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# 2-Amino-4,6-dimethylpyrimidin-1-ium 1-oxo-2,6,7-trioxa-1$\lambda^5$-phosphabicyclo-[2.2.2]octane-4-carboxylate

**Xu-Feng Hou,* Gong-Chun Li and Peng-Yang Lai**

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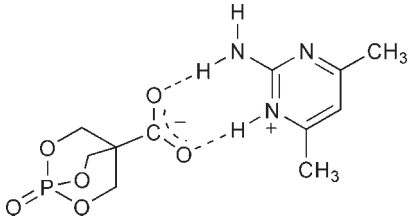
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.001 Å; $R$ factor = 0.039; $wR$ factor = 0.107; data-to-parameter ratio = 32.0.

In the title compound, $C_6H_{10}N_3^+\cdot C_5H_6O_6P^-$, the cation and anion are linked by pairs of N—H···O hydrogen bonds. There are additional intermolecular N—H···N hydrogen bonds., which generate centrosymmetric tetramers of two cations and two anions

## Related literature

For the applications of caged bicyclic phosphates, see: Li *et al.* (2000). For related structures, see: Meng *et al.* (2009); Guo & Zang (2008); Thakur & Desiraju (2008); Wang *et al.* (2007).



## Experimental

### Crystal data

$C_6H_{10}N_3^+\cdot C_5H_6O_6P^-$
$M_r$ = 317.24
Monoclinic, $P2_1/c$
$a$ = 9.5080 (13) Å
$b$ = 6.1870 (8) Å
$c$ = 23.974 (2) Å
$\beta$ = 99.611 (5)°
$V$ = 1390.5 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 113 K
0.24 × 0.22 × 0.14 mm

### Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2009)
$T_{min}$ = 0.947, $T_{max}$ = 0.969
23989 measured reflections
6532 independent reflections
4883 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
$S$ = 1.01
6532 reflections
204 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1 | 0.866 (15) | 1.907 (15) | 2.7719 (11) | 176.4 (14) |
| N1—H2···N3$^{i}$ | 0.900 (14) | 2.113 (15) | 3.0114 (12) | 176.3 (12) |
| N2—H3···O2 | 0.988 (15) | 1.738 (16) | 2.7170 (10) | 170.4 (15) |

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

Data collection: *CrystalClear-SM Expert* (Rigaku/MSC, 2009); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2009); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2308).

## References

Guo, M.-L. & Zang, H.-J. (2008). *Acta Cryst.* C**64**, m173–m175.
Li, X., Ou, Y.-X., Zhang, Y.-H. & Lian, D.-J. (2000). *Chin. Chem. Lett.* **11**, 887–890.
Meng, A.-L., Huang, J.-E., Zheng, B. & Li, Z.-J. (2009). *Acta Cryst.* E**65**, o1595.
Rigaku/MSC (2009). *CrystalClear-SM Expert* and *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Thakur, T. S. & Desiraju, G. R. (2008). *Cryst. Growth Des.* **8**, 4031–4044.
Wang, Z., Zang, H.-J. & Guo, M.-L. (2007). *Acta Cryst.* E**63**, o3418.

# supporting information

*Acta Cryst.* (2010). E**66**, o1528 [doi:10.1107/S1600536810019896]

## 2-Amino-4,6-dimethylpyrimidin-1-ium 1-oxo-2,6,7-trioxa-1$\lambda^5$-phosphabicyclo-[2.2.2]octane-4-carboxylate

**Xu-Feng Hou, Gong-Chun Li and Peng-Yang Lai**

### S1. Comment

Caged bicyclic phosphates are widely used as flame retardants or pesticides (Li *et al.* 2000). It can also serve as host–guest systems and have been studied in the context of hydrogen-bond patterns (Guo & Zang, 2008; Wang *et al.*, 2007). Aminopyrimidine derivatives are biologically important compounds as they occur in nature as components of nucleic acids (Meng *et al.*, 2009). The crystal structures of aminopyrimidine carboxylates have been reported (Thakur *et al.*, 2008). We report here the crystal structure of a new bicyclic phosphate cage compound.

In the title compound, $[C_6H_{10}N_3]^+$ $[C_5H_6O_6P]^-$, The cation and anion in the asymmetric unit are linked by N—H···O hydrogen bonds. There is also addition intermolecular N—H···N hydrogen bonds. (Fig. 2).

### S2. Experimental

The title compound was obtained by reaction of 1-oxo-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane-4-carboxylic acid (0.39 g, 0.2 mmol) and 2-amino-4,6-dimethylpyrimidine(0.25 g, 0.2 mmol) in refluxing acetone (50 ml). The solvent was evaporated *in vacuo*. The title compound was recrystallized from ethanol and single crystals of (I) were obtained by slow evaporation.

### S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.98 Å or 0.99 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}$(H) = 1.2Ueq(C).

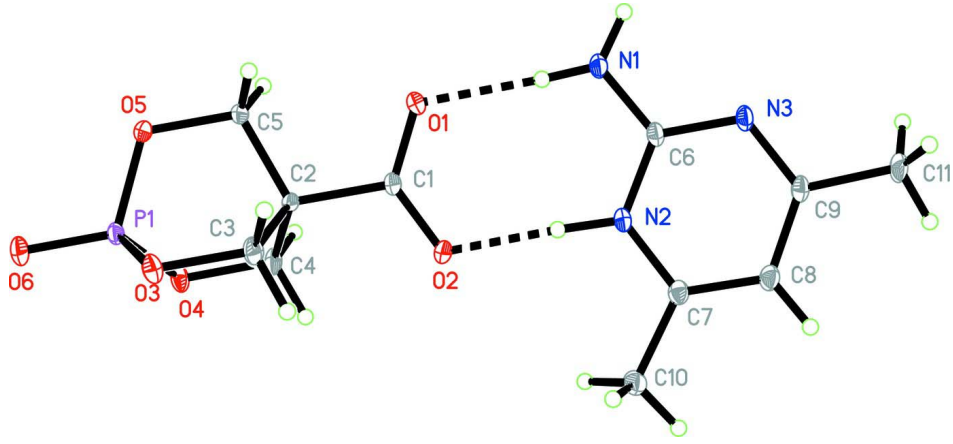


**Figure 1**

The asymmetric unit of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level.

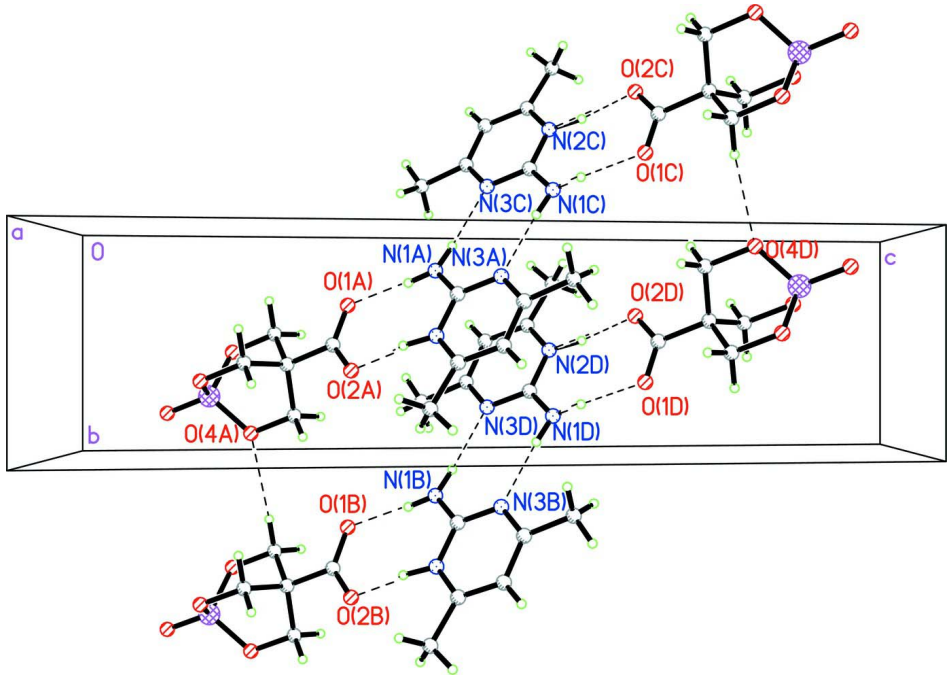


**Figure 2**

The packing diagram of the title compound. Intermolecular hydrogen bonds are shown as dashed line.

### 2-Amino-4,6-dimethylpyrimidin-1-ium 1-oxo-2,6,7-trioxa-1$\lambda^5$-phosphabicyclo[2.2.2]octane-4-carboxylate

*Crystal data*

$C_6H_{10}N_3^+ \cdot C_5H_6O_6P^-$
$M_r = 317.24$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.5080\ (13)$ Å
$b = 6.1870\ (8)$ Å
$c = 23.974\ (2)$ Å
$\beta = 99.611\ (5)°$
$V = 1390.5\ (3)$ Å$^3$
$Z = 4$

$F(000) = 664$
$D_x = 1.515$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 5985 reflections
$\theta = 2.2–36.3°$
$\mu = 0.23$ mm$^{-1}$
$T = 113$ K
Prism, colorless
0.24 × 0.22 × 0.14 mm

*Data collection*

Rigaku Saturn724 CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.222 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2009)
$T_{min} = 0.947$, $T_{max} = 0.969$

23989 measured reflections
6532 independent reflections
4883 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 36.5°$, $\theta_{min} = 1.7°$
$h = -15\rightarrow14$
$k = -10\rightarrow10$
$l = -36\rightarrow39$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.107$
$S = 1.01$
6532 reflections
204 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å$^{-3}$
$\Delta\rho_{min} = -0.38$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| P1 | 0.14090 (2) | 0.74372 (4) | 0.157866 (9) | 0.01584 (6) |
| O1 | 0.32415 (8) | 0.33013 (12) | 0.32735 (3) | 0.02813 (17) |
| O2 | 0.46621 (8) | 0.62093 (12) | 0.33500 (3) | 0.02544 (16) |
| O3 | 0.29862 (7) | 0.67033 (12) | 0.15596 (3) | 0.02097 (14) |
| O4 | 0.15812 (7) | 0.91396 (11) | 0.20765 (3) | 0.02023 (13) |
| O5 | 0.06923 (7) | 0.54214 (12) | 0.18168 (3) | 0.02421 (15) |
| O6 | 0.06557 (8) | 0.82445 (13) | 0.10419 (3) | 0.02619 (16) |
| N1 | 0.45629 (9) | 0.17785 (15) | 0.43177 (4) | 0.02312 (17) |
| N2 | 0.61028 (8) | 0.46847 (12) | 0.43466 (3) | 0.01702 (14) |
| N3 | 0.63811 (8) | 0.21010 (14) | 0.50821 (3) | 0.01949 (15) |
| C1 | 0.36366 (9) | 0.50774 (14) | 0.31115 (4) | 0.01674 (15) |
| C2 | 0.27993 (8) | 0.59650 (13) | 0.25498 (3) | 0.01332 (14) |
| C3 | 0.37600 (9) | 0.58891 (16) | 0.20974 (4) | 0.01990 (17) |
| H3A | 0.4621 | 0.6782 | 0.2219 | 0.024* |
| H3B | 0.4070 | 0.4383 | 0.2049 | 0.024* |
| C4 | 0.23414 (10) | 0.83103 (15) | 0.26188 (4) | 0.02018 (17) |
| H4A | 0.1711 | 0.8386 | 0.2908 | 0.024* |
| H4B | 0.3193 | 0.9214 | 0.2749 | 0.024* |
| C5 | 0.14789 (10) | 0.45860 (16) | 0.23533 (4) | 0.02254 (19) |
| H5A | 0.1769 | 0.3072 | 0.2302 | 0.027* |
| H5B | 0.0854 | 0.4605 | 0.2645 | 0.027* |
| C6 | 0.56840 (9) | 0.28450 (15) | 0.45830 (4) | 0.01698 (15) |
| C7 | 0.72567 (10) | 0.58213 (15) | 0.45997 (4) | 0.01896 (16) |
| C8 | 0.79892 (10) | 0.51036 (16) | 0.51086 (4) | 0.02109 (17) |

| | | | | |
|---|---|---|---|---|
| H8 | 0.8792 | 0.5871 | 0.5300 | 0.025* |
| C9 | 0.75166 (10) | 0.32090 (16) | 0.53356 (4) | 0.01951 (17) |
| C10 | 0.76334 (12) | 0.77807 (16) | 0.42947 (5) | 0.0264 (2) |
| H10A | 0.8040 | 0.7342 | 0.3962 | 0.032* |
| H10B | 0.8334 | 0.8642 | 0.4547 | 0.032* |
| H10C | 0.6774 | 0.8647 | 0.4173 | 0.032* |
| C11 | 0.82793 (13) | 0.22887 (19) | 0.58813 (4) | 0.0295 (2) |
| H11A | 0.7581 | 0.1869 | 0.6120 | 0.035* |
| H11B | 0.8927 | 0.3379 | 0.6079 | 0.035* |
| H11C | 0.8828 | 0.1016 | 0.5803 | 0.035* |
| H1 | 0.4144 (16) | 0.231 (2) | 0.3998 (7) | 0.033 (4)* |
| H2 | 0.4287 (15) | 0.065 (2) | 0.4512 (6) | 0.039 (4)* |
| H3 | 0.5623 (16) | 0.511 (3) | 0.3965 (6) | 0.052 (4)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.01665 (11) | 0.01722 (10) | 0.01235 (10) | 0.00168 (8) | −0.00133 (7) | 0.00215 (7) |
| O1 | 0.0314 (4) | 0.0245 (3) | 0.0237 (3) | −0.0074 (3) | −0.0093 (3) | 0.0116 (3) |
| O2 | 0.0232 (3) | 0.0255 (3) | 0.0229 (3) | −0.0060 (3) | −0.0101 (3) | 0.0070 (3) |
| O3 | 0.0215 (3) | 0.0277 (3) | 0.0142 (3) | 0.0069 (3) | 0.0043 (2) | 0.0034 (2) |
| O4 | 0.0265 (3) | 0.0171 (3) | 0.0155 (3) | 0.0085 (2) | −0.0013 (2) | 0.0013 (2) |
| O5 | 0.0211 (3) | 0.0261 (3) | 0.0213 (3) | −0.0082 (3) | −0.0087 (2) | 0.0080 (3) |
| O6 | 0.0282 (4) | 0.0310 (4) | 0.0167 (3) | 0.0031 (3) | −0.0042 (3) | 0.0060 (3) |
| N1 | 0.0190 (4) | 0.0305 (4) | 0.0177 (4) | −0.0039 (3) | −0.0029 (3) | 0.0094 (3) |
| N2 | 0.0183 (3) | 0.0190 (3) | 0.0127 (3) | 0.0026 (3) | −0.0005 (2) | 0.0021 (2) |
| N3 | 0.0171 (3) | 0.0277 (4) | 0.0127 (3) | 0.0015 (3) | −0.0002 (3) | 0.0054 (3) |
| C1 | 0.0161 (4) | 0.0180 (4) | 0.0149 (4) | 0.0020 (3) | −0.0012 (3) | 0.0028 (3) |
| C2 | 0.0126 (3) | 0.0130 (3) | 0.0134 (3) | 0.0002 (3) | −0.0007 (3) | 0.0011 (3) |
| C3 | 0.0157 (4) | 0.0266 (4) | 0.0171 (4) | 0.0057 (3) | 0.0018 (3) | 0.0032 (3) |
| C4 | 0.0240 (4) | 0.0190 (4) | 0.0151 (4) | 0.0073 (3) | −0.0040 (3) | −0.0018 (3) |
| C5 | 0.0200 (4) | 0.0239 (4) | 0.0203 (4) | −0.0077 (3) | −0.0065 (3) | 0.0090 (3) |
| C6 | 0.0151 (4) | 0.0231 (4) | 0.0125 (3) | 0.0028 (3) | 0.0016 (3) | 0.0034 (3) |
| C7 | 0.0219 (4) | 0.0185 (4) | 0.0157 (4) | 0.0021 (3) | 0.0009 (3) | −0.0016 (3) |
| C8 | 0.0231 (4) | 0.0231 (4) | 0.0154 (4) | 0.0002 (3) | −0.0018 (3) | −0.0015 (3) |
| C9 | 0.0187 (4) | 0.0273 (4) | 0.0116 (3) | 0.0031 (3) | −0.0002 (3) | 0.0010 (3) |
| C10 | 0.0334 (5) | 0.0182 (4) | 0.0247 (5) | −0.0026 (4) | −0.0033 (4) | 0.0018 (3) |
| C11 | 0.0280 (5) | 0.0417 (6) | 0.0151 (4) | −0.0023 (4) | −0.0070 (4) | 0.0075 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| P1—O6 | 1.4529 (7) | C2—C3 | 1.5310 (12) |
| P1—O5 | 1.5734 (7) | C2—C4 | 1.5318 (12) |
| P1—O3 | 1.5748 (7) | C3—H3A | 0.9900 |
| P1—O4 | 1.5798 (7) | C3—H3B | 0.9900 |
| O1—C1 | 1.2443 (11) | C4—H4A | 0.9900 |
| O2—C1 | 1.2578 (11) | C4—H4B | 0.9900 |
| O3—C3 | 1.4631 (11) | C5—H5A | 0.9900 |

| | | | |
|---|---|---|---|
| O4—C4 | 1.4703 (10) | C5—H5B | 0.9900 |
| O5—C5 | 1.4694 (11) | C7—C8 | 1.3737 (12) |
| N1—C6 | 1.3227 (12) | C7—C10 | 1.4901 (14) |
| N1—H1 | 0.866 (15) | C8—C9 | 1.3977 (14) |
| N1—H2 | 0.900 (14) | C8—H8 | 0.9500 |
| N2—C7 | 1.3580 (12) | C9—C11 | 1.4983 (13) |
| N2—C6 | 1.3603 (12) | C10—H10A | 0.9800 |
| N2—H3 | 0.988 (15) | C10—H10B | 0.9800 |
| N3—C9 | 1.3363 (12) | C10—H10C | 0.9800 |
| N3—C6 | 1.3484 (11) | C11—H11A | 0.9800 |
| C1—C2 | 1.5460 (11) | C11—H11B | 0.9800 |
| C2—C5 | 1.5260 (12) | C11—H11C | 0.9800 |

| | | | |
|---|---|---|---|
| O6—P1—O5 | 114.50 (4) | O4—C4—H4B | 109.7 |
| O6—P1—O3 | 113.86 (4) | C2—C4—H4B | 109.7 |
| O5—P1—O3 | 104.73 (4) | H4A—C4—H4B | 108.2 |
| O6—P1—O4 | 114.43 (4) | O5—C5—C2 | 110.24 (7) |
| O5—P1—O4 | 104.52 (4) | O5—C5—H5A | 109.6 |
| O3—P1—O4 | 103.59 (4) | C2—C5—H5A | 109.6 |
| C3—O3—P1 | 114.52 (5) | O5—C5—H5B | 109.6 |
| C4—O4—P1 | 114.14 (5) | C2—C5—H5B | 109.6 |
| C5—O5—P1 | 114.11 (5) | H5A—C5—H5B | 108.1 |
| C6—N1—H1 | 116.8 (10) | N1—C6—N3 | 119.58 (8) |
| C6—N1—H2 | 114.7 (9) | N1—C6—N2 | 119.05 (8) |
| H1—N1—H2 | 128.2 (13) | N3—C6—N2 | 121.37 (8) |
| C7—N2—C6 | 121.20 (7) | N2—C7—C8 | 118.78 (8) |
| C7—N2—H3 | 119.3 (10) | N2—C7—C10 | 116.39 (8) |
| C6—N2—H3 | 119.1 (10) | C8—C7—C10 | 124.83 (9) |
| C9—N3—C6 | 117.95 (8) | C7—C8—C9 | 117.94 (8) |
| O1—C1—O2 | 126.96 (8) | C7—C8—H8 | 121.0 |
| O1—C1—C2 | 116.56 (7) | C9—C8—H8 | 121.0 |
| O2—C1—C2 | 116.46 (7) | N3—C9—C8 | 122.75 (8) |
| C5—C2—C3 | 108.75 (7) | N3—C9—C11 | 116.02 (9) |
| C5—C2—C4 | 109.20 (7) | C8—C9—C11 | 121.23 (9) |
| C3—C2—C4 | 108.63 (7) | C7—C10—H10A | 109.5 |
| C5—C2—C1 | 110.36 (7) | C7—C10—H10B | 109.5 |
| C3—C2—C1 | 108.95 (7) | H10A—C10—H10B | 109.5 |
| C4—C2—C1 | 110.90 (7) | C7—C10—H10C | 109.5 |
| O3—C3—C2 | 110.00 (7) | H10A—C10—H10C | 109.5 |
| O3—C3—H3A | 109.7 | H10B—C10—H10C | 109.5 |
| C2—C3—H3A | 109.7 | C9—C11—H11A | 109.5 |
| O3—C3—H3B | 109.7 | C9—C11—H11B | 109.5 |
| C2—C3—H3B | 109.7 | H11A—C11—H11B | 109.5 |
| H3A—C3—H3B | 108.2 | C9—C11—H11C | 109.5 |
| O4—C4—C2 | 109.99 (7) | H11A—C11—H11C | 109.5 |
| O4—C4—H4A | 109.7 | H11B—C11—H11C | 109.5 |
| C2—C4—H4A | 109.7 | | |

| | | | |
|---|---|---|---|
| O6—P1—O3—C3 | 179.91 (6) | C5—C2—C4—O4 | −59.68 (9) |
| O5—P1—O3—C3 | −54.29 (7) | C3—C2—C4—O4 | 58.79 (9) |
| O4—P1—O3—C3 | 55.00 (7) | C1—C2—C4—O4 | 178.50 (7) |
| O6—P1—O4—C4 | 179.86 (6) | P1—O5—C5—C2 | 1.39 (11) |
| O5—P1—O4—C4 | 53.84 (7) | C3—C2—C5—O5 | −60.03 (10) |
| O3—P1—O4—C4 | −55.60 (7) | C4—C2—C5—O5 | 58.35 (10) |
| O6—P1—O5—C5 | 178.68 (7) | C1—C2—C5—O5 | −179.49 (7) |
| O3—P1—O5—C5 | 53.28 (8) | C9—N3—C6—N1 | 179.42 (9) |
| O4—P1—O5—C5 | −55.34 (8) | C9—N3—C6—N2 | −1.06 (13) |
| O1—C1—C2—C5 | 8.87 (11) | C7—N2—C6—N1 | −179.24 (9) |
| O2—C1—C2—C5 | −172.46 (9) | C7—N2—C6—N3 | 1.24 (13) |
| O1—C1—C2—C3 | −110.46 (9) | C6—N2—C7—C8 | −1.19 (13) |
| O2—C1—C2—C3 | 68.20 (10) | C6—N2—C7—C10 | 178.60 (8) |
| O1—C1—C2—C4 | 130.02 (9) | N2—C7—C8—C9 | 0.99 (13) |
| O2—C1—C2—C4 | −51.31 (11) | C10—C7—C8—C9 | −178.78 (9) |
| P1—O3—C3—C2 | 0.12 (9) | C6—N3—C9—C8 | 0.90 (14) |
| C5—C2—C3—O3 | 59.14 (9) | C6—N3—C9—C11 | −178.44 (9) |
| C4—C2—C3—O3 | −59.61 (9) | C7—C8—C9—N3 | −0.89 (14) |
| C1—C2—C3—O3 | 179.47 (7) | C7—C8—C9—C11 | 178.42 (9) |
| P1—O4—C4—C2 | 1.10 (9) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.866 (15) | 1.907 (15) | 2.7719 (11) | 176.4 (14) |
| N1—H2···N3$^{i}$ | 0.900 (14) | 2.113 (15) | 3.0114 (12) | 176.3 (12) |
| N2—H3···O2 | 0.988 (15) | 1.738 (16) | 2.7170 (10) | 170.4 (15) |

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.