

Crystal structure of dimethyl 2,5-bis[(diphenoxyphosphoryl)oxy]cyclohexa-1,4-diene-1,4-dicarboxylate

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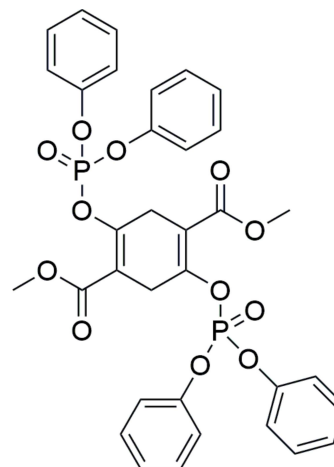
In the title compound, $C_{34}H_{30}O_{12}P_2$, which was synthesized *via* the esterification of dimethyl 2,5-dioxo-1,4-cyclohexanedicarboxylate with diphenyl chlorophosphate, the molecule has crystallographic inversion symmetry. The dihedral angles between the plane of the cyclohexa-1,4-diene ring and those of the two benzene rings of the substituent phosphate groups are 41.0 (1) and 89.5 (1)°, while that with the ester group is 3.1 (3)°. In the crystal, only weak intermolecular C—H...O hydrogen bonds are present.

Keywords: crystal structure; cyclohexa-1,4-diene; C—H...O hydrogen bonds.

CCDC reference: 1057648

1. Related literature

For background information on cyclohexa-1,4-dienes, see: El-Rayyes & Al-Hajjar (1978). For the synthesis of the title compound, see: Chaignaud *et al.* (2008).



2. Experimental

2.1. Crystal data

$C_{34}H_{30}O_{12}P_2$	$V = 1574 (2) \text{ \AA}^3$
$M_r = 692.52$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.272 (10) \text{ \AA}$	$\mu = 0.21 \text{ mm}^{-1}$
$b = 10.629 (8) \text{ \AA}$	$T = 113 \text{ K}$
$c = 13.174 (10) \text{ \AA}$	$0.20 \times 0.18 \times 0.12 \text{ mm}$
$\beta = 113.644 (10)^\circ$	

2.2. Data collection

Rigaku Saturn724 CCD diffractometer	15948 measured reflections
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 2005)	3758 independent reflections
$T_{\min} = 0.960$, $T_{\max} = 0.976$	2264 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.100$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	218 parameters
$wR(F^2) = 0.099$	H-atom parameters constrained
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.54 \text{ e \AA}^{-3}$
3758 reflections	$\Delta\rho_{\text{min}} = -0.62 \text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C6-H6\cdots O3^i$	0.95	2.50	3.345 (4)	148
$C9-H9\cdots O5^{ii}$	0.95	2.59	3.405 (4)	144
$C10-H10\cdots O3^{iii}$	0.95	2.46	3.381 (4)	163
$C15-H15B\cdots O1^{iv}$	0.99	2.56	3.409 (4)	144

Symmetry codes: (i) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $x + 1, -y + \frac{3}{2}, z + \frac{1}{2}$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2005).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: ZS2331).

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supporting information

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Crystal structure of dimethyl 2,5-bis[(diphenoxyphosphoryl)oxy]cyclohexa-1,4-diene-1,4-dicarboxylate

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S1. Comment

1,4-Cyclohexadiene is a useful and fundamental structural motif found in a wide range of organic materials and biologically active molecules (El-Rayyes & Al-Hajjar, 1978). The synthetic routes for the preparation of derivatives of this parent compound have been reported (Chaignaud *et al.*, 2008) but their crystal structures were not described.

The title compound, C₃₄H₃₀O₁₂P₂, was synthesized by the esterification of dimethyl 2,5-dioxo-1,4-cyclohexanedicarboxylate with diphenyl chlorophosphate using the reported procedure of Chaignaud *et al.* (2008) and the structure is reported herein.

The molecule of the title compound has crystallographic inversion symmetry (Fig. 1), with dihedral angles between the cyclohexa-1,4-diene ring and the two benzene rings of the substituent phosphate group of 41.0 (1) [C1–C6] and 89.5 (1)° [C7–C12]. The ester group is essentially coplanar with the cyclohexadiene group [dihedral angle = 3.1 (3)°]. In the crystal, only weak intermolecular C—H⋯O hydrogen bonds are present (Table 1).

S2. Experimental

The title compound was synthesized using the basic procedure of Chaignaud *et al.* (2008) (Fig. 2), as follows: A solution of LiHMDS (1 M in THF, 7.9 mL) in THF (20 mL) was cooled to -78 °C under nitrogen. Subsequently, a mixture of dimethyl 2,5-dioxo-1,4-cyclohexanedicarboxylate (3.19 mmol), diphenyl chlorophosphate (6.67 mmol) and HMPA (8.90 mmol) in anhydrous THF (5 mL) were added dropwise over 5 min. The mixture was stirred at -78 °C for 1h under nitrogen and after completion of the reaction, the mixture was diluted with water (30 mL) and extracted with ethyl acetate (3×15 mL), dried with anhydrous MgSO₄ and filtered. Subsequently, the product obtained by evaporation of the solvent was recrystallized from ethyl acetate giving a white solid in 10% yield (m.p. 118–120 °C).

S3. Refinement

H atoms were positioned geometrically and refined using a riding model with C—H = 0.95–0.99 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ (aromatic) or $1.5U_{\text{eq}}(\text{C})$ (methyl).

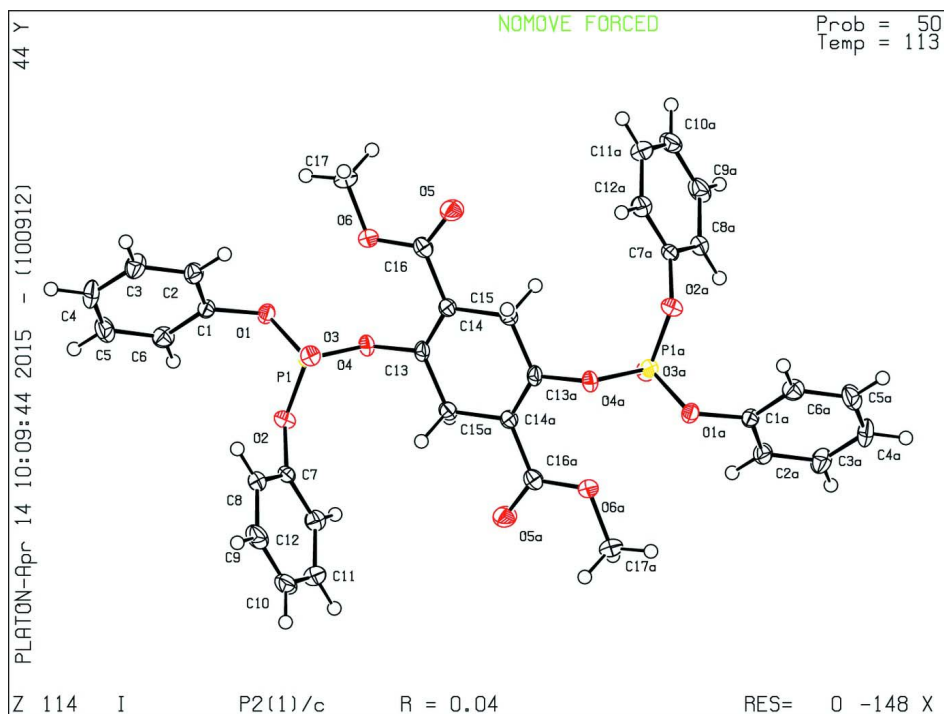


Figure 1

The molecular conformation and atom numbering scheme for the title compound, with probability ellipsoids drawn at the 50% level. For symmetry code (a): $-x, -y + 1, -z$.

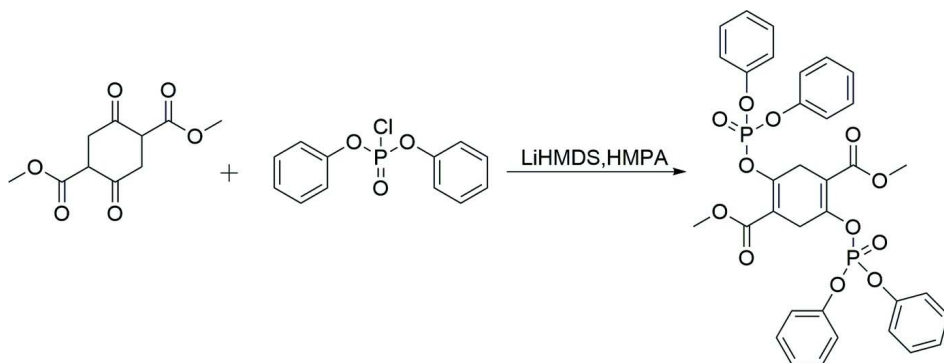


Figure 2

Synthetic route for the title compound.

Dimethyl 2,5-bis[(diphenoxyphosphoryl)oxy]cyclohexa-1,4-diene-1,4-dicarboxylate

Crystal data

$C_{34}H_{30}O_{12}P_2$

$M_r = 692.52$

Monoclinic, $P2_1/c$

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

$a = 12.272$ (10) Å

$b = 10.629$ (8) Å

$c = 13.174$ (10) Å

$\beta = 113.644$ (10)°

$V = 1574$ (2) Å³

$Z = 2$

$F(000) = 720$

$D_x = 1.461$ Mg m⁻³

Melting point = 391–393 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5446 reflections

$\theta = 1.7$ – 28.3 °

$\mu = 0.21 \text{ mm}^{-1}$
 $T = 113 \text{ K}$

Prism, colorless
 $0.20 \times 0.18 \times 0.12 \text{ mm}$

Data collection

Rigaku Saturn724 CCD
 diffractometer
 Radiation source: rotating anode
 Multilayer monochromator
 Detector resolution: $14.22 \text{ pixels mm}^{-1}$
 ω and φ scans
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2005)
 $T_{\min} = 0.960$, $T_{\max} = 0.976$

15948 measured reflections
 3758 independent reflections
 2264 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.100$
 $\theta_{\max} = 28.0^\circ$, $\theta_{\min} = 1.8^\circ$
 $h = -16 \rightarrow 16$
 $k = -13 \rightarrow 13$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.099$
 $S = 1.00$
 3758 reflections
 218 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
 $w = 1/[\sigma^2(F_o^2) + (0.012P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.62 \text{ e } \text{\AA}^{-3}$

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
P1	0.17401 (5)	0.72276 (5)	0.24500 (4)	0.01714 (15)
O1	0.12748 (11)	0.81381 (12)	0.31240 (10)	0.0189 (3)
O2	0.26861 (12)	0.64338 (12)	0.34149 (11)	0.0211 (3)
O3	0.21532 (12)	0.77428 (12)	0.16508 (10)	0.0194 (3)
O4	0.06126 (12)	0.63451 (12)	0.19634 (10)	0.0187 (3)
O5	-0.16106 (13)	0.79217 (13)	-0.10725 (11)	0.0285 (4)
O6	-0.06056 (12)	0.82652 (13)	0.07360 (11)	0.0259 (4)
C1	0.20189 (18)	0.91573 (18)	0.36916 (16)	0.0181 (5)
C2	0.20083 (19)	1.02272 (19)	0.30979 (17)	0.0229 (5)
H2	0.1545	1.0266	0.2323	0.027*
C3	0.2684 (2)	1.1239 (2)	0.36526 (18)	0.0288 (6)
H3	0.2690	1.1986	0.3259	0.035*
C4	0.3353 (2)	1.1172 (2)	0.47791 (18)	0.0310 (6)

H4	0.3818	1.1873	0.5159	0.037*
C5	0.3350 (2)	1.0088 (2)	0.53572 (18)	0.0298 (6)
H5	0.3816	1.0046	0.6132	0.036*
C6	0.26714 (19)	0.90613 (19)	0.48111 (17)	0.0237 (5)
H6	0.2659	0.8313	0.5201	0.028*
C7	0.37059 (18)	0.58701 (19)	0.33647 (16)	0.0193 (5)
C8	0.45474 (17)	0.6591 (2)	0.31964 (15)	0.0221 (5)
H8	0.4432	0.7469	0.3063	0.027*
C9	0.55660 (19)	0.6006 (2)	0.32263 (17)	0.0294 (6)
H9	0.6158	0.6483	0.3105	0.035*
C10	0.5728 (2)	0.4722 (2)	0.34328 (17)	0.0317 (6)
H10	0.6431	0.4326	0.3455	0.038*
C11	0.4874 (2)	0.4024 (2)	0.36046 (17)	0.0290 (6)
H11	0.4987	0.3147	0.3747	0.035*
C12	0.38516 (19)	0.46028 (19)	0.35698 (17)	0.0247 (5)
H12	0.3256	0.4128	0.3687	0.030*
C13	0.02855 (17)	0.57494 (18)	0.09354 (16)	0.0173 (5)
C14	-0.04157 (18)	0.62776 (18)	-0.00080 (16)	0.0167 (5)
C15	-0.07850 (18)	0.55461 (17)	-0.10704 (15)	0.0186 (5)
H15A	-0.1664	0.5490	-0.1412	0.022*
H15B	-0.0532	0.6015	-0.1588	0.022*
C16	-0.09356 (18)	0.75651 (19)	-0.01748 (16)	0.0196 (5)
C17	-0.11425 (19)	0.95035 (18)	0.05728 (18)	0.0302 (6)
H17A	-0.0905	0.9985	0.0061	0.045*
H17B	-0.0876	0.9943	0.1286	0.045*
H17C	-0.2011	0.9420	0.0262	0.045*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0148 (3)	0.0166 (3)	0.0186 (3)	-0.0009 (2)	0.0052 (2)	-0.0017 (2)
O1	0.0177 (8)	0.0178 (8)	0.0225 (8)	-0.0025 (6)	0.0093 (7)	-0.0050 (6)
O2	0.0168 (8)	0.0239 (8)	0.0207 (8)	0.0035 (7)	0.0056 (7)	0.0029 (6)
O3	0.0193 (8)	0.0208 (8)	0.0194 (7)	-0.0011 (6)	0.0090 (7)	0.0005 (6)
O4	0.0166 (7)	0.0197 (8)	0.0182 (8)	-0.0054 (6)	0.0055 (6)	-0.0040 (6)
O5	0.0344 (9)	0.0248 (9)	0.0226 (8)	0.0067 (7)	0.0078 (8)	0.0036 (7)
O6	0.0235 (8)	0.0227 (8)	0.0258 (9)	0.0062 (7)	0.0038 (7)	-0.0043 (7)
C1	0.0165 (11)	0.0177 (11)	0.0200 (11)	-0.0006 (9)	0.0070 (9)	-0.0040 (9)
C2	0.0272 (13)	0.0221 (12)	0.0168 (11)	0.0012 (10)	0.0060 (10)	-0.0016 (9)
C3	0.0354 (14)	0.0208 (13)	0.0301 (13)	-0.0050 (11)	0.0131 (12)	-0.0028 (10)
C4	0.0334 (14)	0.0261 (14)	0.0310 (14)	-0.0123 (11)	0.0103 (12)	-0.0132 (11)
C5	0.0276 (13)	0.0379 (15)	0.0179 (12)	-0.0024 (11)	0.0029 (10)	-0.0045 (10)
C6	0.0271 (13)	0.0225 (13)	0.0217 (12)	0.0013 (10)	0.0101 (10)	0.0023 (10)
C7	0.0143 (11)	0.0238 (12)	0.0158 (11)	0.0044 (9)	0.0017 (9)	-0.0044 (9)
C8	0.0171 (11)	0.0216 (12)	0.0237 (12)	-0.0007 (10)	0.0041 (10)	-0.0038 (9)
C9	0.0161 (12)	0.0398 (15)	0.0307 (14)	-0.0035 (11)	0.0077 (11)	-0.0036 (11)
C10	0.0184 (12)	0.0442 (16)	0.0264 (13)	0.0096 (12)	0.0026 (11)	-0.0099 (11)
C11	0.0289 (13)	0.0248 (13)	0.0296 (13)	0.0069 (11)	0.0077 (11)	-0.0034 (11)

C12	0.0216 (12)	0.0228 (13)	0.0275 (12)	-0.0006 (10)	0.0074 (10)	-0.0010 (10)
C13	0.0147 (10)	0.0186 (11)	0.0189 (11)	-0.0052 (9)	0.0071 (9)	-0.0058 (9)
C14	0.0144 (10)	0.0169 (11)	0.0188 (11)	-0.0012 (9)	0.0066 (9)	-0.0009 (9)
C15	0.0154 (11)	0.0201 (12)	0.0182 (11)	-0.0005 (9)	0.0046 (9)	-0.0002 (9)
C16	0.0158 (11)	0.0240 (13)	0.0199 (11)	-0.0025 (9)	0.0079 (10)	0.0003 (9)
C17	0.0270 (13)	0.0246 (13)	0.0355 (14)	0.0094 (11)	0.0088 (12)	-0.0039 (11)

Geometric parameters (Å, °)

P1—O1	1.5677 (19)	C11—C12	1.382 (4)
P1—O2	1.5785 (19)	C13—C14	1.320 (3)
P1—O3	1.4469 (19)	C13—C15 ⁱ	1.489 (3)
P1—O4	1.579 (2)	C14—C15	1.503 (3)
O1—C1	1.421 (3)	C14—C16	1.489 (3)
O2—C7	1.413 (3)	C2—H2	0.9500
O4—C13	1.400 (3)	C3—H3	0.9500
O5—C16	1.201 (3)	C4—H4	0.9500
O6—C16	1.330 (3)	C5—H5	0.9500
O6—C17	1.449 (3)	C6—H6	0.9500
C1—C2	1.377 (3)	C8—H8	0.9500
C1—C6	1.371 (3)	C9—H9	0.9500
C2—C3	1.376 (3)	C10—H10	0.9500
C3—C4	1.380 (3)	C11—H11	0.9500
C4—C5	1.382 (3)	C12—H12	0.9500
C5—C6	1.386 (3)	C15—H15A	0.9900
C7—C8	1.374 (3)	C15—H15B	0.9900
C7—C12	1.371 (3)	C17—H17A	0.9800
C8—C9	1.383 (3)	C17—H17B	0.9800
C9—C10	1.390 (3)	C17—H17C	0.9800
C10—C11	1.375 (4)		
O1—P1—O2	101.02 (7)	O5—C16—C14	121.40 (18)
O1—P1—O3	119.47 (8)	O6—C16—C14	115.08 (17)
O1—P1—O4	97.92 (8)	C1—C2—H2	121.00
O2—P1—O3	115.41 (9)	C3—C2—H2	121.00
O2—P1—O4	104.54 (8)	C2—C3—H3	120.00
O3—P1—O4	115.79 (8)	C4—C3—H3	120.00
P1—O1—C1	117.75 (13)	C3—C4—H4	120.00
P1—O2—C7	124.62 (13)	C5—C4—H4	120.00
P1—O4—C13	121.73 (14)	C4—C5—H5	120.00
C16—O6—C17	114.76 (16)	C6—C5—H5	120.00
O1—C1—C2	118.23 (17)	C1—C6—H6	121.00
O1—C1—C6	118.96 (17)	C5—C6—H6	121.00
C2—C1—C6	122.74 (19)	C7—C8—H8	121.00
C1—C2—C3	118.52 (19)	C9—C8—H8	121.00
C2—C3—C4	120.2 (2)	C8—C9—H9	120.00
C3—C4—C5	120.3 (2)	C10—C9—H9	120.00
C4—C5—C6	120.3 (2)	C9—C10—H10	120.00

C1—C6—C5	118.03 (19)	C11—C10—H10	120.00
O2—C7—C8	120.56 (18)	C10—C11—H11	120.00
O2—C7—C12	117.1 (2)	C12—C11—H11	120.00
C8—C7—C12	122.2 (2)	C7—C12—H12	120.00
C7—C8—C9	118.3 (2)	C11—C12—H12	120.00
C8—C9—C10	120.3 (2)	C14—C15—H15A	109.00
C9—C10—C11	120.2 (2)	C14—C15—H15B	109.00
C10—C11—C12	119.8 (2)	H15A—C15—H15B	108.00
C7—C12—C11	119.3 (2)	C13 ⁱ —C15—H15A	109.00
O4—C13—C14	122.97 (18)	C13 ⁱ —C15—H15B	109.00
O4—C13—C15 ⁱ	110.99 (16)	O6—C17—H17A	109.00
C14—C13—C15 ⁱ	125.99 (18)	O6—C17—H17B	109.00
C13—C14—C15	119.73 (18)	O6—C17—H17C	109.00
C13—C14—C16	127.52 (18)	H17A—C17—H17B	109.00
C15—C14—C16	112.75 (16)	H17A—C17—H17C	109.00
C13 ⁱ —C15—C14	114.28 (16)	H17B—C17—H17C	109.00
O5—C16—O6	123.51 (19)		
O2—P1—O1—C1	75.66 (14)	C3—C4—C5—C6	-0.3 (4)
O3—P1—O1—C1	-52.09 (15)	C4—C5—C6—C1	0.4 (4)
O4—P1—O1—C1	-177.76 (12)	O2—C7—C8—C9	175.83 (17)
O1—P1—O2—C7	-151.58 (15)	C12—C7—C8—C9	0.6 (3)
O3—P1—O2—C7	-21.23 (17)	O2—C7—C12—C11	-175.66 (18)
O4—P1—O2—C7	107.15 (15)	C8—C7—C12—C11	-0.3 (3)
O1—P1—O4—C13	149.57 (14)	C7—C8—C9—C10	-0.6 (3)
O2—P1—O4—C13	-106.81 (14)	C8—C9—C10—C11	0.3 (3)
O3—P1—O4—C13	21.34 (17)	C9—C10—C11—C12	0.1 (3)
P1—O1—C1—C2	81.9 (2)	C10—C11—C12—C7	-0.1 (3)
P1—O1—C1—C6	-101.1 (2)	O4—C13—C14—C15	-176.33 (19)
P1—O2—C7—C8	59.5 (2)	O4—C13—C14—C16	2.7 (4)
P1—O2—C7—C12	-125.04 (17)	C15 ⁱ —C13—C14—C15	0.7 (4)
P1—O4—C13—C14	-88.2 (2)	C15 ⁱ —C13—C14—C16	179.7 (2)
P1—O4—C13—C15 ⁱ	94.39 (18)	O4—C13—C15 ⁱ —C14 ⁱ	176.67 (18)
C17—O6—C16—O5	1.1 (3)	C14—C13—C15 ⁱ —C14 ⁱ	-0.7 (3)
C17—O6—C16—C14	-178.27 (19)	C13—C14—C15—C13 ⁱ	-0.6 (3)
O1—C1—C2—C3	177.0 (2)	C16—C14—C15—C13 ⁱ	-179.77 (19)
C6—C1—C2—C3	0.2 (4)	C13—C14—C16—O5	-176.4 (2)
O1—C1—C6—C5	-177.2 (2)	C13—C14—C16—O6	2.9 (4)
C2—C1—C6—C5	-0.4 (4)	C15—C14—C16—O5	2.7 (3)
C1—C2—C3—C4	0.0 (4)	C15—C14—C16—O6	-177.98 (19)
C2—C3—C4—C5	0.1 (4)		

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O5 ⁱⁱ	0.95	2.56	3.191 (4)	124

C6—H6···O3 ⁱⁱⁱ	0.95	2.50	3.345 (4)	148
C9—H9···O5 ^{iv}	0.95	2.59	3.405 (4)	144
C10—H10···O3 ^v	0.95	2.46	3.381 (4)	163
C15—H15B···O1 ^{vi}	0.99	2.56	3.409 (4)	144

Symmetry codes: (ii) $-x, -y+2, -z$; (iii) $x, -y+3/2, z+1/2$; (iv) $x+1, -y+3/2, z+1/2$; (v) $-x+1, y-1/2, -z+1/2$; (vi) $x, -y+3/2, z-1/2$.