Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,4′-Bis(acetylamino)-1,1′-ethylenedipyridinium bis(tetrafluoridoborate)

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Received 23 November 2007; accepted 23 November 2007

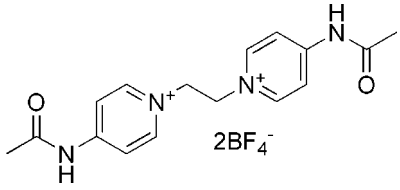
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.144; data-to-parameter ratio = 12.9.

In the organic cation of the title compound, $C_{16}H_{20}N_4O_2^{2+}\cdot 2BF_4^-$, the pyridinium rings are nearly parallel, with a dihedral angle of 12.54 (12)°. The crystal packing is stabilized by N—H···F, C—H···F and C—H···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

$C_{16}H_{20}N_4O_2^{2+}\cdot 2BF_4^-$
M_r = 473.98
Monoclinic, $P2_1/c$
a = 11.368 (2) Å
b = 19.422 (4) Å
c = 9.0959 (18) Å
β = 101.12 (3)°
V = 1970.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 113 (2) K
0.32 × 0.20 × 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_{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···A	D—H	H···A	D···A	D—H···A
N2—H2A···F7	0.90 (3)	1.98 (3)	2.862 (3)	168 (3)
N4—H4A···F4^{i}	0.80 (3)	2.08 (3)	2.868 (3)	170 (3)
C1—H1···F1	0.95	2.41	3.269 (3)	150
C1—H1···F4	0.95	2.53	3.358 (3)	145
C4—H4···O2^{ii}	0.95	2.50	3.404 (3)	159
C5—H5···F6^{iii}	0.95	2.37	3.251 (3)	153
C10—H10···F3	0.95	2.33	3.285 (3)	179
C11—H11···O1^{iv}	0.95	2.58	3.496 (3)	162
C13—H13···F2^{i}	0.95	2.48	3.391 (3)	162
C14—H14···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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supporting information

Acta Cryst. (2008). E**64**, o35 [https://doi.org/10.1107/S1600536807062617]

4,4′-Bis(acetylamino)-1,1′-ethylenedipyridinium bis(tetrafluoridoborate)

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S1. 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 $N1^{+}\cdots N3^{+}$ 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).

S2. Experimental

The title compound was prepared using the method of Li (2007). Colourless single crystals were grown by vapor diffusion of $(^{i}Pr)_2O$ into its acetonitrile solution.

S3. 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 $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

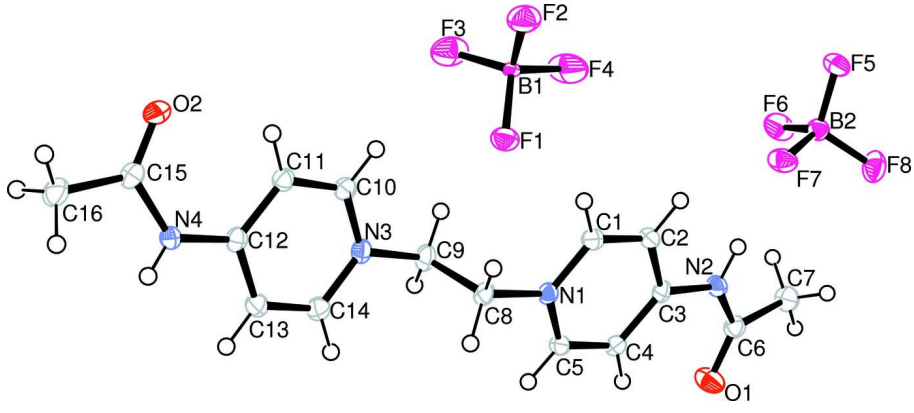

Figure 1

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

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Crystal data

$C_{16}H_{20}N_4O_2^{2+}\cdot 2BF_4^-$
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Hall symbol: -P 2ybc
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$b = 19.422\ (4)$ Å
$c = 9.0959\ (18)$ Å
$\beta = 101.12\ (3)°$
$V = 1970.6\ (7)$ Å^3
$Z = 4$
$F(000) = 968$
$D_x = 1.598$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4669 reflections
$\theta = 2.5–25.0°$
$\mu = 0.16$ mm^{-1}
$T = 113$ K
Prism, colorless
0.32 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: Rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω scans
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 $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -14\rightarrow13$
$k = -23\rightarrow23$
$l = -11\rightarrow11$

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
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
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2 + 1.1885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

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	0.32100 (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)
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 (Å²)

	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 (Å, º)

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
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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···F7	0.90 (3)	1.98 (3)	2.862 (3)	168 (3)
N4—H4*A*···F4^{i}	0.80 (3)	2.08 (3)	2.868 (3)	170 (3)
C1—H1···F1	0.95	2.41	3.269 (3)	150
C1—H1···F4	0.95	2.53	3.358 (3)	145
C4—H4···O2^{ii}	0.95	2.50	3.404 (3)	159
C5—H5···F6^{iii}	0.95	2.37	3.251 (3)	153
C10—H10···F3	0.95	2.33	3.285 (3)	179
C11—H11···O1^{iv}	0.95	2.58	3.496 (3)	162
C13—H13···F2^{i}	0.95	2.48	3.391 (3)	162
C14—H14···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.