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4-[(2′-Cyanobiphenyl-4-yl)methyl]-morpholin-4-ium hexafluoridophosphate

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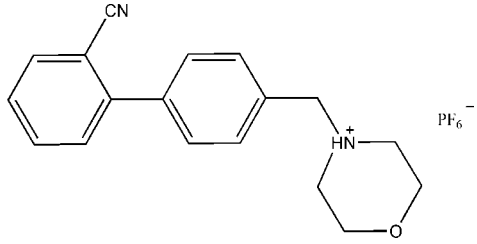
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.084; wR factor = 0.218; data-to-parameter ratio = 14.6.

In the cation of the title compound, $C_{18}H_{19}N_2O^+\cdot PF_6^-$, the morpholine ring adopts the usual chair conformation and the dihedral angle between the benzene rings is 67.55 (11)°. The F atoms of the anion are disordered over two orientations with a refined occupancy ratio of 0.65 (2):0.35 (2). In the crystal, intermolecular N—H···N hydrogen bonds link the cations into chains parallel to the c axis. The crystal packing is further enforced by interionic C—H···F hydrogen bonds.

Related literature

For the screening of molecular salts with physicochemical properties, see: Tong & Whitesell (1998); Shanker (1994). For the structures of related salts, see: SiMa (2010); Li *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{19}N_2O^+\cdot PF_6^-$ M_r = 424.32
Monoclinic, $C2/c$
a = 24.912 (11) Å
b = 10.757 (5) Å
c = 14.925 (7) Å
β = 91.07 (3)°
V = 3999 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.813, T_{max} = 1.000
21155 measured reflections
4512 independent reflections
3216 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.218
S = 1.19
4512 reflections
308 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.91	2.04	2.942 (4)	171
C10—H10A···F1^{ii}	0.93	2.43	3.296 (9)	155
C14—H14A···F3	0.97	2.39	3.355 (12)	171
C15—H15A···F6	0.97	2.46	3.377 (8)	158
C15—H15B···F3^{ii}	0.97	2.48	3.412 (10)	161
C15—H15B···F3′^{ii}	0.97	2.54	3.51 (2)	172
C10—H10A···F1′^{ii}	0.93	2.45	3.26 (2)	145
C14—H14B···F1′^{ii}	0.97	2.38	3.097 (16)	130
C5—H5A···F2′^{iii}	0.93	2.48	3.41 (2)	178
C17—H17B···F6′^{iv}	0.97	2.47	3.29 (3)	143

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

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: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2727).

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Shanker, R. (1994). *Pharm. Res.* A**11**, S–236.
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supplementary materials

Acta Cryst. (2012). E**68**, o1382 [doi:10.1107/S160053681201358X]

4-[(2′-Cyanobiphenyl-4-yl)methyl]morpholin-4-ium hexafluoridophosphate

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Comment

The title compound was prepared as part of our ongoing studies of hydrogen-bonding interactions in the crystal structure of protonated amines. The importance of molecular salts in pharmaceutical formulations is well known. For a given active ingredient, the isolation and selection of a salt with the appropriate physicochemical properties involves significant screening activity, as discussed at some length in the literature (Tong & Whitesell, 1998; Shanker, 1994). Here we report the synthesis and crystal structure of the title compound, 4-[(2′-cyanobiphenyl-4-yl)methyl]morpholin-4-ium hexafluorophosphate.

In the title compound (Fig. 1), bond distances and angles agree very well with those reported for a closely related nitrate (SiMa, 2010) and tetrafluoridoborate (Li *et al.*, 2011) derivatives. In the cation, the morpholine ring adopts the usual chair conformation, and the dihedral angle formed by the phenyl rings is 67.55 (11)°. The hexafluorophosphate anion displays a distorted octahedral geometry, the fluorine atoms being disordered over two orientations with site occupancies of 0.65 (2) and 0.35 (2) for the major and minor components of disorder, respectively. In the structure, the cations interact through intermolecular N–H···N hydrogen bonds (Table 1) to form chains parallel to the *c* axis (Fig. 2). Crystal packing is further consolidated by interionic C–H···O hydrogen bonds.

Experimental

To a stirred solution of 4′-(morpholinomethyl)biphenyl-2-carbonitrile (5.56 g, 0.02 mol) in methanol (30 mL), hexafluorophosphoric acid (4.17 g, 0.02 mol) was added at the room temperature. The precipitate was filtered and washed with a small amount of ethanol 95%. Single crystals suitable for X-ray diffraction analysis were obtained from slow evaporation of a solution of the title compound in water at room temperature.

Refinement

All H-atoms were positioned geometrically and refined using a riding model, with N—H = 0.91 Å, C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2 U_{eq}(N, C). The fluorine atoms of the anion are disoreder over two orientations with a refined occupancy ratio of 0.65 (2):0.35 (2).

Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); 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: *SHELXTL* (Sheldrick, 2008).

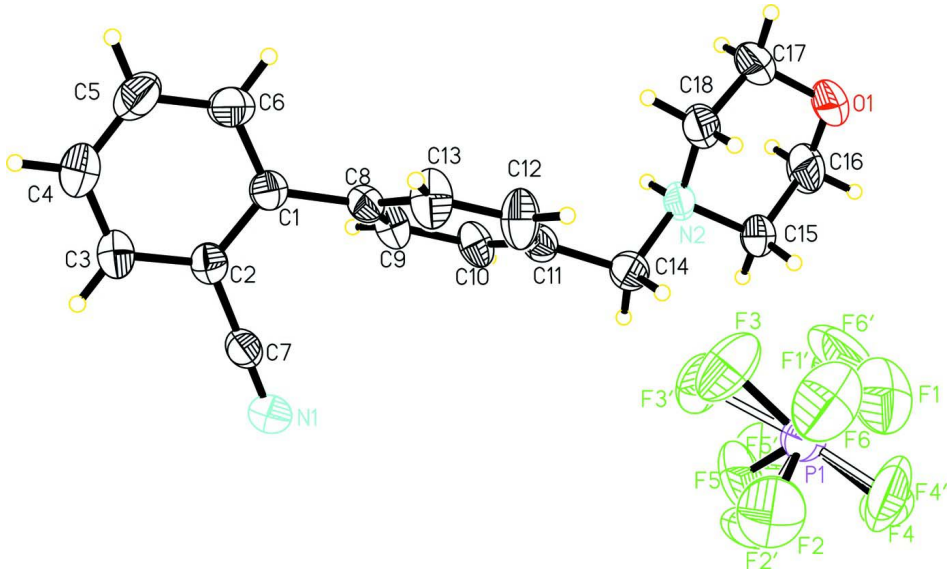

Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

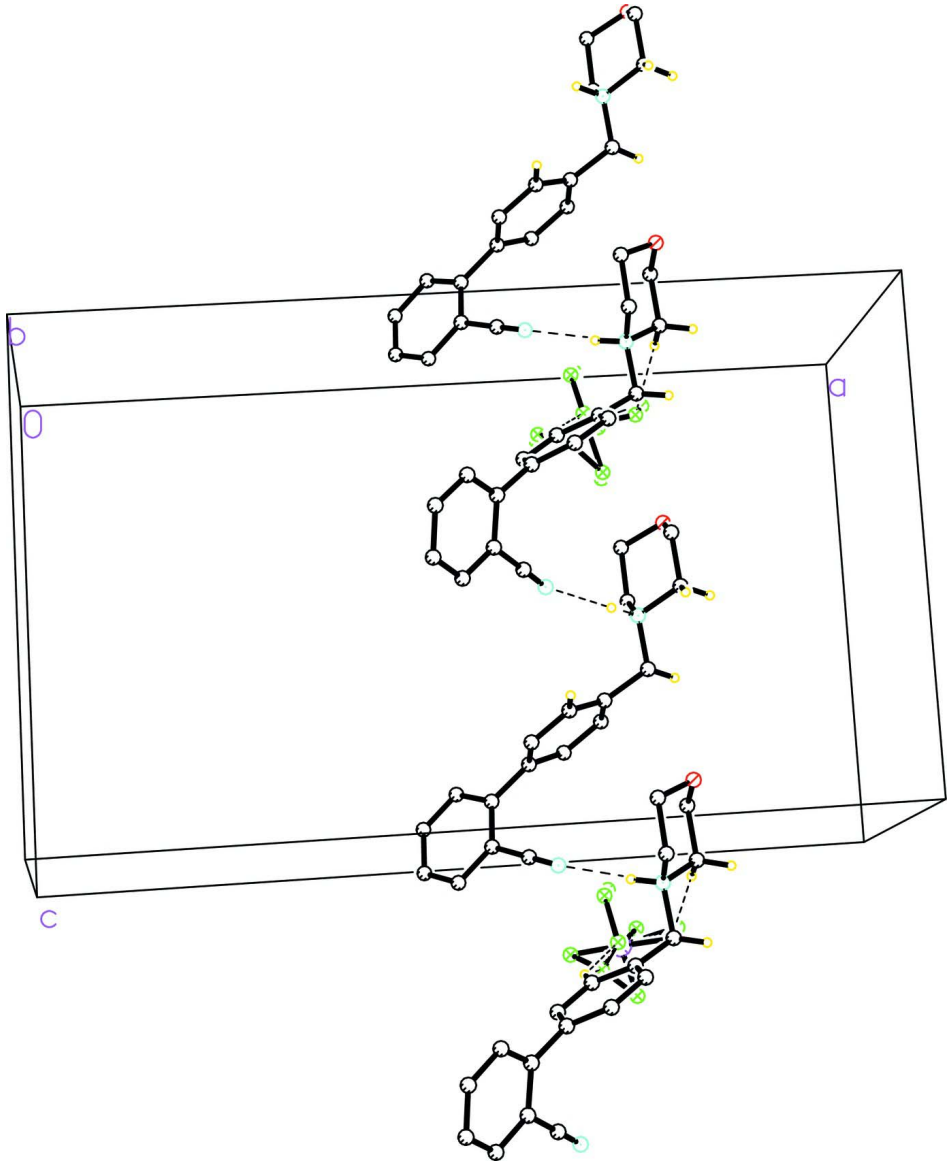

Figure 2

Partial crystal packing of the title compound showing a chain of cations interacting *via* intermolecular N—H···N hydrogen bonds (dashed lines).

4-[(2′-Cyanobiphenyl-4-yl)methyl]morpholin-4-ium hexafluoridophosphate

Crystal data

$C_{18}H_{19}N_2O^+·PF^{6-}$
M_r = 424.32
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 24.912 (11) Å
b = 10.757 (5) Å
c = 14.925 (7) Å
β = 91.07 (3)°
V = 3999 (3) Å^3
Z = 8
F(000) = 1744
D_x = 1.410 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4512 reflections
θ = 2.6–27.4°
μ = 0.20 mm^{-1}
T = 293 K
Prism, colourless
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.813, T_{max} = 1.000
21155 measured reflections
4512 independent reflections
3216 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 27.4°, θ_{min} = 2.1°
h = −32→31
k = −13→13
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.218
S = 1.19
4512 reflections
308 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0935P)^2 + 1.2795P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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}	Occ. (<1)
N2	0.32167 (9)	0.0538 (2)	0.37953 (14)	0.0586 (6)	
H2A	0.3533	0.0143	0.3918	0.070*	
C11	0.36122 (12)	0.1175 (3)	0.23215 (17)	0.0587 (7)	
C2	0.49042 (11)	0.2243 (3)	−0.01594 (18)	0.0597 (7)	
C8	0.44407 (11)	0.2199 (3)	0.13211 (17)	0.0568 (7)	
N1	0.42775 (12)	0.0475 (3)	−0.07023 (19)	0.0804 (8)	
C1	0.48586 (12)	0.2708 (3)	0.07186 (18)	0.0598 (7)	
C3	0.52800 (13)	0.2724 (3)	−0.0749 (2)	0.0750 (9)	
H3A	0.5302	0.2411	−0.1328	0.090*	
C15	0.27767 (13)	−0.0213 (3)	0.4206 (2)	0.0729 (9)	
H15A	0.2431	0.0145	0.4041	0.088*	
H15B	0.2787	−0.1056	0.3977	0.088*	
C7	0.45498 (12)	0.1267 (3)	−0.04641 (19)	0.0624 (7)	
C10	0.40494 (13)	0.0482 (3)	0.21080 (19)	0.0679 (8)	
H10A	0.4072	−0.0341	0.2296	0.082*	
C9	0.44606 (13)	0.0986 (3)	0.16145 (19)	0.0685 (8)	

H9A	0.4756	0.0497	0.1478	0.082*	
C14	0.31444 (13)	0.0585 (3)	0.27939 (19)	0.0697 (8)	
H14A	0.2821	0.1050	0.2649	0.084*	
H14B	0.3095	−0.0255	0.2570	0.084*	
C12	0.35927 (15)	0.2401 (3)	0.2056 (3)	0.0877 (11)	
H12A	0.3301	0.2892	0.2210	0.105*	
O1	0.28375 (13)	0.0972 (4)	0.55657 (19)	0.1302 (13)	
C13	0.40029 (15)	0.2908 (3)	0.1561 (3)	0.0877 (11)	
H13A	0.3984	0.3738	0.1388	0.105*	
C6	0.52083 (15)	0.3653 (3)	0.0969 (2)	0.0810 (10)	
H6A	0.5191	0.3980	0.1545	0.097*	
C4	0.56173 (15)	0.3664 (3)	−0.0467 (3)	0.0850 (10)	
H4A	0.5869	0.3986	−0.0856	0.102*	
C18	0.32429 (16)	0.1780 (4)	0.4223 (3)	0.0940 (12)	
H18A	0.2924	0.2252	0.4062	0.113*	
H18B	0.3553	0.2229	0.4009	0.113*	
C16	0.28390 (18)	−0.0235 (5)	0.5209 (2)	0.1058 (14)	
H16A	0.2547	−0.0710	0.5462	0.127*	
H16B	0.3174	−0.0644	0.5373	0.127*	
C5	0.55830 (15)	0.4125 (4)	0.0386 (3)	0.0916 (11)	
H5A	0.5813	0.4759	0.0574	0.110*	
C17	0.3284 (2)	0.1644 (5)	0.5233 (3)	0.140 (2)	
H17A	0.3613	0.1211	0.5394	0.168*	
H17B	0.3296	0.2461	0.5507	0.168*	
P1	0.15365 (4)	0.14226 (9)	0.20740 (6)	0.0750 (3)	
F1	0.1241 (5)	0.2534 (10)	0.2540 (7)	0.141 (3)	0.65 (2)
F2	0.1364 (4)	0.1889 (13)	0.1147 (8)	0.152 (4)	0.65 (2)
F3	0.2064 (5)	0.2159 (11)	0.2041 (10)	0.136 (4)	0.65 (2)
F4	0.0987 (4)	0.0652 (11)	0.2203 (5)	0.113 (2)	0.65 (2)
F5	0.1803 (6)	0.0238 (11)	0.1705 (8)	0.135 (4)	0.65 (2)
F6	0.1702 (3)	0.0918 (8)	0.3061 (6)	0.108 (2)	0.65 (2)
F1′	0.1419 (7)	0.2894 (14)	0.208 (3)	0.161 (9)	0.35 (2)
F2′	0.1432 (9)	0.147 (2)	0.1016 (11)	0.144 (8)	0.35 (2)
F3′	0.2163 (6)	0.186 (2)	0.1825 (12)	0.106 (5)	0.35 (2)
F4′	0.0981 (6)	0.116 (3)	0.2162 (15)	0.168 (10)	0.35 (2)
F5′	0.1754 (15)	0.0133 (19)	0.192 (2)	0.183 (12)	0.35 (2)
F6′	0.1687 (9)	0.147 (4)	0.3025 (11)	0.185 (10)	0.35 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0516 (13)	0.0768 (16)	0.0475 (12)	0.0046 (12)	0.0073 (9)	0.0004 (11)
C11	0.0619 (17)	0.0708 (18)	0.0434 (14)	0.0016 (14)	0.0008 (12)	0.0058 (12)
C2	0.0577 (16)	0.0639 (17)	0.0575 (16)	0.0037 (13)	0.0061 (13)	0.0023 (13)
C8	0.0634 (17)	0.0610 (17)	0.0461 (14)	0.0001 (13)	0.0020 (12)	0.0002 (12)
N1	0.0799 (19)	0.094 (2)	0.0675 (17)	−0.0107 (16)	−0.0001 (14)	−0.0165 (15)
C1	0.0620 (17)	0.0611 (17)	0.0566 (16)	−0.0026 (14)	0.0022 (13)	0.0024 (13)
C3	0.072 (2)	0.084 (2)	0.070 (2)	−0.0006 (17)	0.0195 (16)	0.0039 (16)
C15	0.071 (2)	0.085 (2)	0.0637 (18)	−0.0106 (17)	0.0155 (15)	0.0033 (15)

C7	0.0638 (18)	0.076 (2)	0.0481 (15)	0.0040 (16)	0.0055 (13)	−0.0039 (14)
C10	0.087 (2)	0.0641 (17)	0.0537 (16)	0.0120 (16)	0.0176 (15)	0.0115 (13)
C9	0.077 (2)	0.0720 (19)	0.0575 (17)	0.0198 (16)	0.0156 (15)	0.0090 (14)
C14	0.0677 (19)	0.091 (2)	0.0504 (16)	−0.0039 (17)	−0.0038 (13)	0.0087 (15)
C12	0.078 (2)	0.085 (2)	0.101 (3)	0.0250 (19)	0.032 (2)	0.026 (2)
O1	0.123 (2)	0.188 (3)	0.0812 (18)	−0.057 (2)	0.0535 (16)	−0.049 (2)
C13	0.097 (3)	0.0618 (19)	0.106 (3)	0.0170 (18)	0.034 (2)	0.0198 (18)
C6	0.091 (2)	0.083 (2)	0.069 (2)	−0.0196 (19)	−0.0070 (18)	−0.0045 (17)
C4	0.077 (2)	0.085 (2)	0.094 (3)	−0.0058 (19)	0.0180 (19)	0.017 (2)
C18	0.095 (3)	0.093 (3)	0.096 (3)	−0.028 (2)	0.040 (2)	−0.034 (2)
C16	0.103 (3)	0.153 (4)	0.062 (2)	−0.017 (3)	0.027 (2)	0.012 (2)
C5	0.080 (2)	0.088 (3)	0.107 (3)	−0.029 (2)	−0.001 (2)	0.011 (2)
C17	0.140 (4)	0.196 (5)	0.085 (3)	−0.075 (4)	0.052 (3)	−0.065 (3)
P1	0.0695 (6)	0.0775 (6)	0.0778 (6)	0.0104 (4)	−0.0032 (4)	−0.0038 (4)
F1	0.158 (7)	0.082 (4)	0.184 (7)	0.038 (4)	0.042 (4)	−0.015 (4)
F2	0.140 (5)	0.199 (9)	0.116 (7)	0.038 (6)	−0.024 (4)	0.072 (6)
F3	0.095 (5)	0.089 (4)	0.223 (10)	−0.024 (4)	−0.005 (5)	0.038 (5)
F4	0.097 (4)	0.146 (6)	0.096 (4)	−0.045 (4)	−0.004 (3)	−0.003 (3)
F5	0.157 (6)	0.112 (7)	0.138 (5)	0.028 (6)	0.075 (5)	−0.029 (5)
F6	0.095 (4)	0.136 (5)	0.093 (4)	0.011 (3)	−0.012 (2)	0.032 (4)
F1′	0.129 (10)	0.071 (7)	0.28 (3)	0.023 (6)	0.021 (10)	−0.022 (10)
F2′	0.167 (14)	0.198 (15)	0.068 (6)	−0.089 (13)	0.002 (7)	−0.033 (9)
F3′	0.061 (5)	0.143 (13)	0.113 (7)	0.024 (6)	−0.004 (5)	0.031 (7)
F4′	0.059 (6)	0.22 (3)	0.224 (16)	−0.005 (9)	0.043 (7)	−0.003 (13)
F5′	0.22 (2)	0.063 (8)	0.27 (3)	0.026 (9)	0.080 (17)	0.050 (12)
F6′	0.195 (14)	0.30 (3)	0.059 (8)	0.041 (16)	−0.016 (7)	−0.055 (11)

Geometric parameters (Å, º)

N2—C18	1.482 (4)	O1—C16	1.403 (5)
N2—C15	1.502 (4)	O1—C17	1.423 (5)
N2—C14	1.503 (3)	C13—H13A	0.9300
N2—H2A	0.9100	C6—C5	1.385 (5)
C11—C10	1.362 (4)	C6—H6A	0.9300
C11—C12	1.378 (4)	C4—C5	1.370 (5)
C11—C14	1.513 (4)	C4—H4A	0.9300
C2—C3	1.396 (4)	C18—C17	1.516 (5)
C2—C1	1.409 (4)	C18—H18A	0.9700
C2—C7	1.440 (4)	C18—H18B	0.9700
C8—C9	1.377 (4)	C16—H16A	0.9700
C8—C13	1.384 (4)	C16—H16B	0.9700
C8—C1	1.492 (4)	C5—H5A	0.9300
N1—C7	1.142 (4)	C17—H17A	0.9700
C1—C6	1.386 (4)	C17—H17B	0.9700
C3—C4	1.375 (5)	P1—F4′	1.421 (17)
C3—H3A	0.9300	P1—F6′	1.463 (16)
C15—C16	1.502 (5)	P1—F5′	1.51 (2)
C15—H15A	0.9700	P1—F2	1.527 (8)
C15—H15B	0.9700	P1—F3	1.536 (9)
C10—C9	1.384 (4)	P1—F5	1.543 (9)

C10—H10A	0.9300	P1—F1	1.574 (7)
C9—H9A	0.9300	P1—F2′	1.597 (15)
C14—H14A	0.9700	P1—F1′	1.610 (14)
C14—H14B	0.9700	P1—F4	1.615 (9)
C12—C13	1.384 (5)	P1—F6	1.616 (7)
C12—H12A	0.9300	P1—F3′	1.678 (17)
C18—N2—C15	109.6 (2)	C6—C5—H5A	119.8
C18—N2—C14	113.7 (3)	O1—C17—C18	111.0 (3)
C15—N2—C14	110.5 (2)	O1—C17—H17A	109.4
C18—N2—H2A	107.6	C18—C17—H17A	109.4
C15—N2—H2A	107.6	O1—C17—H17B	109.4
C14—N2—H2A	107.6	C18—C17—H17B	109.4
C10—C11—C12	118.7 (3)	H17A—C17—H17B	108.0
C10—C11—C14	120.4 (3)	F4′—P1—F6′	98.6 (13)
C12—C11—C14	120.8 (3)	F4′—P1—F5′	100.7 (18)
C3—C2—C1	121.4 (3)	F6′—P1—F5′	95.1 (17)
C3—C2—C7	119.0 (3)	F4′—P1—F2	83.7 (11)
C1—C2—C7	119.5 (3)	F6′—P1—F2	158.7 (14)
C9—C8—C13	117.6 (3)	F5′—P1—F2	105.3 (13)
C9—C8—C1	121.2 (3)	F4′—P1—F3	160.1 (12)
C13—C8—C1	121.1 (3)	F6′—P1—F3	79.0 (11)
C6—C1—C2	116.7 (3)	F5′—P1—F3	99.2 (14)
C6—C1—C8	123.3 (3)	F2—P1—F3	91.6 (6)
C2—C1—C8	120.0 (3)	F4′—P1—F5	107.3 (14)
C4—C3—C2	119.5 (3)	F6′—P1—F5	105.6 (15)
C4—C3—H3A	120.2	F2—P1—F5	93.7 (7)
C2—C3—H3A	120.2	F3—P1—F5	92.3 (8)
C16—C15—N2	110.7 (3)	F4′—P1—F1	69.1 (11)
C16—C15—H15A	109.5	F6′—P1—F1	70.1 (14)
N2—C15—H15A	109.5	F5′—P1—F1	159.6 (10)
C16—C15—H15B	109.5	F2—P1—F1	91.4 (6)
N2—C15—H15B	109.5	F3—P1—F1	91.8 (5)
H15A—C15—H15B	108.1	F5—P1—F1	173.4 (5)
N1—C7—C2	178.5 (3)	F4′—P1—F2′	87.5 (11)
C11—C10—C9	120.9 (3)	F6′—P1—F2′	173.3 (14)
C11—C10—H10A	119.6	F5′—P1—F2′	86.4 (14)
C9—C10—H10A	119.6	F3—P1—F2′	94.3 (8)
C8—C9—C10	121.2 (3)	F5—P1—F2′	74.8 (10)
C8—C9—H9A	119.4	F1—P1—F2′	110.0 (9)
C10—C9—H9A	119.4	F4′—P1—F1′	90.9 (12)
N2—C14—C11	113.5 (2)	F6′—P1—F1′	90.5 (12)
N2—C14—H14A	108.9	F5′—P1—F1′	166.2 (12)
C11—C14—H14A	108.9	F2—P1—F1′	68.3 (10)
N2—C14—H14B	108.9	F3—P1—F1′	69.4 (7)
C11—C14—H14B	108.9	F5—P1—F1′	153.1 (13)
H14A—C14—H14B	107.7	F2′—P1—F1′	86.7 (11)
C11—C12—C13	120.6 (3)	F6′—P1—F4	96.0 (13)
C11—C12—H12A	119.7	F5′—P1—F4	81.5 (13)

C13—C12—H12A	119.7	F2—P1—F4	93.0 (6)
C16—O1—C17	109.3 (3)	F3—P1—F4	175.0 (6)
C8—C13—C12	120.9 (3)	F5—P1—F4	89.4 (7)
C8—C13—H13A	119.5	F1—P1—F4	86.1 (6)
C12—C13—H13A	119.5	F2′—P1—F4	90.7 (7)
C5—C6—C1	121.8 (3)	F1′—P1—F4	110.5 (8)
C5—C6—H6A	119.1	F4′—P1—F6	94.7 (11)
C1—C6—H6A	119.1	F5′—P1—F6	74.9 (13)
C5—C4—C3	120.1 (3)	F2—P1—F6	178.3 (5)
C5—C4—H4A	119.9	F3—P1—F6	90.0 (5)
C3—C4—H4A	119.9	F5—P1—F6	86.8 (6)
N2—C18—C17	110.0 (3)	F1—P1—F6	88.0 (4)
N2—C18—H18A	109.7	F2′—P1—F6	161.3 (9)
C17—C18—H18A	109.7	F1′—P1—F6	111.8 (12)
N2—C18—H18B	109.7	F4—P1—F6	85.4 (4)
C17—C18—H18B	109.7	F4′—P1—F3′	170.8 (13)
H18A—C18—H18B	108.2	F6′—P1—F3′	89.0 (11)
O1—C16—C15	111.3 (3)	F5′—P1—F3′	83.6 (14)
O1—C16—H16A	109.4	F2—P1—F3′	87.4 (7)
C15—C16—H16A	109.4	F5—P1—F3′	75.2 (9)
O1—C16—H16B	109.4	F1—P1—F3′	109.2 (8)
C15—C16—H16B	109.4	F2′—P1—F3′	84.6 (9)
H16A—C16—H16B	108.0	F1′—P1—F3′	83.9 (9)
C4—C5—C6	120.4 (3)	F4—P1—F3′	164.7 (8)
C4—C5—H5A	119.8	F6—P1—F3′	94.3 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N1^{i}	0.91	2.04	2.942 (4)	171
C10—H10*A*···F1^{ii}	0.93	2.43	3.296 (9)	155
C14—H14*A*···F3	0.97	2.39	3.355 (12)	171
C15—H15*A*···F6	0.97	2.46	3.377 (8)	158
C15—H15*B*···F3^{ii}	0.97	2.48	3.412 (10)	161
C15—H15*B*···F3′^{ii}	0.97	2.54	3.51 (2)	172
C10—H10*A*···F1′^{ii}	0.93	2.45	3.26 (2)	145
C14—H14*B*···F1′^{ii}	0.97	2.38	3.097 (16)	130
C5—H5*A*···F2′^{iii}	0.93	2.48	3.41 (2)	178
C17—H17*B*···F6′^{iv}	0.97	2.47	3.29 (3)	143

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