8-28-2018

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IUCrData

ISSN 2414-3146

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

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Received 21 August 2018
Accepted 22 August 2018

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

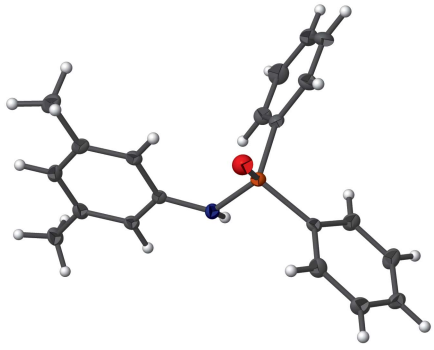
Keywords: crystal structure; hydrogen bonding; phosphinamide.

CCDC reference: 1863429

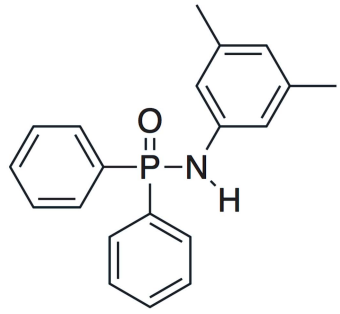
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{20}NOP$, the P atom, with a distorted tetrahedral geometry, is attached to an O atom, two phenyl groups, and a 3,5-dimethylaniline 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.

3D view



Chemical scheme



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 $[Ph_2P(O)NH(2,6\text{-}(CH_3)_2(C_6H_3)]$ structural isomer (Naktode *et al.*, 2012) and related $[Ph_2P(O)NHPh]$ (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 $[Ph_2P(O)NH(2,6\text{-}(CH_3)_2(C_6H_3)]$ and $[Ph_2P(O)NHPh]$ 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

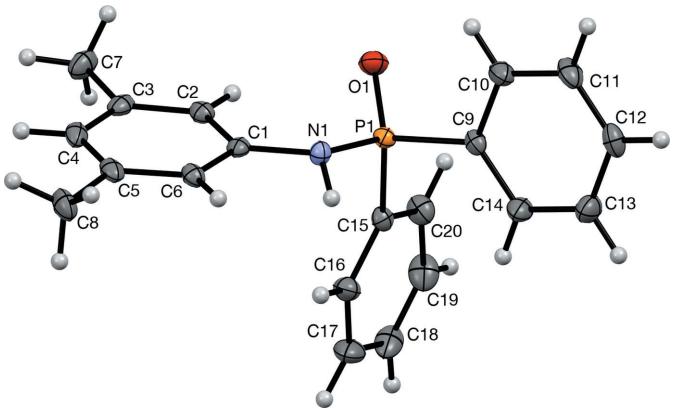


Figure 1
Molecular structure of $[Ph_2P(O)NH(3,5\text{-}(CH_3)_2(C_6H_3)]$ with displacement ellipsoids drawn at the 50% probability level.

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

Synthesis and crystallization

The title compound was obtained during our attempt to crystallize $[(Ph_2P)_2N(3,5\text{-}(CH_3)_2(C_6H_3)]$, which had been prepared by a literature method (Shozi & Friedrich, 2012). A dichloromethane solution of $[(Ph_2P)_2N(3,5\text{-}(CH_3)_2(C_6H_3)]$ was allowed to evaporate slowly at room temperature under argon. After 24 h, crystals suitable for single-crystal structure determination were obtained. However, $[Ph_2P(O)NH(3,5\text{-}(CH_3)_2(C_6H_3)]$ rather than the expected $[(Ph_2P)_2N(3,5\text{-}(CH_3)_2(C_6H_3)]$ was serendipitously isolated. The title compound may have formed as a result of the adventitious exposure of the sample to moisture and/or oxygen.

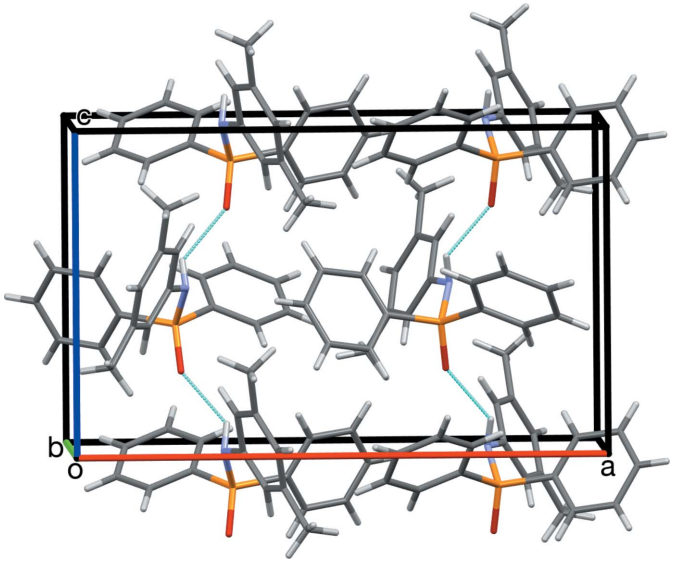


Figure 2
Unit-cell packing viewed along the *b* axis showing N—H···O hydrogen-bonding contacts as dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1	0.95	2.48	3.148 (3)	128
N1—H1···O1^{i}	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	
Chemical formula	$C_{20}H_{20}NOP$
M_r	321.34
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	100
a, b, c (Å)	15.9713 (9), 10.7495 (7), 9.8286 (6)
V (Å^3)	1687.41 (18)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.17
Crystal size (mm)	0.36 × 0.28 × 0.11
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.829, 0.942
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25376, 5327, 4160
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.725
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	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
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.38
Absolute structure	Flack x determined using 1497 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.07 (5)

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

Refinement

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

Acknowledgements

The authors thank Mr Trevahn M. Williams for his assistance in preparing some of the starting materials for this work.

Funding information

Funding for this research was provided by: National Science Foundation, Division of Chemistry (award No. MRI, CHE-0420497 to UMSL); College of Arts and Sciences, Southern Illinois University Edwardsville; Graduate School, Southern Illinois University Edwardsville.

References

Bruker (2013). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2016). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Gusev, O. V., Ustynyuk, N. A., Peganova, T. A., Gonchar, A. V., Petrovskii, P. V. & Lyssenko, K. A. (2009). *Phosphorus Sulfur Silicon*, **184**, 322–331.

Hong, G., Zhu, X., Hu, C., Aruma, A. N., Wu, S. & Wang, L. (2016). *J. Org. Chem.* **81**, 6867–6874.

Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.

Naktode, K., Kottalanka, R. K., Jana, S. K. & Panda, T. K. (2013). *Z. Anorg. Allg. Chem.* **639**, 999–1003.

Naktode, K., Kottalanka, R. K. & Panda, T. K. (2012). *New J. Chem.* **36**, 2280–2285.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Priya, S., Balakrishna, M. S. & Mobin, S. M. (2005). *Polyhedron*, **24**, 1641–1650.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Shozi, M. L. & Friedrich, H. B. (2012). *S. Afr. J. Chem.* **65**, 214–222.

Sun, Y. & Cramer, N. (2017). *Angew. Chem. Int. Ed.* **56**, 364–367.

Xu, Y., Su, Q., Dong, W., Peng, Z. & An, D. (2017). *Tetrahedron*, **73**, 4602–4609.

full crystallographic data

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

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Crystal data

$C_{20}H_{20}NOP$
M_r = 321.34
Orthorhombic, $Pca2_1$
a = 15.9713 (9) Å
b = 10.7495 (7) Å
c = 9.8286 (6) Å
V = 1687.41 (18) Å^3
Z = 4
$F(000)$ = 680
D_x = 1.265 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5345 reflections
θ = 3.1–29.8°
μ = 0.17 mm^{-1}
T = 100 K
Rectangular, colourless
0.36 × 0.28 × 0.11 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: sealed tube
Detector resolution: 8 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.829, T_{max} = 0.942
25376 measured reflections
5327 independent reflections
4160 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 31.0°, θ_{min} = 1.9°
h = −16→23
k = −15→15
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.108
S = 1.04
5327 reflections
210 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.1102P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Absolute structure: Flack x determined using 1497 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
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 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.95	2.48	3.148 (3)	128
N1—H1···O1^{i}	0.88	2.12	2.788 (3)	133

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