Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis[1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato]magnesium(II) hexahydrate

Ji-Feng Wen,[a] Wen-Zhe Yin[a]* and Ya-Xian Qiao[b]

[a]The Second Affiliated Hospital, Harbin Medical University, Harbin, 150086, People's Republic of China, and [b]Scientific and Technical Department, Harbin Medical University, Harbin, 150086, People's Republic of China
Correspondence e-mail: yinwenzhe@126.com

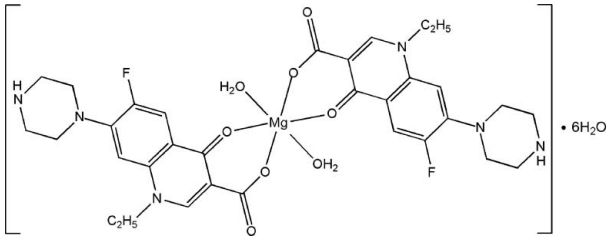
Received 11 September 2010; accepted 1 October 2010

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.065; wR factor = 0.249; data-to-parameter ratio = 11.5.

In the title compound, $[Mg(C_{16}H_{17}FN_3O_3)_2(H_2O)_2]\cdot 6H_2O$, the Mg^{2+} ion (site symmetry $\overline{1}$) exhibits a distorted MgO_6 octahedral geometry defined by two *O*,*O*-bidentate 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylate (norf) anions and two water molecules. In the crystal, O—H···O and O—H···N hydrogen bonds help to establish the packing.

Related literature

For the cadmium, zinc and cobalt(II) complexes of the norf anion, see: Chen *et al.* (2001), Wang *et al.* (2004) and An *et al.* (2007), respectively. For background to the medicinal uses of Norfloxacin [H-norf or 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinoline carboxylic acid], which is used to treat infections, see: Mizuki *et al.* (1996).



Experimental

Crystal data

$[Mg(C_{16}H_{17}FN_3O_3)_2(H_2O)_2]\cdot 6H_2O$
M_r = 805.09
Triclinic, $P\overline{1}$
a = 5.0944 (10) Å
b = 13.785 (3) Å
c = 14.351 (3) Å
α = 112.06 (3)°
β = 97.59 (3)°
γ = 93.74 (3)°
V = 918.6 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 295 K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.984, T_{max} = 0.989
7196 measured reflections
3203 independent reflections
1774 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.249
S = 1.00
3203 reflections
278 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mg1—O2	2.001 (3)	Mg1—O1*W*	2.094 (3)
Mg1—O1	2.085 (3)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2*W*^{i}	0.86	2.20	2.787 (7)	126
O1*W*—H1*W*···O2*W*	0.82 (1)	1.97 (1)	2.786 (6)	175 (3)
O1*W*—H2*W*···O1^{ii}	0.82 (2)	2.09 (2)	2.901 (5)	175 (2)
O2*W*—H3*W*···O3^{iii}	0.82 (5)	1.98 (5)	2.749 (6)	156 (4)
O2*W*—H4*W*···N1^{iv}	0.82 (2)	2.36 (4)	3.121 (7)	154 (5)
O3*W*—H5*W*···O3^{iii}	0.82 (4)	2.18 (4)	2.835 (6)	137 (5)
O3*W*—H6*W*···O4*W*	0.81 (15)	2.3 (2)	2.890 (8)	131 (19)
O4*W*—H8*W*···O3*W*^{v}	0.82 (4)	2.31 (4)	2.888 (8)	128 (4)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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*.

The authors acknowledge financial support by Harbin Medical University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5638).

References

An, Z., Xu, W. & Wang, R.-S. (2007). *Acta Cryst.* E**63**, m507–m508.
Bruker (2001). *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Z.-F., Xiong, R.-G., Zhang, J., Chen, X.-T., Xue, Z.-L. & You, X.-Z. (2001). *Inorg. Chem.* **40**, 4075–4077.
Mizuki, Y., Fujiwara, I. & Yamaguchi, T. (1996). *J. Antimicrob. Chemother.* **37** Suppl. A, 41–55.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, Y.-C., Zhao, H., Ye, Q., Chen, Z.-F., Xiong, R.-G. & Fun, H.-K. (2004). *Inorg. Chim. Acta.* **357**, 4303–4308.

supporting information

Acta Cryst. (2010). E**66**, m1388 [https://doi.org/10.1107/S1600536810039437]

Diaquabis[1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato]magnesium(II) hexahydrate

Ji-Feng Wen, Wen-Zhe Yin and Ya-Xian Qiao

S1. Comment

Norfloxacin (*H*-norf, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl) -3-quinoline carboxylic acid) is member of the class of quinolones that is used to treat infections (Mizuki *et al.*, 1996). Cadmium(II), zinc(II) and cobalt(II) derivatives of norf have been reported (Chen *et al.*, 2001; Wang *et al.*, 2004; An *et al.*,2007).

The title magnesium(II)-containing complex of norf, (I), is reported here.(Fig. 1).

The structure of (I) is built up from Mg^{2+} cations, norf ligands, coordinated water molecules, uncoordinated water molecules (Fig. 1). The manganese geometry is a slightly distorted octahedron.

The components of (I) are linked by O—H···O and O—H···N hydrogen bonds involving all the potential donors, generating a three-dimensional supramolecular network.

S2. Experimental

A mixture of $Mg(NO_3)_2.2H_2O$ (0.5 mmol), H-norf(0.6 mmol), and water (12 ml) was stirred for 30 min in air. The mixture was then transferred to a 25 ml Teflon reactor and kept at 433 K for 72 h under autogenous pressure. Upon cooling, colorless blocks of (I) were obtained from the reaction mixture.

S3. Refinement

The carbon-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The H atoms on the N and water molecules were located in a difference map and refined with a distance restraint of N—H = 0.90 (1) Å, O—H = 0.85 (1) Å,and the constraint U_{iso}(H) = 1.5U_{eq}(N,*O*).

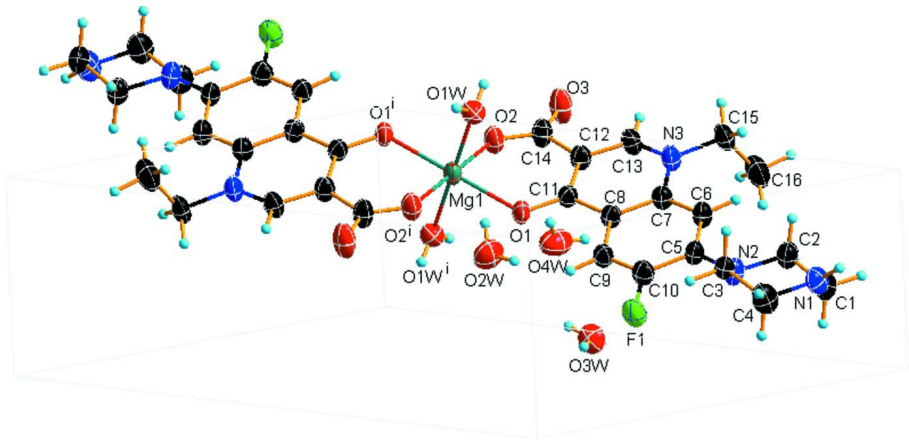


Figure 1

The molecular structure of (I), showing the Mg coordination with 50% displacement ellipsoids. Symmetry code: (i) -*x*, -*y*, 1 - *z*.

Diaquabis[1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato]magnesium(II) hexahydrate

Crystal data

$[Mg(C_{16}H_{17}FN_3O_3)_2(H_2O)_2]\cdot 6H_2O$
$M_r = 805.09$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.0944\ (10)$ Å
$b = 13.785\ (3)$ Å
$c = 14.351\ (3)$ Å
$\alpha = 112.06\ (3)°$
$\beta = 97.59\ (3)°$
$\gamma = 93.74\ (3)°$
$V = 918.6\ (3)$ Å^3
$Z = 1$
$F(000) = 426$
$D_x = 1.455$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3203 reflections
$\theta = 3.1–25.0°$
$\mu = 0.14$ mm^{-1}
$T = 295$ K
Block, colorless
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.984$, $T_{max} = 0.989$
7196 measured reflections
3203 independent reflections
1774 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.1°$
$h = -5\rightarrow6$
$k = -16\rightarrow15$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.249$
$S = 1.00$
3203 reflections
278 parameters
14 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

$w = 1/[\sigma^2(F_o^2) + (0.130P)^2 + 1.1685P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ 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	0.6643 (11)	1.0494 (5)	0.1860 (4)	0.0542 (15)
H1A	0.8374	1.0250	0.1780	0.065*
H1B	0.5932	1.0600	0.1249	0.065*
C2	0.4804 (10)	0.9679 (4)	0.1990 (4)	0.0434 (12)
H2A	0.3051	0.9910	0.2043	0.052*
H2B	0.4622	0.9021	0.1399	0.052*
C3	0.6286 (11)	1.0513 (4)	0.3807 (4)	0.0485 (13)
H3A	0.7095	1.0396	0.4401	0.058*
H3B	0.4582	1.0765	0.3932	0.058*
C4	0.8076 (12)	1.1339 (4)	0.3651 (5)	0.0563 (15)
H4A	0.8267	1.2000	0.4239	0.068*
H4B	0.9833	1.1117	0.3584	0.068*
C5	0.4638 (9)	0.8637 (3)	0.3026 (3)	0.0347 (11)
C6	0.2314 (9)	0.8028 (4)	0.2407 (4)	0.0379 (11)
H6	0.1484	0.8213	0.1891	0.046*
C7	0.1195 (9)	0.7150 (3)	0.2534 (3)	0.0336 (11)
C8	0.2283 (9)	0.6871 (3)	0.3335 (3)	0.0333 (11)
C9	0.4682 (9)	0.7473 (4)	0.3948 (3)	0.0360 (11)
H9	0.5519	0.7296	0.4469	0.043*
C10	0.5770 (9)	0.8300 (4)	0.3787 (4)	0.0385 (11)
C11	0.1060 (8)	0.6013 (3)	0.3537 (3)	0.0324 (10)
C12	−0.1318 (9)	0.5427 (4)	0.2836 (3)	0.0370 (11)
C13	−0.2237 (10)	0.5729 (4)	0.2062 (4)	0.0390 (12)
H13	−0.3732	0.5321	0.1601	0.047*
C14	−0.2863 (10)	0.4475 (4)	0.2873 (4)	0.0413 (12)
C15	−0.2428 (10)	0.6777 (4)	0.1028 (4)	0.0435 (12)
H15A	−0.2341	0.7535	0.1229	0.052*
H15B	−0.4297	0.6488	0.0853	0.052*
C16	−0.1147 (13)	0.6332 (5)	0.0103 (4)	0.0629 (16)
H16A	0.0675	0.6649	0.0255	0.094*
H16B	−0.2094	0.6480	−0.0444	0.094*
H16C	−0.1201	0.5583	−0.0097	0.094*

F1	0.8150 (5)	0.8827 (2)	0.4368 (2)	0.0517 (8)
Mg1	0.0000	0.5000	0.5000	0.0334 (6)
N1	0.6945 (10)	1.1490 (3)	0.2742 (4)	0.0570 (13)
H1	0.6518	1.2077	0.2725	0.068*
N2	0.5853 (8)	0.9511 (3)	0.2908 (3)	0.0410 (10)
N3	−0.1186 (8)	0.6557 (3)	0.1905 (3)	0.0392 (10)
O1	0.2033 (6)	0.5828 (3)	0.4305 (2)	0.0373 (8)
O2	−0.2364 (6)	0.4254 (3)	0.3645 (2)	0.0440 (9)
O3	−0.4641 (8)	0.3955 (3)	0.2116 (3)	0.0572 (11)
O1W	0.2550 (7)	0.3831 (3)	0.4608 (3)	0.0438 (9)
O2W	0.2443 (8)	0.2500 (3)	0.2582 (3)	0.0632 (12)
O3W	0.5868 (10)	0.2135 (4)	0.0401 (3)	0.0759 (13)
O4W	0.0637 (12)	0.1102 (5)	0.0279 (6)	0.1083 (19)
H3W	0.292 (7)	0.302 (3)	0.247 (5)	0.080*
H7W	0.027 (14)	0.105 (5)	−0.0312 (14)	0.080*
H1W	0.241 (5)	0.3441 (18)	0.4005 (5)	0.080*
H5W	0.660 (10)	0.263 (3)	0.092 (3)	0.080*
H4W	0.0823 (16)	0.237 (4)	0.253 (5)	0.080*
H6W	0.51 (5)	0.166 (11)	0.050 (5)	0.080*
H2W	0.407 (2)	0.3970 (11)	0.4929 (19)	0.08 (2)*
H8W	−0.008 (8)	0.155 (3)	0.069 (3)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.052 (3)	0.070 (4)	0.059 (4)	0.008 (3)	0.013 (3)	0.045 (3)
C2	0.049 (3)	0.044 (3)	0.041 (3)	0.000 (2)	0.006 (2)	0.022 (2)
C3	0.056 (3)	0.042 (3)	0.039 (3)	−0.008 (3)	0.000 (2)	0.011 (2)
C4	0.059 (3)	0.047 (3)	0.059 (4)	−0.009 (3)	−0.006 (3)	0.025 (3)
C5	0.040 (3)	0.034 (2)	0.030 (3)	−0.002 (2)	0.004 (2)	0.015 (2)
C6	0.047 (3)	0.036 (3)	0.034 (3)	0.000 (2)	0.004 (2)	0.018 (2)
C7	0.038 (3)	0.030 (2)	0.030 (3)	−0.002 (2)	0.000 (2)	0.011 (2)
C8	0.036 (2)	0.034 (2)	0.028 (2)	−0.003 (2)	0.0006 (19)	0.012 (2)
C9	0.035 (2)	0.042 (3)	0.032 (3)	−0.001 (2)	0.000 (2)	0.018 (2)
C10	0.041 (3)	0.040 (3)	0.033 (3)	0.000 (2)	0.001 (2)	0.014 (2)
C11	0.031 (2)	0.037 (2)	0.029 (2)	−0.002 (2)	0.0013 (19)	0.015 (2)
C12	0.040 (3)	0.037 (3)	0.033 (3)	−0.004 (2)	−0.001 (2)	0.016 (2)
C13	0.044 (3)	0.039 (3)	0.033 (3)	0.002 (2)	−0.004 (2)	0.017 (2)
C14	0.053 (3)	0.038 (3)	0.030 (3)	−0.006 (2)	−0.001 (2)	0.015 (2)
C15	0.049 (3)	0.048 (3)	0.037 (3)	0.004 (2)	−0.007 (2)	0.024 (2)
C16	0.076 (4)	0.073 (4)	0.045 (3)	0.023 (3)	0.001 (3)	0.030 (3)
F1	0.0444 (16)	0.0568 (18)	0.0516 (19)	−0.0141 (14)	−0.0135 (13)	0.0289 (15)
Mg1	0.0354 (12)	0.0384 (12)	0.0304 (12)	−0.0011 (10)	0.0002 (9)	0.0205 (10)
N1	0.068 (3)	0.041 (3)	0.068 (3)	0.006 (2)	0.007 (3)	0.030 (2)
N2	0.053 (3)	0.039 (2)	0.033 (2)	−0.0024 (19)	0.0064 (19)	0.0177 (19)
N3	0.045 (2)	0.039 (2)	0.035 (2)	−0.0019 (19)	−0.0020 (18)	0.0209 (19)
O1	0.0381 (17)	0.0481 (19)	0.0322 (18)	0.0006 (15)	0.0023 (14)	0.0247 (15)
O2	0.0458 (19)	0.049 (2)	0.038 (2)	−0.0101 (16)	−0.0070 (15)	0.0251 (16)

O3	0.072 (3)	0.051 (2)	0.042 (2)	−0.020 (2)	−0.0172 (19)	0.0236 (18)
O1W	0.042 (2)	0.048 (2)	0.044 (2)	0.0087 (17)	0.0063 (16)	0.0205 (17)
O2W	0.056 (2)	0.059 (3)	0.075 (3)	−0.011 (2)	0.010 (2)	0.030 (2)
O3W	0.089 (3)	0.071 (3)	0.057 (3)	0.015 (3)	0.009 (2)	0.013 (2)
O4W	0.093 (4)	0.090 (4)	0.151 (6)	0.023 (3)	0.041 (4)	0.049 (4)

Geometric parameters (Å, º)

C1—N1	1.458 (8)	C12—C13	1.366 (6)
C1—C2	1.498 (6)	C12—C14	1.508 (6)
C1—H1A	0.9700	C13—N3	1.335 (6)
C1—H1B	0.9700	C13—H13	0.9300
C2—N2	1.461 (6)	C14—O2	1.254 (5)
C2—H2A	0.9700	C14—O3	1.259 (6)
C2—H2B	0.9700	C15—N3	1.476 (6)
C3—N2	1.472 (6)	C15—C16	1.495 (8)
C3—C4	1.512 (7)	C15—H15A	0.9700
C3—H3A	0.9700	C15—H15B	0.9700
C3—H3B	0.9700	C16—H16A	0.9600
C4—N1	1.449 (7)	C16—H16B	0.9600
C4—H4A	0.9700	C16—H16C	0.9600
C4—H4B	0.9700	Mg1—O2^{i}	2.001 (3)
C5—C6	1.389 (6)	Mg1—O2	2.001 (3)
C5—N2	1.394 (5)	Mg1—O1^{i}	2.085 (3)
C5—C10	1.412 (6)	Mg1—O1	2.085 (3)
C6—C7	1.388 (6)	Mg1—O1W^{i}	2.094 (3)
C6—H6	0.9300	Mg1—O1W	2.094 (3)
C7—C8	1.403 (6)	N1—H1	0.8600
C7—N3	1.408 (6)	O1W—H1W	0.820 (10)
C8—C9	1.411 (6)	O1W—H2W	0.818 (17)
C8—C11	1.443 (6)	O2W—H3W	0.82 (5)
C9—C10	1.345 (6)	O2W—H4W	0.821 (16)
C9—H9	0.9300	O3W—H5W	0.82 (4)
C10—F1	1.362 (5)	O3W—H6W	0.81 (15)
C11—O1	1.268 (5)	O4W—H8W	0.82 (4)
C11—C12	1.439 (6)	O4W—H7W	0.82 (3)
N1—C1—C2	110.5 (4)	N3—C13—C12	126.0 (4)
N1—C1—H1A	109.5	N3—C13—H13	117.0
C2—C1—H1A	109.5	C12—C13—H13	117.0
N1—C1—H1B	109.5	O2—C14—O3	123.8 (4)
C2—C1—H1B	109.5	O2—C14—C12	119.4 (4)
H1A—C1—H1B	108.1	O3—C14—C12	116.7 (4)
N2—C2—C1	110.1 (4)	N3—C15—C16	113.9 (4)
N2—C2—H2A	109.6	N3—C15—H15A	108.8
C1—C2—H2A	109.6	C16—C15—H15A	108.8
N2—C2—H2B	109.6	N3—C15—H15B	108.8
C1—C2—H2B	109.6	C16—C15—H15B	108.8

H2A—C2—H2B	108.1	H15A—C15—H15B	107.7
N2—C3—C4	111.2 (4)	C15—C16—H16A	109.5
N2—C3—H3A	109.4	C15—C16—H16B	109.5
C4—C3—H3A	109.4	H16A—C16—H16B	109.5
N2—C3—H3B	109.4	C15—C16—H16C	109.5
C4—C3—H3B	109.4	H16A—C16—H16C	109.5
H3A—C3—H3B	108.0	H16B—C16—H16C	109.5
N1—C4—C3	110.0 (4)	O2^{i}—Mg1—O2	180.0
N1—C4—H4A	109.7	O2^{i}—Mg1—O1^{i}	86.80 (12)
C3—C4—H4A	109.7	O2—Mg1—O1^{i}	93.20 (13)
N1—C4—H4B	109.7	O2^{i}—Mg1—O1	93.20 (13)
C3—C4—H4B	109.7	O2—Mg1—O1	86.80 (12)
H4A—C4—H4B	108.2	O1^{i}—Mg1—O1	180.0
C6—C5—N2	123.6 (4)	O2^{i}—Mg1—O1W^{i}	90.04 (15)
C6—C5—C10	115.4 (4)	O2—Mg1—O1W^{i}	89.96 (15)
N2—C5—C10	121.0 (4)	O1^{i}—Mg1—O1W^{i}	90.47 (13)
C5—C6—C7	122.0 (4)	O1—Mg1—O1W^{i}	89.53 (13)
C5—C6—H6	119.0	O2^{i}—Mg1—O1W	89.96 (15)
C7—C6—H6	119.0	O2—Mg1—O1W	90.04 (14)
C6—C7—C8	121.3 (4)	O1^{i}—Mg1—O1W	89.53 (13)
C6—C7—N3	120.7 (4)	O1—Mg1—O1W	90.47 (13)
C8—C7—N3	117.9 (4)	O1W^{i}—Mg1—O1W	180.0
C7—C8—C9	116.7 (4)	C4—N1—C1	109.6 (4)
C7—C8—C11	122.8 (4)	C4—N1—H1	125.2
C9—C8—C11	120.5 (4)	C1—N1—H1	125.2
C10—C9—C8	120.6 (4)	C5—N2—C2	116.5 (4)
C10—C9—H9	119.7	C5—N2—C3	116.4 (4)
C8—C9—H9	119.7	C2—N2—C3	110.4 (4)
C9—C10—F1	118.5 (4)	C13—N3—C7	119.1 (4)
C9—C10—C5	123.9 (4)	C13—N3—C15	119.2 (4)
F1—C10—C5	117.6 (4)	C7—N3—C15	121.4 (4)
O1—C11—C12	123.8 (4)	C11—O1—Mg1	125.9 (3)
O1—C11—C8	120.5 (4)	C14—O2—Mg1	132.8 (3)
C12—C11—C8	115.6 (4)	H1W—O1W—H2W	115 (2)
C13—C12—C11	118.4 (4)	H3W—O2W—H4W	115 (5)
C13—C12—C14	116.7 (4)	H5W—O3W—H6W	115 (7)
C11—C12—C14	124.9 (4)	H8W—O4W—H7W	115 (6)

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2*W*^{ii}	0.86	2.20	2.787 (7)	126
O1*W*—H1*W*···O2*W*	0.82 (1)	1.97 (1)	2.786 (6)	175 (3)
O1*W*—H2*W*···O1^{iii}	0.82 (2)	2.09 (2)	2.901 (5)	175 (2)
O2*W*—H3*W*···O3^{iv}	0.82 (5)	1.98 (5)	2.749 (6)	156 (4)
O2*W*—H4*W*···N1^{v}	0.82 (2)	2.36 (4)	3.121 (7)	154 (5)

O3*W*—H5*W*···O3^{iv}	0.82 (4)	2.18 (4)	2.835 (6)	137 (5)
O3*W*—H6*W*···O4*W*	0.81 (15)	2.3 (2)	2.890 (8)	131 (19)
O4*W*—H8*W*···O3*W*^{vi}	0.82 (4)	2.31 (4)	2.888 (8)	128 (4)

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