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2-Aminopyridinium 2,4-dinitrophenolate

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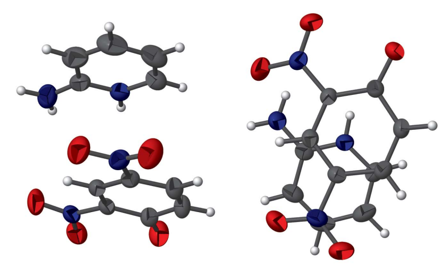
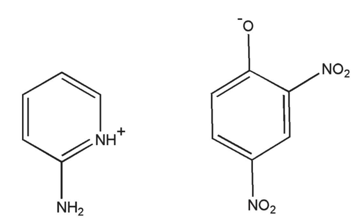
The asymmetric unit of the title organic salt, $C_5H_7N_2^+ \cdot C_6H_3N_2O_5^-$, comprises two 2-aminopyridinium cations and two 2,4-dinitrophenolate anions. The cations are protonated at the pyridine N atoms, while the anions are deprotonated at hydroxyl O atoms. In the crystal, bifurcated N—H···O hydrogen bonds generate two $R_2^1(6)$, two $R_1^2(6)$, and one $R_1^2(4)$ ring motifs. Adjacent anions and cations are linked by N—H···O hydrogen bonds into infinite chains along [110]. Weak C—H···O contacts and π–π interactions further link the components, forming a complex three-dimensional supramolecular network.

3D view



Chemical scheme



Structure description

In order to investigate if pyridine derivatives exhibit biological activities such as antiviral (Hamdouchi *et al.*, 1999) or antibacterial activity (Rival *et al.*, 1992), we synthesized and determined the crystal structure of the title organic salt (Fig. 1). The geometric parameters are in good agreement with those reported for similar structures (Hemamalini & Fun, 2010; Sivakumar *et al.*, 2016). There are two independent 2-aminopyridinium cations and two 2,4-dinitrophenolate anions in the asymmetric unit. The cations are protonated at the pyridine N atoms (N5 and N7) and the anions are deprotonated at the hydroxyl O atoms (O1 and O6).

In the crystal, pairs of bifurcated hydrogen bonds N6—H6*A*···O1^{i}, N5—H5···O1^{i} and N8—H8*A*···O6^{iii}, N7—H7···O6^{iii} generate two $R_2^1(6)$ ring motifs. Pairs of hydrogen bonds N5—H5···O1^{i}, N5—H5···O2^{i} and N7—H7···O6^{iii}, N7—H7···O10^{iii} generate two $R_1^2(6)$ ring motifs. Finally, the N8—H8*B*···O2^{i} and N8—H8*B*···O3^{i} hydrogen bonds generate an $R_1^2(4)$ ring motif (Figs. 2 and 3). Adjacent anions and cations are linked by N—H···O hydrogen bonds (Table 1) into infinite chains along [110]. The crystal also features weak C—H···O hydrogen bonds and π–π interactions between symmetry-

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O1^{i}	0.88 (1)	1.92 (1)	2.7304 (16)	152 (2)
N5—H5···O2^{i}	0.88 (1)	2.31 (2)	2.9553 (17)	130 (2)
N6—H6A···O1^{i}	0.86	2.02	2.7712 (19)	145
N6—H6B···O4^{ii}	0.86	2.15	2.9849 (18)	162
N7—H7···O6^{iii}	0.88 (1)	1.83 (1)	2.6627 (15)	157 (2)
N7—H7···O10^{iii}	0.88 (1)	2.31 (2)	2.8975 (17)	124 (2)
N8—H8A···O6^{iii}	0.86	2.04	2.7727 (16)	143
N8—H8B···O2^{i}	0.86	2.42	3.2740 (17)	175
N8—H8B···O3^{i}	0.86	2.50	3.1445 (17)	132
C3—H3···O8	0.93	2.56	3.1944 (18)	126
C18—H18···O10^{iii}	0.93	2.51	3.034 (2)	116

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

related C7–C12 benzene rings [centroid-to-centroid distance: 3.4949 (7) Å; symmetry code: $2-x, 1-y, -z$], leading to the formation of a three-dimensional network (Fig. 2).

Synthesis and crystallization

The title salt was synthesized from the raw materials 2-aminopyridine (2.353 g) and 2,4-dinitrophenol (4.603 g), which were taken in 1:1 ratio and dissolved in a mixture of water and ethanol, at room temperature. After a period of three weeks, good quality crystals suitable for X-ray diffraction were harvested.

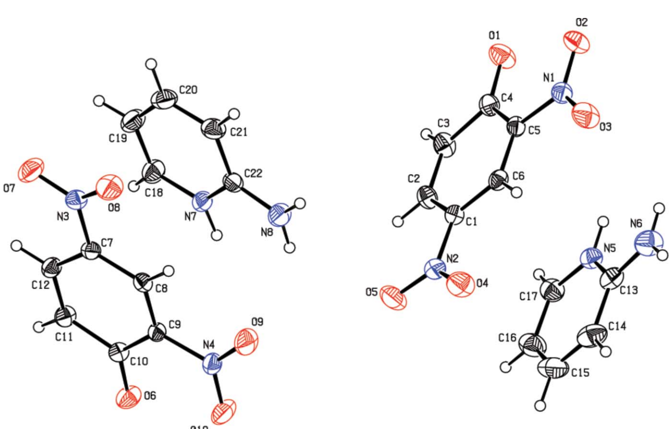


Figure 1
The molecular structure of the title compound, with 30% probability displacement ellipsoids.

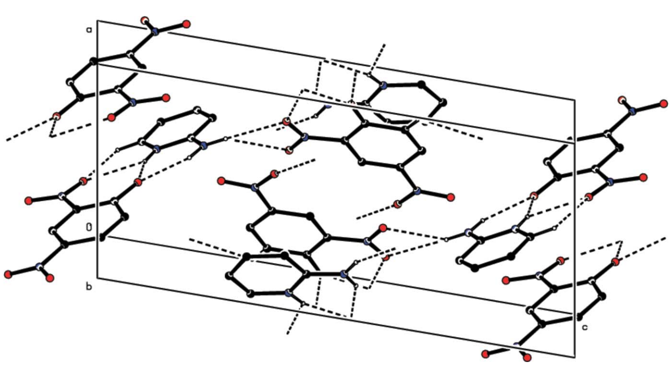


Figure 2
The crystal packing of the title compound viewed along b axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_3N_2O_5·C_5H_7N_2$
M_r	278.23
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	295
a, b, c (Å)	7.6303 (2), 9.3142 (3), 17.2518 (5)
α, β, γ (°)	90.339 (2), 99.468 (2), 99.556 (3)
V (Å^3)	1191.91 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.13
Crystal size (mm)	0.30 × 0.26 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD Diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.963, 0.975
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	44716, 10159, 5393
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.823
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.157, 1.01
No. of reflections	10159
No. of parameters	370
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.26

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

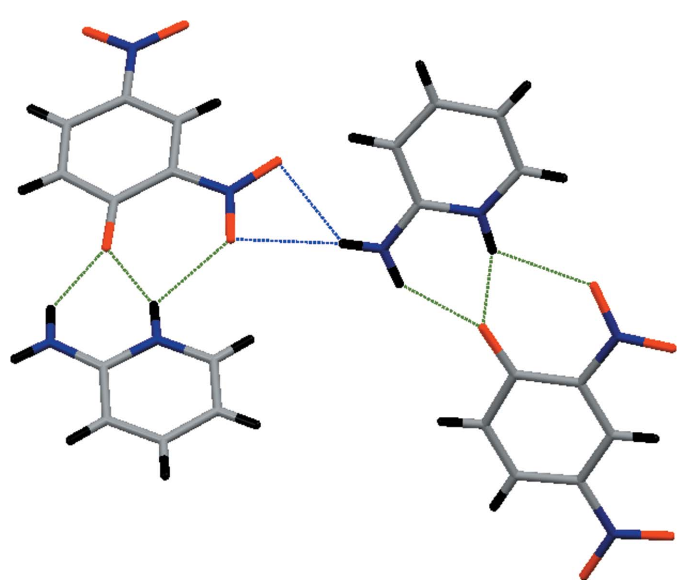


Figure 3
A partial view of the crystal packing of the title compound, showing the ring motifs.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. In the last least-squares cycles, pyridinium N5—H5 and N7—H7 bond lengths were restrained to 0.88 (1) Å.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161489 [doi:10.1107/S2414314616014899]

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2-Aminopyridinium 2,4-dinitrophenolate

Crystal data

$C_5H_7N_2^+ \cdot C_6H_3N_2O_5^-$
$M_r = 278.23$
Triclinic, $P\bar{1}$
Hall symbol: -P 1
$a = 7.6303$ (2) Å
$b = 9.3142$ (3) Å
$c = 17.2518$ (5) Å
$\alpha = 90.339$ (2)°
$\beta = 99.468$ (2)°
$\gamma = 99.556$ (3)°
$V = 1191.91$ (6) Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.550$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9905 reflections
$\theta = 2.3–32.4°$
$\mu = 0.13$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD Diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min} = 0.963$, $T_{max} = 0.975$
44716 measured reflections
10159 independent reflections
5393 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 35.8°$, $\theta_{min} = 1.2°$
$h = -11 \rightarrow 12$
$k = -15 \rightarrow 15$
$l = -28 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.157$
$S = 1.01$
10159 reflections
370 parameters
2 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.2916P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.026 (2)

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

	x	y	z	U_{iso}*/U_{eq}
C1	1.37352 (17)	0.62615 (14)	0.36601 (8)	0.0331 (3)
C2	1.25635 (19)	0.51343 (16)	0.32011 (8)	0.0394 (3)
H2	1.2510	0.5088	0.2659	0.047*
C3	1.1515 (2)	0.41180 (17)	0.35563 (8)	0.0424 (3)
H3	1.0741	0.3383	0.3244	0.051*
C4	1.15318 (18)	0.41126 (15)	0.43895 (8)	0.0360 (3)
C5	1.27290 (17)	0.53107 (14)	0.48189 (7)	0.0317 (3)
C6	1.38030 (18)	0.63512 (14)	0.44565 (8)	0.0332 (3)
H6	1.4570	0.7110	0.4754	0.040*
C7	0.92604 (16)	0.28396 (13)	0.06858 (7)	0.0306 (2)
C8	0.89794 (17)	0.41705 (13)	0.09385 (7)	0.0307 (2)
H8	0.9471	0.4525	0.1446	0.037*
C9	0.79599 (16)	0.49808 (13)	0.04331 (7)	0.0291 (2)
C10	0.71871 (17)	0.44915 (13)	−0.03568 (7)	0.0316 (2)
C11	0.75481 (19)	0.30915 (14)	−0.05728 (8)	0.0366 (3)
H11	0.7077	0.2714	−0.1078	0.044*
C12	0.85390 (18)	0.22925 (14)	−0.00781 (8)	0.0352 (3)
H12	0.8738	0.1390	−0.0244	0.042*
C13	1.1666 (2)	0.92922 (16)	0.43826 (10)	0.0431 (3)
C14	1.2566 (2)	1.03100 (18)	0.39219 (12)	0.0578 (4)
H14	1.3414	1.1086	0.4161	0.069*
C15	1.2192 (3)	1.0155 (2)	0.31277 (13)	0.0631 (5)
H15	1.2790	1.0829	0.2824	0.076*
C16	1.0930 (2)	0.9006 (2)	0.27611 (11)	0.0572 (4)
H16	1.0683	0.8900	0.2216	0.069*
C17	1.0067 (2)	0.80451 (18)	0.32117 (9)	0.0458 (3)
H17	0.9213	0.7269	0.2976	0.055*
C18	0.4901 (2)	0.10146 (16)	0.09284 (10)	0.0461 (3)
H18	0.4265	0.0764	0.0425	0.055*
C19	0.5773 (2)	0.00349 (16)	0.13340 (11)	0.0519 (4)
H19	0.5766	−0.0879	0.1113	0.062*
C20	0.6681 (2)	0.04270 (17)	0.20908 (11)	0.0500 (4)
H20	0.7276	−0.0238	0.2382	0.060*
C21	0.6711 (2)	0.17668 (17)	0.24104 (9)	0.0454 (3)
H21	0.7319	0.2018	0.2918	0.055*
C22	0.58139 (18)	0.27768 (15)	0.19663 (8)	0.0355 (3)
N1	1.29096 (16)	0.54893 (13)	0.56547 (6)	0.0377 (3)
N2	1.49156 (17)	0.73176 (13)	0.33004 (7)	0.0404 (3)
N3	1.03421 (16)	0.20195 (13)	0.12121 (7)	0.0384 (3)
N4	0.77467 (16)	0.63762 (12)	0.07403 (7)	0.0365 (2)
N5	1.04392 (16)	0.82054 (13)	0.40076 (7)	0.0392 (3)
N6	1.1972 (2)	0.93352 (16)	0.51656 (9)	0.0579 (4)
H6A	1.1389	0.8676	0.5418	0.069*
H6B	1.2752	1.0022	0.5419	0.069*
N7	0.49370 (16)	0.23546 (12)	0.12421 (7)	0.0354 (2)

N8	0.5821 (2)	0.41215 (14)	0.22250 (7)	0.0487 (3)
H8A	0.5269	0.4704	0.1929	0.058*
H8B	0.6377	0.4411	0.2688	0.058*
O1	1.05465 (16)	0.31141 (13)	0.46840 (6)	0.0534 (3)
O2	1.21387 (16)	0.45502 (13)	0.60378 (6)	0.0512 (3)
O3	1.38712 (18)	0.65870 (13)	0.59828 (6)	0.0585 (3)
O4	1.58993 (18)	0.83193 (13)	0.37099 (7)	0.0587 (3)
O5	1.4934 (2)	0.71793 (14)	0.25978 (7)	0.0644 (4)
O6	0.62580 (15)	0.51757 (11)	−0.08511 (6)	0.0467 (3)
O7	1.05377 (18)	0.08143 (13)	0.09936 (7)	0.0594 (3)
O8	1.10477 (18)	0.25497 (14)	0.18655 (7)	0.0577 (3)
O9	0.82825 (19)	0.66899 (13)	0.14377 (7)	0.0600 (3)
O10	0.70515 (18)	0.72215 (12)	0.02972 (7)	0.0575 (3)
H5	0.993 (2)	0.7560 (17)	0.4309 (10)	0.062 (6)*
H7	0.441 (2)	0.3037 (17)	0.0994 (10)	0.061 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0341 (6)	0.0327 (6)	0.0338 (6)	0.0077 (5)	0.0072 (5)	0.0015 (5)
C2	0.0420 (7)	0.0463 (8)	0.0291 (6)	0.0057 (6)	0.0059 (5)	−0.0037 (5)
C3	0.0403 (7)	0.0467 (8)	0.0361 (7)	−0.0020 (6)	0.0039 (6)	−0.0083 (6)
C4	0.0329 (6)	0.0400 (7)	0.0351 (6)	0.0052 (5)	0.0062 (5)	−0.0006 (5)
C5	0.0327 (6)	0.0373 (6)	0.0260 (5)	0.0119 (5)	0.0021 (5)	−0.0002 (5)
C6	0.0347 (6)	0.0324 (6)	0.0321 (6)	0.0098 (5)	0.0005 (5)	−0.0021 (5)
C7	0.0297 (6)	0.0315 (6)	0.0311 (6)	0.0059 (5)	0.0058 (5)	0.0055 (5)
C8	0.0319 (6)	0.0329 (6)	0.0269 (5)	0.0038 (5)	0.0055 (5)	0.0006 (4)
C9	0.0309 (6)	0.0270 (5)	0.0298 (6)	0.0049 (4)	0.0062 (5)	−0.0008 (4)
C10	0.0306 (6)	0.0306 (6)	0.0320 (6)	0.0042 (5)	0.0020 (5)	0.0007 (5)
C11	0.0420 (7)	0.0334 (6)	0.0311 (6)	0.0041 (5)	−0.0009 (5)	−0.0043 (5)
C12	0.0402 (7)	0.0285 (6)	0.0364 (6)	0.0057 (5)	0.0053 (5)	−0.0021 (5)
C13	0.0402 (7)	0.0353 (7)	0.0533 (9)	0.0097 (6)	0.0031 (6)	0.0023 (6)
C14	0.0493 (9)	0.0417 (8)	0.0791 (13)	0.0018 (7)	0.0064 (9)	0.0119 (8)
C15	0.0569 (11)	0.0608 (11)	0.0753 (13)	0.0133 (9)	0.0178 (9)	0.0323 (10)
C16	0.0553 (10)	0.0705 (11)	0.0495 (9)	0.0182 (9)	0.0107 (8)	0.0196 (8)
C17	0.0432 (8)	0.0506 (8)	0.0433 (8)	0.0104 (6)	0.0037 (6)	0.0052 (6)
C18	0.0510 (9)	0.0380 (7)	0.0481 (8)	0.0072 (6)	0.0057 (7)	−0.0044 (6)
C19	0.0586 (10)	0.0324 (7)	0.0671 (11)	0.0108 (7)	0.0143 (8)	0.0026 (7)
C20	0.0476 (9)	0.0439 (8)	0.0628 (10)	0.0149 (7)	0.0138 (7)	0.0207 (7)
C21	0.0465 (8)	0.0513 (8)	0.0400 (7)	0.0138 (7)	0.0057 (6)	0.0130 (6)
C22	0.0367 (7)	0.0397 (7)	0.0322 (6)	0.0083 (5)	0.0098 (5)	0.0059 (5)
N1	0.0418 (6)	0.0428 (6)	0.0289 (5)	0.0126 (5)	0.0017 (5)	0.0020 (5)
N2	0.0474 (7)	0.0342 (6)	0.0405 (6)	0.0065 (5)	0.0099 (5)	0.0018 (5)
N3	0.0412 (6)	0.0394 (6)	0.0365 (6)	0.0121 (5)	0.0067 (5)	0.0080 (5)
N4	0.0408 (6)	0.0334 (5)	0.0363 (6)	0.0081 (5)	0.0071 (5)	−0.0035 (4)
N5	0.0383 (6)	0.0377 (6)	0.0418 (6)	0.0079 (5)	0.0055 (5)	0.0044 (5)
N6	0.0649 (9)	0.0474 (8)	0.0534 (8)	−0.0024 (7)	−0.0011 (7)	−0.0038 (6)
N7	0.0373 (6)	0.0340 (5)	0.0361 (6)	0.0102 (4)	0.0055 (5)	0.0019 (4)

N8	0.0681 (9)	0.0452 (7)	0.0327 (6)	0.0187 (6)	−0.0007 (6)	−0.0024 (5)
O1	0.0567 (7)	0.0550 (7)	0.0433 (6)	−0.0106 (5)	0.0131 (5)	0.0001 (5)
O2	0.0595 (7)	0.0593 (7)	0.0341 (5)	0.0055 (5)	0.0098 (5)	0.0095 (5)
O3	0.0782 (9)	0.0574 (7)	0.0315 (5)	−0.0041 (6)	0.0004 (5)	−0.0069 (5)
O4	0.0673 (8)	0.0462 (6)	0.0553 (7)	−0.0109 (5)	0.0102 (6)	−0.0036 (5)
O5	0.0933 (10)	0.0556 (7)	0.0434 (6)	−0.0069 (6)	0.0284 (6)	0.0014 (5)
O6	0.0559 (6)	0.0421 (5)	0.0390 (5)	0.0170 (5)	−0.0097 (5)	−0.0001 (4)
O7	0.0781 (8)	0.0454 (6)	0.0590 (7)	0.0306 (6)	0.0033 (6)	0.0051 (5)
O8	0.0703 (8)	0.0623 (7)	0.0386 (6)	0.0235 (6)	−0.0084 (5)	0.0035 (5)
O9	0.0920 (10)	0.0498 (6)	0.0380 (6)	0.0194 (6)	0.0027 (6)	−0.0121 (5)
O10	0.0790 (8)	0.0413 (6)	0.0545 (7)	0.0296 (6)	−0.0014 (6)	−0.0027 (5)

Geometric parameters (Å, º)

C1—C6	1.3679 (18)	C15—H15	0.9300
C1—C2	1.4050 (19)	C16—C17	1.349 (2)
C1—N2	1.4356 (18)	C16—H16	0.9300
C2—C3	1.352 (2)	C17—N5	1.3579 (19)
C2—H2	0.9300	C17—H17	0.9300
C3—C4	1.4354 (19)	C18—C19	1.349 (2)
C3—H3	0.9300	C18—N7	1.3517 (18)
C4—O1	1.2600 (17)	C18—H18	0.9300
C4—C5	1.4344 (18)	C19—C20	1.390 (2)
C5—C6	1.3834 (19)	C19—H19	0.9300
C5—N1	1.4317 (16)	C20—C21	1.356 (2)
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.3731 (17)	C21—C22	1.4109 (19)
C7—C12	1.3999 (18)	C21—H21	0.9300
C7—N3	1.4353 (16)	C22—N8	1.3260 (18)
C8—C9	1.3837 (17)	C22—N7	1.3398 (17)
C8—H8	0.9300	N1—O3	1.2294 (16)
C9—C10	1.4324 (17)	N1—O2	1.2296 (15)
C9—N4	1.4446 (15)	N2—O5	1.2207 (16)
C10—O6	1.2623 (16)	N2—O4	1.2322 (16)
C10—C11	1.4361 (18)	N3—O7	1.2222 (16)
C11—C12	1.3550 (18)	N3—O8	1.2288 (16)
C11—H11	0.9300	N4—O9	1.2224 (15)
C12—H12	0.9300	N4—O10	1.2240 (16)
C13—N6	1.332 (2)	N5—H5	0.882 (9)
C13—N5	1.3406 (19)	N6—H6A	0.8600
C13—C14	1.405 (2)	N6—H6B	0.8600
C14—C15	1.355 (3)	N7—H7	0.883 (9)
C14—H14	0.9300	N8—H8A	0.8600
C15—C16	1.386 (3)	N8—H8B	0.8600
C6—C1—C2	120.75 (12)	C17—C16—C15	118.64 (17)
C6—C1—N2	118.96 (12)	C17—C16—H16	120.7
C2—C1—N2	120.27 (12)	C15—C16—H16	120.7

C3—C2—C1	119.28 (12)	C16—C17—N5	120.29 (16)
C3—C2—H2	120.4	C16—C17—H17	119.9
C1—C2—H2	120.4	N5—C17—H17	119.9
C2—C3—C4	123.55 (13)	C19—C18—N7	121.02 (15)
C2—C3—H3	118.2	C19—C18—H18	119.5
C4—C3—H3	118.2	N7—C18—H18	119.5
O1—C4—C5	125.60 (13)	C18—C19—C20	118.29 (14)
O1—C4—C3	120.25 (13)	C18—C19—H19	120.9
C5—C4—C3	114.14 (12)	C20—C19—H19	120.9
C6—C5—N1	115.74 (11)	C21—C20—C19	120.91 (14)
C6—C5—C4	122.36 (12)	C21—C20—H20	119.5
N1—C5—C4	121.89 (12)	C19—C20—H20	119.5
C1—C6—C5	119.88 (12)	C20—C21—C22	119.47 (15)
C1—C6—H6	120.1	C20—C21—H21	120.3
C5—C6—H6	120.1	C22—C21—H21	120.3
C8—C7—C12	120.97 (11)	N8—C22—N7	118.71 (12)
C8—C7—N3	119.05 (11)	N8—C22—C21	123.35 (13)
C12—C7—N3	119.97 (11)	N7—C22—C21	117.93 (13)
C7—C8—C9	119.61 (11)	O3—N1—O2	120.69 (12)
C7—C8—H8	120.2	O3—N1—C5	118.79 (12)
C9—C8—H8	120.2	O2—N1—C5	120.52 (12)
C8—C9—C10	122.42 (11)	O5—N2—O4	121.99 (13)
C8—C9—N4	116.20 (11)	O5—N2—C1	118.74 (12)
C10—C9—N4	121.36 (11)	O4—N2—C1	119.26 (12)
O6—C10—C9	125.87 (11)	O7—N3—O8	122.03 (12)
O6—C10—C11	119.81 (12)	O7—N3—C7	118.77 (12)
C9—C10—C11	114.31 (11)	O8—N3—C7	119.19 (11)
C12—C11—C10	123.39 (12)	O9—N4—O10	121.52 (12)
C12—C11—H11	118.3	O9—N4—C9	119.03 (11)
C10—C11—H11	118.3	O10—N4—C9	119.45 (11)
C11—C12—C7	119.28 (12)	C13—N5—C17	122.72 (14)
C11—C12—H12	120.4	C13—N5—H5	116.1 (13)
C7—C12—H12	120.4	C17—N5—H5	121.1 (13)
N6—C13—N5	118.30 (14)	C13—N6—H6A	120.0
N6—C13—C14	123.98 (16)	C13—N6—H6B	120.0
N5—C13—C14	117.71 (15)	H6A—N6—H6B	120.0
C15—C14—C13	119.64 (17)	C22—N7—C18	122.36 (12)
C15—C14—H14	120.2	C22—N7—H7	113.5 (13)
C13—C14—H14	120.2	C18—N7—H7	124.1 (13)
C14—C15—C16	120.98 (17)	C22—N8—H8A	120.0
C14—C15—H15	119.5	C22—N8—H8B	120.0
C16—C15—H15	119.5	H8A—N8—H8B	120.0

C6—C1—C2—C3	−1.0 (2)	C14—C15—C16—C17	0.4 (3)
N2—C1—C2—C3	177.39 (13)	C15—C16—C17—N5	−0.2 (2)
C1—C2—C3—C4	−0.4 (2)	N7—C18—C19—C20	1.3 (2)
C2—C3—C4—O1	−178.48 (14)	C18—C19—C20—C21	−0.9 (3)
C2—C3—C4—C5	1.7 (2)	C19—C20—C21—C22	−0.2 (2)

O1—C4—C5—C6	178.49 (13)	C20—C21—C22—N8	−177.98 (15)
C3—C4—C5—C6	−1.68 (19)	C20—C21—C22—N7	0.9 (2)
O1—C4—C5—N1	−0.4 (2)	C6—C5—N1—O3	5.60 (18)
C3—C4—C5—N1	179.45 (12)	C4—C5—N1—O3	−175.45 (13)
C2—C1—C6—C5	1.00 (19)	C6—C5—N1—O2	−173.28 (12)
N2—C1—C6—C5	−177.42 (11)	C4—C5—N1—O2	5.67 (19)
N1—C5—C6—C1	179.36 (11)	C6—C1—N2—O5	175.34 (13)
C4—C5—C6—C1	0.42 (19)	C2—C1—N2—O5	−3.1 (2)
C12—C7—C8—C9	0.38 (19)	C6—C1—N2—O4	−3.44 (19)
N3—C7—C8—C9	179.11 (11)	C2—C1—N2—O4	178.14 (13)
C7—C8—C9—C10	−0.63 (19)	C8—C7—N3—O7	177.56 (13)
C7—C8—C9—N4	−179.24 (11)	C12—C7—N3—O7	−3.70 (19)
C8—C9—C10—O6	−179.39 (13)	C8—C7—N3—O8	−2.72 (19)
N4—C9—C10—O6	−0.8 (2)	C12—C7—N3—O8	176.02 (13)
C8—C9—C10—C11	0.54 (18)	C8—C9—N4—O9	−8.16 (18)
N4—C9—C10—C11	179.09 (11)	C10—C9—N4—O9	173.21 (13)
O6—C10—C11—C12	179.70 (13)	C8—C9—N4—O10	171.16 (13)
C9—C10—C11—C12	−0.2 (2)	C10—C9—N4—O10	−7.47 (19)
C10—C11—C12—C7	0.0 (2)	N6—C13—N5—C17	−178.19 (14)
C8—C7—C12—C11	−0.1 (2)	C14—C13—N5—C17	1.1 (2)
N3—C7—C12—C11	−178.80 (12)	C16—C17—N5—C13	−0.6 (2)
N6—C13—C14—C15	178.41 (16)	N8—C22—N7—C18	178.45 (14)
N5—C13—C14—C15	−0.8 (2)	C21—C22—N7—C18	−0.5 (2)
C13—C14—C15—C16	0.1 (3)	C19—C18—N7—C22	−0.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O1^{i}	0.88 (1)	1.92 (1)	2.7304 (16)	152 (2)
N5—H5···O2^{i}	0.88 (1)	2.31 (2)	2.9553 (17)	130 (2)
N6—H6*A*···O1^{i}	0.86	2.02	2.7712 (19)	145
N6—H6*B*···O4^{ii}	0.86	2.15	2.9849 (18)	162
N7—H7···O6^{iii}	0.88 (1)	1.83 (1)	2.6627 (15)	157 (2)
N7—H7···O10^{iii}	0.88 (1)	2.31 (2)	2.8975 (17)	124 (2)
N8—H8*A*···O6^{iii}	0.86	2.04	2.7727 (16)	143
N8—H8*B*···O2^{i}	0.86	2.42	3.2740 (17)	175
N8—H8*B*···O3^{i}	0.86	2.50	3.1445 (17)	132
C3—H3···O8	0.93	2.56	3.1944 (18)	126
C18—H18···O10^{iii}	0.93	2.51	3.034 (2)	116

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