Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diisopropyl [(benzoylamino)(phenyl)-methyl]phosphonate

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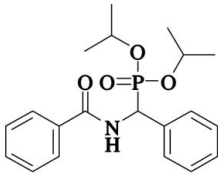
Received 13 February 2009; accepted 21 February 2009

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.006 Å; R factor = 0.065; wR factor = 0.174; data-to-parameter ratio = 14.5.

The title compound, $C_{20}H_{26}NO_4P$, has been obtained by the reaction of benzoyl chloride and diisopropyl[amino(phenyl)-methyl]phosphonate. The dihedral angle between the planes of the benzoylamino group and the phenyl ring is 77.0 (2)°. The crystal structure is stabilized by strong intermolecular N—H···O hydrogen bonds between the doubly bonded phosphoryl O atom and the amide N atom which link the molecules into pairs about a center of symmetry.

Related literature

For the biological activity and pharmaceutical interest of α-hydroxyphosphonic acid esters, see: Stowasser *et al.* (1992); Chen *et al.* (1995). For their use as reagents in the synthesis of enol ethers and α-ketophosphonates, see: Babak & Rahman (2001). For the synthesis, see: Drescher *et al.* (1995). For bond lengths and angles in related compunds, see: Smaardijk *et al.* (1985).



Experimental

Crystal data

$C_{20}H_{26}NO_4P$
M_r = 375.39
Triclinic, $P\overline{1}$
a = 10.839 (4) Å
b = 10.925 (5) Å
c = 11.057 (5) Å
α = 61.364 (8)°
β = 83.362 (8)°
γ = 60.470 (6)°
V = 987.3 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 273 K
0.28 × 0.21 × 0.05 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.956, T_{max} = 0.992
4991 measured reflections
3411 independent reflections
2509 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.174
S = 0.98
3411 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.86	2.05	2.895 (3)	165

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

This work was supported by the National Natural Science Foundation of China (No. 40806032) and the Scientific Research Foundation of the Third Institute of Oceanography, SOA (No. 2009005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2235).

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supporting information

Acta Cryst. (2009). E**65**, o642 [doi:10.1107/S1600536809006382]

Diisopropyl [(benzoylamino)(phenyl)methyl]phosphonate

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S1. Comment

In recent years α-hydroxyphosphonic acids esters have attracted much attention due to their wide biological activity (Stowasser *et al.*, 1992) and pharmaceutical interest (Chen *et al.*, 1995). They are useful reagents for the synthesis of enol ethers and α-ketophosphonates (Babak *et al.*, 2001). Bond lengths and angles in the title compound, (I), are in agreement with the values reported for related compounds (Smaardijk *et al.*, 1985). The dihedral angle between the planes of the benzoylamino group and phenyl ring is 103.0 (2)° (Fig. 1). The amide N atom is involved in a hydrogen-bonding interaction with the phosphoryl O atom of a neighboring molecule linking the molecules into pairs around a centerof symmetry (Table 1 and Fig. 2).

S2. Experimental

A solution of dry dichloromethane (20 ml) containing (amino-phenyl-methyl)-phosphonic acid diisopropyl ester (1 mmol, 0.27 g) and triethylamine (0.4 ml) was added dropwise to a solution of dichloromethane (10 ml) containing benzoyl chloride (1.2 mmol, 0.17 g). The reaction mixture was stirred for 6 h at room temperature and the solvent was then removed under reduced pressure to give a residue, which was extracted with ethyl acetate (3 × 15 ml). The solution was dried over anhydrous $MgSO_4$ and concentrated under vacuum to obtain a slurry residue, which was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 2:1) to give (I) as a colorless amorphous solid (Drescher, *et al.*, 1995). Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a petroleum ether /dichloro-methane solution (1:1 *v*/*v*).

S3. Refinement

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.93 (aromatic), 0.96 (CH_3) or 0.98 (CH), N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}$ (aromatic C, CH and N) or $1.5U_{eq}$ (methyl C).

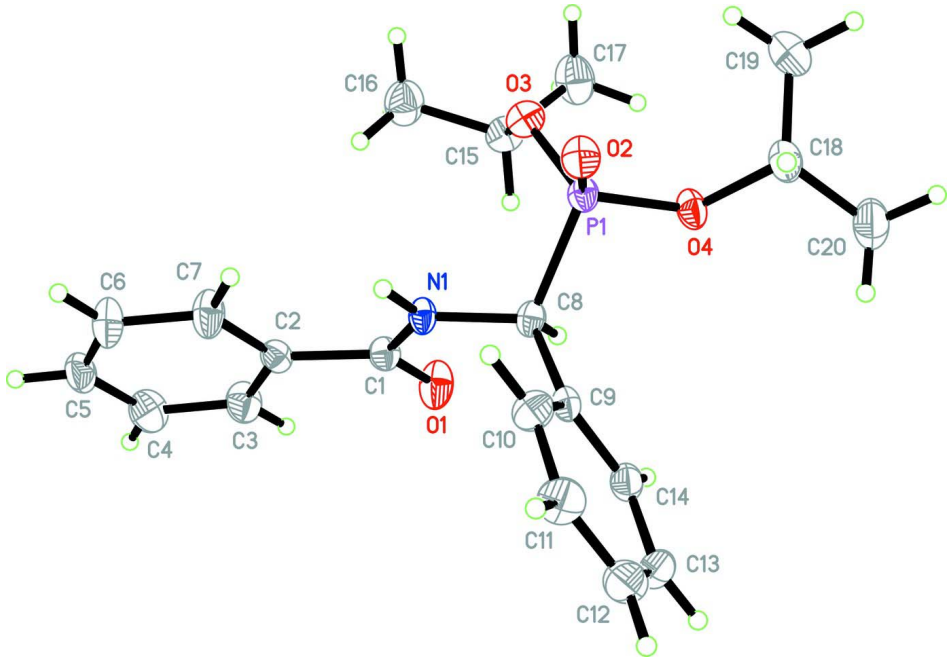

Figure 1

The title molecule showing the anisotropic displacement parameters of the non-hydrogen atoms at the 30% probability level. The H atoms are drawn as spheres of arbitrary radii.

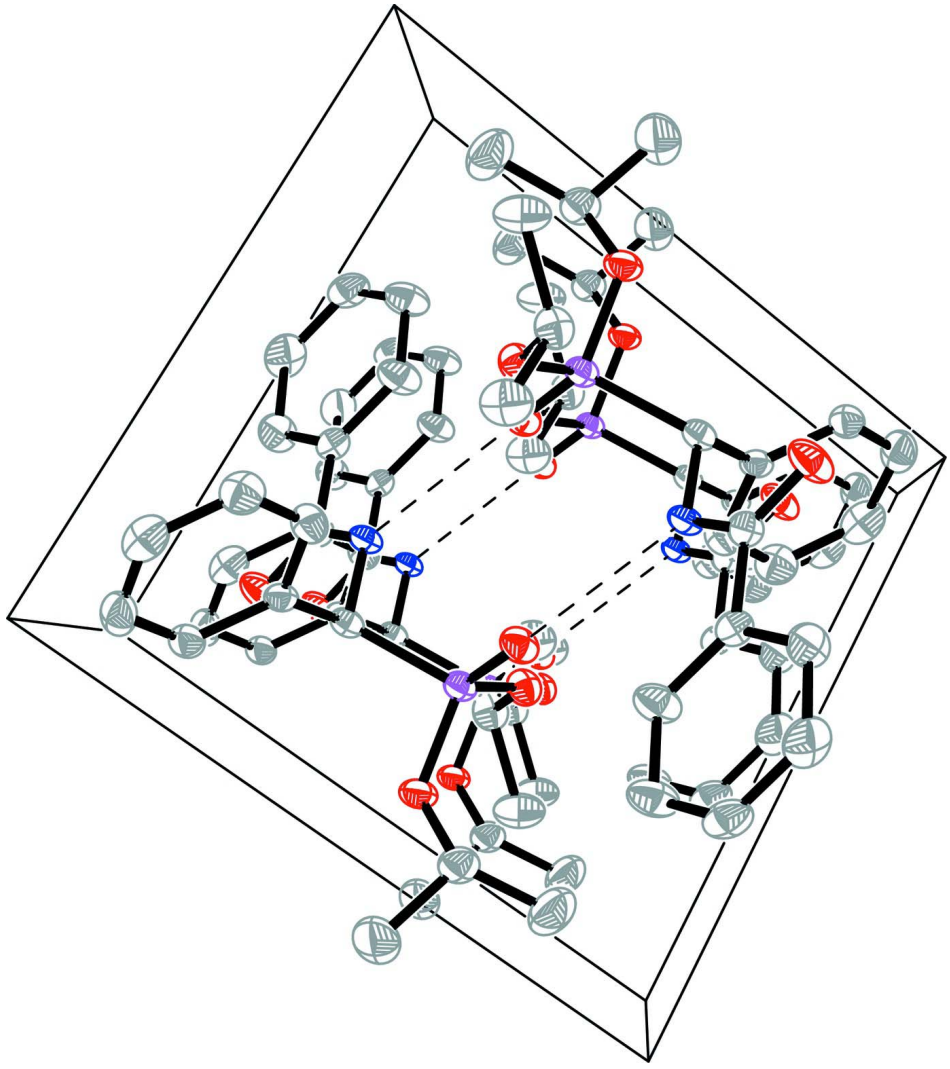

Figure 2

Packing diagram of title compound, showing the N—H···O hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (i) -*x* + 1, -*y* + 2, -*z* + 1)].

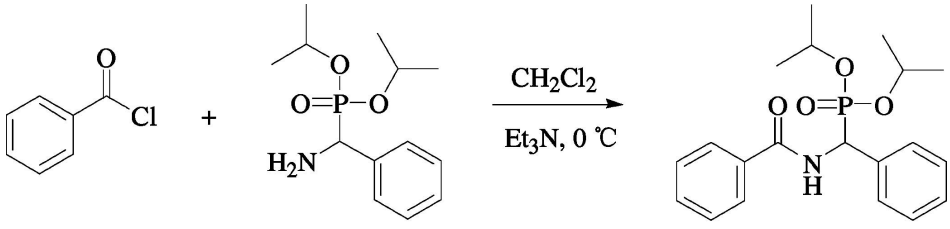

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Figure 3

The formation of the title compound.

Diisopropyl [(benzoylamino)(phenyl)methyl]phosphonate

Crystal data

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$\gamma = 60.470\ (6)°$
$V = 987.3\ (7)$ Å^3
$Z = 2$
$F(000) = 400$
$D_x = 1.263$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1689 reflections
$\theta = 2.3–27.7°$
$\mu = 0.16$ mm^{-1}
$T = 273$ K
Chunk, colorless
0.28 × 0.21 × 0.05 mm

Data collection

Bruker APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.956$, $T_{max} = 0.992$
4991 measured reflections
3411 independent reflections
2509 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -12\rightarrow12$
$k = -12\rightarrow12$
$l = -10\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.174$
$S = 0.98$
3411 reflections
235 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
$w = 1/[\sigma^2(F_o^2) + (0.097P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.73254 (8)	0.85680 (9)	0.47527 (8)	0.0311 (3)
N1	0.6453 (2)	0.6827 (3)	0.6988 (3)	0.0310 (6)
H1A	0.5566	0.7577	0.6718	0.037*

O1	0.8049 (2)	0.4184 (2)	0.8105 (3)	0.0546 (7)
C1	0.6797 (3)	0.5282 (4)	0.7762 (3)	0.0339 (7)
O2	0.6331 (2)	1.0278 (2)	0.4252 (2)	0.0412 (6)
C2	0.5598 (3)	0.4933 (3)	0.8226 (3)	0.0336 (7)
O3	0.6811 (2)	0.7980 (2)	0.3986 (2)	0.0400 (6)
C3	0.5965 (4)	0.3371 (4)	0.9147 (4)	0.0505 (9)
H3A	0.6928	0.2572	0.9424	0.061*
O4	0.8922 (2)	0.8119 (2)	0.4564 (2)	0.0401 (6)
C4	0.4921 (4)	0.2969 (5)	0.9671 (4)	0.0602 (11)
H4A	0.5182	0.1906	1.0313	0.072*
C5	0.3507 (4)	0.4130 (5)	0.9247 (4)	0.0514 (9)
H5A	0.2804	0.3859	0.9603	0.062*
C6	0.3123 (4)	0.5681 (4)	0.8304 (4)	0.0549 (10)
H6A	0.2158	0.6472	0.8006	0.066*
C7	0.4171 (3)	0.6079 (4)	0.7792 (4)	0.0505 (9)
H7A	0.3905	0.7142	0.7142	0.061*
C8	0.7582 (3)	0.7231 (3)	0.6607 (3)	0.0305 (7)
H8A	0.8470	0.6220	0.6812	0.037*
C9	0.7819 (3)	0.7826 (3)	0.7489 (3)	0.0307 (7)
C10	0.6722 (3)	0.9170 (4)	0.7536 (3)	0.0431 (8)
H10A	0.5844	0.9768	0.6961	0.052*
C11	0.6917 (4)	0.9627 (4)	0.8423 (4)	0.0531 (9)
H11A	0.6166	1.0523	0.8456	0.064*
C12	0.8210 (4)	0.8774 (5)	0.9261 (4)	0.0562 (10)
H12A	0.8336	0.9095	0.9856	0.067*
C13	0.9309 (4)	0.7456 (5)	0.9221 (4)	0.0526 (9)
H13A	1.0191	0.6879	0.9784	0.063*
C14	0.9111 (3)	0.6979 (4)	0.8344 (3)	0.0398 (8)
H14A	0.9862	0.6070	0.8329	0.048*
C15	0.7424 (4)	0.6316 (4)	0.4291 (4)	0.0435 (8)
H15A	0.7990	0.5581	0.5230	0.052*
C16	0.6184 (4)	0.6079 (5)	0.4248 (4)	0.0608 (10)
H16A	0.5615	0.6255	0.4942	0.091*
H16B	0.6538	0.5000	0.4432	0.091*
H16C	0.5604	0.6832	0.3342	0.091*
C17	0.8383 (4)	0.6056 (5)	0.3243 (4)	0.0635 (11)
H17A	0.9161	0.6209	0.3328	0.095*
H17B	0.7841	0.6815	0.2319	0.095*
H17C	0.8758	0.4979	0.3409	0.095*
C18	0.9332 (4)	0.9289 (4)	0.3580 (4)	0.0458 (8)
H18A	0.8731	1.0307	0.3593	0.055*
C19	0.9101 (5)	0.9581 (6)	0.2149 (4)	0.0810 (14)
H19A	0.8101	1.0015	0.1875	0.121*
H19B	0.9658	0.8583	0.2131	0.121*
H19C	0.9393	1.0334	0.1513	0.121*
C20	1.0845 (4)	0.8639 (6)	0.4093 (5)	0.0816 (14)
H20A	1.0916	0.8510	0.5009	0.122*
H20B	1.1162	0.9373	0.3470	0.122*

H20C	1.1438	0.7612	0.4133	0.122*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0254 (4)	0.0278 (5)	0.0360 (5)	−0.0115 (3)	0.0062 (3)	−0.0149 (4)
N1	0.0210 (12)	0.0262 (13)	0.0398 (14)	−0.0105 (10)	0.0066 (11)	−0.0139 (12)
O1	0.0308 (12)	0.0297 (13)	0.0752 (18)	−0.0100 (10)	0.0017 (12)	−0.0102 (13)
C1	0.0348 (17)	0.0299 (17)	0.0363 (17)	−0.0170 (14)	0.0064 (14)	−0.0150 (15)
O2	0.0342 (11)	0.0288 (12)	0.0497 (13)	−0.0118 (9)	0.0050 (10)	−0.0155 (11)
C2	0.0407 (17)	0.0328 (17)	0.0343 (17)	−0.0228 (15)	0.0099 (14)	−0.0176 (15)
O3	0.0379 (12)	0.0357 (12)	0.0442 (12)	−0.0141 (10)	0.0030 (10)	−0.0217 (11)
C3	0.049 (2)	0.036 (2)	0.054 (2)	−0.0231 (17)	0.0061 (18)	−0.0111 (18)
O4	0.0284 (11)	0.0367 (12)	0.0448 (13)	−0.0162 (10)	0.0120 (10)	−0.0142 (11)
C4	0.075 (3)	0.050 (2)	0.055 (2)	−0.046 (2)	0.011 (2)	−0.011 (2)
C5	0.059 (2)	0.073 (3)	0.052 (2)	−0.051 (2)	0.0245 (19)	−0.035 (2)
C6	0.0391 (19)	0.055 (2)	0.077 (3)	−0.0298 (18)	0.0200 (19)	−0.032 (2)
C7	0.0383 (18)	0.0377 (19)	0.070 (2)	−0.0226 (16)	0.0128 (18)	−0.0197 (19)
C8	0.0236 (14)	0.0258 (16)	0.0400 (17)	−0.0107 (12)	0.0052 (13)	−0.0164 (15)
C9	0.0266 (15)	0.0321 (17)	0.0336 (16)	−0.0164 (13)	0.0097 (13)	−0.0155 (15)
C10	0.0386 (18)	0.0392 (19)	0.0472 (19)	−0.0152 (15)	0.0013 (16)	−0.0216 (17)
C11	0.057 (2)	0.050 (2)	0.059 (2)	−0.0245 (19)	0.012 (2)	−0.035 (2)
C12	0.080 (3)	0.068 (3)	0.052 (2)	−0.053 (2)	0.019 (2)	−0.036 (2)
C13	0.052 (2)	0.066 (2)	0.044 (2)	−0.040 (2)	0.0010 (18)	−0.018 (2)
C14	0.0338 (17)	0.0424 (19)	0.0400 (17)	−0.0211 (15)	0.0077 (15)	−0.0163 (16)
C15	0.0454 (19)	0.0363 (18)	0.048 (2)	−0.0177 (15)	0.0026 (17)	−0.0213 (17)
C16	0.064 (2)	0.068 (3)	0.072 (3)	−0.041 (2)	0.019 (2)	−0.043 (2)
C17	0.058 (2)	0.068 (3)	0.082 (3)	−0.033 (2)	0.033 (2)	−0.052 (3)
C18	0.0456 (19)	0.044 (2)	0.049 (2)	−0.0285 (17)	0.0128 (17)	−0.0182 (18)
C19	0.095 (3)	0.108 (4)	0.050 (2)	−0.073 (3)	0.020 (2)	−0.023 (3)
C20	0.063 (3)	0.094 (3)	0.074 (3)	−0.056 (3)	0.006 (2)	−0.013 (3)

Geometric parameters (Å, º)

P1—O2	1.456 (2)	C10—H10A	0.9300
P1—O3	1.559 (2)	C11—C12	1.369 (5)
P1—O4	1.567 (2)	C11—H11A	0.9300
P1—C8	1.809 (3)	C12—C13	1.361 (5)
N1—C1	1.337 (4)	C12—H12A	0.9300
N1—C8	1.451 (4)	C13—C14	1.379 (5)
N1—H1A	0.8600	C13—H13A	0.9300
O1—C1	1.226 (3)	C14—H14A	0.9300
C1—C2	1.498 (4)	C15—C16	1.498 (5)
C2—C3	1.365 (4)	C15—C17	1.500 (5)
C2—C7	1.370 (4)	C15—H15A	0.9800
O3—C15	1.460 (4)	C16—H16A	0.9600
C3—C4	1.380 (5)	C16—H16B	0.9600
C3—H3A	0.9300	C16—H16C	0.9600

O4—C18	1.460 (4)	C17—H17A	0.9600
C4—C5	1.363 (5)	C17—H17B	0.9600
C4—H4A	0.9300	C17—H17C	0.9600
C5—C6	1.358 (5)	C18—C20	1.482 (5)
C5—H5A	0.9300	C18—C19	1.483 (5)
C6—C7	1.380 (5)	C18—H18A	0.9800
C6—H6A	0.9300	C19—H19A	0.9600
C7—H7A	0.9300	C19—H19B	0.9600
C8—C9	1.507 (4)	C19—H19C	0.9600
C8—H8A	0.9800	C20—H20A	0.9600
C9—C14	1.378 (4)	C20—H20B	0.9600
C9—C10	1.382 (4)	C20—H20C	0.9600
C10—C11	1.370 (4)		

O2—P1—O3	109.31 (12)	C10—C11—H11A	119.7
O2—P1—O4	114.66 (12)	C13—C12—C11	119.9 (3)
O3—P1—O4	108.59 (12)	C13—C12—H12A	120.0
O2—P1—C8	116.66 (13)	C11—C12—H12A	120.0
O3—P1—C8	107.29 (13)	C12—C13—C14	119.7 (3)
O4—P1—C8	99.67 (12)	C12—C13—H13A	120.1
C1—N1—C8	119.7 (2)	C14—C13—H13A	120.1
C1—N1—H1A	120.1	C9—C14—C13	121.2 (3)
C8—N1—H1A	120.1	C9—C14—H14A	119.4
O1—C1—N1	121.6 (3)	C13—C14—H14A	119.4
O1—C1—C2	120.7 (3)	O3—C15—C16	106.6 (3)
N1—C1—C2	117.7 (3)	O3—C15—C17	108.8 (3)
C3—C2—C7	118.6 (3)	C16—C15—C17	113.3 (3)
C3—C2—C1	117.3 (3)	O3—C15—H15A	109.4
C7—C2—C1	124.1 (3)	C16—C15—H15A	109.4
C15—O3—P1	126.33 (19)	C17—C15—H15A	109.4
C2—C3—C4	120.6 (3)	C15—C16—H16A	109.5
C2—C3—H3A	119.7	C15—C16—H16B	109.5
C4—C3—H3A	119.7	H16A—C16—H16B	109.5
C18—O4—P1	123.20 (19)	C15—C16—H16C	109.5
C5—C4—C3	120.0 (3)	H16A—C16—H16C	109.5
C5—C4—H4A	120.0	H16B—C16—H16C	109.5
C3—C4—H4A	120.0	C15—C17—H17A	109.5
C6—C5—C4	120.1 (3)	C15—C17—H17B	109.5
C6—C5—H5A	119.9	H17A—C17—H17B	109.5
C4—C5—H5A	119.9	C15—C17—H17C	109.5
C5—C6—C7	119.7 (3)	H17A—C17—H17C	109.5
C5—C6—H6A	120.2	H17B—C17—H17C	109.5
C7—C6—H6A	120.2	O4—C18—C20	106.7 (3)
C2—C7—C6	121.0 (3)	O4—C18—C19	110.1 (3)
C2—C7—H7A	119.5	C20—C18—C19	113.7 (4)
C6—C7—H7A	119.5	O4—C18—H18A	108.7
N1—C8—C9	112.6 (2)	C20—C18—H18A	108.7
N1—C8—P1	112.04 (18)	C19—C18—H18A	108.7

C9—C8—P1	113.18 (19)	C18—C19—H19A	109.5
N1—C8—H8A	106.1	C18—C19—H19B	109.5
C9—C8—H8A	106.1	H19A—C19—H19B	109.5
P1—C8—H8A	106.1	C18—C19—H19C	109.5
C14—C9—C10	118.1 (3)	H19A—C19—H19C	109.5
C14—C9—C8	120.7 (3)	H19B—C19—H19C	109.5
C10—C9—C8	121.0 (2)	C18—C20—H20A	109.5
C11—C10—C9	120.5 (3)	C18—C20—H20B	109.5
C11—C10—H10A	119.7	H20A—C20—H20B	109.5
C9—C10—H10A	119.7	C18—C20—H20C	109.5
C12—C11—C10	120.5 (3)	H20A—C20—H20C	109.5
C12—C11—H11A	119.7	H20B—C20—H20C	109.5
C8—N1—C1—O1	−3.5 (4)	O2—P1—C8—N1	82.0 (2)
C8—N1—C1—C2	175.2 (2)	O3—P1—C8—N1	−40.9 (2)
O1—C1—C2—C3	6.2 (4)	O4—P1—C8—N1	−153.99 (19)
N1—C1—C2—C3	−172.5 (3)	O2—P1—C8—C9	−46.6 (2)
O1—C1—C2—C7	−174.3 (3)	O3—P1—C8—C9	−169.52 (19)
N1—C1—C2—C7	7.0 (4)	O4—P1—C8—C9	77.4 (2)
O2—P1—O3—C15	−173.2 (2)	N1—C8—C9—C14	116.7 (3)
O4—P1—O3—C15	61.0 (3)	P1—C8—C9—C14	−115.0 (3)
C8—P1—O3—C15	−45.8 (3)	N1—C8—C9—C10	−58.9 (4)
C7—C2—C3—C4	−2.5 (5)	P1—C8—C9—C10	69.4 (3)
C1—C2—C3—C4	177.0 (3)	C14—C9—C10—C11	−0.7 (5)
O2—P1—O4—C18	−19.8 (3)	C8—C9—C10—C11	174.9 (3)
O3—P1—O4—C18	102.8 (2)	C9—C10—C11—C12	1.0 (5)
C8—P1—O4—C18	−145.1 (2)	C10—C11—C12—C13	−0.4 (6)
C2—C3—C4—C5	1.4 (6)	C11—C12—C13—C14	−0.5 (6)
C3—C4—C5—C6	0.3 (6)	C10—C9—C14—C13	−0.2 (5)
C4—C5—C6—C7	−0.8 (5)	C8—C9—C14—C13	−175.8 (3)
C3—C2—C7—C6	2.0 (5)	C12—C13—C14—C9	0.8 (5)
C1—C2—C7—C6	−177.4 (3)	P1—O3—C15—C16	136.8 (3)
C5—C6—C7—C2	−0.4 (6)	P1—O3—C15—C17	−100.8 (3)
C1—N1—C8—C9	−101.9 (3)	P1—O4—C18—C20	156.8 (3)
C1—N1—C8—P1	129.2 (2)	P1—O4—C18—C19	−79.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.86	2.05	2.895 (3)	165

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