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# 2-Aminopyridinium 5-(5-chloro-2,4-dinitrophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-6-olate

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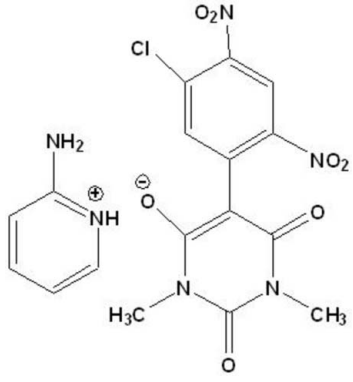
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.044; $wR$ factor = 0.124; data-to-parameter ratio = 12.9.

In the title molecular salt, $C_5H_7N_2^+\cdot C_{12}H_8ClN_4O_7^-$, the dihedral angle between the aromatic rings of the anion is 51.88 (6)°. One of the nitro groups is disordered over two orientations in a 0.710 (6):0.290 (6) ratio. In the crystal, the cations and anions are linked by N—H···O hydrogen bonds, generating infinite ribbons extending along [100] which incorporate $R_4^4(22)$ ring motifs. Weak C—H···O interactions also occur.

## Related literature

For our previous work in this area and background to barbiturate drugs, see: Kalaivani & Buvaneswari (2010); Kalaivani *et al.* (2008). For a related structure, see: Swamy *et al.* (2008).




## Experimental

### Crystal data

$C_5H_7N_2^+\cdot C_{12}H_8ClN_4O_7^-$
$M_r$ = 450.80
Monoclinic, $P2_1/c$
$a$ = 8.578 (5) Å
$b$ = 11.229 (5) Å
$c$ = 19.952 (5) Å
$\beta$ = 94.952 (5)°
$V$ = 1914.7 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.26 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.20 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.882, $T_{max}$ = 0.941
19182 measured reflections
4053 independent reflections
2996 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.124
$S$ = 1.06
4053 reflections
315 parameters
28 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5$A$···O1$^{i}$ | 0.856 (19) | 1.882 (19) | 2.730 (3) | 170.8 (19) |
| N6—H6$A$···O2$^{ii}$ | 0.85 (2) | 1.976 (19) | 2.805 (3) | 163 (3) |
| N6—H6$B$···O3 | 0.85 (2) | 2.12 (2) | 2.883 (3) | 150 (2) |
| C9—H9···O2$^{iii}$ | 0.93 | 2.51 | 3.097 (3) | 121 |
| C9—H9···O7$^{iv}$ | 0.93 | 2.57 | 3.285 (3) | 134 |
| C11—H11$C$···O5$^{v}$ | 0.96 | 2.59 | 3.241 (4) | 126 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

The authors are thankful to the SAIF, IIT Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6510).

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# supporting information

*Acta Cryst.* (2011). E**67**, o3475 [https://doi.org/10.1107/S1600536811049518]

## 2-Aminopyridinium 5-(5-chloro-2,4-dinitrophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-6-olate

**Vaduganathan Manickkam and Doraisamyraja Kalaivani**

### S1. Comment

As part of our ongoing studies of water soluble barbiturates (Kalaivani *et al.*,2008; Kalaivani & Buvaneswari, 2010), we now report the title barbiturate salt, (I), which has reasonable solubility in polar solvents (water 0.5 g/100 ml; ethanol 1.3 g/100 ml; DMSO 10.1 g/100 ml). As single-crystal X-ray diffraction studies help to understand drug-target interaction (Swamy *et al.*, 2008), the present study may probably help to understand the mechanism of action of barbiturates with biological systems. The cation and anion parts of the title molecule are shown in the Scheme. Fig.1 and Fig.2 are the *ORTEP* and packing views of the title molecular salt respectively. The dihedral angle between the chlorodinitrophenyl ring and 1,3-dimethylbarbiturate ring is observed to be 51.88 (6)°. The nitro group at the *para* position is disordered over two positions with percentage of occupancy 71 and 29.

### S2. Experimental

1,3-Dichloro-4,6-dinitrobenzene (1.18 g, 0.005 mol) was dissolved in 20 ml of absolute alcohol. To this, 0.78 g (0.005 mol) of 1,3-dimethylbarbituric acid was added and the temperature of the mixture was raised to 50°C. To this mixture 1.88 g (0.02 mol) of 2-aminopyridine in 20 ml of absolute alcohol was added. This mixture was shaken well for 2–5 h and kept as such at 25°C for 2 days. On standing, crystals came out from the solution which were filtered and dried. The dry orange colored crystals obtained were powdered well, washed with absolute alcohol and dry ether and then recrystallized from absolute alcohol (yield: 70%; m.pt: 233°C (decomposes at its melting point). Colourless blocks of (I) were obtained by slow evaporation of ethanol at room temperature.

### S3. Refinement

The H atoms of the pyridine nitrogen atoms (H5A, H6A & H6B) were located in difference Fourier maps and refined as riding in their as-found relative positions. The other H atoms were positioned geometrically and were refined using a riding model.

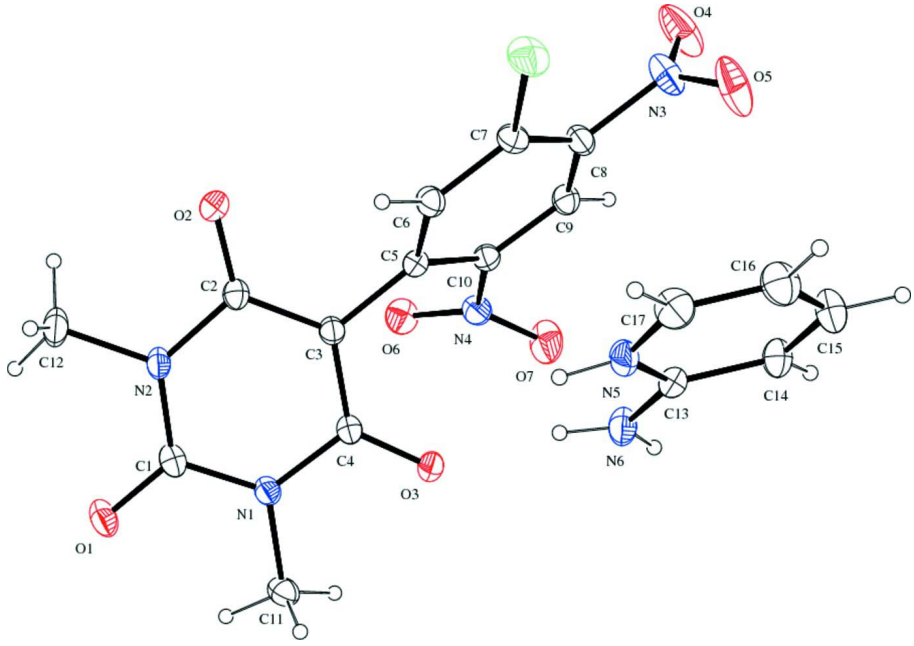


**Figure 1**

The molecular structure of the title compound showing 30% displacement ellipsoids. Only one orientation of the disordered nitro group is shown.

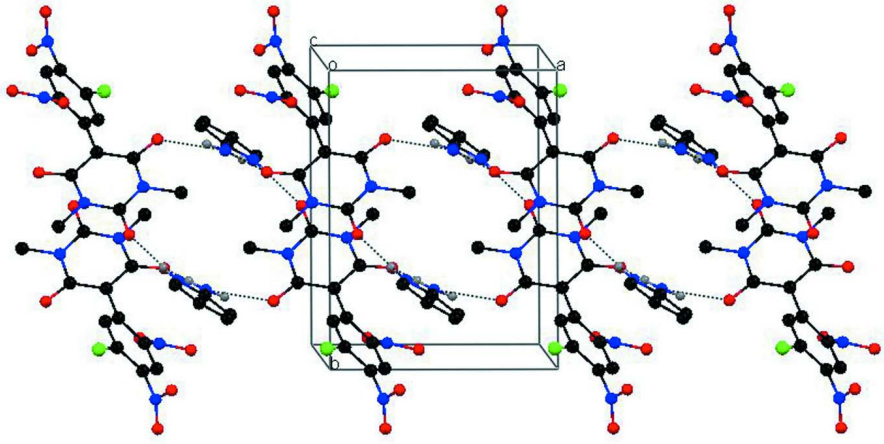


**Figure 2**

Packing view of (I).

## 2-Aminopyridinium 5-(5-chloro-2,4-dinitrophenyl)-1,3-dimethyl-2,4-dioxo- 1,2,3,4-tetrahydropyrimidin-6-olate

*Crystal data*

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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.578$ (5) Å
$b = 11.229$ (5) Å
$c = 19.952$ (5) Å
$\beta = 94.952$ (5)°
$V = 1914.7$ (15) Å$^3$
$Z = 4$
$F(000) = 928$
$D_x = 1.564$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4951 reflections

$\theta$ = 2.4–25.1°
$\mu$ = 0.26 mm$^{-1}$
$T$ = 293 K

Block, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.882, $T_{max}$ = 0.941

19182 measured reflections
4053 independent reflections
2996 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
$\theta_{max}$ = 26.7°, $\theta_{min}$ = 2.1°
$h$ = −9→10
$k$ = −14→14
$l$ = −18→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.124
$S$ = 1.06
4053 reflections
315 parameters
28 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
$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.6796P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), FC$^*$=KFC[1+0.001XFC$^2$Λ$^3$/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.0051 (11)

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted $R$-factors $wR$ and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -$R$-factor-obs *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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Cl1 | 1.03304 (8) | 0.08804 (7) | 0.22906 (3) | 0.0650 (2) | |
| O1 | 1.11087 (18) | 0.53725 (16) | −0.12650 (8) | 0.0532 (6) | |
| O2 | 1.24783 (16) | 0.23068 (14) | 0.01566 (8) | 0.0460 (5) | |
| O3 | 0.72232 (15) | 0.33672 (15) | −0.03589 (7) | 0.0459 (5) | |
| O4 | 0.7709 (6) | −0.1850 (3) | 0.15232 (19) | 0.1030 (18) | 0.710 (6) |
| O5 | 0.7145 (5) | −0.0500 (3) | 0.22061 (16) | 0.0947 (14) | 0.710 (6) |
| O6 | 0.8277 (2) | 0.09835 (17) | −0.09732 (8) | 0.0562 (6) | |
| O7 | 0.6060 (2) | 0.0610 (2) | −0.05967 (10) | 0.0784 (8) | |
| N1 | 0.91735 (19) | 0.43435 (15) | −0.08264 (8) | 0.0365 (5) | |
| N2 | 1.17873 (18) | 0.38319 (16) | −0.05623 (8) | 0.0388 (5) | |
| N3 | 0.7806 (3) | −0.0840 (2) | 0.17169 (11) | 0.0648 (9) | |
| N4 | 0.7452 (2) | 0.08402 (17) | −0.05157 (9) | 0.0448 (6) | |

| | | | | | |
|---|---|---|---|---|---|
| C1 | 1.0719 (2) | 0.4558 (2) | −0.09035 (10) | 0.0381 (6) | |
| C2 | 1.1398 (2) | 0.29008 (19) | −0.01345 (10) | 0.0365 (6) | |
| C3 | 0.9800 (2) | 0.27172 (18) | −0.00748 (10) | 0.0350 (6) | |
| C4 | 0.8653 (2) | 0.34440 (18) | −0.04092 (9) | 0.0351 (6) | |
| C5 | 0.9311 (2) | 0.17671 (18) | 0.03654 (10) | 0.0345 (6) | |
| C6 | 0.9943 (2) | 0.1711 (2) | 0.10340 (10) | 0.0398 (6) | |
| C7 | 0.9474 (2) | 0.0883 (2) | 0.14804 (10) | 0.0408 (7) | |
| C8 | 0.8320 (2) | 0.00736 (19) | 0.12644 (11) | 0.0423 (7) | |
| C9 | 0.7662 (2) | 0.00879 (19) | 0.06162 (11) | 0.0417 (7) | |
| C10 | 0.8161 (2) | 0.09193 (18) | 0.01787 (10) | 0.0355 (6) | |
| C11 | 0.8007 (3) | 0.5095 (2) | −0.11964 (11) | 0.0456 (7) | |
| C12 | 1.3446 (2) | 0.4019 (2) | −0.06582 (13) | 0.0545 (8) | |
| O4′ | 0.6703 (16) | −0.1204 (15) | 0.1656 (8) | 0.152 (5) | 0.290 (6) |
| O5′ | 0.8902 (10) | −0.1336 (8) | 0.2104 (5) | 0.102 (3) | 0.290 (6) |
| N5 | 0.6809 (2) | 0.31348 (18) | 0.17967 (10) | 0.0481 (6) | |
| N6 | 0.5498 (2) | 0.2728 (2) | 0.07658 (10) | 0.0532 (7) | |
| C13 | 0.5615 (2) | 0.2616 (2) | 0.14244 (11) | 0.0400 (7) | |
| C14 | 0.4528 (3) | 0.1982 (2) | 0.17685 (12) | 0.0495 (8) | |
| C15 | 0.4704 (3) | 0.1919 (3) | 0.24481 (13) | 0.0594 (9) | |
| C16 | 0.5962 (3) | 0.2470 (3) | 0.28138 (13) | 0.0619 (9) | |
| C17 | 0.6990 (3) | 0.3063 (2) | 0.24771 (13) | 0.0575 (9) | |
| H6 | 1.07120 | 0.22570 | 0.11820 | 0.0480* | |
| H11B | 0.71160 | 0.46200 | −0.13510 | 0.0680* | |
| H11C | 0.84510 | 0.54440 | −0.15760 | 0.0680* | |
| H12A | 1.35390 | 0.43670 | −0.10920 | 0.0820* | |
| H12B | 1.39840 | 0.32690 | −0.06300 | 0.0820* | |
| H12C | 1.39000 | 0.45440 | −0.03150 | 0.0820* | |
| H9 | 0.68870 | −0.04570 | 0.04740 | 0.0500* | |
| H11A | 0.76860 | 0.57140 | −0.09060 | 0.0680* | |
| H5A | 0.744 (2) | 0.3561 (18) | 0.1589 (10) | 0.049 (7)* | |
| H6A | 0.467 (2) | 0.249 (3) | 0.0536 (13) | 0.073 (9)* | |
| H6B | 0.623 (2) | 0.302 (2) | 0.0556 (12) | 0.069 (8)* | |
| H14 | 0.36870 | 0.16050 | 0.15310 | 0.0590* | |
| H15 | 0.39740 | 0.15020 | 0.26750 | 0.0710* | |
| H16 | 0.60800 | 0.24250 | 0.32810 | 0.0740* | |
| H17 | 0.78410 | 0.34320 | 0.27120 | 0.0690* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0728 (4) | 0.0825 (5) | 0.0377 (3) | −0.0051 (3) | −0.0068 (3) | 0.0101 (3) |
| O1 | 0.0544 (9) | 0.0594 (11) | 0.0458 (9) | −0.0187 (8) | 0.0043 (7) | 0.0157 (8) |
| O2 | 0.0325 (7) | 0.0504 (9) | 0.0544 (9) | −0.0007 (6) | 0.0004 (6) | 0.0074 (8) |
| O3 | 0.0312 (7) | 0.0556 (10) | 0.0516 (9) | 0.0007 (7) | 0.0071 (6) | 0.0137 (8) |
| O4 | 0.186 (4) | 0.0408 (19) | 0.091 (3) | −0.016 (2) | 0.063 (3) | 0.0045 (17) |
| O5 | 0.149 (3) | 0.082 (2) | 0.0616 (19) | −0.041 (2) | 0.058 (2) | −0.0098 (17) |
| O6 | 0.0605 (10) | 0.0705 (12) | 0.0379 (9) | −0.0008 (8) | 0.0061 (7) | −0.0040 (8) |
| O7 | 0.0489 (10) | 0.1158 (18) | 0.0668 (12) | −0.0312 (11) | −0.0159 (8) | 0.0137 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0365 (8) | 0.0383 (10) | 0.0345 (9) | −0.0047 (7) | 0.0023 (7) | 0.0049 (8) |
| N2 | 0.0319 (8) | 0.0457 (11) | 0.0397 (9) | −0.0083 (7) | 0.0079 (7) | 0.0043 (8) |
| N3 | 0.0844 (17) | 0.0585 (16) | 0.0519 (14) | −0.0244 (13) | 0.0078 (12) | 0.0123 (12) |
| N4 | 0.0436 (10) | 0.0453 (11) | 0.0443 (10) | −0.0049 (8) | −0.0024 (8) | 0.0028 (9) |
| C1 | 0.0434 (11) | 0.0418 (12) | 0.0292 (10) | −0.0116 (9) | 0.0035 (8) | −0.0015 (9) |
| C2 | 0.0334 (10) | 0.0394 (12) | 0.0368 (11) | −0.0061 (8) | 0.0030 (8) | −0.0013 (9) |
| C3 | 0.0322 (10) | 0.0380 (11) | 0.0347 (10) | −0.0040 (8) | 0.0027 (8) | 0.0035 (9) |
| C4 | 0.0349 (10) | 0.0370 (11) | 0.0338 (10) | −0.0045 (8) | 0.0049 (8) | 0.0015 (9) |
| C5 | 0.0285 (9) | 0.0361 (11) | 0.0390 (11) | 0.0009 (8) | 0.0040 (8) | 0.0023 (9) |
| C6 | 0.0370 (10) | 0.0408 (12) | 0.0408 (11) | −0.0062 (9) | −0.0003 (8) | 0.0027 (10) |
| C7 | 0.0460 (11) | 0.0416 (12) | 0.0345 (11) | 0.0016 (9) | 0.0015 (9) | 0.0038 (10) |
| C8 | 0.0479 (12) | 0.0378 (12) | 0.0426 (12) | −0.0017 (9) | 0.0113 (9) | 0.0075 (10) |
| C9 | 0.0379 (10) | 0.0377 (12) | 0.0495 (12) | −0.0060 (9) | 0.0047 (9) | 0.0010 (10) |
| C10 | 0.0330 (9) | 0.0382 (11) | 0.0349 (10) | −0.0002 (8) | 0.0011 (8) | 0.0017 (9) |
| C11 | 0.0496 (12) | 0.0420 (13) | 0.0441 (12) | −0.0024 (10) | −0.0028 (9) | 0.0092 (10) |
| C12 | 0.0361 (11) | 0.0690 (17) | 0.0598 (15) | −0.0140 (11) | 0.0121 (10) | 0.0068 (13) |
| O4′ | 0.117 (7) | 0.166 (9) | 0.170 (9) | −0.057 (7) | −0.003 (6) | 0.078 (8) |
| O5′ | 0.096 (5) | 0.092 (6) | 0.116 (6) | 0.000 (4) | −0.007 (4) | 0.078 (5) |
| N5 | 0.0361 (9) | 0.0528 (12) | 0.0555 (12) | −0.0102 (8) | 0.0046 (8) | 0.0082 (10) |
| N6 | 0.0390 (11) | 0.0754 (15) | 0.0458 (12) | −0.0071 (10) | 0.0080 (9) | 0.0075 (11) |
| C13 | 0.0328 (10) | 0.0425 (12) | 0.0451 (12) | 0.0019 (9) | 0.0066 (8) | 0.0022 (10) |
| C14 | 0.0414 (11) | 0.0566 (15) | 0.0512 (14) | −0.0118 (10) | 0.0081 (10) | −0.0022 (12) |
| C15 | 0.0610 (15) | 0.0685 (18) | 0.0508 (14) | −0.0150 (13) | 0.0166 (12) | 0.0058 (13) |
| C16 | 0.0702 (16) | 0.0725 (18) | 0.0429 (13) | −0.0057 (14) | 0.0048 (12) | 0.0003 (13) |
| C17 | 0.0535 (14) | 0.0628 (17) | 0.0542 (15) | −0.0091 (12) | −0.0064 (11) | −0.0014 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C7 | 1.717 (2) | C3—C4 | 1.402 (3) |
| O1—C1 | 1.229 (3) | C3—C5 | 1.466 (3) |
| O2—C2 | 1.244 (3) | C5—C6 | 1.397 (3) |
| O3—C4 | 1.242 (2) | C5—C10 | 1.398 (3) |
| O4—N3 | 1.199 (4) | C6—C7 | 1.372 (3) |
| O4′—N3 | 1.028 (15) | C7—C8 | 1.385 (3) |
| O5—N3 | 1.231 (4) | C8—C9 | 1.366 (3) |
| O5′—N3 | 1.290 (10) | C9—C10 | 1.372 (3) |
| O6—N4 | 1.213 (3) | C6—H6 | 0.9300 |
| O7—N4 | 1.219 (3) | C9—H9 | 0.9300 |
| N1—C4 | 1.406 (3) | C11—H11C | 0.9600 |
| N1—C1 | 1.369 (3) | C11—H11A | 0.9600 |
| N1—C11 | 1.460 (3) | C11—H11B | 0.9600 |
| N2—C12 | 1.467 (2) | C12—H12A | 0.9600 |
| N2—C2 | 1.408 (3) | C12—H12B | 0.9600 |
| N2—C1 | 1.364 (3) | C12—H12C | 0.9600 |
| N3—C8 | 1.460 (3) | C13—C14 | 1.399 (3) |
| N4—C10 | 1.467 (3) | C14—C15 | 1.353 (4) |
| N5—C13 | 1.345 (3) | C15—C16 | 1.394 (4) |
| N5—C17 | 1.355 (3) | C16—C17 | 1.332 (4) |

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| N6—C13 | 1.315 (3) | C14—H14 | 0.9300 |
| N5—H5A | 0.856 (19) | C15—H15 | 0.9300 |
| N6—H6B | 0.85 (2) | C16—H16 | 0.9300 |
| N6—H6A | 0.85 (2) | C17—H17 | 0.9300 |
| C2—C3 | 1.401 (3) | | |

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| C1—N1—C4 | 123.57 (17) | C6—C7—C8 | 118.99 (19) |
| C1—N1—C11 | 118.01 (17) | N3—C8—C7 | 121.0 (2) |
| C4—N1—C11 | 118.42 (16) | N3—C8—C9 | 118.15 (19) |
| C1—N2—C2 | 124.21 (16) | C7—C8—C9 | 120.85 (19) |
| C1—N2—C12 | 117.82 (17) | C8—C9—C10 | 118.98 (18) |
| C2—N2—C12 | 117.96 (16) | C5—C10—C9 | 123.07 (19) |
| O4—N3—O5 | 121.7 (3) | N4—C10—C5 | 121.22 (18) |
| O4—N3—C8 | 118.8 (3) | N4—C10—C9 | 115.67 (17) |
| O5—N3—C8 | 117.2 (2) | C5—C6—H6 | 119.00 |
| O4′—N3—C8 | 122.0 (9) | C7—C6—H6 | 119.00 |
| O5′—N3—C8 | 115.5 (4) | C10—C9—H9 | 121.00 |
| O4′—N3—O5′ | 121.0 (10) | C8—C9—H9 | 120.00 |
| O6—N4—O7 | 123.84 (19) | H11A—C11—H11C | 110.00 |
| O6—N4—C10 | 118.78 (17) | N1—C11—H11A | 109.00 |
| O7—N4—C10 | 117.37 (17) | N1—C11—H11B | 109.00 |
| C13—N5—C17 | 122.9 (2) | H11A—C11—H11B | 110.00 |
| C17—N5—H5A | 119.7 (13) | H11B—C11—H11C | 109.00 |
| C13—N5—H5A | 117.3 (13) | N1—C11—H11C | 109.00 |
| C13—N6—H6B | 122.2 (15) | H12B—C12—H12C | 109.00 |
| C13—N6—H6A | 119.6 (17) | H12A—C12—H12C | 109.00 |
| H6A—N6—H6B | 118 (2) | N2—C12—H12A | 109.00 |
| O1—C1—N1 | 120.80 (18) | N2—C12—H12B | 109.00 |
| N1—C1—N2 | 117.01 (18) | N2—C12—H12C | 109.00 |
| O1—C1—N2 | 122.19 (17) | H12A—C12—H12B | 109.00 |
| O2—C2—N2 | 118.36 (16) | N5—C13—C14 | 117.2 (2) |
| O2—C2—C3 | 125.17 (19) | N6—C13—C14 | 122.84 (19) |
| N2—C2—C3 | 116.47 (17) | N5—C13—N6 | 119.95 (19) |
| C4—C3—C5 | 118.91 (16) | C13—C14—C15 | 119.8 (2) |
| C2—C3—C4 | 121.69 (18) | C14—C15—C16 | 121.0 (3) |
| C2—C3—C5 | 119.38 (17) | C15—C16—C17 | 118.3 (2) |
| O3—C4—C3 | 125.33 (18) | N5—C17—C16 | 120.8 (2) |
| O3—C4—N1 | 117.64 (17) | C13—C14—H14 | 120.00 |
| N1—C4—C3 | 117.02 (16) | C15—C14—H14 | 120.00 |
| C3—C5—C10 | 124.59 (18) | C14—C15—H15 | 120.00 |
| C6—C5—C10 | 115.49 (18) | C16—C15—H15 | 119.00 |
| C3—C5—C6 | 119.82 (17) | C15—C16—H16 | 121.00 |
| C5—C6—C7 | 122.62 (18) | C17—C16—H16 | 121.00 |
| Cl1—C7—C8 | 121.88 (17) | N5—C17—H17 | 120.00 |
| Cl1—C7—C6 | 119.14 (15) | C16—C17—H17 | 120.00 |

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| C4—N1—C1—O1 | −178.55 (19) | O2—C2—C3—C5 | 0.7 (3) |
| C11—N1—C1—O1 | 1.2 (3) | C2—C3—C4—O3 | −176.86 (19) |

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| C4—N1—C1—N2 | 1.4 (3) | C4—C3—C5—C10 | 50.9 (3) |
| C11—N1—C1—N2 | −178.89 (18) | C2—C3—C5—C10 | −131.1 (2) |
| C1—N1—C4—C3 | −1.9 (3) | C4—C3—C5—C6 | −125.3 (2) |
| C11—N1—C4—C3 | 178.34 (18) | C5—C3—C4—O3 | 1.1 (3) |
| C1—N1—C4—O3 | 177.10 (18) | C2—C3—C5—C6 | 52.7 (3) |
| C11—N1—C4—O3 | −2.6 (3) | C2—C3—C4—N1 | 2.1 (3) |
| C1—N2—C2—O2 | −179.13 (19) | C5—C3—C4—N1 | −179.97 (18) |
| C2—N2—C1—N1 | −1.0 (3) | C6—C5—C10—N4 | −177.07 (17) |
| C12—N2—C1—N1 | 177.76 (18) | C3—C5—C10—N4 | 6.6 (3) |
| C2—N2—C1—O1 | 178.9 (2) | C3—C5—C10—C9 | −175.78 (18) |
| C12—N2—C1—O1 | −2.3 (3) | C6—C5—C10—C9 | 0.5 (3) |
| C12—N2—C2—C3 | −177.59 (19) | C10—C5—C6—C7 | 0.0 (3) |
| C12—N2—C2—O2 | 2.2 (3) | C3—C5—C6—C7 | 176.49 (18) |
| C1—N2—C2—C3 | 1.1 (3) | C5—C6—C7—Cl1 | 179.60 (16) |
| O5—N3—C8—C9 | −116.6 (3) | C5—C6—C7—C8 | −0.5 (3) |
| O4—N3—C8—C9 | 46.4 (4) | C6—C7—C8—C9 | 0.5 (3) |
| O5—N3—C8—C7 | 65.2 (3) | Cl1—C7—C8—C9 | −179.60 (16) |
| O4—N3—C8—C7 | −131.8 (3) | C6—C7—C8—N3 | 178.68 (19) |
| O6—N4—C10—C5 | 38.9 (3) | Cl1—C7—C8—N3 | −1.4 (3) |
| O7—N4—C10—C5 | −142.5 (2) | N3—C8—C9—C10 | −178.23 (19) |
| O7—N4—C10—C9 | 39.8 (3) | C7—C8—C9—C10 | 0.0 (3) |
| O6—N4—C10—C9 | −138.9 (2) | C8—C9—C10—C5 | −0.5 (3) |
| C13—N5—C17—C16 | −0.6 (4) | C8—C9—C10—N4 | 177.19 (17) |
| C17—N5—C13—C14 | 0.1 (3) | N5—C13—C14—C15 | 0.4 (3) |
| C17—N5—C13—N6 | 179.4 (2) | N6—C13—C14—C15 | −178.9 (2) |
| N2—C2—C3—C5 | −179.65 (17) | C13—C14—C15—C16 | −0.5 (4) |
| O2—C2—C3—C4 | 178.6 (2) | C14—C15—C16—C17 | 0.0 (5) |
| N2—C2—C3—C4 | −1.7 (3) | C15—C16—C17—N5 | 0.5 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N5—H5*A*···O1$^{i}$ | 0.856 (19) | 1.882 (19) | 2.730 (3) | 170.8 (19) |
| N6—H6*A*···O2$^{ii}$ | 0.85 (2) | 1.976 (19) | 2.805 (3) | 163 (3) |
| N6—H6*B*···O3 | 0.85 (2) | 2.12 (2) | 2.883 (3) | 150 (2) |
| C9—H9···O2$^{iii}$ | 0.93 | 2.51 | 3.097 (3) | 121 |
| C9—H9···O7$^{iv}$ | 0.93 | 2.57 | 3.285 (3) | 134 |
| C11—H11*C*···O5$^{v}$ | 0.96 | 2.59 | 3.241 (4) | 126 |

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