Crystal structure of 3-amino-1-propylpyridinium bromide

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The title molecular salt, $C_8H_{13}N_2^+ \cdot Br^-$, crystallizes with two independent 3-aminopyridinium cations and two bromide anions in the asymmetric unit ($Z' = 2$). In the pyridine ring, the N atom is alkylated by a propyl group. The dihedral angle between the mean planes of the pyridinium ring and the propyl group is 84.84 (2)° in cation A, whereas the corresponding angle is 89.23 (2)° in cation B. In the crystal, the anions and cations are linked via N—H···Br and C—H···Br hydrogen bonds, forming chains propagating along [100].

1. Chemical context

Aminopyridinium and 1-alkyl-aminopyridinium salts display a wide range of antimicrobial activity (Sundararaman et al., 2013; Ilangovan et al., 2012). They have found many applications such as surfactants (Gama et al., 1981), ionic liquids (Muldoon et al., 2010; Petkovic et al., 2011), liquid-crystal display mediums (Ezaki & Kokeguchi, 2006), ionic crystals for second-order non-linear optics (Anwar et al., 2001), phase-transfer catalysts in organic transformations (Kupetis et al., 2002) and additives for protein refolding processes (Yamamoto et al., 2011). In addition, the amino group in the pyridinium ring participates through hydrogen bonds with wool proteins (Zhao & Sun, 2007; Calas et al., 2007).

2. Structural commentary

The asymmetric unit of the title salt, consists of two 3-aminopyrdinium cations and two bromide anions, as shown in Fig. 1. The geometrical parameters of the cation moiety are comparable with those of a related structure, 3-amino-1-(4-nitrobenzyl)pyridinium bromide (Sundar et al., 2006). The molecular structure of the two cations are very similar with weighted and unit-weight r.m.s. fits of 0.089 and 0.081 Å, respectively, for ten fitted atoms (Fig. 2). The dihedral angle
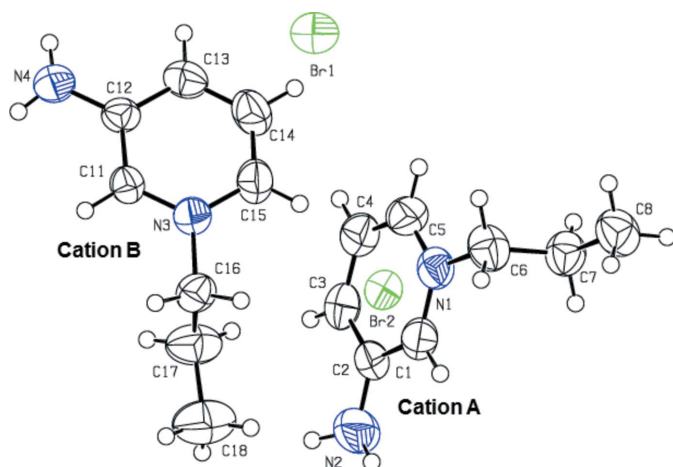

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Figure 1
The molecular structure of the title salt, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

between the mean planes of the pyridinium ring (N2/C1–C5) and the propyl group (N1/C6–C8) is 84.84 (2)° in cation A, whereas the corresponding angle is 89.23 (2)° in cation B.

3. Supramolecular features

The crystal structure of the title salt, is stabilized by a network of intermolecular N—H···Br and C—H···Br hydrogen bonds (Table 1 and Fig. 3). Anion Br2 is involved in five hydrogen bonds as an acceptor while anion Br1 is involved in only two hydrogen bonds. The dimerization of cation A mediates through two bromide anions with the aid of two N—H···Br and C—H···Br hydrogen bonds. As shown in Fig. 4, these interactions generate an $R_4^2(12)$ loop. Atom C16 (via H16A) forms a C—H···Br^i hydrogen bond with bromide anion Br2
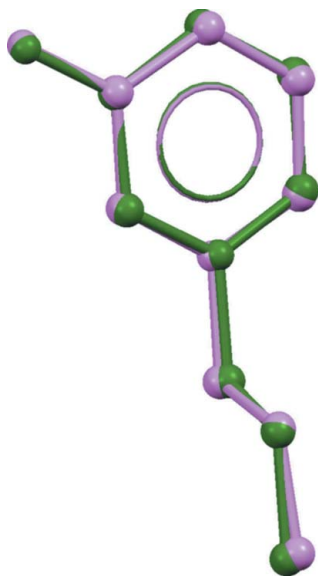
Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Br2^i	0.90 (2)	2.47 (2)	3.364 (3)	177 (4)
N2—H2B···Br2^{ii}	0.90 (2)	2.54 (2)	3.419 (3)	168 (4)
N4—H4A···Br1^{iii}	0.83 (2)	2.58 (2)	3.406 (3)	172 (3)
N4—H4B···Br2^{iv}	0.87 (2)	2.57 (2)	3.434 (3)	171 (3)
C6—H6A···Br2	0.97	2.88	3.655 (4)	138
C6—H6B···Br1^{ii}	0.97	2.84	3.775 (4)	163
C16—H16A···Br2^v	0.97	2.91	3.866 (3)	167

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

[symmetry code: (i) $x + 1, y, z$]. The same Br2 anion acts as an acceptor for an N—H···Br hydrogen bond with atom N4 of cation B. These interactions form a chain which runs parallel to the a axis (Fig. 5).
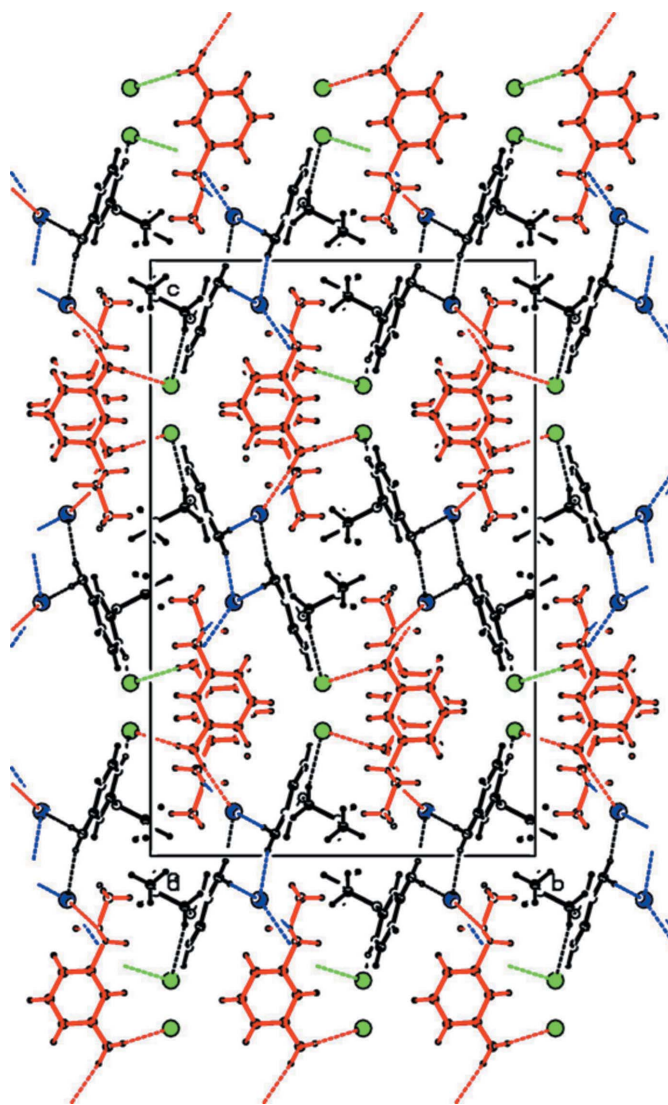

Figure 3
The crystal packing of the title salt projected onto the bc plane. The N—H···Br and C—H···Br hydrogen bonds are shown as dashed lines (see Table 1 for details).

Figure 2
Structural superimposition of the non-H atoms of the pyridinium cations (green: cation A; violet: cation B).
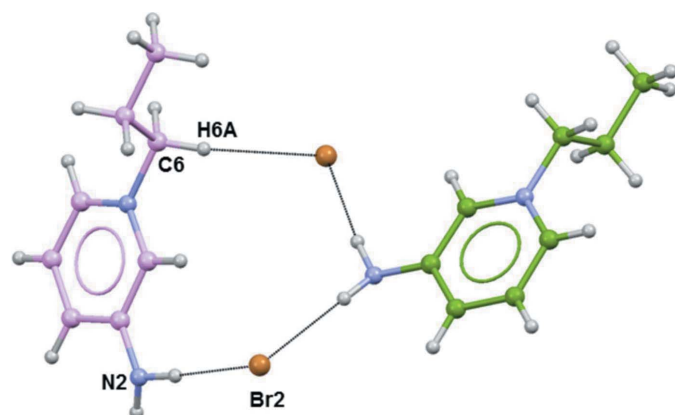
Figure 4
Part of the crystal structure of the title salt, showing the formation of an $R_2^4(12)$ ring motif (see Table 1 for details; only the interacting atoms are labelled).

4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update May 2014; Groom & Allen, 2014) for 4-amino-pyridinium halide salts gave nine hits, while a search for 3-aminopyridinium salts yielded eight hits. They all have different substituents at the pyridine ring N position, and include for example, 2-(3-aminopyridinium-1-yl)propanoate hydrobromide hemihydrate (CCDC refcode: IVAWUY; Kowalczyk *et al.*, 2011), 2-(3-aminopyridinium-1-yl)-3-carboxypropanoate monohydrate (CCDC refcode: LAQGAN; Millán Corrales *et al.*, 2012), 3-amino-1-(carboxymethyl)-pyridinium chloride (CCDC refcode: PABTIX; Kowalczyk *et al.*, 2010) and 3-Amino-1-(4-nitrobenzyl)pyridinium bromide (CCDC refcode: XEBFUG; Sundar *et al.*, 2006). The mean planes of the substituent groups at the ring N atom make dihedral angles of *ca* 80.3° with the 3-aminopyridinium ring in IVAWUY and *ca* 86.6° in PABTIX. In LAQGAN, the propanoate moiety is inclined at an angle of *ca* 86.6°, and the
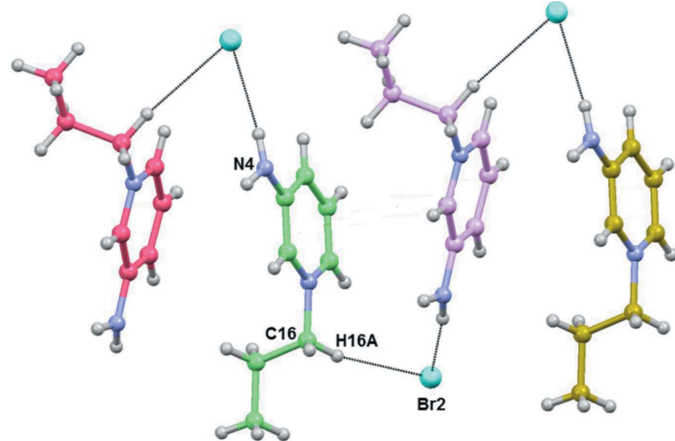

Figure 5
Part of the crystal structure of the title salt, showing the formation of a hydrogen-bonded chain that runs parallel to the *a* axis (see Table 1 for details; only the interacting atoms are labelled).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_{13}N_2^+ \cdot Br^-$
M_r	217.11
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, *b*, *c* (Å)	8.2937 (1), 17.4137 (3), 26.9626 (4)
V (Å^3)	3894.05 (10)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.17
Crystal size (mm)	$0.12 \times 0.10 \times 0.10$
Data collection	
Diffractometer	Bruker *SMART* CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.635, 0.681
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21922, 4491, 2698
R_{int}	0.043
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.085, 1.00
No. of reflections	4491
No. of parameters	214
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.32

Computer programs: *SMART* and *SAINT* (Bruker, 2008), *SHELXS2014* and *SHELXL2014* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

carboxy moiety by *ca* 68.4°, with respect to the 3-aminopyridinium ring. In XEBFUG, the 4-nitrobenzyl ring makes a dihedral angle of *ca* 88.7 ° with the 3-aminopyridinium ring.

5. Synthesis and crystallization

The title salt was prepared by dissolving 3-aminopyridine (0.94 g, 10 m*M*) in dried acetone (20 ml) and adding *n*-propyl bromide (1.48g, 12 m*M*). The reaction mixture was stirred at room temperature for 8 h. The title salt precipitated as a white solid, which was filtered and washed with cold acetone and dried in vacuum to afford the stable salt. It was recrystallized from an aqueous ethanol solution giving colourless prismatic crystals.

6. Refinement

The details of crystal data, data collection and structure refinement are summarized in Table 2. The N-bound H atoms were located in a difference Fourier map and freely refined. In the final cycles of refinement, the H atoms bound to atom N2 were refined with $U_{iso}(H) = 1.1U_{eq}(N)$. The C-bound H atoms were included in calculated positions and treated as riding atoms: C—H = 0.93–0.97 Å with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $= 1.2U_{eq}(C)$ for other H atoms.

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supporting information

Crystal structure of 3-amino-1-propylpyridinium bromide

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Computing details

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

3-Amino-1-propylpyridinium bromide

Crystal data

$C_8H_{13}N_2{}^+\cdot Br^-$	$D_x = 1.481$ Mg m^{-3}
$M_r = 217.11$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 5144 reflections
$a = 8.2937$ (1) Å	$\theta = 2.8–23.4°$
$b = 17.4137$ (3) Å	$\mu = 4.17$ mm^{-1}
$c = 26.9626$ (4) Å	$T = 296$ K
$V = 3894.05$ (10) Å^3	Prismolourec, colourless
$Z = 16$	$0.12 \times 0.10 \times 0.10$ mm
$F(000) = 1760$	

Data collection

Bruker SMART CCD area-detector diffractometer	21922 measured reflections
Radiation source: sealed tube	4491 independent reflections
Graphite monochromator	2698 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{int} = 0.043$
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)	$\theta_{max} = 27.6°$, $\theta_{min} = 2.8°$
	$h = -10 \rightarrow 10$
	$k = -22 \rightarrow 22$
$T_{min} = 0.635$, $T_{max} = 0.681$	$l = -35 \rightarrow 30$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 1.288P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.085$	
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
4491 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
214 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
4 restraints	Extinction correction: *SHELXL2014* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Hydrogen site location: mixed	
	Extinction coefficient: 0.00312 (18)

Special details

Experimental. The minimum and maximum absorption values stated above are those calculated in *SHELXL2014*/6 from the given crystal dimensions. The ratio of minimum to maximum apparent transmission was determined experimentally as 0.639091.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.82809 (4)	0.05269 (2)	0.70989 (2)	0.06468 (14)
N1	−0.0380 (3)	0.39600 (15)	0.40238 (10)	0.0563 (7)
N2	−0.3901 (4)	0.3230 (2)	0.46352 (12)	0.0885 (10)
H2A	−0.472 (3)	0.2941 (19)	0.4526 (13)	0.097*
H2B	−0.341 (4)	0.305 (2)	0.4909 (10)	0.097*
C1	−0.1328 (4)	0.36563 (18)	0.43751 (12)	0.0566 (8)
H1	−0.0897	0.3536	0.4684	0.068*
C4	−0.2546 (4)	0.4017 (2)	0.34649 (13)	0.0644 (9)
H4	−0.2950	0.4143	0.3154	0.077*
C2	−0.2949 (4)	0.35190 (19)	0.42823 (12)	0.0556 (8)
C7	0.1580 (4)	0.4864 (2)	0.43960 (13)	0.0626 (9)
H7A	0.0959	0.4875	0.4701	0.075*
H7B	0.1185	0.5272	0.4183	0.075*
C3	−0.3540 (4)	0.37094 (18)	0.38170 (12)	0.0601 (9)
H3	−0.4622	0.3627	0.3744	0.072*
C8	0.3336 (4)	0.5006 (2)	0.45141 (14)	0.0739 (10)
H8A	0.3448	0.5494	0.4675	0.111*
H8B	0.3724	0.4608	0.4730	0.111*
H8C	0.3951	0.5005	0.4212	0.111*
C6	0.1340 (4)	0.4116 (2)	0.41464 (13)	0.0653 (9)
H6A	0.1739	0.3711	0.4360	0.078*
H6B	0.1969	0.4108	0.3843	0.078*
C5	−0.0945 (5)	0.4141 (2)	0.35731 (13)	0.0658 (9)
H5	−0.0260	0.4348	0.3335	0.079*
Br2	0.29379 (4)	0.21682 (2)	0.42595 (2)	0.06172 (14)
N3	0.9614 (3)	0.15602 (14)	0.30646 (8)	0.0478 (6)
N4	0.8705 (4)	0.1118 (2)	0.17923 (11)	0.0678 (8)
H4A	0.815 (3)	0.0725 (14)	0.1844 (13)	0.064 (11)*
H4B	0.859 (4)	0.1350 (18)	0.1507 (8)	0.072 (11)*
C11	0.9112 (3)	0.11840 (17)	0.26620 (10)	0.0455 (7)
H11	0.8716	0.0687	0.2694	0.055*
C16	0.9419 (4)	0.1197 (2)	0.35593 (10)	0.0558 (8)
H16A	1.0258	0.1379	0.3780	0.067*
H16B	0.9528	0.0644	0.3528	0.067*
C13	0.9756 (4)	0.22690 (19)	0.21730 (12)	0.0612 (9)
H13	0.9786	0.2522	0.1869	0.073*

C15	1.0220 (4)	0.22732 (19)	0.30409 (13)	0.0605 (9)
H15	1.0591	0.2517	0.3326	0.073*
C12	0.9171 (3)	0.15187 (18)	0.21987 (10)	0.0477 (7)
C14	1.0285 (4)	0.26351 (19)	0.25917 (14)	0.0679 (9)
H14	1.0690	0.3132	0.2570	0.081*
C18	0.7575 (5)	0.1097 (3)	0.42914 (14)	0.1018 (15)
H18A	0.6522	0.1233	0.4411	0.153*
H18B	0.7691	0.0549	0.4294	0.153*
H18C	0.8379	0.1323	0.4502	0.153*
C17	0.7780 (4)	0.1388 (3)	0.37761 (13)	0.0812 (12)
H17A	0.7637	0.1940	0.3775	0.097*
H17B	0.6949	0.1166	0.3567	0.097*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0623 (2)	0.0678 (3)	0.0640 (2)	−0.01030 (16)	0.00528 (16)	−0.00851 (18)
N1	0.0529 (16)	0.0501 (16)	0.0659 (18)	−0.0015 (13)	0.0095 (14)	−0.0127 (14)
N2	0.083 (2)	0.111 (3)	0.072 (2)	−0.037 (2)	−0.0128 (18)	0.011 (2)
C1	0.061 (2)	0.053 (2)	0.056 (2)	−0.0037 (16)	−0.0051 (16)	−0.0058 (16)
C4	0.070 (2)	0.061 (2)	0.062 (2)	−0.0034 (19)	0.0026 (19)	−0.0106 (18)
C2	0.056 (2)	0.053 (2)	0.058 (2)	−0.0156 (15)	0.0041 (16)	−0.0062 (17)
C7	0.057 (2)	0.063 (2)	0.068 (2)	0.0004 (17)	0.0003 (16)	−0.0092 (19)
C3	0.056 (2)	0.061 (2)	0.063 (2)	−0.0030 (17)	−0.0124 (17)	−0.0115 (18)
C8	0.059 (2)	0.079 (3)	0.084 (3)	−0.0115 (19)	−0.0043 (18)	0.002 (2)
C6	0.0474 (19)	0.064 (2)	0.085 (2)	−0.0005 (17)	0.0056 (17)	−0.008 (2)
C5	0.080 (3)	0.060 (2)	0.057 (2)	−0.0028 (19)	0.0154 (19)	−0.0059 (18)
Br2	0.0741 (3)	0.0604 (2)	0.0506 (2)	−0.01163 (16)	0.00011 (15)	−0.00427 (16)
N3	0.0482 (14)	0.0465 (16)	0.0486 (15)	0.0023 (12)	−0.0029 (11)	0.0027 (12)
N4	0.087 (2)	0.072 (2)	0.0449 (18)	−0.0176 (18)	−0.0075 (16)	0.0096 (17)
C11	0.0466 (17)	0.0398 (17)	0.0500 (17)	−0.0013 (13)	−0.0030 (14)	0.0008 (15)
C16	0.057 (2)	0.063 (2)	0.0474 (17)	−0.0012 (16)	−0.0069 (15)	0.0026 (16)
C13	0.069 (2)	0.056 (2)	0.058 (2)	−0.0019 (17)	0.0035 (17)	0.0141 (18)
C15	0.068 (2)	0.049 (2)	0.064 (2)	−0.0054 (17)	−0.0065 (17)	−0.0074 (17)
C12	0.0483 (17)	0.0518 (19)	0.0430 (18)	−0.0003 (14)	−0.0023 (14)	0.0074 (15)
C14	0.079 (2)	0.045 (2)	0.080 (3)	−0.0076 (17)	−0.001 (2)	0.0045 (19)
C18	0.086 (3)	0.141 (4)	0.078 (3)	0.011 (3)	0.015 (2)	0.017 (3)
C17	0.066 (2)	0.115 (3)	0.063 (2)	0.003 (2)	0.0002 (18)	0.022 (2)

Geometric parameters (Å, º)

N1—C5	1.340 (4)	N3—C11	1.334 (3)
N1—C1	1.340 (4)	N3—C15	1.341 (4)
N1—C6	1.489 (4)	N3—C16	1.485 (3)
N2—C2	1.336 (4)	N4—C12	1.356 (4)
N2—H2A	0.896 (18)	N4—H4A	0.834 (18)
N2—H2B	0.897 (18)	N4—H4B	0.874 (18)
C1—C2	1.388 (4)	C11—C12	1.379 (4)

C1—H1	0.9300	C11—H11	0.9300
C4—C3	1.366 (4)	C16—C17	1.517 (4)
C4—C5	1.377 (5)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C2—C3	1.387 (4)	C13—C14	1.369 (4)
C7—C6	1.479 (4)	C13—C12	1.395 (4)
C7—C8	1.511 (4)	C13—H13	0.9300
C7—H7A	0.9700	C15—C14	1.366 (4)
C7—H7B	0.9700	C15—H15	0.9300
C3—H3	0.9300	C14—H14	0.9300
C8—H8A	0.9600	C18—C17	1.488 (5)
C8—H8B	0.9600	C18—H18A	0.9600
C8—H8C	0.9600	C18—H18B	0.9600
C6—H6A	0.9700	C18—H18C	0.9600
C6—H6B	0.9700	C17—H17A	0.9700
C5—H5	0.9300	C17—H17B	0.9700
C5—N1—C1	121.9 (3)	C11—N3—C15	122.2 (3)
C5—N1—C6	119.6 (3)	C11—N3—C16	119.2 (3)
C1—N1—C6	118.5 (3)	C15—N3—C16	118.6 (3)
C2—N2—H2A	115 (3)	C12—N4—H4A	116 (2)
C2—N2—H2B	117 (2)	C12—N4—H4B	120 (2)
H2A—N2—H2B	115 (4)	H4A—N4—H4B	118 (3)
N1—C1—C2	120.6 (3)	N3—C11—C12	121.2 (3)
N1—C1—H1	119.7	N3—C11—H11	119.4
C2—C1—H1	119.7	C12—C11—H11	119.4
C3—C4—C5	119.7 (3)	N3—C16—C17	110.5 (2)
C3—C4—H4	120.1	N3—C16—H16A	109.6
C5—C4—H4	120.1	C17—C16—H16A	109.6
N2—C2—C3	121.7 (3)	N3—C16—H16B	109.6
N2—C2—C1	120.6 (3)	C17—C16—H16B	109.6
C3—C2—C1	117.7 (3)	H16A—C16—H16B	108.1
C6—C7—C8	111.6 (3)	C14—C13—C12	120.4 (3)
C6—C7—H7A	109.3	C14—C13—H13	119.8
C8—C7—H7A	109.3	C12—C13—H13	119.8
C6—C7—H7B	109.3	N3—C15—C14	119.0 (3)
C8—C7—H7B	109.3	N3—C15—H15	120.5
H7A—C7—H7B	108.0	C14—C15—H15	120.5
C4—C3—C2	120.6 (3)	N4—C12—C11	120.3 (3)
C4—C3—H3	119.7	N4—C12—C13	122.8 (3)
C2—C3—H3	119.7	C11—C12—C13	116.9 (3)
C7—C8—H8A	109.5	C15—C14—C13	120.2 (3)
C7—C8—H8B	109.5	C15—C14—H14	119.9
H8A—C8—H8B	109.5	C13—C14—H14	119.9
C7—C8—H8C	109.5	C17—C18—H18A	109.5
H8A—C8—H8C	109.5	C17—C18—H18B	109.5
H8B—C8—H8C	109.5	H18A—C18—H18B	109.5
C7—C6—N1	113.0 (3)	C17—C18—H18C	109.5

C7—C6—H6A	109.0	H18A—C18—H18C	109.5
N1—C6—H6A	109.0	H18B—C18—H18C	109.5
C7—C6—H6B	109.0	C18—C17—C16	112.8 (3)
N1—C6—H6B	109.0	C18—C17—H17A	109.0
H6A—C6—H6B	107.8	C16—C17—H17A	109.0
N1—C5—C4	119.6 (3)	C18—C17—H17B	109.0
N1—C5—H5	120.2	C16—C17—H17B	109.0
C4—C5—H5	120.2	H17A—C17—H17B	107.8
C5—N1—C1—C2	−0.1 (5)	C15—N3—C11—C12	−1.1 (4)
C6—N1—C1—C2	178.3 (3)	C16—N3—C11—C12	175.7 (3)
N1—C1—C2—N2	−178.7 (3)	C11—N3—C16—C17	−88.0 (3)
N1—C1—C2—C3	−0.2 (5)	C15—N3—C16—C17	88.9 (3)
C5—C4—C3—C2	−0.1 (5)	C11—N3—C15—C14	1.9 (5)
N2—C2—C3—C4	178.8 (3)	C16—N3—C15—C14	−174.9 (3)
C1—C2—C3—C4	0.3 (5)	N3—C11—C12—N4	177.9 (3)
C8—C7—C6—N1	−179.9 (3)	N3—C11—C12—C13	−0.9 (4)
C5—N1—C6—C7	94.3 (4)	C14—C13—C12—N4	−176.8 (3)
C1—N1—C6—C7	−84.2 (4)	C14—C13—C12—C11	1.9 (4)
C1—N1—C5—C4	0.4 (5)	N3—C15—C14—C13	−0.8 (5)
C6—N1—C5—C4	−178.0 (3)	C12—C13—C14—C15	−1.1 (5)
C3—C4—C5—N1	−0.3 (5)	N3—C16—C17—C18	−174.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Br2[i]	0.90 (2)	2.47 (2)	3.364 (3)	177 (4)
N2—H2*B*···Br2[ii]	0.90 (2)	2.54 (2)	3.419 (3)	168 (4)
N4—H4*A*···Br1[iii]	0.83 (2)	2.58 (2)	3.406 (3)	172 (3)
N4—H4*B*···Br2[iv]	0.87 (2)	2.57 (2)	3.434 (3)	171 (3)
C6—H6*A*···Br2	0.97	2.88	3.655 (4)	138
C6—H6*B*···Br1[ii]	0.97	2.84	3.775 (4)	163
C16—H16*A*···Br2[v]	0.97	2.91	3.866 (3)	167

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