

## [2-(4-Methylpiperazin-1-ylmethyl)-phenyl]diphenylphosphane

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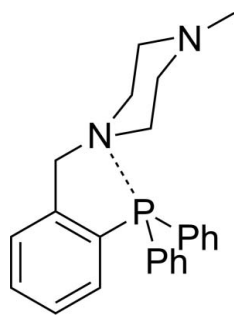
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 Key indicators: single-crystal X-ray study;  $T = 297$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.085;  $wR$  factor = 0.178; data-to-parameter ratio = 15.0.

In the title compound,  $\text{C}_{24}\text{H}_{27}\text{N}_2\text{P}$ , the P atom is bonded to three C atoms in a trigonal-pyramidal geometry. The overall  $\Psi$ -trigonal-bipyramidal coordination of the P atom is established when the contribution of the electron lone pair and of the N–P donor–acceptor distance of 3.051 (3) Å are considered. The 4-methylpiperazinyl ring adopts a chair conformation. Intra- and intermolecular C–H $\cdots\pi$  hydrogen bonding leads to the consolidation of the structure.

### Related literature

For organophosphorus compounds containing substituents with the capability of intramolecular donor $\cdots$ acceptor interactions, see: Alberico *et al.* (2007); Chandrasekaran *et al.* (2002); Chuit *et al.* (1993); Pretorius *et al.* (2004). For the structures of triclinic polymorphs of triphenylphosphine, see: Ziemer *et al.* (2000).



### Experimental

#### Crystal data

$\text{C}_{24}\text{H}_{27}\text{N}_2\text{P}$	$V = 2084.2$ (4) Å <sup>3</sup>
$M_r = 374.45$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.3689$ (10) Å	$\mu = 0.14$ mm <sup>-1</sup>
$b = 14.6735$ (16) Å	$T = 297$ K
$c = 15.4362$ (16) Å	$0.30 \times 0.26 \times 0.21$ mm
$\beta = 100.849$ (2)°	

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer	14906 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	3667 independent reflections
$T_{\min} = 0.959$ , $T_{\max} = 0.971$	2811 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.064$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.085$	245 parameters
$wR(F^2) = 0.178$	H-atom parameters constrained
$S = 1.20$	$\Delta\rho_{\text{max}} = 0.25$ e Å <sup>-3</sup>
3667 reflections	$\Delta\rho_{\text{min}} = -0.25$ e Å <sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

C1–P1	1.841 (4)	C19–P1	1.839 (4)
C13–P1	1.829 (4)		
C13–P1–C19	101.62 (16)	C19–P1–C1	100.26 (16)
C13–P1–C1	103.38 (16)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9–H9B $\cdots$ Cg3	0.97	2.91	3.835 (4)	160
C14–H14 $\cdots$ Cg4 <sup>i</sup>	0.97	2.74	3.651 (5)	166
C23–H23 $\cdots$ Cg2 <sup>ii</sup>	0.97	2.98	3.830 (5)	154

Symmetry codes: (i)  $-x + 2, -y + 1, -z$ ; (ii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ . Cg2, Cg3, and Cg4 are the centroids of the C1–C6, C13–C18, and C19–C24 benzene rings, respectively.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2009); software used to prepare material for publication: publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2285).

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## supporting information

*Acta Cryst.* (2009). E65, o3193 [doi:10.1107/S1600536809049526]

**[2-(4-Methylpiperazin-1-ylmethyl)phenyl]diphenylphosphane**

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**S1. Comment**

We report here on the preparation and structural characterization in solution and the crystalline state of an asymmetric triphosphane,  $\text{PPh}_2[\text{C}_6\text{H}_4\{\text{CH}_2\text{N}(\text{CH}_2\text{CH}_2)_2\text{NMe}\}-2]$  (**I**).

Asymmetric organophosphorus(III) derivatives of the type  $\text{PPh}_2R$ , where  $R$  is a substituent capable of intramolecular coordination, were reported in the literature (Pretorius *et al.*, 2004; Alberico *et al.*, 2007). Nevertheless, only in the symmetrical triorganophosphane  $\text{P}[\text{C}_6\text{H}_4(\text{CH}_2\text{NMe}_2)-2]_3$  the nitrogen atom is coordinated to the phosphorous atom via N—P donor...acceptor interactions (Chuit *et al.*, 1993; Chandrasekaran *et al.*, 2002).

In the structure of (**I**) the nitrogen atom bonded to the benzyl fragment is coordinated to the phosphorous atom *trans* to a phenyl group. This induces chirality at the  $\Psi$ -trigonal-bipyramidal phosphorus centre, in addition to the planar chirality (the nitrogen atom acts as the pilot atom and the phenyl group as the chiral plane). (**I**) crystallizes in the racemic form. The ( $R_NA_P$ ) isomer is shown in Fig. 1. The ( $S_NC_P$ ) isomer is generated by symmetry with respect to the inversion centre.

The P—C bond lengths and C—P—C angles (Table 1) are in the range of those of triclinic  $\text{PPh}_3$  (Ziemer *et al.*, 2000). As expected, the P—C<sub>Ph</sub> bond in *trans*-position to the P—N bond is slightly longer than the other P—C bond. The length of the P—N bond donor...acceptor interaction is in the range of values found in  $\text{P}[\text{C}_6\text{H}_4(\text{CH}_2\text{NMe}_2)-2]_3$  (Chandrasekaran *et al.*, 2002).

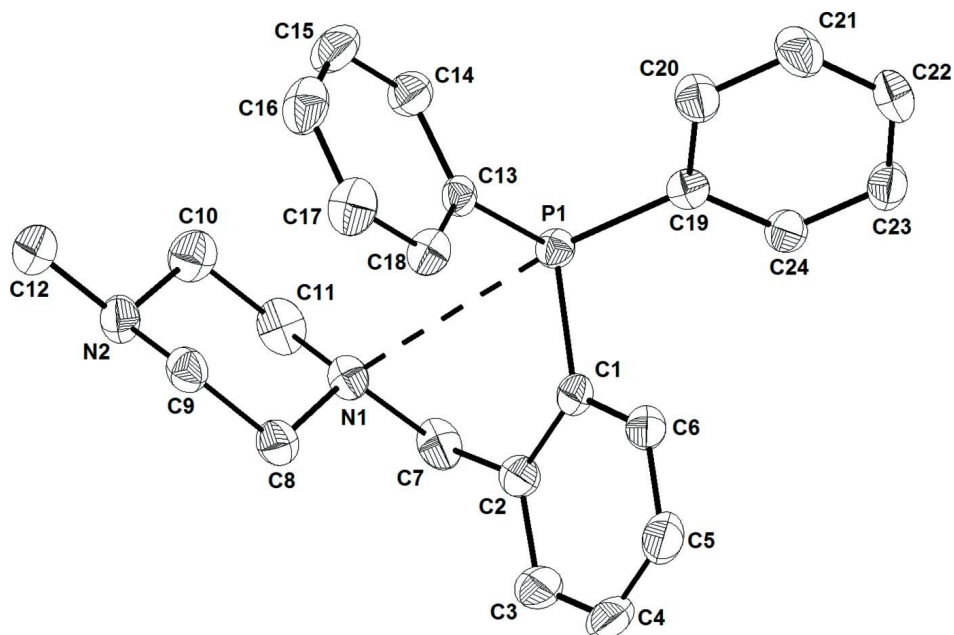
The structure displays intramolecular C—H... $\pi$  bonds between one hydrogen atom of the piperazinyl group and a phenyl group (Fig. 2). Four intermolecular C—H... $\pi$  bonds are established between the hydrogen atoms of the phenyl groups and  $\pi$  electrons of the benzene rings of neighbouring molecules. Geometrical parameters of the hydrogen bonds are listed in Table 2.

**S2. Experimental**

To a cooled solution of [2-{4-MeN(CH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>NCH<sub>2</sub>}C<sub>6</sub>H<sub>4</sub>]Li (2.55 g, 13 mmol) in tetrahydrofuran (thf) (203 K) was added dropwise a solution of  $\text{PPh}_2\text{Cl}$  (2.40 ml,  $\rho = 1.23$  g/ml, 13 mmol) in thf. The reaction mixture was stirred at 203 K for 2 h and was allowed to warm to room temperature. The solvent was removed under reduced pressure and over the resulting oily product was added dichloromethane. The obtained suspension was filtered and the dichloromethane was removed under reduced pressure. The remaining oily product solidified on addition of hexane. (**I**) was isolated as a colourless solid. Colourless crystals were obtained by the diffusion method from a dichloromethane/hexane mixture. Yield: 2.87 g (59%). mp 69 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  1.96 (s, 3H, NMe), 2.26 (s,br, 8H, H<sub>8,11</sub>+H<sub>9,10</sub>), 3.62 (d, 2H, H<sub>7</sub>, <sup>4</sup>J<sub>PH</sub> = 0.8 Hz), 6.88 (m, 1H, H<sub>6</sub>), 7.09 (ddd, 1H, H<sub>4</sub>, <sup>3</sup>J<sub>HH</sub> = 7.5 Hz, <sup>4</sup>J<sub>HH</sub> = 1.3 Hz), 7.18 (m, 11H, P—C<sub>6</sub>H<sub>5</sub> + H<sub>5</sub>), 7.29 (m, 1H, H<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  45.86 (s, NMe), 52.15 (s, C<sub>8,11</sub>), 54.24 (s, C<sub>9,10</sub>), 61.95 (d, C<sub>7</sub>, <sup>3</sup>J<sub>PC</sub> = 15.5 Hz), 127.17 (s, C<sub>4</sub>), 128.14 (m, C<sub>6</sub>H<sub>5</sub>-*meta+para*), 128.32 (s, C<sub>5</sub>), 129.48 (d, C<sub>3</sub>, <sup>3</sup>J<sub>PC</sub> = 5.8 Hz), 133.55 (d, C<sub>6</sub>H<sub>5</sub>-*ortho*, <sup>2</sup>J<sub>PC</sub> = 19.6 Hz), 134.89 (s, C<sub>6</sub>), 137.03 (d, C<sub>2</sub>, <sup>2</sup>J<sub>PC</sub> = 15.9 Hz), 138.45 (d, C<sub>6</sub>H<sub>5</sub>-*ipso*, <sup>1</sup>J<sub>PC</sub> = 9.9 Hz), 143.76 (d, C<sub>1</sub>, <sup>1</sup>J<sub>PC</sub> = 24.2 Hz). <sup>31</sup>P NMR (162 MHz, CDCl<sub>3</sub>):  $\delta$  -16.1 (s).

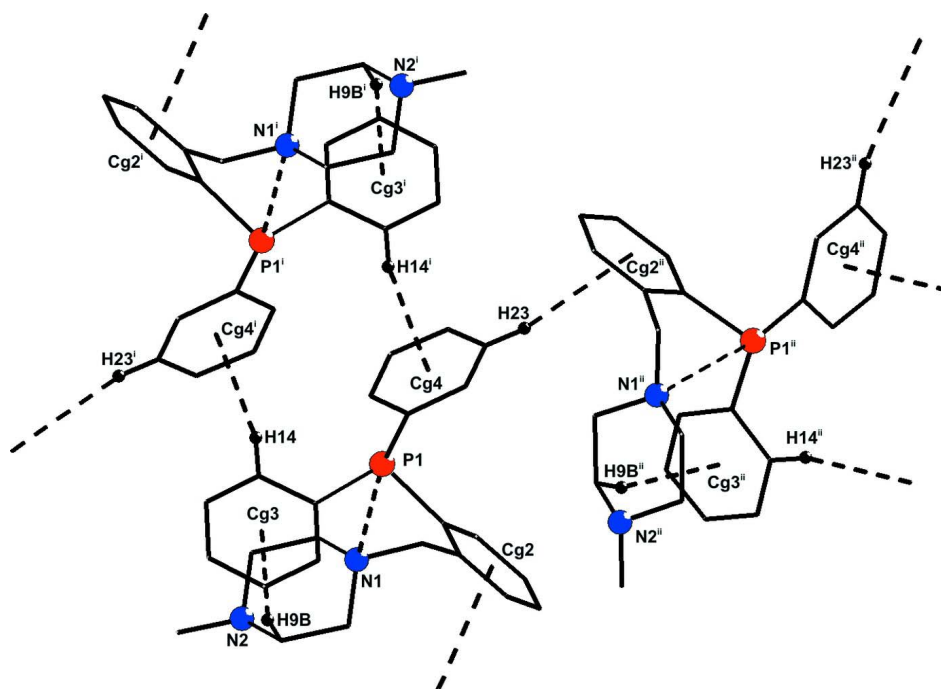
### S3. Refinement

Hydrogen atoms were placed in calculated positions with isotropic displacement parameters set at 1.2 times of those of the parent carbon atoms for aromatic and methylene hydrogen atoms, and at 1.5 times for hydrogen atoms of the methyl group.



**Figure 1**

Graphical representation of the molecular structure of  $R_{N_4P}$ -I. Hydrogen atoms were omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.



**Figure 2**

Intramolecular  $H\cdots\pi$  and  $N\cdots P$  interactions in the structure of **I** (shown as dashed lines). All the hydrogen atoms, except for those involved in hydrogen bonds, were omitted for clarity. *Cg2*, *Cg3*, and *Cg4* are the centroids of the benzene rings C1—C6, C13—C18, and C19—C24, respectively. Symmetry codes: (i)  $-x + 2, -y + 1, -z$ ; (ii)  $-x + 3/2, y - 1/2, -z + 1/2$ .

### [2-(4-Methylpiperazin-1-ylmethyl)phenyl]diphenylphosphane

#### Crystal data

$C_{24}H_{27}N_2P$

$M_r = 374.45$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P 2_1n$

$a = 9.3689$  (10) Å

$b = 14.6735$  (16) Å

$c = 15.4362$  (16) Å

$\beta = 100.849$  (2)°

$V = 2084.2$  (4) Å<sup>3</sup>

$Z = 4$

$F(000) = 800$

$D_x = 1.193$  Mg m<sup>-3</sup>

Melting point: 342 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3207 reflections

$\theta = 2.4$ – $23.9^\circ$

$\mu = 0.14$  mm<sup>-1</sup>

$T = 297$  K

Block, colourless

$0.30 \times 0.26 \times 0.21$  mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2000)

$T_{\min} = 0.959$ ,  $T_{\max} = 0.971$

14906 measured reflections

3667 independent reflections

2811 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.064$

$\theta_{\max} = 25^\circ$ ,  $\theta_{\min} = 1.9^\circ$

$h = -11 \rightarrow 11$

$k = -17 \rightarrow 17$

$l = -18 \rightarrow 18$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.085$   
 $wR(F^2) = 0.178$   
 $S = 1.20$   
 3667 reflections  
 245 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 1.2183P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.25 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.25 \text{ e } \text{Å}^{-3}$

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 ( $\text{Å}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6682 (4)	0.5851 (2)	0.1668 (3)	0.0428 (9)
C2	0.5236 (4)	0.6120 (2)	0.1377 (3)	0.0486 (10)
C3	0.4311 (5)	0.6148 (3)	0.1980 (4)	0.0666 (13)
H3	0.3349	0.6325	0.1794	0.08*
C4	0.4792 (6)	0.5920 (3)	0.2845 (4)	0.0783 (16)
H4	0.4153	0.5936	0.3239	0.094*
C5	0.6207 (6)	0.5670 (3)	0.3133 (3)	0.0731 (14)
H5	0.6535	0.5525	0.3724	0.088*
C6	0.7139 (5)	0.5633 (3)	0.2549 (3)	0.0542 (11)
H6	0.8099	0.5459	0.2749	0.065*
C7	0.4705 (4)	0.6395 (3)	0.0433 (3)	0.0541 (11)
H7A	0.4805	0.5884	0.0049	0.065*
H7B	0.3683	0.6554	0.0348	0.065*
C8	0.5243 (4)	0.7993 (2)	0.0655 (3)	0.0516 (10)
H8A	0.5466	0.7889	0.1287	0.062*
H8B	0.4223	0.8152	0.0494	0.062*
C9	0.6161 (4)	0.8769 (2)	0.0421 (3)	0.0493 (10)
H9A	0.5953	0.9316	0.0726	0.059*
H9B	0.7181	0.8623	0.0615	0.059*
C10	0.6156 (5)	0.8106 (3)	-0.0969 (3)	0.0603 (12)
H10A	0.7175	0.7946	-0.0799	0.072*
H10B	0.5951	0.8207	-0.1602	0.072*
C11	0.5246 (5)	0.7335 (3)	-0.0750 (3)	0.0610 (12)
H11A	0.4226	0.7479	-0.0948	0.073*
H11B	0.5463	0.679	-0.1055	0.073*

C12	0.6772 (5)	0.9677 (3)	-0.0734 (3)	0.0725 (14)
H12A	0.6606	1.021	-0.0406	0.109*
H12B	0.6525	0.9807	-0.1354	0.109*
H12C	0.7777	0.9507	-0.0584	0.109*
C13	0.8981 (4)	0.6775 (2)	0.1019 (2)	0.0374 (9)
C14	0.9778 (4)	0.6993 (3)	0.0381 (3)	0.0526 (10)
H14	0.9738	0.6612	-0.0105	0.063*
C15	1.0624 (5)	0.7758 (3)	0.0448 (3)	0.0672 (13)
H15	1.1167	0.7885	0.0016	0.081*
C16	1.0676 (5)	0.8335 (3)	0.1143 (3)	0.0666 (13)
H16	1.1241	0.886	0.1183	0.08*
C17	0.9895 (5)	0.8137 (3)	0.1778 (3)	0.0626 (12)
H17	0.9931	0.853	0.2255	0.075*
C18	0.9055 (4)	0.7367 (3)	0.1725 (3)	0.0485 (10)
H18	0.8532	0.7241	0.2167	0.058*
C19	0.9139 (4)	0.4871 (2)	0.1368 (2)	0.0400 (9)
C20	1.0627 (4)	0.4962 (3)	0.1523 (3)	0.0554 (11)
H20	1.1033	0.5516	0.1405	0.066*
C21	1.1529 (5)	0.4251 (3)	0.1850 (3)	0.0639 (12)
H21	1.2532	0.4328	0.1942	0.077*
C22	1.0960 (5)	0.3439 (3)	0.2037 (3)	0.0582 (11)
H22	1.157	0.2964	0.2269	0.07*
C23	0.9485 (5)	0.3325 (3)	0.1881 (3)	0.0546 (11)
H23	0.9091	0.2769	0.2004	0.065*
C24	0.8585 (4)	0.4026 (2)	0.1544 (2)	0.0461 (10)
H24	0.7585	0.3935	0.143	0.055*
N1	0.5526 (3)	0.7170 (2)	0.0195 (2)	0.0432 (8)
N2	0.5876 (4)	0.8936 (2)	-0.0522 (2)	0.0534 (9)
P1	0.78585 (10)	0.57472 (7)	0.08427 (6)	0.0391 (3)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.044 (2)	0.032 (2)	0.054 (2)	-0.0038 (17)	0.0124 (18)	0.0048 (17)
C2	0.041 (2)	0.032 (2)	0.075 (3)	-0.0081 (17)	0.017 (2)	-0.0027 (19)
C3	0.053 (3)	0.046 (3)	0.109 (4)	-0.011 (2)	0.037 (3)	0.001 (3)
C4	0.101 (4)	0.046 (3)	0.109 (5)	-0.006 (3)	0.073 (4)	0.006 (3)
C5	0.109 (4)	0.048 (3)	0.072 (3)	0.010 (3)	0.043 (3)	0.013 (2)
C6	0.069 (3)	0.044 (2)	0.055 (3)	0.009 (2)	0.025 (2)	0.007 (2)
C7	0.037 (2)	0.044 (2)	0.075 (3)	-0.0056 (18)	-0.007 (2)	-0.005 (2)
C8	0.056 (3)	0.041 (2)	0.059 (3)	0.0023 (19)	0.014 (2)	-0.0035 (19)
C9	0.049 (2)	0.036 (2)	0.062 (3)	-0.0010 (18)	0.010 (2)	-0.0048 (19)
C10	0.071 (3)	0.064 (3)	0.045 (2)	-0.002 (2)	0.008 (2)	0.001 (2)
C11	0.065 (3)	0.056 (3)	0.054 (3)	0.001 (2)	-0.007 (2)	-0.009 (2)
C12	0.072 (3)	0.059 (3)	0.091 (4)	0.003 (2)	0.029 (3)	0.021 (3)
C13	0.034 (2)	0.037 (2)	0.039 (2)	0.0023 (16)	0.0011 (16)	0.0081 (17)
C14	0.050 (2)	0.054 (3)	0.054 (2)	-0.002 (2)	0.011 (2)	0.004 (2)
C15	0.059 (3)	0.070 (3)	0.076 (3)	-0.015 (2)	0.022 (3)	0.018 (3)

C16	0.055 (3)	0.056 (3)	0.082 (3)	-0.019 (2)	-0.003 (3)	0.012 (3)
C17	0.066 (3)	0.055 (3)	0.061 (3)	-0.018 (2)	-0.004 (2)	-0.006 (2)
C18	0.048 (2)	0.050 (2)	0.045 (2)	-0.0071 (19)	0.0030 (18)	0.0022 (19)
C19	0.043 (2)	0.041 (2)	0.035 (2)	-0.0044 (17)	0.0066 (16)	-0.0081 (16)
C20	0.047 (2)	0.049 (3)	0.068 (3)	-0.001 (2)	0.005 (2)	0.002 (2)
C21	0.042 (2)	0.061 (3)	0.084 (3)	0.006 (2)	0.001 (2)	0.003 (3)
C22	0.062 (3)	0.047 (3)	0.063 (3)	0.015 (2)	0.003 (2)	0.005 (2)
C23	0.073 (3)	0.040 (2)	0.053 (3)	0.001 (2)	0.018 (2)	0.0044 (19)
C24	0.045 (2)	0.040 (2)	0.054 (2)	-0.0047 (18)	0.0112 (19)	-0.0038 (18)
N1	0.0405 (18)	0.0381 (18)	0.0483 (19)	-0.0022 (14)	0.0012 (14)	-0.0042 (14)
N2	0.055 (2)	0.046 (2)	0.058 (2)	0.0053 (16)	0.0083 (17)	0.0103 (17)
P1	0.0366 (5)	0.0398 (6)	0.0404 (6)	-0.0027 (4)	0.0058 (4)	0.0008 (4)

*Geometric parameters (Å, °)*

C1—C6	1.384 (5)	C12—N2	1.448 (5)
C1—C2	1.402 (5)	C12—H12A	0.96
C1—P1	1.841 (4)	C12—H12B	0.96
C2—C3	1.386 (6)	C12—H12C	0.96
C2—C7	1.504 (6)	C13—C14	1.381 (5)
C3—C4	1.368 (7)	C13—C18	1.386 (5)
C3—H3	0.93	C13—P1	1.829 (4)
C4—C5	1.367 (7)	C14—C15	1.366 (6)
C4—H4	0.93	C14—H14	0.93
C5—C6	1.369 (6)	C15—C16	1.360 (6)
C5—H5	0.93	C15—H15	0.93
C6—H6	0.93	C16—C17	1.361 (6)
C7—N1	1.458 (5)	C16—H16	0.93
C7—H7A	0.97	C17—C18	1.370 (5)
C7—H7B	0.97	C17—H17	0.93
C8—N1	1.452 (5)	C18—H18	0.93
C8—C9	1.510 (5)	C19—C20	1.376 (5)
C8—H8A	0.97	C19—C24	1.391 (5)
C8—H8B	0.97	C19—P1	1.839 (4)
C9—N2	1.450 (5)	C20—C21	1.376 (5)
C9—H9A	0.97	C20—H20	0.93
C9—H9B	0.97	C21—C22	1.359 (6)
C10—N2	1.449 (5)	C21—H21	0.93
C10—C11	1.493 (6)	C22—C23	1.368 (6)
C10—H10A	0.97	C22—H22	0.93
C10—H10B	0.97	C23—C24	1.368 (5)
C11—N1	1.453 (5)	C23—H23	0.93
C11—H11A	0.97	C24—H24	0.93
C11—H11B	0.97	N1—P1	3.051 (3)
C6—C1—C2	118.8 (4)	H12A—C12—H12B	109.5
C6—C1—P1	123.1 (3)	N2—C12—H12C	109.5
C2—C1—P1	118.0 (3)	H12A—C12—H12C	109.5

C3—C2—C1	118.8 (4)	H12B—C12—H12C	109.5
C3—C2—C7	120.6 (4)	C14—C13—C18	117.5 (4)
C1—C2—C7	120.6 (4)	C14—C13—P1	117.3 (3)
C4—C3—C2	121.0 (5)	C18—C13—P1	125.2 (3)
C4—C3—H3	119.5	C15—C14—C13	121.4 (4)
C2—C3—H3	119.5	C15—C14—H14	119.3
C5—C4—C3	120.3 (4)	C13—C14—H14	119.3
C5—C4—H4	119.9	C16—C15—C14	120.3 (4)
C3—C4—H4	119.9	C16—C15—H15	119.8
C4—C5—C6	119.7 (5)	C14—C15—H15	119.8
C4—C5—H5	120.1	C15—C16—C17	119.4 (4)
C6—C5—H5	120.1	C15—C16—H16	120.3
C5—C6—C1	121.4 (4)	C17—C16—H16	120.3
C5—C6—H6	119.3	C16—C17—C18	120.9 (4)
C1—C6—H6	119.3	C16—C17—H17	119.5
N1—C7—C2	111.1 (3)	C18—C17—H17	119.5
N1—C7—H7A	109.4	C17—C18—C13	120.5 (4)
C2—C7—H7A	109.4	C17—C18—H18	119.8
N1—C7—H7B	109.4	C13—C18—H18	119.8
C2—C7—H7B	109.4	C20—C19—C24	117.0 (4)
H7A—C7—H7B	108	C20—C19—P1	124.4 (3)
N1—C8—C9	110.2 (3)	C24—C19—P1	118.2 (3)
N1—C8—H8A	109.6	C19—C20—C21	121.6 (4)
C9—C8—H8A	109.6	C19—C20—H20	119.2
N1—C8—H8B	109.6	C21—C20—H20	119.2
C9—C8—H8B	109.6	C22—C21—C20	120.2 (4)
H8A—C8—H8B	108.1	C22—C21—H21	119.9
N2—C9—C8	111.3 (3)	C20—C21—H21	119.9
N2—C9—H9A	109.4	C21—C22—C23	119.6 (4)
C8—C9—H9A	109.4	C21—C22—H22	120.2
N2—C9—H9B	109.4	C23—C22—H22	120.2
C8—C9—H9B	109.4	C22—C23—C24	120.3 (4)
H9A—C9—H9B	108	C22—C23—H23	119.8
N2—C10—C11	111.5 (4)	C24—C23—H23	119.8
N2—C10—H10A	109.3	C23—C24—C19	121.2 (4)
C11—C10—H10A	109.3	C23—C24—H24	119.4
N2—C10—H10B	109.3	C19—C24—H24	119.4
C11—C10—H10B	109.3	C8—N1—C11	109.7 (3)
H10A—C10—H10B	108	C8—N1—C7	111.9 (3)
N1—C11—C10	110.6 (3)	C11—N1—C7	112.3 (3)
N1—C11—H11A	109.5	C12—N2—C10	111.1 (3)
C10—C11—H11A	109.5	C12—N2—C9	110.5 (3)
N1—C11—H11B	109.5	C10—N2—C9	108.7 (3)
C10—C11—H11B	109.5	C13—P1—C19	101.62 (16)
H11A—C11—H11B	108.1	C13—P1—C1	103.38 (16)
N2—C12—H12A	109.5	C19—P1—C1	100.26 (16)
N2—C12—H12B	109.5		



C6—C1—C2—C3	-0.8 (5)	C21—C22—C23—C24	-0.4 (6)
P1—C1—C2—C3	176.2 (3)	C22—C23—C24—C19	-1.2 (6)
C6—C1—C2—C7	177.8 (3)	C20—C19—C24—C23	1.9 (5)
P1—C1—C2—C7	-5.3 (5)	P1—C19—C24—C23	175.7 (3)
C1—C2—C3—C4	0.1 (6)	C9—C8—N1—C11	-57.1 (4)
C7—C2—C3—C4	-178.4 (4)	C9—C8—N1—C7	177.6 (3)
C2—C3—C4—C5	0.8 (7)	C10—C11—N1—C8	57.5 (4)
C3—C4—C5—C6	-1.1 (7)	C10—C11—N1—C7	-177.4 (3)
C4—C5—C6—C1	0.4 (7)	C2—C7—N1—C8	-67.7 (4)
C2—C1—C6—C5	0.5 (6)	C2—C7—N1—C11	168.4 (3)
P1—C1—C6—C5	-176.2 (3)	C11—C10—N2—C12	179.6 (3)
C3—C2—C7—N1	118.9 (4)	C11—C10—N2—C9	57.9 (4)
C1—C2—C7—N1	-59.6 (5)	C8—C9—N2—C12	-179.6 (3)
N1—C8—C9—N2	58.3 (4)	C8—C9—N2—C10	-57.6 (4)
N2—C10—C11—N1	-58.8 (5)	C14—C13—P1—C19	89.3 (3)
C18—C13—C14—C15	0.9 (6)	C18—C13—P1—C19	-93.1 (3)
P1—C13—C14—C15	178.7 (3)	C14—C13—P1—C1	-167.1 (3)
C13—C14—C15—C16	-1.3 (7)	C18—C13—P1—C1	10.5 (4)
C14—C15—C16—C17	1.0 (7)	C20—C19—P1—C13	-21.0 (4)
C15—C16—C17—C18	-0.2 (7)	C24—C19—P1—C13	165.6 (3)
C16—C17—C18—C13	-0.3 (6)	C20—C19—P1—C1	-127.1 (3)
C14—C13—C18—C17	-0.1 (6)	C24—C19—P1—C1	59.5 (3)
P1—C13—C18—C17	-177.7 (3)	C6—C1—P1—C13	-79.7 (3)
C24—C19—C20—C21	-0.9 (6)	C2—C1—P1—C13	103.5 (3)
P1—C19—C20—C21	-174.3 (3)	C6—C1—P1—C19	25.0 (3)
C19—C20—C21—C22	-0.7 (7)	C2—C1—P1—C19	-151.8 (3)
C20—C21—C22—C23	1.4 (7)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C9—H9B...Cg3	0.97	2.91	3.835 (4)	160
C14—H14...Cg4 <sup>i</sup>	0.97	2.74	3.651 (5)	166
C23—H23...Cg2 <sup>ii</sup>	0.97	2.98	3.830 (5)	154

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