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# 3-Carboxyquinolin-1-ium-2-carboxylate monohydrate

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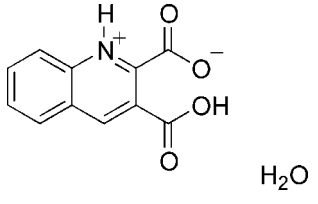
Key indicators: single-crystal X-ray study; $T$ = 153 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.101; data-to-parameter ratio = 10.8.

The title compound, $C_{11}H_7NO_4\cdot H_2O$, contains a 3-carboxyquinolin-1-ium-2-carboxylate (qda) zwitterion and one water molecule. In the crystal, pairs of N—H···O hydrogen bonds link the molecules into inversion dimers, and these dimers are further connected by O—H···O hydrogen bonds into a three-dimensional supramolecular architecture. In addition, $\pi$–$\pi$ interactions occur between pyridine and benzene rings from different qda ligands [centroid–centroid distance = 3.749 (1) Å] and the dihedral angles of the $-CO_2H$ and $-CO_2$ groups to the quinoline system are 8.47 (3) and 88.16 (6)°, respectively.

## Related literature

For background on the use of quinoline carboxylic acid derivatives in metal organic frameworks, see: Dobrzyńska *et al.* (2004, 2005); Hu *et al.* (2007); Li & Liu (2010). For background on the role of noncovalent intermolecular interactions, see: Wang *et al.* (2011). For related structures, see: Dobrzyńska *et al.* (2004); Dobrzyńska & Jerzykiewicz (2008); Odoko *et al.* (2001); Zurowska *et al.* (2007).




## Experimental

### Crystal data

$C_{11}H_7NO_4\cdot H_2O$
$M_r$ = 235.19
Monoclinic, $P2_1/c$
$a$ = 7.5424 (15) Å
$b$ = 14.422 (3) Å
$c$ = 9.755 (2) Å
$\beta$ = 108.17 (3)°
$V$ = 1008.3 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 153 K
0.15 × 0.13 × 0.11 mm

### Data collection

Rigaku CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
$T_{min}$ = 0.981, $T_{max}$ = 1
4586 measured reflections
1817 independent reflections
1547 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
$S$ = 1.05
1817 reflections
168 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 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$A$···O2$^{i}$ | 0.93 (2) | 1.71 (2) | 2.6392 (16) | 170.7 (17) |
| O1$W$—H1$C$···O1$^{ii}$ | 0.86 (2) | 1.93 (2) | 2.7589 (16) | 161 (2) |
| O1$W$—H1$D$···O1 | 0.87 (2) | 1.90 (2) | 2.7597 (16) | 175 (2) |
| O4—H4$A$···O1$W^{iii}$ | 0.89 (2) | 1.70 (2) | 2.5950 (17) | 175.6 (19) |

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

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalClear* (Rigaku, 2007) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2053).

## References

Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Dobrzyńska, D., Duczmal, M., Jerzykiewicz, L. B., Warchulska, J. & Drabent, K. (2004). *Eur. J. Inorg. Chem.* pp. 110–117.
Dobrzyńska, D. & Jerzykiewicz, L. B. (2008). *Acta Cryst.* E**64**, m1383–m1384.
Dobrzyńska, D., Jerzykiewicz, L. B., Jezierska, J. & Duczmal, M. (2005). *Cryst. Growth Des.* **5**, 1945–1951.
Hu, S., Zhang, S.-H. & Zeng, M.-H. (2007). *Acta Cryst.* E**63**, m2565.
Li, X. L. & Liu, G. Z. (2010). *Z. Kristallogr. New Cryst. Struct.* **225**, 761–762.
Odoko, M., Muranishi, Y. & Okabe, N. (2001). *Acta Cryst.* E**57**, m267–m269.
Rigaku (2007). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, X. L., Zhang, J. X., Liu, G. C. & Lin, H. Y. (2011). *J. Solid State Chem.* **184**, 280–288.
Zurowska, B., Mrozinski, J. & Ciunik, Z. (2007). *Polyhedron*, **26**, 3085–3091.

# supplementary materials

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## 3-Carboxyquinolin-1-ium-2-carboxylate monohydrate

**Xing Wang, Chun-Bo Liu, Yong-Sheng Yan, Shen-Tang Wang and Qing Zhang**

### Comment

Quinoline carboxylic acid derivatives have been explored in the synthesis of metal organic frameworks due to their abundant coordination modes which lead to the construction of metal organic frameworks with intriguing structures and functional properties (Dobrzyńska *et al.* 2004; Hu *et al.* 2007; Dobrzyńska *et al.* 2005; Li & Liu 2010). It is well known that noncovalent intermolecular interactions such as hydrogen bonding interactions and $\pi$–$\pi$ interactions, play crucial role in the design and construction of supramolecular architecture (Wang *et al.* 2011). Taking quinoline-2-carboxylic acid for example, the crystal structures of its metal complexes have been determined for several metal ions, including $Cu^{II}$ (Zurowska *et al.* 2007), $Mn^{II}$ (Dobrzyńska & Jerzykiewicz, 2008), $Ni^{II}$ (Odoko *et al.* 2001), $Co^{II}$ and $Fe^{II}$ (Dobrzyńska *et al.* 2004). Of these complexes, the magnetic properties of $Cu^{II}$, $Co^{II}$ and $Fe^{II}$ complexes have also been investigated. Herein, the structurally similar quinoline-2,3-dicarboxylic acid (qda) is a good choice for constructing a framework with novel physical properties, and the crystal structure of its monohydrate is reported now.

In this report, the title compound was prepared by using quinoline-2,3-dicarboxylic acid (qda) ligand under hydrothermal conditions. The analysis of crystal structure shows that one proton of carboxyl group of qda is transferred to N atom from pyridine ring, and one water molecule exists in the crystal lattice (Fig. 1). As shown in Fig. 2, the N—H···O hydrogen bond (yellow dotted line) links the molecules into dimers, and these dimers are further connected by O–H···O hydrogen bond (black dotted line) to a 3D supramolecular architecture. In addition, the $\pi$–$\pi$ interactions (blue dotted line) occur between pyridine ring and benzene ring from different qda ligands with the distance of 3.749 (1) Å, making the supramolecular network more stable (Fig. 3).

### Experimental

The quinoline-2,3-dicarboxylic acid (qda) was purchased commercially and used without further purification. A mixture of $ZnCl_2$ (13.4 mg, 0.1 mmol), and qda (43.8 mg, 0.2 mmol) was dissolved in a 15 mL of water, and the pH was adjusted to 7 by 1 mol $L^{-1}$ sodium hydroxide solution. Then the mixture was placed in a 25 mL autoclave with Teflon-liner. The autoclave was heated to 433 K and held at this temperature for three days. It was then cooled to room temperature under spontaneous conditions. The colourless block crystals were obtained with a yield of 60 %, however, X-ray crystallographic study shows that this crystal is not zinc complex but the title compound.

### Refinement

All H atoms on C atoms were placed in an ideal position using a riding model th with C—H distances of 0.93 Å and $U_{iso}$(H)=1.2$U_{eq}$(C). The pyridinium NH and hydroxy H-atoms were located in a difference Fourier map with N—H distance of 0.933 Å and O—H distance of 0.893 Å, and their temperature factors were freely refined. Water hydrogen atoms were also located in a difference Fourier map with a distance restraint to their parent O atoms (0.867 and 0.858 Å, respectively) and $U_{iso}$(H)=1.5$U_{eq}$(O).

### Computing details

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear* (Rigaku, 2007); data reduction: *CrystalClear* (Rigaku, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalClear* (Rigaku, 2007) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

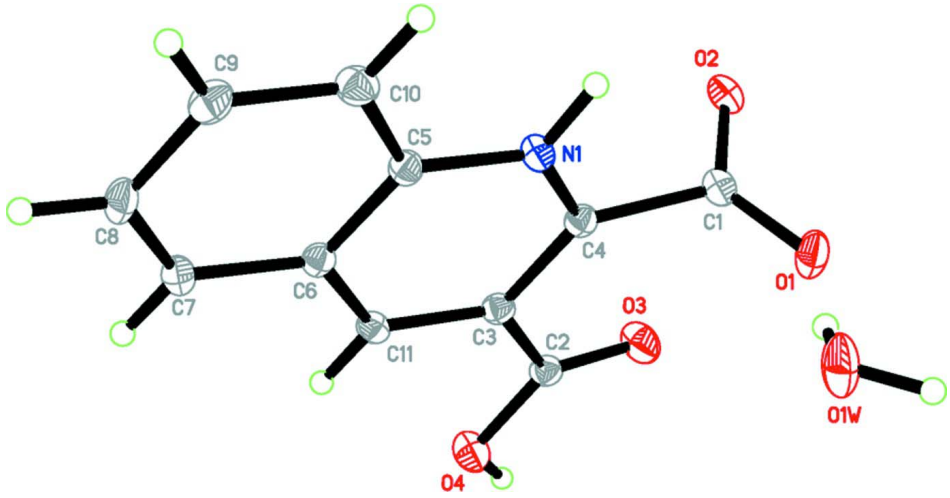


**Figure 1**

The crystal structure of the title compound with atom-labelling scheme, showing 30% probability displacement ellipsoids. H atoms are presented as a small spheres of arbitrary radius.

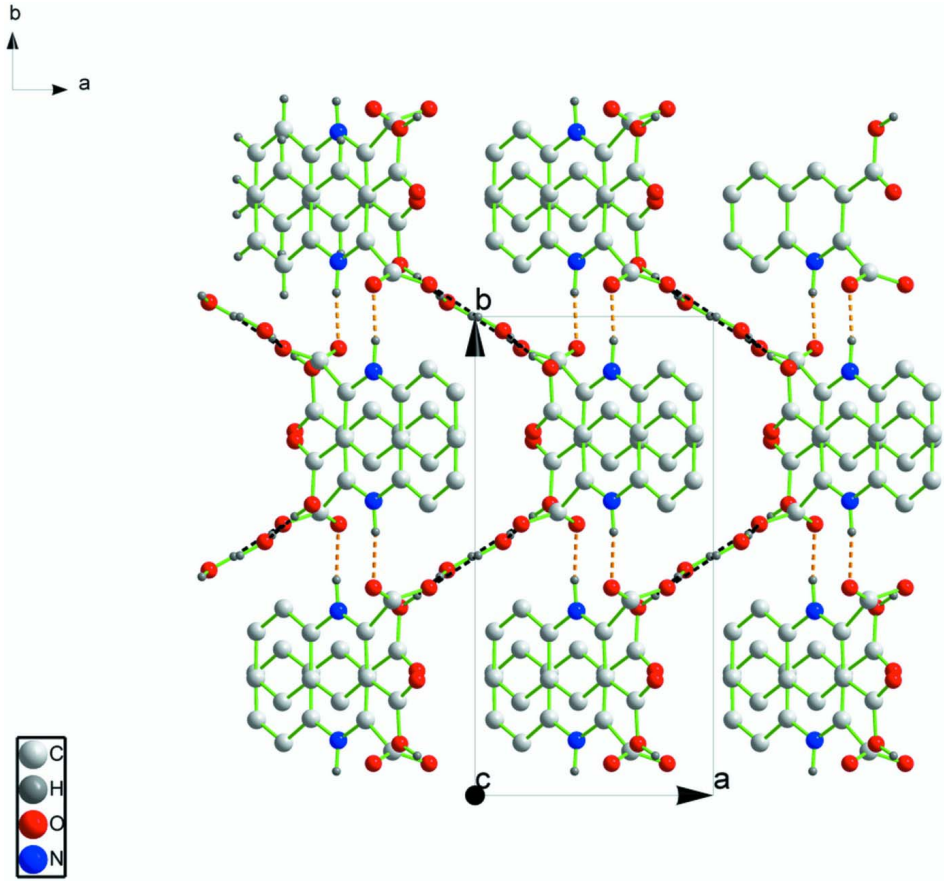


**Figure 2**

A view of 3D supramolecular architecture formed by N—H···O hydrogen bond (yellow dotted line) and O—H···O hydrogen bond (black dotted line) along c axis.

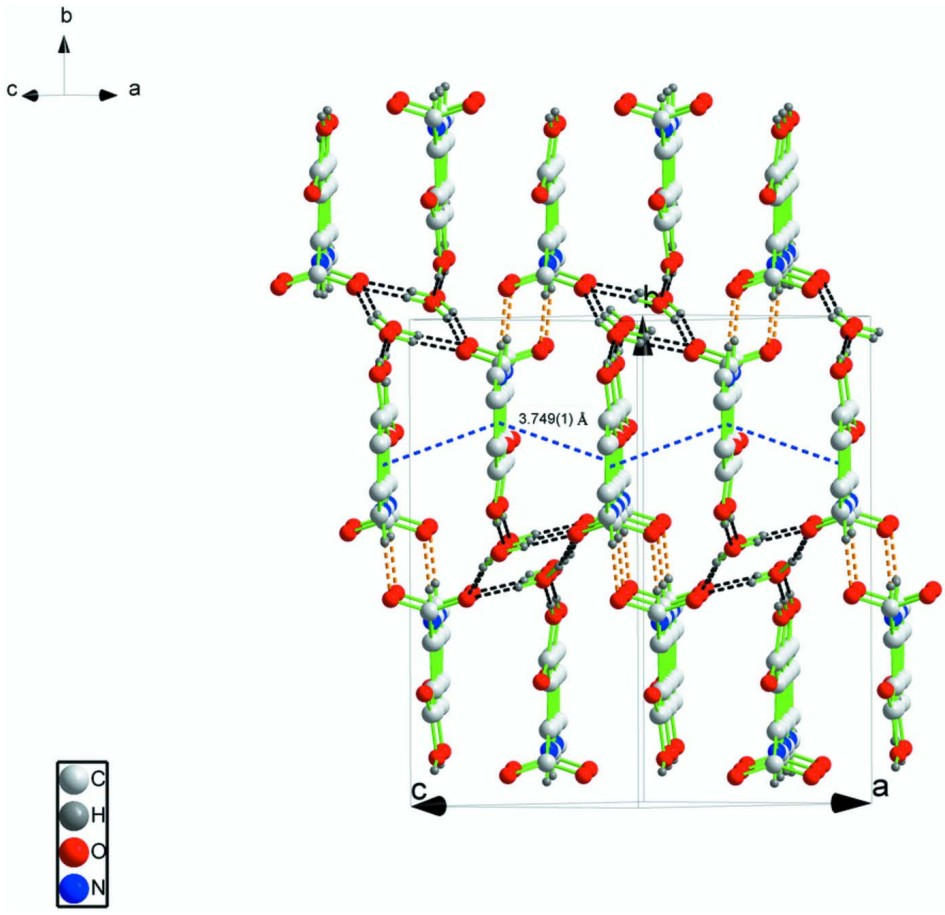


**Figure 3**

A view of the formation of the O—H···O interactions and $\pi$–$\pi$ interactions.

### 3-Carboxyquinolin-1-ium-2-carboxylate monohydrate

*Crystal data*

$C_{11}H_7NO_4 \cdot H_2O$
$M_r = 235.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.5424$ (15) Å
$b = 14.422$ (3) Å
$c = 9.755$ (2) Å
$\beta = 108.17$ (3)°
$V = 1008.3$ (4) Å$^3$
$Z = 4$
$F(000) = 488$
$D_x = 1.549$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4018 reflections
$\theta = 4.0$–$28.9°$
$\mu = 0.13$ mm$^{-1}$
$T = 153$ K
Prism, colourless
0.15 × 0.13 × 0.11 mm

*Data collection*

Rigaku CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 28.5714 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
$T_{min} = 0.981$, $T_{max} = 1$
4586 measured reflections
1817 independent reflections
1547 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$

$\theta_{max}$ = 25.3°, $\theta_{min}$ = 4.0°
$h$ = −8→7
$k$ = −17→15
$l$ = −8→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
$S$ = 1.05
1817 reflections
168 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.0617P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 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 $F^2 > 2$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 | 0.65319 (19) | 0.09213 (9) | 1.05483 (14) | 0.0216 (3) |
| C2 | 0.67451 (18) | 0.30200 (9) | 1.06906 (15) | 0.0216 (3) |
| C3 | 0.54746 (17) | 0.25508 (9) | 0.93895 (14) | 0.0195 (3) |
| C4 | 0.54008 (17) | 0.15740 (9) | 0.93584 (14) | 0.0194 (3) |
| C5 | 0.31108 (17) | 0.16028 (10) | 0.70347 (14) | 0.0199 (3) |
| C6 | 0.31153 (18) | 0.25796 (9) | 0.70374 (14) | 0.0192 (3) |
| C7 | 0.19098 (18) | 0.30475 (10) | 0.58263 (14) | 0.0231 (3) |
| H7 | 0.1883 | 0.3692 | 0.5804 | 0.028* |
| C8 | 0.07928 (19) | 0.25556 (10) | 0.46975 (16) | 0.0255 (3) |
| H8 | 0.0000 | 0.2867 | 0.3909 | 0.031* |
| C9 | 0.08227 (19) | 0.15775 (10) | 0.47086 (15) | 0.0266 (3) |
| H9 | 0.0054 | 0.1253 | 0.3923 | 0.032* |
| C10 | 0.19651 (19) | 0.10985 (10) | 0.58570 (15) | 0.0254 (3) |
| H10 | 0.1983 | 0.0454 | 0.5858 | 0.031* |
| C11 | 0.43333 (17) | 0.30389 (9) | 0.82448 (14) | 0.0197 (3) |
| H11 | 0.4362 | 0.3684 | 0.8265 | 0.024* |
| O1 | 0.80640 (13) | 0.06645 (7) | 1.04539 (11) | 0.0322 (3) |
| O2 | 0.57317 (13) | 0.06656 (6) | 1.14257 (10) | 0.0241 (3) |
| O3 | 0.75594 (15) | 0.25971 (7) | 1.17666 (11) | 0.0346 (3) |
| N1 | 0.42599 (15) | 0.11485 (8) | 0.82176 (11) | 0.0206 (3) |
| H1A | 0.418 (2) | 0.0503 (15) | 0.8245 (19) | 0.046 (5)* |
| O1W | 0.88294 (16) | 0.02969 (8) | 0.79197 (12) | 0.0380 (3) |
| H1C | 0.987 (2) | 0.0010 (13) | 0.825 (2) | 0.057* |

| | | | | |
|---|---|---|---|---|
| H1D | 0.853 (3) | 0.0434 (14) | 0.8685 (19) | 0.057* |
| O4 | 0.68389 (15) | 0.39253 (7) | 1.05383 (12) | 0.0300 (3) |
| H4A | 0.757 (3) | 0.4174 (13) | 1.136 (3) | 0.059 (6)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0257 (7) | 0.0190 (7) | 0.0174 (7) | 0.0003 (5) | 0.0030 (6) | −0.0014 (5) |
| C2 | 0.0206 (7) | 0.0246 (7) | 0.0197 (8) | −0.0019 (6) | 0.0061 (6) | 0.0011 (6) |
| C3 | 0.0197 (7) | 0.0212 (7) | 0.0184 (7) | −0.0010 (5) | 0.0070 (6) | 0.0002 (5) |
| C4 | 0.0184 (7) | 0.0224 (7) | 0.0181 (7) | 0.0003 (5) | 0.0067 (5) | 0.0004 (5) |
| C5 | 0.0193 (7) | 0.0224 (7) | 0.0180 (7) | 0.0006 (5) | 0.0060 (5) | 0.0014 (5) |
| C6 | 0.0185 (7) | 0.0214 (7) | 0.0183 (7) | 0.0006 (5) | 0.0067 (6) | 0.0002 (5) |
| C7 | 0.0234 (7) | 0.0226 (7) | 0.0225 (8) | 0.0031 (6) | 0.0059 (6) | 0.0028 (6) |
| C8 | 0.0210 (7) | 0.0319 (8) | 0.0197 (7) | 0.0040 (6) | 0.0006 (6) | 0.0032 (6) |
| C9 | 0.0231 (7) | 0.0326 (8) | 0.0209 (7) | −0.0040 (6) | 0.0022 (6) | −0.0049 (6) |
| C10 | 0.0280 (8) | 0.0223 (7) | 0.0251 (8) | −0.0034 (6) | 0.0068 (6) | −0.0021 (6) |
| C11 | 0.0224 (7) | 0.0183 (7) | 0.0199 (8) | 0.0001 (5) | 0.0087 (6) | 0.0007 (5) |
| O1 | 0.0256 (5) | 0.0411 (6) | 0.0285 (6) | 0.0120 (5) | 0.0063 (4) | 0.0085 (5) |
| O2 | 0.0345 (6) | 0.0186 (5) | 0.0198 (5) | 0.0016 (4) | 0.0092 (4) | 0.0012 (4) |
| O3 | 0.0391 (6) | 0.0319 (6) | 0.0220 (6) | −0.0069 (5) | −0.0061 (5) | 0.0050 (5) |
| N1 | 0.0240 (6) | 0.0173 (6) | 0.0193 (6) | 0.0012 (5) | 0.0050 (5) | 0.0010 (4) |
| O1W | 0.0426 (7) | 0.0441 (7) | 0.0249 (6) | 0.0210 (5) | 0.0073 (5) | 0.0095 (5) |
| O4 | 0.0367 (6) | 0.0217 (5) | 0.0243 (6) | −0.0046 (4) | −0.0011 (5) | −0.0029 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.2439 (17) | C6—C7 | 1.4170 (18) |
| C1—O2 | 1.2470 (17) | C7—C8 | 1.359 (2) |
| C1—C4 | 1.5310 (18) | C7—H7 | 0.9300 |
| C2—O3 | 1.2038 (16) | C8—C9 | 1.411 (2) |
| C2—O4 | 1.3184 (17) | C8—H8 | 0.9300 |
| C2—C3 | 1.4929 (18) | C9—C10 | 1.369 (2) |
| C3—C11 | 1.3727 (18) | C9—H9 | 0.9300 |
| C3—C4 | 1.4098 (19) | C10—H10 | 0.9300 |
| C4—N1 | 1.3260 (17) | C11—H11 | 0.9300 |
| C5—N1 | 1.3741 (17) | N1—H1A | 0.93 (2) |
| C5—C10 | 1.4059 (19) | O1W—H1C | 0.858 (15) |
| C5—C6 | 1.409 (2) | O1W—H1D | 0.868 (15) |
| C6—C11 | 1.4126 (19) | O4—H4A | 0.89 (2) |
| | | | |
| O1—C1—O2 | 128.49 (13) | C8—C7—H7 | 120.0 |
| O1—C1—C4 | 115.97 (12) | C6—C7—H7 | 120.0 |
| O2—C1—C4 | 115.32 (11) | C7—C8—C9 | 120.75 (13) |
| O3—C2—O4 | 124.70 (13) | C7—C8—H8 | 119.6 |
| O3—C2—C3 | 121.96 (12) | C9—C8—H8 | 119.6 |
| O4—C2—C3 | 113.32 (12) | C10—C9—C8 | 121.03 (13) |
| C11—C3—C4 | 118.97 (12) | C10—C9—H9 | 119.5 |
| C11—C3—C2 | 122.18 (12) | C8—C9—H9 | 119.5 |
| C4—C3—C2 | 118.81 (11) | C9—C10—C5 | 118.53 (13) |

| | | | |
|---|---|---|---|
| N1—C4—C3 | 119.43 (11) | C9—C10—H10 | 120.7 |
| N1—C4—C1 | 114.47 (11) | C5—C10—H10 | 120.7 |
| C3—C4—C1 | 126.09 (11) | C3—C11—C6 | 121.18 (13) |
| N1—C5—C10 | 120.37 (13) | C3—C11—H11 | 119.4 |
| N1—C5—C6 | 118.34 (12) | C6—C11—H11 | 119.4 |
| C10—C5—C6 | 121.29 (12) | C4—N1—C5 | 123.95 (12) |
| C5—C6—C11 | 118.10 (12) | C4—N1—H1A | 118.0 (11) |
| C5—C6—C7 | 118.30 (12) | C5—N1—H1A | 118.0 (11) |
| C11—C6—C7 | 123.60 (13) | H1C—O1W—H1D | 104.2 (18) |
| C8—C7—C6 | 120.10 (13) | C2—O4—H4A | 109.7 (13) |
| | | | |
| O3—C2—C3—C11 | 170.11 (13) | C5—C6—C7—C8 | −0.28 (18) |
| O4—C2—C3—C11 | −8.67 (17) | C11—C6—C7—C8 | 179.25 (13) |
| O3—C2—C3—C4 | −7.72 (19) | C6—C7—C8—C9 | −0.4 (2) |
| O4—C2—C3—C4 | 173.51 (12) | C7—C8—C9—C10 | 0.4 (2) |
| C11—C3—C4—N1 | 1.20 (18) | C8—C9—C10—C5 | 0.2 (2) |
| C2—C3—C4—N1 | 179.10 (11) | N1—C5—C10—C9 | 179.13 (12) |
| C11—C3—C4—C1 | −178.47 (11) | C6—C5—C10—C9 | −0.88 (19) |
| C2—C3—C4—C1 | −0.57 (18) | C4—C3—C11—C6 | −0.89 (18) |
| O1—C1—C4—N1 | 89.54 (14) | C2—C3—C11—C6 | −178.72 (12) |
| O2—C1—C4—N1 | −85.51 (14) | C5—C6—C11—C3 | −0.38 (18) |
| O1—C1—C4—C3 | −90.78 (16) | C7—C6—C11—C3 | −179.91 (12) |
| O2—C1—C4—C3 | 94.17 (15) | C3—C4—N1—C5 | −0.20 (18) |
| N1—C5—C6—C11 | 1.36 (18) | C1—C4—N1—C5 | 179.51 (11) |
| C10—C5—C6—C11 | −178.63 (11) | C10—C5—N1—C4 | 178.89 (12) |
| N1—C5—C6—C7 | −179.09 (11) | C6—C5—N1—C4 | −1.10 (18) |
| C10—C5—C6—C7 | 0.92 (18) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O2$^{i}$ | 0.93 (2) | 1.71 (2) | 2.6392 (16) | 170.7 (17) |
| O1*W*—H1*C*···O1$^{ii}$ | 0.86 (2) | 1.93 (2) | 2.7589 (16) | 161 (2) |
| O4—H4*A*···O1*W*$^{iii}$ | 0.89 (2) | 1.70 (2) | 2.5950 (17) | 175.6 (19) |
| O1*W*—H1*D*···O1 | 0.87 (2) | 1.90 (2) | 2.7597 (16) | 175 (2) |

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