Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[bis(μ-3-amino-5-carboxybenzoato-κ²*N*:*O*¹)diaquazinc] dihydrate]

Kou-Lin Zhang,[a] Ting-Ting Qiu[a] and Seik Weng Ng[b,c]*

[a]College of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou 225002, People's Republic of China, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

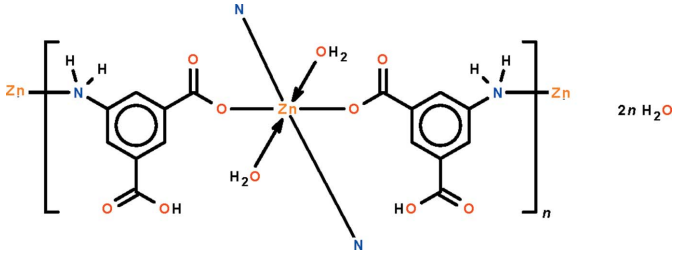
Received 2 July 2012; accepted 12 July 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.098; data-to-parameter ratio = 14.8.

The Zn^{II} atom in the title polymeric compound, $\{[Zn(C_8H_6NO_4)_2(H_2O)_2]\cdot 2H_2O\}_n$, lies on a center of inversion and is coordinated by two amine N atoms and two carboxylate O atoms from two 3-amino-5-carboxybenzoate anions along with two water molecules in a distorted octahedral geometry. The bridging nature of the anion generates a layer motif parallel to (100). Hydrogen bonds of the N—H···O and O—H···O types exist in the structure. One H atom of the coordinated water molecule and one H atom of the solvent water molecule are each disordered over two positions in a 1:1 ratio.

Related literature

For *catena*-poly[(5-aminoisophthalato)aquazinc], see: Wu *et al.* (2002).



Experimental

Crystal data

$[Zn(C_8H_6NO_4)_2(H_2O)_2]\cdot 2H_2O$
M_r = 497.71
Monoclinic, $C2/c$
a = 14.2209 (10) Å
b = 11.2252 (8) Å
c = 12.7139 (9) Å
β = 113.286 (1)°
V = 1864.2 (2) Å³
Z = 4
Mo $K\alpha$ radiation
μ = 1.39 mm⁻¹
T = 293 K
0.30 × 0.26 × 0.18 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.680, T_{max} = 0.788
8005 measured reflections
2130 independent reflections
1843 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.098
S = 1.07
2130 reflections
144 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å⁻³
$\Delta\rho_{min}$ = −0.37 e Å⁻³

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1···O2W^{i}	0.84	1.84	2.675 (3)	172
O1W—H2···O2^{ii}	0.84	1.97	2.695 (3)	143
O2W—H4···O2	0.84	1.79	2.619 (3)	170
O2W—H5···O2W^{iii}	0.84	2.03	2.869 (5)	171
O2W—H5′···O1^{iv}	0.84	2.31	3.106 (3)	158
O2W—H5′···O1W^{iv}	0.84	2.35	2.910 (3)	125
N1—H6···O4^{v}	0.88	2.14	3.013 (3)	172
N1—H7···O4^{vi}	0.88	2.21	3.059 (2)	161

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX* (Dolomanov *et al.*, 2003) and *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This study is a project funded by the Priority Academic Development Program of Jiangsu Higher Education Institution. We thank Yangzhou University and the Ministry of Higher Education of Malaysia (grant No. UM.C/HIR/MOHE/SC/12) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5588).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dolomanov, O. V., Blake, A. J., Champness, N. R. & Schröder, M. (2003). *J. Appl. Cryst.* **36**, 1283–1284.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Wu, C.-D., Lu, C.-Z., Yang, W.-B., Zhuang, H.-H. & Huang, J.-S. (2002). *Inorg. Chem.* **41**, 3302–3307.

supporting information

Acta Cryst. (2012). E**68**, m1088 [https://doi.org/10.1107/S1600536812031789]

Poly[[bis(*μ*-3-amino-5-carboxybenzoato-κ^2N:O^1)diaquazinc] dihydrate]

Kou-Lin Zhang, Ting-Ting Qiu and Seik Weng Ng

S1. Comment

5-Aminoisophthalic acid furnishes a zinc derivative in which the ligand is dibasic; the dianion functions in a u3-bridging mode in monoaqua compound, which adopts a chain structure (Wu *et al.*, 2002). The title compound (Scheme I) was the unexpected when nicotinamide was added to the reaction.

The Zn^{II} atom in of polymeric $[Zn(H_2O)_2(C_8H_6NO_4)2{\cdot}2H_2O]_n$ lies in a octahedron that is composed of two amino N atoms and two carboxyl O atoms (from two 5-aminoisophthalate anions) along with two water molecules (Fig. 1). The bridging nature of the anion generates a layer motif parallel to [1 0 0] (Fig. 2). Hydrogen bonds of the N–H···O and O–H···O type exist within the layer (Table 1).

S2. Experimental

5-Aminoisophthalic acid (0.030 g, 0.165 mmol) and sodium hydroxide (0.013 g, 0.330 mmol) were dissolved in a water/methanol (1:1 *v*/*v*; 10 ml) mixture. Zinc acetate hexahydrate (0.049 g, 0.165 mmol) dissolved in a water/methanol (1:1 *v*/*v*; 3 ml) mixture and nicotinamide (0.050 g, 0.33 mmol) dissolved in water (3 ml) were added. The solution was filtered. Light brown crystals were isolated after several days.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(*C*). The amino, water and acid H atoms were similarly positioned [N–H 0.88, O–H 0.84 Å; *U*(H) 1.2–1.5*U*(*N*,*O*)].

One H-atom of the coordinated water molecule and one H-atom of the lattice water molecule are each disordered over two positions in a 1:1 ratio. In the disorder model, the unprimed H-atoms are not within 2 Å of the primed ones.

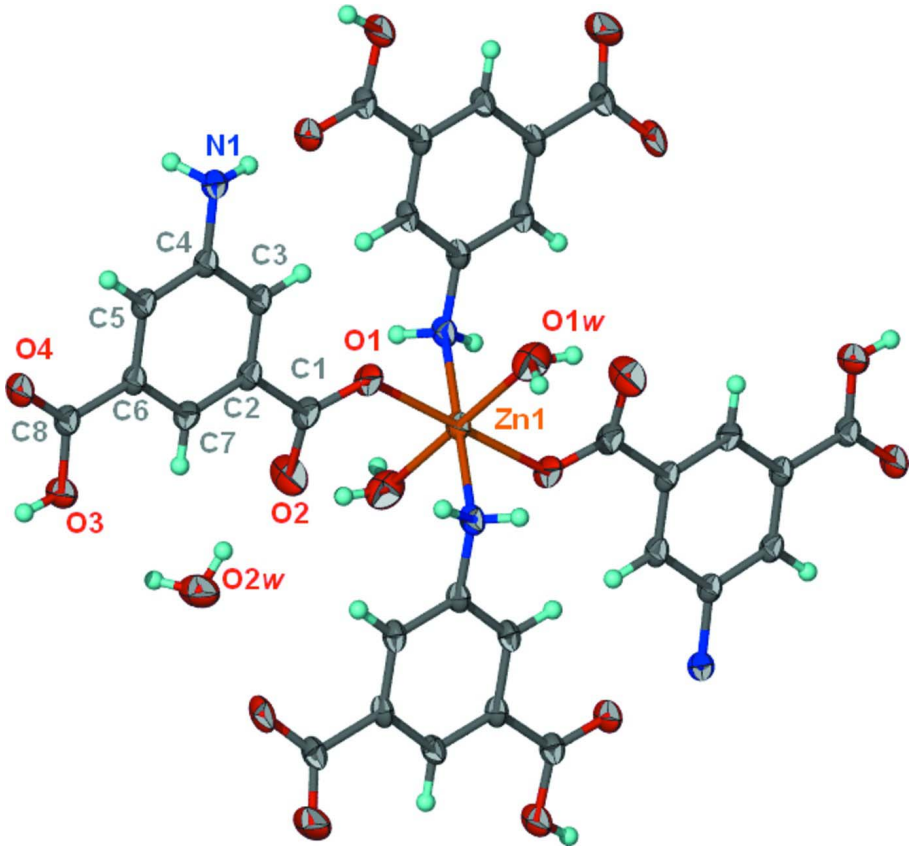


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of a portion of polymeric $Zn(H_2O)_2(C_8H_6NO_4)2{\cdot}2H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in the hydrogen atoms of the coordinated and lattice water molecules is not shown.

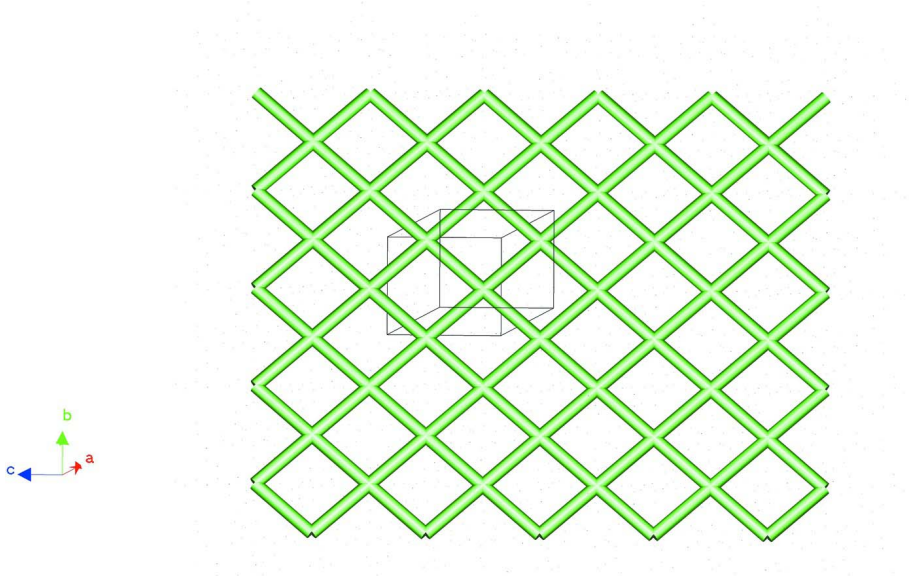


Figure 2

Layer motif represented as an OLEX-type (Dolomanov *et al.*, 2003) of network.

Poly[[bis(μ-3-amino-5-carboxybenzoato- κ²*N*:*O*¹)diaquazinc] dihydrate]

Crystal data

$[Zn(C_8H_6NO_4)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 497.71$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 14.2209\ (10)$ Å
$b = 11.2252\ (8)$ Å
$c = 12.7139\ (9)$ Å
$\beta = 113.286\ (1)°$
$V = 1864.2\ (2)$ Å^3
$Z = 4$
$F(000) = 1024$
$D_x = 1.773$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4815 reflections
$\theta = 2.4–28.2°$
$\mu = 1.39$ mm^{-1}
$T = 293$ K
Prism, light brown
0.30 × 0.26 × 0.18 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.680$, $T_{max} = 0.788$
8005 measured reflections
2130 independent reflections
1843 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -18\rightarrow15$
$k = -14\rightarrow14$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.098$
$S = 1.07$
2130 reflections
144 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 3.2779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.2500	0.2500	0.0000	0.02950 (14)	
O1	0.20751 (15)	0.32463 (16)	0.12770 (14)	0.0412 (4)	
O2	0.1529 (2)	0.1571 (2)	0.1754 (2)	0.0655 (7)	
O3	0.09628 (17)	0.14472 (16)	0.53610 (16)	0.0436 (4)	
H1	0.0885	0.1154	0.5929	0.065*	
O4	0.07472 (15)	0.31377 (16)	0.61500 (15)	0.0408 (4)	
O1W	0.35790 (16)	0.38916 (19)	0.03707 (18)	0.0531 (5)	
H2	0.3743	0.3994	−0.0189	0.080*	
H3	0.4102	0.3714	0.0953	0.080*	0.50
H3′	0.3322	0.4522	0.0496	0.080*	0.50

O2W	0.0898 (2)	−0.04635 (18)	0.22475 (18)	0.0594 (6)	
H4	0.1052	0.0229	0.2118	0.089*	
H5	0.0334	−0.0439	0.2320	0.089*	0.50
H5′	0.1397	−0.0755	0.2797	0.089*	0.50
N1	0.12864 (15)	0.64309 (17)	0.36983 (16)	0.0312 (4)	
H6	0.0705	0.6633	0.3742	0.037*	
H7	0.1250	0.6675	0.3025	0.037*	
C1	0.1718 (2)	0.2655 (2)	0.1878 (2)	0.0349 (5)	
C2	0.15207 (17)	0.3304 (2)	0.28176 (18)	0.0291 (4)	
C3	0.15228 (17)	0.4538 (2)	0.28397 (18)	0.0294 (5)	
H3A	0.1667	0.4963	0.2293	0.035*	
C4	0.13087 (16)	0.5152 (2)	0.36787 (17)	0.0274 (4)	
C5	0.11166 (17)	0.4506 (2)	0.45058 (18)	0.0295 (5)	
H5A	0.0982	0.4904	0.5073	0.035*	
C6	0.11247 (17)	0.3261 (2)	0.44894 (17)	0.0277 (4)	
C7	0.13167 (19)	0.2662 (2)	0.3638 (2)	0.0302 (5)	
H7A	0.1309	0.1834	0.3618	0.036*	
C8	0.09264 (19)	0.2626 (2)	0.54063 (19)	0.0309 (5)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0412 (2)	0.0297 (2)	0.0248 (2)	−0.00028 (15)	0.02079 (16)	−0.00161 (13)
O1	0.0631 (12)	0.0436 (10)	0.0312 (9)	0.0127 (9)	0.0339 (8)	0.0038 (7)
O2	0.121 (2)	0.0466 (12)	0.0583 (13)	−0.0156 (13)	0.0664 (14)	−0.0190 (10)
O3	0.0725 (13)	0.0354 (9)	0.0375 (9)	0.0045 (9)	0.0374 (9)	0.0025 (7)
O4	0.0639 (12)	0.0404 (10)	0.0321 (9)	−0.0022 (9)	0.0340 (8)	−0.0024 (7)
O1W	0.0501 (11)	0.0531 (12)	0.0538 (12)	−0.0046 (9)	0.0181 (9)	−0.0207 (10)
O2W	0.1023 (18)	0.0426 (11)	0.0469 (11)	0.0111 (11)	0.0441 (12)	0.0074 (9)
N1	0.0419 (11)	0.0334 (10)	0.0242 (9)	0.0046 (8)	0.0194 (8)	0.0030 (7)
C1	0.0436 (13)	0.0414 (14)	0.0258 (11)	0.0043 (10)	0.0203 (10)	−0.0048 (9)
C2	0.0323 (11)	0.0388 (12)	0.0199 (9)	0.0037 (9)	0.0142 (8)	−0.0027 (8)
C3	0.0324 (11)	0.0394 (12)	0.0203 (9)	0.0035 (9)	0.0148 (8)	0.0011 (8)
C4	0.0290 (10)	0.0343 (11)	0.0208 (9)	0.0016 (9)	0.0118 (8)	−0.0011 (8)
C5	0.0340 (11)	0.0367 (12)	0.0227 (10)	0.0037 (9)	0.0165 (9)	−0.0024 (8)
C6	0.0295 (11)	0.0366 (11)	0.0200 (9)	0.0015 (9)	0.0129 (8)	0.0000 (8)
C7	0.0376 (12)	0.0323 (11)	0.0256 (10)	0.0033 (9)	0.0178 (9)	−0.0022 (8)
C8	0.0356 (11)	0.0380 (12)	0.0233 (10)	0.0028 (9)	0.0160 (9)	0.0013 (8)

Geometric parameters (Å, º)

Zn1—O1W	2.108 (2)	O2W—H5′	0.8407
Zn1—O1W^{i}	2.108 (2)	N1—C4	1.436 (3)
Zn1—O1	2.1163 (16)	N1—Zn1^{iv}	2.214 (2)
Zn1—O1^{i}	2.1163 (16)	N1—H6	0.8800
Zn1—N1^{ii}	2.214 (2)	N1—H7	0.8800
Zn1—N1^{iii}	2.214 (2)	C1—C2	1.517 (3)
O1—C1	1.261 (3)	C2—C7	1.390 (3)

O2—C1	1.243 (3)	C2—C3	1.386 (3)
O3—C8	1.326 (3)	C3—C4	1.401 (3)
O3—H1	0.8400	C3—H3A	0.9300
O4—C8	1.217 (3)	C4—C5	1.390 (3)
O1W—H2	0.8400	C5—C6	1.398 (3)
O1W—H3	0.8400	C5—H5A	0.9300
O1W—H3′	0.8400	C6—C7	1.390 (3)
O2W—H4	0.8408	C6—C8	1.486 (3)
O2W—H5	0.8425	C7—H7A	0.9300

O1W—Zn1—O1W^{i}	180.00 (9)	Zn1^{iv}—N1—H6	106.7
O1W—Zn1—O1	86.47 (8)	C4—N1—H7	106.7
O1W^{i}—Zn1—O1	93.53 (8)	Zn1^{iv}—N1—H7	106.7
O1W—Zn1—O1^{i}	93.53 (8)	H6—N1—H7	106.6
O1W^{i}—Zn1—O1^{i}	86.47 (8)	O2—C1—O1	123.9 (2)
O1—Zn1—O1^{i}	180.00 (8)	O2—C1—C2	118.2 (2)
O1W—Zn1—N1^{ii}	92.80 (8)	O1—C1—C2	117.9 (2)
O1W^{i}—Zn1—N1^{ii}	87.20 (8)	C7—C2—C3	120.2 (2)
O1—Zn1—N1^{ii}	89.10 (7)	C7—C2—C1	120.1 (2)
O1^{i}—Zn1—N1^{ii}	90.90 (7)	C3—C2—C1	119.8 (2)
O1W—Zn1—N1^{iii}	87.20 (8)	C2—C3—C4	120.5 (2)
O1W^{i}—Zn1—N1^{iii}	92.80 (8)	C2—C3—H3A	119.7
O1—Zn1—N1^{iii}	90.90 (7)	C4—C3—H3A	119.7
O1^{i}—Zn1—N1^{iii}	89.10 (7)	C5—C4—C3	119.1 (2)
N1^{ii}—Zn1—N1^{iii}	180.00 (18)	C5—C4—N1	119.72 (19)
C1—O1—Zn1	124.19 (16)	C3—C4—N1	121.18 (19)
C8—O3—H1	109.5	C4—C5—C6	120.31 (19)
Zn1—O1W—H2	109.5	C4—C5—H5A	119.8
Zn1—O1W—H3	109.5	C6—C5—H5A	119.8
H2—O1W—H3	109.5	C7—C6—C5	120.1 (2)
Zn1—O1W—H3′	109.5	C7—C6—C8	122.4 (2)
H2—O1W—H3′	109.5	C5—C6—C8	117.58 (19)
H3—O1W—H3′	109.5	C2—C7—C6	119.8 (2)
H4—O2W—H5	108.9	C2—C7—H7A	120.1
H4—O2W—H5′	108.8	C6—C7—H7A	120.1
H5—O2W—H5′	116.7	O4—C8—O3	121.9 (2)
C4—N1—Zn1^{iv}	122.60 (14)	O4—C8—C6	123.1 (2)
C4—N1—H6	106.7	O3—C8—C6	114.96 (19)

O1W—Zn1—O1—C1	−150.9 (2)	Zn1^{iv}—N1—C4—C5	72.4 (2)
O1W^{i}—Zn1—O1—C1	29.1 (2)	Zn1^{iv}—N1—C4—C3	−107.5 (2)
N1^{ii}—Zn1—O1—C1	116.2 (2)	C3—C4—C5—C6	−0.8 (3)
N1^{iii}—Zn1—O1—C1	−63.8 (2)	N1—C4—C5—C6	179.3 (2)
Zn1—O1—C1—O2	−3.4 (4)	C4—C5—C6—C7	−0.6 (3)
Zn1—O1—C1—C2	175.68 (15)	C4—C5—C6—C8	179.3 (2)
O2—C1—C2—C7	11.5 (4)	C3—C2—C7—C6	−0.7 (3)
O1—C1—C2—C7	−167.7 (2)	C1—C2—C7—C6	−179.2 (2)
O2—C1—C2—C3	−167.1 (3)	C5—C6—C7—C2	1.3 (3)

O1—C1—C2—C3	13.8 (3)	C8—C6—C7—C2	−178.5 (2)
C7—C2—C3—C4	−0.7 (3)	C7—C6—C8—O4	−179.2 (2)
C1—C2—C3—C4	177.9 (2)	C5—C6—C8—O4	1.0 (3)
C2—C3—C4—C5	1.4 (3)	C7—C6—C8—O3	1.0 (3)
C2—C3—C4—N1	−178.7 (2)	C5—C6—C8—O3	−178.8 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1···O2*W*^{v}	0.84	1.84	2.675 (3)	172
O1*W*—H2···O2^{i}	0.84	1.97	2.695 (3)	143
O2*W*—H4···O2	0.84	1.79	2.619 (3)	170
O2*W*—H5···O2*W*^{vi}	0.84	2.03	2.869 (5)	171
O2*W*—H5′···O1^{iii}	0.84	2.31	3.106 (3)	158
O2*W*—H5′···O1*W*^{iii}	0.84	2.35	2.910 (3)	125
N1—H6···O4^{vii}	0.88	2.14	3.013 (3)	172
N1—H7···O4^{ii}	0.88	2.21	3.059 (2)	161

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