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Bis(3-azoniapentane-1,5-diaminium) cyclohexaphosphate dihydrate: a monoclinic polymorph

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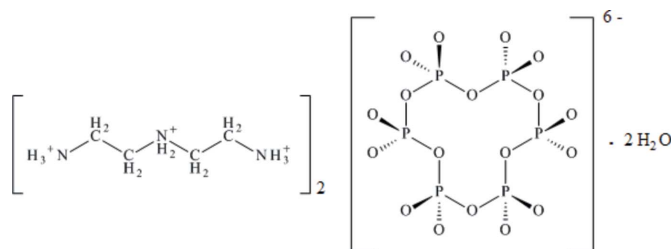
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.034; wR factor = 0.099; data-to-parameter ratio = 33.3.

In the title hydrated molecular salt, $2\text{C}_4\text{H}_{16}\text{N}_3^{3+} \cdot \text{P}_6\text{O}_{18}^{6-} \cdot 2\text{H}_2\text{O}$, the complete cyclohexaphosphate anion is generated by crystallographic inversion symmetry. The six P atoms of the $\text{P}_6\text{O}_{18}^{6-}$ anion form a chair conformation and the organic cation has a corrugated linear geometry. In the crystal, the cations and the anions are connected by $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds into slabs propagating in the ac plane. The water molecules link the slabs by accepting $\text{N}-\text{H} \cdots \text{O}$ links and forming $\text{O}-\text{H} \cdots \text{O}$ links. The triclinic polymorph was reported by Gharbi *et al.* [(1995). *J. Solid State Chem.* **114**, 42–51].

Related literature

For the triclinic polymorph of the title compound, see: Gharbi *et al.* (1995). For related structures, see: Averbuch-Pouchot & Durif (1991); Bridi & Jouini (1989); Kamoun *et al.* (1990); Khedhiri *et al.* (2007); Schülke & Kayser (1985); Khedhiri *et al.* (2003).



Experimental

Crystal data

$2\text{C}_4\text{H}_{16}\text{N}_3^{3+} \cdot \text{P}_6\text{O}_{18}^{6-} \cdot 2\text{H}_2\text{O}$
 $M_r = 722.25$
Monoclinic, $P2_1/c$

$a = 10.033$ (4) Å
 $b = 16.597$ (2) Å
 $c = 8.007$ (3) Å

$\beta = 105.07$ (2)°
 $V = 1287.6$ (7) Å³
 $Z = 2$
Ag $K\alpha$ radiation

$\lambda = 0.56087$ Å
 $\mu = 0.27$ mm⁻¹
 $T = 293$ K
 $0.32 \times 0.27 \times 0.21$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
9091 measured reflections
6303 independent reflections

5211 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$
2 standard reflections every 120 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.099$
 $S = 1.07$
6303 reflections
189 parameters
3 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.47$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.97$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1W}-\text{H1W1} \cdots \text{O5}$	0.84 (1)	2.12 (1)	2.9274 (17)	163 (2)
$\text{O1W}-\text{H2W1} \cdots \text{O2}^{\text{i}}$	0.85 (1)	1.85 (1)	2.6938 (16)	175 (2)
$\text{N1}-\text{H1B} \cdots \text{O1W}^{\text{ii}}$	0.89	1.99	2.7817 (15)	147
$\text{N1}-\text{H1C} \cdots \text{O1}$	0.89	1.96	2.8054 (14)	159
$\text{N1}-\text{H1A} \cdots \text{O6}^{\text{iii}}$	0.89	1.96	2.8013 (15)	156
$\text{N2}-\text{H2A} \cdots \text{O8}^{\text{iii}}$	0.90	2.10	2.8049 (16)	135
$\text{N2}-\text{H2A} \cdots \text{O9}^{\text{ii}}$	0.90	2.36	3.0891 (15)	138
$\text{N2}-\text{H2B} \cdots \text{O9}$	0.90	2.14	2.7973 (16)	130
$\text{N2}-\text{H2B} \cdots \text{O8}^{\text{ii}}$	0.90	2.15	2.8706 (13)	137
$\text{N3}-\text{H3B} \cdots \text{O5}^{\text{iv}}$	0.89	1.99	2.8414 (17)	159
$\text{N3}-\text{H3C} \cdots \text{O1}^{\text{v}}$	0.89	1.93	2.7973 (16)	164
$\text{N3}-\text{H3A} \cdots \text{O6}^{\text{vi}}$	0.89	1.96	2.8008 (16)	157

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6809).

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supplementary materials

Acta Cryst. (2012). E68, o2038–o2039 [doi:10.1107/S1600536812025172]

Bis(3-azoniapentane-1,5-diaminium) cyclohexaphosphate dihydrate: a monoclinic polymorph

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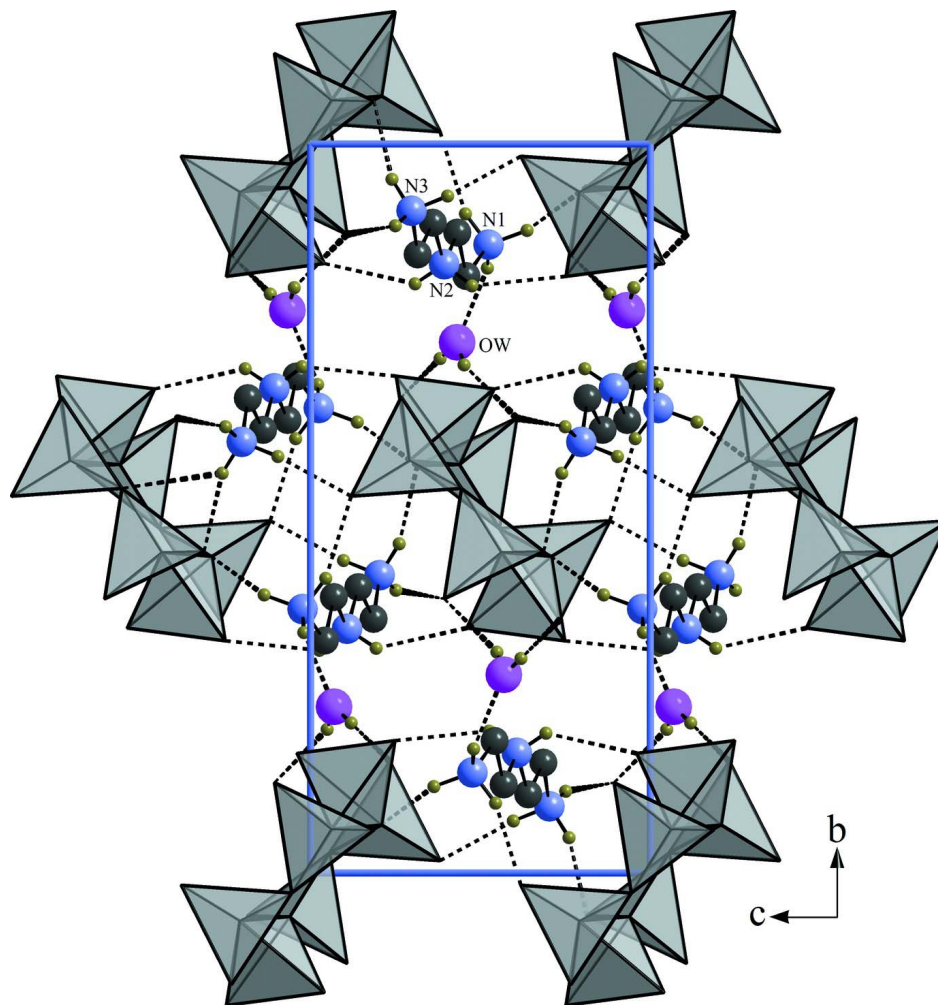
Comment

The title compound (I), was prepared as part of our ongoing structural studies of inorganic-organic cyclohexaphosphates systems. Its chemical composition includes three entities, P_6O_{18} ring, water molecules and organic cations $[C_4N_3H_{16}]^{3+}$ and is polymorphic with a previously described triclinic phase (Gharbi *et al.*, 1995). The geometrical configuration of these entities is depicted in Figure 1, whereas Figure 2 shows the complete atomic arrangement.

The packing of (I) consists of hybrid layers where the organic and inorganic species are alternated. These layers, extended perpendicularly to the *b* axis, are also connected between them in the two other directions *via* H-bonds assuring the cohesion of the network. The P_6O_{18} rings are located around the inversion centers (0, 0, 0) and (1/2, 1/2, 1/2) and are built up by only three independent PO_4 tetrahedra. The P—P—P angles of 98.85 (1), 109.09 (1) and 138.42 (1)° show that the rings are significantly distorted from the ideal threefold symmetry. It should be noted that these large deviations are commonly observed in cyclohexaphosphates with a ring of low local symmetry (Khedhiri *et al.*, 2003, Khedhiri *et al.*, 2007), as in the title compound. Nevertheless, this distortion is comparatively less important than that observed in $Cs_6P_6O_{18} \cdot 6H_2O$, which shows the greatest distortion for the same angles, ranging between 93.2 and 145.5° (Averbuch-Pouchot and Durif, 1991). The great flexibility of the hexamembered P_6O_{18} rings can probably explain the pronounced distortion observed for the big rings compared with their smaller ring analogues. Examination of the main geometrical features of the three independent PO_4 tetrahedra (P—O and P—P distances as well as P—O—P or O—P—O angles) shows clearly that, in spite of the P—P—P angles deformation, they are in accordance with values generally observed in condensed phosphate anions.

In the organic entity, N—C and C—C distances and N—C—C and C—N—C angles, spreading within the respective ranges 1.477 (1) - 1.512 (2) Å and 109 (1) - 111.5 (9)°, are similar to those observed in others compounds (Kamoun *et al.*, 1990; Bridi *et al.*, 1989). All nitrogen atoms of the used amine are protonated and so it is formulated by $[C_4N_3H_{16}]^{3+}$. Among the eight hydrogen atoms of this group, only one, H1B, establishes a hydrogen bond with a water molecule, the remaining ones are connected to the external oxygen atoms of three phosphoric rings to form an anionic entity of formula $[C_4N_3H_{16}(P_6O_{18})_3]^{15-}$. The two hydrogen atoms of the water molecule act as a link between successive anions. A three dimensional network of N—H...O and O—H...O hydrogen bonds interconnects the structural arrangement.

This study shows that (I) is a polymorph of the triclinic structure published elsewhere (Gharbi *et al.*, 1995). Both phases have the same chemical formula and some structural analogues but they present several differences in their crystal data, H-bonding scheme, internal symmetry of the cyclohexaphosphoric anions and particularly the aza-3 pentanediy-1,5 diaminium which has different conformations where the torsion angles N2—C3—C4—N3, C2—N2—C3—C4, N1—C1—C2—N2 and C3—N2—C2—C1 exhibit the following values -175.34 (9)°, -178.34 (9)°, 171.15 (9)° and 177.79 (9)° in the title compound and 177.67°, 175.32°, 66.45° and -69.92° in the bibliography one.


Figure 2

Structure projection of (I) along the a axis. The H-atoms not involved in H-bonding are omitted.

Bis(3-azoniapentane-1,5-diaminium) cyclohexaphosphate dihydrate

Crystal data

$2\text{C}_4\text{H}_{16}\text{N}_3^{3+} \cdot \text{P}_6\text{O}_{18}^{6-} \cdot 2\text{H}_2\text{O}$

$M_r = 722.25$

Monoclinic, $P2_1/c$

$a = 10.033$ (4) Å

$b = 16.597$ (2) Å

$c = 8.007$ (3) Å

$\beta = 105.07$ (2)°

$V = 1287.6$ (7) Å³

$Z = 2$

$F(000) = 752$

$D_x = 1.863$ Mg m⁻³

Ag $K\alpha$ radiation, $\lambda = 0.56087$ Å

Cell parameters from 25 reflections

$\theta = 9\text{--}11^\circ$

$\mu = 0.27$ mm⁻¹

$T = 293$ K

Prism, colorless

$0.32 \times 0.27 \times 0.21$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

non-profiled ω scans

9091 measured reflections

6303 independent reflections

5211 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$
 $\theta_{\text{max}} = 28.0^\circ$, $\theta_{\text{min}} = 2.3^\circ$
 $h = -16 \rightarrow 3$
 $k = -27 \rightarrow 2$

$l = -13 \rightarrow 13$
 2 standard reflections every 120 min
 intensity decay: 2%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.099$
 $S = 1.07$
 6303 reflections
 189 parameters
 3 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
 $w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.1509P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.003$
 $\Delta\rho_{\text{max}} = 0.47 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.97 \text{ e } \text{\AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
P1	0.20977 (2)	0.430603 (15)	0.26986 (3)	0.01668 (6)
P2	0.22574 (3)	0.561419 (16)	0.52233 (3)	0.01743 (6)
P3	0.50730 (2)	0.627794 (15)	0.61516 (3)	0.01533 (5)
O1	0.14711 (9)	0.48310 (6)	0.11911 (10)	0.02688 (16)
O2	0.15970 (10)	0.34709 (5)	0.26697 (13)	0.03036 (18)
O3	0.37237 (8)	0.43405 (4)	0.29127 (10)	0.01950 (13)
O4	0.19351 (8)	0.47242 (5)	0.44433 (9)	0.01962 (13)
O5	0.16446 (10)	0.62392 (5)	0.39346 (12)	0.02936 (17)
O6	0.18261 (11)	0.55876 (6)	0.68613 (12)	0.03256 (19)
O7	0.38893 (8)	0.56033 (5)	0.56188 (13)	0.02876 (18)
O8	0.47732 (10)	0.68151 (5)	0.74802 (10)	0.02667 (16)
O9	0.53563 (11)	0.66399 (6)	0.46030 (11)	0.0340 (2)
O1W	0.00786 (13)	0.72797 (7)	0.5688 (2)	0.0500 (3)
H1W1	0.061 (2)	0.6947 (11)	0.540 (3)	0.060*
H2W1	-0.0488 (19)	0.7066 (13)	0.618 (3)	0.060*
N1	0.13894 (10)	0.63794 (6)	-0.02369 (13)	0.02486 (17)
H1A	0.1317	0.6212	-0.1313	0.037*
H1B	0.0692	0.6709	-0.0228	0.037*
H1C	0.1363	0.5957	0.0438	0.037*
N2	0.52234 (9)	0.66493 (5)	0.10700 (11)	0.01944 (14)
H2A	0.5252	0.6967	0.0169	0.023*

H2B	0.5298	0.6966	0.2003	0.023*
N3	0.88883 (10)	0.59139 (7)	0.20294 (12)	0.02576 (18)
H3A	0.8737	0.5500	0.2663	0.039*
H3B	0.9692	0.6143	0.2545	0.039*
H3C	0.8911	0.5739	0.0986	0.039*
C1	0.27111 (11)	0.68116 (7)	0.04148 (16)	0.02540 (19)
H1D	0.2726	0.7076	0.1499	0.030*
H1E	0.2810	0.7220	-0.0411	0.030*
C2	0.38863 (11)	0.62149 (6)	0.06828 (14)	0.02173 (17)
H2C	0.3865	0.5857	0.1634	0.026*
H2D	0.3784	0.5891	-0.0351	0.026*
C3	0.63924 (10)	0.60786 (6)	0.14047 (14)	0.02126 (17)
H3D	0.6324	0.5748	0.0387	0.026*
H3E	0.6344	0.5725	0.2352	0.026*
C4	0.77604 (12)	0.65144 (8)	0.18517 (19)	0.0315 (2)
H4A	0.7791	0.6898	0.0948	0.038*
H4B	0.7874	0.6807	0.2928	0.038*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.01475 (10)	0.01827 (10)	0.01602 (10)	-0.00204 (7)	0.00221 (8)	-0.00203 (7)
P2	0.01514 (10)	0.01911 (11)	0.01686 (10)	0.00136 (8)	0.00204 (8)	-0.00171 (7)
P3	0.01797 (10)	0.01535 (10)	0.01216 (9)	0.00046 (7)	0.00302 (7)	0.00027 (7)
O1	0.0259 (4)	0.0339 (4)	0.0167 (3)	0.0062 (3)	-0.0019 (3)	0.0011 (3)
O2	0.0304 (4)	0.0226 (4)	0.0406 (5)	-0.0104 (3)	0.0137 (4)	-0.0089 (3)
O3	0.0149 (3)	0.0209 (3)	0.0223 (3)	0.0003 (2)	0.0043 (2)	0.0044 (2)
O4	0.0214 (3)	0.0203 (3)	0.0178 (3)	-0.0036 (2)	0.0063 (2)	-0.0028 (2)
O5	0.0276 (4)	0.0240 (4)	0.0311 (4)	0.0032 (3)	-0.0020 (3)	0.0059 (3)
O6	0.0412 (5)	0.0361 (5)	0.0248 (4)	-0.0009 (4)	0.0165 (4)	-0.0082 (3)
O7	0.0154 (3)	0.0231 (3)	0.0438 (5)	-0.0011 (3)	0.0005 (3)	-0.0097 (3)
O8	0.0383 (4)	0.0210 (3)	0.0211 (3)	0.0043 (3)	0.0083 (3)	-0.0055 (3)
O9	0.0430 (5)	0.0408 (5)	0.0204 (3)	0.0056 (4)	0.0121 (3)	0.0133 (3)
O1W	0.0487 (7)	0.0299 (5)	0.0854 (9)	0.0048 (4)	0.0424 (7)	0.0120 (6)
N1	0.0197 (4)	0.0278 (4)	0.0272 (4)	0.0013 (3)	0.0063 (3)	-0.0007 (3)
N2	0.0197 (3)	0.0188 (3)	0.0203 (3)	0.0004 (3)	0.0059 (3)	0.0006 (3)
N3	0.0182 (4)	0.0354 (5)	0.0225 (4)	-0.0010 (3)	0.0031 (3)	-0.0015 (3)
C1	0.0205 (4)	0.0232 (4)	0.0324 (5)	0.0012 (3)	0.0067 (4)	-0.0026 (4)
C2	0.0188 (4)	0.0215 (4)	0.0241 (4)	0.0003 (3)	0.0042 (3)	0.0004 (3)
C3	0.0183 (4)	0.0207 (4)	0.0242 (4)	0.0011 (3)	0.0044 (3)	0.0010 (3)
C4	0.0209 (4)	0.0270 (5)	0.0436 (7)	-0.0024 (4)	0.0031 (4)	-0.0081 (5)

Geometric parameters (\AA , $^\circ$)

P1—O2	1.4725 (9)	N2—C3	1.4769 (14)
P1—O1	1.4889 (9)	N2—C2	1.4831 (14)
P1—O3	1.5964 (10)	N2—H2A	0.9000
P1—O4	1.6058 (9)	N2—H2B	0.9000
P2—O5	1.4796 (9)	N3—C4	1.4867 (16)
P2—O6	1.4847 (10)	N3—H3A	0.8900

P2—O7	1.5849 (11)	N3—H3B	0.8900
P2—O4	1.6037 (8)	N3—H3C	0.8900
P3—O9	1.4706 (9)	C1—C2	1.5119 (15)
P3—O8	1.4776 (9)	C1—H1D	0.9700
P3—O7	1.6072 (9)	C1—H1E	0.9700
P3—O3 ⁱ	1.6132 (8)	C2—H2C	0.9700
O3—P3 ⁱ	1.6132 (8)	C2—H2D	0.9700
O1W—H1W1	0.840 (9)	C3—C4	1.5099 (16)
O1W—H2W1	0.849 (9)	C3—H3D	0.9700
N1—C1	1.4783 (15)	C3—H3E	0.9700
N1—H1A	0.8900	C4—H4A	0.9700
N1—H1B	0.8900	C4—H4B	0.9700
N1—H1C	0.8900		
O2—P1—O1	117.88 (6)	C2—N2—H2B	109.4
O2—P1—O3	111.74 (5)	H2A—N2—H2B	108.0
O1—P1—O3	105.69 (5)	C4—N3—H3A	109.5
O2—P1—O4	108.01 (5)	C4—N3—H3B	109.5
O1—P1—O4	109.60 (5)	H3A—N3—H3B	109.5
O3—P1—O4	102.90 (4)	C4—N3—H3C	109.5
O5—P2—O6	118.24 (6)	H3A—N3—H3C	109.5
O5—P2—O7	111.58 (6)	H3B—N3—H3C	109.5
O6—P2—O7	110.27 (6)	N1—C1—C2	109.10 (9)
O5—P2—O4	111.65 (5)	N1—C1—H1D	109.9
O6—P2—O4	103.95 (5)	C2—C1—H1D	109.9
O7—P2—O4	99.24 (4)	N1—C1—H1E	109.9
O9—P3—O8	118.73 (6)	C2—C1—H1E	109.9
O9—P3—O7	110.62 (6)	H1D—C1—H1E	108.3
O8—P3—O7	109.68 (6)	N2—C2—C1	109.94 (9)
O9—P3—O3 ⁱ	111.48 (5)	N2—C2—H2C	109.7
O8—P3—O3 ⁱ	108.51 (5)	C1—C2—H2C	109.7
O7—P3—O3 ⁱ	95.29 (5)	N2—C2—H2D	109.7
P1—O3—P3 ⁱ	130.36 (5)	C1—C2—H2D	109.7
P2—O4—P1	132.93 (5)	H2C—C2—H2D	108.2
P2—O7—P3	134.33 (6)	N2—C3—C4	111.46 (9)
H1W1—O1W—H2W1	113.7 (19)	N2—C3—H3D	109.3
C1—N1—H1A	109.5	C4—C3—H3D	109.3
C1—N1—H1B	109.5	N2—C3—H3E	109.3
H1A—N1—H1B	109.5	C4—C3—H3E	109.3
C1—N1—H1C	109.5	H3D—C3—H3E	108.0
H1A—N1—H1C	109.5	N3—C4—C3	108.90 (10)
H1B—N1—H1C	109.5	N3—C4—H4A	109.9
C3—N2—C2	111.02 (9)	C3—C4—H4A	109.9
C3—N2—H2A	109.4	N3—C4—H4B	109.9
C2—N2—H2A	109.4	C3—C4—H4B	109.9
C3—N2—H2B	109.4	H4A—C4—H4B	108.3
O2—P1—O3—P3 ⁱ	-28.76 (9)	O6—P2—O7—P3	-82.21 (10)
O1—P1—O3—P3 ⁱ	-158.18 (6)	O4—P2—O7—P3	169.10 (9)

O4—P1—O3—P3 ⁱ	86.88 (7)	O9—P3—O7—P2	-89.73 (10)
O5—P2—O4—P1	50.02 (9)	O8—P3—O7—P2	43.13 (11)
O6—P2—O4—P1	178.57 (7)	O3 ⁱ —P3—O7—P2	154.95 (9)
O7—P2—O4—P1	-67.73 (8)	C3—N2—C2—C1	177.79 (9)
O2—P1—O4—P2	-178.70 (7)	N1—C1—C2—N2	171.15 (9)
O1—P1—O4—P2	-49.08 (8)	C2—N2—C3—C4	-178.34 (9)
O3—P1—O4—P2	63.01 (8)	N2—C3—C4—N3	-175.34 (9)
O5—P2—O7—P3	51.30 (11)		

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

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

<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>
O1 <i>W</i> —H1 <i>W</i> 1 \cdots O5	0.84 (1)	2.12 (1)	2.9274 (17)	163 (2)
O1 <i>W</i> —H2 <i>W</i> 1 \cdots O2 ⁱⁱ	0.85 (1)	1.85 (1)	2.6938 (16)	175 (2)
N1—H1 <i>B</i> \cdots O1 <i>W</i> ⁱⁱⁱ	0.89	1.99	2.7817 (15)	147
N1—H1 <i>C</i> \cdots O1	0.89	1.96	2.8054 (14)	159
N1—H1 <i>A</i> \cdots O6 ^{iv}	0.89	1.96	2.8013 (15)	156
N2—H2 <i>A</i> \cdots O8 ^{iv}	0.90	2.10	2.8049 (16)	135
N2—H2 <i>A</i> \cdots O9 ⁱⁱⁱ	0.90	2.36	3.0891 (15)	138
N2—H2 <i>B</i> \cdots O9	0.90	2.14	2.7973 (16)	130
N2—H2 <i>B</i> \cdots O8 ⁱⁱⁱ	0.90	2.15	2.8706 (13)	137
N3—H3 <i>B</i> \cdots O5 ^v	0.89	1.99	2.8414 (17)	159
N3—H3 <i>C</i> \cdots O1 ^{vi}	0.89	1.93	2.7973 (16)	164
N3—H3 <i>A</i> \cdots O6 ⁱ	0.89	1.96	2.8008 (16)	157

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