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5-Bromo-5-bromomethyl-2-phenoxy-1,3,2-dioxaphosphorinan-2-one

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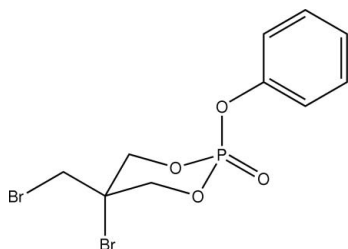
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.047; wR factor = 0.142; data-to-parameter ratio = 24.4.

In the title 1,3,2-dioxaphosphorinane derivative, $\text{C}_{10}\text{H}_{11}\text{Br}_2\text{O}_4\text{P}$, the 1,3,2-dioxaphosphorinane ring adopts a chair conformation, having the $\text{P}=\text{O}$ bond equatorially oriented and the phenoxy group axially oriented. The bromo substituent is in an axial position opposite to the phenoxy group and the bromomethyl group is in an equatorial position opposite to the $\text{P}=\text{O}$ bond. In the crystal packing, molecules are linked through weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Br}$ interactions to form chains along the b axis. The chains are arranged into sheets parallel to the ab plane. In adjacent sheets, molecules are arranged in an antiparallel fashion. Intermolecular $\text{C}-\text{H}\cdots\pi$ interactions are also observed.

Related literature

For values of bond lengths and angles, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For ring conformations, see: Cremer & Pople (1975). For related structures, see, for example: Jones *et al.* (1984); Polozov *et al.* (1995). For related literature and applications of dioxaphosphorinane derivatives, see, for example: Goswami (1993); Goswami & Adak (2002); Pilato *et al.* (1991); Taylor & Goswami (1992).



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Experimental

Crystal data

$\text{C}_{10}\text{H}_{11}\text{Br}_2\text{O}_4\text{P}$
 $M_r = 385.96$
 Monoclinic, $P2_1/c$
 $a = 12.1315$ (3) Å
 $b = 6.3095$ (1) Å
 $c = 16.8901$ (3) Å
 $\beta = 92.196$ (2)°
 $V = 1291.88$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 6.40$ mm⁻¹
 $T = 296$ (2) K
 $0.45 \times 0.10 \times 0.05$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.156$, $T_{\max} = 0.726$
 16007 measured reflections
 3756 independent reflections
 1952 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.072$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.142$
 $S = 0.99$
 3756 reflections
 154 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.67$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.91$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the phenyl ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}2-\text{H}2\text{A}\cdots\text{O}3^{\text{i}}$	0.97	2.35	3.217 (6)	148
$\text{C}4-\text{H}4\text{A}\cdots\text{O}3^{\text{i}}$	0.97	2.53	3.362 (6)	144
$\text{C}2-\text{H}2\text{B}\cdots\text{C}g1^{\text{ii}}$	0.97	2.81	3.755 (5)	166
$\text{C}3-\text{H}3\text{C}\cdots\text{C}g1^{\text{iii}}$	0.97	2.70	3.560 (5)	148

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 2, -y + 1, -z$.

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: SAINT (Bruker, 2005); program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2349).

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supporting information

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5-Bromo-5-bromomethyl-2-phenoxy-1,3,2-dioxaphosphorinan-2-one

Hoong-Kun Fun, Suchada Chantrapromma, Avijit Kr. Adak, Annada C. Maity and Shyamaprosad Goswami

S1. Comment

Six-membered cyclic phosphates are important constituents present in a number of biologically important molecules *e.g.* cyclic adenosine monophosphate (cAMP) and the Compound Z, a precursor of the molybdenum cofactor (Moco) (Goswami, 1993). They especially play key roles in many biosynthetic pathways and comprise structural sub-units of many physiologically important materials. In our synthetic studies (Pilato *et al.*, 1991; Taylor & Goswami, 1992) on the molybdenum cofactor, we are interested to have an efficient synthesis of cyclic dihydroxyacetone phosphate (CDHAP) (Goswami & Adak, 2002). Reaction of phosphate triesters with *N*-bromosuccinimide (NBS) results in the formation of a dibromo derivative (Fig. 1).

In the title 1,3,2-dioxaphosphorinane derivative (Fig. 1), C₁₀H₁₁Br₂O₄P, the 1,3,2-dioxaphosphorinane ring adopts a slightly flattened chair conformation with the puckering parameter (Cremer & Pople, 1975) $Q = 0.496$ (4) Å, $\theta = 7.4$ (5)° and $\varphi = 177$ (4)°, having the P=O bond equatorially attached and the phenoxy substituent axially attached with the torsion angle O1—P1—O4—O5 = 82.6 (4)°. The orientation of the phenoxy group is not co-planar to the 1,3,2-dioxaphosphorinane ring as can be indicated by the torsion angle P1—O4—C5—C6 of -108.2 (4)°. The bromo substituent is in the opposite axial position to the phenoxy substituent and the methylbromo group is in an opposite equatorial position to the P=O bond. The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and are comparable to related structures (Jones *et al.*, 1984; Polozov *et al.*, 1995). The closest Br···Br distance is 3.5484 (9) Å.

In the crystal packing shown in Fig. 2, the molecules are linked through weak C—H···O interactions (Table 1) to form chains along the *b* axis which generate *S*(6) ring motifs (Bernstein *et al.*, 1995). The chains are arranged into sheets parallel to the *ab* plane. In the adjacent sheets, the molecules are arranged in an anti-parallel fashion (Fig. 3). The adjacent sheets are connected through weak C—H···O interactions (Table 1) and Br···Br short contacts with the Br···Br distance of 3.8771 (9) Å (symmetry code: 1 - *x*, 1/2 + *y*, 1/2 - *z*). The crystal is stabilized by weak C—H···O, C—H···Br interactions and C—H··· π interactions (Table 1); *Cg*1 is the centroid of the C5—C10 ring.

S2. Experimental

A solution of 5-methylene-2-oxo-2-phenoxy-[1,3,2]-dioxaphosphorinane (0.4 g, 1.76 mmol), doubly crystallized *N*-bromosuccinimide (0.38 g, 1.78 mmol) and azobisisobutyronitrile (10 mg) in dry CCl₄ (40 ml) was heated under reflux in the presence of a 60 W lamp for 4 h. By this time, a maximum of 80% of the starting materials were converted into the product. Upon prolonged heating for a period of 8 h, no improvement has been observed with respect to yield nor new spot was observed as monitored by thin layer chromatography. The CCl₄ layer was then stripped off and the gummy material was dissolved in dichloromethane (100 ml) and washed well with water (2 × 100 ml) and then with brine. The organic layer was dried (Na₂SO₄) and concentrated to afford the crude product as a light brown gum which was passed through a silica gel (100–200 mesh) column eluting with dichloromethane to get the pure title compound as a white

crystalline solid (0.32 g, 60%; m.p. 361–362 K).

S3. Refinement

All H atoms were constrained in a riding motion approximation, with $C_{\text{aryl}}\text{—H} = 0.93 \text{ \AA}$ and 0.97 \AA for CH_2 . The $U_{\text{iso}}(\text{H})$ values were constrained to be $1.2U_{\text{eq}}$ of the carrier atom. The highest residual electron density peak is located at 0.72 \AA from Br1 and the deepest hole is located at 0.61 \AA from Br2.

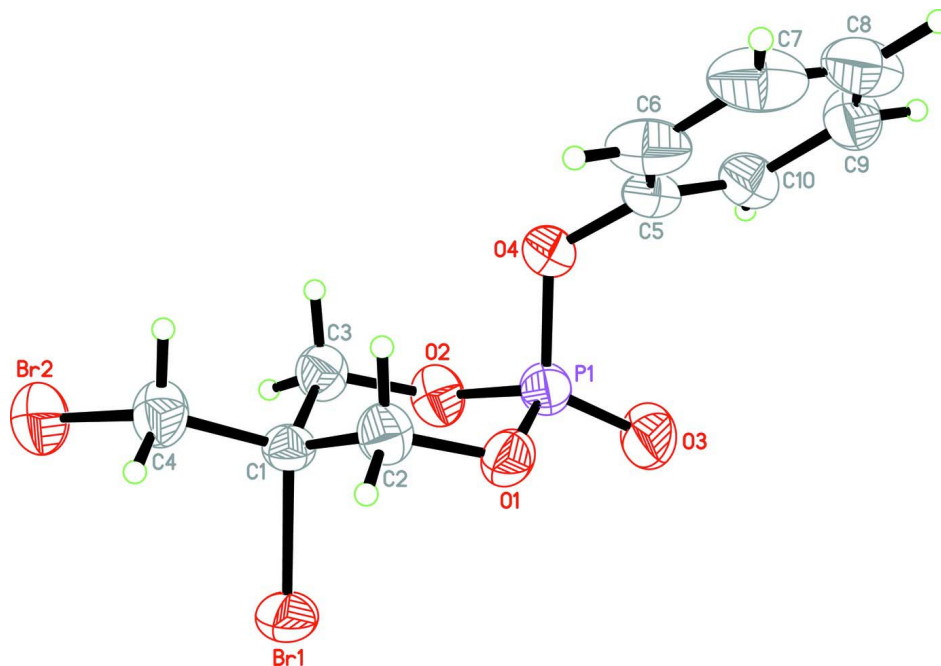


Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

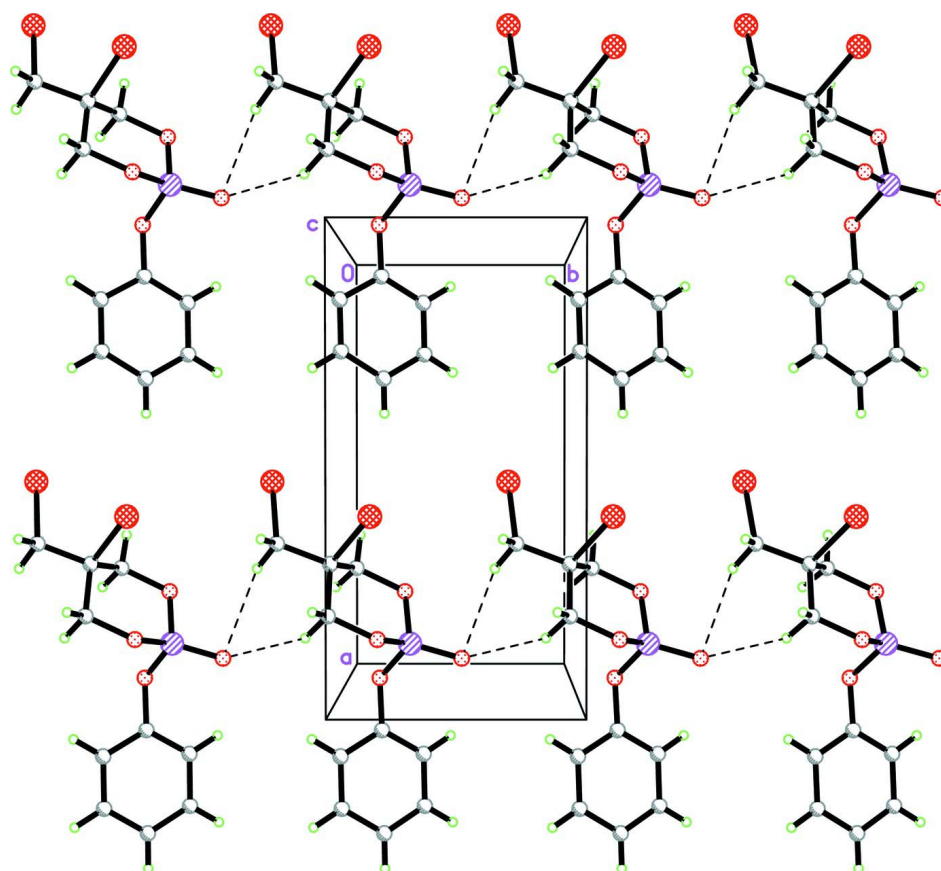


Figure 2

The crystal packing of (I), viewed along the *c* axis showing chains along the *b* axis. Hydrogen bonds were shown as dash lines.

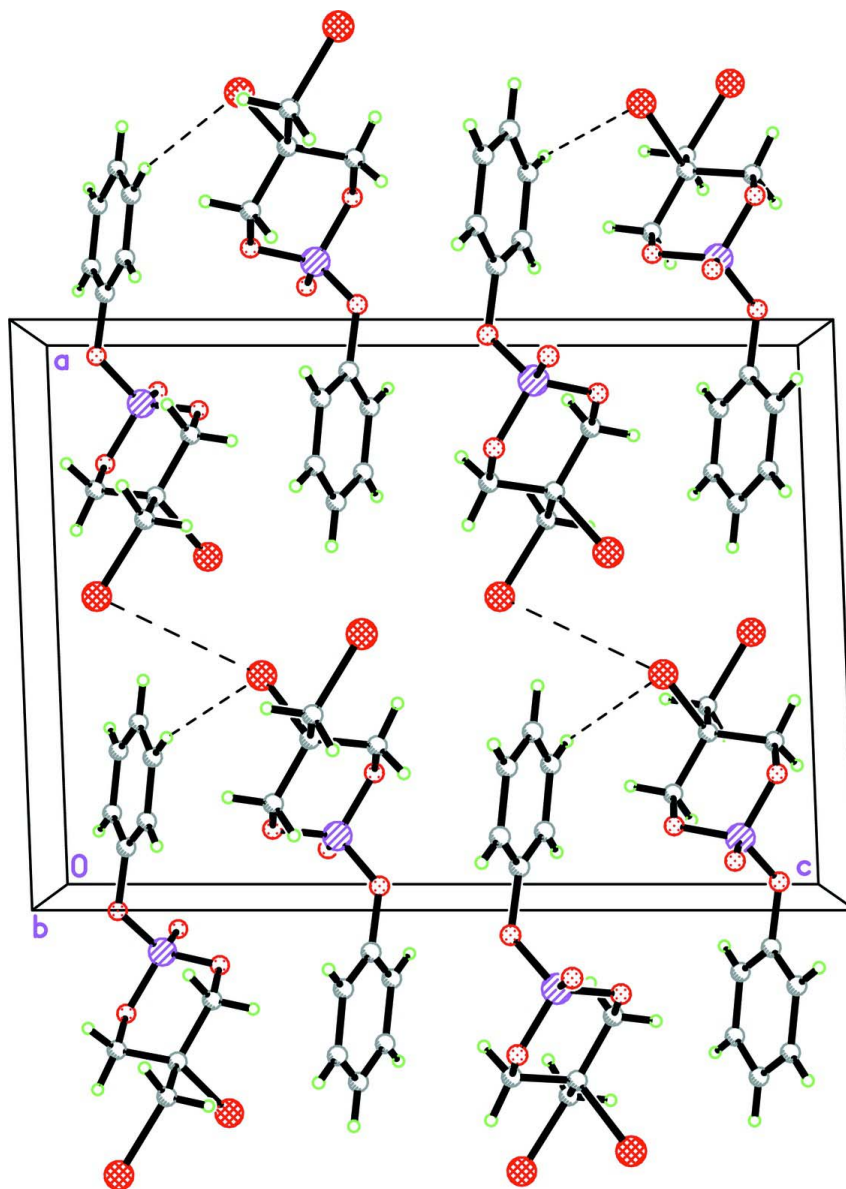


Figure 3

The crystal packing of (I), viewed along the *b* axis showing the anti-parallel arrangement of the adjacent sheets. Hydrogen bonds and Br...Br short contact were shown as dash lines.

5-Bromo-5-bromomethyl-2-phenoxy-1,3,2-dioxaphosphorinan-2-one

Crystal data

$C_{10}H_{11}Br_2O_4P$

$M_r = 385.96$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 12.1315\ (3)\ \text{\AA}$

$b = 6.3095\ (1)\ \text{\AA}$

$c = 16.8901\ (3)\ \text{\AA}$

$\beta = 92.196\ (2)^\circ$

$V = 1291.88\ (4)\ \text{\AA}^3$

$Z = 4$

$F(000) = 752$

$D_x = 1.984\ \text{Mg m}^{-3}$

Melting point = 361–362 K

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3756 reflections

$\theta = 2.4\text{--}30.0^\circ$

$\mu = 6.40 \text{ mm}^{-1}$
 $T = 296 \text{ K}$

Needle, colourless
 $0.45 \times 0.10 \times 0.05 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: $8.33 \text{ pixels mm}^{-1}$
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\min} = 0.156$, $T_{\max} = 0.726$

16007 measured reflections
 3756 independent reflections
 1952 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.072$
 $\theta_{\max} = 30.0^\circ$, $\theta_{\min} = 2.4^\circ$
 $h = -15 \rightarrow 17$
 $k = -8 \rightarrow 8$
 $l = -22 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.142$
 $S = 0.99$
 3756 reflections
 154 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
 $w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.3299P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.67 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.91 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.60424 (5)	0.36096 (9)	0.21315 (3)	0.0610 (2)
Br2	0.53167 (5)	0.78769 (10)	0.08461 (4)	0.0719 (2)
P1	0.88523 (11)	0.20179 (19)	0.12969 (8)	0.0438 (3)
O1	0.8686 (3)	0.3316 (5)	0.20749 (18)	0.0463 (8)
O2	0.7744 (3)	0.2261 (5)	0.0802 (2)	0.0495 (8)
O3	0.9159 (3)	-0.0157 (5)	0.1448 (3)	0.0677 (11)
O4	0.9665 (3)	0.3340 (5)	0.0784 (2)	0.0504 (8)
C1	0.7093 (4)	0.5327 (6)	0.1542 (3)	0.0376 (10)
C2	0.8186 (4)	0.5375 (7)	0.2016 (3)	0.0443 (11)
H2A	0.8687	0.6340	0.1764	0.053*
H2B	0.8063	0.5908	0.2544	0.053*
C3	0.7229 (4)	0.4330 (7)	0.0740 (3)	0.0453 (11)
H3B	0.6511	0.4192	0.0472	0.054*

H3C	0.7677	0.5250	0.0422	0.054*
C4	0.6653 (4)	0.7573 (7)	0.1467 (3)	0.0519 (13)
H4A	0.7214	0.8449	0.1235	0.062*
H4B	0.6535	0.8115	0.1994	0.062*
C5	1.0807 (4)	0.3235 (7)	0.0921 (3)	0.0408 (11)
C6	1.1335 (5)	0.4950 (9)	0.1258 (3)	0.0619 (15)
H6A	1.0939	0.6132	0.1413	0.074*
C7	1.2469 (6)	0.4884 (12)	0.1362 (3)	0.077 (2)
H7A	1.2841	0.6040	0.1585	0.092*
C8	1.3055 (5)	0.3123 (14)	0.1139 (3)	0.077 (2)
H8A	1.3817	0.3087	0.1217	0.092*
C9	1.2510 (5)	0.1428 (10)	0.0803 (3)	0.0640 (16)
H9A	1.2904	0.0241	0.0651	0.077*
C10	1.1368 (4)	0.1479 (8)	0.0688 (3)	0.0494 (12)
H10A	1.0993	0.0336	0.0458	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0439 (3)	0.0719 (4)	0.0680 (4)	-0.0032 (3)	0.0128 (3)	0.0258 (3)
Br2	0.0560 (4)	0.0786 (4)	0.0810 (5)	0.0177 (3)	0.0001 (3)	0.0093 (3)
P1	0.0372 (7)	0.0360 (6)	0.0585 (8)	-0.0025 (5)	0.0049 (6)	0.0049 (5)
O1	0.0419 (19)	0.0494 (18)	0.0472 (19)	0.0009 (15)	-0.0047 (15)	0.0109 (14)
O2	0.048 (2)	0.0423 (17)	0.058 (2)	0.0006 (15)	-0.0007 (17)	-0.0115 (15)
O3	0.056 (2)	0.0374 (18)	0.110 (3)	0.0033 (17)	0.011 (2)	0.0135 (19)
O4	0.0383 (19)	0.0516 (19)	0.062 (2)	0.0020 (15)	0.0096 (16)	0.0124 (16)
C1	0.038 (3)	0.035 (2)	0.040 (2)	-0.0041 (19)	0.006 (2)	0.0020 (18)
C2	0.041 (3)	0.047 (3)	0.044 (3)	0.001 (2)	-0.003 (2)	-0.004 (2)
C3	0.040 (3)	0.052 (3)	0.043 (3)	0.001 (2)	-0.005 (2)	0.000 (2)
C4	0.044 (3)	0.041 (3)	0.070 (4)	-0.001 (2)	-0.002 (3)	-0.001 (2)
C5	0.039 (3)	0.046 (3)	0.037 (2)	-0.007 (2)	0.008 (2)	0.0027 (19)
C6	0.076 (4)	0.056 (3)	0.055 (3)	-0.022 (3)	0.020 (3)	-0.009 (3)
C7	0.082 (5)	0.097 (5)	0.050 (3)	-0.048 (4)	-0.001 (3)	-0.007 (3)
C8	0.048 (4)	0.137 (6)	0.045 (3)	-0.029 (4)	-0.008 (3)	0.022 (4)
C9	0.049 (3)	0.088 (4)	0.055 (3)	0.010 (3)	0.004 (3)	0.014 (3)
C10	0.043 (3)	0.058 (3)	0.048 (3)	-0.005 (2)	0.004 (2)	-0.003 (2)

Geometric parameters (Å, °)

Br1—C1	1.971 (4)	C3—H3C	0.9700
Br2—C4	1.907 (5)	C4—H4A	0.9700
P1—O3	1.442 (4)	C4—H4B	0.9700
P1—O2	1.563 (4)	C5—C10	1.365 (7)
P1—O1	1.568 (3)	C5—C6	1.371 (7)
P1—O4	1.576 (3)	C6—C7	1.380 (9)
O1—C2	1.436 (5)	C6—H6A	0.9300
O2—C3	1.450 (6)	C7—C8	1.380 (10)
O4—C5	1.398 (6)	C7—H7A	0.9300

C1—C3	1.509 (6)	C8—C9	1.369 (9)
C1—C4	1.518 (6)	C8—H8A	0.9300
C1—C2	1.523 (6)	C9—C10	1.392 (8)
C2—H2A	0.9700	C9—H9A	0.9300
C2—H2B	0.9700	C10—H10A	0.9300
C3—H3B	0.9700		
O3—P1—O2	113.5 (2)	H3B—C3—H3C	107.9
O3—P1—O1	112.9 (2)	C1—C4—Br2	115.4 (3)
O2—P1—O1	105.14 (18)	C1—C4—H4A	108.4
O3—P1—O4	116.0 (2)	Br2—C4—H4A	108.4
O2—P1—O4	101.35 (19)	C1—C4—H4B	108.4
O1—P1—O4	106.73 (19)	Br2—C4—H4B	108.4
C2—O1—P1	118.8 (3)	H4A—C4—H4B	107.5
C3—O2—P1	119.1 (3)	C10—C5—C6	122.0 (5)
C5—O4—P1	121.4 (3)	C10—C5—O4	119.5 (4)
C3—C1—C4	111.3 (4)	C6—C5—O4	118.4 (5)
C3—C1—C2	110.9 (4)	C5—C6—C7	118.5 (6)
C4—C1—C2	108.8 (4)	C5—C6—H6A	120.8
C3—C1—Br1	108.6 (3)	C7—C6—H6A	120.8
C4—C1—Br1	108.9 (3)	C8—C7—C6	120.7 (6)
C2—C1—Br1	108.2 (3)	C8—C7—H7A	119.6
O1—C2—C1	112.0 (4)	C6—C7—H7A	119.6
O1—C2—H2A	109.2	C9—C8—C7	119.8 (6)
C1—C2—H2A	109.2	C9—C8—H8A	120.1
O1—C2—H2B	109.2	C7—C8—H8A	120.1
C1—C2—H2B	109.2	C8—C9—C10	120.1 (6)
H2A—C2—H2B	107.9	C8—C9—H9A	120.0
O2—C3—C1	111.8 (4)	C10—C9—H9A	120.0
O2—C3—H3B	109.3	C5—C10—C9	118.9 (5)
C1—C3—H3B	109.3	C5—C10—H10A	120.5
O2—C3—H3C	109.3	C9—C10—H10A	120.5
C1—C3—H3C	109.3		
O3—P1—O1—C2	-168.7 (3)	C2—C1—C3—O2	53.4 (5)
O2—P1—O1—C2	-44.4 (4)	Br1—C1—C3—O2	-65.5 (4)
O4—P1—O1—C2	62.7 (4)	C3—C1—C4—Br2	54.6 (5)
O3—P1—O2—C3	168.0 (3)	C2—C1—C4—Br2	177.1 (3)
O1—P1—O2—C3	44.1 (4)	Br1—C1—C4—Br2	-65.2 (4)
O4—P1—O2—C3	-66.9 (4)	P1—O4—C5—C10	74.5 (5)
O3—P1—O4—C5	-44.2 (4)	P1—O4—C5—C6	-108.2 (4)
O2—P1—O4—C5	-167.6 (3)	C10—C5—C6—C7	0.0 (8)
O1—P1—O4—C5	82.6 (4)	O4—C5—C6—C7	-177.3 (4)
P1—O1—C2—C1	52.5 (5)	C5—C6—C7—C8	-0.6 (9)
C3—C1—C2—O1	-54.0 (5)	C6—C7—C8—C9	0.7 (9)
C4—C1—C2—O1	-176.7 (4)	C7—C8—C9—C10	-0.2 (9)
Br1—C1—C2—O1	65.1 (4)	C6—C5—C10—C9	0.4 (7)
P1—O2—C3—C1	-52.0 (5)	O4—C5—C10—C9	177.7 (4)

C4—C1—C3—O2

174.6 (4)

C8—C9—C10—C5

-0.4 (8)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C2—H2 <i>A</i> \cdots O3 ⁱ	0.97	2.35	3.217 (6)	148
C3—H3 <i>B</i> \cdots Br2	0.97	2.82	3.233 (5)	106
C4—H4 <i>A</i> \cdots O3 ⁱ	0.97	2.53	3.362 (6)	144
C2—H2 <i>B</i> \cdots Cg1 ⁱⁱ	0.97	2.81	3.755 (5)	166
C3—H3 <i>C</i> \cdots Cg1 ⁱⁱⁱ	0.97	2.70	3.560 (5)	148

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+2, y+1/2, -z+1/2$; (iii) $-x+2, -y+1, -z$.