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Ethyl 5-{[(*E*)-2-(isonicotinoyl)hydrazinylidene]methyl}-3,4-dimethyl-1*H*-pyrrole-2-carboxylate dihydrate

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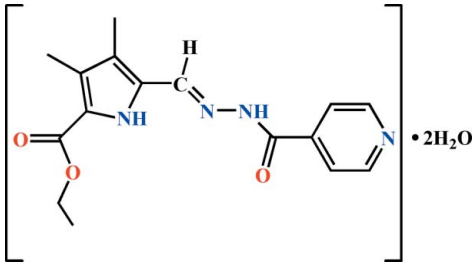
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.074; wR factor = 0.176; data-to-parameter ratio = 15.9.

In the title compound, $C_{16}H_{18}N_4O_3\cdot 2H_2O$, the dihedral angle between the pyrrole and pyridine rings in the hydrazone molecule is 7.12 (3)°. In the crystal structure, intermolecular N—H···O, O—H···N and O—H···O hydrogen bonds link the hydrazone and water molecules into double layers parallel to (101). The crystal packing exhibits weak π–π interactions between the pyrrole and pyridine rings of neighbouring hydrazone molecules [centroid–centroid distance = 3.777 (3) Å]. The crystal studied was a non-merohedral twin, the refined ratio of twin domains being 0.73 (3):0.27 (3).

Related literature

For the antioxidant and DNA-binding properties of hydrazone complexes, see: Liu & Yang (2009). For the synthesis and structure of 5-formyl-3,4-dimethyl-1*H*-pyrrole-2-carboxylate, see: Wu *et al.* (2009). For the similar structure of ethyl 5-[(3,4-dimethyl-1*H*-pyrrole-2-carboxylimino)-methyl]-3,4-dimethyl-1*H*-pyrrole-2-carboxylate monohydrate, see: Wang *et al.* (2009).



Experimental

Crystal data

$C_{16}H_{18}N_4O_3\cdot 2H_2O$
M_r = 350.38
Monoclinic, $P2_1/n$
a = 8.297 (4) Å
b = 18.120 (6) Å
c = 11.834 (4) Å
β = 91.814 (4)°
V = 1778.3 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.23 × 0.21 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.977, T_{max} = 0.984
10998 measured reflections
3839 independent reflections
2671 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.176
S = 1.02
3839 reflections
241 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1W^{i}	0.86	2.08	2.919 (4)	164
N4—H4A···O2W	0.86	2.24	3.084 (4)	165
O1W—H1C···N1	0.69 (5)	2.18 (5)	2.854 (4)	164 (6)
O1W—H1D···O2W^{ii}	0.91 (5)	1.88 (5)	2.790 (5)	174 (5)
O2W—H2C···O2^{iii}	0.92 (5)	2.06 (5)	2.941 (4)	160 (4)
O2W—H2D···O1	0.82 (5)	2.27 (5)	3.048 (4)	159 (5)
O2W—H2D···N3	0.82 (5)	2.43 (5)	3.014 (4)	129 (4)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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: CV5084).

References

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Wang, Y., Wu, W.-N., Zhao, R.-Q., Wang, Q.-F. & Qin, B.-F. (2009). *Z. Kristallogr. New Cryst. Struct.* **224**, 625–626.
Wu, W.-N., Wang, Y. & Wang, Q.-F. (2009). *Acta Cryst.* E**65**, o1661.

supporting information

Acta Cryst. (2011). E**67**, o1413 [doi:10.1107/S1600536811017132]

Ethyl 5-{[(*E*)-2-(isonicotinoyl)hydrazinylidene]methyl}-3,4-dimethyl-1*H*-pyrrole-2-carboxylate dihydrate

Zhao-Po Zhang, Yuan Wang, Ming-Jia Lu, Lei-Wei Jia and Hong-Chang Qiao

S1. Comment

In recent years, hydrazone complexes have received extensive attention due to their biological and pharmaceutical activities (Liu *et al.*, 2009). As a part of our studies of hydrazone ligands bearing pyrrole unit (Wang *et al.*, 2009), we present here the crystal structure of the title compound.

In the title compound (Fig. 1), the imine C=N double bond has an E configuration. The dihedral angle between pyrrole (N4/C8–C11, r.m.s. deviation 0.0030 Å) and pyridine rings (N1/C1–C5, r.m.s. deviation 0.0038 Å) in the hydrazone molecule is 7.12 (3)°. In the crystal structure, intermolecular N—H···O, O—H···N and O—H···O hydrogen bonds link the hydrazone and water molecules into doubled layers parallel to (101) plane. The crystal packing exhibits weak π–π interactions between the pyrrole and pyridine rings from the neighbouring hydrazone molecules [centroid-to-centroid distance of 3.777 (3) Å].

S2. Experimental

Isonicotinohydrazide (0.137 g, 1 mmol) and ethyl 5-formyl-3,4-dimethyl-1*H*-pyrrole-2-carboxylate (0.167 g, 1 mmol) (Wu *et al.*, 2009) was dissolved in an ethanol solution. The mixture was stirred for 4 h at room temperture. The resulting solution was left in air for a few days, yielding yellow prism-shaped crystals.

S3. Refinement

The water H atoms were located in a difference Fourier map and refined with U_{iso}(H)=1.5Ueq(O). Other H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and were thereafter treated as riding, with U_{iso}(H) values of 1.5Ueq(C) for methyl groups and 1.2Ueq(C,*N*) for others. The crystal studied was a twin.

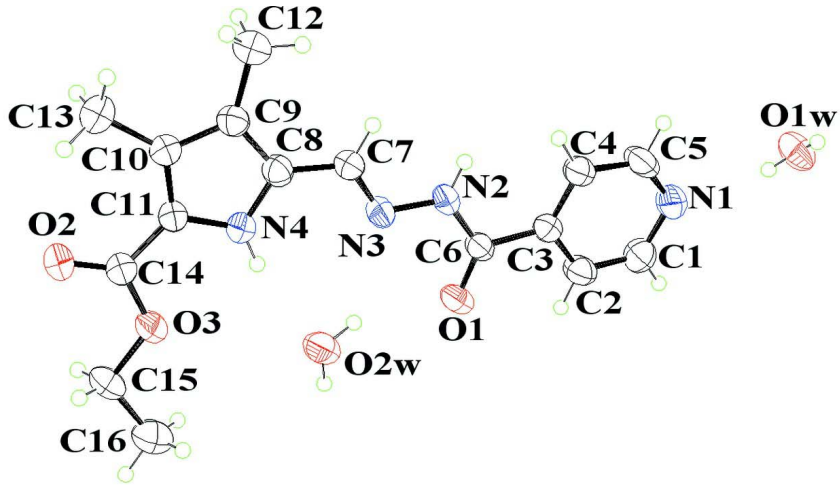

Figure 1

The title compound with the displacement ellipsoids shown at the 50% probability level.

Ethyl 5-{[(*E*)-2-(isonicotinoyl)hydrazinylidene]methyl}- 3,4-dimethyl-1*H*-pyrrole-2-carboxylate dihydrate

Crystal data

$C_{16}H_{18}N_4O_3\cdot 2H_2O$
$M_r = 350.38$
Monoclinic, $P2_1/n$
$a = 8.297$ (4) Å
$b = 18.120$ (6) Å
$c = 11.834$ (4) Å
$\beta = 91.814$ (4)°
$V = 1778.3$ (11) Å^3
$Z = 4$
$F(000) = 744$
$D_x = 1.309$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 2.7$–25.3°
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Prism, yellow
0.23 × 0.21 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.977$, $T_{max} = 0.984$
10998 measured reflections
3839 independent reflections
2671 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.1°$
$h = -10\rightarrow10$
$k = -9\rightarrow24$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.176$
$S = 1.02$
3839 reflections
241 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 3.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.069$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6319 (3)	0.46189 (12)	0.4160 (2)	0.0530 (6)
O2	1.1091 (4)	0.29040 (14)	0.9756 (2)	0.0660 (8)
O3	0.9696 (3)	0.27423 (12)	0.8122 (2)	0.0564 (7)
N1	0.4775 (4)	0.68078 (16)	0.1780 (2)	0.0532 (8)
N2	0.7766 (3)	0.55247 (14)	0.5019 (2)	0.0406 (6)
H2A	0.8043	0.5982	0.5024	0.049*
N3	0.8374 (3)	0.50452 (14)	0.5828 (2)	0.0420 (6)
N4	0.9761 (3)	0.41573 (14)	0.7584 (2)	0.0415 (6)
H4A	0.9158	0.3892	0.7141	0.050*
C1	0.4299 (4)	0.6106 (2)	0.1836 (3)	0.0545 (9)
H1	0.3507	0.5946	0.1319	0.065*
C2	0.4901 (4)	0.56074 (19)	0.2606 (3)	0.0498 (8)
H2	0.4522	0.5124	0.2604	0.060*
C3	0.6076 (4)	0.58255 (17)	0.3388 (3)	0.0385 (7)
C4	0.6579 (5)	0.65506 (18)	0.3348 (3)	0.0531 (9)
H4	0.7355	0.6730	0.3861	0.064*
C5	0.5898 (5)	0.70012 (19)	0.2527 (3)	0.0605 (10)
H5	0.6267	0.7485	0.2500	0.073*
C6	0.6727 (4)	0.52615 (16)	0.4219 (3)	0.0380 (7)
C7	0.9388 (4)	0.53192 (17)	0.6540 (3)	0.0418 (7)
H7A	0.9686	0.5811	0.6471	0.050*
C8	1.0084 (4)	0.48875 (17)	0.7448 (3)	0.0412 (7)
C9	1.1112 (4)	0.51125 (18)	0.8322 (3)	0.0428 (8)
C10	1.1406 (4)	0.44984 (18)	0.9021 (3)	0.0423 (7)
C11	1.0555 (4)	0.39167 (17)	0.8543 (3)	0.0411 (7)
C12	1.1778 (5)	0.5870 (2)	0.8501 (3)	0.0654 (11)
H12A	1.1754	0.6131	0.7795	0.098*
H12B	1.2870	0.5837	0.8789	0.098*
H12C	1.1137	0.6129	0.9033	0.098*
C13	1.2480 (5)	0.4481 (2)	1.0061 (3)	0.0589 (10)
H13A	1.1894	0.4654	1.0695	0.088*
H13B	1.3398	0.4792	0.9954	0.088*
H13C	1.2835	0.3984	1.0201	0.088*
C14	1.0502 (4)	0.31492 (18)	0.8893 (3)	0.0452 (8)
C15	0.9548 (5)	0.19650 (18)	0.8342 (3)	0.0609 (10)

H15A	0.8978	0.1883	0.9034	0.073*
H15B	1.0605	0.1738	0.8420	0.073*
C16	0.8642 (7)	0.1652 (2)	0.7371 (4)	0.0830 (15)
H16A	0.7623	0.1900	0.7281	0.125*
H16B	0.8461	0.1135	0.7498	0.125*
H16C	0.9247	0.1715	0.6700	0.125*
O1W	0.4291 (4)	0.80318 (15)	0.0290 (3)	0.0654 (8)
H1C	0.428 (7)	0.770 (3)	0.059 (5)	0.098*
H1D	0.528 (6)	0.813 (3)	0.001 (4)	0.098*
O2W	0.7783 (3)	0.34071 (15)	0.5656 (2)	0.0588 (7)
H2C	0.704 (6)	0.305 (3)	0.544 (4)	0.088*
H2D	0.744 (6)	0.380 (3)	0.541 (4)	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0688 (16)	0.0297 (12)	0.0598 (15)	−0.0029 (11)	−0.0066 (12)	0.0035 (10)
O2	0.102 (2)	0.0431 (14)	0.0513 (15)	0.0040 (14)	−0.0203 (15)	0.0099 (12)
O3	0.0790 (18)	0.0327 (12)	0.0562 (15)	−0.0080 (12)	−0.0160 (13)	0.0066 (11)
N1	0.0622 (19)	0.0453 (17)	0.0512 (18)	0.0079 (14)	−0.0106 (15)	0.0081 (14)
N2	0.0489 (15)	0.0314 (13)	0.0412 (15)	0.0009 (11)	−0.0045 (12)	0.0071 (11)
N3	0.0514 (16)	0.0334 (14)	0.0412 (15)	0.0061 (12)	0.0007 (12)	0.0060 (11)
N4	0.0479 (15)	0.0373 (14)	0.0388 (14)	−0.0002 (12)	−0.0063 (12)	0.0009 (11)
C1	0.055 (2)	0.056 (2)	0.051 (2)	−0.0028 (17)	−0.0150 (17)	0.0018 (17)
C2	0.053 (2)	0.0374 (18)	0.058 (2)	−0.0064 (15)	−0.0077 (17)	0.0021 (16)
C3	0.0430 (17)	0.0327 (16)	0.0396 (17)	0.0022 (13)	0.0000 (13)	−0.0006 (13)
C4	0.069 (2)	0.0373 (18)	0.052 (2)	−0.0048 (16)	−0.0192 (18)	0.0029 (15)
C5	0.079 (3)	0.0298 (18)	0.072 (3)	−0.0034 (17)	−0.017 (2)	0.0099 (17)
C6	0.0437 (17)	0.0295 (16)	0.0410 (17)	0.0023 (13)	0.0040 (14)	0.0027 (13)
C7	0.0525 (19)	0.0333 (16)	0.0396 (17)	0.0013 (14)	0.0019 (15)	0.0003 (13)
C8	0.0459 (18)	0.0379 (17)	0.0399 (17)	0.0056 (14)	0.0024 (14)	0.0016 (14)
C9	0.0515 (19)	0.0367 (17)	0.0404 (17)	0.0011 (14)	0.0029 (15)	−0.0014 (13)
C10	0.0501 (19)	0.0384 (17)	0.0383 (17)	0.0027 (14)	−0.0022 (14)	−0.0018 (14)
C11	0.0502 (18)	0.0368 (17)	0.0359 (16)	0.0040 (14)	−0.0030 (14)	0.0018 (13)
C12	0.092 (3)	0.042 (2)	0.061 (2)	−0.008 (2)	−0.011 (2)	0.0002 (18)
C13	0.072 (3)	0.056 (2)	0.047 (2)	0.0001 (19)	−0.0138 (18)	−0.0002 (17)
C14	0.057 (2)	0.0384 (18)	0.0404 (18)	0.0043 (15)	−0.0020 (15)	0.0007 (14)
C15	0.086 (3)	0.0304 (18)	0.065 (2)	−0.0057 (18)	−0.004 (2)	0.0070 (16)
C16	0.118 (4)	0.043 (2)	0.086 (3)	−0.005 (2)	−0.025 (3)	−0.005 (2)
O1W	0.0706 (18)	0.0443 (16)	0.081 (2)	0.0111 (14)	−0.0049 (16)	0.0186 (14)
O2W	0.0681 (18)	0.0384 (14)	0.0692 (18)	0.0038 (12)	−0.0093 (14)	−0.0031 (13)

Geometric parameters (Å, º)

O1—C6	1.214 (4)	C7—H7A	0.9300
O2—C14	1.204 (4)	C8—C9	1.382 (5)
O3—C14	1.336 (4)	C9—C10	1.403 (4)
O3—C15	1.438 (4)	C9—C12	1.492 (5)

N1—C5	1.312 (5)	C10—C11	1.380 (4)
N1—C1	1.334 (5)	C10—C13	1.497 (5)
N2—C6	1.347 (4)	C11—C14	1.452 (4)
N2—N3	1.377 (3)	C12—H12A	0.9600
N2—H2A	0.8600	C12—H12B	0.9600
N3—C7	1.273 (4)	C12—H12C	0.9600
N4—C8	1.361 (4)	C13—H13A	0.9600
N4—C11	1.366 (4)	C13—H13B	0.9600
N4—H4A	0.8600	C13—H13C	0.9600
C1—C2	1.366 (5)	C15—C16	1.468 (5)
C1—H1	0.9300	C15—H15A	0.9700
C2—C3	1.380 (4)	C15—H15B	0.9700
C2—H2	0.9300	C16—H16A	0.9600
C3—C4	1.380 (4)	C16—H16B	0.9600
C3—C6	1.506 (4)	C16—H16C	0.9600
C4—C5	1.376 (5)	O1W—H1C	0.69 (5)
C4—H4	0.9300	O1W—H1D	0.91 (5)
C5—H5	0.9300	O2W—H2C	0.92 (5)
C7—C8	1.435 (4)	O2W—H2D	0.82 (5)

C14—O3—C15	117.4 (3)	C11—C10—C9	106.7 (3)
C5—N1—C1	115.2 (3)	C11—C10—C13	127.2 (3)
C6—N2—N3	118.5 (3)	C9—C10—C13	126.1 (3)
C6—N2—H2A	120.7	N4—C11—C10	108.9 (3)
N3—N2—H2A	120.7	N4—C11—C14	121.6 (3)
C7—N3—N2	115.7 (3)	C10—C11—C14	129.4 (3)
C8—N4—C11	108.5 (3)	C9—C12—H12A	109.5
C8—N4—H4A	125.8	C9—C12—H12B	109.5
C11—N4—H4A	125.8	H12A—C12—H12B	109.5
N1—C1—C2	124.1 (3)	C9—C12—H12C	109.5
N1—C1—H1	117.9	H12A—C12—H12C	109.5
C2—C1—H1	117.9	H12B—C12—H12C	109.5
C1—C2—C3	119.6 (3)	C10—C13—H13A	109.5
C1—C2—H2	120.2	C10—C13—H13B	109.5
C3—C2—H2	120.2	H13A—C13—H13B	109.5
C4—C3—C2	117.2 (3)	C10—C13—H13C	109.5
C4—C3—C6	124.5 (3)	H13A—C13—H13C	109.5
C2—C3—C6	118.3 (3)	H13B—C13—H13C	109.5
C3—C4—C5	118.1 (3)	O2—C14—O3	123.9 (3)
C3—C4—H4	120.9	O2—C14—C11	125.5 (3)
C5—C4—H4	120.9	O3—C14—C11	110.7 (3)
N1—C5—C4	125.7 (3)	O3—C15—C16	106.3 (3)
N1—C5—H5	117.1	O3—C15—H15A	110.5
C4—C5—H5	117.1	C16—C15—H15A	110.5
O1—C6—N2	123.4 (3)	O3—C15—H15B	110.5
O1—C6—C3	121.3 (3)	C16—C15—H15B	110.5
N2—C6—C3	115.3 (3)	H15A—C15—H15B	108.7
N3—C7—C8	121.7 (3)	C15—C16—H16A	109.5

N3—C7—H7A	119.2	C15—C16—H16B	109.5
C8—C7—H7A	119.2	H16A—C16—H16B	109.5
N4—C8—C9	108.5 (3)	C15—C16—H16C	109.5
N4—C8—C7	122.9 (3)	H16A—C16—H16C	109.5
C9—C8—C7	128.6 (3)	H16B—C16—H16C	109.5
C8—C9—C10	107.4 (3)	H1C—O1W—H1D	112 (5)
C8—C9—C12	126.5 (3)	H2C—O2W—H2D	107 (4)
C10—C9—C12	126.1 (3)		

C6—N2—N3—C7	177.9 (3)	C7—C8—C9—C10	177.6 (3)
C5—N1—C1—C2	0.3 (6)	N4—C8—C9—C12	179.8 (3)
N1—C1—C2—C3	0.1 (6)	C7—C8—C9—C12	−1.8 (6)
C1—C2—C3—C4	0.3 (5)	C8—C9—C10—C11	0.4 (4)
C1—C2—C3—C6	−179.4 (3)	C12—C9—C10—C11	179.9 (3)
C2—C3—C4—C5	−1.0 (5)	C8—C9—C10—C13	178.8 (3)
C6—C3—C4—C5	178.7 (3)	C12—C9—C10—C13	−1.8 (6)
C1—N1—C5—C4	−1.1 (6)	C8—N4—C11—C10	−0.5 (4)
C3—C4—C5—N1	1.5 (7)	C8—N4—C11—C14	−177.4 (3)
N3—N2—C6—O1	−1.4 (5)	C9—C10—C11—N4	0.0 (4)
N3—N2—C6—C3	178.1 (3)	C13—C10—C11—N4	−178.3 (3)
C4—C3—C6—O1	−174.7 (3)	C9—C10—C11—C14	176.6 (3)
C2—C3—C6—O1	5.0 (5)	C13—C10—C11—C14	−1.7 (6)
C4—C3—C6—N2	5.8 (5)	C15—O3—C14—O2	−0.7 (5)
C2—C3—C6—N2	−174.5 (3)	C15—O3—C14—C11	179.5 (3)
N2—N3—C7—C8	178.2 (3)	N4—C11—C14—O2	−175.6 (3)
C11—N4—C8—C9	0.8 (4)	C10—C11—C14—O2	8.2 (6)
C11—N4—C8—C7	−177.7 (3)	N4—C11—C14—O3	4.3 (5)
N3—C7—C8—N4	2.6 (5)	C10—C11—C14—O3	−172.0 (3)
N3—C7—C8—C9	−175.5 (3)	C14—O3—C15—C16	−179.3 (4)
N4—C8—C9—C10	−0.8 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1*W*^{i}	0.86	2.08	2.919 (4)	164
N4—H4*A*···O2*W*	0.86	2.24	3.084 (4)	165
O1*W*—H1*C*···N1	0.69 (5)	2.18 (5)	2.854 (4)	164 (6)
O1*W*—H1*D*···O2*W*^{ii}	0.91 (5)	1.88 (5)	2.790 (5)	174 (5)
O2*W*—H2*C*···O2^{iii}	0.92 (5)	2.06 (5)	2.941 (4)	160 (4)
O2*W*—H2*D*···O1	0.82 (5)	2.27 (5)	3.048 (4)	159 (5)
O2*W*—H2*D*···N3	0.82 (5)	2.43 (5)	3.014 (4)	129 (4)

Symmetry codes: (i) *x*+1/2, −*y*+3/2, *z*+1/2; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iii) *x*−1/2, −*y*+1/2, *z*−1/2.