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# 2-Amino-5-methylpyridinium 4-carboxybutanoate

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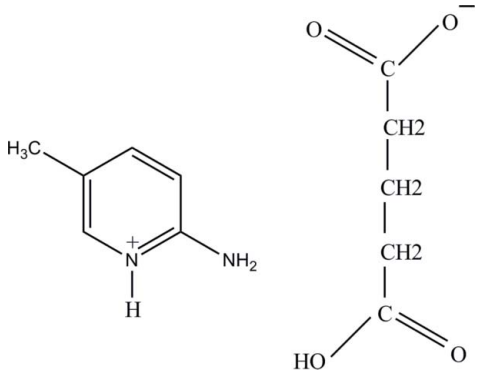
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.037; $wR$ factor = 0.109; data-to-parameter ratio = 13.0.

In the title salt, $C_6H_9N_2^+\cdot C_5H_7O_4^-$, the 2-amino-5-methylpyridinium cation is essentially planar, with a maximum deviation of 0.008 (1) Å. In the crystal, the protonated N atom and the 2-amino group are hydrogen bonded to the carboxylate O atoms *via* a pair of N—H···O hydrogen bonds, forming an $R_2^2(8)$ ring motif. The 4-carboxybutanoate anions are linked *via* O—H···O hydrogen bonds. The crystal structure is further stabilized by weak C—H···O interactions.

## Related literature

For background to the chemistry of substituted pyridines, see: Pozharski *et al.* (1997); Katritzky *et al.* (1996). For applications of glutaric acid, see: Windholz (1976); Saraswathi *et al.* (2001). For details of hydrogen bonding, see: Jeffrey & Saenger (1991); Jeffrey (1997); Scheiner (1997). For related structures, see: Hemamalini & Fun (2010*a*,*b*); Fun *et al.* (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_6H_9N_2^+\cdot C_5H_7O_4^-$
$M_r$ = 240.26
Orthorhombic, $P2_12_12_1$
$a$ = 5.3159 (10) Å
$b$ = 14.383 (3) Å
$c$ = 15.625 (3) Å
$V$ = 1194.7 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 100 K
0.29 × 0.17 × 0.10 mm

### Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.971, $T_{max}$ = 0.990
7996 measured reflections
2028 independent reflections
1752 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
$S$ = 1.05
2028 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.86 | 1.82 | 2.672 (2) | 170 |
| N2—H2$A$···O2$^{i}$ | 0.86 | 2.00 | 2.853 (3) | 174 |
| N2—H2$B$···O2 | 0.86 | 2.08 | 2.854 (2) | 149 |
| O4—H4···O1$^{ii}$ | 0.82 | 1.76 | 2.5729 (19) | 169 |
| C2—H2···O3$^{iii}$ | 0.93 | 2.59 | 3.441 (2) | 152 |
| C5—H5···O3$^{iv}$ | 0.93 | 2.50 | 3.379 (2) | 158 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2141).

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# supporting information

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## 2-Amino-5-methylpyridinium 4-carboxybutanoate

**Madhukar Hemamalini and Hoong-Kun Fun**

### S1. Comment

Pyridine and its derivatives play an important role in heterocyclic chemistry (Pozharski *et al.*, 1997; Katritzky *et al.*, 1996). They are often involved in hydrogen-bond interactions (Jeffrey & Saenger, 1991; Jeffrey, 1997; Scheiner, 1997). Glutaric acid (pentanedioic acid) is a dicarboxylic acid with five carbon atoms, occurring in plant and animal tissues. Glutaric acid is found in the blood and urine. It is used in the synthesis of pharmaceuticals, surfactants and metal finishing compounds. Alpha-ketoglutaric acid is used in dietary supplements to improve protein synthesis (Windholz, 1976). We have recently reported the crystal structures of 2-amino-5-methylpyridinium 4-nitrobenzoate (Hemamalini & Fun, 2010*a*), 2-amino-5-methylpyridinium nicotinate (Fun *et al.*, 2010) and 2-amino-5-methylpyridinium 3-amino-benzoate (Hemamalini & Fun, 2010*b*). In continuation of our studies of pyridinium derivatives, the crystal structure determination of the title compound has been undertaken.

The asymmetric unit (Fig. 1) contains a 2-amino-5-methylpyridinium cation and a 4-carboxybutanoate anion. The 2-amino-5-methylpyridinium cation is essentially planar, with a maximum deviation of 0.008 (1) Å for atom N1. In the 2-amino-5-methylpyridinium cation, a wide angle (123.09 (16)°) is subtended at the protonated N1 atom. The backbone conformation of the 4-carboxybutanoate anion can be described by the two torsion angles C11-C10-C9-C8 of -179.18 (14)° and C10-C9-C8-C7 of -72.74 (19)°. As evident from the torsion angles, the backbone is in a fully extended conformation (Saraswathi *et al.*, 2001) of the two carboxyl groups, one is deprotonated while the other is not. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges.

In the crystal packing (Fig. 2), the protonated N1 atom and the 2-amino group (N2) is hydrogen-bonded to the carboxylate oxygen atoms (O1 and O2) via a pair of intermolecular N1—H1···O1 and N2—H2A···O2 hydrogen bonds forming a ring motif $R_2^2(8)$ (Bernstein *et al.*, 1995). The 4-carboxybutanoate anions self-assemble via O4—H4···O1 hydrogen bonds. The crystal structure is further stabilized by weak C2—H2···O3 and C5—H5···O3 (Table 1) hydrogen bonds.

### S2. Experimental

A hot methanol solution (20 ml) of 2-amino-5-methylpyridine (27 mg, Aldrich) and glutaric acid (33 mg, Merck) were mixed and warmed over a heating magnetic stirrer for a few minutes. The resulting solution was allowed to cool slowly at room temperature and crystals of the title compound appeared after a few days.

### S3. Refinement

All hydrogen atoms were positioned geometrically [C–H = 0.93–0.97 Å, N–H = 0.86 Å and O–H = 0.82 Å] and were refined using a riding model, with $U_{iso}$(H) = 1.2 $U_{eq}$(C, N) or 1.5 $U_{eq}$(O). The methyl H atoms were positioned geometrically and were refined using a riding model, with $U_{iso}$(H) = 1.5$U_{eq}$(C). A rotating group model was used for the methyl group. In the absence of significant anomalous scattering effects, 1457 Friedel pairs were merged.

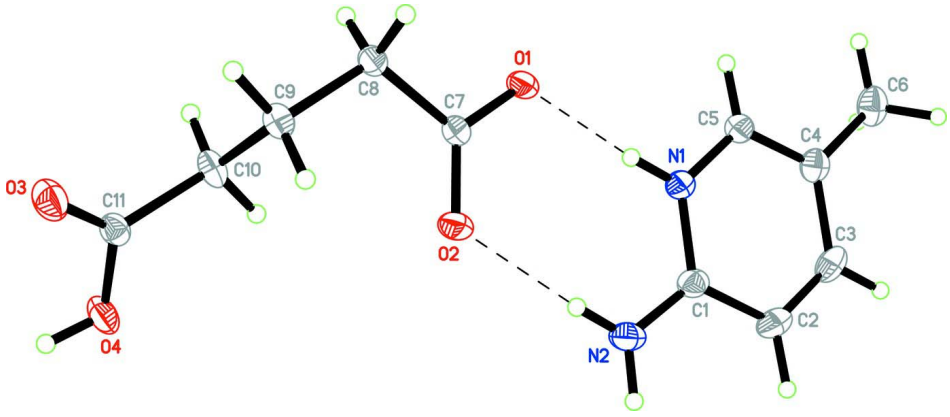


**Figure 1**

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

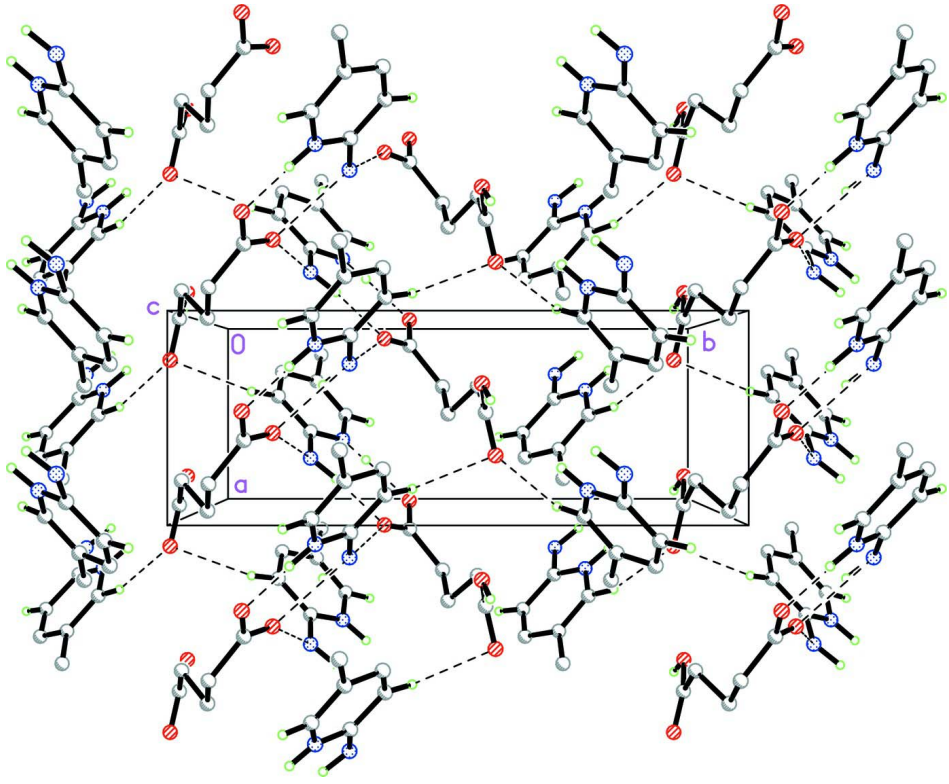


**Figure 2**

The crystal packing of the title compound, showing hydrogen-bonded (dashed lines) networks. H atoms are not involing the hydrogen bond interactions are omitted for clarity.

### 2-Amino-5-methylpyridinium 4-carboxybutanoate

*Crystal data*

$C_6H_9N_2^+·C_5H_7O_4^-$
$M_r$ = 240.26
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab

$a$ = 5.3159 (10) Å
$b$ = 14.383 (3) Å
$c$ = 15.625 (3) Å
$V$ = 1194.7 (4) Å$^3$

$Z = 4$
$F(000) = 512$
$D_x = 1.336$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2351 reflections
$\theta = 3.1$–$29.9°$
$\mu = 0.10$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.29 × 0.17 × 0.10 mm

*Data collection*

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.971$, $T_{max} = 0.990$
7996 measured reflections
2028 independent reflections
1752 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 30.1°$, $\theta_{min} = 2.8°$
$h = -7 \rightarrow 7$
$k = -13 \rightarrow 20$
$l = -21 \rightarrow 21$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.109$
$S = 1.05$
2028 reflections
156 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.0024P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.1366 (3) | 0.23633 (10) | 0.72155 (9) | 0.0178 (3) |
| H1 | 0.2568 | 0.1970 | 0.7149 | 0.021* |
| N2 | 0.2291 (4) | 0.29299 (12) | 0.58707 (9) | 0.0238 (4) |
| H2A | 0.3451 | 0.2516 | 0.5828 | 0.029* |
| H2B | 0.2030 | 0.3313 | 0.5457 | 0.029* |
| C1 | 0.0899 (4) | 0.29783 (12) | 0.65773 (10) | 0.0187 (4) |
| C2 | −0.1037 (4) | 0.36383 (13) | 0.67157 (11) | 0.0232 (4) |
| H2 | −0.1392 | 0.4084 | 0.6301 | 0.028* |
| C3 | −0.2378 (4) | 0.36172 (14) | 0.74603 (12) | 0.0237 (4) |

| | | | | |
|---|---|---|---|---|
| H3 | −0.3653 | 0.4051 | 0.7543 | 0.028* |
| C4 | −0.1888 (4) | 0.29528 (12) | 0.81139 (11) | 0.0198 (4) |
| C5 | 0.0019 (4) | 0.23393 (12) | 0.79573 (10) | 0.0184 (3) |
| H5 | 0.0408 | 0.1894 | 0.8368 | 0.022* |
| C6 | −0.3412 (4) | 0.29045 (14) | 0.89247 (13) | 0.0266 (4) |
| H6A | −0.5064 | 0.2673 | 0.8797 | 0.040* |
| H6B | −0.3544 | 0.3514 | 0.9170 | 0.040* |
| H6C | −0.2601 | 0.2495 | 0.9324 | 0.040* |
| O1 | −0.0252 (3) | 0.40052 (9) | 0.28998 (7) | 0.0196 (3) |
| O2 | 0.0882 (3) | 0.35424 (10) | 0.42007 (7) | 0.0238 (3) |
| O3 | 0.7031 (3) | 0.57159 (10) | 0.58440 (8) | 0.0245 (3) |
| O4 | 0.3325 (3) | 0.54500 (10) | 0.64750 (8) | 0.0240 (3) |
| H4 | 0.4108 | 0.5588 | 0.6909 | 0.036* |
| C7 | 0.1204 (4) | 0.40279 (12) | 0.35520 (10) | 0.0160 (3) |
| C8 | 0.3451 (4) | 0.46878 (12) | 0.34924 (10) | 0.0172 (3) |
| H8A | 0.4587 | 0.4460 | 0.3054 | 0.021* |
| H8B | 0.2852 | 0.5294 | 0.3311 | 0.021* |
| C9 | 0.4914 (4) | 0.48016 (12) | 0.43228 (10) | 0.0177 (3) |
| H9A | 0.6509 | 0.5102 | 0.4205 | 0.021* |
| H9B | 0.5261 | 0.4194 | 0.4565 | 0.021* |
| C10 | 0.3435 (4) | 0.53813 (13) | 0.49684 (10) | 0.0191 (4) |
| H10A | 0.3062 | 0.5982 | 0.4717 | 0.023* |
| H10B | 0.1847 | 0.5074 | 0.5086 | 0.023* |
| C11 | 0.4815 (4) | 0.55288 (11) | 0.58018 (10) | 0.0167 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0184 (8) | 0.0183 (7) | 0.0169 (6) | 0.0033 (6) | −0.0006 (6) | 0.0006 (5) |
| N2 | 0.0275 (9) | 0.0264 (8) | 0.0176 (6) | 0.0062 (7) | −0.0001 (7) | 0.0053 (5) |
| C1 | 0.0203 (9) | 0.0176 (7) | 0.0181 (7) | −0.0002 (7) | −0.0050 (7) | 0.0006 (6) |
| C2 | 0.0236 (9) | 0.0193 (8) | 0.0268 (8) | 0.0038 (8) | −0.0040 (8) | 0.0049 (7) |
| C3 | 0.0194 (9) | 0.0179 (8) | 0.0339 (9) | 0.0052 (8) | −0.0008 (9) | −0.0002 (7) |
| C4 | 0.0185 (9) | 0.0177 (7) | 0.0233 (8) | −0.0028 (7) | 0.0012 (8) | −0.0017 (6) |
| C5 | 0.0206 (9) | 0.0175 (7) | 0.0170 (7) | −0.0001 (7) | −0.0010 (7) | −0.0002 (5) |
| C6 | 0.0259 (10) | 0.0230 (9) | 0.0308 (9) | −0.0021 (9) | 0.0070 (9) | −0.0045 (7) |
| O1 | 0.0215 (7) | 0.0246 (6) | 0.0126 (5) | −0.0056 (6) | −0.0017 (5) | 0.0022 (4) |
| O2 | 0.0298 (8) | 0.0269 (6) | 0.0146 (5) | −0.0080 (6) | −0.0044 (6) | 0.0058 (5) |
| O3 | 0.0200 (7) | 0.0339 (7) | 0.0195 (6) | −0.0022 (6) | −0.0026 (6) | −0.0033 (5) |
| O4 | 0.0230 (7) | 0.0354 (7) | 0.0136 (5) | −0.0054 (6) | −0.0003 (6) | −0.0058 (5) |
| C7 | 0.0175 (8) | 0.0166 (7) | 0.0138 (6) | −0.0002 (7) | 0.0006 (7) | −0.0015 (5) |
| C8 | 0.0176 (8) | 0.0204 (8) | 0.0136 (6) | −0.0029 (7) | 0.0003 (7) | −0.0017 (6) |
| C9 | 0.0172 (8) | 0.0196 (7) | 0.0163 (7) | 0.0013 (7) | −0.0008 (7) | −0.0027 (6) |
| C10 | 0.0182 (9) | 0.0236 (8) | 0.0155 (7) | 0.0037 (7) | −0.0045 (7) | −0.0054 (6) |
| C11 | 0.0198 (8) | 0.0154 (7) | 0.0150 (6) | 0.0028 (7) | −0.0022 (7) | −0.0012 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.356 (2) | C6—H6C | 0.9600 |
| N1—C5 | 1.363 (2) | O1—C7 | 1.280 (2) |
| N1—H1 | 0.8600 | O2—C7 | 1.243 (2) |
| N2—C1 | 1.331 (2) | O3—C11 | 1.210 (2) |
| N2—H2A | 0.8600 | O4—C11 | 1.321 (2) |
| N2—H2B | 0.8600 | O4—H4 | 0.8200 |
| C1—C2 | 1.417 (3) | C7—C8 | 1.528 (3) |
| C2—C3 | 1.365 (3) | C8—C9 | 1.522 (2) |
| C2—H2 | 0.9300 | C8—H8A | 0.9700 |
| C3—C4 | 1.423 (3) | C8—H8B | 0.9700 |
| C3—H3 | 0.9300 | C9—C10 | 1.527 (2) |
| C4—C5 | 1.366 (3) | C9—H9A | 0.9700 |
| C4—C6 | 1.505 (3) | C9—H9B | 0.9700 |
| C5—H5 | 0.9300 | C10—C11 | 1.509 (2) |
| C6—H6A | 0.9600 | C10—H10A | 0.9700 |
| C6—H6B | 0.9600 | C10—H10B | 0.9700 |
| | | | |
| C1—N1—C5 | 123.09 (16) | H6B—C6—H6C | 109.5 |
| C1—N1—H1 | 118.5 | C11—O4—H4 | 109.5 |
| C5—N1—H1 | 118.5 | O2—C7—O1 | 123.48 (17) |
| C1—N2—H2A | 120.0 | O2—C7—C8 | 120.42 (15) |
| C1—N2—H2B | 120.0 | O1—C7—C8 | 116.09 (14) |
| H2A—N2—H2B | 120.0 | C9—C8—C7 | 114.48 (13) |
| N2—C1—N1 | 118.31 (16) | C9—C8—H8A | 108.6 |
| N2—C1—C2 | 124.45 (16) | C7—C8—H8A | 108.6 |
| N1—C1—C2 | 117.24 (16) | C9—C8—H8B | 108.6 |
| C3—C2—C1 | 119.66 (16) | C7—C8—H8B | 108.6 |
| C3—C2—H2 | 120.2 | H8A—C8—H8B | 107.6 |
| C1—C2—H2 | 120.2 | C8—C9—C10 | 111.04 (15) |
| C2—C3—C4 | 122.08 (18) | C8—C9—H9A | 109.4 |
| C2—C3—H3 | 119.0 | C10—C9—H9A | 109.4 |
| C4—C3—H3 | 119.0 | C8—C9—H9B | 109.4 |
| C5—C4—C3 | 116.18 (16) | C10—C9—H9B | 109.4 |
| C5—C4—C6 | 121.36 (16) | H9A—C9—H9B | 108.0 |
| C3—C4—C6 | 122.44 (17) | C11—C10—C9 | 113.37 (15) |
| N1—C5—C4 | 121.73 (16) | C11—C10—H10A | 108.9 |
| N1—C5—H5 | 119.1 | C9—C10—H10A | 108.9 |
| C4—C5—H5 | 119.1 | C11—C10—H10B | 108.9 |
| C4—C6—H6A | 109.5 | C9—C10—H10B | 108.9 |
| C4—C6—H6B | 109.5 | H10A—C10—H10B | 107.7 |
| H6A—C6—H6B | 109.5 | O3—C11—O4 | 123.98 (16) |
| C4—C6—H6C | 109.5 | O3—C11—C10 | 123.45 (17) |
| H6A—C6—H6C | 109.5 | O4—C11—C10 | 112.56 (15) |
| | | | |
| C5—N1—C1—N2 | −178.57 (16) | C3—C4—C5—N1 | −0.2 (3) |
| C5—N1—C1—C2 | 2.0 (3) | C6—C4—C5—N1 | 178.30 (16) |

| | | | |
|---|---|---|---|
| N2—C1—C2—C3 | 178.99 (19) | O2—C7—C8—C9 | −9.4 (2) |
| N1—C1—C2—C3 | −1.7 (3) | O1—C7—C8—C9 | 171.50 (15) |
| C1—C2—C3—C4 | 0.4 (3) | C7—C8—C9—C10 | −72.74 (19) |
| C2—C3—C4—C5 | 0.5 (3) | C8—C9—C10—C11 | −179.18 (14) |
| C2—C3—C4—C6 | −177.97 (18) | C9—C10—C11—O3 | 42.8 (2) |
| C1—N1—C5—C4 | −1.1 (3) | C9—C10—C11—O4 | −138.56 (16) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.86 | 1.82 | 2.672 (2) | 170 |
| N2—H2*A*···O2$^{i}$ | 0.86 | 2.00 | 2.853 (3) | 174 |
| N2—H2*B*···O2 | 0.86 | 2.08 | 2.854 (2) | 149 |
| O4—H4···O1$^{ii}$ | 0.82 | 1.76 | 2.5729 (19) | 169 |
| C2—H2···O3$^{iii}$ | 0.93 | 2.59 | 3.441 (2) | 152 |
| C5—H5···O3$^{iv}$ | 0.93 | 2.50 | 3.379 (2) | 158 |

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1; (ii) −*x*+1/2, −*y*+1, *z*+1/2; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, *y*−1/2, −*z*+3/2.