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Crystal structure of diethyl [(4-nitrophenylamino)(2-hydroxyphenyl)methyl]-phosphonate methanol monosolvate

QingMing Wang,[a] Feng Su,[b] TingTing Yang,[a] LiPing Lu[b] and MiaoLi Zhu[b]*

[a]School of Pharmacy, Yancheng Teachers' University, Yancheng, Jiangsu 224051, People's Republic of China, and [b]Institute of Molecular Science, Key Laboratory of Chemical Biology and Molecular Engineering of the Education Ministry, Shanxi University, Taiyuan, Shanxi 030006, People's Republic of China. *Correspondence e-mail: miaoli@sxu.edu.cn

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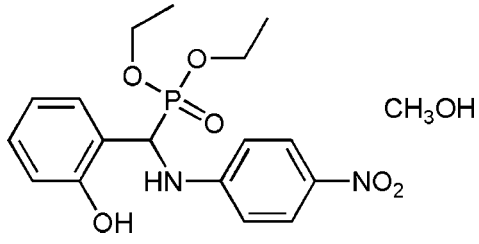
In the title compound, $C_{17}H_{21}N_2O_6P\cdot CH_3OH$, the planes of the 4-nitroaniline and 2-hydroxyphenyl groups form a dihedral angle of 84.04 (8)°. The P atom exhibits tetrahedral geometry involving two *O*-ethyl groups, a Cα atom and a double-bonded O atom. In the crystal, O—H···O, N—H···O and C—H···O hydrogen bonds link the α-aminophosphonic acid and methanol molecules into chains that propagate parallel to the *a* axis.

Keywords: crystal structure; α-aminophosphonic acids; phosphonate salts; hydrogen bonding.

CCDC reference: 1019639

1. Related literature

For background to the synthesis and properties of α-aminophosphonic acids, see: Allen *et al.* (1978); Arizpe *et al.* (2011); Cherkasov & Galkin (1998); Sieńczyk & Oleksyszyn (2009). For structures of related compounds, see: Li *et al.* (2008); Wang *et al.* (2012).



2. Experimental

2.1. Crystal data

$C_{17}H_{21}N_2O_6P\cdot CH_4O$
M_r = 412.37
Triclinic, $P\overline{1}$
a = 9.401 (6) Å
b = 10.061 (6) Å
c = 11.963 (7) Å
α = 101.328 (10)°
β = 94.183 (10)°
γ = 104.549 (9)°
V = 1065.0 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 296 K
0.40 × 0.34 × 0.30 mm

2.2. Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.935, T_{max} = 0.951
14569 measured reflections
5230 independent reflections
2934 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.138
S = 1.01
5230 reflections
262 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O4^{i}	0.82	2.00	2.819 (3)	172
O1—H1···O7	0.82	1.95	2.757 (3)	170
C10—H10···O5^{ii}	0.93	2.53	3.308 (4)	141
N1—H1A···O4^{iii}	0.82 (2)	2.14 (2)	2.959 (3)	171 (2)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: PK2529).

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supporting information

Acta Cryst. (2014). E**70**, o1053–o1054 [doi:10.1107/S1600536814018649]

Crystal structure of diethyl [(4-nitrophenylamino)(2-hydroxyphenyl)methyl]-phosphonate methanol monosolvate

QingMing Wang, Feng Su, TingTing Yang, LiPing Lu and MiaoLi Zhu

S1. Introduction

As mimics of natural amino acids, α-aminophosphonic acids and related derivatives are currently attracting a great deal of interest in medicinal chemistry due to their important biological effects (Arizpe, *et al.*, 2011). They have been reported to possess a wide range of biological functions. These include antibacterial activities (Allen *et al.*, 1978), action as inhibitors of enzymes such as rennin, HIV proteases, serine proteases and so on (Sieńczyk, *et al.*, 2009).

S2. Experimental

S2.1. Synthesis and crystallization

The synthesis of o-cresol α-aminophosphonate N-derivatives with rigid structures was achieved through the Pudovik reaction reaction (Cherkasov *et al.*, 1998). We obtained the title compound following our earlier report (Wang *et al.*, 2012). The synthesis involved two steps: a) the Schiff bases were first prepared in a condensation of 4-nitroaniline and salicylaldehyde in methanol solvent by refluxing equimolar amounts of reagents; b) reaction of Schiff base with a diethyl phosphonate in methanol solvent under reflux. The title compound was obtained from the filtrate after three days.

S2.2. Refinement

The amine H atom was located in a difference Fourier map and refined freely. All other H atoms were placed in geometrically idealized positions and refined as riding, with C–H = 0.93-0.98 Å, O–H = 0.82 Å, and the Uiso(H) = 1.2Ueq (C) for benzene ring, C7, C14, C16 and Uiso(H) = 1.5Ueq (O, C) for O—H groups and C15, C17, C18.

S3. Results and discussion

The crystal structure of the title compound is triclinic, with space group $P\bar{1}$. As seen from Fig. 1, the P atom has tetrahedral geometry involving two O-ethyl groups (O2, O3), one Cα atom (C7), and a double bond O atom (O4), which is the same as our earlier reports (Li *et al.*, 2008; Wang *et al.*, 2012). The C—P and P═O bond lengths are comparable to those in similar structures (Li *et al.* 2008; Wang *et al.*, 2012). Several hydrogen bonding interactions [O7—H7A···O4^{i} (i = x+1,y,z), O1—H1···O7, C10—H10···O5^{ii} (ii=-x, -y, -z-1), N1—H1A···O4^{iii} (iii=-x, -y+1, -z)] exist within in the crystal structure. The dihedral angle formed by the planes of the 4-nitroaniline and 2-hydroxyphenyl groups is 84.08 (8)°.

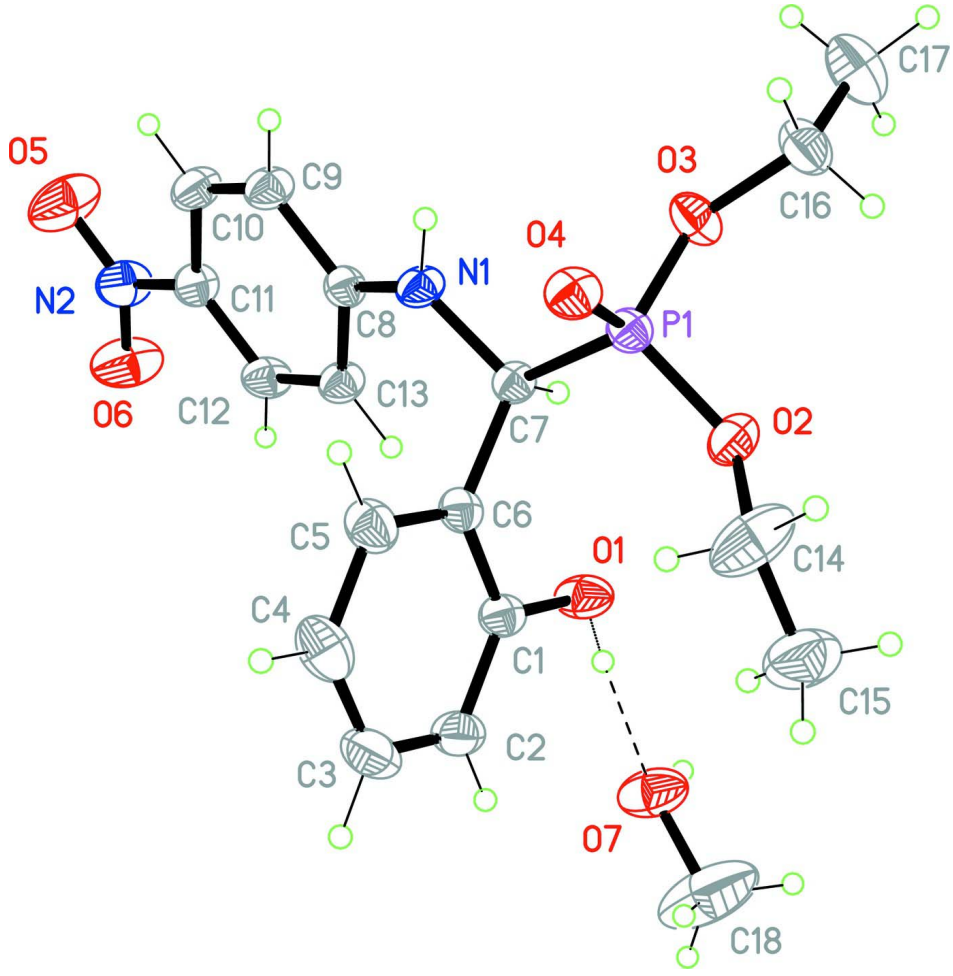

Figure 1

A view of the structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

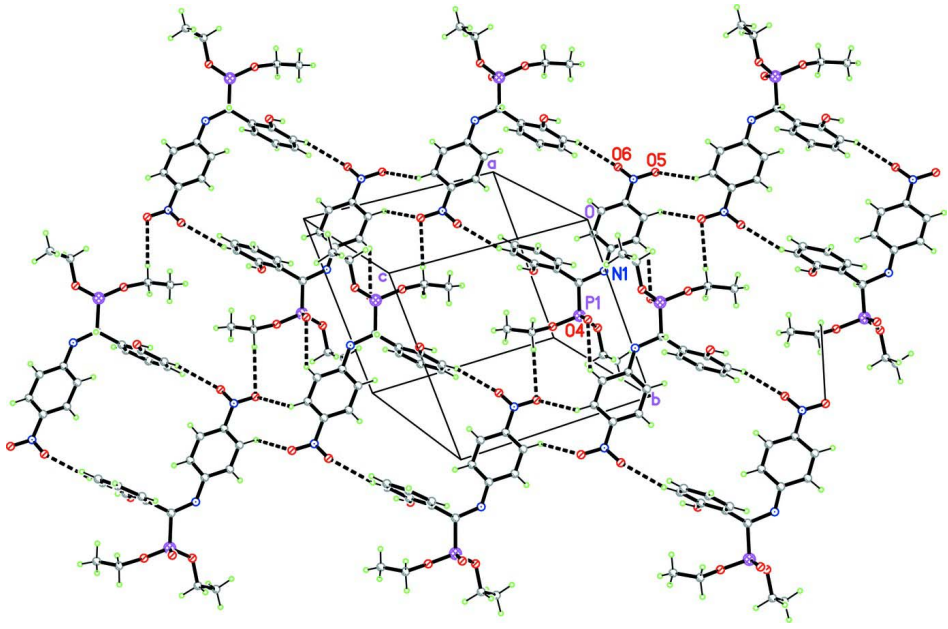

Figure 2

Crystal packing of the title compound, drawn so as to highlight the hydrogen-bonding interactions between molecules.

Diethyl [(4-nitrophenylamino)(2-hydroxyphenyl)methyl]phosphonate methanol monosolvate

Crystal data

$C_{17}H_{21}N_2O_6P\cdot CH_4O$
$M_r = 412.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.401$ (6) Å
$b = 10.061$ (6) Å
$c = 11.963$ (7) Å
$\alpha = 101.328$ (10)°
$\beta = 94.183$ (10)°
$\gamma = 104.549$ (9)°
$V = 1065.0$ (12) Å^3
$Z = 2$
$F(000) = 436$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1930 reflections
$\theta = 1.8$–28.3°
$\mu = 0.17$ mm^{-1}
$T = 296$ K
Block, yellow
0.4 × 0.34 × 0.3 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min} = 0.935$, $T_{max} = 0.951$
14569 measured reflections
5230 independent reflections
2934 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 28.2°$, $\theta_{min} = 1.8°$
$h = -12\rightarrow12$
$k = -13\rightarrow13$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.138$
$S = 1.01$
5230 reflections
262 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.0659P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H atoms treated by a mixture of independent and constrained refinement	$\Delta\rho_{max} = 0.31$ e Å^{-3}
	$\Delta\rho_{min} = -0.27$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4255 (3)	0.3224 (2)	0.17400 (19)	0.0408 (5)
C2	0.4364 (3)	0.2362 (3)	0.2493 (2)	0.0538 (7)
H2	0.5292	0.2347	0.2808	0.065*
C3	0.3111 (4)	0.1532 (3)	0.2778 (2)	0.0655 (8)
H3	0.3192	0.0962	0.3291	0.079*
C4	0.1720 (4)	0.1538 (3)	0.2302 (3)	0.0692 (8)
H4	0.0868	0.0979	0.2497	0.083*
C5	0.1618 (3)	0.2385 (3)	0.1535 (2)	0.0538 (7)
H5	0.0688	0.2379	0.1207	0.065*
C6	0.2871 (3)	0.3241 (2)	0.12431 (18)	0.0378 (5)
C7	0.2760 (2)	0.4232 (2)	0.04485 (17)	0.0348 (5)
H7	0.3749	0.4597	0.0239	0.042*
C8	0.2056 (2)	0.2631 (2)	−0.14895 (19)	0.0372 (5)
C9	0.1083 (3)	0.2150 (2)	−0.2517 (2)	0.0467 (6)
H9	0.0257	0.2492	−0.2595	0.056*
C10	0.1327 (3)	0.1185 (3)	−0.3410 (2)	0.0526 (7)
H10	0.0681	0.0884	−0.4092	0.063*
C11	0.2548 (3)	0.0660 (2)	−0.3287 (2)	0.0449 (6)
C12	0.3527 (3)	0.1124 (3)	−0.2294 (2)	0.0472 (6)
H12	0.4347	0.0772	−0.2227	0.057*
C13	0.3303 (3)	0.2105 (2)	−0.1397 (2)	0.0428 (6)
H13	0.3976	0.2422	−0.0729	0.051*
C14	0.3182 (4)	0.6256 (4)	0.3468 (2)	0.0941 (12)
H14A	0.2782	0.7004	0.3841	0.113*
H14B	0.2476	0.5363	0.3455	0.113*
C15	0.4561 (4)	0.6334 (4)	0.4116 (3)	0.0989 (12)
H15A	0.5020	0.5674	0.3700	0.148*
H15B	0.4377	0.6111	0.4846	0.148*
H15C	0.5206	0.7269	0.4237	0.148*

C16	0.2262 (3)	0.8152 (3)	0.0724 (2)	0.0600 (7)
H16A	0.2731	0.8615	0.1500	0.072*
H16B	0.1208	0.8069	0.0696	0.072*
C17	0.2894 (4)	0.8987 (3)	−0.0089 (3)	0.0853 (10)
H17A	0.3945	0.9110	−0.0026	0.128*
H17B	0.2697	0.9891	0.0087	0.128*
H17C	0.2453	0.8505	−0.0858	0.128*
C18	0.8676 (5)	0.4263 (6)	0.3596 (3)	0.154 (2)
H18A	0.9379	0.3743	0.3716	0.232*
H18B	0.7854	0.3987	0.4010	0.232*
H18C	0.9143	0.5253	0.3868	0.232*
N1	0.1748 (2)	0.3567 (2)	−0.06050 (16)	0.0415 (5)
N2	0.2802 (3)	−0.0373 (3)	−0.4225 (2)	0.0650 (7)
O1	0.54719 (18)	0.4078 (2)	0.14493 (15)	0.0566 (5)
H1	0.6220	0.4018	0.1811	0.085*
O2	0.33759 (18)	0.63846 (17)	0.22920 (13)	0.0518 (4)
O3	0.25022 (19)	0.67641 (16)	0.04156 (14)	0.0525 (5)
O4	0.06458 (17)	0.53339 (17)	0.14848 (13)	0.0478 (4)
O5	0.1927 (3)	−0.0771 (3)	−0.51111 (19)	0.1029 (9)
O6	0.3885 (3)	−0.0818 (2)	−0.41134 (17)	0.0919 (8)
O7	0.8177 (2)	0.3987 (3)	0.24407 (17)	0.0785 (6)
H7A	0.8843	0.4359	0.2104	0.118*
P1	0.21847 (7)	0.57045 (6)	0.12230 (5)	0.03809 (18)
H1A	0.107 (3)	0.391 (2)	−0.077 (2)	0.045 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0458 (14)	0.0433 (14)	0.0362 (12)	0.0202 (11)	0.0041 (11)	0.0060 (11)
C2	0.0633 (18)	0.0542 (16)	0.0482 (15)	0.0253 (14)	−0.0009 (13)	0.0122 (13)
C3	0.092 (2)	0.0552 (18)	0.0595 (18)	0.0284 (17)	0.0110 (17)	0.0260 (14)
C4	0.073 (2)	0.0569 (18)	0.081 (2)	0.0077 (16)	0.0271 (17)	0.0307 (16)
C5	0.0478 (16)	0.0494 (16)	0.0677 (18)	0.0133 (12)	0.0112 (13)	0.0202 (14)
C6	0.0427 (13)	0.0345 (12)	0.0383 (12)	0.0170 (10)	0.0074 (10)	0.0043 (10)
C7	0.0304 (12)	0.0384 (12)	0.0371 (12)	0.0127 (10)	0.0051 (10)	0.0069 (10)
C8	0.0386 (13)	0.0356 (12)	0.0384 (12)	0.0127 (10)	0.0057 (10)	0.0070 (10)
C9	0.0420 (14)	0.0532 (15)	0.0473 (14)	0.0244 (12)	−0.0002 (11)	0.0041 (12)
C10	0.0521 (16)	0.0589 (16)	0.0433 (14)	0.0201 (13)	−0.0072 (12)	0.0010 (12)
C11	0.0521 (15)	0.0439 (14)	0.0401 (13)	0.0229 (12)	0.0043 (11)	0.0008 (11)
C12	0.0491 (15)	0.0530 (15)	0.0478 (15)	0.0301 (12)	0.0070 (12)	0.0093 (12)
C13	0.0401 (13)	0.0476 (14)	0.0421 (13)	0.0196 (11)	0.0015 (11)	0.0047 (11)
C14	0.077 (2)	0.154 (4)	0.0440 (17)	0.040 (2)	0.0036 (17)	−0.005 (2)
C15	0.131 (3)	0.117 (3)	0.0546 (19)	0.058 (3)	−0.007 (2)	0.008 (2)
C16	0.0649 (18)	0.0428 (15)	0.0774 (19)	0.0221 (14)	0.0101 (15)	0.0153 (14)
C17	0.102 (3)	0.0560 (19)	0.106 (3)	0.0203 (18)	0.030 (2)	0.0333 (19)
C18	0.090 (3)	0.273 (6)	0.081 (3)	−0.008 (3)	−0.006 (2)	0.074 (4)
N1	0.0372 (11)	0.0475 (12)	0.0416 (11)	0.0229 (10)	−0.0020 (9)	0.0017 (9)
N2	0.0834 (18)	0.0676 (16)	0.0481 (14)	0.0422 (14)	−0.0002 (13)	−0.0021 (12)

O1	0.0382 (10)	0.0749 (13)	0.0640 (12)	0.0186 (9)	0.0022 (9)	0.0298 (10)
O2	0.0484 (10)	0.0560 (11)	0.0440 (10)	0.0116 (8)	−0.0047 (8)	0.0020 (8)
O3	0.0708 (12)	0.0400 (9)	0.0556 (11)	0.0256 (9)	0.0171 (9)	0.0143 (8)
O4	0.0395 (9)	0.0560 (10)	0.0531 (10)	0.0234 (8)	0.0092 (8)	0.0094 (8)
O5	0.1169 (19)	0.120 (2)	0.0634 (14)	0.0713 (16)	−0.0256 (14)	−0.0358 (13)
O6	0.1136 (18)	0.1124 (18)	0.0664 (14)	0.0860 (16)	−0.0014 (13)	−0.0079 (12)
O7	0.0485 (12)	0.1205 (19)	0.0717 (14)	0.0160 (12)	0.0039 (10)	0.0441 (13)
P1	0.0382 (3)	0.0382 (3)	0.0402 (3)	0.0168 (3)	0.0047 (3)	0.0059 (3)

Geometric parameters (Å, º)

C1—O1	1.360 (3)	C14—C15	1.438 (4)
C1—C2	1.382 (3)	C14—O2	1.458 (3)
C1—C6	1.396 (3)	C14—H14A	0.9700
C2—C3	1.370 (4)	C14—H14B	0.9700
C2—H2	0.9300	C15—H15A	0.9600
C3—C4	1.390 (4)	C15—H15B	0.9600
C3—H3	0.9300	C15—H15C	0.9600
C4—C5	1.383 (4)	C16—O3	1.451 (3)
C4—H4	0.9300	C16—C17	1.469 (4)
C5—C6	1.386 (3)	C16—H16A	0.9700
C5—H5	0.9300	C16—H16B	0.9700
C6—C7	1.522 (3)	C17—H17A	0.9600
C7—N1	1.454 (3)	C17—H17B	0.9600
C7—P1	1.812 (2)	C17—H17C	0.9600
C7—H7	0.9800	C18—O7	1.377 (4)
C8—N1	1.371 (3)	C18—H18A	0.9600
C8—C9	1.401 (3)	C18—H18B	0.9600
C8—C13	1.407 (3)	C18—H18C	0.9600
C9—C10	1.371 (3)	N1—H1A	0.82 (2)
C9—H9	0.9300	N2—O6	1.219 (3)
C10—C11	1.389 (3)	N2—O5	1.225 (3)
C10—H10	0.9300	O1—H1	0.8200
C11—C12	1.372 (3)	O2—P1	1.5557 (18)
C11—N2	1.450 (3)	O3—P1	1.5638 (18)
C12—C13	1.376 (3)	O4—P1	1.4734 (18)
C12—H12	0.9300	O7—H7A	0.8200
C13—H13	0.9300		

O1—C1—C2	122.1 (2)	O2—C14—H14A	109.3
O1—C1—C6	117.4 (2)	C15—C14—H14B	109.3
C2—C1—C6	120.6 (2)	O2—C14—H14B	109.3
C3—C2—C1	120.4 (3)	H14A—C14—H14B	108.0
C3—C2—H2	119.8	C14—C15—H15A	109.5
C1—C2—H2	119.8	C14—C15—H15B	109.5
C2—C3—C4	120.2 (3)	H15A—C15—H15B	109.5
C2—C3—H3	119.9	C14—C15—H15C	109.5
C4—C3—H3	119.9	H15A—C15—H15C	109.5

C5—C4—C3	119.2 (3)	H15B—C15—H15C	109.5
C5—C4—H4	120.4	O3—C16—C17	109.0 (2)
C3—C4—H4	120.4	O3—C16—H16A	109.9
C4—C5—C6	121.5 (3)	C17—C16—H16A	109.9
C4—C5—H5	119.3	O3—C16—H16B	109.9
C6—C5—H5	119.3	C17—C16—H16B	109.9
C5—C6—C1	118.2 (2)	H16A—C16—H16B	108.3
C5—C6—C7	121.6 (2)	C16—C17—H17A	109.5
C1—C6—C7	120.2 (2)	C16—C17—H17B	109.5
N1—C7—C6	113.91 (19)	H17A—C17—H17B	109.5
N1—C7—P1	109.45 (15)	C16—C17—H17C	109.5
C6—C7—P1	108.85 (14)	H17A—C17—H17C	109.5
N1—C7—H7	108.2	H17B—C17—H17C	109.5
C6—C7—H7	108.2	O7—C18—H18A	109.5
P1—C7—H7	108.2	O7—C18—H18B	109.5
N1—C8—C9	119.2 (2)	H18A—C18—H18B	109.5
N1—C8—C13	122.4 (2)	O7—C18—H18C	109.5
C9—C8—C13	118.4 (2)	H18A—C18—H18C	109.5
C10—C9—C8	121.1 (2)	H18B—C18—H18C	109.5
C10—C9—H9	119.5	C8—N1—C7	123.21 (19)
C8—C9—H9	119.5	C8—N1—H1A	115.2 (17)
C9—C10—C11	119.4 (2)	C7—N1—H1A	119.4 (17)
C9—C10—H10	120.3	O6—N2—O5	121.8 (2)
C11—C10—H10	120.3	O6—N2—C11	119.1 (2)
C12—C11—C10	120.7 (2)	O5—N2—C11	119.1 (2)
C12—C11—N2	119.7 (2)	C1—O1—H1	109.5
C10—C11—N2	119.6 (2)	C14—O2—P1	125.58 (18)
C11—C12—C13	120.4 (2)	C16—O3—P1	121.48 (16)
C11—C12—H12	119.8	C18—O7—H7A	109.5
C13—C12—H12	119.8	O4—P1—O2	114.76 (10)
C12—C13—C8	120.0 (2)	O4—P1—O3	114.66 (10)
C12—C13—H13	120.0	O2—P1—O3	104.51 (10)
C8—C13—H13	120.0	O4—P1—C7	114.21 (10)
C15—C14—O2	111.4 (3)	O2—P1—C7	105.37 (10)
C15—C14—H14A	109.3	O3—P1—C7	101.94 (10)

O1—C1—C2—C3	179.0 (2)	C9—C8—C13—C12	−1.3 (3)
C6—C1—C2—C3	−1.2 (4)	C9—C8—N1—C7	−173.7 (2)
C1—C2—C3—C4	0.7 (4)	C13—C8—N1—C7	7.8 (3)
C2—C3—C4—C5	0.4 (4)	C6—C7—N1—C8	−72.5 (3)
C3—C4—C5—C6	−0.9 (4)	P1—C7—N1—C8	165.39 (18)
C4—C5—C6—C1	0.4 (4)	C12—C11—N2—O6	0.2 (4)
C4—C5—C6—C7	−176.7 (2)	C10—C11—N2—O6	179.3 (3)
O1—C1—C6—C5	−179.6 (2)	C12—C11—N2—O5	−179.4 (3)
C2—C1—C6—C5	0.6 (3)	C10—C11—N2—O5	−0.3 (4)
O1—C1—C6—C7	−2.4 (3)	C15—C14—O2—P1	150.2 (2)
C2—C1—C6—C7	177.8 (2)	C17—C16—O3—P1	170.2 (2)
C5—C6—C7—N1	−49.0 (3)	C14—O2—P1—O4	21.6 (3)

C1—C6—C7—N1	133.9 (2)	C14—O2—P1—O3	148.0 (2)
C5—C6—C7—P1	73.4 (2)	C14—O2—P1—C7	−104.9 (2)
C1—C6—C7—P1	−103.7 (2)	C16—O3—P1—O4	58.8 (2)
N1—C8—C9—C10	−178.1 (2)	C16—O3—P1—O2	−67.7 (2)
C13—C8—C9—C10	0.5 (4)	C16—O3—P1—C7	−177.30 (19)
C8—C9—C10—C11	0.9 (4)	N1—C7—P1—O4	56.04 (18)
C9—C10—C11—C12	−1.6 (4)	C6—C7—P1—O4	−69.04 (17)
C9—C10—C11—N2	179.3 (2)	N1—C7—P1—O2	−177.09 (14)
C10—C11—C12—C13	0.8 (4)	C6—C7—P1—O2	57.82 (17)
N2—C11—C12—C13	179.9 (2)	N1—C7—P1—O3	−68.20 (17)
C11—C12—C13—C8	0.6 (4)	C6—C7—P1—O3	166.71 (15)
N1—C8—C13—C12	177.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···O4^{i}	0.82	2.00	2.819 (3)	172
O1—H1···O7	0.82	1.95	2.757 (3)	170
C10—H10···O5^{ii}	0.93	2.53	3.308 (4)	141
N1—H1*A*···O4^{iii}	0.82 (2)	2.14 (2)	2.959 (3)	171 (2)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*, −*y*, −*z*−1; (iii) −*x*, −*y*+1, −*z*.