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4,4'-Bis(acetylamino)-1,1'-ethylene-dipyridinium bis(tetrafluoridoborate)

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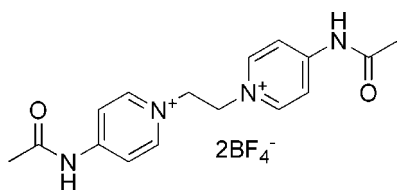
Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.046; wR factor = 0.144; data-to-parameter ratio = 12.9.

In the organic cation of the title compound, $\text{C}_{16}\text{H}_{20}\text{N}_4\text{O}_2^{2+} \cdot 2\text{BF}_4^-$, the pyridinium rings are nearly parallel, with a dihedral angle of 12.54 (12)°. The crystal packing is stabilized by $\text{N}-\text{H} \cdots \text{F}$, $\text{C}-\text{H} \cdots \text{F}$ and $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds.

Related literature

For the 1,2-bis(aminopyridinium)ethane dication, see: Xu *et al.* (2007); Fan *et al.* (2007).

For related literature, see: Allen *et al.* (1987); Li (2007); Loeb & Wisner (1998).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{20}\text{N}_4\text{O}_2^{2+} \cdot 2\text{BF}_4^-$ $M_r = 473.98$ Monoclinic, $P2_1/c$ $a = 11.368$ (2) Å $b = 19.422$ (4) Å $c = 9.0959$ (18) Å $\beta = 101.12$ (3)° $V = 1970.6$ (7) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.16$ mm⁻¹ $T = 113$ (2) K $0.32 \times 0.20 \times 0.18$ mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku/MSC,
2005)

 $T_{\min} = 0.952$, $T_{\max} = 0.973$

21399 measured reflections
3846 independent reflections
3138 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.046$ $wR(F^2) = 0.144$ $S = 1.15$

3846 reflections

299 parameters

H atoms treated by a mixture of
independent and constrained
refinement

 $\Delta\rho_{\max} = 0.33$ e Å⁻³ $\Delta\rho_{\min} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N2}-\text{H2A} \cdots \text{F7}$	0.90 (3)	1.98 (3)	2.862 (3)	168 (3)
$\text{N4}-\text{H4A} \cdots \text{F4}^i$	0.80 (3)	2.08 (3)	2.868 (3)	170 (3)
$\text{C1}-\text{H1} \cdots \text{F1}$	0.95	2.41	3.269 (3)	150
$\text{C1}-\text{H1} \cdots \text{F4}$	0.95	2.53	3.358 (3)	145
$\text{C4}-\text{H4} \cdots \text{O2}^{ii}$	0.95	2.50	3.404 (3)	159
$\text{C5}-\text{H5} \cdots \text{F6}^{iii}$	0.95	2.37	3.251 (3)	153
$\text{C10}-\text{H10} \cdots \text{F3}$	0.95	2.33	3.285 (3)	179
$\text{C11}-\text{H11} \cdots \text{O1}^{iv}$	0.95	2.58	3.496 (3)	162
$\text{C13}-\text{H13} \cdots \text{F2}^i$	0.95	2.48	3.391 (3)	162
$\text{C14}-\text{H14} \cdots \text{F8}^{iii}$	0.95	2.22	3.050 (3)	145

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2653).

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supplementary materials

Acta Cryst. (2008). E64, o35 [doi:10.1107/S1600536807062617]

4,4'-Bis(acetylamino)-1,1'-ethylenedipyridinium bis(tetrafluoroborate)

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Comment

As part of our continuous studies of derivatives of 1,2-bis(pyridinium)ethane dications (Xu *et al.*, 2007; Fan *et al.*, 2007), which can thread through the 24-membered crown ether (Loeb & Wisner, 1998), we herein report the crystal structure of the title compound (Fig. 1).

The organic dication has two pyridinium rings with a dihedral angle of 12.54 (12) Å. The C3—N2 and C12—N4 bond lengths of 1.382 (3) and 1.379 (3) Å, respectively, are between typical C=N (1.34–1.38 Å) and C—N bond lengths (1.47–1.50 Å; Allen *et al.*, 1987), suggesting significant double-bond character. The N1⁺...N3⁺ distance is 3.765 (3) Å, similar to those reported for the related analogues (Xu *et al.*, 2007; Fan *et al.*, 2007; Loeb & Wisner, 1998).

The crystal structure is stabilized by a series of inter-molecular N—H...F, C—H...F and C—H...O hydrogen bonds (Table 1).

Experimental

The title compound was prepared using the method of Li (2007). Colourless single crystals were grown by vapor diffusion of (iPr)₂O into its acetonitrile solution.

Refinement

The N-bound H atoms were refined freely while the other H atoms were positioned geometrically (C—H = 0.95, 0.98 and 0.99 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

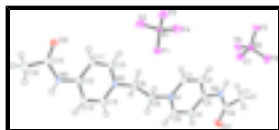


Fig. 1. The molecular structure of (I) with the atom-numbering scheme and 50% probability displacement ellipsoids.

4,4'-Bis(acetylamino)-1,1'-ethylenedipyridinium bis(tetrafluoroborate)

Crystal data

C₁₆H₂₀N₄O₂²⁺·2BF₄⁻

$M_r = 473.98$

Monoclinic, $P2_1/c$

$F_{000} = 968$

$D_x = 1.598 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

supplementary materials

Hall symbol: -P 2₁yc

$a = 11.368 (2) \text{ \AA}$

$b = 19.422 (4) \text{ \AA}$

$c = 9.0959 (18) \text{ \AA}$

$\beta = 101.12 (3)^\circ$

$V = 1970.6 (7) \text{ \AA}^3$

$Z = 4$

Cell parameters from 4669 reflections

$\theta = 2.5\text{--}25.0^\circ$

$\mu = 0.16 \text{ mm}^{-1}$

$T = 113 (2) \text{ K}$

Prism, colorless

$0.32 \times 0.20 \times 0.18 \text{ mm}$

Data collection

Rigaku Saturn
diffractometer

Radiation source: Rotating anode

Monochromator: confocal

$T = 113(2) \text{ K}$

ω scans

Absorption correction: multi-scan
(CrystalClear; Rigaku/MS, 2005)

$T_{\min} = 0.952, T_{\max} = 0.973$

21399 measured reflections

3846 independent reflections

3138 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\text{max}} = 26.0^\circ$

$\theta_{\text{min}} = 1.8^\circ$

$h = -14 \rightarrow 13$

$k = -23 \rightarrow 23$

$l = -11 \rightarrow 11$

Standard reflections: ?

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.144$

$S = 1.15$

3846 reflections

299 parameters

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

$$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2 + 1.1885P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$

Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.32100 (17)	0.51691 (10)	0.6784 (2)	0.0170 (4)
N2	0.56501 (18)	0.63875 (11)	0.9608 (2)	0.0198 (5)
N3	0.15074 (17)	0.44990 (10)	0.3099 (2)	0.0185 (4)
N4	-0.11675 (18)	0.34400 (11)	0.0245 (2)	0.0193 (5)
O1	0.72991 (16)	0.57022 (9)	1.0292 (2)	0.0329 (5)
O2	-0.23344 (15)	0.42922 (9)	-0.09946 (19)	0.0256 (4)
C1	0.2934 (2)	0.58226 (12)	0.7114 (3)	0.0189 (5)
H1	0.2172	0.6007	0.6685	0.023*
C2	0.3735 (2)	0.62158 (12)	0.8049 (3)	0.0191 (5)
H2	0.3525	0.6672	0.8275	0.023*
C3	0.4868 (2)	0.59555 (12)	0.8686 (2)	0.0165 (5)
C4	0.5144 (2)	0.52784 (12)	0.8323 (2)	0.0182 (5)
H4	0.5902	0.5082	0.8728	0.022*
C5	0.4291 (2)	0.49065 (12)	0.7369 (2)	0.0176 (5)
H5	0.4473	0.4449	0.7117	0.021*
C6	0.6832 (2)	0.62699 (13)	1.0264 (3)	0.0214 (5)
C7	0.7466 (2)	0.69017 (13)	1.0942 (3)	0.0261 (6)
H7A	0.8307	0.6791	1.1350	0.039*
H7B	0.7082	0.7070	1.1749	0.039*
H7C	0.7426	0.7259	1.0172	0.039*
C8	0.2312 (2)	0.47529 (12)	0.5753 (2)	0.0181 (5)
H8A	0.1493	0.4893	0.5848	0.022*
H8B	0.2415	0.4259	0.6019	0.022*
C9	0.2478 (2)	0.48615 (13)	0.4140 (3)	0.0215 (5)
H9A	0.2453	0.5360	0.3904	0.026*
H9B	0.3267	0.4680	0.4020	0.026*
C10	0.0551 (2)	0.48478 (13)	0.2363 (3)	0.0192 (5)
H10	0.0509	0.5331	0.2512	0.023*
C11	-0.0370 (2)	0.45266 (12)	0.1399 (3)	0.0182 (5)
H11	-0.1039	0.4783	0.0893	0.022*
C12	-0.0302 (2)	0.38156 (12)	0.1180 (2)	0.0179 (5)
C13	0.0700 (2)	0.34627 (13)	0.1969 (3)	0.0206 (5)
H13	0.0767	0.2980	0.1843	0.025*
C14	0.1577 (2)	0.38076 (13)	0.2913 (3)	0.0217 (5)
H14	0.2247	0.3562	0.3449	0.026*
C15	-0.2133 (2)	0.36836 (13)	-0.0805 (3)	0.0203 (5)
C16	-0.2881 (2)	0.31331 (14)	-0.1681 (3)	0.0276 (6)
H16A	-0.3716	0.3287	-0.1938	0.041*
H16B	-0.2834	0.2713	-0.1077	0.041*
H16C	-0.2581	0.3039	-0.2602	0.041*
B1	0.0229 (2)	0.65645 (12)	0.4308 (3)	0.0138 (5)
B2	0.5204 (3)	0.83160 (14)	0.9965 (3)	0.0203 (6)
F1	0.02861 (13)	0.59066 (7)	0.49479 (16)	0.0253 (4)
F2	-0.09234 (14)	0.68388 (8)	0.43197 (18)	0.0347 (4)
F3	0.03702 (16)	0.65177 (9)	0.28453 (19)	0.0407 (5)

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F4	0.10691 (17)	0.69772 (9)	0.5142 (2)	0.0533 (6)
F5	0.44339 (13)	0.88840 (7)	0.97263 (16)	0.0284 (4)
F6	0.60218 (15)	0.83575 (8)	0.90042 (18)	0.0344 (4)
F7	0.45540 (13)	0.77098 (7)	0.96911 (17)	0.0289 (4)
F8	0.58269 (13)	0.83141 (8)	1.14353 (17)	0.0337 (4)
H4A	-0.110 (2)	0.3030 (16)	0.024 (3)	0.025 (8)*
H2A	0.541 (2)	0.6827 (15)	0.963 (3)	0.026 (7)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0198 (10)	0.0167 (10)	0.0145 (9)	-0.0025 (8)	0.0037 (8)	0.0001 (8)
N2	0.0203 (11)	0.0165 (11)	0.0206 (10)	-0.0009 (9)	-0.0008 (8)	-0.0030 (8)
N3	0.0212 (10)	0.0190 (10)	0.0152 (9)	-0.0043 (9)	0.0031 (8)	-0.0012 (8)
N4	0.0209 (11)	0.0158 (11)	0.0191 (10)	-0.0011 (9)	-0.0017 (8)	-0.0017 (8)
O1	0.0231 (10)	0.0234 (10)	0.0467 (12)	0.0029 (8)	-0.0072 (9)	-0.0055 (9)
O2	0.0256 (10)	0.0233 (10)	0.0242 (9)	0.0037 (8)	-0.0043 (7)	0.0023 (7)
C1	0.0191 (12)	0.0186 (12)	0.0191 (11)	0.0012 (10)	0.0041 (9)	0.0013 (9)
C2	0.0226 (13)	0.0157 (12)	0.0192 (12)	0.0017 (10)	0.0050 (10)	-0.0010 (9)
C3	0.0164 (12)	0.0194 (12)	0.0135 (11)	-0.0040 (10)	0.0020 (9)	-0.0001 (9)
C4	0.0188 (12)	0.0192 (12)	0.0160 (11)	0.0006 (10)	0.0017 (9)	0.0019 (9)
C5	0.0199 (12)	0.0159 (11)	0.0173 (11)	0.0013 (10)	0.0043 (9)	0.0009 (9)
C6	0.0217 (13)	0.0215 (13)	0.0194 (12)	-0.0034 (11)	0.0000 (10)	0.0002 (10)
C7	0.0209 (13)	0.0249 (14)	0.0287 (14)	-0.0047 (11)	-0.0047 (11)	-0.0040 (11)
C8	0.0162 (12)	0.0192 (12)	0.0168 (11)	-0.0049 (10)	-0.0015 (9)	-0.0003 (9)
C9	0.0226 (13)	0.0237 (13)	0.0171 (12)	-0.0070 (10)	0.0010 (10)	-0.0028 (10)
C10	0.0231 (13)	0.0192 (12)	0.0159 (11)	0.0005 (10)	0.0051 (10)	0.0012 (9)
C11	0.0193 (12)	0.0187 (12)	0.0166 (11)	-0.0007 (10)	0.0033 (9)	0.0005 (9)
C12	0.0181 (12)	0.0209 (12)	0.0152 (11)	-0.0029 (10)	0.0043 (9)	-0.0006 (9)
C13	0.0202 (13)	0.0193 (12)	0.0212 (12)	0.0020 (10)	0.0014 (10)	-0.0024 (9)
C14	0.0209 (13)	0.0225 (13)	0.0206 (12)	0.0030 (10)	0.0014 (10)	-0.0006 (10)
C15	0.0189 (12)	0.0254 (14)	0.0166 (11)	-0.0012 (10)	0.0033 (10)	0.0008 (10)
C16	0.0266 (14)	0.0269 (14)	0.0249 (13)	-0.0052 (11)	-0.0062 (11)	0.0008 (11)
B1	0.0190 (13)	0.0070 (12)	0.0138 (12)	0.0019 (10)	-0.0013 (10)	0.0015 (9)
B2	0.0228 (14)	0.0180 (14)	0.0208 (13)	-0.0001 (11)	0.0058 (11)	0.0009 (11)
F1	0.0282 (8)	0.0186 (7)	0.0283 (8)	0.0002 (6)	0.0031 (6)	0.0028 (6)
F2	0.0340 (9)	0.0373 (9)	0.0337 (9)	0.0130 (7)	0.0087 (7)	0.0055 (7)
F3	0.0468 (10)	0.0440 (10)	0.0365 (9)	0.0125 (8)	0.0209 (8)	0.0144 (8)
F4	0.0494 (11)	0.0233 (9)	0.0726 (14)	-0.0099 (8)	-0.0250 (10)	0.0009 (8)
F5	0.0339 (9)	0.0204 (8)	0.0316 (8)	0.0070 (6)	0.0081 (7)	-0.0004 (6)
F6	0.0409 (10)	0.0280 (9)	0.0403 (9)	0.0029 (7)	0.0231 (8)	0.0036 (7)
F7	0.0277 (8)	0.0187 (8)	0.0374 (9)	-0.0036 (6)	-0.0004 (7)	0.0015 (6)
F8	0.0268 (8)	0.0462 (10)	0.0257 (8)	0.0029 (7)	-0.0010 (6)	-0.0096 (7)

Geometric parameters (\AA , $^\circ$)

N1—C5	1.342 (3)	C8—C9	1.529 (3)
N1—C1	1.355 (3)	C8—H8A	0.9900
N1—C8	1.485 (3)	C8—H8B	0.9900

N2—C6	1.380 (3)	C9—H9A	0.9900
N2—C3	1.382 (3)	C9—H9B	0.9900
N2—H2A	0.90 (3)	C10—C11	1.378 (3)
N3—C10	1.345 (3)	C10—H10	0.9500
N3—C14	1.358 (3)	C11—C12	1.400 (3)
N3—C9	1.485 (3)	C11—H11	0.9500
N4—C12	1.379 (3)	C12—C13	1.403 (3)
N4—C15	1.391 (3)	C13—C14	1.360 (3)
N4—H4A	0.80 (3)	C13—H13	0.9500
O1—C6	1.222 (3)	C14—H14	0.9500
O2—C15	1.210 (3)	C15—C16	1.496 (3)
C1—C2	1.355 (3)	C16—H16A	0.9800
C1—H1	0.9500	C16—H16B	0.9800
C2—C3	1.401 (3)	C16—H16C	0.9800
C2—H2	0.9500	B1—F4	1.361 (3)
C3—C4	1.406 (3)	B1—F3	1.373 (3)
C4—C5	1.375 (3)	B1—F1	1.401 (3)
C4—H4	0.9500	B1—F2	1.416 (3)
C5—H5	0.9500	B2—F7	1.387 (3)
C6—C7	1.495 (3)	B2—F8	1.387 (3)
C7—H7A	0.9800	B2—F6	1.396 (3)
C7—H7B	0.9800	B2—F5	1.399 (3)
C7—H7C	0.9800		
C5—N1—C1	120.1 (2)	N3—C9—C8	109.43 (19)
C5—N1—C8	120.6 (2)	N3—C9—H9A	109.8
C1—N1—C8	119.3 (2)	C8—C9—H9A	109.8
C6—N2—C3	128.4 (2)	N3—C9—H9B	109.8
C6—N2—H2A	114.9 (18)	C8—C9—H9B	109.8
C3—N2—H2A	115.4 (18)	H9A—C9—H9B	108.2
C10—N3—C14	119.8 (2)	N3—C10—C11	122.1 (2)
C10—N3—C9	120.6 (2)	N3—C10—H10	119.0
C14—N3—C9	119.6 (2)	C11—C10—H10	119.0
C12—N4—C15	128.2 (2)	C10—C11—C12	118.7 (2)
C12—N4—H4A	118 (2)	C10—C11—H11	120.6
C15—N4—H4A	114 (2)	C12—C11—H11	120.6
N1—C1—C2	120.7 (2)	N4—C12—C11	123.9 (2)
N1—C1—H1	119.6	N4—C12—C13	118.0 (2)
C2—C1—H1	119.6	C11—C12—C13	118.1 (2)
C1—C2—C3	120.6 (2)	C14—C13—C12	120.4 (2)
C1—C2—H2	119.7	C14—C13—H13	119.8
C3—C2—H2	119.7	C12—C13—H13	119.8
N2—C3—C2	117.7 (2)	N3—C14—C13	120.8 (2)
N2—C3—C4	124.3 (2)	N3—C14—H14	119.6
C2—C3—C4	118.0 (2)	C13—C14—H14	119.6
C5—C4—C3	118.5 (2)	O2—C15—N4	122.2 (2)
C5—C4—H4	120.7	O2—C15—C16	123.3 (2)
C3—C4—H4	120.7	N4—C15—C16	114.5 (2)
N1—C5—C4	122.1 (2)	C15—C16—H16A	109.5
N1—C5—H5	119.0	C15—C16—H16B	109.5

supplementary materials

C4—C5—H5	119.0	H16A—C16—H16B	109.5
O1—C6—N2	122.8 (2)	C15—C16—H16C	109.5
O1—C6—C7	124.0 (2)	H16A—C16—H16C	109.5
N2—C6—C7	113.2 (2)	H16B—C16—H16C	109.5
C6—C7—H7A	109.5	F4—B1—F3	112.2 (2)
C6—C7—H7B	109.5	F4—B1—F1	109.50 (19)
H7A—C7—H7B	109.5	F3—B1—F1	109.73 (19)
C6—C7—H7C	109.5	F4—B1—F2	109.0 (2)
H7A—C7—H7C	109.5	F3—B1—F2	108.29 (19)
H7B—C7—H7C	109.5	F1—B1—F2	108.0 (2)
N1—C8—C9	109.54 (19)	F7—B2—F8	109.0 (2)
N1—C8—H8A	109.8	F7—B2—F6	109.4 (2)
C9—C8—H8A	109.8	F8—B2—F6	109.0 (2)
N1—C8—H8B	109.8	F7—B2—F5	110.2 (2)
C9—C8—H8B	109.8	F8—B2—F5	109.9 (2)
H8A—C8—H8B	108.2	F6—B2—F5	109.2 (2)
C5—N1—C1—C2	-0.9 (3)	C14—N3—C9—C8	-78.7 (3)
C8—N1—C1—C2	-179.9 (2)	N1—C8—C9—N3	-174.58 (18)
N1—C1—C2—C3	0.5 (4)	C14—N3—C10—C11	-0.7 (3)
C6—N2—C3—C2	-174.5 (2)	C9—N3—C10—C11	-179.4 (2)
C6—N2—C3—C4	4.2 (4)	N3—C10—C11—C12	-0.2 (3)
C1—C2—C3—N2	178.8 (2)	C15—N4—C12—C11	11.1 (4)
C1—C2—C3—C4	0.0 (3)	C15—N4—C12—C13	-169.5 (2)
N2—C3—C4—C5	-178.8 (2)	C10—C11—C12—N4	-179.9 (2)
C2—C3—C4—C5	-0.1 (3)	C10—C11—C12—C13	0.6 (3)
C1—N1—C5—C4	0.7 (3)	N4—C12—C13—C14	-179.6 (2)
C8—N1—C5—C4	179.8 (2)	C11—C12—C13—C14	-0.2 (4)
C3—C4—C5—N1	-0.2 (3)	C10—N3—C14—C13	1.2 (3)
C3—N2—C6—O1	-11.9 (4)	C9—N3—C14—C13	179.9 (2)
C3—N2—C6—C7	168.7 (2)	C12—C13—C14—N3	-0.7 (4)
C5—N1—C8—C9	-89.3 (3)	C12—N4—C15—O2	-1.4 (4)
C1—N1—C8—C9	89.7 (3)	C12—N4—C15—C16	177.8 (2)
C10—N3—C9—C8	100.0 (2)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A \cdots F7	0.90 (3)	1.98 (3)	2.862 (3)	168 (3)
N4—H4A \cdots F4 ⁱ	0.80 (3)	2.08 (3)	2.868 (3)	170 (3)
C1—H1 \cdots F1	0.95	2.41	3.269 (3)	150
C1—H1 \cdots F4	0.95	2.53	3.358 (3)	145
C4—H4 \cdots O2 ⁱⁱ	0.95	2.50	3.404 (3)	159
C5—H5 \cdots F6 ⁱⁱⁱ	0.95	2.37	3.251 (3)	153
C10—H10 \cdots F3	0.95	2.33	3.285 (3)	179
C11—H11 \cdots O1 ^{iv}	0.95	2.58	3.496 (3)	162
C13—H13 \cdots F2 ⁱ	0.95	2.48	3.391 (3)	162
C14—H14 \cdots F8 ⁱⁱⁱ	0.95	2.22	3.050 (3)	145

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

Fig. 1

