# research communications

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# Crystal structure of bis(2-aminoanilinium) hydrogen phosphate

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The asymmetric unit of the title compound, $2C_6H_9N_2^+ \cdot HPO_4^{2-}$, comprises two 2-aminoanilinium cations and one hydrogen phosphate dianion. In the crystal, the HPO_4^{2-} dianions are linked by O—H···O hydrogen bonds into chains along [100]. The inorganic anionic chains and organic cations are linked by N—H···O and N—H···N hydrogen bonds, forming a two-dimensional supramolecular network extending parallel to (001).

1. Chemical context

Inorganic–organic hybrid compounds are of current interest due to their fascinating architectures and potential applications in crystal engineering and supramolecular chemistry (Singh *et al.*, 2011; Direm *et al.*, 2015). Among the explored hybrid compounds, organic phosphates formed as a result of the reaction with inorganic oxy acids such as orthophosphoric acid (H_3PO_4) and organic amines and amides are particularly interesting. Organic monohydrogen (HPO_4^{2-}) and dihydrogen phosphate ($H_2PO_4^-$) compounds provide a class of materials with numerous practical and potential uses in various fields such as biomolecular sciences, catalysis, liquid-crystal-material development, ferroelectrics, non-linear optical and supramolecular studies (Khan *et al.*, 2009; Evans *et al.*, 2008; Balamurugan *et al.*, 2010). Non-covalent interactions, such as hydrogen bonding and other weak interactions, represent the basic set of tools for the construction of elaborate supramolecular architectures of organic or inorganic–organic compounds. In this respect, the potential of monohydrogen and dihydrogen phosphate anions as useful building blocks has been investigated structurally (Shylaja *et al.*, 2008; Oueslati *et al.*, 2007; Jagan *et al.*, 2015; Trojette *et al.*, 1998; Soumhi & Jouini, 1995). Here we report the structure and the self-assembled supramolecular architecture exhibited through the formation of O—H···O, N—H···O and N—H···N hydrogen bonds in bis(2-aminoanilinium) hydrogen phosphate.

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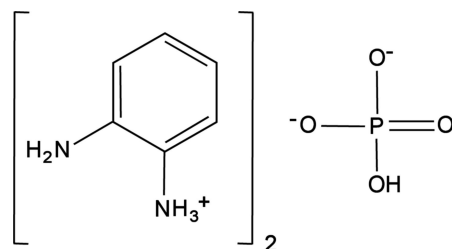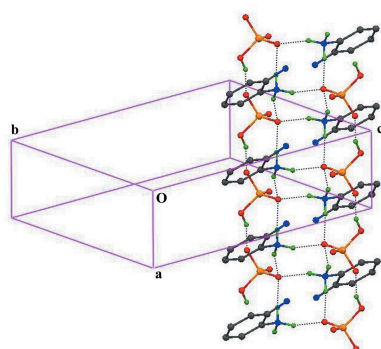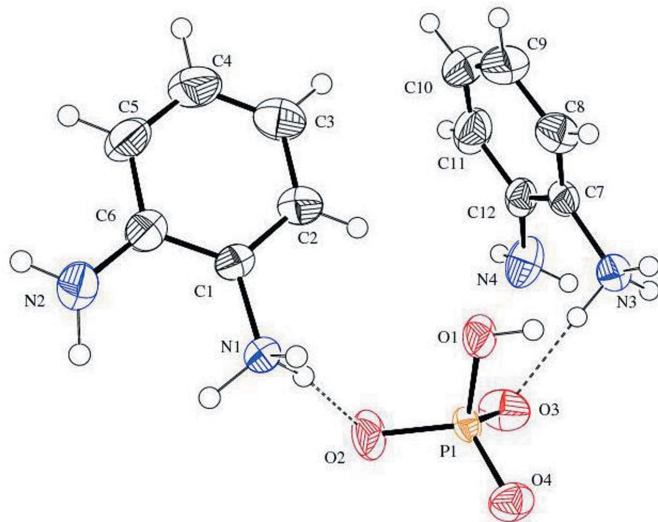
Figure 1
The asymmetric unit of the title compound with displacement ellipsoid drawn at the 40% probability level. The dashed lines represent hydrogen bonds.

2. Structural commentary

The asymmetric unit of the title compound comprises two 2-aminoanilinium cations and one hydrogen phosphate dianion (Fig. 1). The existence of the hydrogen phosphate anion is confirmed by the P—O bond distances, and the presence of a relevant density peak at a distance from the oxygen atom O1 confirms the hydroxyl group of the anion. The bond distance P1—O1 = 1.561 (2) Å indicates single-bond character, while the bond distances P1—O2 = 1.504 (2), P1—O3 = 1.504 (2) and P1—O4 = 1.497 (2) Å reveal the resonating P—O bonds of the hydrogen phosphate anion. As expected (Rao *et al.*, 2010; Peng & Zhao, 2010), in both cations the C—N bond [C1—N1 = 1.450 (3), C7—N3 = 1.450 (4) Å] involving the ammonium group is longer than that in the amine group [C6—N2 = 1.384 (4), C12—N4 = 1.383 (4) Å]. The phenyl rings of the *o*-phenylenediammonium cations are almost perpendicular to one another [dihedral angle 86.53 (2)°].

3. Supramolecular features

In the title structure, the hydrogen phosphate anion and 2-aminoanilinium cations possess a number of donor and acceptor sites, which leads to the formation of a variety of hydrogen bonds *viz.* O—H···O, N—H···O and N—H···N (Table 1). The O1—H1D···O2^i hydrogen bond [symmetry code: (i) $x + 1$, y, z] connects adjacent hydrogen phosphate anions, forming anionic chains extending along [100]. The oxygen atom O3 acts as a trifurcated hydrogen-bond acceptor for the donor nitrogen atom N1 at (x, y, z), ($-1 + x, y, z$) and ($1 - x, 1 - y, 2 - z$), forming a one-dimensional supramolecular ladder extending along [100] as shown in Fig. 2. In the ladder, centrosymmetrically related anions and cations are interlinked through N3—H3C···O3, N3—H3A···O3^i and N3—H3B···O3^{iv} [symmetry code: (iv) $-x + 1$, $-y + 1$, $-z + 2$]

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1D···O2^i	0.85 (1)	1.65 (1)	2.470 (3)	164 (4)
N3—H3A···O3^i	0.90 (2)	2.06 (2)	2.928 (3)	160 (3)
N1—H1A···O4^{ii}	0.92 (2)	1.81 (2)	2.720 (3)	171 (3)
N1—H1C···O4^{iii}	0.93 (2)	2.02 (2)	2.953 (3)	179 (3)
N2—H2A···O4^{iii}	0.92 (2)	1.99 (2)	2.904 (4)	170 (3)
N4—H4A···O4^{iv}	0.88 (2)	2.45 (3)	3.188 (4)	142 (3)
N3—H3B···O3^{iv}	0.91 (2)	1.87 (2)	2.740 (3)	159 (3)
N3—H3C···O3	0.91 (2)	1.87 (2)	2.778 (3)	176 (3)
N1—H1B···O2	0.92 (2)	1.83 (2)	2.734 (3)	169 (3)
N4—H4B···N2^v	0.89 (2)	2.33 (2)	3.210 (4)	172 (3)

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

hydrogen bonds, forming two types of fused rings of $R_4^2(8)$ graph-set motif. The association of O—H···O hydrogen bonds in the anionic chains with the N—H···O hydrogen bonds in the ladder forms heteromeric $R_3^3(10)$ hydrogen-bonded motifs. Adjacent ladders are further bridged by N1—H1B···O2, N1—H1A···O4^{ii} and N1—H1C···O4^{iii} [symmetry codes: (ii) $-x + 1$, $-y + 2$, $-z + 2$; (iii) $-x$, $-y + 2$, $-z + 2$] hydrogen bonds, resulting in the formation of a two-dimensional organic–inorganic supramolecular layered network parallel to (001) (Fig. 3). In the (001) network, the bridging cations make rings of $R_3^3(10)$ and $R_5^3(12)$ motifs through the three charge-assisted N—H···O and the O1—H1D···O2^i hydrogen bonds. In addition, the N2—H2A···O4^{iii}, N1—H1C···O4^{iii} and N4—H4B···N2^v [symmetry codes: (iii) $-x$, $-y + 2$, $-z + 2$; (v) x, $-1 + y$, z] hydrogen bonds stabilize the (001) network. In
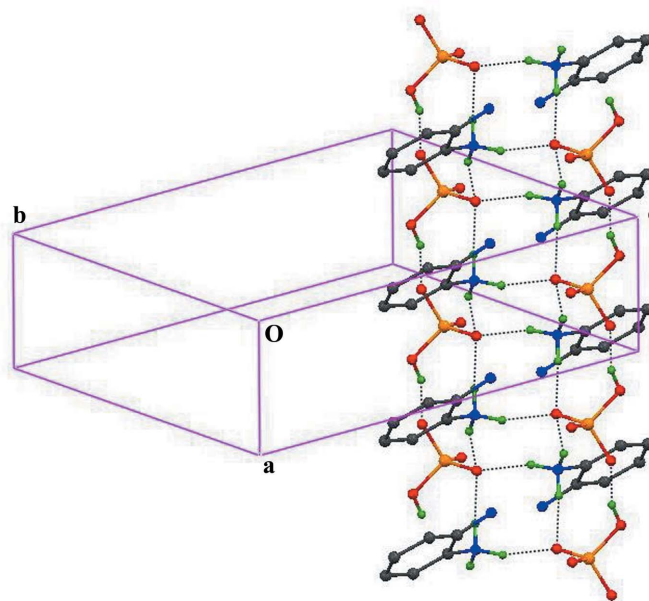
Figure 2
Partial packing diagram of the title compound showing the formation of an organic–inorganic supramolecular ladder through N—H···O and O—H···O hydrogen bonds extending along [100]. The formation of rings with $R_4^2(8)$ and $R_3^3(10)$ graph-set motifs is also shown. Hydrogen atoms not involved in hydrogen bonding are omitted for clarity.
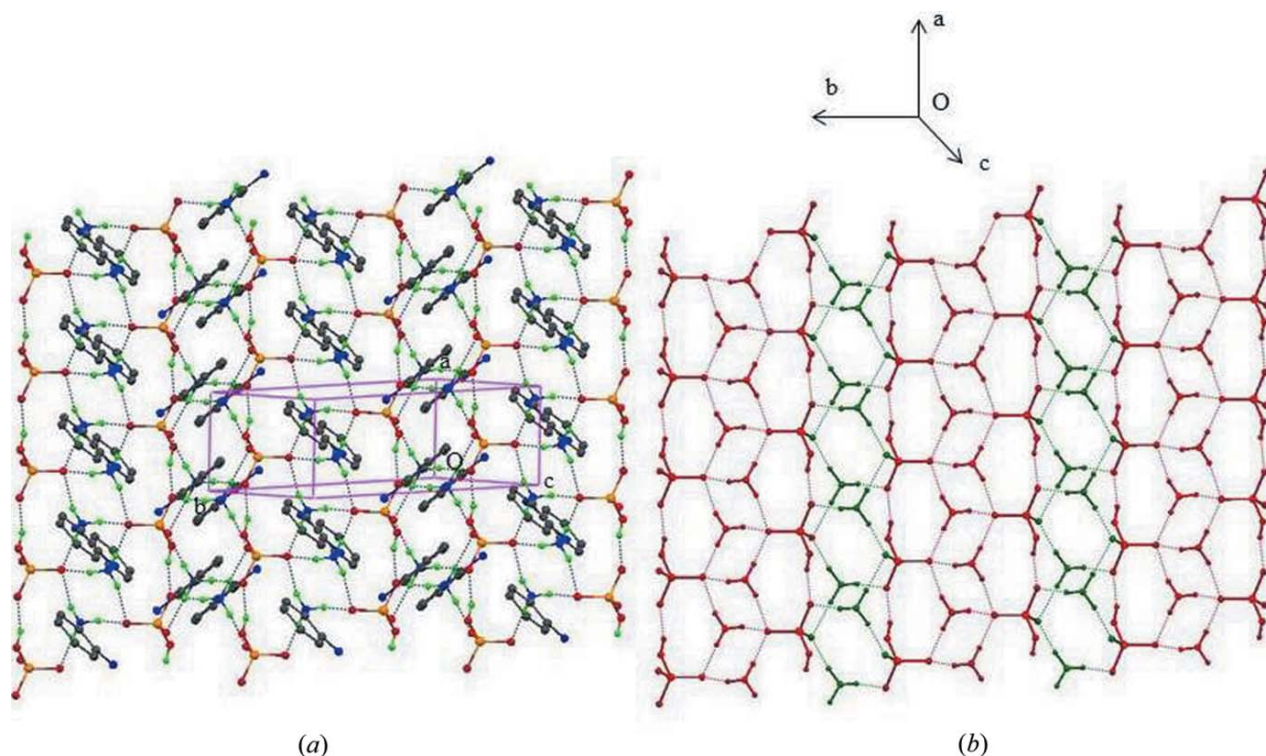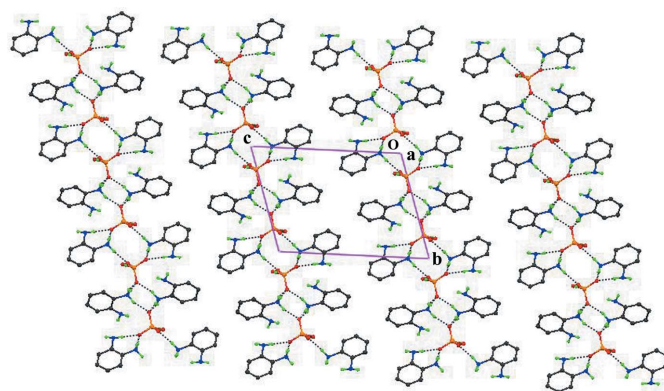
Figure 3
Crystal packing of the title compound showing (*a*) the formation through hydrogen bonds (dashed lines) of an organic–inorganic supramolecular sheet extending parallel to (001) and (*b*) the (001) network in which red represents the [100] ladder, bridged by the cations (represented in green) through N—H···O hydrogen bonds.

the crystal structure (Fig. 4), adjacent organic–inorganic layers are separated by a distance equal to the length of the *c* axis.

4. Database Survey

A CSD database search (*ConQuest* 1.17; Groom & Allen, 2014) showed 48 entries for hydrogen phosphate salts formed with various amino cations. It is interesting to observe that most of the reported structures of hydrogen phosphate salts are hydrated (33 structures) compared to the reported structures of dihydrogen phosphate and phosphate salts. Most of the hydrogen phosphate structures reported contain alkyl cations (Ilioudis *et al.*, 2002; Mrad *et al.*, 2012; Li *et al.*, 2010), in which the alkyl cations encapsulated between chains of hydrogen phosphate are flexible with respect to the nature of the cations, which may induce a change in physical properties (Baouab & Jouini, 1998). As observed in the title compound, in the crystal structure of 2-aminoanilinium dihydrogen phosphate (CSD refcode: SAYWAQ; Trojette *et al.*, 1998), the dihydrogen phosphate anions form chains, which are bridged by 2-aminoanilinium cations through N—H···O hydrogen bonds, generating a two-dimensional inorganic–organic network. Conversely, in the crystal structure of 1,2-phenylenediammonium bis(dihydrogen phosphate) (ZAYPAQ; Soumhi & Jouini, 1995), the anions form inorganic sheets interlinked by 1,2-phenylenediammonium cations, thus generating a three-dimensional inorganic–organic framework.

This can be attributed to the double protonation of the cations in ZAYPAQ compared to the title compound and SAYWAQ. In the crystal structure of 2-aminoanilinium perchlorate monohydrate (KAJGUY; Raghavaiah *et al.*, 2005), the 2-aminoanilinium cation, the perchlorate anion and the lattice water molecule assemble into a unique hydrogen-bonded supramolecular framework, forming alternate hydrophobic and hydrophilic zones.

Figure 4
Packing of the title compound, viewed down the *a* axis, showing the arrangement of the (001) two-dimensional supramolecular networks stacked along the *c* axis. Dashed lines indicate hydrogen bonds.

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_6H_9N_2{}^+ \cdot HPO_4{}^{2-}$
M_r	314.28
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	296
a, b, c (Å)	4.7613 (7), 10.8925 (17), 15.054 (2)
α, β, γ (°)	107.263 (3), 94.060 (3), 94.549 (3)
V (Å^3)	739.6 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	$0.30 \times 0.20 \times 0.20$
Data collection	
Diffractometer	Bruker Kappa APEXII CCD Diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.865, 0.902
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16948, 2841, 2271
R_{int}	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.119, 1.16
No. of reflections	2841
No. of parameters	242
No. of restraints	11
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.49, −0.34

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2012), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

5. Synthesis and crystallization

The title compound was prepared by dissolving in water *o*-phenylenediamine and orthophosphoric acid in a 2:1 molar ratio. The resulting mixture was stirred continuously for 3 h with constant heating maintained at 333 K. The solution was then cooled, filtered and kept for crystallization without any disturbance. Good diffraction-quality crystals were obtained after one week.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms associated with the N and O atoms were localized in a difference electron-density map and refined with the N—H and O—H distances constrained to values of 0.90 (2) and 0.85 (1) Å, respectively. All other hydrogen atoms were placed in calculated positions and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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supporting information

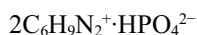## Crystal structure of bis(2-aminoanilinium) hydrogen phosphate

Reena Ittyachan, Melesuparambil Sundaram Ahigna and Rajamony Jagan

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *APEX2* and *SAINT* (Bruker, 2012); data reduction: *SAINT* and *XPREP* (Bruker, 2012); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

Bis(2-aminoanilinium) hydrogen phosphate

Crystal data

$2C_6H_9N_2{}^+ \cdot HPO_4{}^{2-}$	$Z = 2$
$M_r = 314.28$	$F(000) = 332$
Triclinic, $P\overline{1}$	$D_x = 1.411$ Mg m^{-3}
$a = 4.7613$ (7) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 10.8925$ (17) Å	Cell parameters from 7191 reflections
$c = 15.054$ (2) Å	$\theta = 2.8$–26.1°
$\alpha = 107.263$ (3)°	$\mu = 0.21$ mm^{-1}
$\beta = 94.060$ (3)°	$T = 296$ K
$\gamma = 94.549$ (3)°	Block, brown
$V = 739.6$ (2) Å^3	$0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD Diffractometer	2271 reflections with $I > 2\sigma(I)$
ω and φ scan	$R_{int} = 0.039$
Absorption correction: multi-scan	$\theta_{max} = 26.0°$, $\theta_{min} = 2.0°$
(*SADABS*; Bruker, 2012)	$h = -5 \rightarrow 5$
$T_{min} = 0.865$, $T_{max} = 0.902$	$k = -13 \rightarrow 13$
16948 measured reflections	$l = -18 \rightarrow 18$
2841 independent reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent
Least-squares matrix: full	and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 0.8089P]$
$wR(F^2) = 0.119$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.16$	$(\Delta/\sigma)_{max} < 0.001$
2841 reflections	$\Delta\rho_{max} = 0.49$ e Å^{-3}
242 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
11 restraints	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0716 (5)	0.9348 (3)	0.75677 (17)	0.0294 (6)
C2	0.2315 (7)	0.8319 (3)	0.7246 (2)	0.0430 (7)
H2	0.3277	0.7991	0.7669	0.042 (9)*
C3	0.2477 (8)	0.7789 (4)	0.6308 (2)	0.0589 (10)
H3	0.3532	0.7097	0.6090	0.068 (11)*
C4	0.1069 (8)	0.8290 (4)	0.5698 (2)	0.0618 (10)
H4	0.1203	0.7942	0.5061	0.082 (13)*
C5	−0.0531 (7)	0.9289 (4)	0.6000 (2)	0.0546 (9)
H5	−0.1503	0.9597	0.5566	0.059 (10)*
C6	−0.0730 (6)	0.9859 (3)	0.6957 (2)	0.0375 (7)
N1	0.0743 (5)	0.9908 (2)	0.85708 (15)	0.0290 (5)
H1A	0.238 (5)	1.046 (3)	0.881 (2)	0.060 (10)*
H1B	0.079 (6)	0.928 (2)	0.8862 (19)	0.039 (8)*
H1C	−0.080 (5)	1.037 (3)	0.8734 (19)	0.040 (8)*
N2	−0.2164 (6)	1.0939 (3)	0.7268 (2)	0.0492 (7)
H2A	−0.300 (7)	1.106 (3)	0.7814 (17)	0.064 (11)*
H2B	−0.337 (7)	1.100 (4)	0.680 (2)	0.071 (12)*
C7	0.6532 (6)	0.4711 (3)	0.79919 (19)	0.0321 (6)
C8	0.7961 (7)	0.5283 (3)	0.7439 (2)	0.0493 (8)
H8	0.9487	0.5905	0.7699	0.049 (9)*
C9	0.7133 (9)	0.4933 (4)	0.6491 (3)	0.0683 (11)
H9	0.8085	0.5322	0.6110	0.076 (12)*
C10	0.4896 (9)	0.4008 (4)	0.6120 (3)	0.0694 (12)
H10	0.4328	0.3768	0.5483	0.071 (11)*
C11	0.3490 (8)	0.3432 (3)	0.6677 (2)	0.0551 (9)
H11	0.1989	0.2799	0.6410	0.061 (11)*
C12	0.4257 (6)	0.3773 (3)	0.7630 (2)	0.0371 (7)
N3	0.7285 (5)	0.5133 (2)	0.89942 (16)	0.0321 (5)
H3A	0.895 (5)	0.564 (3)	0.917 (2)	0.052 (10)*
H3B	0.745 (6)	0.449 (2)	0.9267 (19)	0.043 (9)*
H3C	0.588 (5)	0.558 (3)	0.926 (2)	0.046 (9)*
N4	0.2718 (6)	0.3266 (3)	0.8209 (2)	0.0508 (7)
H4A	0.372 (7)	0.311 (4)	0.867 (2)	0.076 (13)*
H4B	0.135 (6)	0.266 (3)	0.790 (2)	0.065 (11)*
O1	0.5217 (4)	0.8037 (2)	0.92225 (14)	0.0429 (5)
H1D	0.692 (3)	0.799 (3)	0.940 (2)	0.064 (11)*
O2	0.0401 (4)	0.8199 (2)	0.95819 (16)	0.0524 (6)
O3	0.2896 (5)	0.63962 (19)	0.98533 (15)	0.0475 (6)
O4	0.4165 (4)	0.86357 (19)	1.08978 (13)	0.0407 (5)

P1	0.31296 (13)	0.78084 (6)	0.99259 (5)	0.02434 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0285 (14)	0.0316 (15)	0.0257 (13)	−0.0056 (11)	0.0010 (11)	0.0076 (11)
C2	0.0474 (18)	0.0450 (18)	0.0349 (16)	0.0065 (15)	0.0069 (14)	0.0084 (14)
C3	0.067 (2)	0.059 (2)	0.045 (2)	0.0181 (19)	0.0133 (17)	0.0015 (17)
C4	0.065 (2)	0.080 (3)	0.0335 (19)	0.011 (2)	0.0065 (16)	0.0061 (18)
C5	0.051 (2)	0.081 (3)	0.0347 (17)	0.0056 (19)	−0.0001 (15)	0.0248 (18)
C6	0.0325 (16)	0.0440 (17)	0.0370 (16)	−0.0026 (13)	0.0014 (12)	0.0161 (13)
N1	0.0293 (13)	0.0301 (13)	0.0267 (12)	0.0017 (10)	0.0011 (10)	0.0080 (10)
N2	0.0471 (17)	0.0611 (18)	0.0478 (17)	0.0145 (14)	0.0051 (14)	0.0270 (15)
C7	0.0321 (15)	0.0303 (15)	0.0350 (15)	0.0118 (12)	0.0032 (12)	0.0093 (12)
C8	0.0430 (19)	0.059 (2)	0.051 (2)	0.0094 (17)	0.0126 (15)	0.0215 (17)
C9	0.069 (3)	0.100 (3)	0.053 (2)	0.029 (2)	0.025 (2)	0.039 (2)
C10	0.075 (3)	0.098 (3)	0.035 (2)	0.034 (3)	0.0019 (19)	0.015 (2)
C11	0.060 (2)	0.053 (2)	0.0439 (19)	0.0135 (18)	−0.0113 (17)	0.0038 (16)
C12	0.0409 (17)	0.0309 (15)	0.0377 (16)	0.0121 (13)	−0.0036 (13)	0.0075 (12)
N3	0.0308 (14)	0.0290 (13)	0.0353 (13)	0.0021 (11)	0.0013 (10)	0.0083 (11)
N4	0.0484 (17)	0.0438 (17)	0.0583 (19)	−0.0114 (14)	−0.0164 (15)	0.0215 (15)
O1	0.0187 (10)	0.0748 (16)	0.0457 (12)	0.0028 (10)	0.0043 (9)	0.0346 (11)
O2	0.0195 (10)	0.0860 (18)	0.0641 (15)	0.0096 (10)	0.0061 (9)	0.0404 (13)
O3	0.0651 (15)	0.0264 (11)	0.0524 (13)	0.0050 (10)	0.0176 (11)	0.0115 (9)
O4	0.0401 (11)	0.0419 (12)	0.0329 (11)	−0.0036 (9)	0.0010 (9)	0.0031 (9)
P1	0.0160 (3)	0.0270 (4)	0.0319 (4)	0.0021 (2)	0.0026 (2)	0.0116 (3)

Geometric parameters (Å, º)

C1—C6	1.380 (4)	C8—C9	1.382 (5)
C1—C2	1.391 (4)	C8—H8	0.9300
C1—N1	1.450 (3)	C9—C10	1.369 (6)
C2—C3	1.368 (4)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.367 (5)
C3—C4	1.363 (5)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.385 (4)
C4—C5	1.363 (5)	C11—H11	0.9300
C4—H4	0.9300	C12—N4	1.383 (4)
C5—C6	1.403 (4)	N3—H3A	0.902 (18)
C5—H5	0.9300	N3—H3B	0.913 (18)
C6—N2	1.384 (4)	N3—H3C	0.906 (18)
N1—H1A	0.923 (19)	N4—H4A	0.880 (19)
N1—H1B	0.915 (17)	N4—H4B	0.885 (19)
N1—H1C	0.931 (17)	O1—P1	1.561 (2)
N2—H2A	0.919 (18)	O1—H1D	0.846 (10)
N2—H2B	0.901 (19)	O2—P1	1.504 (2)
C7—C8	1.366 (4)	O3—P1	1.504 (2)
C7—C12	1.387 (4)	O4—P1	1.497 (2)

C7—N3	1.450 (4)		
C6—C1—C2	121.3 (3)	C7—C8—H8	120.1
C6—C1—N1	121.2 (2)	C9—C8—H8	120.1
C2—C1—N1	117.5 (2)	C10—C9—C8	119.3 (4)
C3—C2—C1	120.2 (3)	C10—C9—H9	120.4
C3—C2—H2	119.9	C8—C9—H9	120.4
C1—C2—H2	119.9	C11—C10—C9	120.6 (3)
C4—C3—C2	119.0 (3)	C11—C10—H10	119.7
C4—C3—H3	120.5	C9—C10—H10	119.7
C2—C3—H3	120.5	C10—C11—C12	121.3 (4)
C5—C4—C3	121.6 (3)	C10—C11—H11	119.3
C5—C4—H4	119.2	C12—C11—H11	119.3
C3—C4—H4	119.2	N4—C12—C11	121.7 (3)
C4—C5—C6	120.8 (3)	N4—C12—C7	121.0 (3)
C4—C5—H5	119.6	C11—C12—C7	117.1 (3)
C6—C5—H5	119.6	C7—N3—H3A	113 (2)
C1—C6—N2	121.9 (3)	C7—N3—H3B	116.0 (19)
C1—C6—C5	117.1 (3)	H3A—N3—H3B	105 (3)
N2—C6—C5	120.8 (3)	C7—N3—H3C	107 (2)
C1—N1—H1A	110 (2)	H3A—N3—H3C	110 (3)
C1—N1—H1B	110.7 (19)	H3B—N3—H3C	105 (3)
H1A—N1—H1B	105 (3)	C12—N4—H4A	116 (3)
C1—N1—H1C	112.3 (18)	C12—N4—H4B	113 (2)
H1A—N1—H1C	109 (3)	H4A—N4—H4B	116 (4)
H1B—N1—H1C	110 (3)	P1—O1—H1D	113 (2)
C6—N2—H2A	118 (2)	O4—P1—O2	111.69 (13)
C6—N2—H2B	110 (2)	O4—P1—O3	111.37 (12)
H2A—N2—H2B	112 (3)	O2—P1—O3	111.93 (14)
C8—C7—C12	121.9 (3)	O4—P1—O1	110.20 (12)
C8—C7—N3	119.8 (3)	O2—P1—O1	103.14 (11)
C12—C7—N3	118.2 (3)	O3—P1—O1	108.14 (12)
C7—C8—C9	119.8 (4)		
C6—C1—C2—C3	−0.1 (5)	C12—C7—C8—C9	0.4 (5)
N1—C1—C2—C3	−177.0 (3)	N3—C7—C8—C9	−176.2 (3)
C1—C2—C3—C4	0.5 (5)	C7—C8—C9—C10	−0.5 (5)
C2—C3—C4—C5	−1.1 (6)	C8—C9—C10—C11	0.0 (6)
C3—C4—C5—C6	1.5 (6)	C9—C10—C11—C12	0.7 (6)
C2—C1—C6—N2	−175.3 (3)	C10—C11—C12—N4	175.2 (3)
N1—C1—C6—N2	1.4 (4)	C10—C11—C12—C7	−0.8 (5)
C2—C1—C6—C5	0.4 (4)	C8—C7—C12—N4	−175.7 (3)
N1—C1—C6—C5	177.2 (3)	N3—C7—C12—N4	0.9 (4)
C4—C5—C6—C1	−1.1 (5)	C8—C7—C12—C11	0.3 (4)
C4—C5—C6—N2	174.7 (3)	N3—C7—C12—C11	176.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*D*···O2[i]	0.85 (1)	1.65 (1)	2.470 (3)	164 (4)
N3—H3*A*···O3[i]	0.90 (2)	2.06 (2)	2.928 (3)	160 (3)
N1—H1*A*···O4[ii]	0.92 (2)	1.81 (2)	2.720 (3)	171 (3)
N1—H1*C*···O4[iii]	0.93 (2)	2.02 (2)	2.953 (3)	179 (3)
N2—H2*A*···O4[iii]	0.92 (2)	1.99 (2)	2.904 (4)	170 (3)
N4—H4*A*···O4[iv]	0.88 (2)	2.45 (3)	3.188 (4)	142 (3)
N3—H3*B*···O3[iv]	0.91 (2)	1.87 (2)	2.740 (3)	159 (3)
N3—H3*C*···O3	0.91 (2)	1.87 (2)	2.778 (3)	176 (3)
N1—H1*B*···O2	0.92 (2)	1.83 (2)	2.734 (3)	169 (3)
N4—H4*B*···N2[v]	0.89 (2)	2.33 (2)	3.210 (4)	172 (3)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+2, −*z*+2; (iii) −*x*, −*y*+2, −*z*+2; (iv) −*x*+1, −*y*+1, −*z*+2; (v) *x*, *y*−1, *z*.