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2-Amino-4-methylpyridinium 2-hydroxybenzoate

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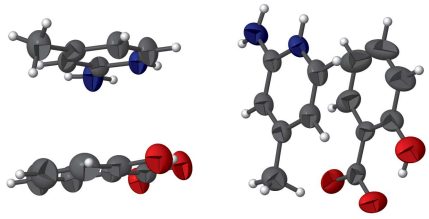
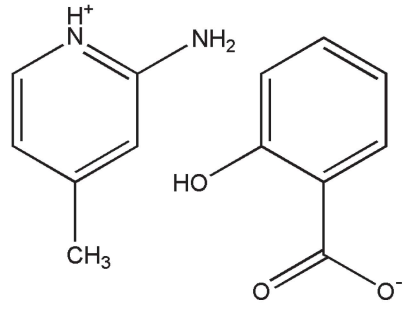
The title molecular salt, $C_6H_9N_2^+\cdot C_7H_5O_3^-$, contains two ion pairs in the asymmetric unit. Both anions feature an intramolecular O—H···O hydrogen bond, which closes an $S(6)$ ring. In the crystal, N—H···O hydogen bonds link the components into [010] chains, which feature $R_2^2(8)$ loops. The crystal structure is consolidated by weak C—H···O and π–π [centroid-to-centroid distance = 3.7528 (16) Å] interactions, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

As part of our ongoing studies of pyridinium molecular salts (Sivakumar *et al.*, 2016*a*,*b*), we now report the synthesis and the crystal structure of the title molecular salt (Fig. 1), whose asymmetric unit contains two 2-amino-4-methylpyridinium cations and two 2-hydroxybenzoate anions. The cations are protonated at the pyridine N (N1 and N3) atoms as usual. In both anions, intramolecular O1—H1*A*···O3 and O4—H4*C*···O6 hydrogen bonds (Table 1) generate $S(6)$ rings.

In the crystal, N1—H1···O3^{i}, N2—H2*B*···O2^{i}, N3—H3*A*···O5^{ii} and N4—H4*A*···O6^{ii} hydrogen bonds link adjacent anions and cations, generating $R_2^2(8)$ ring-set motifs (Fig. 2); these units are further connected by N4—H4*B*···O2 (Table 1) hydrogen bonds into chains propagating along [010]. The crystal structure also features weak C12—H12···O4^{iii} (Table 1) and π–π [*Cg*1···*Cg*1^{iv} = 3.7528 (16) Å; symmetry code: (iv) $1-x$, $1-y$, $-z$; *Cg*1 is the centroid of the N1/C8–C12 ring] interactions, which cross-link the chains, forming a three-dimensional network (Fig. 3).

Synthesis and crystallization

An equimolar ratio of 2-hydroxy benzoic acid (0.69 g) and 2-amino-4-methylpyridine (0.54 g) was dissolved in 10 ml of methanol and a white precipitate formed. The preci-

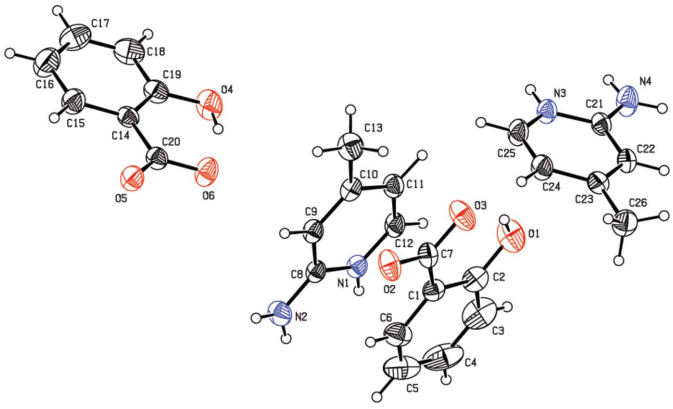


Figure 1
The molecular structure of the title molecular salt, with atom labelling and 30% probability displacement ellipsoids.

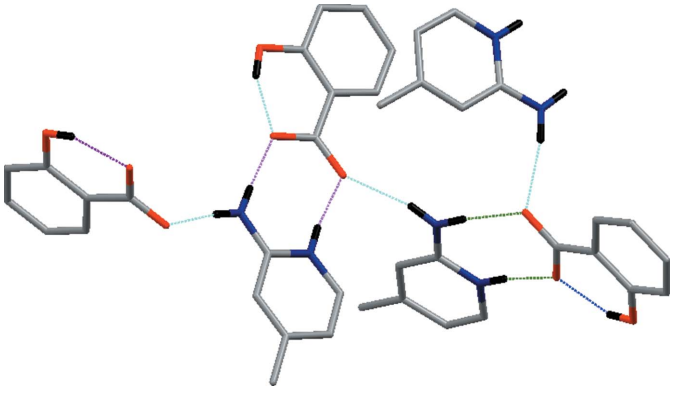


Figure 2
A partial view of the crystal packing showing the ring motifs.

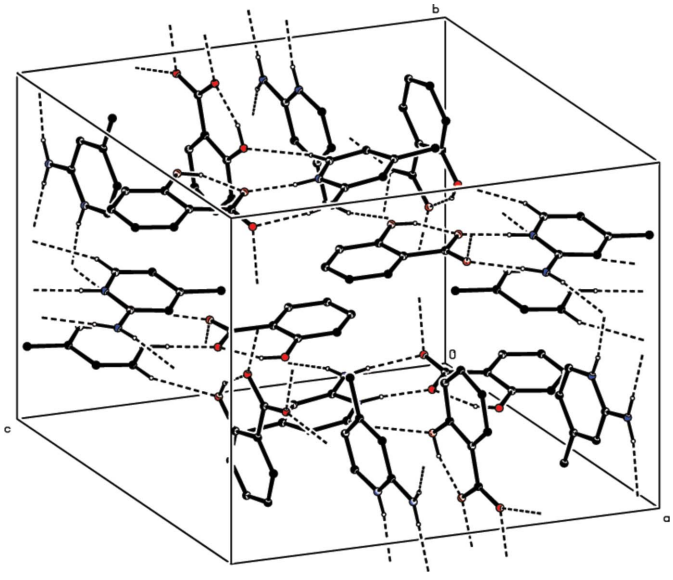


Figure 3
The crystal packing of the title molecular salt viewed along the *bc* plane. Hydrogen bonds are shown as dashed lines. H atoms not involving in hydrogen bonding have been omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*A*···O3	0.83 (1)	1.81 (2)	2.546 (3)	149 (4)
O4—H4*C*···O6	0.83 (1)	1.74 (2)	2.508 (3)	154 (4)
N1—H1···O3^{i}	0.86	1.79	2.648 (3)	173
N2—H2*B*···O2^{i}	0.86 (1)	2.00 (1)	2.858 (4)	175 (3)
N2—H2*A*···O5^{ii}	0.85 (1)	2.05 (1)	2.890 (3)	168 (3)
N3—H3*A*···O5^{ii}	0.86 (1)	1.89 (1)	2.743 (3)	172 (3)
N4—H4*A*···O6^{ii}	0.86 (1)	1.96 (1)	2.814 (4)	177 (3)
N4—H4*B*···O2^{ii}	0.86 (1)	2.05 (1)	2.891 (4)	170 (4)
C12—H12···O4^{iii}	0.93	2.52	3.390 (4)	156

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_9N_2^+\cdot C_7H_5O_3^-$
M_r	246.26
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	12.6615 (9), 13.8008 (11), 15.4039 (14)
β (°)	111.225 (2)
V (Å^3)	2509.1 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.26 × 0.24 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.678, 0.745
No. of measured, independent and observed reflections	27359, 5010, 2989
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.621
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.161, 1.08
No. of reflections	5010
No. of parameters	359
No. of restraints	8
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.22

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

pitate was dissolved in 20 ml of water and kept at room temperature for slow evaporation. After 30 days, colourless blocks of the title salt were isolated.

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**, x161443 [doi:10.1107/S2414314616014437]

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Crystal data

$C_6H_9N_2^+·C_7H_5O_3^-$
M_r = 246.26
Monoclinic, $P2_1/c$
a = 12.6615 (9) Å
b = 13.8008 (11) Å
c = 15.4039 (14) Å
β = 111.225 (2)°
V = 2509.1 (4) Å^3
Z = 8
$F(000)$ = 1040
D_x = 1.304 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6612 reflections
θ = 2.3–23.6°
μ = 0.09 mm^{-1}
T = 295 K
Block, colourless
0.26 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.678, T_{max} = 0.745
27359 measured reflections
5010 independent reflections
R_{int} = 0.034
θ_{max} = 26.2°, θ_{min} = 1.7°
h = −15→15
k = −17→17
l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.161
S = 1.08
5010 reflections
359 parameters
8 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 2.845P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.3683 (3)	0.1420 (2)	0.0863 (2)	0.0459 (7)

C6	0.2754 (3)	0.1418 (2)	0.0040 (3)	0.0673 (10)
H6	0.203120	0.146580	0.006113	0.081*
C5	0.2876 (5)	0.1348 (3)	−0.0803 (3)	0.0926 (14)
H5	0.224383	0.135931	−0.135172	0.111*
C4	0.3943 (6)	0.1260 (3)	−0.0829 (3)	0.1019 (17)
H4	0.402933	0.120288	−0.140142	0.122*
C3	0.4884 (4)	0.1255 (3)	−0.0027 (3)	0.0886 (13)
H3	0.560097	0.119550	−0.005858	0.106*
C2	0.4768 (3)	0.1339 (2)	0.0828 (2)	0.0574 (9)
C7	0.3514 (2)	0.1503 (2)	0.1759 (2)	0.0495 (8)
C8	0.3182 (2)	0.3869 (2)	−0.0761 (2)	0.0429 (7)
C9	0.3187 (2)	0.4032 (2)	0.0137 (2)	0.0454 (7)
H9	0.250654	0.414888	0.022009	0.055*
C10	0.4166 (2)	0.4021 (2)	0.0888 (2)	0.0465 (7)
C11	0.5197 (3)	0.3858 (2)	0.0753 (2)	0.0504 (8)
C12	0.5169 (2)	0.3711 (2)	−0.0118 (2)	0.0505 (8)
H12	0.584292	0.359920	−0.021349	0.061*
C13	0.4198 (3)	0.4157 (3)	0.1863 (2)	0.0668 (10)
H13A	0.345547	0.432604	0.184730	0.100*
H13B	0.472013	0.466614	0.216086	0.100*
H13C	0.443824	0.356553	0.220642	0.100*
C14	0.1061 (2)	0.6973 (2)	0.1147 (2)	0.0439 (7)
C15	0.0309 (3)	0.7700 (3)	0.1141 (3)	0.0623 (9)
H15	−0.040918	0.753619	0.112752	0.075*
C16	0.0598 (4)	0.8659 (3)	0.1155 (3)	0.0831 (12)
H16	0.007493	0.913827	0.114029	0.100*
C17	0.1663 (4)	0.8908 (3)	0.1192 (3)	0.0840 (12)
H17	0.186402	0.955820	0.121303	0.101*
C18	0.2425 (3)	0.8214 (3)	0.1198 (3)	0.0737 (11)
H18	0.314367	0.839136	0.122314	0.088*
C19	0.2136 (3)	0.7240 (3)	0.1167 (2)	0.0536 (8)
C20	0.0747 (2)	0.5936 (2)	0.1145 (2)	0.0474 (7)
C21	−0.0130 (2)	0.6937 (2)	−0.1326 (2)	0.0460 (7)
C22	0.0192 (2)	0.7896 (2)	−0.1379 (2)	0.0484 (8)
H22	−0.031505	0.839371	−0.141032	0.058*
C23	0.1235 (2)	0.8113 (2)	−0.1388 (2)	0.0486 (8)
C24	0.1985 (2)	0.7350 (2)	−0.1345 (2)	0.0562 (9)
H24	0.270064	0.747788	−0.135866	0.067*
C25	0.1660 (2)	0.6435 (2)	−0.1286 (3)	0.0595 (9)
H25	0.215866	0.592996	−0.125625	0.071*
C26	0.1601 (3)	0.9135 (2)	−0.1424 (3)	0.0679 (10)
H26A	0.095063	0.952753	−0.174757	0.102*
H26B	0.212228	0.915961	−0.174700	0.102*
H26C	0.196441	0.937671	−0.080238	0.102*
N1	0.41871 (18)	0.37204 (17)	−0.08565 (18)	0.0449 (6)
H1	0.420195	0.362938	−0.140423	0.054*
N2	0.2249 (2)	0.3872 (2)	−0.1522 (2)	0.0576 (7)
N3	0.0624 (2)	0.62292 (19)	−0.12671 (19)	0.0492 (6)

N4	−0.1142 (2)	0.6683 (2)	−0.1317 (3)	0.0685 (9)
O1	0.5718 (2)	0.1361 (2)	0.1601 (2)	0.0791 (8)
O2	0.25347 (17)	0.15946 (19)	0.17682 (17)	0.0679 (7)
O3	0.43864 (17)	0.1485 (2)	0.25005 (16)	0.0690 (7)
O4	0.2911 (2)	0.6573 (2)	0.1163 (2)	0.0736 (8)
O5	−0.01976 (16)	0.57100 (16)	0.11794 (16)	0.0586 (6)
O6	0.14672 (18)	0.53092 (16)	0.11156 (18)	0.0660 (7)
H1A	0.552 (3)	0.140 (3)	0.2055 (19)	0.103 (16)*
H2A	0.1614 (15)	0.391 (2)	−0.145 (2)	0.061 (10)*
H2B	0.230 (3)	0.371 (2)	−0.2043 (13)	0.067 (11)*
H3A	0.044 (3)	0.5637 (10)	−0.122 (2)	0.058 (10)*
H4A	−0.127 (3)	0.6079 (10)	−0.126 (3)	0.080 (13)*
H4B	−0.160 (2)	0.7161 (18)	−0.141 (3)	0.081 (13)*
H4C	0.259 (3)	0.6048 (17)	0.114 (3)	0.108 (18)*
H11	0.593 (2)	0.384 (2)	0.131 (2)	0.046 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0556 (18)	0.0360 (16)	0.0472 (19)	−0.0029 (14)	0.0200 (15)	0.0055 (14)
C6	0.079 (2)	0.057 (2)	0.058 (2)	−0.0116 (19)	0.014 (2)	0.0039 (18)
C5	0.135 (4)	0.072 (3)	0.058 (3)	−0.035 (3)	0.021 (3)	−0.005 (2)
C4	0.177 (5)	0.082 (3)	0.065 (3)	−0.035 (4)	0.066 (4)	−0.016 (3)
C3	0.119 (4)	0.089 (3)	0.088 (3)	−0.012 (3)	0.073 (3)	−0.002 (3)
C2	0.069 (2)	0.053 (2)	0.060 (2)	−0.0050 (17)	0.0352 (19)	0.0029 (17)
C7	0.0419 (17)	0.0506 (19)	0.058 (2)	0.0062 (14)	0.0198 (16)	0.0095 (16)
C8	0.0367 (15)	0.0387 (16)	0.059 (2)	−0.0004 (13)	0.0240 (15)	−0.0010 (14)
C9	0.0358 (15)	0.0468 (17)	0.062 (2)	0.0011 (13)	0.0271 (15)	0.0003 (15)
C10	0.0499 (17)	0.0398 (16)	0.058 (2)	0.0008 (14)	0.0291 (16)	0.0024 (15)
C11	0.0403 (17)	0.0522 (19)	0.060 (2)	0.0037 (15)	0.0191 (16)	0.0012 (16)
C12	0.0336 (15)	0.0514 (19)	0.073 (2)	0.0040 (14)	0.0264 (16)	−0.0015 (17)
C13	0.063 (2)	0.078 (3)	0.067 (2)	0.0048 (19)	0.0328 (19)	0.002 (2)
C14	0.0360 (15)	0.0543 (19)	0.0413 (17)	−0.0023 (14)	0.0139 (13)	−0.0021 (14)
C15	0.0512 (19)	0.058 (2)	0.080 (3)	−0.0002 (17)	0.0265 (18)	−0.0047 (19)
C16	0.082 (3)	0.059 (2)	0.113 (4)	0.003 (2)	0.040 (3)	−0.006 (2)
C17	0.098 (3)	0.055 (2)	0.101 (3)	−0.020 (2)	0.037 (3)	−0.009 (2)
C18	0.062 (2)	0.080 (3)	0.082 (3)	−0.025 (2)	0.029 (2)	−0.004 (2)
C19	0.0444 (17)	0.068 (2)	0.051 (2)	−0.0070 (16)	0.0192 (15)	−0.0012 (17)
C20	0.0392 (16)	0.0555 (19)	0.0497 (19)	0.0003 (15)	0.0187 (14)	−0.0012 (15)
C21	0.0357 (15)	0.0540 (19)	0.0486 (19)	0.0037 (14)	0.0156 (14)	0.0019 (15)
C22	0.0392 (16)	0.0510 (19)	0.055 (2)	0.0090 (14)	0.0172 (14)	0.0030 (15)
C23	0.0423 (16)	0.0520 (19)	0.0492 (19)	0.0001 (14)	0.0138 (14)	0.0012 (15)
C24	0.0350 (15)	0.057 (2)	0.079 (2)	−0.0003 (15)	0.0241 (16)	−0.0008 (18)
C25	0.0378 (16)	0.056 (2)	0.088 (3)	0.0065 (15)	0.0273 (17)	−0.0015 (19)
C26	0.060 (2)	0.054 (2)	0.091 (3)	−0.0061 (17)	0.028 (2)	0.0001 (19)
N1	0.0391 (13)	0.0483 (15)	0.0545 (16)	0.0014 (11)	0.0257 (12)	−0.0031 (12)
N2	0.0388 (15)	0.079 (2)	0.060 (2)	0.0019 (14)	0.0237 (15)	−0.0076 (16)
N3	0.0386 (13)	0.0442 (16)	0.0672 (18)	0.0021 (12)	0.0221 (12)	0.0026 (14)

N4	0.0442 (16)	0.058 (2)	0.112 (3)	0.0045 (16)	0.0378 (17)	0.010 (2)
O1	0.0539 (15)	0.117 (2)	0.082 (2)	0.0055 (15)	0.0422 (15)	0.0129 (18)
O2	0.0421 (12)	0.0922 (18)	0.0738 (17)	0.0151 (12)	0.0262 (12)	0.0163 (14)
O3	0.0417 (12)	0.115 (2)	0.0534 (15)	0.0081 (13)	0.0213 (11)	0.0109 (14)
O4	0.0451 (13)	0.088 (2)	0.099 (2)	−0.0021 (14)	0.0388 (14)	0.0017 (17)
O5	0.0394 (11)	0.0574 (14)	0.0850 (17)	−0.0045 (10)	0.0296 (11)	−0.0071 (12)
O6	0.0515 (13)	0.0573 (14)	0.103 (2)	0.0036 (11)	0.0444 (13)	−0.0021 (13)

Geometric parameters (Å, º)

C1—C6	1.382 (4)	C15—H15	0.9300
C1—C2	1.398 (4)	C16—C17	1.373 (5)
C1—C7	1.477 (4)	C16—H16	0.9300
C6—C5	1.365 (5)	C17—C18	1.357 (5)
C6—H6	0.9300	C17—H17	0.9300
C5—C4	1.371 (7)	C18—C19	1.389 (5)
C5—H5	0.9300	C18—H18	0.9300
C4—C3	1.372 (6)	C19—O4	1.348 (4)
C4—H4	0.9300	C20—O5	1.255 (3)
C3—C2	1.382 (5)	C20—O6	1.271 (3)
C3—H3	0.9300	C21—N4	1.333 (4)
C2—O1	1.352 (4)	C21—N3	1.345 (4)
C7—O2	1.252 (3)	C21—C22	1.396 (4)
C7—O3	1.269 (4)	C22—C23	1.359 (4)
C8—N2	1.329 (4)	C22—H22	0.9300
C8—N1	1.349 (3)	C23—C24	1.403 (4)
C8—C9	1.399 (4)	C23—C26	1.493 (4)
C9—C10	1.355 (4)	C24—C25	1.343 (4)
C9—H9	0.9300	C24—H24	0.9300
C10—C11	1.413 (4)	C25—N3	1.352 (4)
C10—C13	1.501 (4)	C25—H25	0.9300
C11—C12	1.345 (4)	C26—H26A	0.9600
C11—H11	1.01 (3)	C26—H26B	0.9600
C12—N1	1.347 (4)	C26—H26C	0.9600
C12—H12	0.9300	N1—H1	0.8600
C13—H13A	0.9600	N2—H2A	0.853 (10)
C13—H13B	0.9600	N2—H2B	0.859 (10)
C13—H13C	0.9600	N3—H3A	0.861 (10)
C14—C15	1.381 (4)	N4—H4A	0.860 (10)
C14—C19	1.400 (4)	N4—H4B	0.855 (10)
C14—C20	1.484 (4)	O1—H1A	0.825 (10)
C15—C16	1.371 (5)	O4—H4C	0.826 (10)
C6—C1—C2	119.2 (3)	C15—C16—H16	120.2
C6—C1—C7	119.6 (3)	C17—C16—H16	120.2
C2—C1—C7	121.2 (3)	C18—C17—C16	120.6 (4)
C5—C6—C1	121.4 (4)	C18—C17—H17	119.7
C5—C6—H6	119.3	C16—C17—H17	119.7

C1—C6—H6	119.3	C17—C18—C19	120.3 (3)
C6—C5—C4	119.1 (4)	C17—C18—H18	119.8
C6—C5—H5	120.5	C19—C18—H18	119.8
C4—C5—H5	120.5	O4—C19—C18	118.6 (3)
C5—C4—C3	121.2 (4)	O4—C19—C14	121.6 (3)
C5—C4—H4	119.4	C18—C19—C14	119.8 (3)
C3—C4—H4	119.4	O5—C20—O6	122.6 (3)
C4—C3—C2	120.0 (4)	O5—C20—C14	119.9 (3)
C4—C3—H3	120.0	O6—C20—C14	117.5 (2)
C2—C3—H3	120.0	N4—C21—N3	118.0 (3)
O1—C2—C3	118.3 (4)	N4—C21—C22	123.5 (3)
O1—C2—C1	122.5 (3)	N3—C21—C22	118.5 (3)
C3—C2—C1	119.2 (4)	C23—C22—C21	121.0 (3)
O2—C7—O3	122.4 (3)	C23—C22—H22	119.5
O2—C7—C1	119.9 (3)	C21—C22—H22	119.5
O3—C7—C1	117.8 (3)	C22—C23—C24	118.6 (3)
N2—C8—N1	118.5 (3)	C22—C23—C26	121.6 (3)
N2—C8—C9	123.8 (3)	C24—C23—C26	119.8 (3)
N1—C8—C9	117.7 (3)	C25—C24—C23	119.3 (3)
C10—C9—C8	121.2 (3)	C25—C24—H24	120.3
C10—C9—H9	119.4	C23—C24—H24	120.3
C8—C9—H9	119.4	C24—C25—N3	121.5 (3)
C9—C10—C11	119.0 (3)	C24—C25—H25	119.2
C9—C10—C13	122.6 (3)	N3—C25—H25	119.2
C11—C10—C13	118.4 (3)	C23—C26—H26A	109.5
C12—C11—C10	118.6 (3)	C23—C26—H26B	109.5
C12—C11—H11	122.1 (16)	H26A—C26—H26B	109.5
C10—C11—H11	119.3 (16)	C23—C26—H26C	109.5
C11—C12—N1	121.6 (3)	H26A—C26—H26C	109.5
C11—C12—H12	119.2	H26B—C26—H26C	109.5
N1—C12—H12	119.2	C12—N1—C8	121.9 (3)
C10—C13—H13A	109.5	C12—N1—H1	119.1
C10—C13—H13B	109.5	C8—N1—H1	119.1
H13A—C13—H13B	109.5	C8—N2—H2A	118 (2)
C10—C13—H13C	109.5	C8—N2—H2B	119 (2)
H13A—C13—H13C	109.5	H2A—N2—H2B	122 (3)
H13B—C13—H13C	109.5	C21—N3—C25	121.1 (3)
C15—C14—C19	118.1 (3)	C21—N3—H3A	119 (2)
C15—C14—C20	121.1 (3)	C25—N3—H3A	120 (2)
C19—C14—C20	120.8 (3)	C21—N4—H4A	118 (2)
C16—C15—C14	121.5 (3)	C21—N4—H4B	113 (3)
C16—C15—H15	119.2	H4A—N4—H4B	129 (3)
C14—C15—H15	119.2	C2—O1—H1A	108 (3)
C15—C16—C17	119.6 (4)	C19—O4—H4C	105 (3)

C2—C1—C6—C5	−0.6 (5)	C15—C16—C17—C18	1.2 (7)
C7—C1—C6—C5	179.6 (3)	C16—C17—C18—C19	0.0 (6)
C1—C6—C5—C4	1.2 (6)	C17—C18—C19—O4	179.2 (4)

C6—C5—C4—C3	−0.9 (7)	C17—C18—C19—C14	−1.2 (6)
C5—C4—C3—C2	0.0 (7)	C15—C14—C19—O4	−179.2 (3)
C4—C3—C2—O1	−178.0 (4)	C20—C14—C19—O4	1.6 (5)
C4—C3—C2—C1	0.5 (6)	C15—C14—C19—C18	1.2 (5)
C6—C1—C2—O1	178.2 (3)	C20—C14—C19—C18	−178.0 (3)
C7—C1—C2—O1	−2.0 (5)	C15—C14—C20—O5	−3.1 (5)
C6—C1—C2—C3	−0.3 (5)	C19—C14—C20—O5	176.1 (3)
C7—C1—C2—C3	179.5 (3)	C15—C14—C20—O6	177.4 (3)
C6—C1—C7—O2	−1.7 (5)	C19—C14—C20—O6	−3.4 (4)
C2—C1—C7—O2	178.5 (3)	N4—C21—C22—C23	−179.9 (3)
C6—C1—C7—O3	178.8 (3)	N3—C21—C22—C23	1.0 (5)
C2—C1—C7—O3	−1.0 (4)	C21—C22—C23—C24	0.3 (5)
N2—C8—C9—C10	−179.9 (3)	C21—C22—C23—C26	−178.7 (3)
N1—C8—C9—C10	−1.3 (4)	C22—C23—C24—C25	−0.9 (5)
C8—C9—C10—C11	1.0 (4)	C26—C23—C24—C25	178.1 (3)
C8—C9—C10—C13	−177.7 (3)	C23—C24—C25—N3	0.1 (5)
C9—C10—C11—C12	−0.5 (5)	C11—C12—N1—C8	−0.6 (5)
C13—C10—C11—C12	178.3 (3)	N2—C8—N1—C12	179.7 (3)
C10—C11—C12—N1	0.3 (5)	C9—C8—N1—C12	1.1 (4)
C19—C14—C15—C16	−0.1 (5)	N4—C21—N3—C25	179.0 (3)
C20—C14—C15—C16	179.1 (3)	C22—C21—N3—C25	−1.8 (5)
C14—C15—C16—C17	−1.1 (6)	C24—C25—N3—C21	1.2 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O3	0.83 (1)	1.81 (2)	2.546 (3)	149 (4)
O4—H4*C*···O6	0.83 (1)	1.74 (2)	2.508 (3)	154 (4)
N1—H1···O3^{i}	0.86	1.79	2.648 (3)	173
N2—H2*B*···O2^{i}	0.86 (1)	2.00 (1)	2.858 (4)	175 (3)
N2—H2*A*···O5^{ii}	0.85 (1)	2.05 (1)	2.890 (3)	168 (3)
N3—H3*A*···O5^{ii}	0.86 (1)	1.89 (1)	2.743 (3)	172 (3)
N4—H4*A*···O6^{ii}	0.86 (1)	1.96 (1)	2.814 (4)	177 (3)
N4—H4*B*···O2^{ii}	0.86 (1)	2.05 (1)	2.891 (4)	170 (4)
C12—H12···O4^{iii}	0.93	2.52	3.390 (4)	156

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