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# 1-(2-Cyanoethyl)-2-(2-pyridyl)-1*H*,3*H*-benzimidazol-3-ium perchlorate

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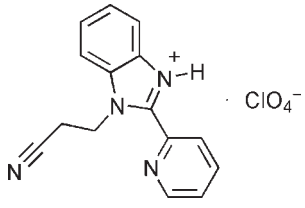
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.047; $wR$ factor = 0.122; data-to-parameter ratio = 13.2.

The title compound, $C_{15}H_{13}N_4^+\cdot ClO_4^-$, comprises a nonplanar 1-(2-cyanoethyl)-2-(2-pyridyl)-1*H*,3*H*-benzimidazol-3-ium cation [dihedral angle between the imidazole and pyridine rings = 22.5 (8)°] and a perchlorate anion. The cation is formed by protonation of the N atom of the benzimidazole ring. A charged N—H···O hydrogen bond connects the anion and cation, and intermolecular C—H···O and C—H···N interactions contribute to the crystal packing.

## Related literature

For the pharmacological activity of benzimidazole and its derivatives, see: Feng & Xu (2001); Ferey (2001); Hossain *et al.* (2001); Howarth & Hanlon (2001); Kazak *et al.* (2006); Li *et al.* (1998).



## Experimental

### Crystal data

$C_{15}H_{13}N_4^+\cdot ClO_4^-$
$M_r$ = 348.74
Triclinic, $P\overline{1}$
$a$ = 8.788 (1) Å
$b$ = 9.4608 (10) Å
$c$ = 10.6013 (11) Å
$\alpha$ = 69.690 (2)°
$\beta$ = 73.844 (2)°
$\gamma$ = 86.193 (2)°
$V$ = 793.52 (15) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.27 mm$^{-1}$
$T$ = 296 K
0.22 × 0.21 × 0.19 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.940, $T_{max}$ = 0.955
4167 measured reflections
2924 independent reflections
2316 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.013

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.122
$S$ = 1.01
2924 reflections
221 parameters
102 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H5···O4 | 0.77 (3) | 2.11 (3) | 2.885 (4) | 179 (4) |
| C11—H11···O3 | 0.93 | 2.54 | 3.343 (5) | 145 |
| C4—H4···O4 | 0.93 | 2.62 | 3.347 (4) | 135 |
| C13—H13*A*···N1 | 0.97 | 2.41 | 2.903 (4) | 111 |
| C10—H10···N4$^{i}$ | 0.93 | 2.64 | 3.423 (4) | 142 |
| C13—H13*B*···O2$^{ii}$ | 0.97 | 2.60 | 3.427 (4) | 144 |
| C14—H14*B*···O2$^{iii}$ | 0.97 | 2.57 | 3.483 (4) | 157 |
| C2—H2···O1$^{iv}$ | 0.93 | 2.62 | 3.552 (4) | 180 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2242).

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# supporting information

*Acta Cryst.* (2010). E**66**, o413 [https://doi.org/10.1107/S1600536809055251]

## 1-(2-Cyanoethyl)-2-(2-pyridyl)-1*H*,3*H*-benzimidazol-3-ium perchlorate

**Yan Li, Xiaoliang Tang, Jiayu Chen, Daxiang Wu and Weisheng Liu**

### S1. Comment

For many years benzimidazole and its derivatives continue to attract attention in chemical synthesis, structural science and applied biological research due to their various pharmacological activities (Li *et al.*, 1998; Howarth & Hanlon, 2001; Feng & Xu, 2001; Ferey, 2001; Kazak *et al.*, 2006). Like the phenanthroline based ligands these compounds are known to chelate metal atoms although their coordination chemistry has not been as extensively explored. To further widen the scope of research on the chemical and physical properties of benzimidazole derivatives, there is a need to prepare a new series of benzimidazole derivatives. In this paper, we present the structure of the title compound as a perchlorate salt.

The compound is composed of $C_{15}H_{13}N_4^+$ cation and a perchlorate anion, in a 1:1 ratio (Fig. 1). In $C_{15}H_{13}N_4^+$ cation, the molecular skeleton of protonated 2-(2-pyridyl)benzimidazole is non-planar and the dihedral angle between benzimidazole ring and pyridine ring is 25.46°. Two of O atoms of the perchlorate anion, link benzimidazole *via* the charged N(2)–H(5)···O(4) and C(11)–H(11)···O(3) hydrogen bonds (Table 1). In addition, intermolecular C–H···O, N–H···O hydrogen bonds and $\pi\cdots\pi$ interactions between benzimidazole groups [$Cg\cdots Cg^{i}$ plane···plane separation = 3.6933 (16) Å, i = 1 - *x*, 1 - *y*, 1 - *z*] link the molecules into a three-dimensional structure (Fig. 2).

### S2. Experimental

The ligand, 1-(cyanoethyl)-2-(2-pyridyl)benzimidazole was prepared according to the method described by Hossain *et al.* (2001), using 2-(2-pyridyl)benzimidazole and acrylonitrile as starting materials (yield: 62%, m.p. 378–383 K).

Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of a methanol solution (6 ml) containing $Fe(ClO_4)_3.10H_2O$ (26.7 mg, 0.05 mmol) and 1-(cyanoethyl)-2-(2-pyridyl)benzimidazole (24.8 mg, 0.10 mmol) after two weeks at room temperature. Our attempt to obtain an iron(III) perchlorate complex of the ligand failed and, instead, the protonated ligand salt was crystallised.

### S3. Refinement

The position of the amine H atom was refined freely, together with its individual isotropic displacement parameter. All other H atoms were positioned geometrically with C—H = 0.93 and 0.97 Å for aromatic, methylene H atoms, respectively, and constrained to ride on their parent atoms with *U*iso(H) = 1.2*U*eq(C).

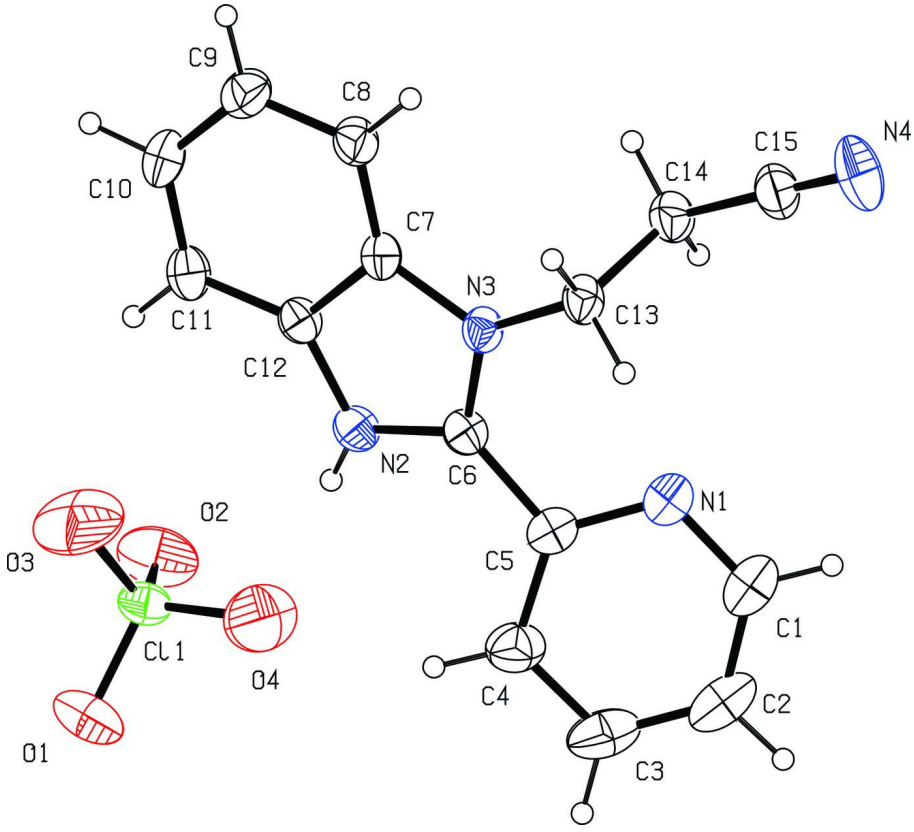


**Figure 1**

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

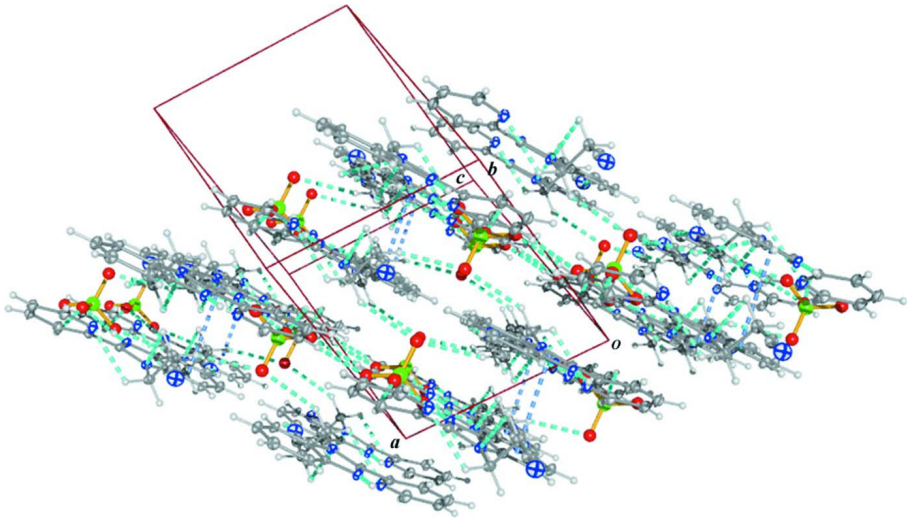


**Figure 2**

The three-dimensional packing diagram of the compound. Hydrogen bonds are shown as turquiose dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. The $\pi\cdots\pi$ interaction between benzimidazole groups are shown as light blue dashed lines.

## 1-(2-Cyanoethyl)-2-(2-pyridyl)-1*H*,3*H*-benzimidazol-3-ium perchlorate

*Crystal data*

$C_{15}H_{13}N_4^+ \cdot ClO_4^-$
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$\alpha = 69.690$ (2)°
$\beta = 73.844$ (2)°
$\gamma = 86.193$ (2)°
$V = 793.52$ (15) Å$^3$
$Z = 2$
$F(000) = 360$
$D_x = 1.460$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1758 reflections
$\theta = 2.4$–$26.4°$
$\mu = 0.27$ mm$^{-1}$
$T = 296$ K
Block, yellow
0.22 × 0.21 × 0.19 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.940$, $T_{max} = 0.955$
4167 measured reflections
2924 independent reflections
2316 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.1°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 6$
$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.122$
$S = 1.01$
2924 reflections
221 parameters
102 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
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.670P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ e Å$^{-3}$

*Special details*

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1586 (4) | −0.0845 (4) | 0.8393 (4) | 0.0755 (9) |
| H1 | 0.1941 | −0.1600 | 0.9072 | 0.091* |
| C2 | 0.0604 (4) | −0.1248 (4) | 0.7774 (4) | 0.0781 (10) |

| | | | | |
|---|---|---|---|---|
| H2 | 0.0314 | −0.2256 | 0.8016 | 0.094* |
| C3 | 0.0053 (4) | −0.0148 (4) | 0.6792 (4) | 0.0797 (10) |
| H3 | −0.0635 | −0.0396 | 0.6369 | 0.096* |
| C4 | 0.0524 (4) | 0.1333 (4) | 0.6431 (3) | 0.0657 (8) |
| H4 | 0.0168 | 0.2102 | 0.5762 | 0.079* |
| C5 | 0.1544 (3) | 0.1638 (3) | 0.7097 (3) | 0.0469 (6) |
| C6 | 0.2150 (3) | 0.3172 (3) | 0.6751 (2) | 0.0409 (6) |
| C7 | 0.3245 (3) | 0.5180 (3) | 0.6825 (2) | 0.0402 (5) |
| C8 | 0.3956 (3) | 0.6193 (3) | 0.7178 (3) | 0.0493 (6) |
| H8 | 0.4122 | 0.5949 | 0.8057 | 0.059* |
| C9 | 0.4403 (4) | 0.7580 (3) | 0.6163 (3) | 0.0578 (7) |
| H9 | 0.4903 | 0.8288 | 0.6354 | 0.069* |
| C10 | 0.4127 (4) | 0.7952 (3) | 0.4854 (3) | 0.0582 (7) |
| H10 | 0.4437 | 0.8908 | 0.4199 | 0.070* |
| C11 | 0.3412 (3) | 0.6949 (3) | 0.4506 (3) | 0.0516 (7) |
| H11 | 0.3223 | 0.7203 | 0.3634 | 0.062* |
| C12 | 0.2988 (3) | 0.5544 (3) | 0.5516 (2) | 0.0410 (6) |
| C13 | 0.2574 (3) | 0.2959 (3) | 0.9067 (2) | 0.0437 (6) |
| H13A | 0.1756 | 0.2165 | 0.9481 | 0.052* |
| H13B | 0.2286 | 0.3688 | 0.9542 | 0.052* |
| C14 | 0.4152 (3) | 0.2296 (3) | 0.9245 (3) | 0.0522 (7) |
| H14A | 0.4470 | 0.1621 | 0.8715 | 0.063* |
| H14B | 0.4953 | 0.3102 | 0.8880 | 0.063* |
| C15 | 0.4052 (4) | 0.1470 (3) | 1.0716 (3) | 0.0591 (7) |
| Cl1 | 0.17292 (8) | 0.51237 (8) | 0.19213 (6) | 0.0485 (2) |
| H5 | 0.207 (3) | 0.416 (3) | 0.491 (3) | 0.044 (8)* |
| N1 | 0.2065 (3) | 0.0574 (3) | 0.8078 (3) | 0.0601 (6) |
| N2 | 0.2311 (3) | 0.4263 (2) | 0.5520 (2) | 0.0449 (5) |
| N3 | 0.2685 (2) | 0.3697 (2) | 0.75719 (19) | 0.0399 (5) |
| N4 | 0.3982 (4) | 0.0807 (4) | 1.1839 (3) | 0.0887 (10) |
| O1 | 0.0518 (3) | 0.5091 (3) | 0.1302 (3) | 0.0896 (8) |
| O2 | 0.3196 (3) | 0.4965 (3) | 0.1030 (3) | 0.0923 (8) |
| O3 | 0.1764 (4) | 0.6462 (4) | 0.2192 (4) | 0.1268 (12) |
| O4 | 0.1453 (4) | 0.3906 (4) | 0.3209 (3) | 0.1253 (12) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.087 (2) | 0.0490 (17) | 0.080 (2) | −0.0088 (16) | −0.0136 (18) | −0.0141 (16) |
| C2 | 0.085 (2) | 0.0587 (19) | 0.081 (2) | −0.0247 (17) | 0.0083 (18) | −0.0317 (17) |
| C3 | 0.084 (2) | 0.088 (2) | 0.075 (2) | −0.0308 (19) | −0.0067 (18) | −0.0423 (19) |
| C4 | 0.0707 (19) | 0.073 (2) | 0.0575 (18) | −0.0127 (16) | −0.0179 (15) | −0.0236 (15) |
| C5 | 0.0466 (14) | 0.0479 (14) | 0.0454 (14) | −0.0034 (11) | −0.0045 (11) | −0.0204 (12) |
| C6 | 0.0433 (14) | 0.0456 (14) | 0.0349 (13) | 0.0033 (11) | −0.0098 (10) | −0.0159 (11) |
| C7 | 0.0443 (13) | 0.0380 (13) | 0.0352 (13) | 0.0049 (10) | −0.0098 (10) | −0.0102 (10) |
| C8 | 0.0652 (17) | 0.0459 (15) | 0.0422 (14) | 0.0035 (12) | −0.0224 (13) | −0.0159 (12) |
| C9 | 0.0699 (19) | 0.0453 (16) | 0.0621 (18) | −0.0032 (13) | −0.0218 (15) | −0.0192 (14) |
| C10 | 0.0704 (19) | 0.0397 (15) | 0.0507 (16) | −0.0021 (13) | −0.0122 (14) | −0.0012 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0604 (17) | 0.0511 (16) | 0.0360 (13) | 0.0034 (13) | −0.0134 (12) | −0.0061 (12) |
| C12 | 0.0418 (13) | 0.0454 (14) | 0.0354 (13) | 0.0038 (11) | −0.0104 (10) | −0.0139 (11) |
| C13 | 0.0563 (15) | 0.0430 (14) | 0.0286 (12) | 0.0020 (11) | −0.0118 (11) | −0.0084 (10) |
| C14 | 0.0564 (16) | 0.0528 (16) | 0.0418 (14) | −0.0002 (13) | −0.0165 (12) | −0.0065 (12) |
| C15 | 0.0691 (19) | 0.0531 (17) | 0.0565 (18) | 0.0111 (14) | −0.0295 (15) | −0.0124 (14) |
| Cl1 | 0.0493 (4) | 0.0606 (4) | 0.0450 (4) | −0.0011 (3) | −0.0169 (3) | −0.0257 (3) |
| N1 | 0.0657 (15) | 0.0470 (13) | 0.0656 (15) | −0.0028 (11) | −0.0196 (12) | −0.0149 (12) |
| N2 | 0.0534 (13) | 0.0508 (13) | 0.0340 (11) | 0.0001 (10) | −0.0164 (10) | −0.0152 (10) |
| N3 | 0.0491 (12) | 0.0382 (11) | 0.0309 (10) | 0.0014 (9) | −0.0115 (9) | −0.0096 (9) |
| N4 | 0.108 (2) | 0.093 (2) | 0.0539 (17) | 0.0245 (18) | −0.0388 (16) | −0.0032 (16) |
| O1 | 0.0684 (15) | 0.122 (2) | 0.1015 (18) | 0.0124 (14) | −0.0503 (14) | −0.0474 (16) |
| O2 | 0.0586 (14) | 0.138 (2) | 0.0961 (18) | 0.0062 (14) | −0.0112 (13) | −0.0667 (17) |
| O3 | 0.139 (3) | 0.116 (2) | 0.172 (3) | 0.0001 (19) | −0.041 (2) | −0.108 (2) |
| O4 | 0.173 (3) | 0.129 (2) | 0.0615 (16) | −0.058 (2) | −0.0465 (18) | 0.0051 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.333 (4) | C9—H9 | 0.9300 |
| C1—C2 | 1.361 (5) | C10—C11 | 1.373 (4) |
| C1—H1 | 0.9300 | C10—H10 | 0.9300 |
| C2—C3 | 1.365 (5) | C11—C12 | 1.382 (3) |
| C2—H2 | 0.9300 | C11—H11 | 0.9300 |
| C3—C4 | 1.377 (4) | C12—N2 | 1.382 (3) |
| C3—H3 | 0.9300 | C13—N3 | 1.471 (3) |
| C4—C5 | 1.384 (4) | C13—C14 | 1.517 (4) |
| C4—H4 | 0.9300 | C13—H13A | 0.9700 |
| C5—N1 | 1.335 (3) | C13—H13B | 0.9700 |
| C5—C6 | 1.465 (3) | C14—C15 | 1.462 (4) |
| C6—N2 | 1.330 (3) | C14—H14A | 0.9700 |
| C6—N3 | 1.336 (3) | C14—H14B | 0.9700 |
| C7—C8 | 1.381 (3) | C15—N4 | 1.123 (4) |
| C7—C12 | 1.389 (3) | Cl1—O3 | 1.396 (3) |
| C7—N3 | 1.393 (3) | Cl1—O1 | 1.404 (2) |
| C8—C9 | 1.374 (4) | Cl1—O2 | 1.404 (2) |
| C8—H8 | 0.9300 | Cl1—O4 | 1.418 (3) |
| C9—C10 | 1.395 (4) | N2—H5 | 0.78 (3) |
| | | | |
| N1—C1—C2 | 123.6 (3) | C10—C11—H11 | 121.7 |
| N1—C1—H1 | 118.2 | C12—C11—H11 | 121.7 |
| C2—C1—H1 | 118.2 | C11—C12—N2 | 132.5 (2) |
| C1—C2—C3 | 118.8 (3) | C11—C12—C7 | 121.5 (2) |
| C1—C2—H2 | 120.6 | N2—C12—C7 | 106.0 (2) |
| C3—C2—H2 | 120.6 | N3—C13—C14 | 109.9 (2) |
| C2—C3—C4 | 119.5 (3) | N3—C13—H13A | 109.7 |
| C2—C3—H3 | 120.2 | C14—C13—H13A | 109.7 |
| C4—C3—H3 | 120.2 | N3—C13—H13B | 109.7 |
| C3—C4—C5 | 117.8 (3) | C14—C13—H13B | 109.7 |
| C3—C4—H4 | 121.1 | H13A—C13—H13B | 108.2 |

| | | | |
|---|---|---|---|
| C5—C4—H4 | 121.1 | C15—C14—C13 | 111.2 (2) |
| N1—C5—C4 | 123.1 (3) | C15—C14—H14A | 109.4 |
| N1—C5—C6 | 115.2 (2) | C13—C14—H14A | 109.4 |
| C4—C5—C6 | 121.7 (3) | C15—C14—H14B | 109.4 |
| N2—C6—N3 | 108.6 (2) | C13—C14—H14B | 109.4 |
| N2—C6—C5 | 124.6 (2) | H14A—C14—H14B | 108.0 |
| N3—C6—C5 | 126.7 (2) | N4—C15—C14 | 178.5 (3) |
| C8—C7—C12 | 121.9 (2) | O3—Cl1—O1 | 111.91 (19) |
| C8—C7—N3 | 131.6 (2) | O3—Cl1—O2 | 109.33 (18) |
| C12—C7—N3 | 106.5 (2) | O1—Cl1—O2 | 109.27 (15) |
| C9—C8—C7 | 116.5 (2) | O3—Cl1—O4 | 108.3 (2) |
| C9—C8—H8 | 121.8 | O1—Cl1—O4 | 108.51 (17) |
| C7—C8—H8 | 121.8 | O2—Cl1—O4 | 109.5 (2) |
| C8—C9—C10 | 121.7 (3) | C1—N1—C5 | 117.2 (3) |
| C8—C9—H9 | 119.2 | C6—N2—C12 | 110.0 (2) |
| C10—C9—H9 | 119.2 | C6—N2—H5 | 123 (2) |
| C11—C10—C9 | 121.9 (2) | C12—N2—H5 | 127 (2) |
| C11—C10—H10 | 119.1 | C6—N3—C7 | 108.90 (19) |
| C9—C10—H10 | 119.1 | C6—N3—C13 | 127.9 (2) |
| C10—C11—C12 | 116.6 (2) | C7—N3—C13 | 122.87 (19) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C3 | −1.0 (5) | N3—C13—C14—C15 | −176.3 (2) |
| C1—C2—C3—C4 | 1.3 (5) | C13—C14—C15—N4 | 118 (13) |
| C2—C3—C4—C5 | −0.3 (5) | C2—C1—N1—C5 | −0.2 (5) |
| C3—C4—C5—N1 | −1.1 (4) | C4—C5—N1—C1 | 1.3 (4) |
| C3—C4—C5—C6 | 178.0 (3) | C6—C5—N1—C1 | −177.8 (3) |
| N1—C5—C6—N2 | 152.9 (2) | N3—C6—N2—C12 | 0.7 (3) |
| C4—C5—C6—N2 | −26.3 (4) | C5—C6—N2—C12 | −176.9 (2) |
| N1—C5—C6—N3 | −24.3 (4) | C11—C12—N2—C6 | 179.1 (3) |
| C4—C5—C6—N3 | 156.6 (3) | C7—C12—N2—C6 | 0.2 (3) |
| C12—C7—C8—C9 | −0.3 (4) | N2—C6—N3—C7 | −1.3 (3) |
| N3—C7—C8—C9 | 178.5 (3) | C5—C6—N3—C7 | 176.3 (2) |
| C7—C8—C9—C10 | 1.1 (4) | N2—C6—N3—C13 | 172.2 (2) |
| C8—C9—C10—C11 | −0.8 (5) | C5—C6—N3—C13 | −10.3 (4) |
| C9—C10—C11—C12 | −0.4 (4) | C8—C7—N3—C6 | −177.6 (3) |
| C10—C11—C12—N2 | −177.5 (3) | C12—C7—N3—C6 | 1.4 (3) |
| C10—C11—C12—C7 | 1.3 (4) | C8—C7—N3—C13 | 8.6 (4) |
| C8—C7—C12—C11 | −0.9 (4) | C12—C7—N3—C13 | −172.5 (2) |
| N3—C7—C12—C11 | 180.0 (2) | C14—C13—N3—C6 | 102.0 (3) |
| C8—C7—C12—N2 | 178.1 (2) | C14—C13—N3—C7 | −85.3 (3) |
| N3—C7—C12—N2 | −1.0 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H5···O4 | 0.77 (3) | 2.11 (3) | 2.885 (4) | 179 (4) |
| C11—H11···O3 | 0.93 | 2.54 | 3.343 (5) | 145 |
| C4—H4···O4 | 0.93 | 2.62 | 3.347 (4) | 135 |

| | | | | |
|---|---|---|---|---|
| C13—H13*A*···N1 | 0.97 | 2.41 | 2.903 (4) | 111 |
| C10—H10···N4$^{i}$ | 0.93 | 2.64 | 3.423 (4) | 142 |
| C13—H13*B*···O2$^{ii}$ | 0.97 | 2.60 | 3.427 (4) | 144 |
| C14—H14*B*···O2$^{iii}$ | 0.97 | 2.57 | 3.483 (4) | 157 |
| C2—H2···O1$^{iv}$ | 0.93 | 2.62 | 3.552 (4) | 180 |

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