Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Methylbenzoyl)benzoic acid monohydrate

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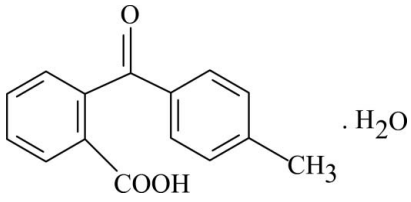
Received 31 March 2008; accepted 17 April 2008

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.061; wR factor = 0.194; data-to-parameter ratio = 14.2.

In the title compound, $C_{15}H_{12}O_3\cdot H_2O$, the two rings are oriented at a dihedral angle of 69.12 (3)°. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules into a three-dimensional framework.

Related literature

For a general background, see: Lin *et al.* (2004). For a related structure, see: Stanescu (1990). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{12}O_3\cdot H_2O$
M_r = 258.26
Triclinic, $P\overline{1}$
a = 7.5410 (15) Å
b = 8.7480 (17) Å
c = 10.728 (2) Å
α = 79.96 (3)°
β = 77.83 (3)°
γ = 85.63 (3)°
V = 680.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.973, T_{max} = 0.982
2638 measured reflections
2435 independent reflections
1840 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.193
S = 1.01
2435 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
OW—H*WA*···O2^{i}	0.85	2.42	2.842 (4)	111
OW—H*WB*···O1^{ii}	0.85	2.38	2.803 (4)	111
O3—H3*B*···*OW*	0.82	1.80	2.601 (4)	165

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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 thank the Center of Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2446).

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North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
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supporting information

Acta Cryst. (2008). E**64**, o894 [doi:10.1107/S1600536808010581]

2-(4-Methylbenzoyl)benzoic acid monohydrate

Guang-Liang Song, Shui-Ping Deng, Shan Liu and Hong-Jun Zhu

S1. Comment

2-(4-methylbenzoyl)benzoic acid (MBBA) is an important dye intermediate used for the synthesis of 2-methylanthraquinone (Lin *et al.*, 2004). We report herein the crystal structure of the title compound, (I).

The asymmetric unit of the title compound, (I), (Fig. 1), contains one MBBA and one water molecules. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C2-C7) and B (C9-C14) are, of course, planar, and they are oriented at a dihedral angle of 69.12 (3)°.

In the crystal structure, intra- and intermolecular O-H···O hydrogen bonds (Table 1) link the molecules to form a three-dimensional framework (Fig. 2), in which they may be effective in the stabilization of the structure.

S2. Experimental

The title compound was prepared according to the method described by Stanescu (1990). Crystals of (I) suitable for X-ray analysis were obtained by dissolving MBBA (2.0 g) in water (100 ml) and evaporating water slowly at room temperature for about 15 d.

S3. Refinement

H atoms were positioned geometrically, with O-H = 0.82 Å (for OH) and 0.85 Å (for H_2O) and C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C,O)$, where x = 1.5 for OH and H_2O H and x = 1.2 for all other H atoms.

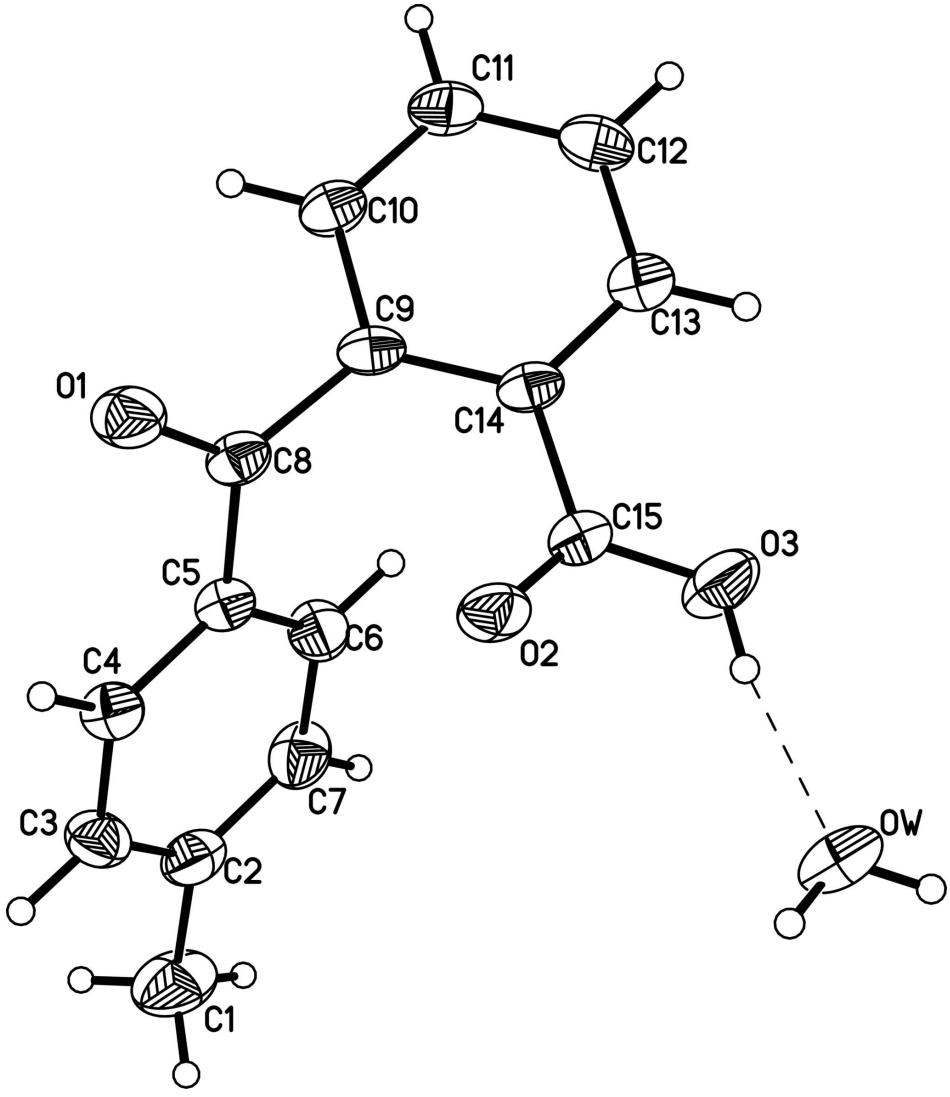

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bond is shown as dashed line.

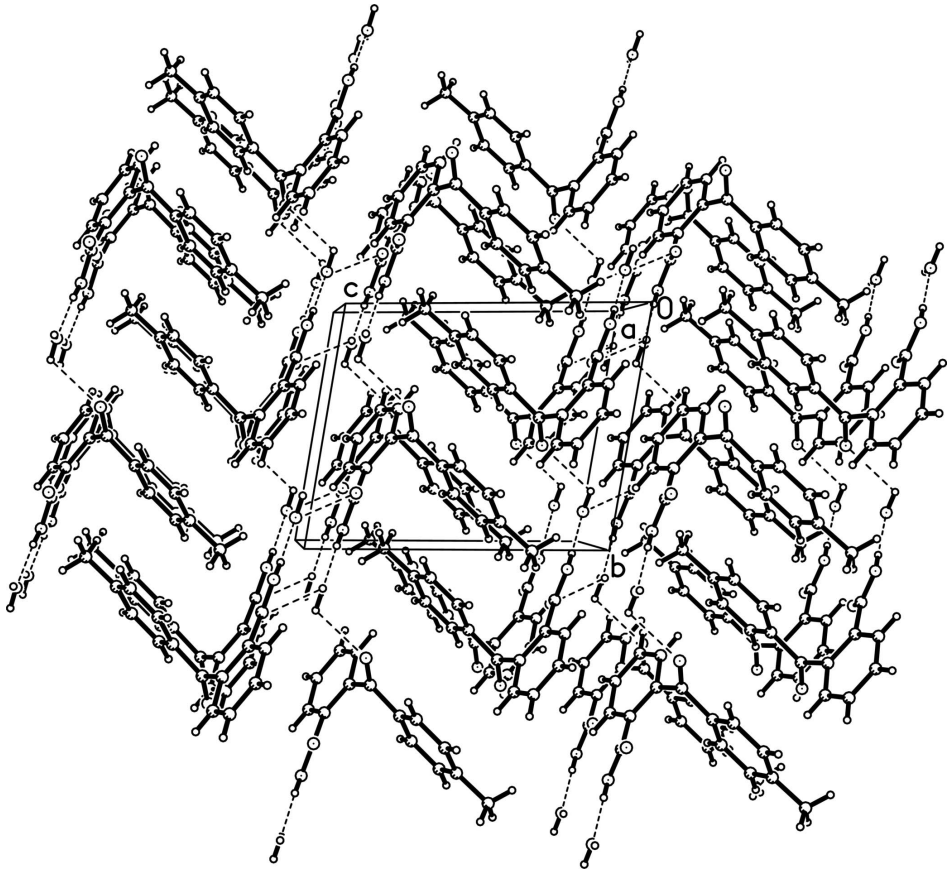

Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2-(4-Methylbenzoyl)benzoic acid monohydrate

Crystal data

$C_{15}H_{12}O_3 \cdot H_2O$
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Triclinic, $P\overline{1}$
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$\gamma = 85.63\ (3)°$
$V = 680.6\ (2)$ Å^3
$Z = 2$
$F(000) = 272$
$D_x = 1.260$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10–13°$
$\mu = 0.09$ mm^{-1}
$T = 294$ K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

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Radiation source: fine-focus sealed tube
Graphite monochromator
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2638 measured reflections
2435 independent reflections
1840 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 25.2°$, $\theta_{min} = 2.0°$
$h = -8 \rightarrow 9$

$k = -10 \rightarrow 10$
$l = 0 \rightarrow 12$

3 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.193$
$S = 1.01$
2435 reflections
172 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.3154 (3)	0.5779 (3)	0.2474 (3)	0.0606 (7)
O2	0.3457 (3)	0.2365 (3)	0.1235 (2)	0.0536 (6)
O3	0.1304 (3)	0.0831 (3)	0.1112 (3)	0.0741 (9)
H3B	0.2170	0.0218	0.0961	0.111*
OW	0.3621 (4)	−0.1469 (3)	0.0679 (3)	0.0649 (7)
HWA	0.4748	−0.1368	0.0625	0.078*
HWB	0.3245	−0.2325	0.0583	0.078*
C1	0.3654 (8)	0.0097 (5)	0.7145 (4)	0.0894 (15)
H1A	0.2658	−0.0581	0.7457	0.134*
H1B	0.3792	0.0646	0.7818	0.134*
H1C	0.4749	−0.0505	0.6892	0.134*
C2	0.3286 (5)	0.1244 (4)	0.6000 (3)	0.0556 (9)
C3	0.4516 (5)	0.2367 (4)	0.5386 (3)	0.0552 (9)
H3A	0.5592	0.2396	0.5672	0.066*
C4	0.4163 (4)	0.3448 (4)	0.4351 (3)	0.0483 (8)
H4A	0.5005	0.4194	0.3948	0.058*
C5	0.2585 (4)	0.3428 (3)	0.3915 (3)	0.0426 (7)
C6	0.1346 (5)	0.2306 (4)	0.4517 (3)	0.0531 (8)
H6A	0.0271	0.2276	0.4229	0.064*
C7	0.1713 (6)	0.1227 (4)	0.5550 (3)	0.0599 (10)
H7A	0.0876	0.0475	0.5947	0.072*
C8	0.2224 (4)	0.4632 (3)	0.2816 (3)	0.0431 (7)
C9	0.0626 (4)	0.4530 (3)	0.2224 (3)	0.0412 (7)

C10	−0.0716 (4)	0.5713 (4)	0.2360 (3)	0.0491 (8)
H10A	−0.0566	0.6524	0.2780	0.059*
C11	−0.2265 (4)	0.5683 (4)	0.1873 (3)	0.0537 (9)
H11A	−0.3156	0.6474	0.1970	0.064*
C12	−0.2500 (4)	0.4501 (4)	0.1250 (3)	0.0539 (9)
H12A	−0.3550	0.4489	0.0928	0.065*
C13	−0.1169 (4)	0.3311 (4)	0.1096 (3)	0.0471 (8)
H13A	−0.1338	0.2506	0.0675	0.056*
C14	0.0391 (4)	0.3326 (3)	0.1566 (3)	0.0410 (7)
C15	0.1881 (4)	0.2129 (3)	0.1288 (3)	0.0438 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0532 (14)	0.0482 (14)	0.0769 (17)	−0.0065 (11)	−0.0189 (12)	0.0089 (12)
O2	0.0396 (13)	0.0515 (14)	0.0682 (15)	0.0127 (10)	−0.0078 (11)	−0.0156 (11)
O3	0.0535 (15)	0.0465 (14)	0.124 (2)	0.0084 (11)	−0.0124 (15)	−0.0292 (15)
OW	0.0646 (16)	0.0387 (13)	0.0809 (18)	0.0083 (11)	0.0040 (13)	−0.0081 (12)
C1	0.128 (4)	0.062 (3)	0.071 (3)	0.016 (3)	−0.027 (3)	0.009 (2)
C2	0.077 (3)	0.0425 (18)	0.0462 (19)	0.0114 (17)	−0.0147 (17)	−0.0077 (15)
C3	0.059 (2)	0.062 (2)	0.0473 (19)	0.0106 (17)	−0.0213 (16)	−0.0103 (16)
C4	0.0482 (19)	0.0444 (18)	0.0505 (18)	0.0008 (14)	−0.0093 (15)	−0.0050 (14)
C5	0.0420 (17)	0.0380 (16)	0.0456 (17)	0.0032 (13)	−0.0067 (13)	−0.0059 (13)
C6	0.058 (2)	0.0505 (19)	0.0506 (19)	−0.0074 (16)	−0.0137 (16)	−0.0015 (15)
C7	0.082 (3)	0.0445 (19)	0.051 (2)	−0.0144 (18)	−0.0119 (18)	0.0037 (15)
C8	0.0378 (16)	0.0369 (16)	0.0499 (18)	0.0034 (13)	−0.0020 (13)	−0.0049 (13)
C9	0.0350 (16)	0.0399 (16)	0.0415 (16)	0.0079 (12)	−0.0010 (12)	0.0007 (13)
C10	0.0444 (18)	0.0440 (18)	0.0552 (19)	0.0105 (14)	−0.0036 (15)	−0.0114 (15)
C11	0.0408 (18)	0.056 (2)	0.058 (2)	0.0182 (15)	−0.0038 (15)	−0.0090 (16)
C12	0.0344 (17)	0.065 (2)	0.057 (2)	0.0076 (15)	−0.0078 (15)	−0.0010 (17)
C13	0.0420 (18)	0.0439 (17)	0.0506 (18)	−0.0004 (14)	−0.0039 (14)	−0.0022 (14)
C14	0.0338 (16)	0.0361 (16)	0.0465 (17)	0.0058 (12)	−0.0004 (13)	−0.0012 (13)
C15	0.0453 (19)	0.0362 (16)	0.0479 (18)	0.0055 (13)	−0.0072 (14)	−0.0068 (13)

Geometric parameters (Å, º)

O1—C8	1.227 (4)	C5—C8	1.494 (4)
O2—C15	1.209 (4)	C6—C7	1.386 (5)
O3—C15	1.303 (4)	C6—H6A	0.9300
O3—H3B	0.8200	C7—H7A	0.9300
OW—HWA	0.8501	C8—C9	1.491 (4)
OW—HWB	0.8500	C9—C10	1.396 (4)
C1—C2	1.505 (5)	C9—C14	1.407 (4)
C1—H1A	0.9600	C10—C11	1.380 (5)
C1—H1B	0.9600	C10—H10A	0.9300
C1—H1C	0.9600	C11—C12	1.366 (5)
C2—C7	1.374 (5)	C11—H11A	0.9300
C2—C3	1.384 (5)	C12—C13	1.396 (5)

C3—C4	1.386 (5)	C12—H12A	0.9300
C3—H3A	0.9300	C13—C14	1.376 (4)
C4—C5	1.370 (4)	C13—H13A	0.9300
C4—H4A	0.9300	C14—C15	1.495 (4)
C5—C6	1.385 (4)		

C15—O3—H3B	109.5	C6—C7—H7A	119.3
HWA—OW—HWB	120.0	O1—C8—C9	119.6 (3)
C2—C1—H1A	109.5	O1—C8—C5	119.7 (3)
C2—C1—H1B	109.5	C9—C8—C5	120.4 (3)
H1A—C1—H1B	109.5	C10—C9—C14	119.1 (3)
C2—C1—H1C	109.5	C10—C9—C8	116.5 (3)
H1A—C1—H1C	109.5	C14—C9—C8	124.4 (3)
H1B—C1—H1C	109.5	C11—C10—C9	120.2 (3)
C7—C2—C3	118.2 (3)	C11—C10—H10A	119.9
C7—C2—C1	121.2 (4)	C9—C10—H10A	119.9
C3—C2—C1	120.6 (4)	C12—C11—C10	120.5 (3)
C2—C3—C4	120.8 (3)	C12—C11—H11A	119.8
C2—C3—H3A	119.6	C10—C11—H11A	119.8
C4—C3—H3A	119.6	C11—C12—C13	120.2 (3)
C5—C4—C3	120.6 (3)	C11—C12—H12A	119.9
C5—C4—H4A	119.7	C13—C12—H12A	119.9
C3—C4—H4A	119.7	C14—C13—C12	120.2 (3)
C4—C5—C6	119.2 (3)	C14—C13—H13A	119.9
C4—C5—C8	119.3 (3)	C12—C13—H13A	119.9
C6—C5—C8	121.5 (3)	C13—C14—C9	119.7 (3)
C5—C6—C7	119.8 (3)	C13—C14—C15	119.7 (3)
C5—C6—H6A	120.1	C9—C14—C15	120.4 (3)
C7—C6—H6A	120.1	O2—C15—O3	124.3 (3)
C2—C7—C6	121.5 (3)	O2—C15—C14	122.5 (3)
C2—C7—H7A	119.3	O3—C15—C14	113.3 (3)

C7—C2—C3—C4	0.3 (5)	C5—C8—C9—C14	−64.3 (4)
C1—C2—C3—C4	−178.5 (3)	C14—C9—C10—C11	1.1 (5)
C2—C3—C4—C5	0.1 (5)	C8—C9—C10—C11	−178.1 (3)
C3—C4—C5—C6	−0.4 (5)	C9—C10—C11—C12	−0.2 (5)
C3—C4—C5—C8	178.6 (3)	C10—C11—C12—C13	−0.2 (5)
C4—C5—C6—C7	0.3 (5)	C11—C12—C13—C14	−0.3 (5)
C8—C5—C6—C7	−178.7 (3)	C12—C13—C14—C9	1.2 (4)
C3—C2—C7—C6	−0.5 (5)	C12—C13—C14—C15	−174.3 (3)
C1—C2—C7—C6	178.3 (4)	C10—C9—C14—C13	−1.6 (4)
C5—C6—C7—C2	0.2 (5)	C8—C9—C14—C13	177.6 (3)
C4—C5—C8—O1	−13.4 (4)	C10—C9—C14—C15	173.9 (3)
C6—C5—C8—O1	165.5 (3)	C8—C9—C14—C15	−7.0 (4)
C4—C5—C8—C9	172.9 (3)	C13—C14—C15—O2	152.2 (3)
C6—C5—C8—C9	−8.1 (4)	C9—C14—C15—O2	−23.2 (5)
O1—C8—C9—C10	−58.8 (4)	C13—C14—C15—O3	−27.6 (4)
C5—C8—C9—C10	114.9 (3)	C9—C14—C15—O3	156.9 (3)

O1—C8—C9—C14	122.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*—H*WA*···O2^{i}	0.85	2.42	2.842 (4)	111
O*W*—H*WB*···O1^{ii}	0.85	2.38	2.803 (4)	111
O3—H3*B*···O*W*	0.82	1.80	2.601 (4)	165

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