

# *N*-(3,5-Dimethylphenyl)-*P,P*-diphenylphosphinic amide

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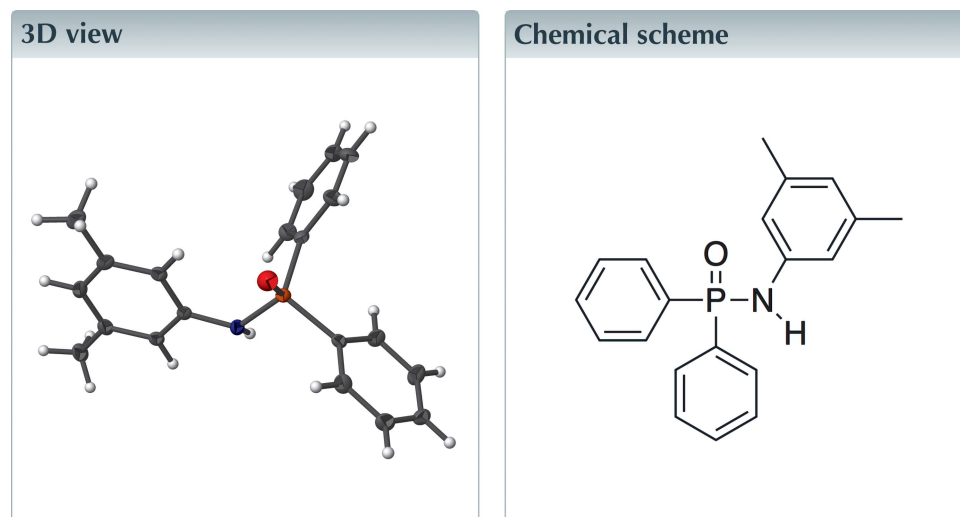
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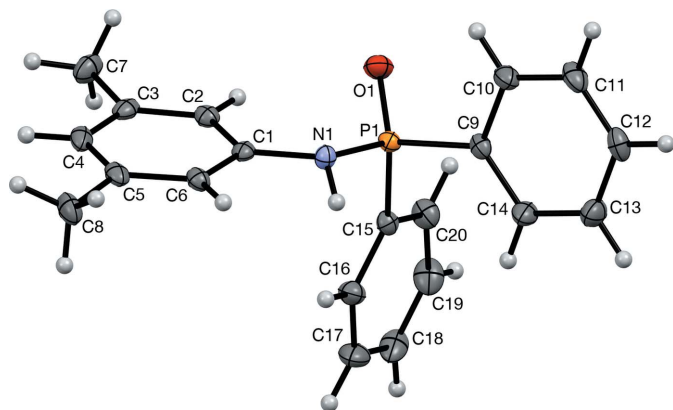
In the title compound, C<sub>20</sub>H<sub>20</sub>NO, the P atom, with a distorted tetrahedral geometry, is attached to an O atom, two phenyl groups, and a 3,5-dimethyl-aniline group. The N–P–C [102.29 (12) and 108.97 (12)°] and C–P–C [107.14 (12)°] bond angles are all smaller than the ideal 109.5° tetrahedral bond angle, whereas the O–P–C [113.07 (12) and 110.62 (12)°] and O–P–N [114.24 (13)°] angles are all larger than 109.5°. A weak intramolecular C–H···O hydrogen bond helps to establish the molecular conformation. In the crystal, the molecules are linked by N–H···O hydrogen bonds, generating [001] chains.



## Structure description

Phosphinamide derivatives have applications as ligands in transition and rare earth metal chemistry and in catalysis (Priya *et al.*, 2005; Gusev *et al.*, 2009; Naktode *et al.*, 2012; Naktode *et al.*, 2013; Sun & Cramer, 2017) and are of general synthetic interest, particularly in the pharmaceutical field (Xu *et al.*, 2017; Hong *et al.*, 2016). As part of our studies in this area, the title compound was serendipitously isolated and its structure is reported here. Structures for the [Ph<sub>2</sub>P(O)NH(2,6-(CH<sub>3</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>3</sub>))] structural isomer (Naktode *et al.*, 2012) and related [Ph<sub>2</sub>P(O)NHPh] (Priya *et al.*, 2005) are known.

The molecular structure of the title compound is shown in Fig. 1. The phosphorus atom exhibits slightly distorted tetrahedral geometry. The four P–X bonds [X = O:1.477 (2), N:1.653 (2), C:1.797 (3) and 1.803 (3) Å] are similar to those found in [Ph<sub>2</sub>P(O)NH(2,6-(CH<sub>3</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>3</sub>))] and [Ph<sub>2</sub>P(O)NHPh] as are the bond angles about the phosphorus atom. The N–P–C [102.29 (12) and 108.97 (12)°] and C–P–C [107.14 (12)°] angles are all slightly smaller than the ideal 109.5° bond angle for tetrahedral geometry, while the O–P–C [113.07 (12) and 110.62 (12)°] and O–P–N [114.24 (13)°] bond angles are all

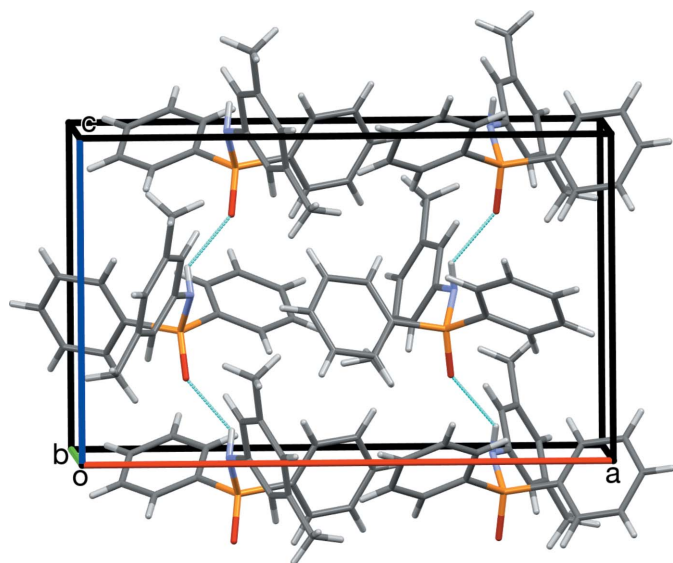


**Figure 1**  
Molecular structure of  $[\text{Ph}_2\text{P}(\text{O})\text{NH}(3,5\text{-(CH}_3)_2\text{C}_6\text{H}_3)]$  with displacement ellipsoids drawn at the 50% probability level.

larger than  $109.5^\circ$ . The N—H and P—O bonds are *anti* to each other, which facilitates the formation of an [001] chain of N—H $\cdots$ O hydrogen bonds (Table 1) in the crystal (Fig. 2). An intramolecular C—H $\cdots$ O hydrogen bond in each molecule helps to position the ring.

### Synthesis and crystallization

The title compound was obtained during our attempt to crystallize  $[(\text{Ph}_2\text{P})_2\text{N}(3,5\text{-(CH}_3)_2\text{C}_6\text{H}_3)]$ , which had been prepared by a literature method (Shozi & Friedrich, 2012). A dichloromethane solution of  $[(\text{Ph}_2\text{P})_2\text{N}(3,5\text{-(CH}_3)_2\text{C}_6\text{H}_3)]$  was allowed to evaporate slowly at room temperature under argon. After 24 h, crystals suitable for single-crystal structure determination were obtained. However,  $[\text{Ph}_2\text{P}(\text{O})\text{NH}(3,5\text{-(CH}_3)_2\text{C}_6\text{H}_3)]$  rather than the expected  $[(\text{Ph}_2\text{P})_2\text{N}(3,5\text{-(CH}_3)_2\text{C}_6\text{H}_3)]$  was serendipitously isolated. The title



**Figure 2**  
Unit-cell packing viewed along the *b* axis showing N—H $\cdots$ O hydrogen-bonding contacts as dotted lines.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C2—H2 $\cdots$ O1	0.95	2.48	3.148 (3)	128
N1—H1 $\cdots$ O1 <sup>i</sup>	0.88	2.12	2.788 (3)	133

Symmetry code: (i)  $-x + \frac{3}{2}, y, z + \frac{1}{2}$ .

**Table 2**  
Experimental details.

Crystal data	$\text{C}_{20}\text{H}_{20}\text{NOP}$
Chemical formula	321.34
$M_r$	Orthorhombic, <i>Pca</i> <sub>21</sub>
Crystal system, space group	100
Temperature (K)	15.9713 (9), 10.7495 (7), 9.8286 (6)
<i>a</i> , <i>b</i> , <i>c</i> ( $\text{\AA}$ )	1687.41 (18)
<i>V</i> ( $\text{\AA}^3$ )	4
<i>Z</i>	Mo $K\alpha$
Radiation type	0.17
$\mu$ ( $\text{mm}^{-1}$ )	0.36 $\times$ 0.28 $\times$ 0.11
Crystal size (mm)	
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2016)
$T_{\text{min}}$ , $T_{\text{max}}$	0.829, 0.942
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	25376, 5327, 4160
$R_{\text{int}}$	0.061
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.725
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.048, 0.108, 1.04
No. of reflections	5327
No. of parameters	210
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	0.37, $-0.38$
Absolute structure	Flack <i>x</i> determined using 1497 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.07 (5)

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2016* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2006) and *SHELXTL* (Sheldrick, 2008).

compound may have formed as a result of the adventitious exposure of the sample to moisture and/or oxygen.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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## full crystallographic data

*IUCrData* (2018). 3, x181192 [https://doi.org/10.1107/S2414314618011926]

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*N*-(3,5-Dimethylphenyl)-*P,P*-diphenylphosphinic amide*Crystal data*

$C_{20}H_{20}NO$	$D_x = 1.265 \text{ Mg m}^{-3}$
$M_r = 321.34$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, $Pca2_1$	Cell parameters from 5345 reflections
$a = 15.9713 (9) \text{ \AA}$	$\theta = 3.1\text{--}29.8^\circ$
$b = 10.7495 (7) \text{ \AA}$	$\mu = 0.17 \text{ mm}^{-1}$
$c = 9.8286 (6) \text{ \AA}$	$T = 100 \text{ K}$
$V = 1687.41 (18) \text{ \AA}^3$	Rectangular, colourless
$Z = 4$	$0.36 \times 0.28 \times 0.11 \text{ mm}$
$F(000) = 680$	

*Data collection*

Bruker SMART APEX CCD diffractometer	25376 measured reflections
Radiation source: sealed tube	5327 independent reflections
Detector resolution: 8 pixels $\text{mm}^{-1}$	4160 reflections with $I > 2\sigma(I)$
$\omega$ and $\varphi$ scans	$R_{\text{int}} = 0.061$
Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2016)	$\theta_{\text{max}} = 31.0^\circ$ , $\theta_{\text{min}} = 1.9^\circ$
$T_{\text{min}} = 0.829$ , $T_{\text{max}} = 0.942$	$h = -16 \rightarrow 23$
	$k = -15 \rightarrow 15$
	$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$	Hydrogen site location: mixed
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.1102P]$
$wR(F^2) = 0.108$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\text{max}} < 0.001$
5327 reflections	$\Delta\rho_{\text{max}} = 0.37 \text{ e \AA}^{-3}$
210 parameters	$\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$
1 restraint	Absolute structure: Flack $x$ determined using
Primary atom site location: dual	1497 quotients $[(I^-)-(I)]/[(I^+)+(I)]$ (Parsons <i>et al.</i> , 2013)
Secondary atom site location: difference Fourier map	Absolute structure parameter: 0.07 (5)

*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.** All H atoms were positioned geometrically and refined using a riding model with C—H = 0.95–0.99  $\text{\AA}$  and with  $U_{\text{iso}}(\text{H}) = 1.2$  (1.5 for methyl groups) times  $U_{\text{eq}}(\text{C})$ .

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
P1	0.69664 (4)	0.49044 (6)	0.38310 (8)	0.01446 (14)
O1	0.70603 (12)	0.5330 (2)	0.2410 (2)	0.0234 (5)
N1	0.71536 (13)	0.5990 (2)	0.4983 (2)	0.0162 (5)
H1	0.709159	0.565487	0.579440	0.019*
C1	0.68182 (15)	0.7201 (2)	0.5019 (3)	0.0154 (5)
C2	0.63941 (14)	0.7720 (2)	0.3912 (3)	0.0171 (5)
H2	0.630838	0.723925	0.311269	0.020*
C3	0.60956 (15)	0.8938 (3)	0.3973 (3)	0.0201 (6)
C4	0.62074 (16)	0.9628 (3)	0.5159 (3)	0.0219 (6)
H4	0.599481	1.045187	0.520752	0.026*
C5	0.66277 (16)	0.9125 (3)	0.6280 (3)	0.0204 (6)
C6	0.69365 (15)	0.7911 (3)	0.6188 (3)	0.0170 (5)
H6	0.723196	0.756459	0.693638	0.020*
C7	0.56648 (18)	0.9491 (3)	0.2749 (3)	0.0276 (7)
H7A	0.601677	0.937469	0.194249	0.041*
H7B	0.557222	1.038154	0.289994	0.041*
H7C	0.512526	0.907574	0.261002	0.041*
C8	0.67299 (19)	0.9845 (3)	0.7585 (3)	0.0267 (7)
H8A	0.667692	1.073669	0.739848	0.040*
H8B	0.728343	0.967449	0.797312	0.040*
H8C	0.629586	0.959041	0.823277	0.040*
C9	0.77031 (15)	0.3712 (2)	0.4290 (3)	0.0162 (5)
C10	0.85145 (16)	0.3818 (3)	0.3759 (4)	0.0230 (6)
H10	0.864781	0.448842	0.316708	0.028*
C11	0.91222 (16)	0.2954 (3)	0.4091 (3)	0.0259 (7)
H11	0.967111	0.303452	0.372958	0.031*
C12	0.89351 (17)	0.1976 (3)	0.4945 (3)	0.0231 (6)
H12	0.935353	0.138266	0.517217	0.028*
C13	0.81298 (18)	0.1860 (3)	0.5474 (3)	0.0273 (7)
H13	0.799857	0.118741	0.606324	0.033*
C14	0.75191 (18)	0.2725 (3)	0.5141 (3)	0.0234 (6)
H14	0.697004	0.263892	0.550083	0.028*
C15	0.59332 (15)	0.4278 (2)	0.4110 (3)	0.0162 (5)
C16	0.54908 (17)	0.4479 (3)	0.5302 (3)	0.0221 (6)
H16	0.572231	0.498776	0.599668	0.026*
C17	0.47006 (18)	0.3932 (3)	0.5484 (4)	0.0313 (7)
H17	0.439077	0.408013	0.629256	0.038*
C18	0.43792 (18)	0.3179 (3)	0.4481 (4)	0.0334 (8)
H18	0.385194	0.278845	0.461449	0.040*
C19	0.48081 (19)	0.2982 (3)	0.3290 (4)	0.0300 (7)
H19	0.457270	0.247131	0.260043	0.036*
C20	0.55888 (17)	0.3533 (3)	0.3091 (3)	0.0236 (6)
H20	0.588524	0.340067	0.226604	0.028*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
P1	0.0130 (2)	0.0162 (3)	0.0142 (3)	−0.0003 (3)	0.0002 (3)	−0.0005 (3)
O1	0.0247 (10)	0.0268 (11)	0.0188 (10)	−0.0004 (9)	0.0030 (8)	0.0033 (9)
N1	0.0179 (10)	0.0146 (11)	0.0159 (11)	0.0010 (9)	−0.0010 (9)	−0.0010 (9)
C1	0.0107 (10)	0.0155 (13)	0.0200 (13)	−0.0019 (10)	0.0017 (10)	0.0025 (11)
C2	0.0134 (10)	0.0191 (12)	0.0187 (12)	−0.0023 (9)	0.0009 (11)	−0.0014 (12)
C3	0.0118 (10)	0.0211 (13)	0.0274 (15)	−0.0015 (10)	0.0026 (11)	0.0083 (12)
C4	0.0133 (11)	0.0161 (13)	0.0363 (17)	0.0004 (10)	0.0060 (12)	0.0008 (12)
C5	0.0135 (12)	0.0194 (14)	0.0283 (15)	−0.0023 (11)	0.0063 (11)	−0.0044 (12)
C6	0.0130 (11)	0.0187 (14)	0.0194 (13)	−0.0005 (10)	0.0010 (10)	−0.0025 (11)
C7	0.0234 (14)	0.0248 (16)	0.0346 (18)	0.0019 (13)	−0.0025 (13)	0.0111 (14)
C8	0.0235 (14)	0.0218 (16)	0.0349 (17)	0.0004 (12)	0.0031 (13)	−0.0110 (14)
C9	0.0133 (11)	0.0161 (13)	0.0192 (13)	−0.0010 (10)	−0.0005 (10)	−0.0052 (11)
C10	0.0190 (11)	0.0216 (13)	0.0285 (14)	−0.0002 (11)	0.0067 (13)	−0.0015 (14)
C11	0.0145 (11)	0.0259 (15)	0.0374 (19)	0.0016 (11)	0.0037 (12)	−0.0072 (14)
C12	0.0199 (13)	0.0233 (15)	0.0260 (15)	0.0070 (12)	−0.0054 (12)	−0.0077 (13)
C13	0.0258 (15)	0.0233 (15)	0.0328 (17)	0.0039 (13)	0.0029 (13)	0.0084 (13)
C14	0.0151 (11)	0.0228 (14)	0.0322 (16)	0.0009 (12)	0.0047 (11)	0.0046 (13)
C15	0.0134 (10)	0.0177 (13)	0.0176 (14)	0.0022 (10)	−0.0019 (9)	0.0004 (10)
C16	0.0206 (13)	0.0248 (15)	0.0209 (14)	0.0001 (12)	0.0035 (11)	0.0010 (12)
C17	0.0227 (14)	0.0325 (18)	0.0387 (19)	0.0000 (14)	0.0128 (14)	0.0061 (15)
C18	0.0132 (13)	0.0242 (16)	0.063 (2)	−0.0020 (12)	0.0027 (14)	0.0056 (17)
C19	0.0181 (13)	0.0279 (18)	0.0439 (19)	−0.0021 (13)	−0.0095 (13)	−0.0053 (15)
C20	0.0204 (13)	0.0248 (16)	0.0256 (14)	−0.0023 (12)	−0.0022 (12)	−0.0057 (12)

*Geometric parameters (Å, °)*

P1—O1	1.477 (2)	C9—C14	1.383 (4)
P1—N1	1.653 (2)	C9—C10	1.402 (4)
P1—C9	1.797 (3)	C10—C11	1.383 (4)
P1—C15	1.803 (3)	C10—H10	0.9500
N1—C1	1.409 (3)	C11—C12	1.378 (4)
N1—H1	0.8805	C11—H11	0.9500
C1—C6	1.393 (4)	C12—C13	1.393 (4)
C1—C2	1.397 (4)	C12—H12	0.9500
C2—C3	1.395 (4)	C13—C14	1.387 (4)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.393 (4)	C14—H14	0.9500
C3—C7	1.507 (4)	C15—C16	1.385 (4)
C4—C5	1.398 (4)	C15—C20	1.395 (4)
C4—H4	0.9500	C16—C17	1.404 (4)
C5—C6	1.398 (4)	C16—H16	0.9500
C5—C8	1.507 (4)	C17—C18	1.374 (5)
C6—H6	0.9500	C17—H17	0.9500
C7—H7A	0.9800	C18—C19	1.373 (5)
C7—H7B	0.9800	C18—H18	0.9500

C7—H7C	0.9800	C19—C20	1.394 (4)
C8—H8A	0.9800	C19—H19	0.9500
C8—H8B	0.9800	C20—H20	0.9500
C8—H8C	0.9800		
O1—P1—N1	114.24 (13)	H8B—C8—H8C	109.5
O1—P1—C9	113.07 (12)	C14—C9—C10	119.0 (2)
N1—P1—C9	102.29 (12)	C14—C9—P1	124.1 (2)
O1—P1—C15	110.62 (12)	C10—C9—P1	117.0 (2)
N1—P1—C15	108.97 (12)	C11—C10—C9	120.4 (3)
C9—P1—C15	107.14 (12)	C11—C10—H10	119.8
C1—N1—P1	126.92 (19)	C9—C10—H10	119.8
C1—N1—H1	108.2	C12—C11—C10	120.3 (3)
P1—N1—H1	108.1	C12—C11—H11	119.9
C6—C1—C2	119.3 (2)	C10—C11—H11	119.9
C6—C1—N1	118.4 (2)	C11—C12—C13	119.7 (3)
C2—C1—N1	122.3 (2)	C11—C12—H12	120.2
C3—C2—C1	120.4 (3)	C13—C12—H12	120.2
C3—C2—H2	119.8	C14—C13—C12	120.1 (3)
C1—C2—H2	119.8	C14—C13—H13	119.9
C4—C3—C2	119.4 (3)	C12—C13—H13	119.9
C4—C3—C7	121.1 (3)	C9—C14—C13	120.5 (3)
C2—C3—C7	119.5 (3)	C9—C14—H14	119.7
C3—C4—C5	121.0 (3)	C13—C14—H14	119.7
C3—C4—H4	119.5	C16—C15—C20	119.7 (2)
C5—C4—H4	119.5	C16—C15—P1	122.5 (2)
C6—C5—C4	118.6 (3)	C20—C15—P1	117.8 (2)
C6—C5—C8	119.7 (3)	C15—C16—C17	120.1 (3)
C4—C5—C8	121.6 (3)	C15—C16—H16	120.0
C1—C6—C5	121.1 (3)	C17—C16—H16	120.0
C1—C6—H6	119.4	C18—C17—C16	119.4 (3)
C5—C6—H6	119.4	C18—C17—H17	120.3
C3—C7—H7A	109.5	C16—C17—H17	120.3
C3—C7—H7B	109.5	C19—C18—C17	121.0 (3)
H7A—C7—H7B	109.5	C19—C18—H18	119.5
C3—C7—H7C	109.5	C17—C18—H18	119.5
H7A—C7—H7C	109.5	C18—C19—C20	120.0 (3)
H7B—C7—H7C	109.5	C18—C19—H19	120.0
C5—C8—H8A	109.5	C20—C19—H19	120.0
C5—C8—H8B	109.5	C19—C20—C15	119.7 (3)
H8A—C8—H8B	109.5	C19—C20—H20	120.1
C5—C8—H8C	109.5	C15—C20—H20	120.1
H8A—C8—H8C	109.5		
O1—P1—N1—C1	49.7 (2)	C14—C9—C10—C11	-0.5 (4)
C9—P1—N1—C1	172.3 (2)	P1—C9—C10—C11	178.5 (2)
C15—P1—N1—C1	-74.5 (2)	C9—C10—C11—C12	0.2 (5)
P1—N1—C1—C6	169.28 (19)	C10—C11—C12—C13	0.0 (5)

P1—N1—C1—C2	-12.5 (4)	C11—C12—C13—C14	0.1 (5)
C6—C1—C2—C3	0.4 (4)	C10—C9—C14—C13	0.6 (4)
N1—C1—C2—C3	-177.9 (2)	P1—C9—C14—C13	-178.4 (2)
C1—C2—C3—C4	-1.4 (4)	C12—C13—C14—C9	-0.4 (5)
C1—C2—C3—C7	178.0 (2)	O1—P1—C15—C16	-141.0 (2)
C2—C3—C4—C5	1.2 (4)	N1—P1—C15—C16	-14.7 (3)
C7—C3—C4—C5	-178.2 (2)	C9—P1—C15—C16	95.3 (2)
C3—C4—C5—C6	0.0 (4)	O1—P1—C15—C20	41.0 (3)
C3—C4—C5—C8	-178.1 (2)	N1—P1—C15—C20	167.4 (2)
C2—C1—C6—C5	0.9 (4)	C9—P1—C15—C20	-82.6 (2)
N1—C1—C6—C5	179.2 (2)	C20—C15—C16—C17	0.2 (4)
C4—C5—C6—C1	-1.1 (4)	P1—C15—C16—C17	-177.7 (2)
C8—C5—C6—C1	177.0 (2)	C15—C16—C17—C18	1.2 (5)
O1—P1—C9—C14	-143.4 (2)	C16—C17—C18—C19	-1.8 (5)
N1—P1—C9—C14	93.3 (3)	C17—C18—C19—C20	1.1 (5)
C15—P1—C9—C14	-21.2 (3)	C18—C19—C20—C15	0.3 (5)
O1—P1—C9—C10	37.7 (3)	C16—C15—C20—C19	-0.9 (4)
N1—P1—C9—C10	-85.7 (2)	P1—C15—C20—C19	177.1 (2)
C15—P1—C9—C10	159.8 (2)		

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C2—H2...O1	0.95	2.48	3.148 (3)	128
N1—H1...O1 <sup>i</sup>	0.88	2.12	2.788 (3)	133

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