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Bis(2-amino-6-methylpyridinium) 3-nitrobenzene-1,2-dicarboxylate

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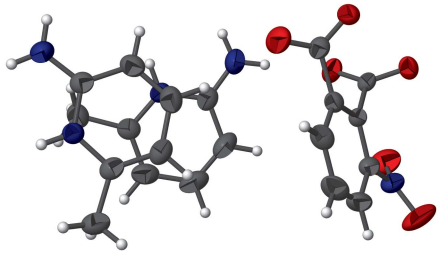
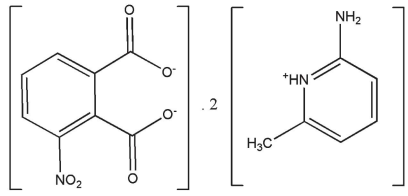
In the title molecular salt, $2C_6H_9N_2^+\cdot C_8H_3NO_6^{2-}$, the cations are protonated at their pyridine N atoms. The cations and anion are linked by N—H···O and C—H···O hydrogen bonds and a π–π interaction [centroid-to-centroid distance = 3.7299 (13) Å]. In the crystal, N—H···O hydrogen bonds link the anions and cations into an infinite two-dimensional network parallel to $(10\overline{1})$. N—H···O hydrogen bonds generate $R_1^2(4)$, $R_2^1(6)$, $R_2^4(18)$ and $R_2^2(11)$ ring motifs. The structure also features weak C—H···O and C—H···π interactions, which lead to the formation of a three-dimensional network.

3D view



Chemical scheme



Structure description

Pyridine derivatives are known to exhibit pharmacological properties such as anti-proliferative, antitubolin (Magedov *et al.*, 2008) and antiviral (Hamdouchi *et al.*, 1999) activities. We report herein the synthesis and the crystal structure of the title molecular salt (Fig. 1). The geometric parameters are in agreement with reported similar structures (Sivakumar *et al.*, 2016*a*,*b*). The asymmetric unit contains two 2-amino-6-methylpyridinium cations and one 3-nitrobenzene-1,2-dicarboxylate anion. The cations are protonated at its pyridine N (N2 and N4) atoms and the anion is deprotonated at hydroxy O (O4 and O6) atoms. The cations and anion are linked by N—H···O and C—H···O hydrogen bonds (Table 1) and a π–π interaction [*Cg*2···*Cg*3 = 3.7299 (13) Å; *Cg*2 and *Cg*3 are the centroids of the rings (N2/C9–C13) and (N4/C15–C19), respectively].

In the crystal, N4—H4*A*···O3^{ii} and N5—H5*A*···O5^{ii} hydrogen bonds (Table 1, Fig. 2) generate an $R_2^2(11)$ ring-motif enclosing the atoms (N5/H5*A*/O5/C8/C3/C2/C7/O3/H4*A*/N4/C19). The N2—H2*A*···O5^{i} and N3—H3*A*···O6^{i} hydrogen bonds (Table 1, Fig. 2) generate a bifurcated $R_1^2(4)$ ring-motif, constituted by the atoms (C8/O5/H2*A*/O6). The

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O5^{i}	0.87 (2)	1.93 (2)	2.777 (2)	167 (2)
N2—H2*A*···O6^{i}	0.87 (2)	2.69 (2)	3.364 (2)	136 (2)
N3—H3*A*···O6^{i}	0.86	1.91	2.755 (2)	167
N3—H3*B*···O4	0.86	1.97	2.825 (2)	171
N4—H4*A*···O3^{ii}	0.87 (2)	1.81 (2)	2.678 (2)	171 (2)
N5—H5*A*···O5^{ii}	0.86	2.16	2.949 (2)	152
N5—H5*B*···O3^{i}	0.86	2.17	2.993 (2)	161
C17—H17···O6	0.93	2.33	3.241 (3)	166
C18—H18···O4^{i}	0.93	2.42	3.293 (2)	156
C14—H14*C*···*Cg*1^{iii}	0.96	2.73	3.490 (2)	137

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

N2—H2*A*···O6^{i} and N3—H3*A*···O6^{i} (Table 1, Fig. 2) hydrogen bonds generate a bifurcated $R_2^1(6)$ ring-motif, constituted by the atoms (C13/N2/H2*A*/O6/H3*A*/N3). A pair of N3—H3*B*···O4 and N3—H3*A*···O6^{i} hydrogen bonds generate an $R_2^4(18)$ ring-motif (Table 1, Fig. 2). The N—H···O hydrogen bonds link the components into an infinite two-dimensional network parallel to the $(10\bar{1})$ plane. A weak C—H···O hydrogen bond and a C—H···π interaction (Table 1) lead to the formation of a three dimensional network (Fig. 3).

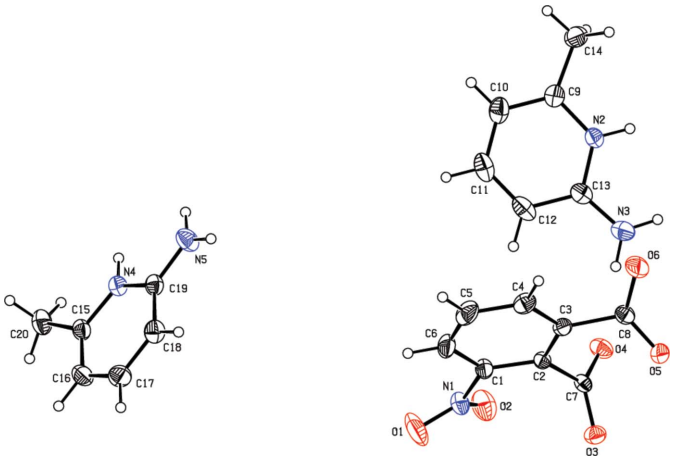

Figure 1
The molecular structure of the title molecular salt, with atom labelling and 30% probability displacement ellipsoids.

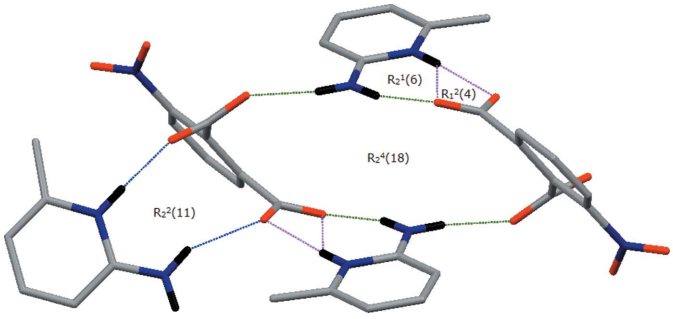

Figure 2
A partial view of the crystal packing of the title molecular salt, showing the ring graph-set motifs. H atoms not involving in hydrogen bonds have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_6H_9N_2^+\cdot C_8H_3NO_6^{2-}$
M_r	427.42
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	295
a, b, c (Å)	13.5461 (15), 7.7453 (9), 19.625 (2)
β (°)	101.486 (4)
V (Å^3)	2017.8 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.24 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.975, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28851, 3776, 2886
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.608
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.123, 1.03
No. of reflections	3776
No. of parameters	290
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})	0.22, −0.21

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

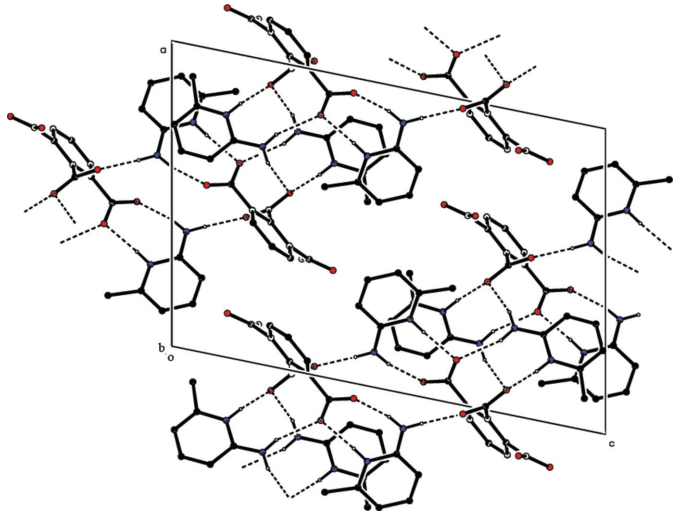

Figure 3
The crystal packing of the title molecular salt viewed along the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms not involving in hydrogen bonds have been omitted for clarity.

Synthesis and crystallization

The title molecular salt was synthesized using the raw materials 3-nitrophthalic acid (2.11 g) and 2-amino-6-methylpyridine (1.08 g) in an equimolar ratio. These reactants were dissolved in 20 ml of methanol and kept for slow evaporation at room temperature. After a span of 30 days, crystals suitable for X-ray diffraction were harvested.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161233 [doi:10.1107/S2414314616012335]

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Crystal data

$2C_6H_9N_2^+·C_8H_3NO_6^{2-}$
M_r = 427.42
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 13.5461 (15) Å
b = 7.7453 (9) Å
c = 19.625 (2) Å
β = 101.486 (4)°
V = 2017.8 (4) Å^3
Z = 4
$F(000)$ = 896
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9996 reflections
θ = 2.8–25.2°
μ = 0.11 mm^{-1}
T = 295 K
Block, colourless
0.24 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.975, T_{max} = 0.981
28851 measured reflections
3776 independent reflections
2886 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.6°, θ_{min} = 2.1°
h = −16→16
k = −9→9
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.123
S = 1.03
3776 reflections
290 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.8038P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.09358 (13)	0.1082 (3)	0.22870 (9)	0.0375 (4)
C2	1.02798 (12)	0.0628 (2)	0.27184 (8)	0.0295 (4)
C3	1.00168 (13)	0.1935 (2)	0.31418 (9)	0.0328 (4)
C4	1.04193 (15)	0.3587 (3)	0.31251 (11)	0.0431 (5)
H4	1.0247	0.4441	0.3414	0.052*
C5	1.10690 (16)	0.3976 (3)	0.26877 (12)	0.0543 (6)
H5	1.1331	0.5084	0.2683	0.065*
C6	1.13264 (15)	0.2732 (3)	0.22620 (11)	0.0509 (6)
H6	1.1756	0.2986	0.1961	0.061*
C7	0.98915 (13)	−0.1210 (2)	0.27654 (8)	0.0305 (4)
C8	0.93033 (14)	0.1621 (2)	0.36309 (9)	0.0352 (4)
C9	1.33900 (14)	0.0667 (3)	0.57066 (10)	0.0398 (4)
C10	1.39045 (17)	0.1214 (3)	0.52207 (12)	0.0532 (6)
H10	1.4536	0.1721	0.5355	0.064*
C11	1.34777 (19)	0.1009 (3)	0.45176 (12)	0.0602 (6)
H11	1.3827	0.1396	0.4184	0.072*
C12	1.25659 (18)	0.0259 (3)	0.43120 (11)	0.0546 (6)
H12	1.2290	0.0133	0.3841	0.066*
C13	1.20386 (15)	−0.0330 (3)	0.48160 (10)	0.0409 (5)
C14	1.37628 (16)	0.0794 (3)	0.64726 (11)	0.0502 (5)
H14A	1.4015	−0.0309	0.6651	0.075*
H14B	1.3220	0.1138	0.6691	0.075*
H14C	1.4293	0.1634	0.6569	0.075*
C15	1.30217 (14)	0.5431 (2)	0.55806 (10)	0.0381 (4)
C16	1.22798 (16)	0.4884 (3)	0.50592 (10)	0.0457 (5)
H16	1.2320	0.5088	0.4598	0.055*
C17	1.14507 (16)	0.4010 (3)	0.52183 (11)	0.0481 (5)
H17	1.0938	0.3637	0.4860	0.058*
C18	1.13860 (14)	0.3698 (3)	0.58871 (10)	0.0434 (5)
H18	1.0841	0.3089	0.5987	0.052*
C19	1.21448 (14)	0.4300 (2)	0.64267 (10)	0.0365 (4)
C20	1.39675 (16)	0.6288 (3)	0.54851 (11)	0.0506 (5)
H20A	1.4491	0.5441	0.5513	0.076*
H20B	1.4163	0.7138	0.5843	0.076*
H20C	1.3858	0.6839	0.5038	0.076*
N1	1.12444 (13)	−0.0224 (3)	0.18282 (9)	0.0506 (5)
N2	1.24708 (11)	−0.0084 (2)	0.54935 (8)	0.0363 (4)
N3	1.11547 (13)	−0.1094 (3)	0.46649 (9)	0.0535 (5)
H3A	1.0863	−0.1428	0.4993	0.064*
H3B	1.0869	−0.1261	0.4238	0.064*

N4	1.29323 (11)	0.5142 (2)	0.62538 (8)	0.0351 (4)
N5	1.21327 (13)	0.4063 (2)	0.70948 (8)	0.0500 (5)
H5A	1.2620	0.4443	0.7408	0.060*
H5B	1.1637	0.3529	0.7214	0.060*
O1	1.14462 (17)	0.0271 (3)	0.12823 (10)	0.0919 (7)
O2	1.12823 (14)	−0.1731 (2)	0.20011 (9)	0.0686 (5)
O3	0.92072 (9)	−0.17215 (17)	0.22829 (6)	0.0407 (3)
O4	1.02835 (10)	−0.20448 (17)	0.32863 (6)	0.0435 (3)
O5	0.85596 (10)	0.0646 (2)	0.34366 (7)	0.0478 (4)
O6	0.94974 (12)	0.2387 (2)	0.41937 (8)	0.0608 (4)
H2A	1.2139 (14)	−0.042 (3)	0.5804 (9)	0.051 (6)*
H4A	1.3394 (12)	0.558 (2)	0.6583 (8)	0.040 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0335 (9)	0.0455 (12)	0.0344 (10)	−0.0022 (8)	0.0091 (8)	0.0049 (8)
C2	0.0290 (8)	0.0322 (9)	0.0268 (8)	−0.0004 (7)	0.0045 (7)	0.0027 (7)
C3	0.0322 (9)	0.0325 (10)	0.0322 (9)	−0.0023 (7)	0.0032 (7)	−0.0001 (7)
C4	0.0443 (11)	0.0329 (10)	0.0501 (11)	−0.0038 (9)	0.0042 (9)	−0.0015 (9)
C5	0.0528 (13)	0.0401 (12)	0.0675 (15)	−0.0170 (10)	0.0057 (11)	0.0095 (11)
C6	0.0429 (11)	0.0609 (15)	0.0504 (12)	−0.0138 (10)	0.0128 (9)	0.0143 (11)
C7	0.0356 (9)	0.0317 (10)	0.0258 (8)	0.0019 (7)	0.0099 (7)	−0.0020 (7)
C8	0.0389 (10)	0.0353 (10)	0.0321 (9)	0.0036 (8)	0.0091 (8)	−0.0033 (8)
C9	0.0400 (10)	0.0340 (10)	0.0464 (11)	0.0029 (8)	0.0108 (8)	0.0027 (8)
C10	0.0491 (12)	0.0514 (13)	0.0623 (14)	−0.0040 (10)	0.0189 (10)	0.0130 (11)
C11	0.0681 (15)	0.0644 (16)	0.0561 (14)	0.0038 (13)	0.0315 (12)	0.0158 (12)
C12	0.0674 (15)	0.0641 (15)	0.0352 (11)	0.0118 (12)	0.0173 (10)	0.0067 (10)
C13	0.0446 (11)	0.0427 (11)	0.0352 (10)	0.0091 (9)	0.0076 (8)	0.0007 (8)
C14	0.0468 (12)	0.0522 (13)	0.0484 (12)	−0.0062 (10)	0.0021 (9)	−0.0003 (10)
C15	0.0446 (10)	0.0344 (10)	0.0382 (10)	0.0049 (8)	0.0154 (8)	0.0004 (8)
C16	0.0551 (12)	0.0496 (13)	0.0334 (10)	0.0020 (10)	0.0113 (9)	−0.0010 (9)
C17	0.0480 (12)	0.0503 (13)	0.0435 (11)	−0.0025 (10)	0.0030 (9)	−0.0076 (9)
C18	0.0396 (10)	0.0422 (12)	0.0497 (12)	−0.0069 (9)	0.0119 (9)	−0.0049 (9)
C19	0.0394 (10)	0.0327 (10)	0.0398 (10)	0.0017 (8)	0.0133 (8)	−0.0012 (8)
C20	0.0509 (12)	0.0539 (13)	0.0531 (12)	−0.0025 (10)	0.0245 (10)	0.0013 (10)
N1	0.0440 (10)	0.0715 (14)	0.0413 (10)	−0.0031 (9)	0.0202 (8)	−0.0031 (9)
N2	0.0375 (8)	0.0402 (9)	0.0328 (8)	0.0024 (7)	0.0110 (7)	0.0012 (7)
N3	0.0526 (11)	0.0705 (13)	0.0353 (9)	−0.0023 (9)	0.0033 (8)	−0.0034 (8)
N4	0.0357 (8)	0.0357 (9)	0.0349 (8)	−0.0020 (7)	0.0094 (7)	−0.0019 (7)
N5	0.0504 (10)	0.0634 (12)	0.0387 (9)	−0.0143 (9)	0.0148 (8)	0.0005 (8)
O1	0.1245 (17)	0.1093 (17)	0.0595 (11)	−0.0101 (13)	0.0608 (12)	0.0005 (11)
O2	0.0831 (12)	0.0595 (12)	0.0740 (11)	0.0119 (9)	0.0418 (9)	−0.0062 (9)
O3	0.0436 (7)	0.0376 (8)	0.0384 (7)	−0.0055 (6)	0.0020 (6)	−0.0036 (6)
O4	0.0609 (9)	0.0361 (8)	0.0319 (7)	0.0006 (6)	0.0056 (6)	0.0037 (6)
O5	0.0398 (7)	0.0659 (10)	0.0404 (7)	−0.0131 (7)	0.0146 (6)	−0.0116 (7)
O6	0.0758 (11)	0.0668 (11)	0.0441 (8)	−0.0194 (9)	0.0221 (8)	−0.0228 (8)

Geometric parameters (Å, º)

C1—C6	1.388 (3)	C13—N2	1.355 (2)
C1—C2	1.389 (2)	C14—H14A	0.9600
C1—N1	1.470 (3)	C14—H14B	0.9600
C2—C3	1.400 (2)	C14—H14C	0.9600
C2—C7	1.526 (3)	C15—C16	1.352 (3)
C3—C4	1.393 (3)	C15—N4	1.369 (2)
C3—C8	1.511 (2)	C15—C20	1.488 (3)
C4—C5	1.380 (3)	C16—C17	1.399 (3)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.365 (3)	C17—C18	1.354 (3)
C5—H5	0.9300	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.401 (3)
C7—O4	1.237 (2)	C18—H18	0.9300
C7—O3	1.250 (2)	C19—N5	1.327 (2)
C8—O6	1.235 (2)	C19—N4	1.350 (2)
C8—O5	1.256 (2)	C20—H20A	0.9600
C9—C10	1.356 (3)	C20—H20B	0.9600
C9—N2	1.363 (2)	C20—H20C	0.9600
C9—C14	1.491 (3)	N1—O2	1.213 (3)
C10—C11	1.395 (3)	N1—O1	1.219 (2)
C10—H10	0.9300	N2—H2A	0.867 (10)
C11—C12	1.352 (3)	N3—H3A	0.8600
C11—H11	0.9300	N3—H3B	0.8600
C12—C13	1.406 (3)	N4—H4A	0.874 (9)
C12—H12	0.9300	N5—H5A	0.8600
C13—N3	1.316 (3)	N5—H5B	0.8600
C6—C1—C2	123.34 (19)	H14A—C14—H14B	109.5
C6—C1—N1	117.10 (17)	C9—C14—H14C	109.5
C2—C1—N1	119.57 (17)	H14A—C14—H14C	109.5
C1—C2—C3	116.58 (17)	H14B—C14—H14C	109.5
C1—C2—C7	122.89 (16)	C16—C15—N4	118.96 (18)
C3—C2—C7	120.47 (15)	C16—C15—C20	125.00 (18)
C4—C3—C2	120.20 (17)	N4—C15—C20	116.00 (17)
C4—C3—C8	117.76 (17)	C15—C16—C17	119.44 (18)
C2—C3—C8	122.04 (16)	C15—C16—H16	120.3
C5—C4—C3	121.1 (2)	C17—C16—H16	120.3
C5—C4—H4	119.5	C18—C17—C16	120.82 (19)
C3—C4—H4	119.5	C18—C17—H17	119.6
C6—C5—C4	119.9 (2)	C16—C17—H17	119.6
C6—C5—H5	120.0	C17—C18—C19	119.61 (19)
C4—C5—H5	120.0	C17—C18—H18	120.2
C5—C6—C1	118.85 (19)	C19—C18—H18	120.2
C5—C6—H6	120.6	N5—C19—N4	118.74 (17)
C1—C6—H6	120.6	N5—C19—C18	123.33 (18)
O4—C7—O3	126.30 (17)	N4—C19—C18	117.92 (17)

O4—C7—C2	116.17 (15)	C15—C20—H20A	109.5
O3—C7—C2	117.52 (15)	C15—C20—H20B	109.5
O6—C8—O5	125.12 (17)	H20A—C20—H20B	109.5
O6—C8—C3	116.18 (17)	C15—C20—H20C	109.5
O5—C8—C3	118.68 (15)	H20A—C20—H20C	109.5
C10—C9—N2	118.93 (19)	H20B—C20—H20C	109.5
C10—C9—C14	124.77 (19)	O2—N1—O1	123.0 (2)
N2—C9—C14	116.29 (17)	O2—N1—C1	119.49 (17)
C9—C10—C11	119.4 (2)	O1—N1—C1	117.6 (2)
C9—C10—H10	120.3	C13—N2—C9	123.43 (17)
C11—C10—H10	120.3	C13—N2—H2A	117.6 (15)
C12—C11—C10	121.2 (2)	C9—N2—H2A	119.0 (15)
C12—C11—H11	119.4	C13—N3—H3A	120.0
C10—C11—H11	119.4	C13—N3—H3B	120.0
C11—C12—C13	119.4 (2)	H3A—N3—H3B	120.0
C11—C12—H12	120.3	C19—N4—C15	123.21 (16)
C13—C12—H12	120.3	C19—N4—H4A	119.1 (13)
N3—C13—N2	118.70 (18)	C15—N4—H4A	117.6 (13)
N3—C13—C12	123.66 (19)	C19—N5—H5A	120.0
N2—C13—C12	117.64 (19)	C19—N5—H5B	120.0
C9—C14—H14A	109.5	H5A—N5—H5B	120.0
C9—C14—H14B	109.5		

C6—C1—C2—C3	0.0 (3)	C14—C9—C10—C11	179.4 (2)
N1—C1—C2—C3	−179.99 (15)	C9—C10—C11—C12	−0.7 (4)
C6—C1—C2—C7	−177.19 (17)	C10—C11—C12—C13	−0.1 (4)
N1—C1—C2—C7	2.8 (3)	C11—C12—C13—N3	−179.1 (2)
C1—C2—C3—C4	−0.9 (2)	C11—C12—C13—N2	1.1 (3)
C7—C2—C3—C4	176.34 (16)	N4—C15—C16—C17	−1.2 (3)
C1—C2—C3—C8	179.48 (15)	C20—C15—C16—C17	176.5 (2)
C7—C2—C3—C8	−3.3 (2)	C15—C16—C17—C18	−0.3 (3)
C2—C3—C4—C5	0.9 (3)	C16—C17—C18—C19	1.7 (3)
C8—C3—C4—C5	−179.45 (17)	C17—C18—C19—N5	179.3 (2)
C3—C4—C5—C6	0.0 (3)	C17—C18—C19—N4	−1.5 (3)
C4—C5—C6—C1	−0.9 (3)	C6—C1—N1—O2	150.7 (2)
C2—C1—C6—C5	0.9 (3)	C2—C1—N1—O2	−29.3 (3)
N1—C1—C6—C5	−179.07 (18)	C6—C1—N1—O1	−29.7 (3)
C1—C2—C7—O4	103.5 (2)	C2—C1—N1—O1	150.3 (2)
C3—C2—C7—O4	−73.6 (2)	N3—C13—N2—C9	178.91 (18)
C1—C2—C7—O3	−77.2 (2)	C12—C13—N2—C9	−1.3 (3)
C3—C2—C7—O3	105.67 (19)	C10—C9—N2—C13	0.4 (3)
C4—C3—C8—O6	−36.3 (2)	C14—C9—N2—C13	−178.47 (18)
C2—C3—C8—O6	143.32 (19)	N5—C19—N4—C15	179.10 (18)
C4—C3—C8—O5	142.41 (18)	C18—C19—N4—C15	−0.1 (3)
C2—C3—C8—O5	−38.0 (3)	C16—C15—N4—C19	1.5 (3)
N2—C9—C10—C11	0.6 (3)	C20—C15—N4—C19	−176.50 (18)

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O5^{i}	0.87 (2)	1.93 (2)	2.777 (2)	167 (2)
N2—H2*A*···O6^{i}	0.87 (2)	2.69 (2)	3.364 (2)	136 (2)
N3—H3*A*···O6^{i}	0.86	1.91	2.755 (2)	167
N3—H3*B*···O4	0.86	1.97	2.825 (2)	171
N4—H4*A*···O3^{ii}	0.87 (2)	1.81 (2)	2.678 (2)	171 (2)
N5—H5*A*···O5^{ii}	0.86	2.16	2.949 (2)	152
N5—H5*B*···O3^{i}	0.86	2.17	2.993 (2)	161
C17—H17···O6	0.93	2.33	3.241 (3)	166
C18—H18···O4^{i}	0.93	2.42	3.293 (2)	156
C14—H14*C*···*Cg*1^{iii}	0.96	2.73	3.490 (2)	137

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