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# Poly[diaqua($\mu_3$-1*H*-benzimidazole-5,6-dicarboxylato-$\kappa^4N^3:O^5,O^6:O^{6'}$)-magnesium(II)]

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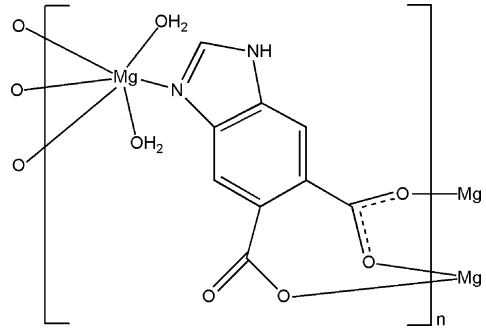
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.036; $wR$ factor = 0.090; data-to-parameter ratio = 7.0.

In the title complex, $[Mg(C_9H_4N_2O_4)(H_2O)_2]_n$, the $Mg^{II}$ atom is six-coordinated by one N and three O atoms from three different 1*H*-benzimidazole-5,6-dicarboxylate ligands and two O atoms from two water molecules, forming a slightly distorted octahedral geometry. The ligand links the $Mg^{II}$ centres into a three-dimensional network. Extensive N—H···O and O—H···O hydrogen bonds exist between the ligands and water molecules, stabilizing the crystal structure.

## Related literature

For related structures of 1*H*-benzimidazole-5,6-dicarboxylate complexes, see: Song, Wang, Hu *et al.* (2009); Song, Wang, Li *et al.* (2009); Song, Wang, Qin *et al.* (2009); Wang *et al.* (2009).




## Experimental

### Crystal data

$[Mg(C_9H_4N_2O_4)(H_2O)_2]$
$M_r$ = 264.48
Monoclinic, *Cc*
$a$ = 7.4793 (15) Å
$b$ = 18.958 (4) Å
$c$ = 7.3132 (15) Å
$\beta$ = 99.38 (3)°
$V$ = 1023.1 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 293 K
0.30 × 0.25 × 0.21 mm

### Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
$T_{min}$ = 0.943, $T_{max}$ = 0.960
4611 measured reflections
1143 independent reflections
1096 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
$S$ = 1.06
1143 reflections
163 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Mg1—N1 | 2.195 (3) | Mg1—O4$^{ii}$ | 2.113 (3) |
| Mg1—O1$^{i}$ | 2.051 (3) | Mg1—O1*W* | 2.063 (3) |
| Mg1—O3$^{i}$ | 2.106 (3) | Mg1—O2*W* | 2.074 (3) |

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

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···O1$^{iii}$ | 0.86 | 2.29 | 2.992 (4) | 138 |
| O1*W*—H1*W*···O2$^{iv}$ | 0.84 | 1.84 | 2.651 (4) | 163 |
| O1*W*—H2*W*···O3$^{ii}$ | 0.84 | 1.92 | 2.734 (4) | 164 |
| O2*W*—H3*W*···O4$^{iv}$ | 0.84 | 2.27 | 3.068 (4) | 160 |
| O2*W*—H4*W*···O2$^{v}$ | 0.84 | 1.87 | 2.685 (4) | 164 |

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

Data collection: *CrystalStructure* (Rigaku/MSC, 2002); cell refinement: *CrystalStructure*; data reduction: *CrystalStructure*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2269).

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# supporting information

*Acta Cryst.* (2010). E**66**, m151 [https://doi.org/10.1107/S1600536810001029]

## Poly[diaqua($\mu_3$-1*H*-benzimidazole-5,6-dicarboxylato-$\kappa^4N^3$:$O^5$,$O^6$:$O^{6'}$)magnesium(II)]

**Hao Wang, Xiao-Fei Li, Wen-Dong Song, Xiao-Tian Ma and Juan-Hua Liu**

### S1. Comment

1*H*-Benzimidazole-5,6-dicarboxylic acid ($H_2L$) can function as a multidentate ligand and several complexes formed from this ligand have been reported recently, including *catena*-poly[[diaqua(1,10-phenanthroline-$\kappa^2N,N'$) nickel(II)]-$\mu$-*L*-$\kappa^2N^3$:$O^6$] (Song, Wang, Hu *et al.*, 2009), pentaaqua(*L*-$\kappa N^3$)cobalt(II) pentahydrate (Song, Wang, Li *et al.*, 2009), pentaaqua(*L*-$\kappa N^3$)nickel(II) pentahydrate (Song, Wang, Qin *et al.*, 2009) and tetraaquabis(*L*-$\kappa N^3$)cobalt(II) dimethylformamide disolvate dihydrate (Wang *et al.*, 2009). However, the Mg complex of the $H_2L$ ligand has not been reported up to now.

As shown in Fig. 1, the $Mg^{II}$ atom is six-coordinated by one N and three O atoms from three different *L* ligands, and two O atoms from two water molecules (Table 1), showing a slightly distorted octahedral geometry. The equatorial plane is defined by O1W, O2W, $O1^{i}$ and $O3^{i}$ atoms, while N1 and $O4^{ii}$ occupy the axial positions [symmetry codes: (i) $x$, 1 - $y$, -1/2 + $z$; (ii) 1/2 + $x$, 1/2 + $y$, $z$]. Intermolecular O—H···O and N—H···O hydrogen bonds between the ligand and the coordinated water molecules stabilize the structure (Table 2 and Fig 2).

### S2. Experimental

A mixture of $MgCl_2$ (1.0 mmol), $H_2L$ (0.6 mmol), $CH_3CN$ (6 ml) and water (4 ml) was added to a 20 ml Teflon-lined stainless container, which was heated to 150°C and held at that temperature for 5 d. After cooling to room temperature, colourless crystals were recovered by filtration.

### S3. Refinement

C– and N-bound H atoms were placed at calculated positions and treated as riding on the parent C or N atoms, with C—H = 0.93 and N—H = 0.86 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C, N). The water H atoms were located in a difference Fourier map and refined as riding with a distance restraint of O—H = 0.84 Å and with $U_{iso}$(H) = 1.5$U_{eq}$(O).

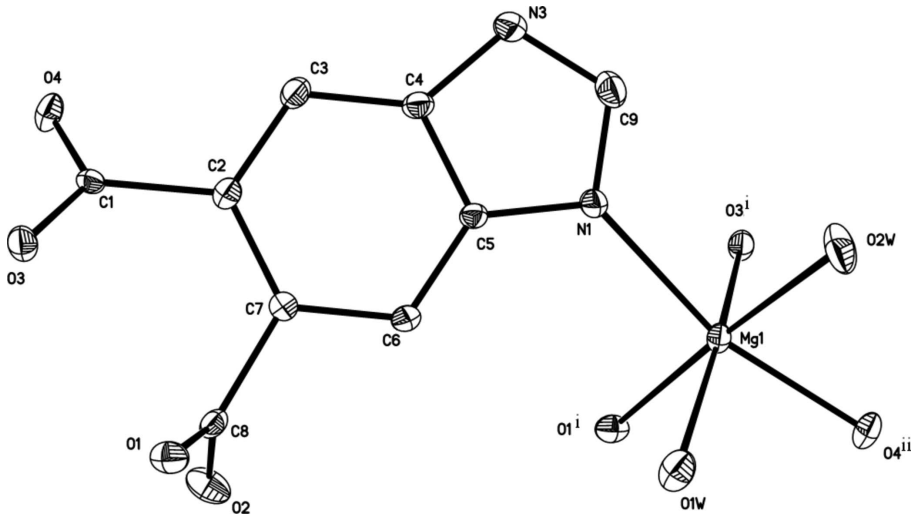


**Figure 1**

The structure of the title compound, showing the 30% probability displacement ellipsoids. [Symmetry codes: (i) *x*, 1 - *y*, -1/2 + *z*; (ii) 1/2 + *x*, 1/2 + *y*, *z*.]

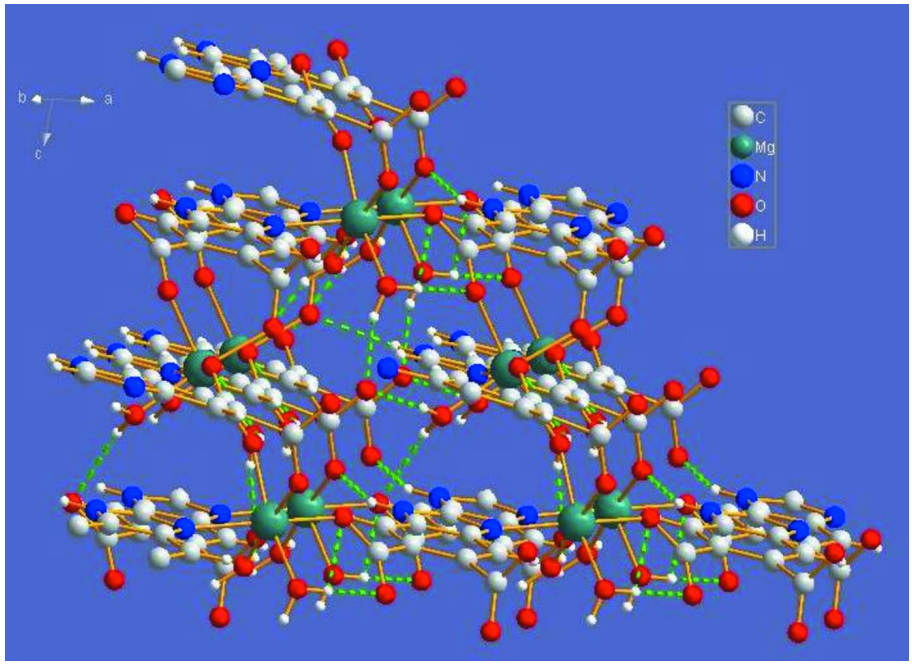


**Figure 2**

A view of the three-dimensional network structure of the title compound. Hydrogen bonds are shown as dashed lines.

**Poly[diaqua($\mu_3$-1*H*-benzimidazole-5,6-dicarboxylato- $\kappa^4N^3$:$O^5$,$O^6$:$O^{6'}$)magnesium(II)]**

*Crystal data*

$[Mg(C_9H_4N_2O_4)(H_2O)_2]$
$M_r$ = 264.48
Monoclinic, *Cc*
Hall symbol: C -2yc
*a* = 7.4793 (15) Å
*b* = 18.958 (4) Å
*c* = 7.3132 (15) Å
*β* = 99.38 (3)°
*V* = 1023.1 (4) Å$^3$
*Z* = 4

$F(000) = 544$
$D_x = 1.717$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4114 reflections
$\theta = 3.6$–$27.5°$
$\mu = 0.20$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.30 × 0.25 × 0.21 mm

*Data collection*

Rigaku/MSC Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (REQAB; Jacobson, 1998)
$T_{min} = 0.943$, $T_{max} = 0.960$
4611 measured reflections
1143 independent reflections
1096 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.6°$
$h = -9 \rightarrow 9$
$k = -24 \rightarrow 24$
$l = -8 \rightarrow 9$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.090$
$S = 1.06$
1143 reflections
163 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 2P]$ 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$^{-3}$

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mg1 | 0.27807 (16) | 0.68928 (5) | 0.63241 (16) | 0.0172 (3) |
| O1 | 0.4349 (4) | 0.37147 (14) | 0.9888 (4) | 0.0234 (5) |
| O2 | 0.5047 (4) | 0.37926 (16) | 0.7087 (4) | 0.0317 (7) |
| O3 | 0.1320 (4) | 0.28489 (12) | 0.8699 (4) | 0.0237 (6) |
| O4 | −0.0733 (4) | 0.28304 (12) | 0.6132 (3) | 0.0236 (6) |
| N1 | 0.0678 (5) | 0.61142 (15) | 0.6633 (5) | 0.0214 (6) |
| N3 | −0.2035 (5) | 0.56134 (16) | 0.6122 (5) | 0.0271 (7) |
| H3 | −0.3196 | 0.5577 | 0.5874 | 0.033* |
| C1 | 0.0380 (5) | 0.31481 (16) | 0.7326 (5) | 0.0173 (6) |
| C2 | 0.0549 (5) | 0.39389 (16) | 0.7123 (5) | 0.0182 (7) |
| C3 | −0.1002 (5) | 0.43318 (18) | 0.6560 (5) | 0.0223 (7) |
| H2 | −0.2127 | 0.4116 | 0.6240 | 0.027* |
| C4 | −0.0816 (5) | 0.50629 (18) | 0.6490 (5) | 0.0206 (7) |
| C5 | 0.0876 (5) | 0.53907 (17) | 0.6828 (5) | 0.0184 (7) |
| C6 | 0.2438 (5) | 0.49930 (18) | 0.7332 (5) | 0.0185 (7) |
| H1 | 0.3574 | 0.5206 | 0.7531 | 0.022* |
| C7 | 0.2259 (4) | 0.42738 (16) | 0.7529 (4) | 0.0154 (6) |
| C8 | 0.3985 (5) | 0.38839 (17) | 0.8204 (5) | 0.0173 (7) |
| C9 | −0.1073 (6) | 0.62155 (18) | 0.6224 (6) | 0.0262 (8) |
| H9 | −0.1599 | 0.6659 | 0.6023 | 0.031* |
| O1W | 0.4663 (4) | 0.65596 (14) | 0.8537 (4) | 0.0289 (6) |

| | | | | |
|---|---|---|---|---|
| H1W | 0.4573 | 0.6408 | 0.9598 | 0.043* |
| H2W | 0.5355 | 0.6911 | 0.8601 | 0.043* |
| O2W | 0.1388 (5) | 0.75021 (15) | 0.7982 (5) | 0.0374 (8) |
| H3W | 0.0660 | 0.7342 | 0.8639 | 0.056* |
| H4W | 0.1176 | 0.7927 | 0.7704 | 0.056* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mg1 | 0.0191 (6) | 0.0134 (4) | 0.0184 (5) | −0.0004 (4) | 0.0009 (4) | 0.0004 (4) |
| O1 | 0.0186 (13) | 0.0310 (13) | 0.0202 (12) | 0.0004 (10) | 0.0019 (11) | 0.0074 (10) |
| O2 | 0.0247 (16) | 0.0462 (17) | 0.0253 (14) | 0.0133 (12) | 0.0075 (12) | 0.0005 (12) |
| O3 | 0.0274 (14) | 0.0165 (11) | 0.0235 (12) | −0.0008 (10) | −0.0074 (11) | 0.0006 (9) |
| O4 | 0.0281 (15) | 0.0195 (12) | 0.0203 (13) | −0.0067 (10) | −0.0045 (11) | 0.0014 (9) |
| N1 | 0.0215 (16) | 0.0167 (13) | 0.0265 (15) | 0.0018 (11) | 0.0058 (12) | 0.0039 (11) |
| N3 | 0.0147 (16) | 0.0249 (14) | 0.0400 (19) | 0.0032 (12) | −0.0009 (14) | 0.0065 (13) |
| C1 | 0.0195 (17) | 0.0151 (13) | 0.0175 (16) | −0.0016 (12) | 0.0043 (14) | −0.0002 (11) |
| C2 | 0.0197 (18) | 0.0150 (14) | 0.0192 (16) | −0.0024 (12) | 0.0008 (14) | 0.0015 (12) |
| C3 | 0.0184 (18) | 0.0204 (16) | 0.0274 (19) | −0.0040 (13) | 0.0011 (15) | 0.0023 (13) |
| C4 | 0.0151 (19) | 0.0216 (16) | 0.0244 (18) | 0.0023 (12) | 0.0011 (14) | 0.0045 (13) |
| C5 | 0.0191 (17) | 0.0160 (14) | 0.0203 (16) | −0.0019 (12) | 0.0035 (14) | 0.0016 (12) |
| C6 | 0.0129 (16) | 0.0198 (15) | 0.0224 (17) | −0.0022 (11) | 0.0018 (14) | 0.0008 (12) |
| C7 | 0.0151 (16) | 0.0178 (14) | 0.0134 (14) | 0.0002 (12) | 0.0027 (13) | −0.0002 (11) |
| C8 | 0.0154 (17) | 0.0154 (14) | 0.0204 (17) | −0.0024 (11) | 0.0007 (14) | −0.0011 (11) |
| C9 | 0.024 (2) | 0.0208 (16) | 0.034 (2) | 0.0068 (14) | 0.0050 (17) | 0.0067 (14) |
| O1W | 0.0340 (15) | 0.0271 (13) | 0.0225 (12) | −0.0071 (11) | −0.0043 (12) | 0.0052 (10) |
| O2W | 0.0486 (19) | 0.0219 (12) | 0.0476 (19) | 0.0063 (12) | 0.0251 (16) | −0.0022 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mg1—N1 | 2.195 (3) | C1—C2 | 1.514 (4) |
| Mg1—O1$^{i}$ | 2.051 (3) | C2—C3 | 1.384 (5) |
| Mg1—O3$^{i}$ | 2.106 (3) | C2—C7 | 1.416 (5) |
| Mg1—O4$^{ii}$ | 2.113 (3) | C3—C4 | 1.395 (5) |
| Mg1—O1W | 2.063 (3) | C3—H2 | 0.9300 |
| Mg1—O2W | 2.074 (3) | C4—C5 | 1.395 (5) |
| O1—C8 | 1.259 (4) | C5—C6 | 1.388 (5) |
| O2—C8 | 1.241 (4) | C6—C7 | 1.380 (5) |
| O3—C1 | 1.263 (4) | C6—H1 | 0.9300 |
| O4—C1 | 1.257 (4) | C7—C8 | 1.499 (5) |
| N1—C9 | 1.310 (5) | C9—H9 | 0.9300 |
| N1—C5 | 1.384 (4) | O1W—H1W | 0.8401 |
| N3—C9 | 1.345 (5) | O1W—H2W | 0.8400 |
| N3—C4 | 1.383 (5) | O2W—H3W | 0.8399 |
| N3—H3 | 0.8600 | O2W—H4W | 0.8400 |
| | | | |
| O1$^{i}$—Mg1—O1W | 81.69 (12) | C7—C2—C1 | 120.7 (3) |
| O1$^{i}$—Mg1—O2W | 174.71 (15) | C2—C3—C4 | 117.5 (3) |

| | | | |
|---|---|---|---|
| O1W—Mg1—O2W | 93.18 (14) | C2—C3—H2 | 121.2 |
| O1$^{i}$—Mg1—O3$^{i}$ | 85.34 (12) | C4—C3—H2 | 121.3 |
| O1W—Mg1—O3$^{i}$ | 166.51 (13) | N3—C4—C3 | 133.6 (3) |
| O2W—Mg1—O3$^{i}$ | 99.68 (13) | N3—C4—C5 | 104.4 (3) |
| O1$^{i}$—Mg1—O4$^{ii}$ | 95.02 (12) | C3—C4—C5 | 122.0 (3) |
| O1W—Mg1—O4$^{ii}$ | 90.61 (11) | N1—C5—C6 | 129.5 (3) |
| O2W—Mg1—O4$^{ii}$ | 83.68 (12) | N1—C5—C4 | 110.1 (3) |
| O3$^{i}$—Mg1—O4$^{ii}$ | 86.80 (11) | C6—C5—C4 | 120.3 (3) |
| O1$^{i}$—Mg1—N1 | 98.87 (12) | C7—C6—C5 | 118.2 (3) |
| O1W—Mg1—N1 | 97.00 (12) | C7—C6—H1 | 120.9 |
| O2W—Mg1—N1 | 82.98 (13) | C5—C6—H1 | 120.9 |
| O3$^{i}$—Mg1—N1 | 88.65 (12) | C6—C7—C2 | 121.4 (3) |
| O4$^{ii}$—Mg1—N1 | 164.98 (12) | C6—C7—C8 | 115.4 (3) |
| C8—O1—Mg1$^{iii}$ | 126.4 (2) | C2—C7—C8 | 123.2 (3) |
| C1—O3—Mg1$^{iii}$ | 139.4 (2) | O2—C8—O1 | 123.3 (3) |
| C1—O4—Mg1$^{iv}$ | 130.8 (2) | O2—C8—C7 | 117.5 (3) |
| C9—N1—C5 | 104.8 (3) | O1—C8—C7 | 119.0 (3) |
| C9—N1—Mg1 | 125.8 (2) | N1—C9—N3 | 113.2 (3) |
| C5—N1—Mg1 | 127.6 (3) | N1—C9—H9 | 123.4 |
| C9—N3—C4 | 107.4 (3) | N3—C9—H9 | 123.4 |
| C9—N3—H3 | 126.3 | Mg1—O1W—H1W | 133.0 |
| C4—N3—H3 | 126.3 | Mg1—O1W—H2W | 97.9 |
| O4—C1—O3 | 123.8 (3) | H1W—O1W—H2W | 111.1 |
| O4—C1—C2 | 117.6 (3) | Mg1—O2W—H3W | 124.6 |
| O3—C1—C2 | 118.6 (3) | Mg1—O2W—H4W | 119.1 |
| C3—C2—C7 | 120.4 (3) | H3W—O2W—H4W | 111.8 |
| C3—C2—C1 | 118.9 (3) | | |

Symmetry codes: (i) $x$, $-y+1$, $z-1/2$; (ii) $x+1/2$, $y+1/2$, $z$; (iii) $x$, $-y+1$, $z+1/2$; (iv) $x-1/2$, $y-1/2$, $z$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···O1$^{v}$ | 0.86 | 2.29 | 2.992 (4) | 138 |
| O1*W*—H1*W*···O2$^{iii}$ | 0.84 | 1.84 | 2.651 (4) | 163 |
| O1*W*—H2*W*···O3$^{ii}$ | 0.84 | 1.92 | 2.734 (4) | 164 |
| O2*W*—H3*W*···O4$^{iii}$ | 0.84 | 2.27 | 3.068 (4) | 160 |
| O2*W*—H4*W*···O2$^{vi}$ | 0.84 | 1.87 | 2.685 (4) | 164 |

Symmetry codes: (ii) $x+1/2$, $y+1/2$, $z$; (iii) $x$, $-y+1$, $z+1/2$; (v) $x-1$, $-y+1$, $z-1/2$; (vi) $x-1/2$, $y+1/2$, $z$.