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# 9-{2-[Bis(pivaloyloxymethoxy)phosphinylmethoxy]ethyl}adenine dihydrate

**Ying Chang, Qi-Tai Zheng and Yang Lu***

Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, 1 Xiannong tan street, Beijing 100050, People's Republic of China

Correspondence e-mail: luy@imm.ac.cn

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**Key indicators**

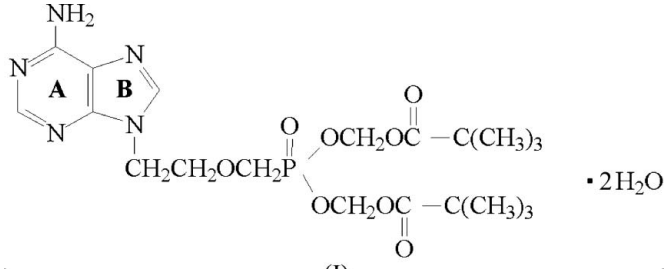
Single-crystal X-ray study
$T$ = 295 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.073
$wR$ factor = 0.146
Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{20}H_{32}N_5O_8P\cdot 2H_2O$, molecules are linked to each other *via* intermolecular N—H···O, N—H···N, O—H···O and O—H···N hydrogen bonds with the water molecules acting as both acceptors and donors.

## Comment

9-{2-[Bis(pivaloyloxymethoxy)phosphinylmethoxy]ethyl}adenine (common name adefovir dipivoxil) has been used to treat adults with chronic hepatitis B (Shepherd *et al.*, 2006). Recently, we obtained single crystals of the dihydrate of adefovir dipivoxil, (I), and determined its crystal structure.




(I)

In (I) (Fig.1), the adenine ring displays the expected planar conformation. The adefovir dipivoxil molecules are linked by an intermolecular N—H···N hydrogen bond and by O—H···O and O—H···N hydrogen-bonding interactions involving the water molecules which act as both acceptors and donors (Table 1 and Fig. 2).

## Experimental

The title compound was synthesized according to Yong *et al.* (2001). Single crystals of (I) were obtained from an ethanol–chloroform solution (1:1) after 10 d.

### *Crystal data*

$C_{20}H_{32}N_5O_8P\cdot 2H_2O$
$M_r$ = 537.51
Triclinic, $P\overline{1}$
$a$ = 6.0590 (12) Å
$b$ = 11.221 (2) Å
$c$ = 20.972 (4) Å
$\alpha$ = 93.88 (3)°
$\beta$ = 97.49 (3)°
$\gamma$ = 102.97 (3)°
$V$ = 1370.7 (5) Å$^3$
$Z$ = 2
$D_x$ = 1.302 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.16 mm$^{-1}$
$T$ = 295 (2) K
Block, colourless
0.60 × 0.40 × 0.40 mm

### *Data collection*

MAC DIP 2030K diffractometer
$\omega$ scans
Absorption correction: none
4874 measured reflections
4873 independent reflections
3870 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 25.5°

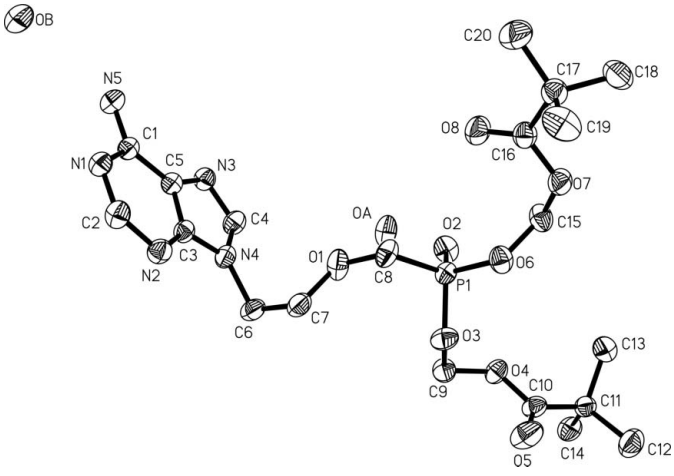



**Figure 1**
The molecular structure of (I), shown with 30% probability displacement ellipsoids. H atoms have been omitted.

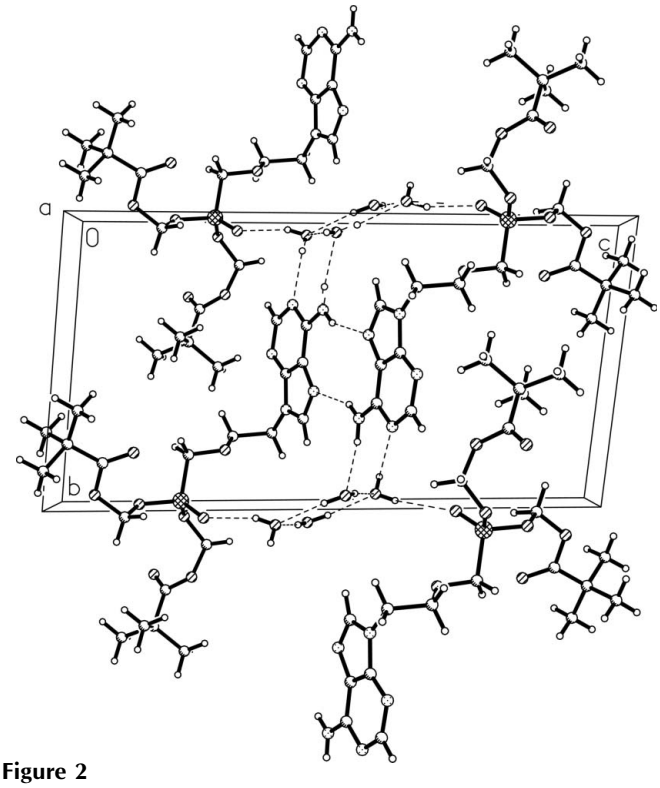



**Figure 2**
The molecular packing of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0129P)^2 + 3.1097P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.073$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.146$ | $\Delta\rho_{max} = 0.26$ e Å$^{-3}$ |
| $S = 1.01$ | $\Delta\rho_{min} = -0.37$ e Å$^{-3}$ |
| 4873 reflections | Extinction correction: *SHELXL97* |
| 338 parameters | Extinction coefficient: 0.0088 (10) |
| H atoms treated by a mixture of independent and constrained refinement | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5$A$···O$B$ | 0.86 | 2.10 | 2.945 (5) | 166 |
| N5—H5$B$···N3$^{i}$ | 0.86 | 2.18 | 2.988 (4) | 156 |
| O$A$—H1$A$···O2$^{ii}$ | 0.83 (3) | 2.008 (19) | 2.801 (4) | 160 (4) |
| O$A$—H1$B$···N1 | 0.82 (4) | 2.12 (3) | 2.867 (4) | 150 (5) |
| O$B$—H2$A$···O$A^{iii}$ | 0.83 (3) | 2.06 (4) | 2.867 (5) | 169 (5) |
| O$B$—H2$B$···O$A^{iv}$ | 0.82 (4) | 2.07 (3) | 2.882 (5) | 174 (6) |

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

The methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, allowed to rotate but not tip, and were refined using a riding model, with $U_{iso}$(H) = 1.5$U_{eq}$(C). The H atoms on water molecules were placed in idealized positions and their coordinates were refined with $U_{iso}$(H) = 1.5$U_{eq}$(O). All other H atoms were placed in geometrically idealized positions, with C—H = 0.92–0.98 Å and N—H = 0.86 Å, and refined in riding mode, with $U_{iso}$(H) = 1.2$U_{eq}$(C,N).

Data collection: *DENZO* (Otwinowski & Minor, 1997); cell refinement: *SCALE* (Otwinowski & Minor, 1997); data reduction: *SCALE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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