Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 2-(quinolin-8-yloxy)acetate monohydrate

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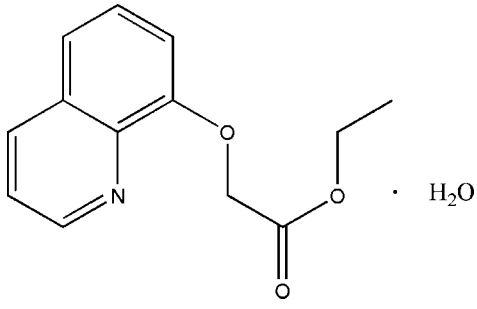
Received 16 March 2013; accepted 24 March 2013

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.123; data-to-parameter ratio = 14.4.

In the title compound, $C_{13}H_{13}NO_3\cdot H_2O$, the dihedral angle between the ethyl ester group [C—C—O—C(=O); maximum deviation = 0.003 (2) Å] and the quinoline ring system is 7.94 (12)°. The water solvent molecule is linked to the title molecule *via* O—H···O and O—H···N hydrogen bonds. In the crystal, molecules are linked by C—H···O hydrogen bonds, forming chains propagating along [100].

Related literature

For related structures see: Sarveswari *et al.* (2010); Ukrainets *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{13}NO_3\cdot H_2O$
M_r = 249.26
Monoclinic, $P2_1/n$
a = 6.9562 (4) Å
b = 17.5050 (9) Å
c = 10.5304 (6) Å
β = 100.124 (5)°
V = 1262.30 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.3 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.715, T_{max} = 1.000
9808 measured reflections
2478 independent reflections
1448 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.123
S = 1.02
2478 reflections
172 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O5	0.85 (3)	2.06 (3)	2.907 (3)	172
O1W—H2W···N16	0.92 (3)	1.96 (3)	2.875 (3)	174
C6—H6A···O1W^{i}	0.97	2.43	3.388 (3)	170

Symmetry code: (i) $x-1, y, z$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

MK acknowledges the help of Bahubali College of Engineering, Shravanabelagola, for his research work. RK acknowledges the Department of Science & Technology for the single-crystal X-ray diffractometer sanctioned as a National Facility under project No. SR/S2/CMP-47/2003.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2575).

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supplementary materials

Acta Cryst. (2013). E**69**, o623 [doi:10.1107/S1600536813008106]

Ethyl 2-(quinolin-8-yloxy)acetate monohydrate

Mohan Kumar, C. Mallikarjunaswamy, M. A. Sridhar, D. G. Bhadregowda, Kamini Kapoor, Vivek K. Gupta and Rajni Kant

Comment

In the title molecule, Fig. 1, the bond lengths (Allen *et al.*, 1987) and angles have normal values and are comparable with those reported for similar structures (Sarveswari *et al.*, 2010; Ukrainets *et al.*, 2009). The dihedral angle between the ethyl ester group (C1/C2/O3/C4/O5) and the quinoline (C8—C15/N16/C17) ring system is 7.94 (12)°. The solvent water molecule is linked to the title molecule via O-H···O and O-H···N hydrogen bonds (Fig. 1 and Table 1).

In the crystal, molecules are linked by C—H···O hydrogen bonds (Table 1) forming chains propagating along the a axis direction (Fig. 2).

Experimental

A mixture of 8-hydroxy quinoline(0.01 mol) and ethyl chloroacetate (0.015 mol) in the presence of dry acetone (50 ml) and anhydrous potassium carbonate (0.015 mol) was refluxed for 8 h. The residual mass was triturated with cold water to remove potassium carbonate and extracted with ether (30 ml). The ether layer was washed with 10% sodium hydroxide solution (350 ml) followed by water (330 ml) and then dried over anhydrous sodium sulfate and evaporated to dryness. The compound was purified by successive recrystallizations from ethanol yielding colourless block-like crystals (Yield 90%, m.p. 350–352 K).

Refinement

The water molecule H atoms were located in a difference Fourier map and freely refined. The C-bound H atoms were positioned geometrically and treated as riding atoms: C—H distances of 0.93–0.97 Å with U_{iso}(H) = 1.5U_{eq}(methyl C) and = 1.2U_{eq}(C) for other H atoms.

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

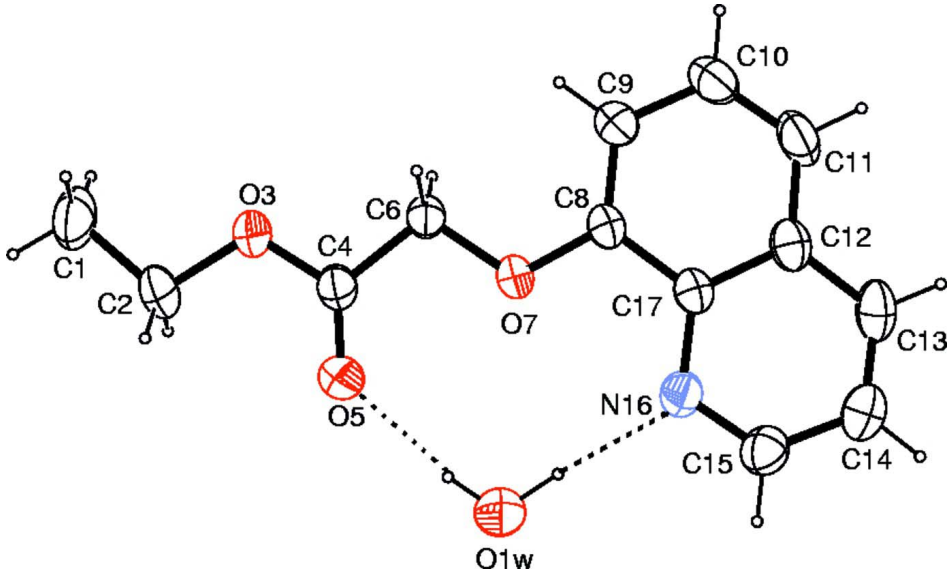

Figure 1

A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 40% probability level. The O-H···O and O-H···N hydrogen bonds are shown as dashed lines (see Table for details).

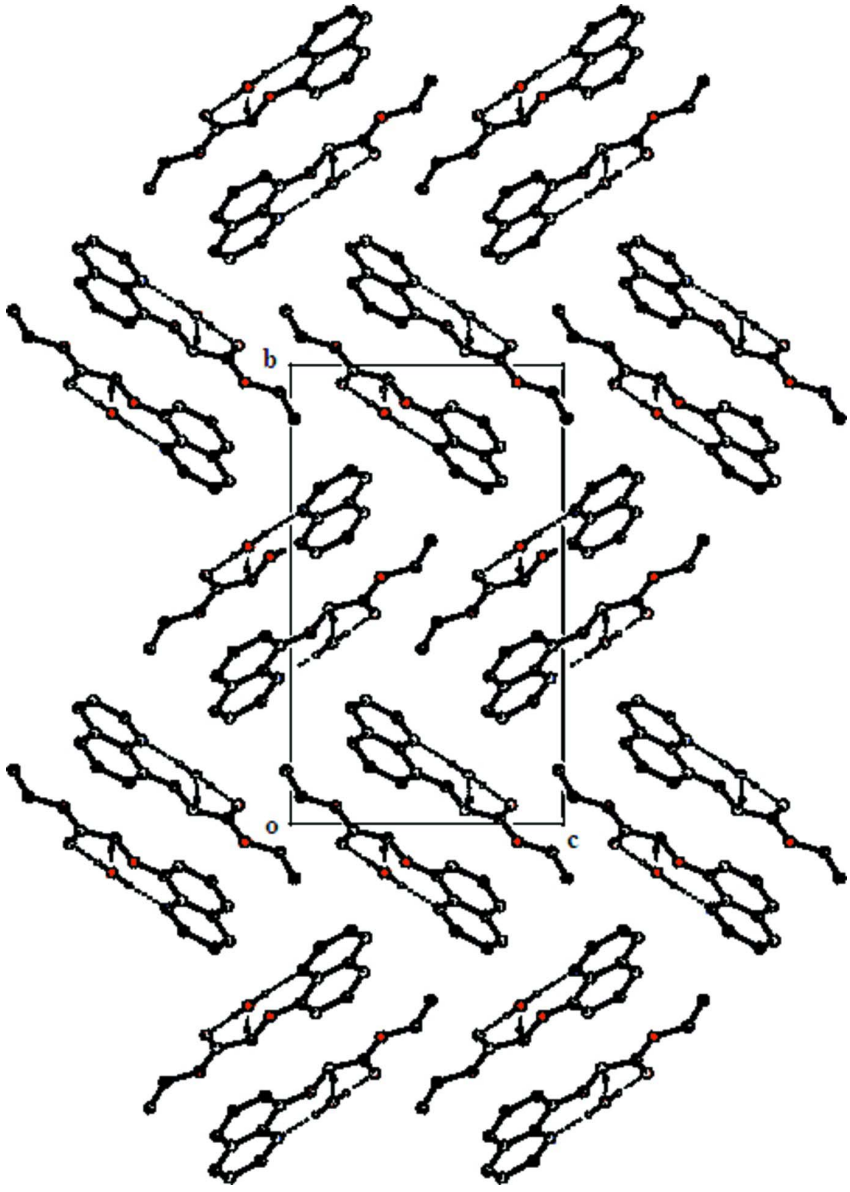

Figure 2

The crystal packing of the title compound view along the *a* axis, showing the O—H···O, O—H···N and C-H···O hydrogen bonds as dashed lines (see Table 1 for details).

Ethyl 2-(quinolin-8-yloxy)acetate monohydrate

Crystal data

$C_{13}H_{13}NO_3·H_2O$
M_r = 249.26
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 6.9562 (4) Å
b = 17.5050 (9) Å
c = 10.5304 (6) Å
β = 100.124 (5)°
V = 1262.30 (12) Å^3
Z = 4
F(000) = 528
D_x = 1.312 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3127 reflections
θ = 3.5–29.0°
μ = 0.10 mm^{-1}

T = 293 K
Block, colourless

0.3 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.715, T_{max} = 1.000

9808 measured reflections
2478 independent reflections
1448 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 26.0°, θ_{min} = 3.5°
h = −8→8
k = −21→21
l = −11→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.123
S = 1.02
2478 reflections
172 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
$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 0.1537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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	0.1064 (4)	−0.11734 (16)	−0.0152 (2)	0.0746 (9)
H1A	0.1136	−0.1608	0.0410	0.112*
H1B	0.1291	−0.1334	−0.0985	0.112*
H1C	−0.0208	−0.0946	−0.0237	0.112*
C2	0.2574 (4)	−0.06026 (15)	0.0399 (2)	0.0605 (7)
H2A	0.3868	−0.0825	0.0481	0.073*
H2B	0.2511	−0.0160	−0.0160	0.073*
O3	0.2179 (2)	−0.03807 (9)	0.16644 (14)	0.0527 (5)
C4	0.3381 (3)	0.01324 (13)	0.2305 (2)	0.0431 (6)
O5	0.4722 (3)	0.04156 (11)	0.19103 (16)	0.0671 (6)
C6	0.2763 (3)	0.03087 (12)	0.35690 (19)	0.0407 (6)
H6A	0.1472	0.0537	0.3421	0.049*
H6B	0.2717	−0.0157	0.4062	0.049*

O7	0.4143 (2)	0.08241 (8)	0.42563 (13)	0.0440 (4)
C8	0.3737 (3)	0.11137 (12)	0.5390 (2)	0.0374 (5)
C9	0.2176 (3)	0.09077 (14)	0.5928 (2)	0.0501 (6)
H9	0.1299	0.0544	0.5529	0.060*
C10	0.1893 (4)	0.12463 (16)	0.7087 (2)	0.0628 (7)
H10	0.0824	0.1100	0.7451	0.075*
C11	0.3136 (4)	0.17809 (16)	0.7690 (2)	0.0630 (8)
H11	0.2902	0.2006	0.8449	0.076*
C12	0.4787 (4)	0.19961 (13)	0.7166 (2)	0.0471 (6)
C13	0.6180 (4)	0.25321 (14)	0.7755 (2)	0.0595 (7)
H13	0.6003	0.2777	0.8510	0.071*
C14	0.7760 (4)	0.26897 (14)	0.7230 (2)	0.0582 (7)
H14	0.8698	0.3035	0.7620	0.070*
C15	0.7960 (4)	0.23238 (13)	0.6085 (2)	0.0538 (7)
H15	0.9056	0.2441	0.5728	0.065*
N16	0.6718 (3)	0.18260 (11)	0.54715 (17)	0.0466 (5)
C17	0.5122 (3)	0.16581 (12)	0.6004 (2)	0.0383 (5)
O1W	0.8236 (3)	0.10488 (13)	0.3454 (2)	0.0723 (6)
H2W	0.770 (5)	0.1318 (18)	0.406 (3)	0.123 (14)*
H1W	0.728 (5)	0.0844 (18)	0.295 (3)	0.109 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.099 (2)	0.0701 (19)	0.0512 (16)	−0.0165 (17)	0.0026 (16)	−0.0184 (14)
C2	0.0763 (19)	0.0683 (18)	0.0396 (14)	−0.0050 (15)	0.0171 (13)	−0.0153 (13)
O3	0.0602 (11)	0.0590 (11)	0.0403 (9)	−0.0135 (9)	0.0124 (8)	−0.0143 (8)
C4	0.0463 (14)	0.0449 (14)	0.0378 (13)	0.0001 (12)	0.0067 (11)	−0.0053 (11)
O5	0.0646 (12)	0.0882 (14)	0.0534 (11)	−0.0269 (11)	0.0243 (9)	−0.0198 (10)
C6	0.0409 (13)	0.0417 (13)	0.0394 (12)	−0.0017 (10)	0.0065 (10)	−0.0068 (10)
O7	0.0484 (9)	0.0490 (10)	0.0359 (8)	−0.0061 (8)	0.0110 (7)	−0.0102 (7)
C8	0.0442 (13)	0.0353 (12)	0.0327 (12)	0.0049 (10)	0.0067 (10)	−0.0018 (10)
C9	0.0499 (15)	0.0598 (17)	0.0424 (14)	−0.0055 (13)	0.0129 (12)	−0.0047 (12)
C10	0.0585 (17)	0.083 (2)	0.0517 (16)	−0.0014 (15)	0.0234 (13)	−0.0074 (15)
C11	0.0686 (18)	0.079 (2)	0.0443 (15)	0.0070 (16)	0.0184 (14)	−0.0182 (14)
C12	0.0577 (15)	0.0410 (14)	0.0413 (13)	0.0083 (12)	0.0054 (12)	−0.0041 (11)
C13	0.0715 (19)	0.0504 (16)	0.0531 (15)	0.0103 (14)	0.0015 (14)	−0.0194 (13)
C14	0.0637 (18)	0.0478 (16)	0.0590 (17)	−0.0028 (13)	−0.0003 (14)	−0.0094 (13)
C15	0.0588 (16)	0.0491 (15)	0.0524 (15)	−0.0068 (13)	0.0073 (13)	0.0025 (13)
N16	0.0512 (12)	0.0438 (12)	0.0446 (11)	−0.0055 (10)	0.0079 (10)	−0.0040 (9)
C17	0.0450 (13)	0.0358 (13)	0.0335 (12)	0.0054 (11)	0.0051 (10)	0.0010 (10)
O1W	0.0525 (12)	0.0896 (16)	0.0786 (15)	−0.0139 (11)	0.0217 (11)	−0.0260 (13)

Geometric parameters (Å, º)

C1—C2	1.492 (3)	C9—H9	0.9300
C1—H1A	0.9600	C10—C11	1.354 (3)
C1—H1B	0.9600	C10—H10	0.9300
C1—H1C	0.9600	C11—C12	1.410 (3)
C2—O3	1.460 (3)	C11—H11	0.9300

C2—H2A	0.9700	C12—C13	1.412 (3)
C2—H2B	0.9700	C12—C17	1.414 (3)
O3—C4	1.328 (2)	C13—C14	1.344 (3)
C4—O5	1.194 (3)	C13—H13	0.9300
C4—C6	1.501 (3)	C14—C15	1.393 (3)
C6—O7	1.420 (2)	C14—H14	0.9300
C6—H6A	0.9700	C15—N16	1.314 (3)
C6—H6B	0.9700	C15—H15	0.9300
O7—C8	1.371 (2)	N16—C17	1.361 (3)
C8—C9	1.359 (3)	O1W—H2W	0.93 (4)
C8—C17	1.427 (3)	O1W—H1W	0.85 (4)
C9—C10	1.401 (3)		

C2—C1—H1A	109.5	C8—C9—C10	119.7 (2)
C2—C1—H1B	109.5	C8—C9—H9	120.1
H1A—C1—H1B	109.5	C10—C9—H9	120.1
C2—C1—H1C	109.5	C11—C10—C9	121.7 (2)
H1A—C1—H1C	109.5	C11—C10—H10	119.2
H1B—C1—H1C	109.5	C9—C10—H10	119.2
O3—C2—C1	107.5 (2)	C10—C11—C12	119.9 (2)
O3—C2—H2A	110.2	C10—C11—H11	120.1
C1—C2—H2A	110.2	C12—C11—H11	120.1
O3—C2—H2B	110.2	C11—C12—C13	123.3 (2)
C1—C2—H2B	110.2	C11—C12—C17	119.8 (2)
H2A—C2—H2B	108.5	C13—C12—C17	117.0 (2)
C4—O3—C2	116.17 (19)	C14—C13—C12	120.2 (2)
O5—C4—O3	124.4 (2)	C14—C13—H13	119.9
O5—C4—C6	125.9 (2)	C12—C13—H13	119.9
O3—C4—C6	109.7 (2)	C13—C14—C15	118.4 (2)
O7—C6—C4	108.00 (18)	C13—C14—H14	120.8
O7—C6—H6A	110.1	C15—C14—H14	120.8
C4—C6—H6A	110.1	N16—C15—C14	125.0 (3)
O7—C6—H6B	110.1	N16—C15—H15	117.5
C4—C6—H6B	110.1	C14—C15—H15	117.5
H6A—C6—H6B	108.4	C15—N16—C17	117.0 (2)
C8—O7—C6	117.01 (17)	N16—C17—C12	122.4 (2)
C9—C8—O7	124.6 (2)	N16—C17—C8	119.47 (19)
C9—C8—C17	120.9 (2)	C12—C17—C8	118.1 (2)
O7—C8—C17	114.56 (19)	H2W—O1W—H1W	107 (3)

C1—C2—O3—C4	−179.6 (2)	C17—C12—C13—C14	−1.4 (3)
C2—O3—C4—O5	0.3 (3)	C12—C13—C14—C15	1.2 (4)
C2—O3—C4—C6	179.04 (19)	C13—C14—C15—N16	−0.4 (4)
O5—C4—C6—O7	−4.6 (3)	C14—C15—N16—C17	−0.1 (3)
O3—C4—C6—O7	176.69 (16)	C15—N16—C17—C12	−0.1 (3)
C4—C6—O7—C8	173.95 (17)	C15—N16—C17—C8	−179.14 (19)
C6—O7—C8—C9	4.0 (3)	C11—C12—C17—N16	−178.0 (2)
C6—O7—C8—C17	−176.90 (17)	C13—C12—C17—N16	0.9 (3)
O7—C8—C9—C10	−179.4 (2)	C11—C12—C17—C8	1.0 (3)

C17—C8—C9—C10	1.5 (3)	C13—C12—C17—C8	179.91 (19)
C8—C9—C10—C11	0.3 (4)	C9—C8—C17—N16	177.0 (2)
C9—C10—C11—C12	−1.4 (4)	O7—C8—C17—N16	−2.2 (3)
C10—C11—C12—C13	−178.1 (2)	C9—C8—C17—C12	−2.1 (3)
C10—C11—C12—C17	0.7 (4)	O7—C8—C17—C12	178.72 (18)
C11—C12—C13—C14	177.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O5	0.85 (3)	2.06 (3)	2.907 (3)	172
O1*W*—H2*W*···N16	0.92 (3)	1.96 (3)	2.875 (3)	174
C6—H6*A*···O1*W*^{i}	0.97	2.43	3.388 (3)	170

Symmetry code: (i) *x*−1, *y*, *z*.