (18)	1.09633 (15)	0.0299 (4)	
C9	0.7812 (3)	0.5310 (2)	1.20691 (18)	0.0383 (5)	
C10	0.7429 (2)	0.31384 (18)	0.95678 (14)	0.0288 (4)	
C11	0.7380 (3)	0.1630 (2)	0.93015 (15)	0.0368 (5)	
C12	0.7507 (2)	0.60362 (18)	1.01258 (15)	0.0291 (4)	
C13	0.7366 (2)	0.43534 (19)	0.87573 (15)	0.0297 (4)	
N5	0.7283 (2)	0.42030 (16)	0.76655 (12)	0.0364 (4)	
C18	0.7235 (3)	0.5492 (2)	0.68715 (16)	0.0519 (6)	
H18A	0.8436	0.5884	0.6720	0.062*	
H18B	0.6299	0.6271	0.7177	0.062*	
C17	0.6766 (10)	0.4927 (6)	0.5828 (4)	0.0567 (15)	0.638 (10)
H17A	0.7199	0.5533	0.5169	0.068*	0.638 (10)
H17B	0.5437	0.4872	0.5884	0.068*	0.638 (10)
C16	0.7840 (11)	0.3389 (7)	0.5805 (4)	0.0657 (18)	0.638 (10)
H16A	0.9162	0.3446	0.5558	0.079*	0.638 (10)
H16B	0.7389	0.2747	0.5310	0.079*	0.638 (10)
C17′	0.7780 (18)	0.4694 (13)	0.5745 (7)	0.068 (3)	0.361 (10)
H17C	0.7346	0.5301	0.5135	0.082*	0.362 (10)
H17D	0.9121	0.4476	0.5566	0.082*	0.362 (10)
C16′	0.6834 (18)	0.3273 (12)	0.5927 (8)	0.061 (3)	0.362 (10)
H16C	0.7328	0.2556	0.5352	0.073*	0.362 (10)
H16D	0.5492	0.3453	0.5982	0.073*	0.362 (10)
N1	0.73637 (19)	0.57681 (15)	0.90682 (12)	0.0323 (4)	
N2	0.7503 (2)	0.74643 (18)	1.03834 (16)	0.0440 (4)	
N3	0.7954 (3)	0.5758 (2)	1.29203 (16)	0.0641 (6)	
N4	0.7312 (3)	0.04021 (19)	0.91349 (15)	0.0589 (5)	
C15	0.7437 (4)	0.2824 (2)	0.70643 (18)	0.0634 (7)	
H15A	0.6287	0.2354	0.7221	0.076*	
H15B	0.8451	0.2130	0.7257	0.076*	
Cl1	0.74935 (9)	−0.10029 (6)	1.45478 (5)	0.0728 (2)	
H2A	0.759 (2)	0.771 (2)	1.1096 (10)	0.048 (6)*	
H2B	0.745 (3)	0.8223 (17)	0.9853 (14)	0.066 (7)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0684 (14)	0.0303 (11)	0.0283 (11)	−0.0027 (10)	−0.0039 (10)	0.0067 (9)
C2	0.0557 (13)	0.0439 (12)	0.0387 (12)	−0.0010 (10)	−0.0146 (10)	0.0077 (10)
C3	0.0415 (11)	0.0378 (11)	0.0385 (12)	−0.0088 (9)	−0.0076 (9)	0.0051 (9)

C4	0.0398 (11)	0.0271 (9)	0.0256 (10)	−0.0039 (8)	−0.0034 (8)	0.0015 (8)
C5	0.0487 (12)	0.0400 (11)	0.0370 (12)	−0.0138 (9)	−0.0116 (9)	0.0056 (9)
C6	0.0612 (13)	0.0420 (12)	0.0434 (13)	−0.0218 (10)	−0.0029 (11)	0.0084 (10)
C7	0.0281 (9)	0.0274 (10)	0.0307 (10)	−0.0048 (7)	−0.0050 (8)	0.0030 (8)
C8	0.0330 (10)	0.0300 (10)	0.0270 (10)	−0.0056 (8)	−0.0044 (8)	−0.0009 (8)
C9	0.0478 (12)	0.0321 (11)	0.0352 (12)	−0.0076 (9)	−0.0064 (9)	0.0022 (9)
C10	0.0337 (10)	0.0251 (9)	0.0274 (10)	−0.0044 (8)	−0.0041 (8)	0.0000 (8)
C11	0.0504 (12)	0.0305 (11)	0.0285 (11)	−0.0044 (9)	−0.0044 (9)	0.0035 (8)
C12	0.0288 (10)	0.0254 (10)	0.0329 (11)	−0.0023 (8)	−0.0047 (8)	−0.0007 (8)
C13	0.0306 (10)	0.0300 (10)	0.0287 (11)	−0.0034 (8)	−0.0054 (8)	−0.0006 (8)
N5	0.0507 (10)	0.0339 (9)	0.0257 (9)	−0.0057 (7)	−0.0090 (7)	−0.0005 (7)
C18	0.0719 (15)	0.0521 (13)	0.0318 (12)	−0.0033 (11)	−0.0136 (11)	0.0086 (10)
C17	0.059 (3)	0.083 (3)	0.031 (2)	−0.018 (3)	−0.015 (3)	0.0128 (19)
C16	0.108 (5)	0.064 (3)	0.029 (2)	−0.019 (4)	−0.011 (3)	−0.007 (2)
C17′	0.076 (8)	0.093 (8)	0.041 (5)	−0.027 (7)	−0.019 (5)	0.014 (4)
C16′	0.073 (7)	0.071 (6)	0.038 (4)	−0.009 (5)	−0.006 (5)	−0.008 (4)
N1	0.0412 (9)	0.0268 (8)	0.0297 (9)	−0.0040 (7)	−0.0089 (7)	0.0027 (7)
N2	0.0700 (12)	0.0262 (9)	0.0384 (11)	−0.0060 (8)	−0.0158 (9)	−0.0027 (8)
N3	0.0930 (15)	0.0639 (13)	0.0390 (12)	−0.0137 (11)	−0.0146 (11)	−0.0101 (10)
N4	0.0976 (15)	0.0308 (10)	0.0480 (12)	−0.0093 (10)	−0.0091 (10)	−0.0003 (9)
C15	0.1068 (19)	0.0471 (14)	0.0404 (14)	−0.0073 (13)	−0.0214 (13)	−0.0100 (11)
Cl1	0.1163 (6)	0.0539 (4)	0.0454 (4)	−0.0100 (3)	−0.0114 (3)	0.0240 (3)

Geometric parameters (Å, º)

C1—C2	1.372 (3)	C13—N1	1.352 (2)
C1—C6	1.374 (3)	N5—C15	1.458 (3)
C1—Cl1	1.7385 (19)	N5—C18	1.472 (2)
C2—C3	1.377 (3)	C18—C17	1.481 (5)
C2—H2	0.9300	C18—C17′	1.538 (8)
C3—C4	1.382 (2)	C18—H18A	0.9700
C3—H3	0.9300	C18—H18B	0.9700
C4—C5	1.388 (2)	C17—C16	1.523 (7)
C4—C7	1.497 (2)	C17—H17A	0.9700
C5—C6	1.374 (3)	C17—H17B	0.9700
C5—H5	0.9300	C16—C15	1.564 (5)
C6—H6	0.9300	C16—H16A	0.9700
C7—C8	1.391 (2)	C16—H16B	0.9700
C7—C10	1.396 (2)	C17′—C16′	1.517 (9)
C8—C12	1.415 (2)	C17′—H17C	0.9700
C8—C9	1.425 (3)	C17′—H17D	0.9700
C9—N3	1.143 (2)	C16′—C15	1.527 (8)
C10—C11	1.424 (3)	C16′—H16C	0.9700
C10—C13	1.435 (2)	C16′—H16D	0.9700
C11—N4	1.147 (2)	N2—H2A	0.907 (9)
C12—N1	1.328 (2)	N2—H2B	0.916 (9)
C12—N2	1.345 (2)	C15—H15A	0.9700
C13—N5	1.337 (2)	C15—H15B	0.9700

C2—C1—C6	120.58 (18)	C17′—C18—H18A	87.7
C2—C1—Cl1	119.71 (16)	N5—C18—H18B	110.6
C6—C1—Cl1	119.71 (16)	C17—C18—H18B	110.6
C1—C2—C3	119.43 (18)	C17′—C18—H18B	136.3
C1—C2—H2	120.3	H18A—C18—H18B	108.8
C3—C2—H2	120.3	C18—C17—C16	100.5 (4)
C2—C3—C4	121.07 (18)	C18—C17—H17A	111.7
C2—C3—H3	119.5	C16—C17—H17A	111.7
C4—C3—H3	119.5	C18—C17—H17B	111.7
C3—C4—C5	118.45 (17)	C16—C17—H17B	111.7
C3—C4—C7	120.55 (16)	H17A—C17—H17B	109.4
C5—C4—C7	120.84 (16)	C17—C16—C15	103.0 (4)
C6—C5—C4	120.70 (18)	C17—C16—H16A	111.2
C6—C5—H5	119.7	C15—C16—H16A	111.2
C4—C5—H5	119.7	C17—C16—H16B	111.2
C1—C6—C5	119.75 (19)	C15—C16—H16B	111.2
C1—C6—H6	120.1	H16A—C16—H16B	109.1
C5—C6—H6	120.1	C16′—C17′—C18	105.0 (7)
C8—C7—C10	119.14 (16)	C16′—C17′—H17C	110.7
C8—C7—C4	118.54 (16)	C18—C17′—H17C	110.7
C10—C7—C4	122.30 (16)	C16′—C17′—H17D	110.7
C7—C8—C12	118.67 (16)	C18—C17′—H17D	110.7
C7—C8—C9	123.41 (16)	H17C—C17′—H17D	108.8
C12—C8—C9	117.90 (16)	C17′—C16′—C15	96.3 (7)
N3—C9—C8	174.5 (2)	C17′—C16′—H16C	112.5
C7—C10—C11	117.62 (15)	C15—C16′—H16C	112.5
C7—C10—C13	118.72 (15)	C17′—C16′—H16D	112.5
C11—C10—C13	123.66 (16)	C15—C16′—H16D	112.5
N4—C11—C10	177.1 (2)	H16C—C16′—H16D	110.0
N1—C12—N2	117.00 (16)	C12—N1—C13	119.72 (15)
N1—C12—C8	122.72 (16)	C12—N2—H2A	120.3 (12)
N2—C12—C8	120.28 (17)	C12—N2—H2B	122.1 (13)
N5—C13—N1	114.88 (15)	H2A—N2—H2B	117.5 (18)
N5—C13—C10	124.18 (16)	N5—C15—C16′	105.3 (5)
N1—C13—C10	120.93 (16)	N5—C15—C16	101.7 (3)
C13—N5—C15	127.41 (16)	C16′—C15—C16	27.8 (3)
C13—N5—C18	121.73 (15)	N5—C15—H15A	111.4
C15—N5—C18	110.50 (16)	C16′—C15—H15A	84.8
N5—C18—C17	105.5 (3)	C16—C15—H15A	111.4
N5—C18—C17′	99.8 (5)	N5—C15—H15B	111.4
C17—C18—C17′	28.3 (4)	C16′—C15—H15B	131.2
N5—C18—H18A	110.6	C16—C15—H15B	111.4
C17—C18—H18A	110.6	H15A—C15—H15B	109.3

C6—C1—C2—C3	1.8 (3)	C7—C10—C13—N1	−3.1 (2)
Cl1—C1—C2—C3	−176.95 (15)	C11—C10—C13—N1	178.08 (16)
C1—C2—C3—C4	−0.8 (3)	N1—C13—N5—C15	173.81 (18)

C2—C3—C4—C5	−0.8 (3)	C10—C13—N5—C15	−7.1 (3)
C2—C3—C4—C7	174.70 (17)	N1—C13—N5—C18	1.3 (2)
C3—C4—C5—C6	1.4 (3)	C10—C13—N5—C18	−179.57 (17)
C7—C4—C5—C6	−174.06 (17)	C13—N5—C18—C17	−168.9 (3)
C2—C1—C6—C5	−1.2 (3)	C15—N5—C18—C17	17.4 (4)
Cl1—C1—C6—C5	177.55 (15)	C13—N5—C18—C17′	162.6 (5)
C4—C5—C6—C1	−0.5 (3)	C15—N5—C18—C17′	−11.1 (5)
C3—C4—C7—C8	−57.7 (2)	N5—C18—C17—C16	−37.2 (6)
C5—C4—C7—C8	117.6 (2)	C17′—C18—C17—C16	44.7 (9)
C3—C4—C7—C10	123.59 (19)	C18—C17—C16—C15	43.0 (8)
C5—C4—C7—C10	−61.0 (2)	N5—C18—C17′—C16′	37.4 (11)
C10—C7—C8—C12	2.1 (2)	C17—C18—C17′—C16′	−67.1 (10)
C4—C7—C8—C12	−176.63 (16)	C18—C17′—C16′—C15	−47.4 (13)
C10—C7—C8—C9	−179.69 (16)	N2—C12—N1—C13	179.75 (15)
C4—C7—C8—C9	1.6 (3)	C8—C12—N1—C13	−0.5 (2)
C8—C7—C10—C11	179.32 (16)	N5—C13—N1—C12	−177.73 (15)
C4—C7—C10—C11	−2.0 (2)	C10—C13—N1—C12	3.1 (2)
C8—C7—C10—C13	0.4 (2)	C13—N5—C15—C16′	168.2 (5)
C4—C7—C10—C13	179.06 (16)	C18—N5—C15—C16′	−18.6 (5)
C7—C8—C12—N1	−2.2 (2)	C13—N5—C15—C16	−163.4 (3)
C9—C8—C12—N1	179.51 (16)	C18—N5—C15—C16	9.8 (4)
C7—C8—C12—N2	177.60 (17)	C17′—C16′—C15—N5	39.5 (11)
C9—C8—C12—N2	−0.7 (2)	C17′—C16′—C15—C16	−46.5 (9)
C7—C10—C13—N5	177.84 (15)	C17—C16—C15—N5	−32.6 (7)
C11—C10—C13—N5	−1.0 (3)	C17—C16—C15—C16′	68.1 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···N4^{i}	0.92 (1)	2.12 (1)	2.992 (3)	160 (2)

Symmetry code: (i) *x*, *y*+1, *z*.