

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

3,3'-Diethyl-1,1'-(1,4-phenylene-dimethylene)diimidazol-3-ium bis(hexafluorophosphate)

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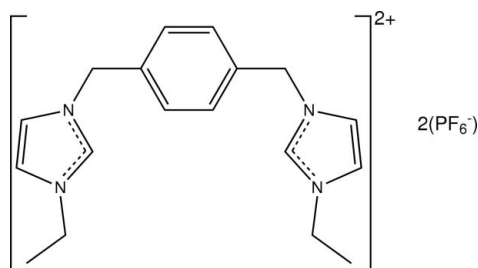
Received 25 June 2012; accepted 26 June 2012

Key indicators: single-crystal X-ray study; $T = 297$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in solvent or counterion; R factor = 0.053; wR factor = 0.170; data-to-parameter ratio = 17.5.

In the title molecular salt, $\text{C}_{18}\text{H}_{24}\text{N}_4^{2+} \cdot 2\text{PF}_6^-$, the complete dication is generated by a crystallographic inversion centre. The central benzene ring makes a dihedral angle of 77.19 (9)° with each of the imidazole rings. In the crystal, $\text{C}-\text{H} \cdots \text{F}$ interactions link the cations and anions into layers lying parallel to the bc plane. The hexafluorophosphate anion is disordered over two sets of sites in a 0.520 (11): 0.480 (11) ratio.

Related literature

For the properties of imidazole derivatives, see: Shargel *et al.* (2006). For related structures, see: Haque *et al.* (2010, 2011).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{24}\text{N}_4^{2+} \cdot 2\text{PF}_6^-$
 $M_r = 586.35$

Triclinic, $P\bar{1}$
 $a = 8.5441$ (5) Å

$b = 8.6018$ (5) Å
 $c = 9.5626$ (6) Å
 $\alpha = 67.913$ (1)°
 $\beta = 77.928$ (1)°
 $\gamma = 67.837$ (1)°
 $V = 601.25$ (6) Å³

$Z = 1$
Mo $K\alpha$ radiation
 $\mu = 0.29$ mm⁻¹
 $T = 297$ K
 $0.28 \times 0.25 \times 0.12$ mm

Data collection

Bruker APEX DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
 $T_{\min} = 0.925$, $T_{\max} = 0.966$

12274 measured reflections
3996 independent reflections
2968 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.170$
 $S = 1.04$
3996 reflections
228 parameters

21 restraints
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.38$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{C3}-\text{H3A} \cdots \text{F1}^{\text{i}}$	0.93	2.49	3.408 (10)	170
$\text{C4}-\text{H4A} \cdots \text{F3}^{\text{ii}}$	0.93	2.48	3.369 (11)	160
$\text{C5}-\text{H5A} \cdots \text{F6}^{\text{iii}}$	0.93	2.32	3.211 (8)	159

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

RAH and SFN thank Universiti Sains Malaysia (USM) for the short-term grant (304/PKIMIA/6311123) and RU grants (1001/PKIMIA/811157), (1001/PKIMIA/813023). HKF thanks USM for the Research University Grant No. 1001/PFIZIK/811160.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6877).

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† Thomson Reuters ResearcherID: A-3561-2009.

supporting information

Acta Cryst. (2012). E68, o2280 [https://doi.org/10.1107/S1600536812028966]

3,3'-Diethyl-1,1'-(1,4-phenylenedimethylene)diimidazol-3-ium bis(hexafluorophosphate)

Rosenani A. Haque, S. Fatimah Nasri, Mohd Mustaqim Rosli and Hoong-Kun Fun

S1. Comment

Substituted imidazole derivatives are valuable in the treatment of many systemic fungal infections (Shargel *et al.*, 2006). Previously, we have reported crystal structures of *para*-xylyl linked bis-imidazolium salts with propyl (Haque *et al.*, 2011) and benzyl (Haque *et al.*, 2010) substitutions. In this report, we describe the crystal structure of a *para*-xylyl linked bis-benzimidazolium salt with ethyl substituents

All parameters in (I) are within normal ranges. The complete dication is generated by a crystallographic inversion centre. The central benzene ring (C7—C9/C7A—C9A) makes a dihedral angle of 77.19 (9)° with the imidazole rings (N1—N2/C3—C5 and N1A—N2A/C3A—C5A). The hexafluorophosphate anions are disordered over two sets of sites with the final refined occupancies of 0.52 (1):0.48 (1).

In the crystal, C3—H3A \cdots F1ⁱ, C4—H4A \cdots F3ⁱⁱ and C5—H5A \cdots F6ⁱⁱⁱ (Table 1) interactions link the molecules into layers lying parallel to the *bc*-plane.

S2. Experimental

To a solution of 1,4-bis((1*H*-imidazol-1-yl)methyl)benzene (1.00 g, 0.004 mol) in 15 ml of acetonitrile, 1-iodoethane (1.31 g, 0.008 mol) was added. The mixture was refluxed at 363 K for 24 h. The resultant white precipitate was filtered, washed with fresh acetonitrile (2 × 5 ml) and converted directly to its hexafluorophosphate counterpart by metathesis reaction using KPF₆ (1.67 g, 0.008 mol) in 40 ml of methanol/water. The white precipitates were collected, washed with fresh acetonitrile (2 × 3 ml) to give the product as a white solid (1.78 g, 67%). *M.p* 467–469 K. Colourless blocks were obtained by slow diffusion method of the salt solution by using diethyl ether and acetonitrile at room temperature.

S3. Refinement

All H atoms attached to C atoms were fixed geometrically and refined as riding with C—H = 0.93–0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. A rotating group model was applied to the methyl group. The hexafluorophosphate anion is disordered over two sets of sites with refined occupancies of 0.52 (1):0.48 (1).

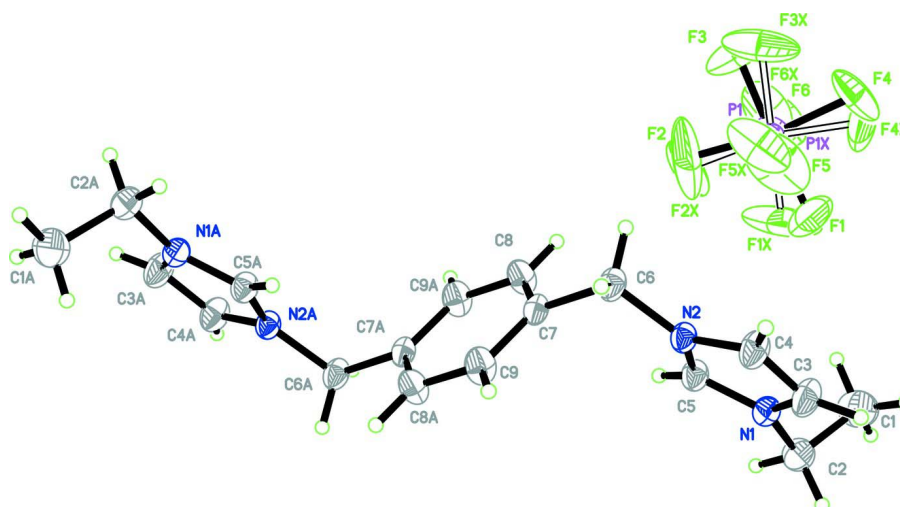


Figure 1

The molecular structure, showing 30% probability displacement ellipsoids. Hydrogen atoms are shown as spheres of arbitrary radius.

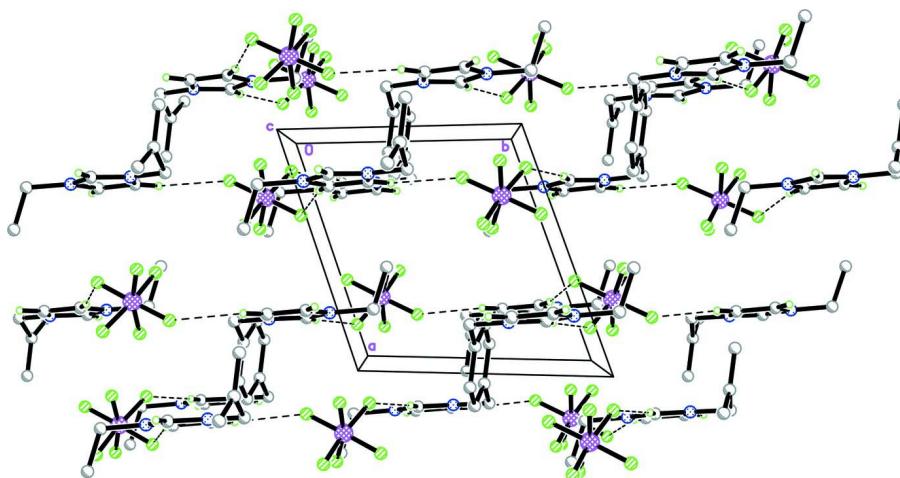


Figure 2

The crystal packing of (I). Dashed lines indicate hydrogen bonds. H atoms not involved in the hydrogen bond interactions have been omitted for clarity.

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Crystal data

$C_{18}H_{24}N_4^{2+} \cdot 2PF_6^-$

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Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 8.5441(5) \text{ \AA}$

$b = 8.6018(5) \text{ \AA}$

$c = 9.5626(6) \text{ \AA}$

$\alpha = 67.913(1)^\circ$

$\beta = 77.928(1)^\circ$

$\gamma = 67.837(1)^\circ$

$V = 601.25(6) \text{ \AA}^3$

$Z = 1$

$F(000) = 298$

$D_x = 1.619 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3921 reflections

$\theta = 2.3\text{--}29.3^\circ$

$\mu = 0.29 \text{ mm}^{-1}$

$T = 297 \text{ K}$

Block, colourless

$0.28 \times 0.25 \times 0.12 \text{ mm}$

Data collection

Bruker APEX DUO CCD diffractometer	12274 measured reflections
Radiation source: fine-focus sealed tube	3996 independent reflections
Graphite monochromator	2968 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.018$
Absorption correction: multi-scan (SADABS; Bruker, 2009)	$\theta_{\text{max}} = 31.7^\circ$, $\theta_{\text{min}} = 2.3^\circ$
$T_{\text{min}} = 0.925$, $T_{\text{max}} = 0.966$	$h = -12 \rightarrow 12$
	$k = -12 \rightarrow 12$
	$l = -14 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.170$	$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 0.1678P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
3996 reflections	$(\Delta/\sigma)_{\text{max}} = 0.026$
228 parameters	$\Delta\rho_{\text{max}} = 0.38 \text{ e } \text{\AA}^{-3}$
21 restraints	$\Delta\rho_{\text{min}} = -0.36 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
P1	0.2804 (5)	0.8326 (6)	0.7615 (5)	0.0638 (15)	0.520 (11)
F1	0.3579 (13)	0.9624 (13)	0.7737 (9)	0.131 (3)	0.520 (11)
F2	0.4136 (13)	0.7509 (17)	0.6579 (12)	0.199 (7)	0.520 (11)
F3	0.2044 (14)	0.6984 (10)	0.7644 (13)	0.163 (4)	0.520 (11)
F4	0.1422 (6)	0.8696 (10)	0.8921 (5)	0.107 (3)	0.520 (11)
F5	0.3982 (12)	0.7149 (17)	0.8932 (9)	0.166 (5)	0.520 (11)
F6	0.1612 (11)	0.9775 (11)	0.6426 (9)	0.114 (3)	0.520 (11)
P1X	0.2841 (4)	0.8298 (4)	0.7654 (4)	0.0360 (7)	0.480 (11)
F1X	0.3854 (13)	0.9578 (14)	0.718 (2)	0.203 (6)	0.480 (11)
F2X	0.4179 (9)	0.7801 (15)	0.6381 (8)	0.125 (4)	0.480 (11)
F3X	0.1751 (10)	0.7065 (9)	0.8061 (13)	0.142 (5)	0.480 (11)
F4X	0.1575 (11)	0.9329 (18)	0.8653 (13)	0.176 (5)	0.480 (11)
F5X	0.3981 (10)	0.6706 (12)	0.8876 (10)	0.124 (3)	0.480 (11)
F6X	0.1650 (13)	0.9487 (15)	0.6319 (9)	0.123 (4)	0.480 (11)
N1	0.7726 (2)	0.9473 (2)	0.78904 (17)	0.0434 (3)	
N2	0.80090 (18)	0.67771 (18)	0.81853 (15)	0.0376 (3)	

C1	0.5791 (3)	1.2530 (3)	0.7237 (4)	0.0789 (8)
H1A	0.5718	1.3735	0.6648	0.118*
H1B	0.5405	1.2453	0.8271	0.118*
H1C	0.5094	1.2165	0.6841	0.118*
C2	0.7574 (3)	1.1356 (3)	0.7159 (3)	0.0580 (5)
H2A	0.8010	1.1559	0.6108	0.070*
H2B	0.8255	1.1650	0.7653	0.070*
C3	0.7587 (3)	0.8606 (3)	0.9407 (2)	0.0568 (5)
H3A	0.7410	0.9089	1.0171	0.068*
C4	0.7751 (3)	0.6920 (3)	0.9598 (2)	0.0512 (5)
H4A	0.7700	0.6025	1.0515	0.061*
C5	0.7975 (2)	0.8345 (2)	0.71706 (19)	0.0424 (4)
H5A	0.8106	0.8607	0.6126	0.051*
C6	0.8154 (3)	0.5168 (2)	0.78841 (19)	0.0460 (4)
H6A	0.7027	0.5143	0.7890	0.055*
H6B	0.8726	0.4127	0.8689	0.055*
C7	0.9118 (2)	0.5083 (2)	0.63878 (17)	0.0375 (3)
C8	0.8268 (2)	0.5812 (3)	0.5089 (2)	0.0513 (5)
H8A	0.7099	0.6362	0.5139	0.062*
C9	1.0854 (3)	0.4272 (3)	0.6285 (2)	0.0512 (5)
H9A	1.1440	0.3775	0.7151	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.061 (2)	0.066 (2)	0.052 (2)	−0.0193 (18)	−0.0073 (16)	−0.0066 (16)
F1	0.183 (8)	0.157 (6)	0.133 (5)	−0.118 (5)	0.029 (4)	−0.093 (5)
F2	0.131 (7)	0.242 (11)	0.180 (9)	0.076 (7)	−0.016 (6)	−0.158 (8)
F3	0.213 (9)	0.120 (5)	0.224 (8)	−0.102 (5)	−0.040 (7)	−0.070 (6)
F4	0.060 (2)	0.168 (5)	0.049 (2)	−0.027 (3)	0.0210 (15)	−0.013 (3)
F5	0.090 (5)	0.284 (12)	0.084 (4)	−0.030 (6)	−0.052 (4)	−0.026 (6)
F6	0.084 (4)	0.078 (3)	0.087 (5)	0.005 (2)	0.005 (3)	0.035 (3)
P1X	0.0345 (13)	0.0375 (13)	0.0373 (15)	−0.0150 (10)	0.0042 (10)	−0.0143 (11)
F1X	0.102 (5)	0.148 (7)	0.343 (16)	−0.096 (5)	−0.007 (7)	−0.013 (8)
F2X	0.073 (4)	0.213 (9)	0.061 (3)	−0.023 (5)	0.027 (3)	−0.055 (4)
F3X	0.088 (3)	0.092 (4)	0.196 (8)	−0.060 (3)	−0.062 (4)	0.064 (5)
F4X	0.115 (5)	0.273 (10)	0.239 (9)	−0.035 (6)	0.011 (5)	−0.231 (9)
F5X	0.070 (4)	0.105 (4)	0.107 (5)	−0.005 (3)	−0.011 (3)	0.041 (3)
F6X	0.089 (5)	0.178 (9)	0.048 (3)	−0.007 (5)	−0.026 (3)	−0.004 (4)
N1	0.0464 (8)	0.0408 (7)	0.0481 (8)	−0.0170 (6)	0.0016 (6)	−0.0202 (6)
N2	0.0450 (7)	0.0383 (7)	0.0311 (6)	−0.0158 (5)	0.0033 (5)	−0.0145 (5)
C1	0.0633 (15)	0.0511 (12)	0.114 (2)	−0.0112 (11)	−0.0112 (14)	−0.0229 (14)
C2	0.0608 (12)	0.0401 (9)	0.0745 (14)	−0.0204 (8)	0.0033 (10)	−0.0211 (9)
C3	0.0789 (14)	0.0595 (12)	0.0443 (10)	−0.0269 (10)	0.0003 (9)	−0.0286 (9)
C4	0.0739 (13)	0.0520 (10)	0.0319 (8)	−0.0240 (9)	−0.0003 (8)	−0.0170 (7)
C5	0.0519 (9)	0.0406 (8)	0.0356 (7)	−0.0179 (7)	0.0035 (6)	−0.0146 (6)
C6	0.0636 (11)	0.0412 (8)	0.0374 (8)	−0.0244 (8)	0.0100 (7)	−0.0177 (7)
C7	0.0481 (9)	0.0326 (7)	0.0328 (7)	−0.0135 (6)	0.0019 (6)	−0.0143 (6)

C8	0.0389 (9)	0.0648 (12)	0.0444 (9)	-0.0058 (8)	-0.0033 (7)	-0.0231 (9)
C9	0.0506 (10)	0.0611 (11)	0.0360 (8)	-0.0064 (8)	-0.0097 (7)	-0.0181 (8)

Geometric parameters (Å, °)

P1—F2	1.490 (7)	C1—H1A	0.9600
P1—F3	1.513 (6)	C1—H1B	0.9600
P1—F6	1.531 (7)	C1—H1C	0.9600
P1—F1	1.545 (6)	C2—H2A	0.9700
P1—F5	1.558 (7)	C2—H2B	0.9700
P1—F4	1.566 (5)	C3—C4	1.347 (3)
P1X—F4X	1.533 (6)	C3—H3A	0.9300
P1X—F1X	1.532 (7)	C4—H4A	0.9300
P1X—F2X	1.553 (6)	C5—H5A	0.9300
P1X—F3X	1.557 (6)	C6—C7	1.507 (2)
P1X—F5X	1.567 (6)	C6—H6A	0.9700
P1X—F6X	1.577 (6)	C6—H6B	0.9700
N1—C5	1.321 (2)	C7—C9	1.381 (3)
N1—C3	1.362 (3)	C7—C8	1.382 (2)
N1—C2	1.469 (2)	C8—C9 ⁱ	1.383 (2)
N2—C5	1.327 (2)	C8—H8A	0.9300
N2—C4	1.367 (2)	C9—C8 ⁱ	1.383 (2)
N2—C6	1.473 (2)	C9—H9A	0.9300
C1—C2	1.482 (3)		
F2—P1—F3	82.7 (7)	C2—C1—H1A	109.5
F2—P1—F6	98.2 (6)	C2—C1—H1B	109.5
F3—P1—F6	90.4 (5)	H1A—C1—H1B	109.5
F2—P1—F1	100.0 (7)	C2—C1—H1C	109.5
F3—P1—F1	175.0 (6)	H1A—C1—H1C	109.5
F6—P1—F1	93.3 (6)	H1B—C1—H1C	109.5
F2—P1—F5	88.9 (6)	N1—C2—C1	111.63 (19)
F3—P1—F5	98.9 (7)	N1—C2—H2A	109.3
F6—P1—F5	169.0 (8)	C1—C2—H2A	109.3
F1—P1—F5	77.1 (6)	N1—C2—H2B	109.3
F2—P1—F4	165.7 (7)	C1—C2—H2B	109.3
F3—P1—F4	86.3 (5)	H2A—C2—H2B	108.0
F6—P1—F4	90.8 (5)	C4—C3—N1	107.53 (16)
F1—P1—F4	90.4 (4)	C4—C3—H3A	126.2
F5—P1—F4	83.8 (5)	N1—C3—H3A	126.2
F4X—P1X—F1X	90.9 (6)	C3—C4—N2	106.79 (17)
F4X—P1X—F2X	163.0 (8)	C3—C4—H4A	126.6
F1X—P1X—F2X	74.1 (7)	N2—C4—H4A	126.6
F4X—P1X—F3X	89.2 (5)	N1—C5—N2	108.71 (15)
F1X—P1X—F3X	176.8 (6)	N1—C5—H5A	125.6
F2X—P1X—F3X	105.3 (6)	N2—C5—H5A	125.6
F4X—P1X—F5X	100.5 (7)	N2—C6—C7	112.44 (14)
F1X—P1X—F5X	99.7 (6)	N2—C6—H6A	109.1

F2X—P1X—F5X	90.0 (5)	C7—C6—H6A	109.1
F3X—P1X—F5X	83.5 (5)	N2—C6—H6B	109.1
F4X—P1X—F6X	88.6 (6)	C7—C6—H6B	109.1
F1X—P1X—F6X	92.3 (7)	H6A—C6—H6B	107.8
F2X—P1X—F6X	84.2 (6)	C9—C7—C8	118.74 (15)
F3X—P1X—F6X	84.5 (5)	C9—C7—C6	121.03 (16)
F5X—P1X—F6X	164.7 (7)	C8—C7—C6	120.23 (17)
C5—N1—C3	108.48 (15)	C9 ⁱ —C8—C7	120.44 (17)
C5—N1—C2	125.15 (17)	C9 ⁱ —C8—H8A	119.8
C3—N1—C2	126.35 (17)	C7—C8—H8A	119.8
C5—N2—C4	108.49 (15)	C7—C9—C8 ⁱ	120.82 (16)
C5—N2—C6	127.06 (14)	C7—C9—H9A	119.6
C4—N2—C6	124.27 (15)	C8 ⁱ —C9—H9A	119.6
C5—N1—C2—C1	104.3 (3)	C6—N2—C5—N1	176.08 (17)
C3—N1—C2—C1	-73.6 (3)	C5—N2—C6—C7	29.1 (3)
C5—N1—C3—C4	-0.2 (3)	C4—N2—C6—C7	-156.30 (18)
C2—N1—C3—C4	178.0 (2)	N2—C6—C7—C9	90.2 (2)
N1—C3—C4—N2	0.6 (3)	N2—C6—C7—C8	-90.3 (2)
C5—N2—C4—C3	-0.9 (2)	C9—C7—C8—C9 ⁱ	-0.1 (3)
C6—N2—C4—C3	-176.35 (19)	C6—C7—C8—C9 ⁱ	-179.61 (18)
C3—N1—C5—N2	-0.4 (2)	C8—C7—C9—C8 ⁱ	0.1 (3)
C2—N1—C5—N2	-178.59 (18)	C6—C7—C9—C8 ⁱ	179.61 (18)
C4—N2—C5—N1	0.8 (2)		

Symmetry code: (i) $-x+2, -y+1, -z+1$.

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C3—H3A \cdots F1 ⁱⁱ	0.93	2.49	3.408 (10)	170
C4—H4A \cdots F3 ⁱⁱⁱ	0.93	2.48	3.369 (11)	160
C5—H5A \cdots F6 ^{iv}	0.93	2.32	3.211 (8)	159

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