2-(2-Azabicyclo[3.2.1]octa-3,6-dien-2-yl)-1,3-dimethoxyimidazolium hexafluoridophosphate

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The title salt, $C_{12}H_{16}N_3O_2{}^+ \cdot PF_6{}^-$, was obtained by the dipolar cycloaddition of norbornadiene to 2-azido-1,3-dimethoxyimidazolium hexafluoridophosphate. The methoxy groups attached to the imidazolium ring of the cation adopt an *anti* conformation [displacements of the C atoms from the ring plane = 1.386 (4) and −1.404 (3) Å]. In the crystal, weak inter-ionic C—H···F contacts are observed. The structure was refined as a two-component twin. Positional disorder of the fluorine atoms of the PF_6 anion was observed, the occupancy ratio being 0.562 (16):0.438 (16).

3D view
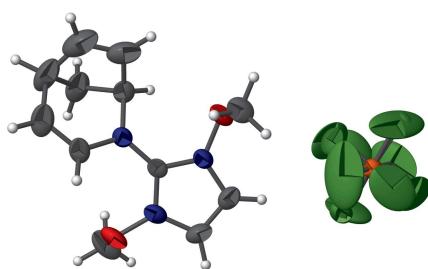
Chemical scheme
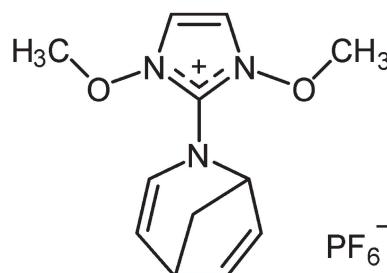
Structure description

The 1,3-dipolar cycloaddition of strained alkenes such as norbornene or norbornadiene to azidoazolium salts with concomitant loss of dinitrogen affords tricyclic aziridines or bicyclic azaoctadienes, respectively (Laus, Kahlenberg *et al.*, 2016; Laus, Kostner *et al.*, 2016). Thus, the title compound was obtained from bicyclo[2.2.1]hepta-2,5-diene (norbornadiene) and 2-azido-1,3-dimethoxyimidazolium hexafluoridophosphate.

Conformational *syn/anti* isomerism in related 1,3-di(alkyloxy)imidazolium salts has been noticed previously (Laus *et al.*, 2007; Laus, Kahlenberg *et al.*, 2010; Laus, Wurst *et al.*, 2010; Froschauer *et al.*, 2013; Rietzler *et al.*, 2015; Partl *et al.*, 2016). Here, the methoxy groups of the norbornadiene adduct adopt an *anti* conformation (Fig. 1). The C4 atom is displaced from the ring plane by 1.386 (4), and C5 by −1.404 (3) Å. A C4—O1···O2—C5 pseudo dihedral angle of 168.4 (3)° is found.

There are no directional classical hydrogen bonds in this structure. At the most, weak C—H···F interactions (H2···F5 = 2.36, H3···F6 = 2.42 and H5*A*···F5 = 2.53 Å) shorter than the sum of van der Waals radii between the imidazole H atoms and negatively polarized F atoms are worth mentioning (Table 1; Fig. 2).
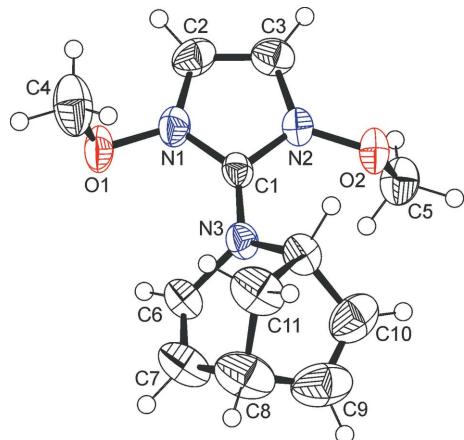
Figure 1
The molecular structure of the cation of the title compound, showing 50% probability displacement ellipsoids. The anion is not shown.

Synthesis and crystallization

A solution of 2-azido-1,3-dimethoxyimidazolium hexafluoridophosphate (0.38 g, 1.2 mmol; Laus *et al.*, 2007) and norbornadiene (0.13 g, 1.4 mmol) in acetone (20 ml) was stirred for 18 h at room temperature. The volatiles were removed under reduced pressure, and the residue was crystallized from H_2O/acetone. ^{1}H NMR (300 MHz, DMSO-d_6): δ 1.86 (*d*, *J* = 10.6 Hz, 1H), 2.00 (*m*, 1H), 2.87 (*m*, 1H), 4.12 (*s*, 6H), 4.76 (*s*, 1H), 5.40 (*td*, *J* = 6.4, 1.3 Hz, 1H), 5.68 (*dd*, *J* = 2.3, 5.5 Hz, 1H), 6.06 (*dd*, *J* = 0.9, 7.7 Hz, 1H), 6.41 (*dd*, *J* = 2.7, 5.4 Hz, 1H), 8.00 (*s*, 2H) p.p.m. ^{13}C NMR (75 MHz, DMSO-d_6): δ 35.2, 36.2, 63.8, 68.0 (2 C), 109.6, 112.4 (2 C), 121.2, 122.4, 134.8, 139.4 p.p.m. IR (neat): ν 3173, 3151, 1627, 1614, 827 cm^{-1}.
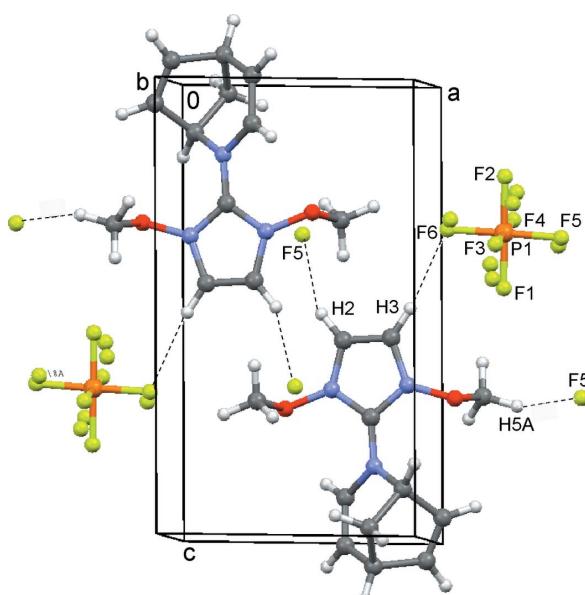

Figure 2
Crystal packing of the title compound. The C—H···F interactions are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···F5^i	0.95	2.36	3.242 (12)	154
C2—H2···F5A^i	0.95	2.36	3.23 (2)	153
C3—H3···F6	0.95	2.42	3.365 (11)	171
C4—H4A···F6A^{ii}	0.98	2.49	3.21 (2)	131
C4—H4B···F2A^{iii}	0.98	2.51	3.383 (17)	148
C5—H5A···F5^{iv}	0.98	2.53	3.134 (11)	120
C5—H5A···F5A^{iv}	0.98	2.34	3.02 (2)	125

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{16}N_3O_2{}^+ \cdot PF_6{}^-$
M_r	379.25
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	173
a, b, c (Å)	7.4207 (6), 8.8159 (7), 12.5246 (10)
α, β, γ (°)	86.873 (3), 87.735 (3), 77.166 (3)
V (Å^3)	797.39 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.25
Crystal size (mm)	0.18 × 0.17 × 0.09
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON 100
Absorption correction	Multi-scan (*DIFABS*; Bruker, 2014)
T_{min}, T_{max}	0.792, 0.862
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2774, 2774, 2501
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.124, 1.12
No. of reflections	2774
No. of parameters	273
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.40, −0.31

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXS2014*/7 (Sheldrick, 2008), *SHELXL2014*/7 (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2006).

Refinement

The structure was refined as a two-component twin with non-merohedral twinning by 180 degrees about the reciprocal axis 0 0 1. In addition, positional disorder of the fluorine atoms of the PF$_6$ anion was observed; the occupancy ratio of 0.562 (16):0.438 (16) for the two orientations was obtained by refinement with a free variable. Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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2-(2-Azabicyclo[3.2.1]octa-3,6-dien-2-yl)-1,3-dimethoxyimidazolium hexafluoridophosphate

Crystal data
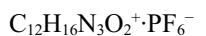
$C_{12}H_{16}N_3O_2{}^+ \cdot PF_6{}^-$	$Z = 2$
$M_r = 379.25$	$F(000) = 388$
Triclinic, $P\bar{1}$	$D_x = 1.580$ Mg m^{-3}
$a = 7.4207$ (6) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 8.8159$ (7) Å	Cell parameters from 4024 reflections
$c = 12.5246$ (10) Å	$\theta = 2.8–25.3°$
$\alpha = 86.873$ (3)°	$\mu = 0.25$ mm^{-1}
$\beta = 87.735$ (3)°	$T = 173$ K
$\gamma = 77.166$ (3)°	Prism, brown
$V = 797.39$ (11) Å^3	$0.18 \times 0.17 \times 0.09$ mm

Data collection

Bruker D8 QUEST PHOTON 100 diffractometer	$T_{min} = 0.792$, $T_{max} = 0.862$
Radiation source: Incoatec Microfocus	2774 measured reflections
Multi layered optics monochromator	2774 independent reflections
Detector resolution: 10.4 pixels mm^{-1}	2501 reflections with $I > 2\sigma(I)$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (DIFABS; Bruker, 2014)	$h = -8 \rightarrow 8$
	$k = -10 \rightarrow 10$
	$l = 0 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o{}^2) + (0.031P)^2 + 0.897P]$
$wR(F^2) = 0.124$	where $P = (F_o{}^2 + 2F_c{}^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
2774 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
273 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
0 restraints	

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. Refined as a 2-component twin with non-merohedral twinning by 180 degrees about the reciprocal axis 0 0 1. Programs like "cell_now" and "twinabs" (Bruker) were used for cell search of twin components and absorption correction. Positional disorder of the fluorine atoms of PF6; ratio of 56:44 was obtained by using refinement with free variable.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.4239 (4)	0.2863 (3)	0.7117 (3)	0.0505 (8)	
O2	1.0715 (3)	0.2143 (3)	0.6834 (3)	0.0429 (7)	
N1	0.6012 (4)	0.2657 (4)	0.6683 (3)	0.0417 (8)	
N2	0.8907 (4)	0.2373 (4)	0.6560 (3)	0.0367 (8)	
N3	0.7628 (4)	0.2455 (4)	0.8350 (2)	0.0372 (8)	
C1	0.7505 (6)	0.2487 (5)	0.7279 (3)	0.0335 (8)	
C2	0.6461 (7)	0.2612 (5)	0.5602 (4)	0.0513 (11)	
H2	0.5639	0.2666	0.5032	0.062*	
C3	0.8300 (7)	0.2476 (5)	0.5526 (3)	0.0470 (11)	
H3	0.9036	0.2454	0.4887	0.056*	
C4	0.3311 (7)	0.4469 (5)	0.6979 (5)	0.0724 (16)	
H4A	0.2053	0.4614	0.7287	0.109*	
H4B	0.3989	0.5117	0.7342	0.109*	
H4C	0.3256	0.4774	0.6215	0.109*	
C5	1.1633 (6)	0.0519 (4)	0.6758 (4)	0.0513 (11)	
H5A	1.2927	0.0374	0.6957	0.077*	
H5B	1.1011	−0.0124	0.7244	0.077*	
H5C	1.1583	0.0208	0.6022	0.077*	
C6	0.6429 (6)	0.1744 (5)	0.9028 (3)	0.0462 (10)	
H6	0.5642	0.1171	0.8733	0.055*	
C7	0.6429 (8)	0.1896 (6)	1.0083 (4)	0.0650 (14)	
H7	0.5667	0.1398	1.0544	0.078*	
C8	0.7627 (11)	0.2851 (7)	1.0546 (4)	0.0775 (17)	
H8	0.7280	0.3147	1.1298	0.093*	
C9	0.9570 (10)	0.1996 (7)	1.0392 (5)	0.0832 (19)	
H9	1.0245	0.1315	1.0923	0.100*	
C10	1.0243 (8)	0.2281 (6)	0.9454 (5)	0.0685 (15)	
H10	1.1462	0.1852	0.9198	0.082*	
C11	0.8821 (6)	0.3375 (5)	0.8847 (3)	0.0428 (10)	
H11	0.9348	0.4058	0.8315	0.051*	
C12	0.7620 (8)	0.4288 (6)	0.9721 (4)	0.0673 (15)	
H12A	0.6363	0.4779	0.9477	0.081*	
H12B	0.8201	0.5082	1.0009	0.081*	
P1	1.26751 (15)	0.24411 (11)	0.32028 (8)	0.0327 (2)	
F1	1.2604 (10)	0.1998 (16)	0.4404 (5)	0.095 (5)	0.562 (16)
F2	1.2768 (14)	0.2929 (17)	0.1975 (5)	0.104 (4)	0.562 (16)
F3	1.2520 (13)	0.4160 (9)	0.3478 (14)	0.115 (5)	0.562 (16)
F4	1.285 (2)	0.0749 (9)	0.2887 (15)	0.137 (7)	0.562 (16)
F5	1.4859 (13)	0.2220 (13)	0.3286 (9)	0.068 (3)	0.562 (16)
F6	1.0517 (15)	0.2681 (14)	0.3144 (8)	0.066 (3)	0.562 (16)

F1A	1.201 (3)	0.1183 (18)	0.387 (2)	0.205 (11)	0.438 (16)
F2A	1.315 (2)	0.382 (2)	0.258 (2)	0.159 (9)	0.438 (16)
F3A	1.232 (2)	0.341 (2)	0.4227 (13)	0.134 (7)	0.438 (16)
F4A	1.305 (2)	0.139 (3)	0.2291 (15)	0.149 (9)	0.438 (16)
F5A	1.470 (2)	0.177 (3)	0.345 (2)	0.184 (11)	0.438 (16)
F6A	1.067 (2)	0.318 (3)	0.2936 (18)	0.135 (8)	0.438 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0267 (15)	0.0486 (17)	0.078 (2)	−0.0131 (13)	−0.0037 (14)	0.0034 (15)
O2	0.0269 (13)	0.0386 (14)	0.0639 (19)	−0.0073 (11)	0.0018 (14)	−0.0100 (15)
N1	0.0323 (17)	0.0449 (18)	0.051 (2)	−0.0143 (14)	−0.0047 (17)	−0.0025 (17)
N2	0.0301 (17)	0.0390 (17)	0.042 (2)	−0.0095 (13)	0.0010 (14)	−0.0058 (14)
N3	0.0345 (19)	0.0411 (19)	0.0392 (17)	−0.0147 (14)	0.0014 (14)	−0.0049 (15)
C1	0.0320 (19)	0.0313 (19)	0.0403 (19)	−0.0141 (15)	−0.0001 (18)	−0.0009 (17)
C2	0.060 (3)	0.055 (3)	0.042 (3)	−0.017 (2)	−0.016 (2)	−0.005 (2)
C3	0.060 (3)	0.047 (2)	0.037 (2)	−0.017 (2)	−0.001 (2)	−0.0073 (19)
C4	0.047 (3)	0.050 (3)	0.121 (5)	−0.011 (2)	0.010 (3)	−0.017 (3)
C5	0.044 (2)	0.035 (2)	0.072 (3)	−0.0010 (17)	−0.001 (2)	−0.010 (2)
C6	0.047 (2)	0.047 (2)	0.047 (3)	−0.017 (2)	0.009 (2)	−0.003 (2)
C7	0.087 (4)	0.055 (3)	0.057 (3)	−0.029 (3)	0.021 (3)	−0.006 (2)
C8	0.120 (5)	0.078 (4)	0.045 (3)	−0.041 (4)	0.012 (4)	−0.023 (3)
C9	0.124 (6)	0.079 (4)	0.058 (4)	−0.044 (4)	−0.029 (4)	0.002 (3)
C10	0.077 (4)	0.059 (3)	0.077 (4)	−0.025 (3)	−0.030 (3)	−0.005 (3)
C11	0.048 (2)	0.039 (2)	0.046 (2)	−0.0162 (18)	0.0029 (19)	−0.0122 (18)
C12	0.093 (4)	0.059 (3)	0.055 (3)	−0.025 (3)	0.014 (3)	−0.024 (3)
P1	0.0377 (5)	0.0274 (4)	0.0329 (5)	−0.0070 (3)	−0.0026 (5)	−0.0024 (5)
F1	0.080 (5)	0.183 (13)	0.025 (3)	−0.041 (6)	−0.002 (3)	0.031 (5)
F2	0.110 (6)	0.161 (12)	0.034 (3)	−0.025 (6)	0.000 (4)	0.028 (5)
F3	0.099 (6)	0.040 (4)	0.210 (15)	−0.021 (4)	0.032 (8)	−0.048 (6)
F4	0.138 (8)	0.028 (4)	0.252 (19)	−0.028 (4)	0.020 (11)	−0.052 (6)
F5	0.040 (4)	0.099 (6)	0.068 (5)	−0.024 (5)	0.001 (3)	−0.010 (4)
F6	0.044 (4)	0.099 (7)	0.064 (4)	−0.028 (4)	0.005 (3)	−0.028 (5)
F1A	0.31 (3)	0.088 (9)	0.22 (2)	−0.074 (12)	0.124 (19)	0.038 (11)
F2A	0.155 (13)	0.109 (12)	0.22 (2)	−0.067 (10)	−0.010 (13)	0.107 (14)
F3A	0.165 (12)	0.127 (15)	0.110 (12)	−0.009 (10)	0.000 (9)	−0.101 (11)
F4A	0.136 (11)	0.19 (2)	0.117 (13)	−0.003 (14)	−0.002 (10)	−0.141 (14)
F5A	0.098 (12)	0.169 (16)	0.24 (2)	0.101 (11)	−0.103 (13)	−0.121 (14)
F6A	0.047 (8)	0.133 (14)	0.208 (17)	0.017 (8)	−0.059 (9)	0.014 (11)

Geometric parameters (Å, º)

O1—N1	1.380 (4)	C8—C9	1.481 (9)
O1—C4	1.435 (5)	C8—C12	1.590 (8)
O2—N2	1.366 (4)	C8—H8	1.0000
O2—C5	1.449 (4)	C9—C10	1.293 (9)
N1—C1	1.336 (5)	C9—H9	0.9500

N1—C2	1.382 (6)	C10—C11	1.467 (7)
N2—C1	1.339 (5)	C10—H10	0.9500
N2—C3	1.379 (5)	C11—C12	1.529 (6)
N3—C1	1.347 (5)	C11—H11	1.0000
N3—C6	1.426 (5)	C12—H12A	0.9900
N3—C11	1.499 (5)	C12—H12B	0.9900
C2—C3	1.343 (6)	P1—F4A	1.489 (9)
C2—H2	0.9500	P1—F2A	1.504 (9)
C3—H3	0.9500	P1—F1A	1.511 (10)
C4—H4A	0.9800	P1—F5A	1.523 (15)
C4—H4B	0.9800	P1—F6A	1.528 (15)
C4—H4C	0.9800	P1—F1	1.535 (5)
C5—H5A	0.9800	P1—F4	1.540 (7)
C5—H5B	0.9800	P1—F3	1.550 (7)
C5—H5C	0.9800	P1—F3A	1.562 (9)
C6—C7	1.335 (6)	P1—F6	1.572 (11)
C6—H6	0.9500	P1—F2	1.577 (6)
C7—C8	1.504 (8)	P1—F5	1.596 (9)
C7—H7	0.9500		
N1—O1—C4	109.6 (3)	C8—C9—H9	123.8
N2—O2—C5	110.5 (3)	C9—C10—C11	109.0 (6)
C1—N1—O1	123.0 (4)	C9—C10—H10	125.5
C1—N1—C2	112.1 (4)	C11—C10—H10	125.5
O1—N1—C2	124.9 (4)	C10—C11—N3	108.0 (4)
C1—N2—O2	123.3 (3)	C10—C11—C12	103.2 (4)
C1—N2—C3	111.7 (3)	N3—C11—C12	106.1 (4)
O2—N2—C3	124.9 (3)	C10—C11—H11	113.0
C1—N3—C6	120.6 (3)	N3—C11—H11	113.0
C1—N3—C11	120.1 (3)	C12—C11—H11	113.0
C6—N3—C11	118.7 (3)	C11—C12—C8	96.9 (4)
N1—C1—N2	104.0 (3)	C11—C12—H12A	112.4
N1—C1—N3	129.5 (4)	C8—C12—H12A	112.4
N2—C1—N3	126.5 (4)	C11—C12—H12B	112.4
C3—C2—N1	105.7 (4)	C8—C12—H12B	112.4
C3—C2—H2	127.2	H12A—C12—H12B	109.9
N1—C2—H2	127.2	F4A—P1—F2A	95.0 (11)
C2—C3—N2	106.4 (4)	F4A—P1—F1A	89.4 (11)
C2—C3—H3	126.8	F2A—P1—F1A	173.8 (11)
N2—C3—H3	126.8	F4A—P1—F5A	84.3 (10)
O1—C4—H4A	109.5	F2A—P1—F5A	91.4 (12)
O1—C4—H4B	109.5	F1A—P1—F5A	93.4 (13)
H4A—C4—H4B	109.5	F4A—P1—F6A	96.4 (10)
O1—C4—H4C	109.5	F2A—P1—F6A	85.9 (10)
H4A—C4—H4C	109.5	F1A—P1—F6A	89.3 (11)
H4B—C4—H4C	109.5	F5A—P1—F6A	177.3 (12)
O2—C5—H5A	109.5	F1—P1—F4	92.9 (7)
O2—C5—H5B	109.5	F1—P1—F3	89.2 (7)

H5A—C5—H5B	109.5	F4—P1—F3	177.9 (8)
O2—C5—H5C	109.5	F4A—P1—F3A	174.9 (11)
H5A—C5—H5C	109.5	F2A—P1—F3A	89.6 (11)
H5B—C5—H5C	109.5	F1A—P1—F3A	86.2 (9)
C7—C6—N3	119.1 (4)	F5A—P1—F3A	93.4 (10)
C7—C6—H6	120.4	F6A—P1—F3A	86.1 (10)
N3—C6—H6	120.4	F1—P1—F6	91.1 (5)
C6—C7—C8	120.4 (4)	F4—P1—F6	88.4 (7)
C6—C7—H7	119.8	F3—P1—F6	92.1 (5)
C8—C7—H7	119.8	F1—P1—F2	178.7 (7)
C9—C8—C7	107.0 (5)	F4—P1—F2	88.3 (7)
C9—C8—C12	99.4 (5)	F3—P1—F2	89.6 (7)
C7—C8—C12	106.2 (4)	F6—P1—F2	89.5 (5)
C9—C8—H8	114.3	F1—P1—F5	88.0 (5)
C7—C8—H8	114.3	F4—P1—F5	92.6 (7)
C12—C8—H8	114.3	F3—P1—F5	87.0 (5)
C10—C9—C8	112.4 (6)	F6—P1—F5	178.7 (5)
C10—C9—H9	123.8	F2—P1—F5	91.3 (5)
C4—O1—N1—C1	103.4 (5)	O2—N2—C3—C2	176.5 (3)
C4—O1—N1—C2	−76.1 (5)	C1—N3—C6—C7	−171.9 (5)
C5—O2—N2—C1	99.9 (4)	C11—N3—C6—C7	−1.1 (7)
C5—O2—N2—C3	−78.3 (5)	N3—C6—C7—C8	2.1 (8)
O1—N1—C1—N2	−178.0 (3)	C6—C7—C8—C9	−69.0 (7)
C2—N1—C1—N2	1.6 (5)	C6—C7—C8—C12	36.5 (7)
O1—N1—C1—N3	1.0 (7)	C7—C8—C9—C10	84.2 (6)
C2—N1—C1—N3	−179.4 (4)	C12—C8—C9—C10	−26.1 (6)
O2—N2—C1—N1	−178.2 (3)	C8—C9—C10—C11	−0.1 (7)
C3—N2—C1—N1	0.2 (5)	C9—C10—C11—N3	−84.2 (5)
O2—N2—C1—N3	2.7 (6)	C9—C10—C11—C12	27.8 (5)
C3—N2—C1—N3	−178.9 (4)	C1—N3—C11—C10	−119.4 (5)
C6—N3—C1—N1	36.2 (6)	C6—N3—C11—C10	69.8 (5)
C11—N3—C1—N1	−134.4 (4)	C1—N3—C11—C12	130.6 (4)
C6—N3—C1—N2	−144.9 (4)	C6—N3—C11—C12	−40.2 (5)
C11—N3—C1—N2	44.4 (6)	C10—C11—C12—C8	−40.5 (5)
C1—N1—C2—C3	−2.7 (5)	N3—C11—C12—C8	72.9 (5)
O1—N1—C2—C3	176.9 (3)	C9—C8—C12—C11	39.0 (5)
N1—C2—C3—N2	2.6 (4)	C7—C8—C12—C11	−71.9 (5)
C1—N2—C3—C2	−1.8 (5)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···F5[i]	0.95	2.36	3.242 (12)	154
C2—H2···F5A[i]	0.95	2.36	3.23 (2)	153
C3—H3···F6	0.95	2.42	3.365 (11)	171
C4—H4A···F6A[ii]	0.98	2.49	3.21 (2)	131
C4—H4B···F2A[iii]	0.98	2.51	3.383 (17)	148

C5—H5*A*···F5^{iv}	0.98	2.53	3.134 (11)	120
C5—H5*A*···F5*A*^{iv}	0.98	2.34	3.02 (2)	125

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