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2,2′-[(1*E*)-3-Phenylprop-2-ene-1,1-diyl]-bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one)

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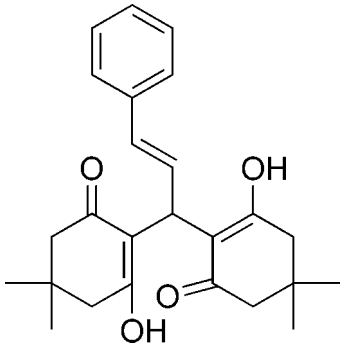
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.071; wR factor = 0.154; data-to-parameter ratio = 15.4.

In the title molecule, $C_{25}H_{30}O_4$, the two cyclohexene rings adopt envelope conformations. The two hydroxy groups are involved in the formation of intramolecular O—H···O hydrogen bonds. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link molecules related by translation along the axis *a* into chains.

Related literature

For related structures, see: Bolte *et al.* (2001); Palakshi Reddy *et al.* (2010); Shi *et al.* (1998). For applications of related compounds, see: Ali *et al.* (2011); Wang *et al.* (2006). For the synthesis of related compounds, see: Ramachary & Mamillapalli (2007); Rohr & Mahrwald (2009).



Experimental

Crystal data

$C_{25}H_{30}O_4$
M_r = 394.49
Triclinic, $P\overline{1}$
a = 5.9465 (15) Å
b = 11.214 (3) Å
c = 17.170 (4) Å
α = 82.804 (3)°
β = 81.062 (3)°
γ = 76.927 (3)°
V = 1096.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.30 × 0.28 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.977, T_{max} = 0.984
11804 measured reflections
4149 independent reflections
3560 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.154
S = 1.02
4149 reflections
269 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O4	0.82	1.82	2.610 (3)	163
O3—H3···O1	0.82	1.85	2.640 (3)	160
C19—H19···O4^{i}	0.93	2.54	3.349 (3)	146
C14—H14*B*···O1^{ii}	0.97	2.59	3.439 (4)	146

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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: CV5137).

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supporting information

Acta Cryst. (2011). E**67**, o2398 [doi:10.1107/S1600536811033745]

2,2′-[(1*E*)-3-Phenylprop-2-ene-1,1-diyl]bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one)

Yu-Lin Zhu, Guo-Lan Xiao, Yan-Fen Chen, Rui-Ting Chen and Ying Zhou

S1. Comment

Tetraketones constitute an important class of organic compounds which can be used as dyes, fluorescent materials for visualization of biomolecules or in laser technologies due to their useful spectroscopic properties (Wang *et al.*, 2006). The title compound is an aldol condensation/Michael addition compound which can be used as an intermediate during the synthesis of oxathene derivatives (Ali *et al.*, 2011). When comes to the unactivated aldehydes such as cinnamaldehyde, the open chain structure can be obtained in a good yield (Ramachary & Mamillapalli, 2007; Rohr & Mahrwald, 2009). The reaction between cinnamaldehyde and 5,5-dimethyl-1,3-cyclohexanedione in the presence palladium(II) chloride proceeded to give the title compound (I) in isolated yield 82%.

In (I) (Fig. 1), the bond lengths and angles are normal and correspond to those observed in related structures (Bolte *et al.*, 2001; Palakshi Reddy *et al.*, 2010; Shi *et al.*, 1998). Two six-membered cyclohexene rings adopt an envelope conformation. The phenyl ring C20–C25 is twisted at 18.1 (1)° from the C18═C19—C20 plane. The hydroxy groups and carbonyl O atoms face each other and form two intramolecular O—H···O hydrogen bonds (Table 1). There are weak intermolecular C19—H19···O4, C14—H14B···O1 and C9—H9···O2 interactions which link molecules into chains.

In the crystal structure, weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules related by translation along axis *a* into chains.

S2. Experimental

The title compound has been synthesized following the known procedures (Ramachary & Mamillapalli, 2007; Rohr & Mahrwald, 2009). A mixture of cinnamaldehyde (0.66 g, 5 mmol), 5,5-dimethyl-1,3-cyclohexanedione (1.40 g, 10 mmol), and palladium (II) chloride (0.0010 g) was refluxed in acetonitrile (10 ml) at 353 K for 6 h (Fig. 2). After being cooled to room temperature, the reaction mixture was poured into water. The white precipitate was filtered off with a silica pad, washed twice with water, and the filtrate was then dried under vacuum to yield the product in yield of 82%. Single crystals of the title compound were obtained by slow evaporation from ethanol at room temperature to yield colourless, block-shaped crystals.

S3. Refinement

The H atoms were positioned geometrically (C—H 0.93–0.98 Å, O—H 0.82 Å) and allowed to ride on their parent atoms, with U_{iso} = 1.2 or 1.5U_{eq}(parent atom).

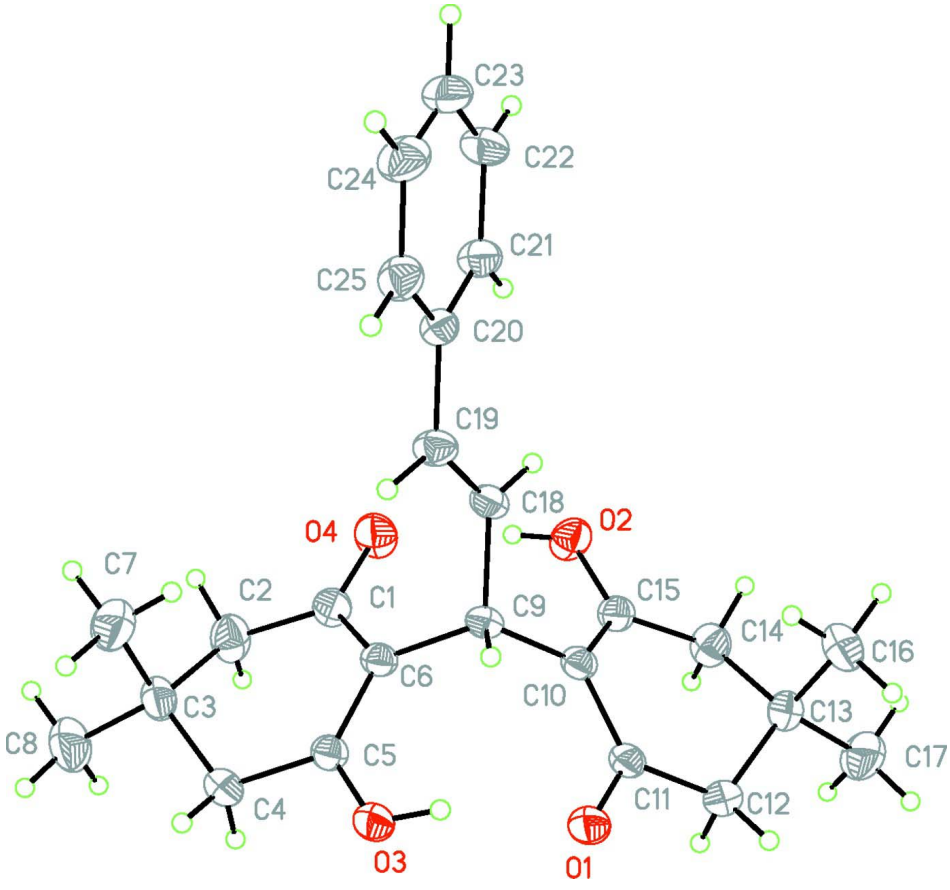

Figure 1

View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

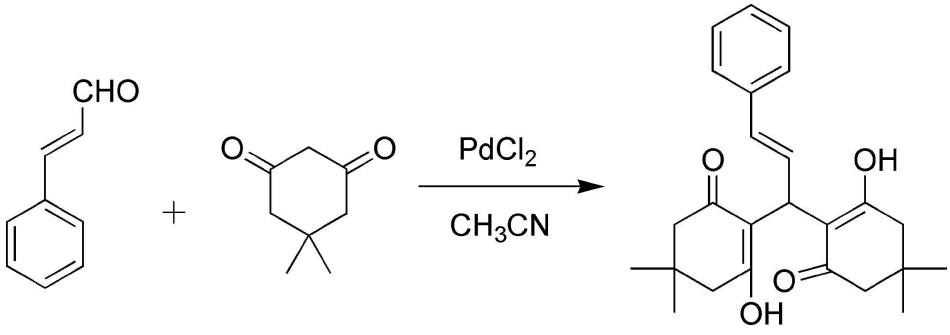

Figure 2

Palladium(II) chloride catalyzed synthesis of the title compound.

2,2′-[(1*E*)-3-Phenylprop-2-ene-1,1-diyl]bis(3-hydroxy-5,5- dimethylcyclohex-2-en-1-one)

Crystal data

$C_{25}H_{30}O_4$
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c = 17.170 (4) Å
α = 82.804 (3)°
β = 81.062 (3)°
γ = 76.927 (3)°

V = 1096.9 (5) Å^3
Z = 2
F(000) = 424
D_x = 1.194 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2118 reflections

θ = 2.3–27.2°
μ = 0.08 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.28 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.977, T_{max} = 0.984

11804 measured reflections
4149 independent reflections
3560 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 26.0°, θ_{min} = 1.9°
h = −7→6
k = −13→13
l = −21→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.154
S = 1.02
4149 reflections
269 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
$w = 1/[\sigma^2(F_o^2) + (0.019P)^2 + 1.9414P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0130 (19)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
C6	0.2857 (5)	0.8045 (2)	0.81379 (16)	0.0357 (6)
C5	0.4316 (5)	0.7081 (2)	0.85206 (16)	0.0374 (6)
C1	0.0541 (5)	0.8394 (3)	0.85021 (17)	0.0429 (7)
C4	0.3647 (6)	0.6518 (3)	0.93287 (17)	0.0506 (8)
H4A	0.5010	0.6299	0.9604	0.061*
H4B	0.3156	0.5764	0.9283	0.061*
C2	−0.0248 (6)	0.7860 (3)	0.93157 (19)	0.0576 (9)
H2A	−0.1034	0.7208	0.9267	0.069*
H2B	−0.1377	0.8494	0.9586	0.069*

C3	0.1700 (6)	0.7341 (3)	0.98281 (17)	0.0514 (8)
C7	0.2611 (8)	0.8383 (4)	1.0080 (2)	0.0740 (11)
H7A	0.3860	0.8043	1.0389	0.111*
H7B	0.1375	0.8896	1.0392	0.111*
H7C	0.3169	0.8863	0.9619	0.111*
C8	0.0803 (8)	0.6583 (4)	1.0562 (2)	0.0821 (13)
H8A	0.0167	0.5950	1.0405	0.123*
H8B	−0.0386	0.7107	1.0883	0.123*
H8C	0.2064	0.6215	1.0861	0.123*
C9	0.3718 (4)	0.8650 (2)	0.73423 (15)	0.0342 (6)
H9	0.5418	0.8459	0.7315	0.041*
C20	0.3317 (5)	1.2099 (2)	0.75974 (16)	0.0379 (6)
C18	0.3039 (5)	1.0046 (2)	0.72762 (16)	0.0398 (6)
H18	0.1955	1.0426	0.6938	0.048*
C19	0.3858 (5)	1.0746 (2)	0.76568 (18)	0.0427 (7)
H19	0.4901	1.0350	0.8005	0.051*
C21	0.1371 (5)	1.2795 (3)	0.72830 (18)	0.0458 (7)
H21	0.0347	1.2401	0.7110	0.055*
C25	0.4806 (6)	1.2720 (3)	0.78509 (18)	0.0482 (7)
H25	0.6132	1.2275	0.8060	0.058*
C23	0.2417 (7)	1.4659 (3)	0.7482 (2)	0.0605 (9)
H23	0.2115	1.5514	0.7444	0.073*
C24	0.4348 (7)	1.3986 (3)	0.7797 (2)	0.0593 (9)
H24	0.5354	1.4387	0.7975	0.071*
C22	0.0926 (6)	1.4064 (3)	0.7221 (2)	0.0573 (9)
H22	−0.0381	1.4516	0.7004	0.069*
C10	0.3235 (5)	0.8101 (2)	0.66340 (15)	0.0355 (6)
C11	0.4927 (5)	0.7122 (2)	0.63160 (16)	0.0395 (6)
C15	0.1190 (5)	0.8469 (3)	0.62977 (16)	0.0404 (6)
C12	0.4642 (6)	0.6603 (3)	0.55792 (18)	0.0521 (8)
H12A	0.3949	0.5890	0.5732	0.063*
H12B	0.6169	0.6329	0.5288	0.063*
C13	0.3140 (6)	0.7512 (3)	0.50335 (17)	0.0494 (7)
C14	0.0882 (5)	0.8041 (3)	0.55416 (18)	0.0523 (8)
H14A	0.0015	0.8728	0.5234	0.063*
H14B	−0.0049	0.7418	0.5664	0.063*
C16	0.4406 (7)	0.8516 (3)	0.4663 (2)	0.0679 (10)
H16A	0.3454	0.9085	0.4320	0.102*
H16B	0.5847	0.8157	0.4362	0.102*
H16C	0.4721	0.8941	0.5072	0.102*
C17	0.2593 (8)	0.6843 (4)	0.4381 (2)	0.0787 (12)
H17A	0.1771	0.6215	0.4618	0.118*
H17B	0.4020	0.6474	0.4077	0.118*
H17C	0.1646	0.7421	0.4040	0.118*
O3	0.6399 (3)	0.65715 (19)	0.81993 (12)	0.0469 (5)
H3	0.6525	0.6755	0.7719	0.070*
O1	0.6739 (4)	0.66073 (19)	0.66454 (12)	0.0501 (5)
O2	−0.0650 (4)	0.9210 (2)	0.66144 (13)	0.0554 (6)

H2	−0.0526	0.9260	0.7078	0.083*
O4	−0.1002 (4)	0.9153 (2)	0.81522 (13)	0.0588 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C6	0.0404 (14)	0.0296 (13)	0.0385 (14)	−0.0068 (11)	−0.0109 (11)	−0.0022 (10)
C5	0.0417 (15)	0.0331 (13)	0.0377 (14)	−0.0070 (11)	−0.0087 (11)	−0.0025 (11)
C1	0.0365 (15)	0.0466 (16)	0.0442 (16)	−0.0036 (12)	−0.0084 (12)	−0.0052 (13)
C4	0.063 (2)	0.0411 (16)	0.0410 (16)	−0.0011 (14)	−0.0069 (14)	0.0042 (13)
C2	0.0456 (18)	0.076 (2)	0.0470 (18)	−0.0086 (16)	−0.0009 (14)	−0.0033 (16)
C3	0.0582 (19)	0.0573 (19)	0.0348 (15)	−0.0079 (15)	−0.0048 (13)	0.0016 (13)
C7	0.090 (3)	0.076 (3)	0.058 (2)	−0.006 (2)	−0.020 (2)	−0.0202 (19)
C8	0.094 (3)	0.092 (3)	0.046 (2)	−0.009 (2)	0.003 (2)	0.008 (2)
C9	0.0320 (13)	0.0282 (12)	0.0403 (14)	−0.0028 (10)	−0.0063 (11)	0.0007 (10)
C20	0.0396 (14)	0.0348 (14)	0.0373 (14)	−0.0053 (11)	−0.0014 (11)	−0.0055 (11)
C18	0.0470 (16)	0.0309 (13)	0.0404 (15)	−0.0041 (12)	−0.0124 (12)	0.0014 (11)
C19	0.0408 (15)	0.0347 (14)	0.0519 (17)	0.0003 (12)	−0.0159 (13)	−0.0048 (12)
C21	0.0474 (17)	0.0377 (15)	0.0522 (17)	−0.0039 (13)	−0.0116 (13)	−0.0069 (13)
C25	0.0503 (17)	0.0484 (17)	0.0492 (17)	−0.0129 (14)	−0.0095 (14)	−0.0087 (14)
C23	0.082 (3)	0.0341 (16)	0.063 (2)	−0.0151 (17)	0.0035 (18)	−0.0068 (15)
C24	0.070 (2)	0.0486 (18)	0.066 (2)	−0.0238 (17)	−0.0063 (18)	−0.0157 (16)
C22	0.064 (2)	0.0383 (16)	0.062 (2)	0.0031 (15)	−0.0098 (17)	0.0021 (14)
C10	0.0381 (14)	0.0300 (13)	0.0369 (14)	−0.0073 (11)	−0.0034 (11)	0.0013 (10)
C11	0.0435 (15)	0.0321 (13)	0.0374 (14)	−0.0052 (12)	0.0009 (12)	0.0043 (11)
C15	0.0406 (15)	0.0373 (14)	0.0420 (15)	−0.0073 (12)	−0.0036 (12)	−0.0031 (12)
C12	0.069 (2)	0.0375 (15)	0.0447 (17)	−0.0006 (14)	−0.0048 (15)	−0.0065 (13)
C13	0.063 (2)	0.0474 (17)	0.0367 (15)	−0.0073 (15)	−0.0066 (14)	−0.0069 (13)
C14	0.0488 (18)	0.061 (2)	0.0493 (18)	−0.0090 (15)	−0.0148 (14)	−0.0093 (15)
C16	0.082 (3)	0.063 (2)	0.049 (2)	−0.0109 (19)	−0.0005 (18)	0.0112 (16)
C17	0.106 (3)	0.076 (3)	0.055 (2)	−0.002 (2)	−0.024 (2)	−0.0255 (19)
O3	0.0456 (12)	0.0445 (11)	0.0429 (11)	0.0047 (9)	−0.0072 (9)	0.0005 (9)
O1	0.0460 (12)	0.0466 (12)	0.0470 (12)	0.0077 (9)	−0.0030 (9)	−0.0001 (9)
O2	0.0422 (12)	0.0646 (14)	0.0536 (13)	0.0089 (10)	−0.0110 (10)	−0.0155 (11)
O4	0.0404 (12)	0.0707 (15)	0.0545 (13)	0.0098 (11)	−0.0093 (10)	−0.0009 (11)

Geometric parameters (Å, º)

C6—C5	1.388 (4)	C21—H21	0.9300
C6—C1	1.411 (4)	C25—C24	1.378 (4)
C6—C9	1.515 (4)	C25—H25	0.9300
C5—O3	1.308 (3)	C23—C24	1.371 (5)
C5—C4	1.485 (4)	C23—C22	1.377 (5)
C1—O4	1.272 (3)	C23—H23	0.9300
C1—C2	1.498 (4)	C24—H24	0.9300
C4—C3	1.528 (4)	C22—H22	0.9300
C4—H4A	0.9700	C10—C15	1.383 (4)
C4—H4B	0.9700	C10—C11	1.413 (4)

C2—C3	1.529 (4)	C11—O1	1.280 (3)
C2—H2A	0.9700	C11—O1	1.280 (3)
C2—H2B	0.9700	C11—C12	1.504 (4)
C3—C8	1.524 (5)	C15—O2	1.304 (3)
C3—C7	1.527 (5)	C15—C14	1.490 (4)
C7—H7A	0.9600	C12—C13	1.524 (4)
C7—H7B	0.9600	C12—H12A	0.9700
C7—H7C	0.9600	C12—H12B	0.9700
C8—H8A	0.9600	C13—C16	1.514 (5)
C8—H8B	0.9600	C13—C14	1.523 (4)
C8—H8C	0.9600	C13—C17	1.536 (4)
C9—C18	1.520 (3)	C14—H14A	0.9700
C9—C10	1.522 (4)	C14—H14B	0.9700
C9—H9	0.9800	C16—H16A	0.9600
C20—C21	1.385 (4)	C16—H16B	0.9600
C20—C25	1.391 (4)	C16—H16C	0.9600
C20—C19	1.472 (4)	C17—H17A	0.9600
C18—C19	1.297 (4)	C17—H17B	0.9600
C18—H18	0.9300	C17—H17C	0.9600
C19—H19	0.9300	O3—H3	0.8200
C21—C22	1.381 (4)	O2—H2	0.8200

C5—C6—C1	117.4 (3)	C20—C21—H21	119.4
C5—C6—C9	120.6 (2)	C24—C25—C20	121.0 (3)
C1—C6—C9	122.0 (2)	C24—C25—H25	119.5
O3—C5—C6	123.2 (2)	C20—C25—H25	119.5
O3—C5—C4	113.6 (2)	C24—C23—C22	119.7 (3)
C6—C5—C4	123.2 (3)	C24—C23—H23	120.2
O4—C1—C6	122.0 (3)	C22—C23—H23	120.2
O4—C1—C2	116.4 (3)	C23—C24—C25	120.3 (3)
C6—C1—C2	121.6 (3)	C23—C24—H24	119.8
C5—C4—C3	114.5 (2)	C25—C24—H24	119.8
C5—C4—H4A	108.6	C23—C22—C21	120.0 (3)
C3—C4—H4A	108.6	C23—C22—H22	120.0
C5—C4—H4B	108.6	C21—C22—H22	120.0
C3—C4—H4B	108.6	C15—C10—C11	117.5 (3)
H4A—C4—H4B	107.6	C15—C10—C9	124.0 (2)
C1—C2—C3	114.7 (3)	C11—C10—C9	118.5 (2)
C1—C2—H2A	108.6	O1—C11—C10	122.4 (3)
C3—C2—H2A	108.6	O1—C11—C10	122.4 (3)
C1—C2—H2B	108.6	O1—C11—C12	116.5 (2)
C3—C2—H2B	108.6	O1—C11—C12	116.5 (2)
H2A—C2—H2B	107.6	C10—C11—C12	121.1 (3)
C8—C3—C7	109.4 (3)	O2—C15—C10	123.4 (3)
C8—C3—C4	109.6 (3)	O2—C15—C14	113.8 (3)
C7—C3—C4	110.1 (3)	C10—C15—C14	122.9 (3)
C8—C3—C2	110.1 (3)	C11—C12—C13	113.9 (2)
C7—C3—C2	110.4 (3)	C11—C12—H12A	108.8

C4—C3—C2	107.3 (3)	C13—C12—H12A	108.8
C3—C7—H7A	109.5	C11—C12—H12B	108.8
C3—C7—H7B	109.5	C13—C12—H12B	108.8
H7A—C7—H7B	109.5	H12A—C12—H12B	107.7
C3—C7—H7C	109.5	C16—C13—C14	111.0 (3)
H7A—C7—H7C	109.5	C16—C13—C12	109.8 (3)
H7B—C7—H7C	109.5	C14—C13—C12	106.9 (3)
C3—C8—H8A	109.5	C16—C13—C17	109.7 (3)
C3—C8—H8B	109.5	C14—C13—C17	109.4 (3)
H8A—C8—H8B	109.5	C12—C13—C17	110.0 (3)
C3—C8—H8C	109.5	C15—C14—C13	114.8 (3)
H8A—C8—H8C	109.5	C15—C14—H14A	108.6
H8B—C8—H8C	109.5	C13—C14—H14A	108.6
C6—C9—C18	113.8 (2)	C15—C14—H14B	108.6
C6—C9—C10	114.3 (2)	C13—C14—H14B	108.6
C18—C9—C10	113.0 (2)	H14A—C14—H14B	107.5
C6—C9—H9	104.8	C13—C16—H16A	109.5
C18—C9—H9	104.8	C13—C16—H16B	109.5
C10—C9—H9	104.8	H16A—C16—H16B	109.5
C21—C20—C25	117.8 (3)	C13—C16—H16C	109.5
C21—C20—C19	122.3 (3)	H16A—C16—H16C	109.5
C25—C20—C19	119.9 (3)	H16B—C16—H16C	109.5
C19—C18—C9	124.9 (3)	C13—C17—H17A	109.5
C19—C18—H18	117.6	C13—C17—H17B	109.5
C9—C18—H18	117.6	H17A—C17—H17B	109.5
C18—C19—C20	127.1 (3)	C13—C17—H17C	109.5
C18—C19—H19	116.4	H17A—C17—H17C	109.5
C20—C19—H19	116.4	H17B—C17—H17C	109.5
C22—C21—C20	121.1 (3)	C5—O3—H3	109.5
C22—C21—H21	119.4	C15—O2—H2	109.5

C1—C6—C5—O3	171.1 (3)	C19—C20—C25—C24	179.5 (3)
C9—C6—C5—O3	−6.2 (4)	C22—C23—C24—C25	0.3 (5)
C1—C6—C5—C4	−7.9 (4)	C20—C25—C24—C23	−0.7 (5)
C9—C6—C5—C4	174.8 (3)	C24—C23—C22—C21	0.4 (5)
C5—C6—C1—O4	−170.8 (3)	C20—C21—C22—C23	−0.6 (5)
C9—C6—C1—O4	6.5 (4)	C6—C9—C10—C15	87.1 (3)
C5—C6—C1—C2	7.5 (4)	C18—C9—C10—C15	−45.1 (4)
C9—C6—C1—C2	−175.2 (3)	C6—C9—C10—C11	−90.3 (3)
O3—C5—C4—C3	159.0 (3)	C18—C9—C10—C11	137.5 (2)
C6—C5—C4—C3	−21.9 (4)	C15—C10—C11—O1	−170.8 (3)
O4—C1—C2—C3	−159.0 (3)	C9—C10—C11—O1	6.7 (4)
C6—C1—C2—C3	22.6 (4)	C15—C10—C11—O1	−170.8 (3)
C5—C4—C3—C8	167.7 (3)	C9—C10—C11—O1	6.7 (4)
C5—C4—C3—C7	−72.0 (4)	C15—C10—C11—C12	7.2 (4)
C5—C4—C3—C2	48.1 (4)	C9—C10—C11—C12	−175.2 (2)
C1—C2—C3—C8	−167.7 (3)	C11—C10—C15—O2	168.1 (3)
C1—C2—C3—C7	71.4 (4)	C9—C10—C15—O2	−9.3 (4)

C1—C2—C3—C4	−48.5 (4)	C11—C10—C15—C14	−11.2 (4)
C5—C6—C9—C18	−135.7 (3)	C9—C10—C15—C14	171.5 (3)
C1—C6—C9—C18	47.1 (3)	O1—C11—C12—C13	−155.9 (3)
C5—C6—C9—C10	92.5 (3)	O1—C11—C12—C13	−155.9 (3)
C1—C6—C9—C10	−84.7 (3)	C10—C11—C12—C13	25.9 (4)
C6—C9—C18—C19	69.0 (4)	C11—C12—C13—C16	69.2 (4)
C10—C9—C18—C19	−158.5 (3)	C11—C12—C13—C14	−51.3 (4)
C9—C18—C19—C20	178.0 (3)	C11—C12—C13—C17	−170.0 (3)
C21—C20—C19—C18	18.1 (5)	O2—C15—C14—C13	162.1 (3)
C25—C20—C19—C18	−160.8 (3)	C10—C15—C14—C13	−18.5 (4)
C25—C20—C21—C22	0.1 (4)	C16—C13—C14—C15	−71.7 (4)
C19—C20—C21—C22	−178.9 (3)	C12—C13—C14—C15	48.0 (4)
C21—C20—C25—C24	0.5 (4)	C17—C13—C14—C15	167.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O4	0.82	1.82	2.610 (3)	163
O3—H3···O1	0.82	1.85	2.640 (3)	160
C19—H19···O4^{i}	0.93	2.54	3.349 (3)	146
C14—H14*B*···O1^{ii}	0.97	2.59	3.439 (4)	146

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