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1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthracene-9,10-dione monohydrate

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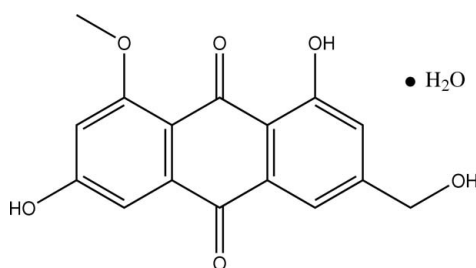
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.055; wR factor = 0.099; data-to-parameter ratio = 11.6.

The title compound, $\text{C}_{16}\text{H}_{12}\text{O}_6 \cdot \text{H}_2\text{O}$, isolated from the halotolerant fungus *Aspergillus varicolor* B-17, is also known as questinol monohydrate. In the crystal structure, $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds link the molecules, forming a three-dimensional network. $\pi-\pi$ stacking interactions consolidate the supramolecular structure [the shortest interplanar distances are 3.456 (3), 3.366 (4) and 3.382 (4) Å].

Related literature

For general background, see: Stickings & Mahmoodian (1962); Slater *et al.* (1971); Kimura *et al.* (1983); Arai *et al.* (1989); Nielsen *et al.* (2004); Wang *et al.* (2007).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{12}\text{O}_6 \cdot \text{H}_2\text{O}$
 $M_r = 318.27$
 Monoclinic, $P2_1/c$
 $a = 11.3317$ (11) Å
 $b = 16.7515$ (19) Å
 $c = 7.2193$ (9) Å
 $\beta = 95.453$ (2)°

$V = 1364.2$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.12$ mm⁻¹
 $T = 298$ (2) K
 $0.18 \times 0.14 \times 0.05$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.978$, $T_{\max} = 0.994$
 7003 measured reflections
 2404 independent reflections
 1108 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.090$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.099$
 $S = 1.01$
 2404 reflections
 208 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1}-\text{H1} \cdots \text{O6}$	0.82	1.82	2.525 (3)	144
$\text{O2}-\text{H2} \cdots \text{O5}^i$	0.82	2.38	2.945 (3)	127
$\text{O2}-\text{H2} \cdots \text{O6}^i$	0.82	2.16	2.919 (3)	154
$\text{O4}-\text{H4} \cdots \text{O7}^{ii}$	0.82	1.85	2.665 (3)	170
$\text{O7}-\text{H7A} \cdots \text{O1}$	0.85	2.03	2.878 (3)	176
$\text{O7}-\text{H7B} \cdots \text{O2}^{iii}$	0.85	1.94	2.771 (3)	165

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP (Siemens, 1994) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2051).

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supporting information

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1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthracene-9,10-dione monohydrate**Wen-Liang Wang, Wei Sun, Qian-Qun Gu and Wei-Ming Zhu****S1. Comment**

Questinol was first isolated from the metabolites of *Penicillium frequentans* (Stickings & Mahmoodian, 1962). This compound and related derivatives arise from their biological activities (Slater et al., 1971; Kimura et al., 1983; Arai et al., 1989; Nielsen et al., 2004). We isolated the title compound (I) as a part of our ongoing study characterizing bioactive metabolites from various halotolerant microorganism (Wang et al., 2007). This was the first report about the X-ray crystallographic study of the title compound.

As shown in Fig. 1, crystal water connected with questinol by a O—H $\cdots$ O hydrogen bond. There is an intramolecular hydrogen bond between a hydroxyl O1 and carbonyl oxygen atom O6. The three six-membered rings adopt a planar conformation with the maximum deviation being 0.070 (3) Å (for atom C13).

In the crystal structure, O—H $\cdots$ O hydrogen bonds (Table 1, Fig. 2) link the molecules to form a three-dimensional network. A supramolecular structure is consolidated by three types (Symmetry codes: (iii) x, 3/2-y, z-1/2; (iv) X, 3/2-Y, z+1/2; (v) 2-X, 1-Y, 2-Z) of π - π stacking interactions (Fig. 3). The shortest interplanar distances for these π - π stacking interactions are 3.456 (3) Å, 3.366 (4) Å and 3.382 (4) Å, respectively.

S2. Experimental

The isolated halotolerant fungal strain *Aspergillus varicolor* B-17, was isolated from the sediments collected in Jilantai salt field, Alashan, Inner Mongolia, China. The working strain was cultured under static conditions at 303 K for 45 days in thirty 1000-ml conical flasks containing the liquid medium (300 ml/flask) composed of maltose (20 g/L), mannitol (20 g/L), glucose (10 g/L), monosodium glutamate (10 g/L), NH₄Cl (10 g/L), MgSO₄ (10 g/L), yeast extract paste (3 g/L), maize paste (3 g/L), NaCl (120 g/L) and KCl (5 g/L) after adjusting its pH to 7.0. The fermented whole broth (9 liters) was filtered through cheese cloth to separate into supernatant and mycelia. The mycelia was extracted three times with acetone and the acetone solution was concentrated under reduced pressure to afford crude extract (7.8 g). The crude extract, which was subjected to chromatography over silica gel column using a stepwise gradient elution of CHCl₃—MeOH, to yield four fractions (Fr.1-Fr.4). Fr.3 was subjected to chromatographing on a silica gel column eluting with CHCl₃—MeOH (93:7), to afford sixteen subfractions (Fr.3-1-Fr.3-16). The title compound (9 mg) was purified by extensive preparative HPLC using MeOH-H₂O from Fr.3-3 and Fr.3-4. The single crystals were obtained by slow evaporation of CHCl₃—MeOH (1:1) solution at 299 K.

S3. Refinement

Water H atoms were found in a difference Fourier map and were treated as riding, with fixed $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93–0.97 (C—H) and 0.82 Å (O—H), and with $U_{\text{iso}}(\text{H})$ values of $1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{C}_{\text{methyl}}, \text{O}_{\text{hydroxyl}})$.

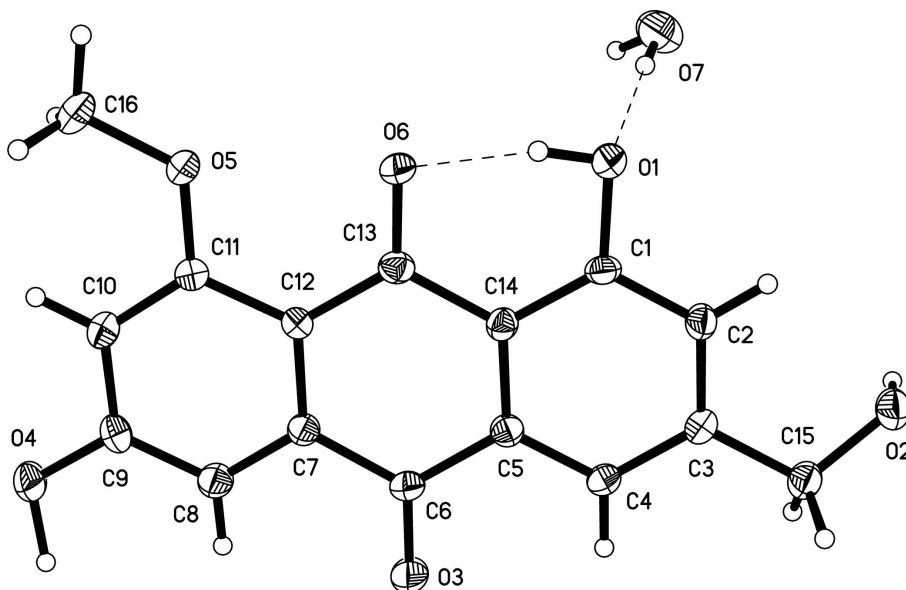
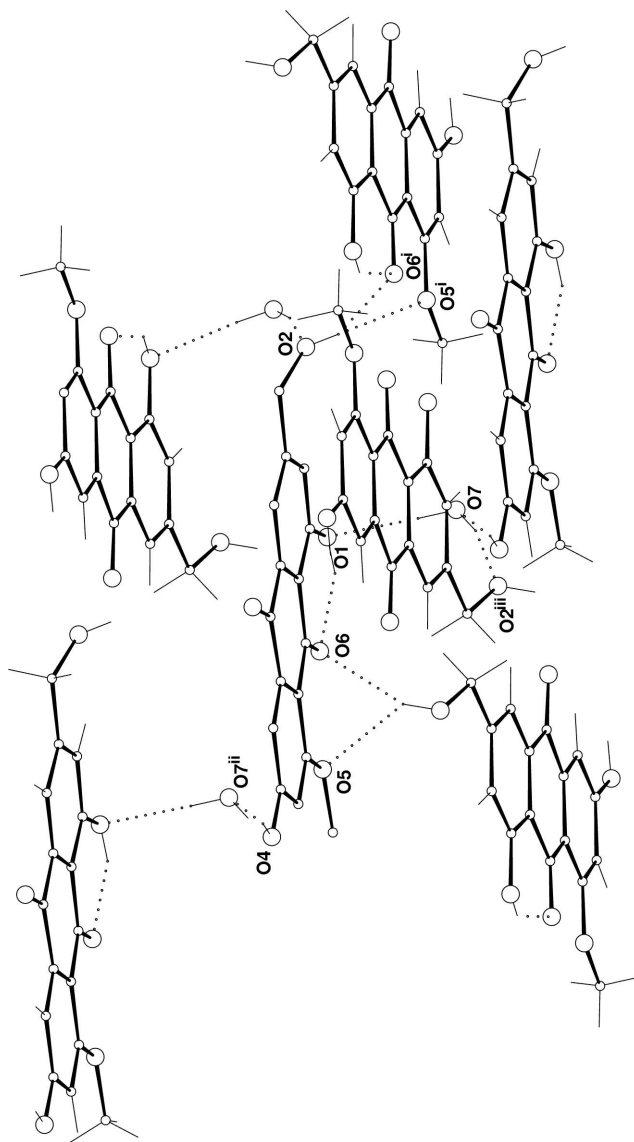


Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering but for non-H atoms. Dashed lines indicate hydrogen bonds.

**Figure 2**

The packing diagram for (I). The H-bonds are shown as dotted lines; H atoms not involved in hydrogen bonding were omitted for clarity. [Symmetry codes: (i) $1 - x, 1/2 + y, 3/2 - z$; (ii) $1 + x, y, z$; (iii) $x, 3/2 - y, z - 1/2$.]

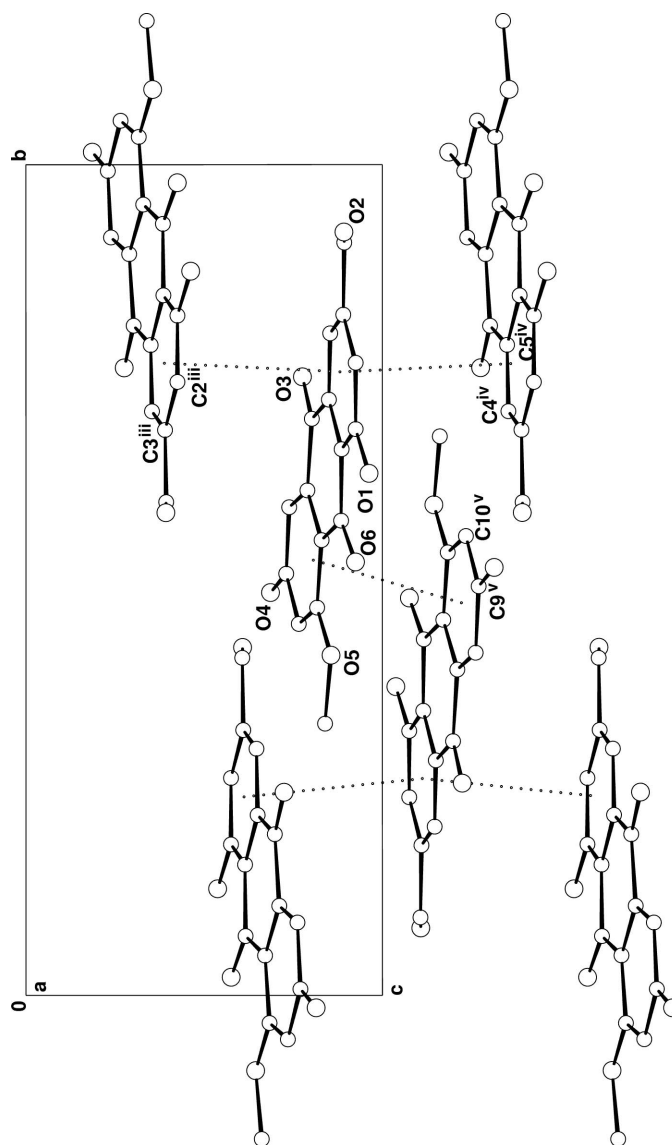


Figure 3

A view showing the π - π stacking interactions, viewed down the a axis. H atoms and H_2O molecules have been omitted for clarity. [Symmetry codes: (iii) $x, 3/2 - y, z - 1/2$; (iv) $x, 3/2 - y, z + 1/2$; (v) $2 - x, 1 - y, 2 - z$.]

1,6-Dihydroxy-3-hydroxymethyl-8-methoxyanthracene-9,10-dione monohydrate

Crystal data

$\text{C}_{16}\text{H}_{12}\text{O}_6 \cdot \text{H}_2\text{O}$

$M_r = 318.27$

Monoclinic, $P2_1/c$

Hall symbol: $-P2_1/c$

$a = 11.3317(11) \text{ \AA}$

$b = 16.7515(19) \text{ \AA}$

$c = 7.2193(9) \text{ \AA}$

$\beta = 95.453(2)^\circ$

$V = 1364.2(3) \text{ \AA}^3$

$Z = 4$

$F(000) = 664$

$D_x = 1.550 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 901 reflections

$\theta = 2.2\text{--}25.2^\circ$

$\mu = 0.12 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Flake, yellow

$0.18 \times 0.14 \times 0.05 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2003)
 $T_{\min} = 0.978$, $T_{\max} = 0.994$

7003 measured reflections
2404 independent reflections
1108 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.090$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 1.8^\circ$
 $h = -13 \rightarrow 10$
 $k = -19 \rightarrow 19$
 $l = -8 \rightarrow 7$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.099$
 $S = 1.01$
2404 reflections
208 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
 $w = 1/[\sigma^2(F_o^2) + (0.0163P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.47014 (19)	0.62825 (13)	0.9624 (3)	0.0409 (7)
H1	0.4927	0.5828	0.9423	0.061*
O2	0.4486 (2)	0.91888 (13)	0.8924 (3)	0.0452 (7)
H2	0.4215	0.9337	0.7887	0.068*
O3	0.9454 (2)	0.74461 (14)	0.7759 (4)	0.0548 (8)
O4	1.1510 (2)	0.48495 (14)	0.6863 (3)	0.0489 (7)
H4	1.1898	0.5246	0.6644	0.073*
O5	0.77278 (19)	0.40952 (13)	0.8557 (3)	0.0446 (7)
O6	0.6237 (2)	0.52178 (13)	0.9245 (3)	0.0419 (7)
O7	0.2909 (2)	0.61113 (14)	0.6547 (3)	0.0609 (8)
H7A	0.3423	0.6145	0.7481	0.073*
H7B	0.3279	0.6016	0.5601	0.073*
C1	0.5559 (3)	0.6817 (2)	0.9249 (4)	0.0302 (9)
C2	0.5248 (3)	0.76155 (18)	0.9251 (4)	0.0316 (9)
H2A	0.4486	0.7763	0.9485	0.038*
C3	0.6068 (3)	0.8194 (2)	0.8904 (4)	0.0303 (9)

C4	0.7203 (3)	0.79692 (18)	0.8534 (4)	0.0314 (9)
H4A	0.7757	0.8358	0.8308	0.038*
C5	0.7514 (3)	0.7171 (2)	0.8500 (4)	0.0290 (8)
C6	0.8705 (3)	0.6940 (2)	0.8020 (4)	0.0334 (9)
C7	0.9000 (3)	0.60779 (19)	0.7896 (4)	0.0294 (9)
C8	1.0101 (3)	0.5876 (2)	0.7384 (4)	0.0363 (9)
H8	1.0626	0.6274	0.7094	0.044*
C9	1.0428 (3)	0.5076 (2)	0.7301 (4)	0.0351 (9)
C10	0.9635 (3)	0.4471 (2)	0.7656 (4)	0.0366 (10)
H10	0.9851	0.3939	0.7549	0.044*
C11	0.8527 (3)	0.4668 (2)	0.8167 (4)	0.0334 (9)
C12	0.8161 (3)	0.54798 (19)	0.8292 (4)	0.0285 (8)
C13	0.7004 (3)	0.5714 (2)	0.8841 (4)	0.0304 (9)
C14	0.6699 (3)	0.65733 (19)	0.8854 (4)	0.0278 (8)
C15	0.5733 (3)	0.90622 (19)	0.8933 (4)	0.0393 (9)
H15A	0.6132	0.9309	1.0036	0.047*
H15B	0.6010	0.9324	0.7856	0.047*
C16	0.8055 (3)	0.3271 (2)	0.8389 (5)	0.0564 (12)
H16A	0.8225	0.3165	0.7135	0.085*
H16B	0.7413	0.2936	0.8694	0.085*
H16C	0.8746	0.3160	0.9226	0.085*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0374 (16)	0.0249 (15)	0.0619 (17)	−0.0027 (12)	0.0123 (13)	−0.0018 (12)
O2	0.0414 (16)	0.0392 (16)	0.0558 (17)	0.0107 (13)	0.0084 (13)	0.0035 (12)
O3	0.0387 (17)	0.0291 (16)	0.100 (2)	−0.0081 (13)	0.0226 (15)	0.0001 (14)
O4	0.0384 (16)	0.0398 (17)	0.0711 (19)	0.0066 (13)	0.0182 (14)	0.0000 (13)
O5	0.0337 (15)	0.0244 (15)	0.0771 (19)	0.0011 (13)	0.0122 (14)	−0.0005 (14)
O6	0.0333 (15)	0.0244 (15)	0.0702 (18)	−0.0049 (12)	0.0167 (13)	0.0007 (12)
O7	0.0491 (18)	0.073 (2)	0.0616 (18)	−0.0052 (15)	0.0096 (14)	−0.0054 (15)
C1	0.029 (2)	0.029 (2)	0.032 (2)	−0.0075 (18)	0.0036 (18)	−0.0010 (16)
C2	0.033 (2)	0.025 (2)	0.038 (2)	0.0050 (18)	0.0069 (18)	0.0032 (16)
C3	0.039 (2)	0.022 (2)	0.030 (2)	0.0024 (19)	0.0027 (18)	−0.0010 (15)
C4	0.033 (2)	0.023 (2)	0.039 (2)	−0.0027 (18)	0.0053 (17)	0.0039 (17)
C5	0.028 (2)	0.030 (2)	0.030 (2)	−0.0011 (18)	0.0053 (17)	0.0013 (16)
C6	0.033 (2)	0.027 (2)	0.041 (2)	−0.0038 (19)	0.0032 (18)	−0.0011 (17)
C7	0.029 (2)	0.028 (2)	0.032 (2)	−0.0014 (18)	0.0073 (17)	0.0002 (16)
C8	0.036 (2)	0.032 (2)	0.043 (2)	−0.001 (2)	0.0117 (18)	0.0018 (18)
C9	0.028 (2)	0.042 (3)	0.036 (2)	0.009 (2)	0.0072 (18)	−0.0001 (18)
C10	0.034 (2)	0.031 (2)	0.045 (2)	0.0034 (18)	0.0025 (19)	−0.0053 (17)
C11	0.028 (2)	0.031 (2)	0.040 (2)	−0.0017 (19)	0.0008 (18)	−0.0001 (17)
C12	0.024 (2)	0.027 (2)	0.035 (2)	0.0004 (18)	0.0047 (17)	−0.0012 (16)
C13	0.029 (2)	0.034 (2)	0.028 (2)	−0.0038 (19)	−0.0002 (17)	−0.0044 (17)
C14	0.030 (2)	0.026 (2)	0.027 (2)	0.0021 (17)	0.0045 (17)	−0.0017 (15)
C15	0.042 (2)	0.035 (2)	0.041 (2)	0.002 (2)	0.0071 (19)	−0.0018 (18)
C16	0.061 (3)	0.020 (2)	0.089 (3)	0.003 (2)	0.013 (2)	0.002 (2)

Geometric parameters (Å, °)

O1—C1	1.368 (3)	C4—H4A	0.9300
O1—H1	0.8200	C5—C14	1.403 (4)
O2—C15	1.428 (3)	C5—C6	1.476 (4)
O2—H2	0.8200	C6—C7	1.486 (4)
O3—C6	1.227 (3)	C7—C8	1.376 (4)
O4—C9	1.349 (3)	C7—C12	1.428 (4)
O4—H4	0.8200	C8—C9	1.394 (4)
O5—C11	1.367 (4)	C8—H8	0.9300
O5—C16	1.439 (4)	C9—C10	1.394 (4)
O6—C13	1.256 (3)	C10—C11	1.382 (4)
O7—H7A	0.8500	C10—H10	0.9300
O7—H7B	0.8500	C11—C12	1.428 (4)
C1—C2	1.382 (4)	C12—C13	1.460 (4)
C1—C14	1.409 (4)	C13—C14	1.481 (4)
C2—C3	1.381 (4)	C15—H15A	0.9700
C2—H2A	0.9300	C15—H15B	0.9700
C3—C4	1.390 (4)	C16—H16A	0.9600
C3—C15	1.504 (4)	C16—H16B	0.9600
C4—C5	1.383 (4)	C16—H16C	0.9600
C1—O1—H1	109.5	O4—C9—C10	117.0 (3)
C15—O2—H2	109.5	C8—C9—C10	120.9 (3)
C9—O4—H4	109.5	C11—C10—C9	119.6 (3)
C11—O5—C16	118.3 (3)	C11—C10—H10	120.2
H7A—O7—H7B	107.3	C9—C10—H10	120.2
O1—C1—C2	116.6 (3)	O5—C11—C10	121.7 (3)
O1—C1—C14	122.1 (3)	O5—C11—C12	116.9 (3)
C2—C1—C14	121.3 (3)	C10—C11—C12	121.4 (3)
C3—C2—C1	120.1 (3)	C11—C12—C7	116.9 (3)
C3—C2—H2A	119.9	C11—C12—C13	123.2 (3)
C1—C2—H2A	119.9	C7—C12—C13	119.9 (3)
C2—C3—C4	119.7 (3)	O6—C13—C12	123.0 (3)
C2—C3—C15	120.0 (3)	O6—C13—C14	118.3 (3)
C4—C3—C15	120.3 (3)	C12—C13—C14	118.6 (3)
C5—C4—C3	120.5 (3)	C5—C14—C1	117.5 (3)
C5—C4—H4A	119.8	C5—C14—C13	122.3 (3)
C3—C4—H4A	119.8	C1—C14—C13	120.2 (3)
C4—C5—C14	120.9 (3)	O2—C15—C3	113.2 (3)
C4—C5—C6	119.9 (3)	O2—C15—H15A	108.9
C14—C5—C6	119.2 (3)	C3—C15—H15A	108.9
O3—C6—C5	121.0 (3)	O2—C15—H15B	108.9
O3—C6—C7	120.0 (3)	C3—C15—H15B	108.9
C5—C6—C7	119.0 (3)	H15A—C15—H15B	107.7
C8—C7—C12	121.3 (3)	O5—C16—H16A	109.5
C8—C7—C6	118.0 (3)	O5—C16—H16B	109.5
C12—C7—C6	120.8 (3)	H16A—C16—H16B	109.5

C7—C8—C9	119.9 (3)	O5—C16—H16C	109.5
C7—C8—H8	120.0	H16A—C16—H16C	109.5
C9—C8—H8	120.0	H16B—C16—H16C	109.5
O4—C9—C8	122.1 (3)		
O1—C1—C2—C3	179.3 (3)	O5—C11—C12—C7	179.6 (3)
C14—C1—C2—C3	−1.6 (5)	C10—C11—C12—C7	−1.0 (5)
C1—C2—C3—C4	0.7 (5)	O5—C11—C12—C13	1.2 (5)
C1—C2—C3—C15	−179.2 (3)	C10—C11—C12—C13	−179.5 (3)
C2—C3—C4—C5	0.4 (5)	C8—C7—C12—C11	1.2 (5)
C15—C3—C4—C5	−179.8 (3)	C6—C7—C12—C11	−179.0 (3)
C3—C4—C5—C14	−0.6 (5)	C8—C7—C12—C13	179.7 (3)
C3—C4—C5—C6	177.2 (3)	C6—C7—C12—C13	−0.5 (4)
C4—C5—C6—O3	4.5 (5)	C11—C12—C13—O6	−0.1 (5)
C14—C5—C6—O3	−177.7 (3)	C7—C12—C13—O6	−178.4 (3)
C4—C5—C6—C7	−176.9 (3)	C11—C12—C13—C14	−177.7 (3)
C14—C5—C6—C7	1.0 (4)	C7—C12—C13—C14	3.9 (4)
O3—C6—C7—C8	−3.5 (5)	C4—C5—C14—C1	−0.2 (5)
C5—C6—C7—C8	177.8 (3)	C6—C5—C14—C1	−178.0 (3)
O3—C6—C7—C12	176.7 (3)	C4—C5—C14—C13	−179.6 (3)
C5—C6—C7—C12	−2.0 (4)	C6—C5—C14—C13	2.6 (4)
C12—C7—C8—C9	−2.0 (5)	O1—C1—C14—C5	−179.6 (3)
C6—C7—C8—C9	178.2 (3)	C2—C1—C14—C5	1.3 (5)
C7—C8—C9—O4	−177.9 (3)	O1—C1—C14—C13	−0.2 (4)
C7—C8—C9—C10	2.7 (5)	C2—C1—C14—C13	−179.3 (3)
O4—C9—C10—C11	178.0 (3)	O6—C13—C14—C5	177.2 (3)
C8—C9—C10—C11	−2.5 (5)	C12—C13—C14—C5	−5.1 (4)
C16—O5—C11—C10	−1.2 (4)	O6—C13—C14—C1	−2.2 (4)
C16—O5—C11—C12	178.1 (3)	C12—C13—C14—C1	175.5 (3)
C9—C10—C11—O5	−178.9 (3)	C2—C3—C15—O2	−13.1 (4)
C9—C10—C11—C12	1.7 (5)	C4—C3—C15—O2	167.1 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H1 $\cdots$ O6	0.82	1.82	2.525 (3)	144
O2—H2 $\cdots$ O5 ⁱ	0.82	2.38	2.945 (3)	127
O2—H2 $\cdots$ O6 ⁱ	0.82	2.16	2.919 (3)	154
O4—H4 $\cdots$ O7 ⁱⁱ	0.82	1.85	2.665 (3)	170
O7—H7A $\cdots$ O1	0.85	2.03	2.878 (3)	176
O7—H7B $\cdots$ O2 ⁱⁱⁱ	0.85	1.94	2.771 (3)	165

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