

# Poly[[silver(I)-bis[ $\mu_2$ -3-(aminomethyl)pyridine]- $\kappa^2 N^1:N^3$ ; $\kappa^2 N^3:N^1$ ] hexafluoridophosphate]

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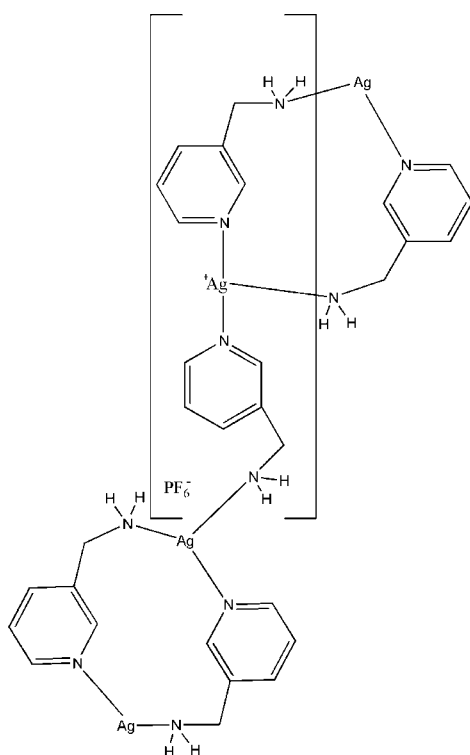
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Key indicators: single-crystal X-ray study;  $T = 110$  K; mean  $\sigma(C-C) = 0.005$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.117; data-to-parameter ratio = 15.6.

In the title compound,  $\{[Ag(C_6H_8N_2)_2]PF_6\}_n$ , a two-dimensional coordination polymer is formed by linking each Ag atom of the  $[Ag(3-AMP)]_2$  rings [3-AMP is 3-(aminomethyl)pyridine] with an additional equivalent of 3-AMP. This polymer exhibits hydrogen bonding to the anion, which sits in channels forming a three-dimensional network. Each Ag atom is ligated by two pyridine and two amine groups.

## Related literature

For related literature, see: Feazell *et al.* (2006a,b,c); Klausmeyer *et al.* (2004).



## Experimental

### Crystal data

$[Ag(C_6H_8N_2)_2]PF_6$   
 $M_r = 469.13$   
 Monoclinic,  $P2_1/n$   
 $a = 6.9563$  (11) Å  
 $b = 11.584$  (2) Å  
 $c = 20.060$  (3) Å  
 $\beta = 90.271$  (5)°

$V = 1616.4$  (4) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.41$  mm<sup>-1</sup>  
 $T = 110$  (2) K  
 $0.25 \times 0.17 \times 0.12$  mm

### Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.740$ ,  $T_{max} = 0.845$   
 16863 measured reflections  
 3387 independent reflections  
 3006 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.031$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.117$   
 $S = 0.96$   
 3387 reflections  
 217 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 1.18$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.67$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Ag1—N1	2.296 (3)	Ag1—N3	2.357 (3)
Ag1—N2 <sup>i</sup>	2.348 (3)	Ag1—N4 <sup>ii</sup>	2.367 (3)
N1—Ag1—N2 <sup>i</sup>	128.98 (10)	N1—Ag1—N4 <sup>ii</sup>	108.13 (9)
N1—Ag1—N3	108.29 (9)	N2 <sup>i</sup> —Ag1—N4 <sup>ii</sup>	93.57 (10)
N2 <sup>i</sup> —Ag1—N3	104.49 (9)	N3—Ag1—N4 <sup>ii</sup>	112.55 (9)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N4—H4A $\cdots$ F1	0.90	2.34	3.135 (4)	147
N4—H4A $\cdots$ F5	0.90	2.52	3.334 (4)	151
N4—H4B $\cdots$ F3 <sup>iii</sup>	0.90	2.61	3.399 (4)	146
N2—H2A $\cdots$ F1 <sup>iv</sup>	0.90	2.38	3.010 (4)	127
N2—H2A $\cdots$ F2 <sup>v</sup>	0.90	2.59	3.217 (3)	127
N2—H2B $\cdots$ F4 <sup>v</sup>	0.90	2.31	2.926 (3)	126

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

Data collection: APEX2 (Bruker, 2003); cell refinement: APEX2; data reduction: SAINT-Plus (Bruker, 2003); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2000); software used to prepare material for publication: SHELXTL.

The Bruker APEXII X8 diffractometer was purchased with funds received from the National Science Foundation Major Research Instrumentation Program grant CHE-0321214. KK thanks the Robert A. Welch Foundation for support (AA-1508).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2026).

## References

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**supplementary materials**

*Acta Cryst.* (2007). E63, m2131-m2132 [ doi:10.1107/S1600536807033430 ]

**Poly[[silver(I)-bis[ $\mu_2$ -3-(aminomethyl)pyridine]- $\kappa^2N^1:N^3$ ;  $\kappa^2N^3:N^1$ ] hexafluoridophosphate]**

**C. E. Carson, R. P. Fezell and K. K. Klausmeyer**

**Comment**

The title compound, (I), is isostructural with  $\text{Ag}(3\text{-aminomethylpyridine})_2\text{BF}_4$  (Klausmeyer *et al.*, 2004). The extended structure reveals that the hexafluorophosphate ions are intercalated between the sheets of 'box-linker-box' units and hydrogen bond with the amine H atoms creating an intricate extended packing structure. The title compound (I) contains silvers in the +1 oxidation state that have distorted tetrahedral geometry with a coordination sphere consisting of two pyridyl N atoms and two amine N atoms from the ligand. The structure displays a "box-linker-box" motif. This motif consists of two 3-AMP ligands binding in a head-to-tail fashion with two silvers. The distance from Ag to Ag across the box is 5.0079 (9) Å. The boxes are then linked by 3-AMP ligands to form the two dimensional polymer.

**Experimental**

The reaction was carried out under an argon atmosphere using a Schlenk line and standard Schlenk techniques. Glassware was dried at 120 °C for several hours prior to use. All reagents were stored in an inert-atmosphere glovebox; solvents were distilled under nitrogen from the appropriate drying agent immediately before use. This reaction used 2 equiv of 3-AMP (0.150 g, 1.40 mmol) in 5 ml  $\text{CH}_3\text{CN}$  added to a solution of  $\text{AgPF}_6$  (0.135 g, 0.69 mmol) in 5 ml  $\text{CH}_3\text{CN}$ . Upon evaporation of the solvent, a white powder was isolated in 84% yield (0.239 g, 0.583 mmol). Colorless plates of (I) were formed at 5 °C by the slow diffusion of ether into a  $\text{CH}_3\text{CN}$  solution of (I)

**Refinement**

Hydrogen atoms were included in calculated positions ( $C_{\text{ring}}\text{—H} = 0.930$  Å); ( $C_{\text{methylene}}\text{—H} = 0.970$  Å); ( $\text{N—H} = 0.900$  Å) isotropic displacement parameters were fixed [ $U_{\text{iso}}(\text{H}) = 1.2U_{\text{iso}}(\text{C})$ ]; [ $U_{\text{iso}}(\text{H}) = 1.2U_{\text{iso}}(\text{N})$ ]; [ $U_{\text{iso}}(\text{H}) = 1.2U_{\text{iso}}(\text{C}_{\text{ring}})$ ].

**Figures**

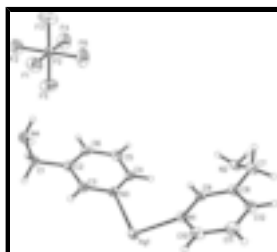


Fig. 1. Thermal ellipsoid plot of the unique portion of 1, ellipsoids are drawn at the 50% probability level.



Fig. 2. The "box-linker-box" motif.

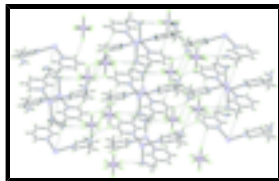


Fig. 3. Extended packing diagram displaying H-bonding.

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### Crystal data

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$M_r = 469.13$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 6.9563$  (11) Å

$b = 11.584$  (2) Å

$c = 20.060$  (3) Å

$\beta = 90.271$  (5)°

$V = 1616.4$  (4) Å<sup>3</sup>

$Z = 4$

$F_{000} = 928$

$D_x = 1.928$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 7201 reflections

$\theta = 2.7$ – $26.6$ °

$\mu = 1.41$  mm<sup>-1</sup>

$T = 110$  (2) K

Block, colorless

$0.25 \times 0.17 \times 0.12$  mm

### Data collection

Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 110$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.740$ ,  $T_{\max} = 0.845$

16863 measured reflections

3387 independent reflections

3006 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\text{max}} = 26.7$ °

$\theta_{\text{min}} = 2.0$ °

$h = -8 \rightarrow 8$

$k = -14 \rightarrow 14$

$l = -25 \rightarrow 25$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.117$

$S = 0.96$

3387 reflections

217 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 1.18$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.67$  e Å<sup>-3</sup>

Primary atom site location: structure-invariant direct methods Extinction correction: none

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.04519 (3)	-0.028628 (19)	0.122801 (11)	0.01880 (13)
N4	0.3921 (4)	0.3978 (2)	0.26917 (13)	0.0221 (6)
H4A	0.4637	0.4383	0.2402	0.026*
H4B	0.4343	0.3244	0.2680	0.026*
N2	0.2897 (4)	0.0347 (2)	-0.13631 (16)	0.0220 (6)
H2A	0.3146	0.0632	-0.1771	0.026*
H2B	0.3382	0.0847	-0.1063	0.026*
N1	0.2333 (4)	-0.1277 (2)	0.04850 (13)	0.0185 (5)
N3	0.1174 (4)	0.1695 (2)	0.11364 (13)	0.0187 (5)
C9	0.2783 (4)	-0.0771 (3)	-0.00970 (15)	0.0174 (6)
H9	0.2622	0.0024	-0.0131	0.021*
C6	0.1799 (4)	0.4065 (3)	0.11783 (17)	0.0214 (6)
H6	0.1999	0.4859	0.1188	0.026*
C4	0.1308 (4)	0.2319 (3)	0.05778 (15)	0.0179 (6)
H4	0.1192	0.1942	0.0170	0.021*
C8	0.3470 (4)	-0.1354 (3)	-0.06464 (16)	0.0184 (6)
C2	0.1688 (4)	0.3443 (3)	0.17690 (15)	0.0184 (6)
C3	0.1356 (4)	0.2257 (3)	0.17155 (15)	0.0187 (6)
H3	0.1255	0.1831	0.2107	0.022*
C12	0.3746 (5)	-0.2542 (3)	-0.05791 (17)	0.0243 (7)
H12	0.4206	-0.2974	-0.0935	0.029*
C5	0.1610 (4)	0.3499 (3)	0.05785 (16)	0.0214 (6)
H5	0.1685	0.3904	0.0179	0.026*
C11	0.3334 (5)	-0.3069 (3)	0.00161 (17)	0.0257 (7)
H11	0.3526	-0.3859	0.0068	0.031*
C10	0.2636 (4)	-0.2420 (3)	0.05352 (17)	0.0225 (7)
H10	0.2363	-0.2786	0.0937	0.027*
C1	0.1937 (5)	0.3985 (3)	0.24467 (16)	0.0232 (7)
H1A	0.1488	0.4777	0.2427	0.028*
H1B	0.1136	0.3575	0.2763	0.028*
C7	0.3925 (5)	-0.0750 (3)	-0.12915 (16)	0.0241 (7)

## supplementary materials

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H7A	0.5297	-0.0607	-0.1312	0.029*
H7B	0.3584	-0.1251	-0.1661	0.029*
P2	0.74018 (13)	0.62393 (7)	0.16233 (4)	0.0247 (2)
F1	0.7579 (4)	0.52866 (18)	0.21854 (13)	0.0396 (6)
F2	0.7217 (3)	0.7249 (2)	0.21651 (12)	0.0419 (6)
F3	0.9663 (3)	0.6428 (2)	0.16267 (13)	0.0476 (6)
F4	0.7170 (4)	0.71905 (19)	0.10383 (12)	0.0463 (6)
F5	0.5096 (3)	0.6095 (2)	0.16439 (13)	0.0484 (6)
F6	0.7550 (5)	0.52789 (19)	0.10652 (14)	0.0519 (8)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.01953 (19)	0.02047 (18)	0.01639 (18)	0.00159 (8)	0.00101 (11)	0.00152 (8)
N4	0.0196 (13)	0.0271 (14)	0.0195 (13)	0.0014 (11)	-0.0016 (10)	-0.0055 (11)
N2	0.0207 (15)	0.0242 (15)	0.0212 (15)	0.0011 (10)	0.0021 (12)	0.0064 (10)
N1	0.0157 (13)	0.0208 (12)	0.0191 (13)	-0.0007 (10)	0.0005 (10)	0.0020 (10)
N3	0.0158 (12)	0.0188 (13)	0.0214 (13)	-0.0008 (10)	-0.0015 (10)	-0.0009 (10)
C9	0.0135 (14)	0.0190 (14)	0.0197 (14)	-0.0008 (12)	-0.0019 (11)	-0.0005 (12)
C6	0.0180 (15)	0.0182 (14)	0.0280 (17)	-0.0018 (12)	-0.0014 (12)	-0.0032 (13)
C4	0.0138 (14)	0.0217 (14)	0.0181 (14)	0.0009 (12)	-0.0021 (11)	-0.0023 (12)
C8	0.0101 (14)	0.0243 (15)	0.0209 (15)	0.0026 (12)	0.0005 (11)	0.0016 (12)
C2	0.0125 (14)	0.0231 (15)	0.0197 (15)	0.0012 (12)	-0.0002 (11)	-0.0061 (12)
C3	0.0173 (15)	0.0217 (14)	0.0172 (14)	0.0008 (12)	-0.0007 (12)	0.0000 (12)
C12	0.0177 (15)	0.0269 (16)	0.0283 (17)	0.0033 (13)	0.0030 (13)	-0.0051 (13)
C5	0.0190 (15)	0.0242 (15)	0.0209 (15)	0.0013 (13)	-0.0011 (12)	0.0043 (12)
C11	0.0246 (17)	0.0200 (15)	0.0325 (18)	0.0065 (13)	0.0012 (14)	0.0021 (14)
C10	0.0166 (15)	0.0220 (15)	0.0287 (17)	0.0031 (12)	0.0004 (13)	0.0076 (13)
C1	0.0210 (16)	0.0270 (16)	0.0216 (16)	0.0013 (13)	0.0009 (13)	-0.0042 (13)
C7	0.0227 (16)	0.0290 (17)	0.0207 (16)	0.0064 (15)	0.0050 (12)	0.0024 (13)
P2	0.0297 (5)	0.0218 (4)	0.0228 (4)	-0.0035 (3)	0.0063 (4)	-0.0012 (3)
F1	0.0413 (14)	0.0420 (14)	0.0356 (13)	0.0008 (9)	0.0004 (11)	0.0163 (9)
F2	0.0488 (14)	0.0400 (13)	0.0368 (12)	0.0031 (11)	0.0051 (10)	-0.0080 (10)
F3	0.0317 (12)	0.0407 (13)	0.0704 (17)	-0.0021 (10)	0.0145 (11)	0.0096 (12)
F4	0.0753 (18)	0.0309 (11)	0.0326 (12)	-0.0017 (11)	-0.0010 (11)	0.0074 (10)
F5	0.0307 (12)	0.0544 (15)	0.0601 (16)	-0.0054 (11)	-0.0093 (11)	0.0077 (13)
F6	0.082 (2)	0.0376 (15)	0.0358 (15)	0.0010 (12)	0.0038 (14)	-0.0110 (10)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Ag1—N1	2.296 (3)	C4—H4	0.9300
Ag1—N2 <sup>i</sup>	2.348 (3)	C8—C12	1.396 (4)
Ag1—N3	2.357 (3)	C8—C7	1.506 (4)
Ag1—N4 <sup>ii</sup>	2.367 (3)	C2—C3	1.397 (4)
N4—C1	1.462 (4)	C2—C1	1.507 (4)
N4—Ag1 <sup>iii</sup>	2.367 (3)	C3—H3	0.9300
N4—H4A	0.9000	C12—C11	1.372 (5)
N4—H4B	0.9000	C12—H12	0.9300

N2—C7	1.465 (4)	C5—H5	0.9300
N2—Ag1 <sup>i</sup>	2.348 (3)	C11—C10	1.375 (5)
N2—H2A	0.9000	C11—H11	0.9300
N2—H2B	0.9000	C10—H10	0.9300
N1—C10	1.344 (4)	C1—H1A	0.9700
N1—C9	1.345 (4)	C1—H1B	0.9700
N3—C3	1.337 (4)	C7—H7A	0.9700
N3—C4	1.337 (4)	C7—H7B	0.9700
C9—C8	1.379 (4)	P2—F6	1.582 (3)
C9—H9	0.9300	P2—F1	1.582 (2)
C6—C5	1.376 (4)	P2—F3	1.588 (2)
C6—C2	1.389 (4)	P2—F2	1.602 (2)
C6—H6	0.9300	P2—F5	1.613 (2)
C4—C5	1.383 (4)	P2—F4	1.617 (2)
N1—Ag1—N2 <sup>i</sup>	128.98 (10)	C2—C3—H3	118.0
N1—Ag1—N3	108.29 (9)	C11—C12—C8	119.6 (3)
N2 <sup>i</sup> —Ag1—N3	104.49 (9)	C11—C12—H12	120.2
N1—Ag1—N4 <sup>ii</sup>	108.13 (9)	C8—C12—H12	120.2
N2 <sup>i</sup> —Ag1—N4 <sup>ii</sup>	93.57 (10)	C6—C5—C4	119.1 (3)
N3—Ag1—N4 <sup>ii</sup>	112.55 (9)	C6—C5—H5	120.5
C1—N4—Ag1 <sup>iii</sup>	118.38 (19)	C4—C5—H5	120.5
C1—N4—H4A	107.7	C12—C11—C10	119.4 (3)
Ag1 <sup>iii</sup> —N4—H4A	107.7	C12—C11—H11	120.3
C1—N4—H4B	107.7	C10—C11—H11	120.3
Ag1 <sup>iii</sup> —N4—H4B	107.7	N1—C10—C11	122.5 (3)
H4A—N4—H4B	107.1	N1—C10—H10	118.7
C7—N2—Ag1 <sup>i</sup>	116.5 (2)	C11—C10—H10	118.7
C7—N2—H2A	108.2	N4—C1—C2	113.9 (3)
Ag1 <sup>i</sup> —N2—H2A	108.2	N4—C1—H1A	108.8
C7—N2—H2B	108.2	C2—C1—H1A	108.8
Ag1 <sup>i</sup> —N2—H2B	108.2	N4—C1—H1B	108.8
H2A—N2—H2B	107.3	C2—C1—H1B	108.8
C10—N1—C9	117.2 (3)	H1A—C1—H1B	107.7
C10—N1—Ag1	122.2 (2)	N2—C7—C8	112.5 (3)
C9—N1—Ag1	118.8 (2)	N2—C7—H7A	109.1
C3—N3—C4	117.3 (3)	C8—C7—H7A	109.1
C3—N3—Ag1	115.16 (19)	N2—C7—H7B	109.1
C4—N3—Ag1	127.4 (2)	C8—C7—H7B	109.1
N1—C9—C8	124.3 (3)	H7A—C7—H7B	107.8
N1—C9—H9	117.9	F6—P2—F1	90.49 (14)
C8—C9—H9	117.9	F6—P2—F3	91.82 (16)
C5—C6—C2	119.5 (3)	F1—P2—F3	91.09 (14)
C5—C6—H6	120.2	F6—P2—F2	177.56 (15)
C2—C6—H6	120.2	F1—P2—F2	91.85 (13)
N3—C4—C5	123.0 (3)	F3—P2—F2	88.81 (13)
N3—C4—H4	118.5	F6—P2—F5	90.78 (16)



## supplementary materials

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C5—C4—H4	118.5	F1—P2—F5	89.07 (13)
C9—C8—C12	117.0 (3)	F3—P2—F5	177.39 (16)
C9—C8—C7	122.3 (3)	F2—P2—F5	88.58 (13)
C12—C8—C7	120.8 (3)	F6—P2—F4	88.41 (13)
C6—C2—C3	117.0 (3)	F1—P2—F4	178.28 (15)
C6—C2—C1	123.1 (3)	F3—P2—F4	90.27 (14)
C3—C2—C1	119.8 (3)	F2—P2—F4	89.24 (13)
N3—C3—C2	124.1 (3)	F5—P2—F4	89.62 (14)
N3—C3—H3	118.0		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N4—H4A $\cdots$ F1	0.90	2.34	3.135 (4)	147
N4—H4A $\cdots$ F5	0.90	2.52	3.334 (4)	151
N4—H4B $\cdots$ F3 <sup>iv</sup>	0.90	2.61	3.399 (4)	146
N2—H2A $\cdots$ F1 <sup>v</sup>	0.90	2.38	3.010 (4)	127
N2—H2A $\cdots$ F2 <sup>vi</sup>	0.90	2.59	3.217 (3)	127
N2—H2B $\cdots$ F4 <sup>vi</sup>	0.90	2.31	2.926 (3)	126

Symmetry codes: (iv)  $-x+3/2, y-1/2, -z+1/2$ ; (v)  $x-1/2, -y+1/2, z-1/2$ ; (vi)  $-x+1, -y+1, -z$ .





Fig. 3

