Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368
Editors: **W. Clegg and D. G. Watson**

5,5′-Diamino-2,2′-bipyridin-1,1′-diium bis(5,5′-diamino-2,2′-bipyridin-1-ium) tetrakis(*rac*-1,1′-binaphthalene-2,2′-diyl phosphate) hexahydrate: a two-dimensional supramolecular hydrogen-bonded network

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5,5′-Diamino-2,2′-bipyridin-1,1′-diium bis(5,5′-diamino-2,2′-bipyridin-1-ium) tetrakis(*rac*-1,1′-binaphthalene-2,2′-diyl phosphate) hexahydrate: a two-dimensional supramolecular hydrogen-bonded network

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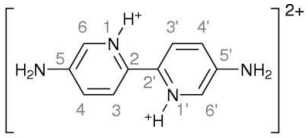
Received 2 April 2007; accepted 3 May 2007

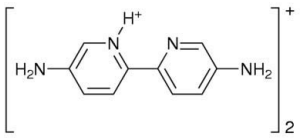
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.138; data-to-parameter ratio = 12.1.

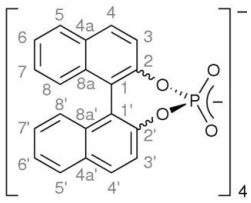
In the title compound, $C_{10}H_{12}N_4^{2+}\cdot 2C_{10}H_{11}N_4^{+}\cdot 4C_{20}H_{12}O_4P^{-}\cdot 6H_2O$, the 1,1′-binaphthalene-2,2′-diyl phosphate anion and 5,5′-diamino-2,2′-bipyridine as hydrogen-acceptor and -donor building blocks, respectively, are combined in a supramolecular two-dimensional hydrogen-bonding network of one centrosymmetric diprotonated diaminobipyridin-1,1′-ium dication, two monoprotonated diaminobipyridinium cations, four phosphate counter-anions and six water molecules of crystallization. Protonation of diaminobipyridine to the bipyridinium mono- or dication enhances the hydrogen bonding due to the primary electrostatic attraction with the anion. The packing can be rationalized by a separation of the hydrophobic binaphthyl backbone from the hydrophilic $(RO)_2PO_2^{-}$ phosphate groups, bipyridinium cation and water components. The binaphthyl tail-to-tail packing in the hydrophobic lamellae as well as the diaminobipyridinium packing is governed by π–π and C—H$\cdots\pi$ interactions.

Related literature

For related literature, see: Dorn *et al.* (2005); Dorn *et al.* (2006); Janiak, Deblon, Wu *et al.* (1999); Janiak, Deblon & Wu (1999); Janiak (2000); Nishio (2004); Yang *et al.* (2003); Yang *et al.* (2004).







·6 H_2O
hexahydrate

Experimental

Crystal data

$C_{10}H_{12}N_4^{2+}\cdot 2C_{10}H_{11}N_4^{+}\cdot 4C_{20}H_{12}O_4P^{-}\cdot 6H_2O$
M_r = 2059.86
Triclinic, $P\overline{1}$
a = 9.7001 (16) Å
b = 14.102 (2) Å
c = 18.244 (3) Å
α = 82.940 (11)°
β = 76.232 (11)°
γ = 85.571 (10)°
V = 2402.5 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 203 (2) K
0.56 × 0.04 × 0.03 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.914, T_{max} = 0.996
24014 measured reflections
8570 independent reflections
4686 reflections with $I > 2\sigma(I)$
R_{int} = 0.098

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.138
S = 0.99
8570 reflections
709 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O2	0.92 (4)	2.33 (4)	3.172 (4)	151 (3)
N3—H3$B\cdots$O8^{i}	0.90 (4)	1.97 (4)	2.830 (4)	161 (4)
N3—H3$C\cdots$O10^{ii}	0.96 (4)	2.08 (5)	3.016 (5)	164 (4)
N4—H4$C\cdots$O9	0.97 (3)	2.18 (4)	3.124 (5)	163 (4)
N5—H5$\cdots$O4^{iii}	0.98 (4)	1.61 (4)	2.581 (4)	167 (3)
N6—H6$B\cdots$O10^{iv}	0.96 (4)	2.05 (4)	3.006 (5)	173 (4)
N6—H6$C\cdots$O11	0.81 (5)	2.34 (5)	3.078 (6)	153 (5)
O9—H9$B\cdots$O3^{v}	0.85 (4)	2.06 (4)	2.875 (4)	159 (4)
O9—H9$C\cdots$O7	0.88 (5)	1.89 (5)	2.753 (4)	164 (4)
O10—H10$A\cdots$O11^{vi}	0.96 (4)	1.85 (4)	2.787 (4)	166 (4)
O10—H10$B\cdots$O9	0.93 (5)	1.98 (5)	2.874 (4)	162 (4)
O11—H11$B\cdots$O3^{v}	0.91 (6)	1.99 (5)	2.817 (4)	151 (5)
O11—H11$A\cdots$O7	0.78 (5)	2.44 (5)	3.046 (4)	136 (5)
O11—H11$A\cdots$O8	0.78 (5)	2.59 (6)	3.264 (5)	147 (6)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

 doi:10.1107/S1600536807021794

DIAMOND (Crystal Impact, 2006); software used to prepare material for publication: *SHELXL97*.

Support through grant Ja466/14-1 is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2222).

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supplementary materials

Acta Cryst. (2007). E**63**, o2871-o2872 [**doi:10.1107/S1600536807021794**]

5,5'-Diamino-2,2'-bipyridin-1,1'-diium bis(5,5'-diamino-2,2'-bipyridin-1-ium) tetrakis(*rac*-1,1'-binaphthalene-2,2'-diyl phosphate) hexahydrate: a two-dimensional supramolecular hydrogen-bonded network

B. Wisser and C. Janiak

Comment

The reaction and crystallization conditions combine one diprotonated diaminobipyridin-1,1'-ium dication with two monoprotonated diaminobipyridinium cations in a network with four phosphate counteranions and six water molecules of crystallization (Dorn *et al.*, 2005; Dorn *et al.*, 2006; Janiak, Deblon & Wu, 1999; Yang *et al.*, 2003; Yang *et al.*, 2004). The dication sits on an inversion center which bisects the central C–C-bond and relates the two pyridinium halves of the molecule. The packing in **1** can be rationalized by a separation of the hydrophobic binaphthyl backbone from the hydrophilic $(RO)_2PO_2^-$ phosphate groups, bipyridinium cation and hydrate components, as seen before (Dorn *et al.*, 2006). Fig. 1 shows a projection of the unit cell crystal packing to illustrate the lamellar or layer-like arrangement of the hydrophobic and hydrophilic regions. The latter are also highlighted by the hydrogen-bonding network as red dashes. Details of part of the hydrogen-bonding network between diaminobipyrdinium, phosphate and crystal water are visualized in Fig. 2 (see Table for bond distances and angles). The binaphthyl tail-to-tail packing in the hydrophobic lamellar as well as the diaminobipyridinium packing is governed by π-π and C–H···π interactions (Dorn *et al.*, 2006; Janiak, 2000; Nishio, 2004).

Experimental

5,5'-Diamino-2,2'-bipyridine (186 mg, 0.10 mmol) (Janiak, Deblon, Wu *et al.*, 1999) was dissolved in 50 ml of hot H_2O. This solution was added to a solution of racemic 1,1'-binaphthalene-2,2'-diyl phosphoric acid (348 mg, 0.10 mmol) (Dorn *et al.*, 2006) in 20 ml of methanol. The solvent was slowly allowed to evaporate. After two weeks yellow needles of **1** were formed and separated by filtration. Crystal yield 334 mg, 65%. Analysis calculated for $C_{110}H_{94}N_{12}O_{22}P_4$ (2058.84): C 64.14, H 4.55, N 8.16%; found: C 63.60, H 4.77, N 8.99%. IR (KBr, ν cm^{-1}): 3345, 1636, 1587, 1550, 1507, 1486, 1464, 1328, 1241, 1218, 1156, 1095, 1069, 992, 961, 836, 750, 717, 656, 568, 535; ^{1}H-NMR (DMSO-d_6): δ 8.03 (d, $H5_{phosphate}$, $^3J_{5,6}$ = 9.0 Hz), 8.02–7.99 (m, $H4_{phosphate}$/$H6_{bipyridine}$), 7.97 (d, $H3_{bipyridine}$, $^3J_{3,4}$ = 8.9 Hz), 7.46–7.40 (m, $H6_{phosphate}$/$H7_{phosphate}$), 7.35–7.27 (m, $H8_{phosphate}$/$H4_{bipyridine}$), 7.23 (d, $H3_{phosphate}$, $^3J_{3,4}$ = 8.1 Hz).

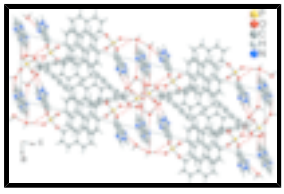
Refinement

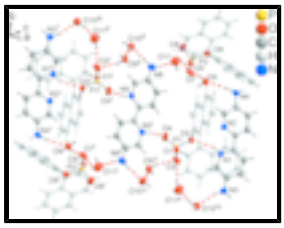
The needle morphology of the crystal gave rise to a somewhat high R_{int} and other R values. Yet, structure solution and refinement proceeded without problems. The quality of the data set enabled the localization and refinement of the protic hydrogen atoms.

Hydrogen atoms on carbon were calculated with appropriate riding models (AFIX 43 for aromatic CH, AFIX 13 for CH, AFIX 23 for CH_2, AFIX 33 for CH_3) and U_{eq}(H) = 1.2 U_{eq}(CH) or 1.5 U_{eq}(CH3), respectively.

Hydrogen atoms on N (NH_2 and NH) and O (H_2O) were found from difference Fourier maps and refined with U_{eq}(H) = 1.5 U_{eq}(N/O)

Figures





Scheme 1: Molecular composition of (5,5'-diamino-2,2'-bipyridin-1,1'-diium) bis(5,5'-diamino-2,2'-bipyridin-1-ium) tetrakis(rac-1,1'-binaphthalene-2,2'-diyl phosphate) hexahydrate, $(C_{10}H_{12}N_4)(C_{10}H_{11}N_4)_2(C_{20}H_{12}PO_4)_4(H_2O)_6$ **1** with nomenclature numbering scheme.
Fig. 1: Projection of the crystal packing in **1** onto the (0 1 0) plane. Hydrogen bonds are indicated as red dashes.
Fig. 2: Part of the hydrogen-bonding network between diaminobipyrdinium, phosphate and crystal water in **1**. Hydrogen bonds are indicated with red dashes (see Table for bond distances and angles). Symmetry code: i = – *x*, 1 – *y*, – *z*; ii = – 1 + *x*, *y*, *z*; iii = – *x*, 2 – *y*, – *z*; iv = *x*, *y* – 1, *z*; v = 1 – *x*, 1 – *y*, – *z*;. The naphthyl groups are depicted transparent for clarity. Displacement ellipsoids are drawn at the 50% probability level, hydrogen atoms with a standard radius of 0.135 Å.

5,5'-Diamino-2,2'-bipyridin-1,1'-dium bis(5,5'-diamino-2,2'-bipyridin-1-ium) tetrakis(*rac*-1,1'-binaphthalene-2,2'-diyl phosphate) hexahydrate

Crystal data

$C_{10}H_{12}N_4^{2+}\cdot 2C_{10}H_{11}N_4^{+}\cdot 4C_{20}H_{12}O_4P^{-}\cdot 6H_2O$	V = 2402.5 (7) Å^3
M_r = 2059.86	Z = 1
Triclinic, $P\overline{1}$	F_{000} = 1074
Hall symbol: -P 1	D_x = 1.424 Mg m^{-3}
a = 9.7001 (16) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 14.102 (2) Å	μ = 0.16 mm^{-1}
c = 18.244 (3) Å	T = 203 (2) K
α = 82.940 (11)°	Needle, yellow
β = 76.232 (11)°	0.56 × 0.04 × 0.03 mm
γ = 85.571 (10)°	

Data collection

Bruker APEXII CCD diffractometer	8570 independent reflections
Radiation source: fine-focus sealed tube	4686 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.098
T = 203(2) K	θ_{max} = 25.3°
ω scans	θ_{min} = 1.5°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.914, T_{max} = 0.996	k = −16→16
24014 measured reflections	l = −21→21

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.138$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.99$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
8570 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
709 parameters	Extinction correction: none
2 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.43917 (11)	0.31213 (7)	0.04758 (5)	0.0382 (3)
O1	0.3322 (2)	0.25002 (15)	0.11340 (11)	0.0332 (6)
O2	0.5291 (2)	0.36183 (14)	0.09484 (12)	0.0328 (5)
O3	0.5400 (3)	0.25075 (18)	−0.00114 (13)	0.0533 (7)
O4	0.3487 (3)	0.38558 (18)	0.01291 (14)	0.0542 (7)
C1	0.4313 (4)	0.2395 (2)	0.22255 (17)	0.0287 (8)
C2	0.3948 (4)	0.1947 (2)	0.16755 (17)	0.0296 (8)
C3	0.4198 (4)	0.0964 (2)	0.16155 (18)	0.0361 (9)
H3A	0.3909	0.0683	0.1239	0.043*
C4	0.4864 (4)	0.0423 (2)	0.21105 (18)	0.0361 (9)
H4A	0.5011	−0.0239	0.2081	0.043*
C5	0.5339 (4)	0.0834 (2)	0.26684 (17)	0.0313 (8)
C6	0.6104 (4)	0.0294 (2)	0.3161 (2)	0.0400 (9)
H6A	0.6261	−0.0369	0.3138	0.048*
C7	0.6615 (4)	0.0710 (2)	0.3665 (2)	0.0438 (10)

H7	0.7109	0.0335	0.3991	0.053*
C8	0.6410 (4)	0.1706 (2)	0.3701 (2)	0.0417 (10)
H8	0.6794	0.1998	0.4039	0.050*
C9	0.5654 (4)	0.2245 (2)	0.32452 (18)	0.0348 (9)
H9A	0.5518	0.2907	0.3277	0.042*
C10	0.5068 (4)	0.1834 (2)	0.27248 (17)	0.0281 (8)
C11	0.4023 (4)	0.3453 (2)	0.22337 (18)	0.0299 (8)
C12	0.4491 (4)	0.4038 (2)	0.15860 (18)	0.0306 (8)
C13	0.4266 (4)	0.5036 (2)	0.1525 (2)	0.0359 (9)
H13	0.4587	0.5406	0.1059	0.043*
C14	0.3582 (4)	0.5458 (2)	0.2145 (2)	0.0390 (9)
H14	0.3453	0.6128	0.2113	0.047*
C15	0.3060 (4)	0.4904 (2)	0.28375 (19)	0.0329 (8)
C16	0.2358 (4)	0.5335 (2)	0.3490 (2)	0.0409 (9)
H16	0.2247	0.6005	0.3463	0.049*
C17	0.1837 (4)	0.4805 (2)	0.4158 (2)	0.0437 (10)
H17	0.1380	0.5108	0.4589	0.052*
C18	0.1983 (4)	0.3805 (2)	0.4203 (2)	0.0401 (9)
H18	0.1620	0.3439	0.4666	0.048*
C19	0.2646 (4)	0.3354 (2)	0.35836 (18)	0.0363 (9)
H19	0.2704	0.2682	0.3619	0.044*
C20	0.3246 (4)	0.3891 (2)	0.28876 (18)	0.0311 (8)
P2	0.17925 (11)	0.83695 (6)	0.24285 (5)	0.0371 (3)
O5	0.0731 (3)	0.76467 (14)	0.30098 (11)	0.0341 (6)
O6	0.2692 (3)	0.87165 (14)	0.29780 (11)	0.0353 (6)
O7	0.2716 (3)	0.77708 (17)	0.18815 (13)	0.0511 (7)
O8	0.1033 (3)	0.92259 (17)	0.21483 (16)	0.0634 (8)
C21	0.0630 (4)	0.8089 (2)	0.42500 (17)	0.0284 (8)
C22	−0.0051 (4)	0.7971 (2)	0.36875 (17)	0.0303 (8)
C23	−0.1514 (4)	0.8136 (2)	0.37639 (19)	0.0348 (8)
H23	−0.1935	0.8025	0.3370	0.042*
C24	−0.2323 (4)	0.8456 (2)	0.44066 (19)	0.0370 (9)
H24	−0.3316	0.8521	0.4474	0.044*
C25	−0.1688 (4)	0.8694 (2)	0.49788 (18)	0.0319 (8)
C26	−0.2476 (4)	0.9113 (2)	0.56202 (19)	0.0382 (9)
H26	−0.3466	0.9211	0.5687	0.046*
C27	−0.1836 (4)	0.9380 (2)	0.6147 (2)	0.0399 (9)
H27	−0.2386	0.9658	0.6572	0.048*
C28	−0.0368 (4)	0.9243 (2)	0.60561 (18)	0.0375 (9)
H28	0.0069	0.9443	0.6415	0.045*
C29	0.0450 (4)	0.8817 (2)	0.54447 (17)	0.0333 (8)
H29	0.1437	0.8724	0.5392	0.040*
C30	−0.0190 (4)	0.8520 (2)	0.48986 (17)	0.0280 (8)
C31	0.2156 (4)	0.7772 (2)	0.41706 (17)	0.0286 (8)
C32	0.3135 (4)	0.8064 (2)	0.35202 (18)	0.0311 (8)
C33	0.4568 (4)	0.7743 (2)	0.3383 (2)	0.0382 (9)
H33	0.5198	0.7952	0.2924	0.046*
C34	0.5044 (4)	0.7130 (2)	0.3912 (2)	0.0417 (9)
H34	0.6008	0.6924	0.3821	0.050*

C35	0.4116 (4)	0.6802 (2)	0.4595 (2)	0.0365 (9)
C36	0.4612 (5)	0.6162 (3)	0.5155 (2)	0.0511 (11)
H36	0.5588	0.5991	0.5082	0.061*
C37	0.3703 (6)	0.5799 (3)	0.5788 (2)	0.0527 (12)
H37	0.4040	0.5378	0.6154	0.063*
C38	0.2246 (5)	0.6055 (2)	0.5896 (2)	0.0493 (11)
H38	0.1609	0.5784	0.6330	0.059*
C39	0.1735 (4)	0.6688 (2)	0.53834 (18)	0.0386 (9)
H39	0.0756	0.6851	0.5474	0.046*
C40	0.2647 (4)	0.7099 (2)	0.47244 (18)	0.0314 (8)
N5	−0.0910 (4)	0.61714 (19)	0.00186 (15)	0.0356 (7)
H5	−0.185 (4)	0.607 (2)	−0.0068 (19)	0.053*
N6	0.0366 (4)	0.8309 (2)	0.0474 (2)	0.0598 (11)
H6B	−0.052 (4)	0.867 (3)	0.048 (3)	0.090*
H6C	0.107 (6)	0.842 (3)	0.060 (3)	0.090*
C51	0.0114 (4)	0.5485 (2)	0.00753 (17)	0.0323 (8)
C52	0.1320 (4)	0.5762 (2)	0.02711 (19)	0.0408 (9)
H52	0.2071	0.5310	0.0308	0.049*
C53	−0.0831 (4)	0.7077 (2)	0.01407 (18)	0.0374 (9)
H53	−0.1583	0.7520	0.0084	0.045*
C54	0.0332 (4)	0.7378 (2)	0.03484 (19)	0.0417 (9)
C55	0.1423 (4)	0.6689 (2)	0.0411 (2)	0.0435 (9)
H55	0.2237	0.6859	0.0550	0.052*
N1	0.8043 (3)	0.2825 (2)	0.15243 (15)	0.0362 (7)
H1	0.738 (4)	0.326 (2)	0.1374 (19)	0.054*
N2	0.7674 (3)	0.46415 (19)	0.17645 (15)	0.0390 (7)
N3	0.8985 (4)	0.0303 (2)	0.14736 (19)	0.0504 (9)
H3B	0.951 (5)	−0.015 (3)	0.169 (2)	0.076*
H3C	0.836 (5)	0.007 (3)	0.121 (2)	0.076*
N4	0.8107 (4)	0.7086 (2)	0.20931 (18)	0.0449 (8)
H4B	0.883 (5)	0.742 (3)	0.210 (2)	0.067*
H4C	0.745 (4)	0.742 (3)	0.181 (2)	0.067*
C41	0.8992 (4)	0.3158 (2)	0.18548 (18)	0.0354 (8)
C42	0.9989 (4)	0.2483 (2)	0.20719 (19)	0.0410 (9)
H42	1.0675	0.2676	0.2302	0.049*
C43	0.9982 (4)	0.1544 (2)	0.19537 (19)	0.0399 (9)
H43	1.0659	0.1102	0.2110	0.048*
C44	0.8984 (4)	0.1225 (2)	0.16032 (19)	0.0386 (9)
C45	0.7994 (4)	0.1913 (2)	0.13969 (19)	0.0374 (9)
H45	0.7293	0.1737	0.1169	0.045*
C46	0.8861 (4)	0.4183 (2)	0.19335 (18)	0.0350 (8)
C47	0.9849 (4)	0.4665 (2)	0.21622 (19)	0.0431 (9)
H47	1.0661	0.4334	0.2279	0.052*
C48	0.9633 (4)	0.5637 (3)	0.22177 (19)	0.0438 (9)
H48	1.0299	0.5972	0.2371	0.053*
C49	0.8424 (4)	0.6115 (2)	0.20454 (18)	0.0383 (9)
C50	0.7481 (4)	0.5573 (2)	0.1819 (2)	0.0422 (9)
H50	0.6661	0.5888	0.1698	0.051*
O9	0.5612 (3)	0.7794 (2)	0.13189 (16)	0.0515 (8)

H9B	0.547 (5)	0.758 (3)	0.093 (3)	0.077*
H9C	0.471 (5)	0.787 (3)	0.155 (3)	0.077*
O10	0.7472 (3)	0.9282 (2)	0.05583 (17)	0.0573 (8)
H10A	0.718 (5)	0.973 (3)	0.018 (2)	0.086*
H10B	0.674 (5)	0.891 (3)	0.084 (3)	0.086*
O11	0.3160 (4)	0.9211 (2)	0.04676 (17)	0.0750 (10)
H11A	0.298 (7)	0.914 (4)	0.091 (3)	0.113*
H11B	0.386 (6)	0.880 (4)	0.025 (3)	0.113*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0350 (6)	0.0509 (6)	0.0303 (5)	−0.0097 (5)	−0.0106 (5)	−0.0004 (4)
O1	0.0283 (15)	0.0428 (13)	0.0287 (12)	−0.0061 (11)	−0.0065 (11)	−0.0014 (10)
O2	0.0252 (14)	0.0410 (12)	0.0327 (13)	−0.0064 (11)	−0.0069 (11)	−0.0031 (10)
O3	0.0499 (19)	0.0655 (17)	0.0447 (15)	−0.0162 (14)	0.0003 (14)	−0.0212 (13)
O4	0.0422 (18)	0.0667 (16)	0.0574 (16)	−0.0151 (14)	−0.0280 (15)	0.0194 (13)
C1	0.026 (2)	0.0312 (17)	0.0271 (17)	−0.0029 (15)	−0.0020 (16)	−0.0048 (14)
C2	0.025 (2)	0.0344 (18)	0.0288 (18)	−0.0005 (15)	−0.0065 (16)	−0.0029 (14)
C3	0.040 (2)	0.0388 (19)	0.0314 (19)	−0.0115 (17)	−0.0061 (18)	−0.0099 (15)
C4	0.042 (2)	0.0248 (16)	0.041 (2)	−0.0055 (16)	−0.0052 (19)	−0.0079 (15)
C5	0.031 (2)	0.0301 (17)	0.0308 (18)	−0.0018 (15)	−0.0034 (17)	−0.0024 (14)
C6	0.041 (2)	0.0291 (17)	0.049 (2)	0.0017 (17)	−0.010 (2)	−0.0052 (16)
C7	0.041 (3)	0.041 (2)	0.052 (2)	0.0053 (18)	−0.020 (2)	−0.0009 (17)
C8	0.045 (3)	0.040 (2)	0.048 (2)	0.0001 (18)	−0.027 (2)	−0.0055 (16)
C9	0.038 (2)	0.0320 (18)	0.0362 (19)	0.0016 (16)	−0.0127 (18)	−0.0063 (15)
C10	0.025 (2)	0.0283 (16)	0.0283 (18)	−0.0039 (14)	−0.0017 (16)	−0.0023 (13)
C11	0.027 (2)	0.0318 (17)	0.0332 (19)	−0.0049 (15)	−0.0119 (17)	−0.0015 (15)
C12	0.022 (2)	0.0377 (18)	0.0317 (19)	−0.0008 (15)	−0.0045 (16)	−0.0041 (15)
C13	0.035 (2)	0.0331 (18)	0.040 (2)	−0.0065 (16)	−0.0120 (18)	0.0046 (16)
C14	0.041 (2)	0.0267 (17)	0.050 (2)	−0.0053 (16)	−0.013 (2)	−0.0008 (16)
C15	0.029 (2)	0.0294 (17)	0.043 (2)	−0.0021 (15)	−0.0121 (18)	−0.0067 (15)
C16	0.042 (3)	0.0281 (17)	0.056 (2)	−0.0003 (17)	−0.013 (2)	−0.0131 (17)
C17	0.046 (3)	0.040 (2)	0.045 (2)	−0.0021 (18)	−0.004 (2)	−0.0179 (18)
C18	0.038 (2)	0.042 (2)	0.039 (2)	−0.0019 (17)	−0.0041 (19)	−0.0093 (16)
C19	0.037 (2)	0.0325 (18)	0.040 (2)	−0.0022 (16)	−0.0065 (18)	−0.0073 (16)
C20	0.031 (2)	0.0306 (17)	0.0340 (19)	−0.0009 (15)	−0.0119 (17)	−0.0038 (15)
P2	0.0438 (7)	0.0362 (5)	0.0303 (5)	−0.0028 (4)	−0.0073 (5)	−0.0013 (4)
O5	0.0390 (16)	0.0327 (12)	0.0299 (12)	−0.0019 (11)	−0.0033 (12)	−0.0093 (10)
O6	0.0426 (16)	0.0315 (12)	0.0305 (12)	−0.0063 (11)	−0.0058 (12)	−0.0001 (10)
O7	0.0531 (19)	0.0622 (16)	0.0335 (14)	−0.0117 (13)	0.0089 (13)	−0.0198 (12)
O8	0.073 (2)	0.0460 (15)	0.0757 (19)	0.0024 (14)	−0.0383 (18)	0.0118 (13)
C21	0.028 (2)	0.0295 (16)	0.0271 (18)	−0.0028 (15)	−0.0041 (16)	−0.0021 (14)
C22	0.030 (2)	0.0299 (17)	0.0287 (18)	−0.0015 (15)	−0.0017 (17)	−0.0061 (14)
C23	0.035 (2)	0.0379 (19)	0.034 (2)	−0.0037 (17)	−0.0120 (18)	−0.0040 (15)
C24	0.028 (2)	0.0383 (19)	0.043 (2)	0.0025 (16)	−0.0074 (19)	−0.0049 (16)
C25	0.032 (2)	0.0264 (17)	0.0321 (19)	−0.0040 (15)	0.0027 (17)	−0.0012 (14)
C26	0.036 (2)	0.0311 (18)	0.041 (2)	−0.0012 (16)	0.0020 (19)	−0.0003 (16)

C27	0.041 (3)	0.0359 (19)	0.037 (2)	−0.0047 (17)	0.0067 (19)	−0.0100 (16)
C28	0.049 (3)	0.0351 (18)	0.0276 (19)	−0.0079 (17)	−0.0031 (18)	−0.0085 (15)
C29	0.036 (2)	0.0316 (17)	0.0339 (19)	0.0014 (16)	−0.0116 (18)	−0.0067 (14)
C30	0.030 (2)	0.0238 (16)	0.0272 (18)	−0.0020 (14)	−0.0003 (16)	−0.0044 (13)
C31	0.031 (2)	0.0269 (16)	0.0306 (18)	−0.0024 (15)	−0.0094 (17)	−0.0094 (14)
C32	0.033 (2)	0.0304 (17)	0.0310 (19)	−0.0046 (16)	−0.0080 (18)	−0.0061 (14)
C33	0.032 (2)	0.0375 (19)	0.045 (2)	−0.0062 (17)	−0.0016 (19)	−0.0120 (16)
C34	0.029 (2)	0.044 (2)	0.057 (2)	0.0032 (17)	−0.015 (2)	−0.0180 (18)
C35	0.041 (2)	0.0311 (18)	0.043 (2)	−0.0008 (17)	−0.015 (2)	−0.0155 (16)
C36	0.058 (3)	0.044 (2)	0.062 (3)	0.012 (2)	−0.035 (3)	−0.016 (2)
C37	0.083 (4)	0.038 (2)	0.046 (2)	0.014 (2)	−0.034 (3)	−0.0069 (18)
C38	0.077 (4)	0.0344 (19)	0.034 (2)	0.001 (2)	−0.010 (2)	−0.0041 (16)
C39	0.046 (3)	0.0368 (19)	0.034 (2)	0.0005 (18)	−0.0095 (19)	−0.0091 (16)
C40	0.038 (2)	0.0281 (17)	0.0313 (19)	−0.0034 (16)	−0.0104 (18)	−0.0091 (14)
N5	0.036 (2)	0.0374 (16)	0.0349 (16)	−0.0057 (15)	−0.0100 (15)	−0.0039 (13)
N6	0.050 (3)	0.049 (2)	0.084 (3)	−0.0069 (18)	−0.013 (2)	−0.0250 (19)
C51	0.031 (2)	0.0375 (18)	0.0270 (18)	−0.0064 (16)	−0.0027 (16)	−0.0028 (14)
C52	0.033 (2)	0.044 (2)	0.047 (2)	−0.0038 (17)	−0.0092 (19)	−0.0076 (17)
C53	0.039 (2)	0.038 (2)	0.034 (2)	−0.0024 (17)	−0.0057 (18)	−0.0051 (15)
C54	0.040 (3)	0.042 (2)	0.041 (2)	−0.0120 (18)	0.0005 (19)	−0.0093 (16)
C55	0.034 (2)	0.050 (2)	0.049 (2)	−0.0087 (19)	−0.007 (2)	−0.0136 (18)
N1	0.0306 (19)	0.0391 (17)	0.0387 (17)	−0.0014 (14)	−0.0097 (15)	−0.0007 (13)
N2	0.033 (2)	0.0403 (17)	0.0443 (18)	−0.0010 (14)	−0.0104 (16)	−0.0060 (13)
N3	0.051 (2)	0.0400 (19)	0.063 (2)	0.0045 (16)	−0.0210 (19)	−0.0071 (16)
N4	0.041 (2)	0.0436 (19)	0.052 (2)	−0.0053 (15)	−0.0072 (18)	−0.0182 (15)
C41	0.032 (2)	0.0420 (19)	0.0311 (19)	−0.0027 (17)	−0.0072 (18)	0.0008 (15)
C42	0.034 (2)	0.050 (2)	0.038 (2)	−0.0044 (18)	−0.0091 (19)	0.0019 (17)
C43	0.036 (2)	0.044 (2)	0.038 (2)	0.0050 (18)	−0.0098 (19)	0.0018 (16)
C44	0.030 (2)	0.046 (2)	0.037 (2)	−0.0005 (18)	−0.0057 (18)	0.0000 (16)
C45	0.030 (2)	0.043 (2)	0.039 (2)	−0.0024 (17)	−0.0080 (18)	−0.0022 (16)
C46	0.032 (2)	0.044 (2)	0.0286 (18)	−0.0074 (17)	−0.0049 (17)	−0.0015 (15)
C47	0.036 (2)	0.050 (2)	0.046 (2)	−0.0046 (19)	−0.014 (2)	−0.0046 (17)
C48	0.038 (3)	0.055 (2)	0.041 (2)	−0.0087 (19)	−0.0097 (19)	−0.0112 (17)
C49	0.039 (2)	0.044 (2)	0.0294 (19)	−0.0045 (18)	−0.0013 (18)	−0.0090 (15)
C50	0.037 (2)	0.044 (2)	0.048 (2)	−0.0004 (18)	−0.013 (2)	−0.0095 (17)
O9	0.0481 (19)	0.0677 (18)	0.0424 (17)	−0.0006 (16)	−0.0129 (15)	−0.0161 (13)
O10	0.055 (2)	0.0572 (18)	0.0596 (19)	−0.0041 (15)	−0.0156 (17)	0.0004 (14)
O11	0.083 (3)	0.086 (2)	0.0466 (18)	0.0059 (18)	−0.008 (2)	0.0079 (17)

Geometric parameters (Å, °)

P1—O3	1.463 (3)	C29—H29	0.9400
P1—O4	1.485 (2)	C31—C32	1.372 (5)
P1—O1	1.605 (2)	C31—C40	1.439 (4)
P1—O2	1.612 (2)	C32—C33	1.402 (5)
O1—C2	1.406 (3)	C33—C34	1.356 (5)
O2—C12	1.405 (4)	C33—H33	0.9400
C1—C2	1.375 (4)	C34—C35	1.401 (5)
C1—C10	1.430 (4)	C34—H34	0.9400

C1—C11	1.498 (4)	C35—C36	1.425 (5)
C2—C3	1.403 (4)	C35—C40	1.427 (5)
C3—C4	1.359 (4)	C36—C37	1.346 (6)
C3—H3A	0.9400	C36—H36	0.9400
C4—C5	1.412 (4)	C37—C38	1.404 (6)
C4—H4A	0.9400	C37—H37	0.9400
C5—C6	1.414 (4)	C38—C39	1.366 (4)
C5—C10	1.426 (4)	C38—H38	0.9400
C6—C7	1.352 (5)	C39—C40	1.402 (5)
C6—H6A	0.9400	C39—H39	0.9400
C7—C8	1.411 (5)	N5—C53	1.333 (4)
C7—H7	0.9400	N5—C51	1.345 (4)
C8—C9	1.362 (4)	N5—H5	0.98 (4)
C8—H8	0.9400	N6—C54	1.364 (5)
C9—C10	1.415 (4)	N6—H6B	0.96 (4)
C9—H9A	0.9400	N6—H6C	0.81 (5)
C11—C12	1.359 (4)	C51—C52	1.397 (5)
C11—C20	1.433 (4)	C51—C51^{i}	1.472 (6)
C12—C13	1.402 (4)	C52—C55	1.377 (5)
C13—C14	1.349 (5)	C52—H52	0.9400
C13—H13	0.9400	C53—C54	1.384 (5)
C14—C15	1.406 (5)	C53—H53	0.9400
C14—H14	0.9400	C54—C55	1.397 (5)
C15—C16	1.407 (5)	C55—H55	0.9400
C15—C20	1.420 (4)	N1—C45	1.342 (4)
C16—C17	1.356 (5)	N1—C41	1.353 (4)
C16—H16	0.9400	N1—H1	0.92 (4)
C17—C18	1.401 (5)	N2—C50	1.324 (4)
C17—H17	0.9400	N2—C46	1.358 (4)
C18—C19	1.365 (5)	N3—C44	1.350 (4)
C18—H18	0.9400	N3—H3B	0.90 (4)
C19—C20	1.416 (5)	N3—H3C	0.96 (4)
C19—H19	0.9400	N4—C49	1.389 (4)
P2—O8	1.467 (2)	N4—H4B	0.87 (4)
P2—O7	1.475 (3)	N4—H4C	0.97 (3)
P2—O5	1.612 (2)	C41—C42	1.395 (4)
P2—O6	1.615 (2)	C41—C46	1.464 (5)
O5—C22	1.397 (4)	C42—C43	1.368 (5)
O6—C32	1.388 (3)	C42—H42	0.9400
C21—C22	1.377 (4)	C43—C44	1.408 (5)
C21—C30	1.434 (4)	C43—H43	0.9400
C21—C31	1.491 (5)	C44—C45	1.394 (5)
C22—C23	1.397 (5)	C45—H45	0.9400
C23—C24	1.354 (5)	C46—C47	1.383 (5)
C23—H23	0.9400	C47—C48	1.383 (5)
C24—C25	1.417 (5)	C47—H47	0.9400
C24—H24	0.9400	C48—C49	1.389 (5)
C25—C26	1.406 (5)	C48—H48	0.9400
C25—C30	1.430 (5)	C49—C50	1.399 (5)

C26—C27	1.363 (5)	C50—H50	0.9400
C26—H26	0.9400	O9—H9B	0.85 (4)
C27—C28	1.395 (5)	O9—H9C	0.88 (5)
C27—H27	0.9400	O10—H10A	0.96 (4)
C28—C29	1.380 (5)	O10—H10B	0.93 (5)
C28—H28	0.9400	O11—H11A	0.78 (5)
C29—C30	1.411 (4)	O11—H11B	0.91 (6)
O3—P1—O4	119.31 (15)	C28—C29—C30	120.3 (4)
O3—P1—O1	111.34 (14)	C28—C29—H29	119.9
O4—P1—O1	105.91 (15)	C30—C29—H29	119.9
O3—P1—O2	106.68 (14)	C29—C30—C25	118.9 (3)
O4—P1—O2	110.01 (14)	C29—C30—C21	121.8 (3)
O1—P1—O2	102.33 (12)	C25—C30—C21	119.3 (3)
C2—O1—P1	115.4 (2)	C32—C31—C40	117.4 (3)
C12—O2—P1	115.8 (2)	C32—C31—C21	119.7 (3)
C2—C1—C10	117.6 (3)	C40—C31—C21	122.7 (3)
C2—C1—C11	119.2 (3)	C31—C32—O6	118.7 (3)
C10—C1—C11	123.0 (3)	C31—C32—C33	122.9 (3)
C1—C2—C3	123.3 (3)	O6—C32—C33	118.4 (3)
C1—C2—O1	118.8 (3)	C34—C33—C32	119.8 (3)
C3—C2—O1	117.9 (3)	C34—C33—H33	120.1
C4—C3—C2	118.9 (3)	C32—C33—H33	120.1
C4—C3—H3A	120.5	C33—C34—C35	120.8 (3)
C2—C3—H3A	120.5	C33—C34—H34	119.6
C3—C4—C5	121.5 (3)	C35—C34—H34	119.6
C3—C4—H4A	119.2	C34—C35—C36	121.1 (4)
C5—C4—H4A	119.2	C34—C35—C40	119.4 (3)
C4—C5—C6	122.4 (3)	C36—C35—C40	119.5 (4)
C4—C5—C10	118.8 (3)	C37—C36—C35	120.9 (4)
C6—C5—C10	118.8 (3)	C37—C36—H36	119.6
C7—C6—C5	121.5 (3)	C35—C36—H36	119.6
C7—C6—H6A	119.2	C36—C37—C38	119.5 (3)
C5—C6—H6A	119.2	C36—C37—H37	120.3
C6—C7—C8	120.2 (3)	C38—C37—H37	120.3
C6—C7—H7	119.9	C39—C38—C37	121.4 (4)
C8—C7—H7	119.9	C39—C38—H38	119.3
C9—C8—C7	119.8 (3)	C37—C38—H38	119.3
C9—C8—H8	120.1	C38—C39—C40	121.1 (4)
C7—C8—H8	120.1	C38—C39—H39	119.5
C8—C9—C10	121.8 (3)	C40—C39—H39	119.5
C8—C9—H9A	119.1	C39—C40—C35	117.5 (3)
C10—C9—H9A	119.1	C39—C40—C31	123.0 (3)
C9—C10—C5	117.8 (3)	C35—C40—C31	119.4 (3)
C9—C10—C1	122.3 (3)	C53—N5—C51	123.8 (3)
C5—C10—C1	119.7 (3)	C53—N5—H5	110 (2)
C12—C11—C20	117.4 (3)	C51—N5—H5	126 (2)
C12—C11—C1	119.0 (3)	C54—N6—H6B	114 (3)
C20—C11—C1	123.6 (3)	C54—N6—H6C	113 (4)
C11—C12—C13	123.9 (3)	H6B—N6—H6C	132 (5)

C11—C12—O2	117.8 (3)	N5—C51—C52	116.5 (3)
C13—C12—O2	118.2 (3)	N5—C51—C51^{i}	118.1 (4)
C14—C13—C12	119.1 (3)	C52—C51—C51^{i}	125.4 (4)
C14—C13—H13	120.4	C55—C52—C51	120.9 (3)
C12—C13—H13	120.4	C55—C52—H52	119.5
C13—C14—C15	120.6 (3)	C51—C52—H52	119.5
C13—C14—H14	119.7	N5—C53—C54	121.6 (3)
C15—C14—H14	119.7	N5—C53—H53	119.2
C14—C15—C16	121.2 (3)	C54—C53—H53	119.2
C14—C15—C20	120.0 (3)	N6—C54—C53	119.7 (4)
C16—C15—C20	118.8 (3)	N6—C54—C55	123.8 (4)
C17—C16—C15	121.5 (3)	C53—C54—C55	116.4 (3)
C17—C16—H16	119.2	C52—C55—C54	120.7 (4)
C15—C16—H16	119.2	C52—C55—H55	119.7
C16—C17—C18	119.7 (3)	C54—C55—H55	119.7
C16—C17—H17	120.1	C45—N1—C41	125.2 (3)
C18—C17—H17	120.1	C45—N1—H1	118 (2)
C19—C18—C17	120.9 (3)	C41—N1—H1	117 (2)
C19—C18—H18	119.5	C50—N2—C46	118.3 (3)
C17—C18—H18	119.5	C44—N3—H3B	120 (3)
C18—C19—C20	120.4 (3)	C44—N3—H3C	124 (2)
C18—C19—H19	119.8	H3B—N3—H3C	115 (4)
C20—C19—H19	119.8	C49—N4—H4B	115 (3)
C19—C20—C15	118.4 (3)	C49—N4—H4C	119 (2)
C19—C20—C11	122.6 (3)	H4B—N4—H4C	114 (4)
C15—C20—C11	118.9 (3)	N1—C41—C42	116.0 (3)
O8—P2—O7	119.53 (16)	N1—C41—C46	116.2 (3)
O8—P2—O5	112.15 (16)	C42—C41—C46	127.7 (3)
O7—P2—O5	105.55 (14)	C43—C42—C41	120.9 (3)
O8—P2—O6	106.54 (14)	C43—C42—H42	119.6
O7—P2—O6	109.94 (15)	C41—C42—H42	119.6
O5—P2—O6	101.72 (12)	C42—C43—C44	121.5 (3)
C22—O5—P2	118.05 (19)	C42—C43—H43	119.2
C32—O6—P2	120.11 (19)	C44—C43—H43	119.2
C22—C21—C30	117.2 (3)	N3—C44—C45	121.8 (4)
C22—C21—C31	120.1 (3)	N3—C44—C43	121.9 (3)
C30—C21—C31	122.7 (3)	C45—C44—C43	116.4 (3)
C21—C22—C23	123.2 (3)	N1—C45—C44	120.0 (3)
C21—C22—O5	119.6 (3)	N1—C45—H45	120.0
C23—C22—O5	117.2 (3)	C44—C45—H45	120.0
C24—C23—C22	119.8 (3)	N2—C46—C47	121.5 (3)
C24—C23—H23	120.1	N2—C46—C41	114.6 (3)
C22—C23—H23	120.1	C47—C46—C41	123.8 (3)
C23—C24—C25	120.6 (3)	C48—C47—C46	119.6 (3)
C23—C24—H24	119.7	C48—C47—H47	120.2
C25—C24—H24	119.7	C46—C47—H47	120.2
C26—C25—C24	122.2 (3)	C47—C48—C49	119.5 (4)
C26—C25—C30	118.5 (3)	C47—C48—H48	120.3

C24—C25—C30	119.2 (3)	C49—C48—H48	120.3
C27—C26—C25	121.5 (4)	C48—C49—N4	123.6 (3)
C27—C26—H26	119.3	C48—C49—C50	117.2 (3)
C25—C26—H26	119.3	N4—C49—C50	119.2 (3)
C26—C27—C28	120.1 (3)	N2—C50—C49	123.9 (3)
C26—C27—H27	119.9	N2—C50—H50	118.0
C28—C27—H27	119.9	C49—C50—H50	118.0
C29—C28—C27	120.7 (3)	H9B—O9—H9C	97 (4)
C29—C28—H28	119.7	H10A—O10—H10B	112 (4)
C27—C28—H28	119.7	H11A—O11—H11B	113 (5)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.92 (4)	2.33 (4)	3.172 (4)	151 (3)
N3—H3B···O8^{ii}	0.90 (4)	1.97 (4)	2.830 (4)	161 (4)
N3—H3C···O10^{iii}	0.96 (4)	2.08 (5)	3.016 (5)	164 (4)
N4—H4C···O9	0.97 (3)	2.18 (4)	3.124 (5)	163 (4)
N5—H5···O4^{i}	0.98 (4)	1.61 (4)	2.581 (4)	167 (3)
N6—H6B···O10^{iv}	0.96 (4)	2.05 (4)	3.006 (5)	173 (4)
N6—H6C···O11	0.81 (5)	2.34 (5)	3.078 (6)	153 (5)
O9—H9B···O3^{v}	0.85 (4)	2.06 (4)	2.875 (4)	159 (4)
O9—H9C···O7	0.88 (5)	1.89 (5)	2.753 (4)	164 (4)
O10—H10A···O11^{vi}	0.96 (4)	1.85 (4)	2.787 (4)	166 (4)
O10—H10B···O9	0.93 (5)	1.98 (5)	2.874 (4)	162 (4)
O11—H11B···O3^{v}	0.91 (6)	1.99 (5)	2.817 (4)	151 (5)
O11—H11A···O7	0.78 (5)	2.44 (5)	3.046 (4)	136 (5)
O11—H11A···O8	0.78 (5)	2.59 (6)	3.264 (5)	147 (6)

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

Fig. 1

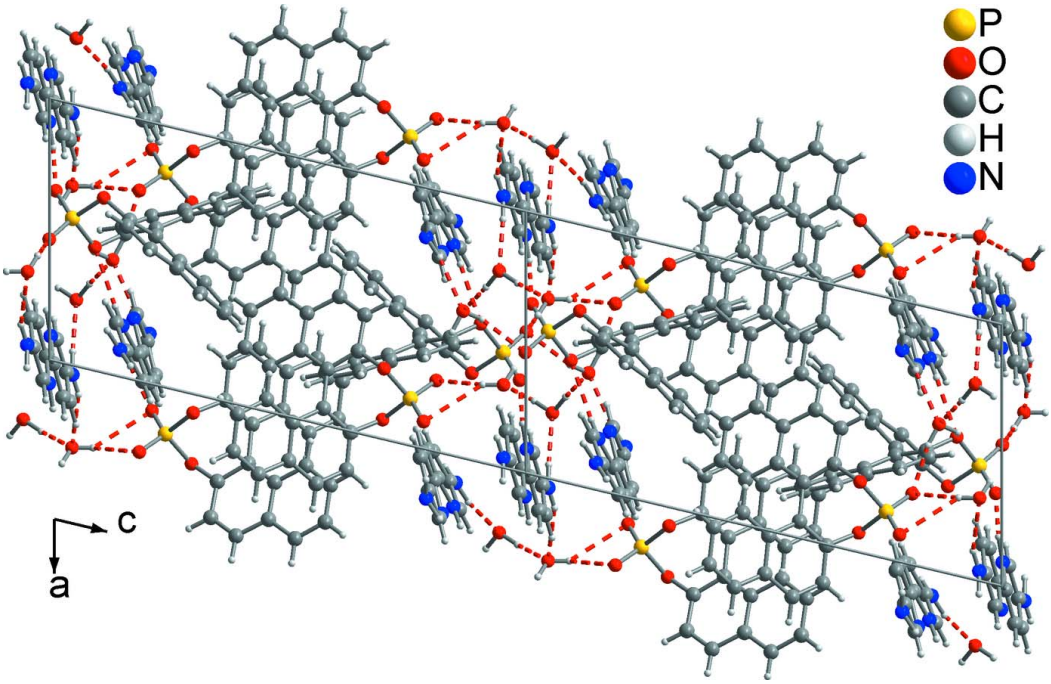


Fig. 2