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Bis(2,6-diaminopyridinium)–adipate–adipic acid–water (2/1/1/2)

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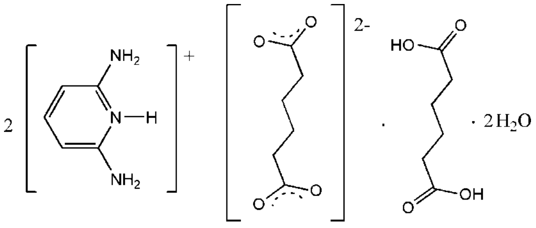
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.118; data-to-parameter ratio = 15.6.

The crystal structure of the title compound, $2C_5H_8N_3^+\cdot C_6H_8O_4^{2-}\cdot C_6H_{10}O_4\cdot 2H_2O$, consists of aminopyridinium cations, adipate dianions, adipic acid molecules and disordered solvent water molecules [occupancies 0.50 (4) and 0.50 (4)]. Both the adipate and adipic acid are located across inversion centres. Eight-membered hydrogen-bonded rings exist involving aminopyridinium and adipate ions. Adipic acid molecules and adipate anions are linked into zigzag supramolecular chains by O—H···O hydrogen bonds.

Related literature

For general background, see: Lah *et al.* (2001); Yang *et al.* (1995); Goswami & Ghosh (1997); Lehn (1990). For related structures, see: Büyükgüngör & Odabaşoğlu (2002, 2006); Odabaşoğlu & Büyükgüngör (2006); Shanmuga Sundara Raj *et al.*, (2000). For synthesis, see: Odabaşoğlu & Büyükgüngör (2006).



Experimental

Crystal data

$2C_5H_8N_3^+\cdot C_6H_8O_4^{2-}\cdot C_6H_{10}O_4\cdot 2H_2O$
M_r = 546.58
Triclinic, $P\bar{1}$
a = 5.0645 (7) Å
b = 7.6261 (11) Å
c = 17.702 (3) Å
α = 87.861 (11)°
β = 85.169 (11)°
γ = 73.323 (11)°
V = 652.55 (18) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 (2) K
0.60 × 0.48 × 0.08 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002) $T_{\min}$ = 0.949, $T_{\max}$ = 0.993
7575 measured reflections
2996 independent reflections
2261 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.118
S = 1.05
2996 reflections
192 parameters
17 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ = 0.21 e Å^{-3}
$\Delta\rho_{\min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	2.03	2.8917 (14)	175
N2—H2A···O4$^{\rm i}$	0.86	2.15	2.8589 (16)	139
N2—H2B···O5	0.86	2.25	3.0892 (18)	166
N3—H3A···O2	0.86	1.91	2.7729 (16)	178
N3—H3B···O2$^{\rm ii}$	0.86	2.06	2.8936 (17)	162
O3—H4A···O1$^{\rm iii}$	0.829 (17)	1.688 (17)	2.5099 (15)	171 (3)
O5—H5A···O4$^{\rm iv}$	0.824 (16)	1.972 (17)	2.7773 (15)	165 (2)
O5—H5B···O5$^{\rm v}$	0.824 (19)	2.00 (2)	2.804 (3)	164 (5)
O5—H5C···O5$^{\rm iv}$	0.823 (19)	2.01 (2)	2.819 (3)	168 (5)

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The author acknowledges the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS II diffractometer (purchased under grant F.279 of the University Research Fund). The author also thanks Professor Dr O. Büyükgüngör for collection of the X-ray data and Professor Dr M. Odabaşoğlu for the synthesis of the title compound.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2332).

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supporting information

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Bis(2,6-diaminopyridinium)–adipate–adipic acid–water (2/1/1/2)

Nevzat Karadayı

S1. Comment

The title crystal is obtained with the reaction of 2-aminopyridine (used in hair and other dyes) and adipic acid (used to esters for plasticizers and as food additive). In addition, The cupper(II) complexes of 2-aminopyridinium carboxylates have important properties in the applications of pharmaceuticals, fungicides, oxygen transfer, oxidative addition, homogenous hydrogenation, gas occlusion compounds, and solvent extractions processes (Lah *et al.*, 2001; Yang *et al.*, 1995). Hydrogen bonding plays a key role in molecular recognition (Goswami & Ghosh, 1997). The design of highly specific solid-state structure is of considerable significance in organic chemistry due to their important applications in the development of new optical, magnetic and electronic systems (Lehn, 1990). This report concerns the *x*-ray structure analysis of the title complex. In the structure investigations show that the 2-aminopyridinium ions are linked to the adipate ions by N1—H1···O1 and N3—H3···O2 hydrogen bonds through the formation of cyclic eight-membered hydrogen bonded rings.

An *ORTEP* diagram of (I) with numbering scheme is shown in Fig. 1. The bond lengths and angles in the structure is within the normally expected ranges. Similar C1—N3 and C5—N2 bonds were observed in other 2-aminopyridine containing molecules (Büyükgüngör & Odabaşoğlu, 2002; Odabaşoğlu & Büyükgüngör, 2006; Shanmuga Sundara Raj *et al.*, 2000). Furthermore, these bond angle and length agrees with that similar bond angle and length values of 2,6-diaminopyridinium hydrogen fumarate complex (Büyükgüngör & Odabaşoğlu, 2006).

2-Aminopyridine and derivatives, are protonated in acidic solution. As for mono-aminopyridinium adipate-adipic acid and in some 2-aminopyridine-containing molecules, the bonding of the H atom to the ring N atom of 2-aminopyridine rather than the amine N atom gives an ion for which an additional resonance structure can be written.

The packing of the molecules is shown in Figure 2. In (I), the 2,6-diaminopyridinium ions are linked to the adipate-adipic ions through N—H···O, O—H···O hydrogen bonds (Table 1). The dihedral angles between the aminopyridinium ring and the O1/O2/C9/C10/C11 and O3/O4/C6/C7/C8 groups are 3.31 (7) and 7.25 (8)° respectively.

The H atoms between the water molecules are distorted because of the mutual repulsive interactions. So, H5B and H5C atoms are the same H-atom in the water molecule, and this H-atom makes a flip-flop motion between the two positions with site occupation factors of 0.50 (4) and 0.50 (4), respectively. The other H-atom (H5A) of the water molecule is localized due to the O5—H5A···O4 intermolecular hydrogen bond between adipic acid molecules (Fig. 3).

S2. Experimental

The title compound was prepared by as described by Odabaşoğlu & Büyükgüngör (2006), using 2,6-diaminopyridine and adipic acid as starting materials. Crystals were obtained by slow evaporation from an aqueous solution.

S3. Refinement

The carboxy H atom was located in a difference Fourier map and refined isotropically. Water H atoms were located in a difference map and refined isotropically with O—H and H···H distances restrained to 0.82 (2) and 1.55 (4) Å, respectively. The site occupancies for disordered H5B and H5C was refined to 0.50 (4) and 0.50 (4), respectively. Other H atoms were refined using the riding model approximation, with C—H = 0.93 (aromatic), 0.97 Å (methylene) and N—H = 0.86 Å, $U_{iso}(H) = 1.2U_{eq}(C,N)$.

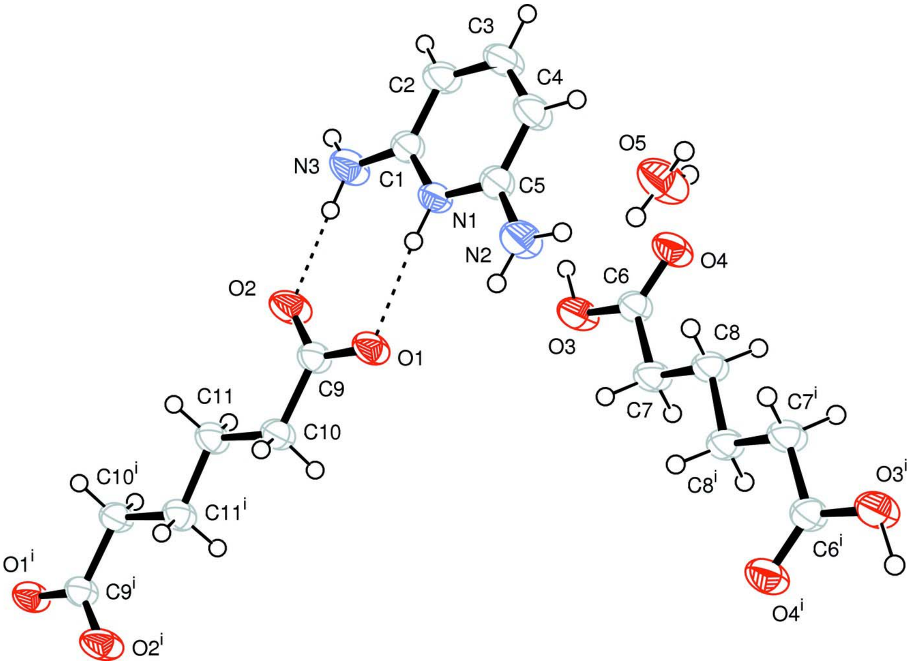

Figure 1

An *ORTEP-3* drawing of the title compound (I) showing the atomic numbering scheme and 50% probability displacement ellipsoids.

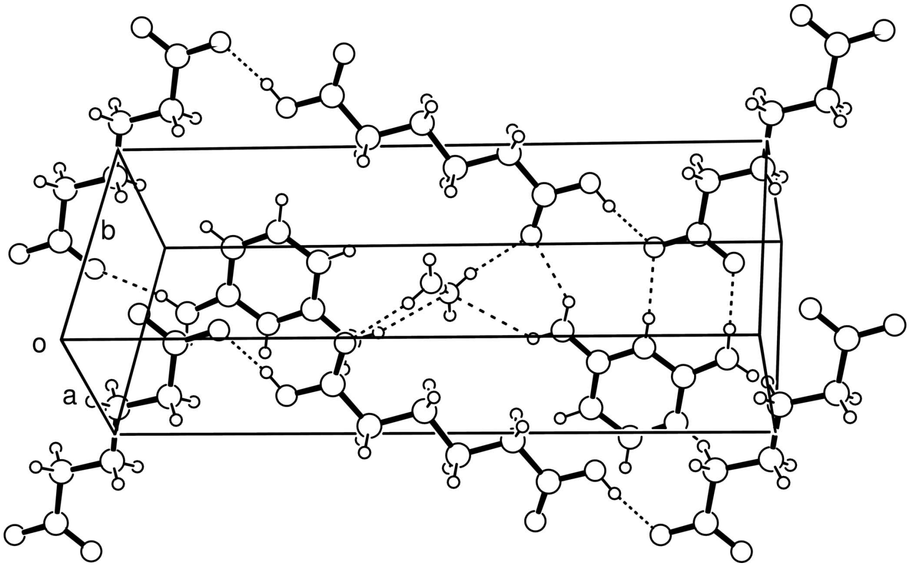

Figure 2

A perspective view of the packing in (I).

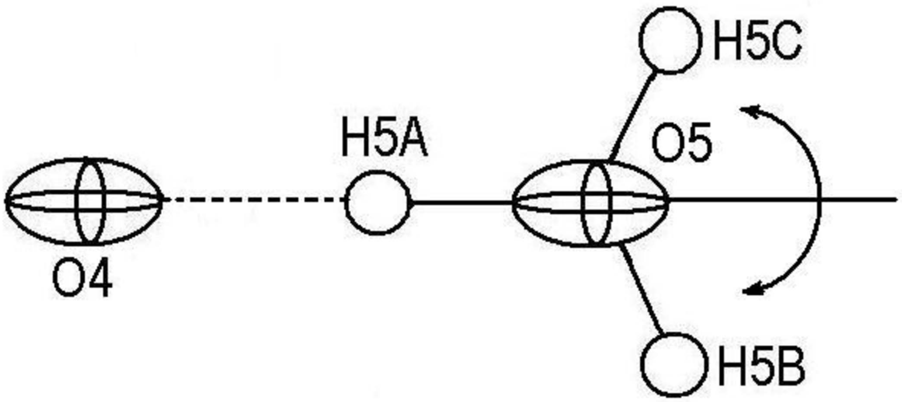

Figure 3

The disordered H atoms of water molecules in the crystal structure.

Bis(2,6-diaminopyridinium)–adipate–adipic acid–water (2/1/1/2)

Crystal data

$2C_5H_8N_3^+\cdot C_6H_8O_4^{2-}\cdot C_6H_{10}O_4\cdot 2H_2O$
M_r = 546.58
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 5.0645 (7) Å
b = 7.6261 (11) Å
c = 17.702 (3) Å
α = 87.861 (11)°
β = 85.169 (11)°
γ = 73.323 (11)°
V = 652.55 (18) Å^3
Z = 1
F(000) = 292
D_x = 1.391 Mg m^{-3}
Melting point = 428–429 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8371 reflections
θ = 2.3–27.9°
μ = 0.11 mm^{-1}
T = 296 K
Plate, colourless
0.60 × 0.48 × 0.08 mm

Data collection

Stoe IPDS 2
diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
ω scans
Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.949$, $T_{\max} = 0.993$

7575 measured reflections
2996 independent reflections
2261 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.043$
$\theta_{\max} = 27.5°$, $\theta_{\min} = 2.3°$
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -20 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.118$
$S = 1.05$
2996 reflections
192 parameters
17 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
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.039P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL* (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.038 (10)

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 (Å^2)

	x	y	z	$U_{\text{iso}}*/U_{\text{eq}}$	Occ. (<1)
O3	1.2490 (2)	0.92346 (16)	0.72447 (6)	0.0543 (3)	
O4	1.5316 (2)	0.79673 (16)	0.62672 (5)	0.0512 (3)	
C6	1.3110 (3)	0.89651 (18)	0.65252 (7)	0.0374 (3)	
N3	1.1687 (3)	0.4528 (2)	0.91704 (7)	0.0546 (4)	
H3A	1.0050	0.5265	0.9243	0.066*	
H3B	1.2601	0.4051	0.9552	0.066*	
C2	1.5414 (3)	0.2937 (2)	0.82983 (8)	0.0460 (3)	
H2	1.6516	0.2374	0.8683	0.055*	
C7	1.0880 (3)	1.00201 (19)	0.60401 (7)	0.0418 (3)	
H7A	1.0818	1.1303	0.6047	0.050*	
H7B	0.9120	0.9916	0.6267	0.050*	
C1	1.2800 (3)	0.41269 (18)	0.84710 (7)	0.0378 (3)	
C11	0.1384 (3)	0.92888 (18)	0.99095 (7)	0.0382 (3)	
H11A	0.1273	0.8107	1.0108	0.046*	
H11B	0.2798	0.9613	1.0164	0.046*	

O2	0.6439 (2)	0.69564 (16)	0.93768 (6)	0.0543 (3)	
C3	1.6345 (3)	0.2603 (2)	0.75544 (9)	0.0501 (4)	
H3	1.8095	0.1809	0.7438	0.060*	
C8	1.1183 (3)	0.94351 (18)	0.52225 (7)	0.0388 (3)	
H8A	1.1244	0.8154	0.5207	0.047*	
H8B	1.2916	0.9562	0.4985	0.047*	
C9	0.5041 (3)	0.77673 (18)	0.88646 (7)	0.0364 (3)	
C10	0.2239 (3)	0.91266 (19)	0.90622 (7)	0.0388 (3)	
H10A	0.0849	0.8764	0.8812	0.047*	
H10B	0.2273	1.0322	0.8862	0.047*	
N1	1.1255 (2)	0.49227 (15)	0.78902 (6)	0.0370 (3)	
H1	0.9640	0.5662	0.7997	0.044*	
C4	1.4745 (3)	0.3419 (2)	0.69719 (8)	0.0498 (4)	
H4	1.5402	0.3177	0.6469	0.060*	
O1	0.58652 (19)	0.75241 (14)	0.81637 (5)	0.0438 (3)	
C5	1.2154 (3)	0.45998 (19)	0.71505 (7)	0.0396 (3)	
N2	1.0457 (3)	0.5462 (2)	0.66285 (7)	0.0553 (4)	
H2A	0.8862	0.6189	0.6767	0.066*	
H2B	1.0960	0.5289	0.6154	0.066*	
O5	1.2848 (3)	0.4164 (2)	0.50152 (7)	0.0631 (4)	
H4A	1.373 (4)	0.865 (3)	0.7510 (13)	0.094 (8)*	
H5A	1.335 (4)	0.338 (3)	0.4684 (11)	0.076 (6)*	
H5B	1.114 (4)	0.448 (7)	0.506 (3)	0.089 (15)*	0.50 (4)
H5C	1.416 (7)	0.457 (6)	0.507 (3)	0.083 (15)*	0.50 (4)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0458 (6)	0.0706 (7)	0.0278 (5)	0.0149 (5)	−0.0071 (4)	−0.0044 (5)
O4	0.0367 (5)	0.0684 (7)	0.0338 (5)	0.0096 (4)	−0.0053 (4)	−0.0049 (4)
C6	0.0346 (6)	0.0427 (7)	0.0292 (6)	−0.0012 (5)	−0.0052 (5)	−0.0017 (5)
N3	0.0456 (7)	0.0723 (8)	0.0295 (6)	0.0086 (6)	−0.0002 (5)	0.0004 (5)
C2	0.0378 (7)	0.0526 (8)	0.0361 (7)	0.0061 (6)	−0.0075 (5)	0.0038 (6)
C7	0.0372 (7)	0.0470 (7)	0.0322 (6)	0.0043 (5)	−0.0076 (5)	−0.0020 (5)
C1	0.0358 (6)	0.0415 (7)	0.0310 (6)	−0.0029 (5)	−0.0029 (5)	0.0011 (5)
C11	0.0341 (6)	0.0455 (7)	0.0288 (6)	−0.0018 (5)	−0.0010 (5)	−0.0020 (5)
O2	0.0410 (5)	0.0729 (7)	0.0315 (5)	0.0124 (5)	−0.0062 (4)	0.0011 (5)
C3	0.0370 (7)	0.0570 (8)	0.0419 (7)	0.0092 (6)	−0.0005 (6)	−0.0042 (6)
C8	0.0343 (6)	0.0441 (7)	0.0309 (6)	0.0016 (5)	−0.0079 (5)	0.0001 (5)
C9	0.0322 (6)	0.0426 (6)	0.0292 (6)	−0.0021 (5)	−0.0027 (5)	−0.0017 (5)
C10	0.0335 (6)	0.0443 (7)	0.0311 (6)	0.0006 (5)	−0.0013 (5)	−0.0006 (5)
N1	0.0298 (5)	0.0424 (6)	0.0312 (5)	0.0016 (4)	−0.0012 (4)	−0.0001 (4)
C4	0.0418 (7)	0.0618 (9)	0.0324 (7)	0.0056 (6)	0.0021 (6)	−0.0043 (6)
O1	0.0373 (5)	0.0547 (6)	0.0274 (5)	0.0052 (4)	0.0000 (4)	−0.0023 (4)
C5	0.0366 (6)	0.0456 (7)	0.0311 (6)	−0.0032 (5)	−0.0031 (5)	0.0016 (5)
N2	0.0421 (7)	0.0760 (9)	0.0331 (6)	0.0073 (6)	−0.0075 (5)	0.0038 (6)
O5	0.0483 (7)	0.0801 (9)	0.0503 (7)	0.0009 (6)	−0.0029 (6)	−0.0218 (6)

Geometric parameters (Å, º)

O3—C6	1.2955 (15)	C3—C4	1.382 (2)
O3—H4A	0.829 (17)	C3—H3	0.9300
O4—C6	1.2196 (16)	C8—C8^{ii}	1.521 (2)
C6—C7	1.5001 (18)	C8—H8A	0.9700
N3—C1	1.3252 (17)	C8—H8B	0.9700
N3—H3A	0.8600	C9—O1	1.2781 (15)
N3—H3B	0.8600	C9—C10	1.5199 (16)
C2—C3	1.369 (2)	C10—H10A	0.9700
C2—C1	1.3901 (18)	C10—H10B	0.9700
C2—H2	0.9300	N1—C5	1.3572 (16)
C7—C8	1.5129 (17)	N1—H1	0.8600
C7—H7A	0.9700	C4—C5	1.3806 (18)
C7—H7B	0.9700	C4—H4	0.9300
C1—N1	1.3617 (17)	C5—N2	1.3375 (17)
C11—C11^{i}	1.524 (2)	N2—H2A	0.8600
C11—C10	1.5253 (17)	N2—H2B	0.8600
C11—H11A	0.9700	O5—H5A	0.824 (16)
C11—H11B	0.9700	O5—H5B	0.824 (19)
O2—C9	1.2332 (16)	O5—H5C	0.823 (19)

C6—O3—H4A	113.2 (17)	C7—C8—H8A	109.2
O4—C6—O3	123.06 (12)	C8^{ii}—C8—H8A	109.2
O4—C6—C7	123.27 (11)	C7—C8—H8B	109.2
O3—C6—C7	113.66 (11)	C8^{ii}—C8—H8B	109.2
C1—N3—H3A	120.0	H8A—C8—H8B	107.9
C1—N3—H3B	120.0	O2—C9—O1	122.48 (11)
H3A—N3—H3B	120.0	O2—C9—C10	119.63 (11)
C3—C2—C1	119.16 (13)	O1—C9—C10	117.89 (11)
C3—C2—H2	120.4	C9—C10—C11	114.35 (11)
C1—C2—H2	120.4	C9—C10—H10A	108.7
C6—C7—C8	115.81 (10)	C11—C10—H10A	108.7
C6—C7—H7A	108.3	C9—C10—H10B	108.7
C8—C7—H7A	108.3	C11—C10—H10B	108.7
C6—C7—H7B	108.3	H10A—C10—H10B	107.6
C8—C7—H7B	108.3	C5—N1—C1	122.82 (11)
H7A—C7—H7B	107.4	C5—N1—H1	118.6
N3—C1—N1	117.35 (12)	C1—N1—H1	118.6
N3—C1—C2	124.09 (13)	C5—C4—C3	118.80 (13)
N1—C1—C2	118.55 (12)	C5—C4—H4	120.6
C11^{i}—C11—C10	113.06 (13)	C3—C4—H4	120.6
C11^{i}—C11—H11A	109.0	N2—C5—N1	117.53 (12)
C10—C11—H11A	109.0	N2—C5—C4	123.31 (12)
C11^{i}—C11—H11B	109.0	N1—C5—C4	119.16 (12)
C10—C11—H11B	109.0	C5—N2—H2A	120.0
H11A—C11—H11B	107.8	C5—N2—H2B	120.0
C2—C3—C4	121.51 (13)	H2A—N2—H2B	120.0

C2—C3—H3	119.2	H5A—O5—H5B	108 (4)
C4—C3—H3	119.2	H5A—O5—H5C	107 (4)
C7—C8—C8$^{\text{ii}}$	112.10 (13)	H5B—O5—H5C	140 (5)

O4—C6—C7—C8	14.8 (2)	C11$^{\text{i}}$—C11—C10—C9	177.91 (14)
O3—C6—C7—C8	−166.16 (13)	N3—C1—N1—C5	−179.08 (13)
C3—C2—C1—N3	179.15 (16)	C2—C1—N1—C5	0.2 (2)
C3—C2—C1—N1	−0.1 (2)	C2—C3—C4—C5	0.2 (3)
C1—C2—C3—C4	−0.1 (3)	C1—N1—C5—N2	−179.90 (13)
C6—C7—C8—C8$^{\text{ii}}$	179.37 (15)	C1—N1—C5—C4	−0.1 (2)
O2—C9—C10—C11	−2.29 (19)	C3—C4—C5—N2	179.70 (16)
O1—C9—C10—C11	178.28 (12)	C3—C4—C5—N1	−0.1 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86	2.03	2.8917 (14)	175
N2—H2*A*···O4$^{\text{iii}}$	0.86	2.15	2.8589 (16)	139
N2—H2*B*···O5	0.86	2.25	3.0892 (18)	166
N3—H3*A*···O2	0.86	1.91	2.7729 (16)	178
N3—H3*B*···O2$^{\text{iv}}$	0.86	2.06	2.8936 (17)	162
O3—H4*A*···O1$^{\text{v}}$	0.83 (2)	1.69 (2)	2.5099 (15)	171 (3)
O5—H5*A*···O4$^{\text{vi}}$	0.82 (2)	1.97 (2)	2.7773 (15)	165 (2)
O5—H5*B*···O5$^{\text{vii}}$	0.82 (2)	2.00 (2)	2.804 (3)	164 (5)
O5—H5*C*···O5$^{\text{vi}}$	0.82 (2)	2.01 (2)	2.819 (3)	168 (5)

Symmetry codes: (iii) *x*−1, *y*, *z*; (iv) −*x*+2, −*y*+1, −*z*+2; (v) *x*+1, *y*, *z*; (vi) −*x*+3, −*y*+1, −*z*+1; (vii) −*x*+2, −*y*+1, −*z*+1.