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4-Ethoxyanilinium hexafluorophosphate monohydrate

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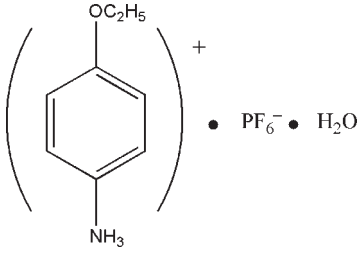
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.059; wR factor = 0.164; data-to-parameter ratio = 12.5.

In the crystal of the title compound, $C_8H_{12}NO^+\cdot PF_6^-\cdot H_2O$, intermolecular N—H···F, N—H···O and O—H···F hydrogen bonds link the molecules into chains along the c axis and C—H···π contacts further stabilize the structure. The F atoms of one of the hexafluorophosphate anions are disordered over two sets of sites with site-occupancy factors of 0.27 (3) and 0.73 (3).

Related literature

For related structures, see: Fu (2009*a*,*b*). The title compound was studied as part of our search for ferroelectric compounds, which usually have a phase transition.For background to phase transition materials, see: Li *et al.* (2008); Zhang *et al.* (2009).



Experimental

Crystal data

$C_8H_{12}NO^+\cdot PF_6^-\cdot H_2O$
M_r = 301.17
Monoclinic, $P2_1/c$
a = 17.498 (4) Å
b = 5.1236 (10) Å
c = 14.793 (3) Å
β = 111.68 (3)°
V = 1232.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 K
0.4 × 0.3 × 0.2 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.900, T_{max} = 0.943
12124 measured reflections
2820 independent reflections
1890 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.164
S = 1.05
2820 reflections
226 parameters
235 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···F2′	0.89	2.16	3.03 (2)	167
N1—H1A···F2	0.89	2.17	3.049 (10)	169
N1—H1B···F1^{i}	0.89	2.22	3.066 (8)	158
N1—H1B···F1′^{i}	0.89	2.28	3.09 (3)	152
N1—H1C···O1W^{ii}	0.89	2.22	2.883 (3)	131
N1—H1C···F3^{ii}	0.89	2.46	3.137 (12)	133
N1—H1C···F3′^{ii}	0.89	2.40	3.01 (3)	126
N1—H1C···F6′^{ii}	0.89	2.51	2.96 (2)	112
O1W—H1WB···F3′^{iii}	0.82 (1)	2.20 (3)	2.97 (3)	156 (4)
O1W—H1WB···F3^{iii}	0.82 (1)	2.28 (3)	3.030 (12)	152 (4)
O1W—H1WA···F4^{i}	0.82 (3)	2.24 (2)	3.040 (12)	164 (4)
O1W—H1WA···F4′^{i}	0.82 (3)	2.11 (3)	2.88 (2)	155 (4)
O1W—H1WA···F5^{i}	0.82 (3)	2.48 (4)	2.951 (16)	117 (3)
C8—H8C···*Cg*1^{iv}	0.96	3.16	4.023 (5)	150

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PRPKAPPA* (Ferguson, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2040).

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supporting information

Acta Cryst. (2010). E**66**, o1461 [https://doi.org/10.1107/S1600536810018404]

4-Ethoxyanilinium hexafluorophosphate monohydrate

Xue-qun Fu

S1. Comment

As a continuation of our study of dielectric-ferroelectric materials, including organic ligands (Li *et al.*, 2008), metal-organic coordination compounds (Zhang *et al.*, 2009), and organic-inorganic hybrids, we studied the dielectric properties of the title compound. Unfortunately, there was no distinct anomaly observed from 93 to 350 K. In this article, the crystal structure of this compound is presented. The crystal structures of 4-ethoxyanilinium together with other anions are known (Fu, 2009a,b).

The asymmetric unit of the crystal structure consists of one almost coplanar protonated 4-ethoxyanilinium cation with the C2—C1—O1—C7 and C1—O1—C7—C8 torsion angles of 172.9 (3) and 177.4 (3)°, respectively, one hexafluorophosphate anion for which the F atoms are disordered over two sets of positions with site-occupancy factors of 0.27 (3) and 0.73 (3), and one water molecule (Fig.1). In the crystal structure, several intermolecular N—H···F and O—H···F hydrogen bonds link all species to chains along the c axis (Fig.2). In addition, C—H···π interactions further stabilize the crystal structure.

S2. Experimental

1.37 g (10 mmol) of 4-Ethoxybenzenamine was firstly dissolved in 50 ml ethanol, to which hexafluorophosphoric acid (70%, w/w) was then added until the solution becomes acidic under stirring. Single crystals of the title compond were prepared by slow evaporation at room temperature of the acidic solution after 3 days.

S3. Refinement

The water H atoms were found in Fourier difference maps and were refined freely. Positional parameters of all other H atoms were calculated geometrically and allowed to ride on the C and N atoms to which they are bonded, with U_{iso}(H) = 1.2U_{eq}(C,N). The F atoms of the hexafluorophosphate anion are disordered in two orientations with site-occupancy factors of 0.73 (3) and 0.27 (3).

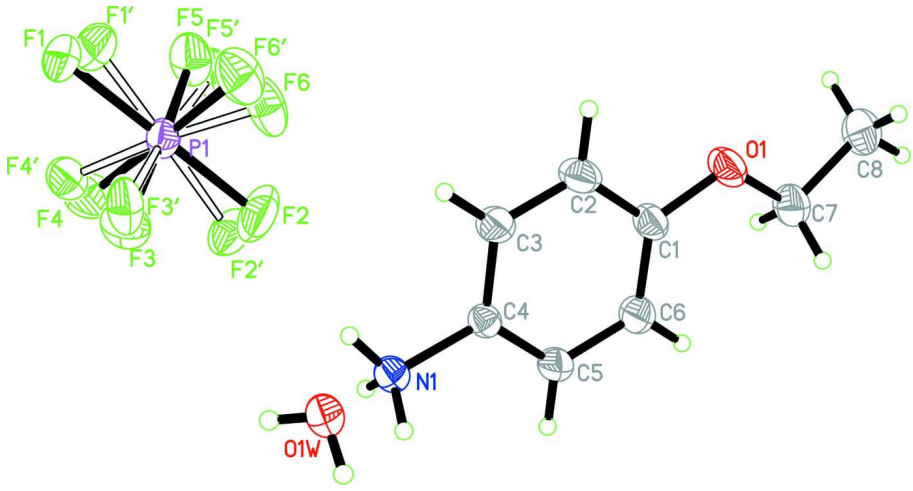

Figure 1

The molecular structure of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level, and all H atoms have been omitted for clarity.

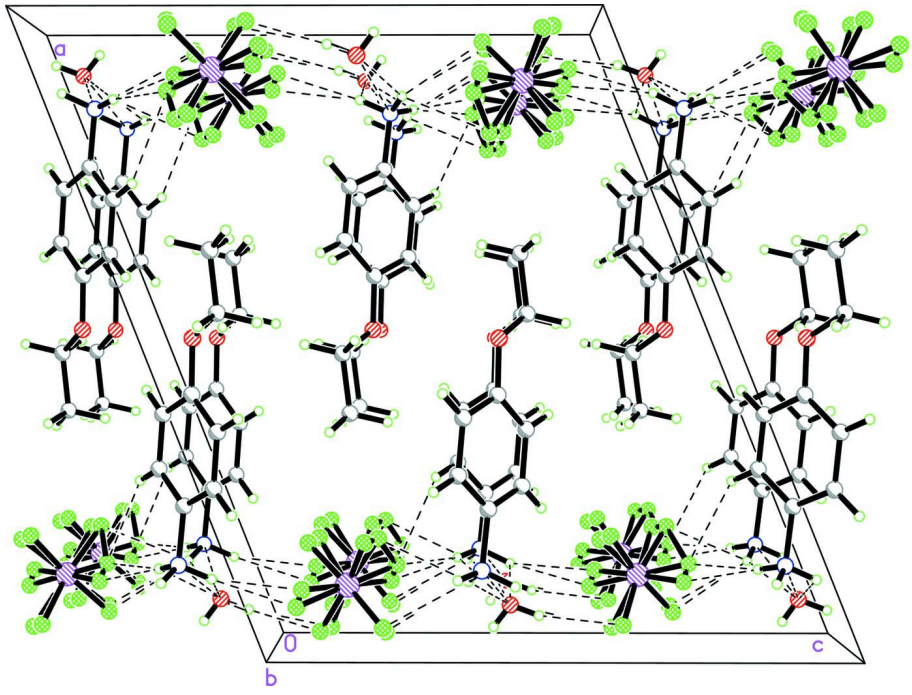

Figure 2

A view of the packing of the title compound, stacking along the *c* axis. Dashed lines indicate hydrogen bonds.

4-Ethoxyanilinium hexafluorophosphate monohydrate

Crystal data

$C_8H_{12}NO^+·PF_6^-·H_2O$
M_r = 301.17
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 17.498 (4) Å
b = 5.1236 (10) Å
c = 14.793 (3) Å
β = 111.68 (3)°
V = 1232.4 (4) Å^3
Z = 4

$F(000) = 616$
$D_x = 1.623$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4774 reflections
$\theta = 3.1$–$27.7°$
$\mu = 0.29$ mm^{-1}
$T = 298$ K
Prism, colourless
0.4 × 0.3 × 0.2 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.900$, $T_{max} = 0.943$
12124 measured reflections
2820 independent reflections
1890 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -22 \rightarrow 22$
$k = -6 \rightarrow 6$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.164$
$S = 1.05$
2820 reflections
226 parameters
235 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
$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2 + 0.6523P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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)
N1	0.15275 (14)	0.3564 (5)	0.42609 (17)	0.0414 (6)	
H1A	0.1427	0.4860	0.3832	0.050*	
H1B	0.1304	0.3936	0.4697	0.050*	
H1C	0.1311	0.2092	0.3953	0.050*	
O1	0.49349 (12)	0.2376 (5)	0.60339 (18)	0.0624 (7)	
C1	0.40946 (18)	0.2556 (6)	0.5644 (2)	0.0458 (7)	
C4	0.24232 (16)	0.3242 (5)	0.47587 (19)	0.0366 (6)	
C3	0.29478 (19)	0.4801 (6)	0.4497 (2)	0.0515 (8)	
H3A	0.2739	0.6074	0.4021	0.062*	
C5	0.27196 (18)	0.1368 (7)	0.5450 (2)	0.0497 (8)	

H5A	0.2360	0.0333	0.5625	0.060*	
C6	0.35635 (19)	0.1007 (7)	0.5895 (2)	0.0558 (9)	
H6A	0.3769	−0.0286	0.6364	0.067*	
C2	0.37808 (19)	0.4465 (7)	0.4943 (3)	0.0561 (9)	
H2A	0.4137	0.5527	0.4773	0.067*	
C8	0.6217 (2)	0.0478 (10)	0.6954 (3)	0.0783 (12)	
H8A	0.6483	−0.0935	0.7380	0.117*	
H8B	0.6405	0.2108	0.7279	0.117*	
H8C	0.6347	0.0396	0.6378	0.117*	
C7	0.5304 (2)	0.0266 (8)	0.6678 (3)	0.0632 (10)	
H7A	0.5107	−0.1390	0.6359	0.076*	
H7B	0.5164	0.0372	0.7254	0.076*	
O1W	0.08195 (12)	0.8613 (5)	0.44539 (16)	0.0473 (5)	
H1WB	0.0467 (16)	0.843 (9)	0.3908 (11)	0.086 (15)*	
H1WA	0.071 (2)	0.856 (9)	0.4948 (14)	0.086 (15)*	
P1	0.11668 (4)	0.96937 (15)	0.18642 (5)	0.0396 (3)	
F3	0.0519 (7)	1.103 (3)	0.2240 (8)	0.064 (2)	0.73 (3)
F5	0.1765 (9)	0.833 (3)	0.1430 (10)	0.065 (2)	0.73 (3)
F4	0.0451 (7)	0.782 (2)	0.1246 (9)	0.072 (2)	0.73 (3)
F1	0.0911 (6)	1.1714 (17)	0.0948 (6)	0.0618 (15)	0.73 (3)
F2	0.1410 (8)	0.783 (2)	0.2777 (7)	0.086 (2)	0.73 (3)
F6	0.1869 (6)	1.169 (2)	0.2477 (7)	0.0704 (18)	0.73 (3)
F6′	0.1908 (13)	1.081 (6)	0.2715 (16)	0.066 (4)	0.27 (3)
F4′	0.0396 (15)	0.830 (6)	0.1040 (17)	0.053 (4)	0.27 (3)
F2′	0.1153 (17)	0.730 (5)	0.256 (2)	0.070 (4)	0.27 (3)
F3′	0.0594 (18)	1.160 (7)	0.2229 (19)	0.056 (4)	0.27 (3)
F5′	0.184 (3)	0.796 (8)	0.164 (3)	0.062 (4)	0.27 (3)
F1′	0.1166 (18)	1.168 (5)	0.1154 (19)	0.075 (4)	0.27 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0383 (13)	0.0429 (13)	0.0428 (13)	−0.0011 (11)	0.0147 (11)	−0.0042 (11)
O1	0.0333 (11)	0.0710 (15)	0.0758 (16)	0.0024 (11)	0.0119 (11)	0.0209 (13)
C1	0.0335 (14)	0.0500 (17)	0.0516 (17)	0.0022 (13)	0.0128 (13)	0.0029 (14)
C4	0.0337 (14)	0.0378 (15)	0.0383 (14)	−0.0002 (12)	0.0132 (12)	−0.0041 (12)
C3	0.0425 (16)	0.0509 (18)	0.0603 (19)	0.0031 (14)	0.0181 (15)	0.0191 (16)
C5	0.0406 (17)	0.0564 (19)	0.0508 (17)	−0.0050 (15)	0.0153 (14)	0.0124 (15)
C6	0.0443 (18)	0.060 (2)	0.0577 (19)	0.0035 (16)	0.0128 (15)	0.0216 (17)
C2	0.0425 (17)	0.0553 (19)	0.073 (2)	−0.0024 (15)	0.0237 (16)	0.0172 (17)
C8	0.045 (2)	0.108 (3)	0.071 (3)	0.018 (2)	0.0099 (19)	0.020 (2)
C7	0.0450 (18)	0.073 (2)	0.064 (2)	0.0094 (18)	0.0113 (16)	0.0147 (19)
O1W	0.0395 (12)	0.0532 (13)	0.0448 (13)	−0.0011 (10)	0.0105 (11)	0.0014 (11)
P1	0.0366 (4)	0.0479 (5)	0.0323 (4)	0.0065 (3)	0.0103 (3)	−0.0011 (3)
F3	0.055 (3)	0.082 (6)	0.065 (3)	0.018 (3)	0.034 (2)	−0.005 (3)
F5	0.055 (3)	0.086 (4)	0.054 (5)	0.022 (2)	0.019 (4)	−0.012 (3)
F4	0.068 (3)	0.074 (4)	0.071 (5)	−0.032 (3)	0.022 (3)	−0.011 (3)
F1	0.054 (4)	0.073 (2)	0.054 (3)	0.014 (3)	0.014 (2)	0.026 (2)

F2	0.092 (6)	0.101 (5)	0.054 (3)	0.027 (4)	0.015 (3)	0.036 (3)
F6	0.057 (2)	0.078 (4)	0.066 (4)	−0.013 (3)	0.011 (2)	−0.025 (3)
F6′	0.042 (4)	0.089 (9)	0.054 (7)	0.011 (6)	0.004 (5)	−0.032 (6)
F4′	0.044 (5)	0.075 (8)	0.040 (6)	−0.004 (5)	0.015 (4)	−0.013 (6)
F2′	0.074 (10)	0.075 (7)	0.060 (8)	0.017 (6)	0.025 (6)	0.029 (6)
F3′	0.048 (6)	0.066 (9)	0.042 (6)	0.022 (6)	0.003 (5)	−0.007 (5)
F5′	0.050 (6)	0.087 (10)	0.049 (10)	0.018 (6)	0.018 (7)	−0.017 (7)
F1′	0.065 (10)	0.081 (6)	0.066 (7)	−0.007 (7)	0.010 (6)	0.035 (6)

Geometric parameters (Å, º)

N1—C4	1.474 (4)	C8—H8B	0.9600
N1—H1A	0.8900	C8—H8C	0.9600
N1—H1B	0.8900	C7—H7A	0.9700
N1—H1C	0.8900	C7—H7B	0.9700
O1—C1	1.370 (4)	O1W—H1WB	0.821 (10)
O1—C7	1.428 (4)	O1W—H1WA	0.82 (3)
C1—C6	1.373 (4)	P1—F1′	1.46 (2)
C1—C2	1.384 (4)	P1—F6′	1.546 (18)
C4—C5	1.358 (4)	P1—F4	1.575 (10)
C4—C3	1.376 (4)	P1—F5	1.578 (13)
C3—C2	1.371 (4)	P1—F2	1.580 (8)
C3—H3A	0.9300	P1—F3	1.590 (11)
C5—C6	1.389 (4)	P1—F6	1.598 (7)
C5—H5A	0.9300	P1—F5′	1.60 (4)
C6—H6A	0.9300	P1—F2′	1.61 (2)
C2—H2A	0.9300	P1—F4′	1.61 (3)
C8—C7	1.500 (5)	P1—F3′	1.63 (3)
C8—H8A	0.9600	P1—F1	1.632 (7)
C4—N1—H1A	109.5	F6′—P1—F3	92.8 (9)
C4—N1—H1B	109.4	F4—P1—F3	87.1 (6)
H1A—N1—H1B	109.5	F5—P1—F3	176.5 (7)
C4—N1—H1C	109.5	F2—P1—F3	87.9 (6)
H1A—N1—H1C	109.5	F1′—P1—F6	76.1 (9)
H1B—N1—H1C	109.5	F4—P1—F6	177.8 (5)
C1—O1—C7	118.8 (3)	F5—P1—F6	91.6 (8)
O1—C1—C6	125.2 (3)	F2—P1—F6	89.7 (3)
O1—C1—C2	115.5 (3)	F3—P1—F6	91.4 (6)
C6—C1—C2	119.4 (3)	F1′—P1—F5′	92.5 (15)
C5—C4—C3	120.9 (3)	F6′—P1—F5′	85.2 (18)
C5—C4—N1	119.7 (3)	F4—P1—F5′	91.5 (18)
C3—C4—N1	119.4 (3)	F2—P1—F5′	81.6 (13)
C2—C3—C4	119.5 (3)	F3—P1—F5′	169.4 (13)
C2—C3—H3A	120.2	F6—P1—F5′	90.3 (18)
C4—C3—H3A	120.2	F1′—P1—F2′	174.5 (15)
C4—C5—C6	119.6 (3)	F6′—P1—F2′	88.1 (9)
C4—C5—H5A	120.2	F4—P1—F2′	73.3 (9)

C6—C5—H5A	120.2	F5—P1—F2′	95.5 (12)
C1—C6—C5	120.1 (3)	F3—P1—F2′	85.4 (12)
C1—C6—H6A	119.9	F6—P1—F2′	108.2 (8)
C5—C6—H6A	119.9	F5′—P1—F2′	84.1 (17)
C3—C2—C1	120.4 (3)	F1′—P1—F4′	89.3 (11)
C3—C2—H2A	119.8	F6′—P1—F4′	174.7 (12)
C1—C2—H2A	119.8	F5—P1—F4′	89.5 (10)
C7—C8—H8A	109.5	F2—P1—F4′	105.3 (9)
C7—C8—H8B	109.5	F3—P1—F4′	87.1 (10)
H8A—C8—H8B	109.5	F6—P1—F4′	164.9 (9)
C7—C8—H8C	109.5	F5′—P1—F4′	94.0 (19)
H8A—C8—H8C	109.5	F2′—P1—F4′	86.7 (10)
H8B—C8—H8C	109.5	F1′—P1—F3′	89.0 (15)
O1—C7—C8	107.4 (3)	F6′—P1—F3′	86.7 (13)
O1—C7—H7A	110.2	F4—P1—F3′	96.0 (12)
C8—C7—H7A	110.2	F5—P1—F3′	169.1 (14)
O1—C7—H7B	110.2	F2—P1—F3′	94.9 (12)
C8—C7—H7B	110.2	F6—P1—F3′	82.3 (12)
H7A—C7—H7B	108.5	F5′—P1—F3′	171.8 (19)
H1WB—O1W—H1WA	122 (2)	F2′—P1—F3′	94.9 (17)
F1′—P1—F6′	96.0 (11)	F4′—P1—F3′	94.1 (14)
F1′—P1—F4	102.6 (9)	F6′—P1—F1	109.3 (11)
F6′—P1—F4	161.3 (10)	F4—P1—F1	89.4 (4)
F1′—P1—F5	80.8 (12)	F5—P1—F1	87.8 (5)
F6′—P1—F5	90.7 (10)	F2—P1—F1	177.8 (5)
F4—P1—F5	89.9 (8)	F3—P1—F1	90.3 (5)
F1′—P1—F2	164.6 (8)	F6—P1—F1	89.0 (3)
F6′—P1—F2	69.4 (10)	F5′—P1—F1	100.2 (13)
F4—P1—F2	91.9 (4)	F2′—P1—F1	162.3 (8)
F5—P1—F2	94.0 (6)	F4′—P1—F1	75.9 (10)
F1′—P1—F3	98.1 (12)	F3′—P1—F1	83.1 (11)
C7—O1—C1—C6	6.9 (5)	C2—C1—C6—C5	−0.3 (5)
C7—O1—C1—C2	−172.9 (3)	C4—C5—C6—C1	0.7 (5)
C5—C4—C3—C2	−0.2 (5)	C4—C3—C2—C1	0.7 (5)
N1—C4—C3—C2	−178.5 (3)	O1—C1—C2—C3	179.3 (3)
C3—C4—C5—C6	−0.5 (5)	C6—C1—C2—C3	−0.4 (5)
N1—C4—C5—C6	177.8 (3)	C1—O1—C7—C8	177.4 (3)
O1—C1—C6—C5	180.0 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F2′	0.89	2.16	3.03 (2)	167
N1—H1*A*···F2	0.89	2.17	3.049 (10)	169
N1—H1*B*···F1^{i}	0.89	2.22	3.066 (8)	158
N1—H1*B*···F1′^{i}	0.89	2.28	3.09 (3)	152

N1—H1*C*···O1*W*^{ii}	0.89	2.22	2.883 (3)	131
N1—H1*C*···F3^{ii}	0.89	2.46	3.137 (12)	133
N1—H1*C*···F3′^{ii}	0.89	2.40	3.01 (3)	126
N1—H1*C*···F6′^{ii}	0.89	2.51	2.96 (2)	112
O1*W*—H1*WB*···F3′^{iii}	0.82 (1)	2.20 (3)	2.97 (3)	156 (4)
O1*W*—H1*WB*···F3^{iii}	0.82 (1)	2.28 (3)	3.030 (12)	152 (4)
O1*W*—H1*WA*···F4^{i}	0.82 (3)	2.24 (2)	3.040 (12)	164 (4)
O1*W*—H1*WA*···F4′^{i}	0.82 (3)	2.11 (3)	2.88 (2)	155 (4)
O1*W*—H1*WA*···F5^{i}	0.82 (3)	2.48 (4)	2.951 (16)	117 (3)
C8—H8*C*···*Cg*1^{iv}	0.96	3.16	4.023 (5)	150

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