Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(propan-2-yl) [(1*S*)-1-(4-fluorophenyl)-1-hydroxy-2-nitroethyl]phosphonate

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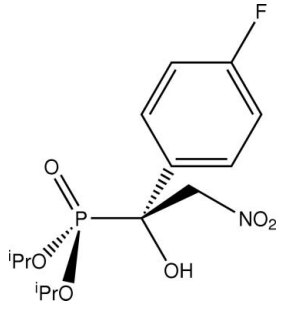
Received 4 December 2009; accepted 7 December 2009

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.049; wR factor = 0.117; data-to-parameter ratio = 16.1.

In the title compound, $C_{14}H_{21}FNO_6P$, a staggered conformation about the central P—C bond occurs, with the oxo and hydroxyl groups occupying diagonally opposite positions. The crystal structure features supramolecular chains mediated by O—H···O hydrogen bonds, which propagate in the *a*-axis direction. A C—H···O interaction consolidates the chains. Disorder was resolved for one of the isopropyl groups with a 0.60 (2):0.40 (2) occupancy ratio for the two components.

Related literature

For background to the enantioselective nitroaldol reaction of α-ketophosphonates and nitromethane and for the synthesis, see: Mandal *et al.* (2007).



Experimental

Crystal data

$C_{14}H_{21}FNO_6P$
M_r = 349.29
Orthorhombic, $P2_12_12_1$
a = 5.8267 (12) Å
b = 15.931 (3) Å
c = 18.273 (4) Å
V = 1696.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 173 K
0.31 × 0.15 × 0.06 mm

Data collection

Rigaku AFC12/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.790, T_{max} = 1
6049 measured reflections
3391 independent reflections
3248 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.117
S = 1.04
3391 reflections
211 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Absolute structure: Flack (1983), 1354 Friedel pairs
Flack parameter: −0.11 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4o···O1^{i}	0.84	1.94	2.728 (3)	156
C10—H10···O5^{ii}	0.95	2.52	3.447 (4)	164

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2009).

CGZ thanks the Welch Foundation (grant No. AX-1593) and the NIH-MBRS program (S06 GM08194) for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5270).

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supporting information

Acta Cryst. (2010). E**66**, o99 [doi:10.1107/S160053680905260X]

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S1. Comment

In connection with previous studies on the enantioselective nitroaldol reaction of α-ketophosphonates and nitromethane for the synthesis of optically active α-hydroxy-β-nitrophosphonates, the title compound, (I), was investigated. The crystal structure analysis of (I), Fig. 1, shows an *S*-configuration about the C7 atom. When viewed down the P–C7 axis, the molecule has a staggered conformation with the P═O and OH groups being diagonally opposite. The presence of O–H···O hydrogen bonding formed between the hydroxyl-O4—H and O═P atoms leads to the formation of supramolecular chains along [1 0 0], Fig. 2 and Table 1. Stability to these chains of linear topology is afforded by C–H···O contacts, Table 1.

S2. Experimental

The title compound was prepared as described in the literature (Mandal *et al.*, 2007).

S3. Refinement

The C-bound H atoms were geometrically placed (C—H = 0.95–1.00 Å) and refined as riding with U_{iso}(H) = 1.2–1.5U_{eq}(C). The methyl H-atoms were rotated to fit the electron density. The O–H H atom was located from a difference map and refined with O–H = 0.840±0.001 Å, and with U_{iso}(H) = 1.5U_{eq}(O). Disorder is evident in the structure as seen in the anisotropic displacement parameters associated with several residues. However, multiple sites were only resolved for the C6 atom. Two distinct sites were resolved from isotropic refinement of C6/C60 with the major component having a site occupancy factor of 0.60 (2).

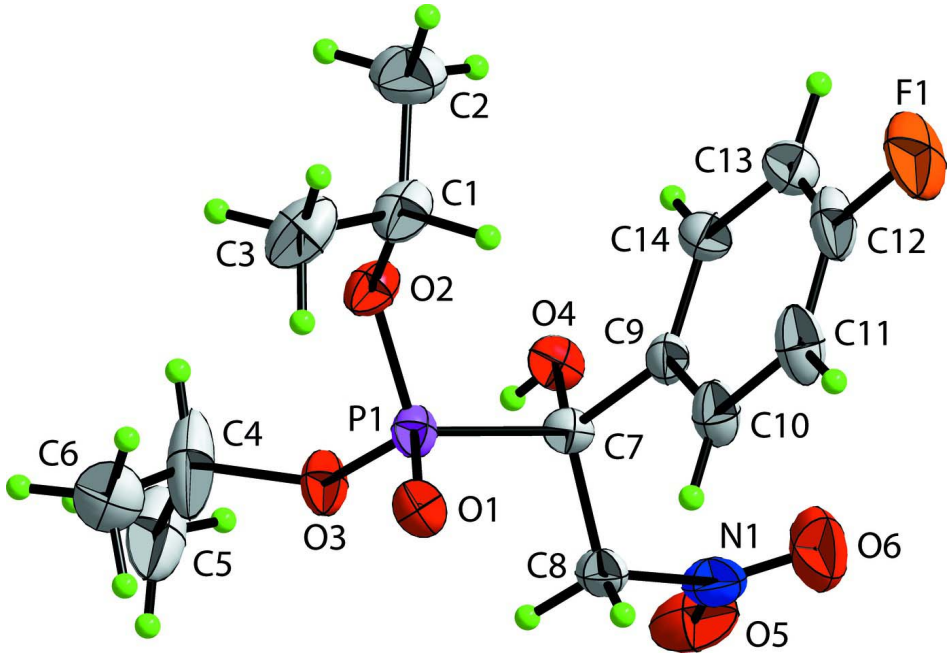

Figure 1

Molecular structure of (I), showing displacement ellipsoids at the 50% probability level. Only the major component of the C6 position is shown (the atom was refined isotropically).

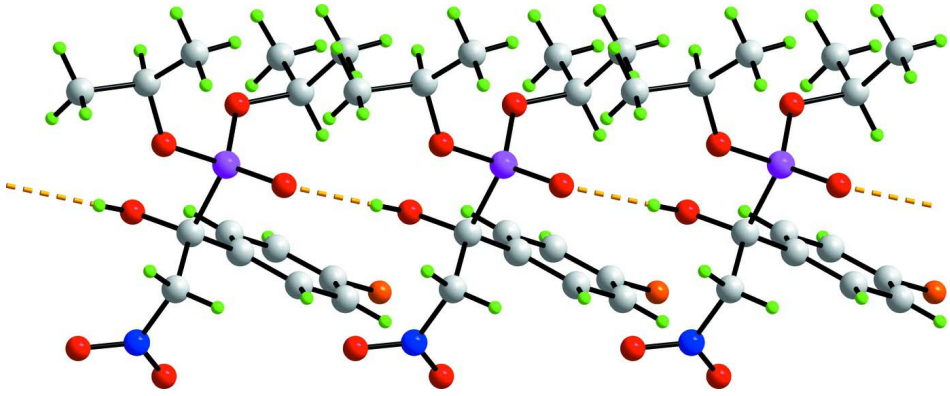

Figure 2

Supramolecular chain along the *a* axis in (I) mediated by O–H···O (orange dashed lines) hydrogen bonding. Colour scheme: P, pink; F, orange; O, red; N, blue; C, grey; and H, green.

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Crystal data

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Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.8267\ (12)$ Å
$b = 15.931\ (3)$ Å
$c = 18.273\ (4)$ Å
$V = 1696.2\ (6)$ Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.368$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6077 reflections
$\theta = 4.2–30.5°$

μ = 0.20 mm^{-1}
T = 173 K

Block, colourless
0.31 × 0.15 × 0.06 mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.790, T_{max} = 1

6049 measured reflections
3391 independent reflections
3248 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.5°, θ_{min} = 4.2°
h = −7→5
k = −20→13
l = −22→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.117
S = 1.04
3391 reflections
211 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.8973P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Absolute structure: Flack (1983), 1354 Friedel pairs
Absolute structure parameter: −0.11 (13)

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}	Occ. (<1)
P1	0.90429 (11)	0.45039 (4)	0.97285 (3)	0.02753 (16)	
F1	1.1808 (4)	0.75747 (13)	0.76550 (11)	0.0698 (7)	
O1	1.1339 (3)	0.41823 (11)	0.95590 (10)	0.0332 (4)	
O2	0.8946 (3)	0.52834 (11)	1.02505 (10)	0.0351 (4)	
O3	0.7358 (3)	0.38649 (12)	1.00898 (10)	0.0367 (5)	
O4	0.5136 (3)	0.50239 (11)	0.90853 (11)	0.0321 (4)	
H4O	0.4245	0.4648	0.9237	0.048*	
O5	0.3934 (4)	0.36867 (16)	0.78091 (14)	0.0629 (7)	
O6	0.6260 (6)	0.45661 (17)	0.73135 (13)	0.0832 (10)	
N1	0.5743 (5)	0.40835 (15)	0.77945 (14)	0.0468 (6)	
C1	1.0726 (5)	0.59419 (18)	1.02606 (16)	0.0428 (7)	
H1	1.1352	0.6024	0.9756	0.051*	

C2	0.9465 (7)	0.6725 (2)	1.0502 (2)	0.0619 (10)	
H2A	0.8252	0.6856	1.0149	0.093*	
H2B	1.0545	0.7196	1.0529	0.093*	
H2C	0.8782	0.6630	1.0985	0.093*	
C3	1.2628 (6)	0.5689 (2)	1.07709 (18)	0.0539 (9)	
H3A	1.3373	0.5180	1.0585	0.081*	
H3B	1.1992	0.5578	1.1258	0.081*	
H3C	1.3758	0.6143	1.0802	0.081*	
C4	0.7057 (8)	0.3642 (3)	1.08354 (19)	0.0803 (15)	0.60 (2)
H4	0.6489	0.4155	1.1092	0.096*	0.60 (2)
C5	0.5148 (8)	0.3014 (3)	1.0862 (2)	0.0710 (12)	0.60 (2)
H5A	0.3931	0.3183	1.0522	0.107*	0.60 (2)
H5B	0.4528	0.2987	1.1360	0.107*	0.60 (2)
H5C	0.5735	0.2460	1.0721	0.107*	0.60 (2)
C6	0.9077 (14)	0.3372 (7)	1.1220 (5)	0.058 (2)*	0.60 (2)
H6A	1.0168	0.3839	1.1251	0.087*	0.60 (2)
H6B	0.9786	0.2903	1.0957	0.087*	0.60 (2)
H6C	0.8655	0.3191	1.1715	0.087*	0.60 (2)
C40	0.7057 (8)	0.3642 (3)	1.08354 (19)	0.0803 (15)	0.40 (2)
H40	0.6132	0.4143	1.0983	0.096*	0.40 (2)
C50	0.5148 (8)	0.3014 (3)	1.0862 (2)	0.0710 (12)	0.40 (2)
H50A	0.3931	0.3183	1.0522	0.107*	0.40 (2)
H50B	0.4528	0.2987	1.1360	0.107*	0.40 (2)
H50C	0.5735	0.2460	1.0721	0.107*	0.40 (2)
C60	0.8713 (15)	0.3703 (8)	1.1382 (5)	0.041 (3)*	0.40 (2)
H60A	0.9949	0.4075	1.1218	0.062*	0.40 (2)
H60B	0.9342	0.3145	1.1485	0.062*	0.40 (2)
H60C	0.8014	0.3932	1.1827	0.062*	0.40 (2)
C7	0.7379 (4)	0.47723 (15)	0.88976 (14)	0.0258 (5)	
C8	0.7355 (5)	0.39729 (16)	0.84242 (14)	0.0328 (6)	
H8A	0.8920	0.3858	0.8239	0.039*	
H8B	0.6863	0.3488	0.8725	0.039*	
C9	0.8523 (4)	0.55250 (16)	0.85275 (12)	0.0274 (5)	
C10	1.0637 (5)	0.54344 (19)	0.81713 (14)	0.0376 (6)	
H10	1.1327	0.4896	0.8134	0.045*	
C11	1.1721 (5)	0.6126 (2)	0.78744 (17)	0.0464 (8)	
H11	1.3149	0.6069	0.7629	0.056*	
C12	1.0702 (6)	0.68921 (19)	0.79409 (16)	0.0457 (8)	
C13	0.8621 (6)	0.70094 (18)	0.82673 (16)	0.0435 (7)	
H13	0.7933	0.7550	0.8285	0.052*	
C14	0.7536 (5)	0.63162 (16)	0.85730 (15)	0.0344 (6)	
H14	0.6106	0.6385	0.8815	0.041*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0271 (3)	0.0296 (3)	0.0259 (3)	−0.0048 (3)	0.0000 (3)	0.0023 (3)
F1	0.0853 (16)	0.0602 (12)	0.0640 (12)	−0.0366 (12)	0.0008 (12)	0.0286 (10)

O1	0.0281 (9)	0.0341 (9)	0.0373 (9)	−0.0007 (8)	−0.0010 (8)	0.0052 (8)
O2	0.0347 (9)	0.0391 (9)	0.0316 (8)	−0.0100 (8)	0.0013 (9)	−0.0067 (8)
O3	0.0377 (10)	0.0416 (10)	0.0307 (9)	−0.0140 (9)	−0.0015 (8)	0.0084 (8)
O4	0.0241 (9)	0.0320 (10)	0.0402 (11)	−0.0023 (8)	0.0052 (8)	0.0023 (9)
O5	0.0469 (13)	0.0661 (15)	0.0756 (16)	0.0048 (13)	−0.0221 (14)	−0.0285 (13)
O6	0.135 (3)	0.0656 (16)	0.0492 (13)	−0.018 (2)	−0.0420 (18)	0.0132 (13)
N1	0.0594 (17)	0.0359 (12)	0.0451 (14)	0.0120 (13)	−0.0185 (14)	−0.0116 (12)
C1	0.0459 (16)	0.0463 (15)	0.0363 (14)	−0.0209 (14)	−0.0003 (15)	−0.0061 (13)
C2	0.076 (3)	0.0427 (17)	0.067 (2)	−0.0038 (18)	−0.015 (2)	−0.0106 (16)
C3	0.0390 (16)	0.076 (2)	0.0469 (17)	−0.0115 (17)	−0.0008 (15)	−0.0171 (17)
C4	0.092 (3)	0.110 (3)	0.0382 (17)	−0.061 (3)	−0.021 (2)	0.032 (2)
C5	0.081 (3)	0.084 (3)	0.0478 (18)	−0.056 (2)	−0.0012 (19)	0.015 (2)
C40	0.092 (3)	0.110 (3)	0.0382 (17)	−0.061 (3)	−0.021 (2)	0.032 (2)
C50	0.081 (3)	0.084 (3)	0.0478 (18)	−0.056 (2)	−0.0012 (19)	0.015 (2)
C7	0.0230 (11)	0.0238 (11)	0.0308 (12)	−0.0007 (9)	0.0024 (10)	−0.0012 (9)
C8	0.0378 (14)	0.0271 (12)	0.0334 (13)	0.0034 (12)	−0.0096 (12)	−0.0024 (10)
C9	0.0310 (13)	0.0290 (12)	0.0223 (10)	−0.0019 (11)	0.0005 (10)	0.0033 (10)
C10	0.0320 (13)	0.0476 (15)	0.0333 (13)	0.0033 (13)	0.0049 (12)	0.0111 (13)
C11	0.0352 (14)	0.062 (2)	0.0421 (15)	−0.0051 (14)	0.0041 (14)	0.0217 (15)
C12	0.0546 (19)	0.0472 (17)	0.0352 (14)	−0.0202 (16)	−0.0075 (15)	0.0172 (13)
C13	0.060 (2)	0.0307 (13)	0.0398 (14)	−0.0088 (14)	−0.0010 (15)	0.0025 (12)
C14	0.0402 (14)	0.0287 (12)	0.0344 (13)	−0.0039 (12)	0.0011 (13)	−0.0005 (11)

Geometric parameters (Å, º)

P1—O1	1.4656 (19)	C5—H5C	0.9800
P1—O3	1.5609 (19)	C6—H6A	0.9800
P1—O2	1.5670 (19)	C6—H6B	0.9800
P1—C7	1.851 (3)	C6—H6C	0.9800
F1—C12	1.368 (3)	C40—C60	1.392 (9)
O2—C1	1.476 (3)	C40—C50	1.496 (5)
O3—C40	1.419 (4)	C40—H40	1.0000
O3—C4	1.419 (4)	C50—H50A	0.9800
O4—C7	1.409 (3)	C50—H50B	0.9800
O4—H4O	0.8401	C50—H50C	0.9800
O5—N1	1.229 (4)	C60—H60A	0.9800
O6—N1	1.206 (4)	C60—H60B	0.9800
N1—C8	1.496 (4)	C60—H60C	0.9800
C1—C3	1.503 (5)	C7—C9	1.529 (3)
C1—C2	1.514 (5)	C7—C8	1.540 (3)
C1—H1	1.0000	C8—H8A	0.9900
C2—H2A	0.9800	C8—H8B	0.9900
C2—H2B	0.9800	C9—C14	1.388 (4)
C2—H2C	0.9800	C9—C10	1.401 (4)
C3—H3A	0.9800	C10—C11	1.382 (4)
C3—H3B	0.9800	C10—H10	0.9500
C3—H3C	0.9800	C11—C12	1.362 (5)
C4—C6	1.436 (8)	C11—H11	0.9500

C4—C5	1.496 (5)	C12—C13	1.364 (5)
C4—H4	1.0000	C13—C14	1.390 (4)
C5—H5A	0.9800	C13—H13	0.9500
C5—H5B	0.9800	C14—H14	0.9500
O1—P1—O3	115.82 (11)	C60—C40—O3	125.8 (5)
O1—P1—O2	116.03 (11)	C60—C40—C50	122.6 (4)
O3—P1—O2	103.69 (10)	O3—C40—C50	106.9 (3)
O1—P1—C7	112.66 (11)	C60—C40—H40	97.2
O3—P1—C7	99.68 (11)	O3—C40—H40	97.2
O2—P1—C7	107.29 (11)	C50—C40—H40	97.2
C1—O2—P1	123.06 (17)	C40—C50—H50A	109.5
C40—O3—P1	130.3 (2)	C40—C50—H50B	109.5
C4—O3—P1	130.3 (2)	H50A—C50—H50B	109.5
C7—O4—H4O	116.8	C40—C50—H50C	109.5
O6—N1—O5	123.9 (3)	H50A—C50—H50C	109.5
O6—N1—C8	118.6 (3)	H50B—C50—H50C	109.5
O5—N1—C8	117.5 (3)	C40—C60—H60A	109.5
O2—C1—C3	109.6 (2)	C40—C60—H60B	109.5
O2—C1—C2	104.4 (3)	H60A—C60—H60B	109.5
C3—C1—C2	113.5 (3)	C40—C60—H60C	109.5
O2—C1—H1	109.8	H60A—C60—H60C	109.5
C3—C1—H1	109.8	H60B—C60—H60C	109.5
C2—C1—H1	109.8	O4—C7—C9	106.77 (19)
C1—C2—H2A	109.5	O4—C7—C8	111.3 (2)
C1—C2—H2B	109.5	C9—C7—C8	113.8 (2)
H2A—C2—H2B	109.5	O4—C7—P1	110.58 (17)
C1—C2—H2C	109.5	C9—C7—P1	108.40 (16)
H2A—C2—H2C	109.5	C8—C7—P1	105.94 (16)
H2B—C2—H2C	109.5	N1—C8—C7	109.9 (2)
C1—C3—H3A	109.5	N1—C8—H8A	109.7
C1—C3—H3B	109.5	C7—C8—H8A	109.7
H3A—C3—H3B	109.5	N1—C8—H8B	109.7
C1—C3—H3C	109.5	C7—C8—H8B	109.7
H3A—C3—H3C	109.5	H8A—C8—H8B	108.2
H3B—C3—H3C	109.5	C14—C9—C10	119.1 (2)
O3—C4—C6	116.3 (5)	C14—C9—C7	120.3 (2)
O3—C4—C5	106.9 (3)	C10—C9—C7	120.5 (2)
C6—C4—C5	113.2 (4)	C11—C10—C9	120.2 (3)
O3—C4—H4	106.6	C11—C10—H10	119.9
C6—C4—H4	106.6	C9—C10—H10	119.9
C5—C4—H4	106.6	C12—C11—C10	118.7 (3)
C4—C5—H5A	109.5	C12—C11—H11	120.6
C4—C5—H5B	109.5	C10—C11—H11	120.6
H5A—C5—H5B	109.5	C11—C12—C13	123.3 (3)
C4—C5—H5C	109.5	C11—C12—F1	118.2 (3)
H5A—C5—H5C	109.5	C13—C12—F1	118.5 (3)
H5B—C5—H5C	109.5	C12—C13—C14	118.1 (3)

C4—C6—H6A	109.5	C12—C13—H13	120.9
C4—C6—H6B	109.5	C14—C13—H13	120.9
H6A—C6—H6B	109.5	C9—C14—C13	120.6 (3)
C4—C6—H6C	109.5	C9—C14—H14	119.7
H6A—C6—H6C	109.5	C13—C14—H14	119.7
H6B—C6—H6C	109.5		

O1—P1—O2—C1	33.2 (2)	O1—P1—C7—C8	55.3 (2)
O3—P1—O2—C1	161.4 (2)	O3—P1—C7—C8	−68.07 (19)
C7—P1—O2—C1	−93.7 (2)	O2—P1—C7—C8	−175.81 (17)
O1—P1—O3—C40	85.5 (4)	O6—N1—C8—C7	69.9 (4)
O2—P1—O3—C40	−42.8 (4)	O5—N1—C8—C7	−108.5 (3)
C7—P1—O3—C40	−153.4 (4)	O4—C7—C8—N1	50.9 (3)
O1—P1—O3—C4	85.5 (4)	C9—C7—C8—N1	−69.8 (3)
O2—P1—O3—C4	−42.8 (4)	P1—C7—C8—N1	171.2 (2)
C7—P1—O3—C4	−153.4 (4)	O4—C7—C9—C14	13.7 (3)
P1—O2—C1—C3	−86.8 (3)	C8—C7—C9—C14	137.0 (2)
P1—O2—C1—C2	151.4 (2)	P1—C7—C9—C14	−105.4 (2)
C40—O3—C4—C6	0 (100)	O4—C7—C9—C10	−169.6 (2)
P1—O3—C4—C6	−54.1 (7)	C8—C7—C9—C10	−46.4 (3)
C40—O3—C4—C5	0 (8)	P1—C7—C9—C10	71.2 (3)
P1—O3—C4—C5	178.4 (3)	C14—C9—C10—C11	0.4 (4)
C4—O3—C40—C60	0 (100)	C7—C9—C10—C11	−176.3 (3)
P1—O3—C40—C60	−25.6 (9)	C9—C10—C11—C12	0.5 (4)
C4—O3—C40—C50	0 (8)	C10—C11—C12—C13	−2.1 (5)
P1—O3—C40—C50	178.4 (3)	C10—C11—C12—F1	179.0 (3)
O1—P1—C7—O4	176.02 (15)	C11—C12—C13—C14	2.7 (5)
O3—P1—C7—O4	52.65 (17)	F1—C12—C13—C14	−178.4 (3)
O2—P1—C7—O4	−55.09 (18)	C10—C9—C14—C13	0.3 (4)
O1—P1—C7—C9	−67.26 (19)	C7—C9—C14—C13	177.0 (2)
O3—P1—C7—C9	169.37 (17)	C12—C13—C14—C9	−1.8 (4)
O2—P1—C7—C9	61.64 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4o···O1^{i}	0.84	1.94	2.728 (3)	156
C10—H10···O5^{ii}	0.95	2.52	3.447 (4)	164

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