Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dimethyl (2-hydroxy-4-phenylbut-3-en-2-yl)phosphonate

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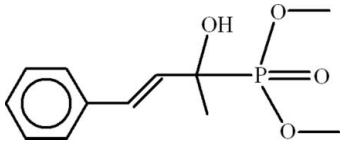
Received 22 October 2009; accepted 23 October 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.061; wR factor = 0.175; data-to-parameter ratio = 13.6.

In the title compound, $C_{12}H_{17}O_4P$, the phenylbutenyl group is disordered over two sets of sites with an occupancy ratio of 0.755 (12):0.245 (12). In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds occur, forming $R_2^2(10)$ ring motifs. The packing is consolidated by weak C—H···π interactions.

Related literature

For related structures, see: Acar *et al.* (2009); Tahir *et al.* (2007, 2009*a*,*b*). For graph-set theory, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{12}H_{17}O_4P$
M_r = 256.23
Monoclinic, $C2/c$
a = 17.1522 (12) Å
b = 8.1571 (13) Å
c = 19.5230 (12) Å
β = 103.771 (10)°
V = 2653.0 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.25 × 0.14 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*MolEN*; Fair, 1990)
T_{min} = 0.885, T_{max} = 0.954
2519 measured reflections
2415 independent reflections
1684 reflections with $I > 2\sigma(I)$
R_{int} = 0.095
3 standard reflections
frequency: 120 min
intensity decay: 0.6%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.175
S = 1.07
2415 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.90	2.721 (3)	176
C6B—H6B···$Cg1^{ii}$	0.93	2.83	3.568 (17)	137
C6B—H6B···$Cg2^{ii}$	0.93	2.94	3.652 (17)	134

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$. $Cg1$ and $Cg2$ are the centroids of the C1A–C6A and C1B–C6B rings, respectively.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1993); cell refinement: *CAD-4 EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *WinGX* (Farrugia, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5172).

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supporting information

Acta Cryst. (2009). E**65**, o2922 [https://doi.org/10.1107/S1600536809044067]

Dimethyl (2-hydroxy-4-phenylbut-3-en-2-yl)phosphonate

M. Nawaz Tahir, Nurcan Acar, Hamza Yilmaz and Riaz H. Tariq

S1. Comment

We have reported the crystal structures which contains α-hydroxy phosphonate such as (II) Dimethyl (1-hydroxy-1,2-diphenylethyl)phosphonate (Tahir *et al.*, 2009*a*), (III) Dimethyl [hydroxy(2-nitrophenyl)methyl]phosphonate (Tahir *et al.*, 2009*b*), (IV) (*R*)-Dimethyl [(2-chlorophenyl)hydroxymethyl]phosphonate (Tahir *et al.*, 2007) and Diethyl (1-hydroxy-1,2-diphenylethyl)phosphonate (Acar *et al.*, 2009). The title compound (I, Fig. 1) is in continuation of synthesizing various α-hydroxy phosphonates.

In the crystal structure of title compound phenylbutan is disordered over two possible sites with occupancy ratio of 0.755 (12):0.245 (12). The benzene rings of disordered moieties A (C1A—C6A) and B (C1B—C6B) are nearly planar to one another as the dihedral angle between A/B is 2.76 (1.35)°. The molecules of title compound are dimerized due to O—H···O type of intermolecular H-bondings (Table 1, Fig. 3) forming $R_2^2(10)$ ring motif (Bernstein *et al.*, 1995). The molecules are stabilized due to C–H···π interactions (Table 1).

S2. Experimental

Benzylacetone (4.45 g, 30 mmol) and dimethylphosphonate (3.30 g, 30 mmol) were dissolved in 50 ml of tetrahydrofuran. The mixture was cooled to 273 K and in it KF (1.74 g, 30 mmol) and γ-Al_2O_3 (1.74 g, 17 mmol) were added and refluxed. The precipitates obtained after 48 h were washed with hot distiled water (50 ml) and dried. The crude material was dissolved in distiled water with few drops of ethyl alcohol and colourless needles of (I) were obtained after 4 days.

S3. Refinement

The H-atoms were positioned geometrically (O–H = 0.82 Å, C–H = 0.93-0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

The incorrect bond distances and higher thermal parameters of phenylbutan lead to disorder. In the disordered group the benzene rings were refined using *AFIX 66*. The benzene ring B (C2B—C6B) was refined using EADP.

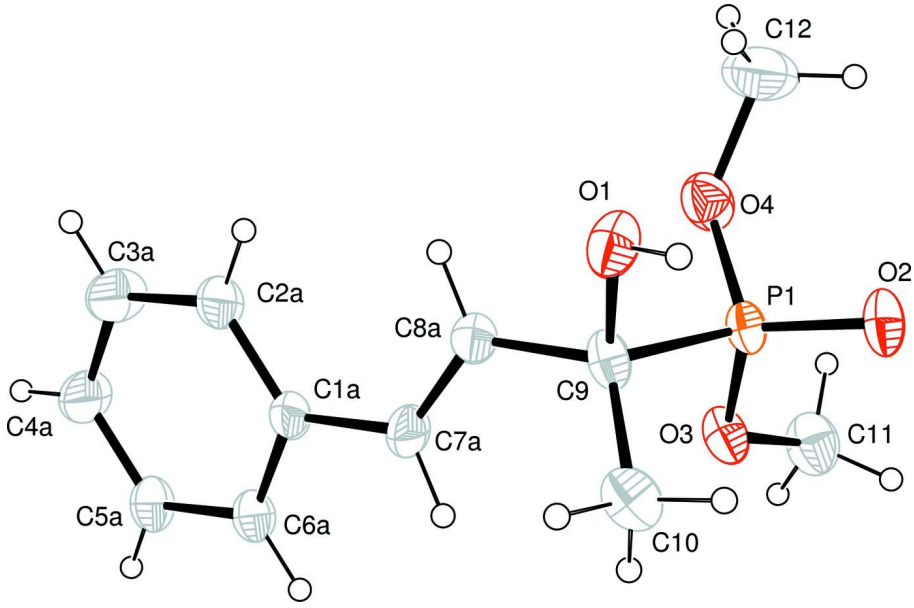

Figure 1

View of (I) with the atom numbering scheme for atoms of greater occupancy ratio. The displacement ellipsoids are drawn at the 30% probability level. H-atoms are shown by small circles of arbitrary radii.

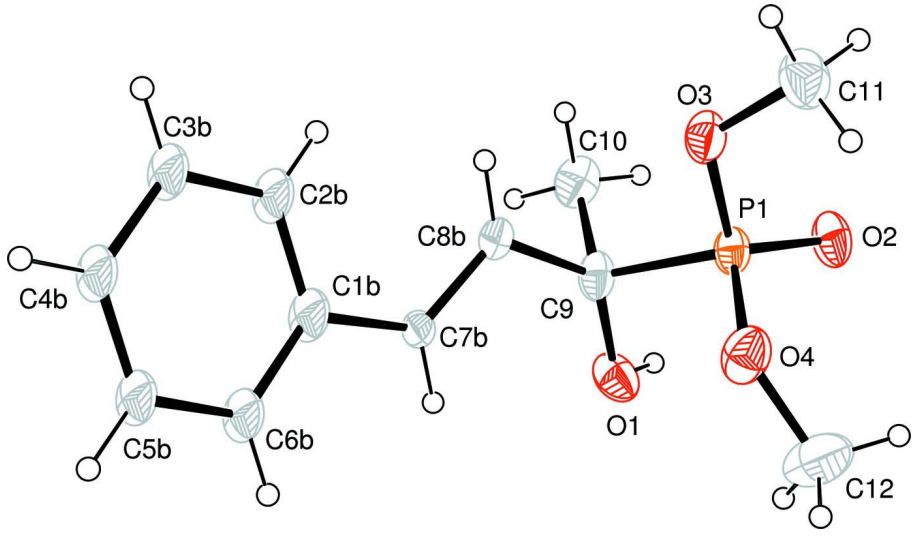

Figure 2

View of the title compound with the atom numbering scheme for atoms of smaller occupancy ratio. The displacement ellipsoids are drawn at the 30% probability level. H-atoms are shown by small circles of arbitrary radii.

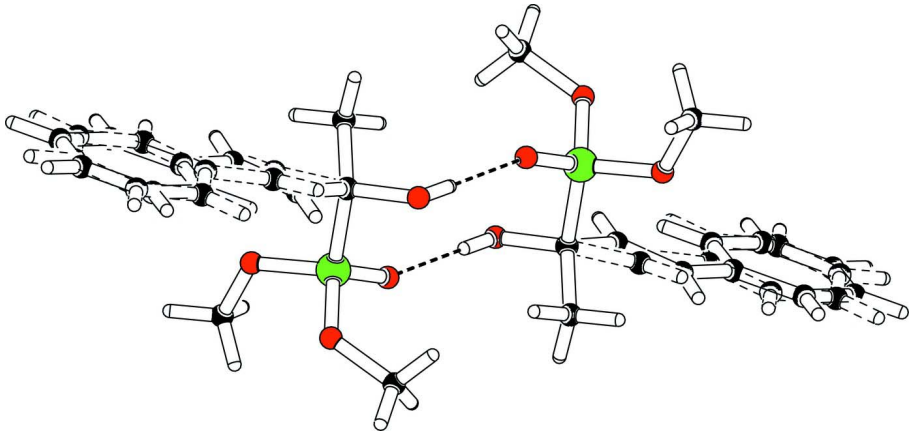

Figure 3

The partial packing of (I), which shows that molecules form inversion dimers.

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Crystal data

$C_{12}H_{17}O_4P$
$M_r = 256.23$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
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$b = 8.1571\ (13)$ Å
$c = 19.5230\ (12)$ Å
$\beta = 103.771\ (10)°$
$V = 2653.0\ (5)$ Å^3
$Z = 8$
$F(000) = 1088$
$D_x = 1.283$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9.9–13.9°$
$\mu = 0.21$ mm^{-1}
$T = 296$ K
Needle, colourless
0.25 × 0.14 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*MolEN*; Fair, 1990)
$T_{min} = 0.885$, $T_{max} = 0.954$
2519 measured reflections
2415 independent reflections
1684 reflections with $I > 2\sigma(I)$
$R_{int} = 0.095$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.8°$
$h = -20\rightarrow20$
$k = 0\rightarrow9$
$l = -23\rightarrow0$
3 standard reflections every 120 min
intensity decay: 0.6%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.175$
$S = 1.07$
2415 reflections
177 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.114P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
P1	0.43961 (4)	0.29251 (9)	0.06739 (4)	0.0399 (3)	
O1	0.43699 (13)	0.6068 (3)	0.08493 (11)	0.0548 (8)	
O2	0.49603 (12)	0.2946 (3)	0.02130 (12)	0.0528 (8)	
O3	0.37510 (12)	0.1526 (2)	0.05085 (11)	0.0500 (7)	
O4	0.48115 (13)	0.2636 (3)	0.14713 (12)	0.0597 (8)	
C1A	0.2124 (3)	0.4228 (6)	0.1674 (2)	0.0453 (16)	0.755 (12)
C2A	0.23963 (19)	0.4970 (7)	0.2329 (3)	0.058 (2)	0.755 (12)
C3A	0.1939 (3)	0.4884 (9)	0.28271 (18)	0.078 (2)	0.755 (12)
C4A	0.1209 (3)	0.4058 (9)	0.2671 (3)	0.072 (2)	0.755 (12)
C5A	0.0937 (2)	0.3316 (6)	0.2017 (3)	0.062 (2)	0.755 (12)
C6A	0.1395 (3)	0.3401 (6)	0.15183 (15)	0.0524 (17)	0.755 (12)
C7A	0.2601 (3)	0.4283 (6)	0.1139 (2)	0.0451 (16)	0.755 (12)
C8A	0.3344 (4)	0.4814 (7)	0.1215 (3)	0.0414 (19)	0.755 (12)
C9	0.37966 (18)	0.4799 (3)	0.06310 (16)	0.0440 (10)	
C10	0.3323 (2)	0.5090 (4)	−0.01138 (18)	0.0584 (11)	
C11	0.4001 (2)	−0.0152 (4)	0.0447 (2)	0.0644 (13)	
C12	0.5626 (2)	0.3125 (6)	0.1775 (2)	0.0896 (19)	
C6B	0.1066 (9)	0.341 (2)	0.1847 (9)	0.061 (3)	0.245 (12)
C7B	0.3065 (12)	0.441 (2)	0.0916 (13)	0.046 (6)	0.245 (12)
C1B	0.1670 (11)	0.380 (2)	0.1509 (5)	0.061 (3)	0.245 (12)
C2B	0.2328 (8)	0.471 (2)	0.1857 (9)	0.061 (3)	0.245 (12)
C3B	0.2381 (8)	0.525 (2)	0.2543 (9)	0.061 (3)	0.245 (12)
C4B	0.1777 (12)	0.486 (3)	0.2880 (7)	0.061 (3)	0.245 (12)
C5B	0.1119 (10)	0.395 (3)	0.2532 (9)	0.061 (3)	0.245 (12)
C8B	0.2981 (10)	0.5086 (19)	0.1470 (10)	0.057 (6)	0.245 (12)
H1	0.45706	0.63143	0.05218	0.0821*	
H2A	0.28844	0.55226	0.24331	0.0697*	0.755 (12)
H10C	0.36812	0.51292	−0.04233	0.0875*	
H11A	0.35594	−0.08762	0.04446	0.0966*	
H11B	0.41720	−0.02795	0.00165	0.0966*	
H11C	0.44381	−0.04117	0.08403	0.0966*	
H12A	0.59764	0.26187	0.15202	0.1344*	
H12B	0.56693	0.42950	0.17485	0.1344*	
H12C	0.57762	0.27862	0.22598	0.1344*	
H3A	0.21203	0.53806	0.32650	0.0928*	0.755 (12)
H4A	0.09026	0.40008	0.30047	0.0865*	0.755 (12)
H5A	0.04489	0.27630	0.19124	0.0741*	0.755 (12)
H6A	0.12130	0.29050	0.10804	0.0629*	0.755 (12)
H7A	0.23485	0.38956	0.06932	0.0541*	0.755 (12)
H8A	0.36086	0.52242	0.16532	0.0500*	0.755 (12)

H10A	0.29444	0.42147	−0.02555	0.0875*	
H10B	0.30398	0.61121	−0.01371	0.0875*	
H1B	0.16342	0.34369	0.10503	0.0729*	0.245 (12)
H3B	0.28213	0.58635	0.27758	0.0729*	0.245 (12)
H4B	0.18126	0.52218	0.33391	0.0729*	0.245 (12)
H5B	0.07147	0.36876	0.27580	0.0729*	0.245 (12)
H6B	0.06255	0.27951	0.16136	0.0729*	0.245 (12)
H7B	0.26815	0.36654	0.06805	0.0543*	0.245 (12)
H8B	0.33514	0.58922	0.16626	0.0680*	0.245 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0354 (4)	0.0436 (5)	0.0463 (5)	0.0019 (3)	0.0206 (3)	0.0024 (3)
O1	0.0676 (15)	0.0482 (12)	0.0568 (13)	−0.0064 (11)	0.0312 (12)	−0.0074 (10)
O2	0.0520 (13)	0.0542 (13)	0.0644 (14)	0.0030 (10)	0.0382 (11)	0.0013 (10)
O3	0.0399 (12)	0.0423 (11)	0.0723 (15)	0.0011 (9)	0.0225 (10)	−0.0003 (10)
O4	0.0499 (13)	0.0785 (15)	0.0530 (14)	0.0069 (12)	0.0167 (11)	0.0118 (11)
C1A	0.037 (3)	0.064 (3)	0.036 (2)	0.007 (2)	0.011 (2)	−0.005 (2)
C2A	0.043 (3)	0.093 (4)	0.045 (4)	−0.002 (2)	0.022 (2)	−0.011 (3)
C3A	0.055 (4)	0.140 (5)	0.047 (3)	−0.025 (4)	0.031 (3)	−0.022 (3)
C4A	0.053 (4)	0.121 (5)	0.051 (3)	−0.013 (3)	0.029 (3)	−0.020 (3)
C5A	0.046 (3)	0.096 (4)	0.054 (4)	0.000 (2)	0.033 (2)	−0.008 (3)
C6A	0.035 (3)	0.078 (3)	0.051 (3)	−0.002 (2)	0.024 (2)	−0.007 (2)
C7A	0.040 (3)	0.061 (3)	0.040 (2)	−0.007 (2)	0.021 (2)	−0.011 (2)
C8A	0.038 (4)	0.047 (3)	0.040 (3)	0.002 (2)	0.011 (3)	−0.005 (2)
C9	0.0388 (16)	0.0440 (16)	0.0560 (18)	0.0029 (13)	0.0245 (14)	0.0051 (13)
C10	0.051 (2)	0.0560 (19)	0.069 (2)	0.0017 (15)	0.0160 (17)	0.0091 (16)
C11	0.066 (2)	0.0462 (18)	0.085 (3)	0.0049 (16)	0.026 (2)	−0.0011 (16)
C12	0.065 (3)	0.119 (4)	0.074 (3)	−0.015 (2)	−0.005 (2)	−0.003 (2)
C6B	0.037 (4)	0.112 (7)	0.040 (5)	−0.002 (4)	0.024 (3)	−0.003 (4)
C7B	0.034 (10)	0.047 (9)	0.058 (13)	0.003 (7)	0.015 (9)	0.002 (7)
C1B	0.037 (4)	0.112 (7)	0.040 (5)	−0.002 (4)	0.024 (3)	−0.003 (4)
C2B	0.037 (4)	0.112 (7)	0.040 (5)	−0.002 (4)	0.024 (3)	−0.003 (4)
C3B	0.037 (4)	0.112 (7)	0.040 (5)	−0.002 (4)	0.024 (3)	−0.003 (4)
C4B	0.037 (4)	0.112 (7)	0.040 (5)	−0.002 (4)	0.024 (3)	−0.003 (4)
C5B	0.037 (4)	0.112 (7)	0.040 (5)	−0.002 (4)	0.024 (3)	−0.003 (4)
C8B	0.036 (8)	0.056 (9)	0.083 (12)	−0.010 (7)	0.023 (9)	−0.028 (8)

Geometric parameters (Å, º)

P1—O2	1.470 (2)	C8A—C9	1.525 (7)
P1—O3	1.569 (2)	C9—C10	1.506 (5)
P1—O4	1.568 (2)	C1B—H1B	0.9300
P1—C9	1.833 (3)	C2A—H2A	0.9300
O1—C9	1.422 (4)	C3A—H3A	0.9300
O3—C11	1.448 (4)	C3B—H3B	0.9300
O4—C12	1.438 (4)	C4A—H4A	0.9300

O1—H1	0.8200	C4B—H4B	0.9300
C1A—C2A	1.391 (7)	C5A—H5A	0.9300
C1A—C7A	1.473 (7)	C5B—H5B	0.9300
C1A—C6A	1.389 (7)	C6A—H6A	0.9300
C1B—C2B	1.39 (2)	C6B—H6B	0.9300
C1B—C6B	1.39 (2)	C7A—H7A	0.9300
C2A—C3A	1.389 (6)	C7B—H7B	0.9300
C2B—C8B	1.52 (2)	C8A—H8A	0.9300
C2B—C3B	1.39 (2)	C8B—H8B	0.9300
C3A—C4A	1.390 (8)	C10—H10B	0.9600
C3B—C4B	1.39 (2)	C10—H10A	0.9600
C4A—C5A	1.390 (8)	C10—H10C	0.9600
C4B—C5B	1.39 (3)	C11—H11A	0.9600
C5A—C6A	1.391 (6)	C11—H11B	0.9600
C5B—C6B	1.39 (2)	C11—H11C	0.9600
C7A—C8A	1.321 (9)	C12—H12A	0.9600
C7B—C8B	1.25 (3)	C12—H12B	0.9600
C7B—C9	1.52 (2)	C12—H12C	0.9600

O2—P1—O3	114.66 (13)	C2A—C3A—H3A	120.00
O2—P1—O4	113.56 (13)	C4A—C3A—H3A	120.00
O2—P1—C9	113.97 (14)	C2B—C3B—H3B	120.00
O3—P1—O4	103.09 (12)	C4B—C3B—H3B	120.00
O3—P1—C9	103.70 (12)	C3A—C4A—H4A	120.00
O4—P1—C9	106.75 (14)	C5A—C4A—H4A	120.00
P1—O3—C11	119.8 (2)	C3B—C4B—H4B	120.00
P1—O4—C12	122.3 (2)	C5B—C4B—H4B	120.00
C9—O1—H1	109.00	C4A—C5A—H5A	120.00
C2A—C1A—C7A	121.1 (4)	C6A—C5A—H5A	120.00
C6A—C1A—C7A	118.9 (4)	C4B—C5B—H5B	120.00
C2A—C1A—C6A	120.0 (4)	C6B—C5B—H5B	120.00
C2B—C1B—C6B	120.1 (12)	C5A—C6A—H6A	120.00
C1A—C2A—C3A	120.0 (4)	C1A—C6A—H6A	120.00
C1B—C2B—C3B	120.0 (14)	C1B—C6B—H6B	120.00
C1B—C2B—C8B	118.3 (14)	C5B—C6B—H6B	120.00
C3B—C2B—C8B	121.7 (14)	C1A—C7A—H7A	116.00
C2A—C3A—C4A	120.0 (5)	C8A—C7A—H7A	116.00
C2B—C3B—C4B	119.8 (15)	C9—C7B—H7B	120.00
C3A—C4A—C5A	120.0 (5)	C8B—C7B—H7B	120.00
C3B—C4B—C5B	120.2 (15)	C7A—C8A—H8A	118.00
C4A—C5A—C6A	120.0 (4)	C9—C8A—H8A	118.00
C4B—C5B—C6B	120.0 (16)	C2B—C8B—H8B	117.00
C1A—C6A—C5A	120.0 (4)	C7B—C8B—H8B	117.00
C1B—C6B—C5B	119.9 (15)	C9—C10—H10C	110.00
C1A—C7A—C8A	127.9 (4)	C9—C10—H10B	109.00
C8B—C7B—C9	119.9 (17)	C9—C10—H10A	109.00
C7A—C8A—C9	124.3 (5)	H10B—C10—H10C	109.00
C2B—C8B—C7B	126.1 (17)	H10A—C10—H10B	109.00

C7B—C9—C10	94.8 (9)	H10A—C10—H10C	110.00
O1—C9—C10	110.5 (2)	H11A—C11—H11B	110.00
O1—C9—C7B	127.9 (8)	O3—C11—H11A	109.00
C8A—C9—C10	117.9 (3)	O3—C11—H11B	109.00
P1—C9—O1	104.7 (2)	O3—C11—H11C	109.00
P1—C9—C8A	110.6 (3)	H11A—C11—H11C	109.00
P1—C9—C10	110.1 (2)	H11B—C11—H11C	109.00
P1—C9—C7B	108.2 (7)	H12B—C12—H12C	109.00
O1—C9—C8A	102.1 (3)	O4—C12—H12A	109.00
C2B—C1B—H1B	120.00	O4—C12—H12B	109.00
C6B—C1B—H1B	120.00	O4—C12—H12C	109.00
C1A—C2A—H2A	120.00	H12A—C12—H12B	110.00
C3A—C2A—H2A	120.00	H12A—C12—H12C	109.00

O2—P1—O3—C11	50.8 (3)	C6A—C1A—C2A—C3A	0.0 (8)
O4—P1—O3—C11	−73.1 (2)	C7A—C1A—C2A—C3A	−179.3 (5)
C9—P1—O3—C11	175.7 (2)	C2A—C1A—C6A—C5A	0.1 (7)
O2—P1—O4—C12	28.4 (3)	C7A—C1A—C6A—C5A	179.3 (4)
O3—P1—O4—C12	153.1 (3)	C2A—C1A—C7A—C8A	8.7 (8)
C9—P1—O4—C12	−98.0 (3)	C6A—C1A—C7A—C8A	−170.6 (5)
O2—P1—C9—O1	−60.4 (2)	C1A—C2A—C3A—C4A	−0.1 (9)
O2—P1—C9—C8A	−169.6 (3)	C2A—C3A—C4A—C5A	0.1 (10)
O2—P1—C9—C10	58.4 (3)	C3A—C4A—C5A—C6A	−0.1 (9)
O3—P1—C9—O1	174.29 (18)	C4A—C5A—C6A—C1A	0.0 (8)
O3—P1—C9—C8A	65.1 (3)	C1A—C7A—C8A—C9	179.0 (4)
O3—P1—C9—C10	−67.0 (2)	C7A—C8A—C9—P1	−93.6 (6)
O4—P1—C9—O1	65.8 (2)	C7A—C8A—C9—O1	155.5 (5)
O4—P1—C9—C8A	−43.4 (3)	C7A—C8A—C9—C10	34.2 (7)
O4—P1—C9—C10	−175.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.90	2.721 (3)	176
C6*B*—H6*B*···*Cg*1^{ii}	0.93	2.83	3.568 (17)	137
C6*B*—H6*B*···*Cg*2^{ii}	0.93	2.94	3.652 (17)	134

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1/2, *y*+1/2, −*z*+1/2.