

Ethyl 2,2-dimethyl-4-oxo-6-phenyl-3,4-dihydro-2H-pyran-5-carboxylate

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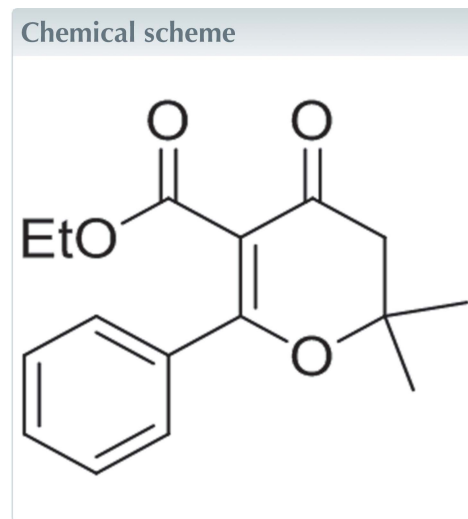
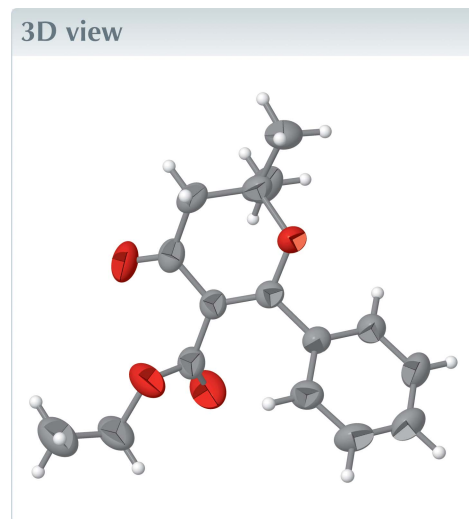
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Keywords: crystal structure; pyran; hydrogen bonding.

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Structural data: full structural data are available from iucrdata.iucr.org

The title compound, C₁₆H₁₈O₄, is a derivative of 3,4-dihydro-2H-pyran-4-one. The plane of the pyranone ring system forms a dihedral angle of 42.76 (10)° with that of the phenyl group. The crystal structure is stabilized by C—H···O interactions that enclose an R₂²(6) ring motif and link the molecules into chains along the *c* axis. A short intramolecular O···O contact [2.942 (3) Å] gives rise to an S(5) motif.



Structure description

Derivatives of the 4H-pyran-4-one heterocyclic system, also known as 4-pyrone or γ -pyrone, are usually quite stable crystalline compounds (Joule *et al.*, 1995). They are reported as compounds acting as melanocortin receptors showing fungicidal, insecticidal, acaricidal, antiviral and anticonvulsant activities (Wang *et al.*, 2006, and references therein). As part of our interest in the structural investigations of 4H-pyran-4-one derivatives, we report herein on the crystal structure determination and the geometry optimization of the title compound ethyl 2,2-dimethyl-4-oxo-6-phenyl-3,4-dihydro-2H-pyran-5-carboxylate, (I). Theoretical calculations of the molecular structure, carried out using MOPAC2012's PM7 geometry optimization algorithm (Stewart, 2012; Maia *et al.*, 2012), are in satisfactory agreement with the results of the X-ray crystal structure analysis.

A perspective view of (I), with the atomic numbering scheme, is illustrated in Fig. 1. The 3,4-dihydro-2H-pyran-4-one moiety (atoms C7–C11/O1/O2) forms a dihedral angle of 42.76 (10)° with the plane of the phenyl group. The phenyl group is almost planar, with an r.m.s. deviation of the fitted atoms of 0.006 Å, whereas the pyran and 3,4-dihydro-2H-pyran-4-one moieties are not planar (r.m.s. deviations = 0.179 and 0.194 Å, respectively).

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C9—H9B···O2 ⁱ	0.97	2.60	3.470 (3)	150
C15—H15A···O2 ⁱ	0.96	2.54	3.406 (3)	151

Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + 1$.

The corresponding bond lengths in the pyran ring are in good agreement with those reported in the literature (Dinçer *et al.*, 2004), except for the O1—C8 and C8—C9 bond lengths [1.476 (2) and 1.519 (3) Å, respectively], which have larger values when compared to the corresponding positions in the related structure (1.367 and 1.342 Å; Dinçer *et al.*, 2004). This is due to the fact that the reported structure is a dihydropyran with two methyl substitutions at C8 of the pyran ring, while the related structure is a tetra-substituted pyran. It could also be evidenced from the fragment overlay (Gans & Shalloway, 2001) of 3,4-dihydro-2*H*-pyran-4-one moieties of (I) with the corresponding moiety in 3,5-bis(4-methylbenzoyl)-2,6-bis(4-methylphenyl)-4*H*-pyran-4-one, (II) (Dinçer *et al.*, 2004) (r.m.s deviation = 1.072 Å). The corresponding positions in (I) is also superimposed with 4-(4-fluorophenyl)-6-methylamino-5-nitro-2-phenyl-4*H*-pyran-3-carbonitrile, (III) (Vishnupriya *et al.*, 2013), gave an r.m.s deviation of 1.401 Å (Fig. 2).

Also, the pyran ring of (I) is puckered (puckering parameters: $Q = 0.439$ (2) Å, $q_2 = 0.348$ (2) Å, $q_3 = 0.269$ (2) Å $\theta = 52.3$ (3)° and $\varphi = 271.6$ (4)°, with atom C8 deviating by 0.576 (2) Å from the C7/C9—C11/O1 plane; the ring is in a half-chair conformation. The relative conformation about the bond joining the 3,4-dihydro-2*H*-pyran-4-one moiety with the benzyl group of (I), defined by the C1—C6—C7—O1 and C5—C6—C7—C11 torsion angles, is (–)synclinal in both the

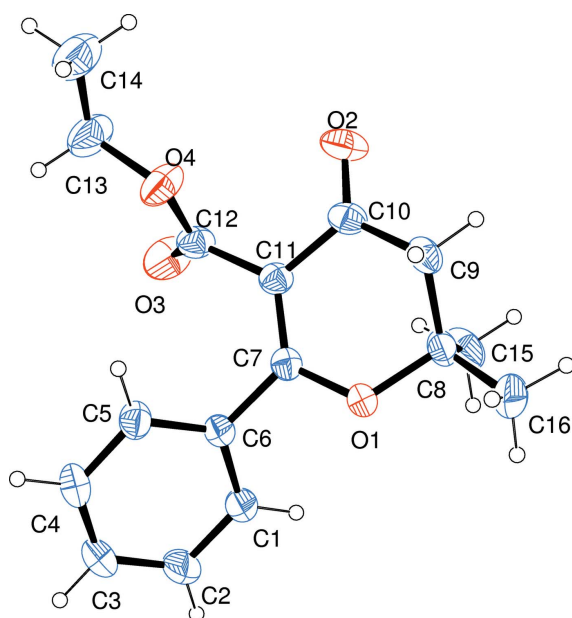


Figure 1
The molecular structure of (I), with displacement ellipsoids for the non-H atoms drawn at the 30% probability level.

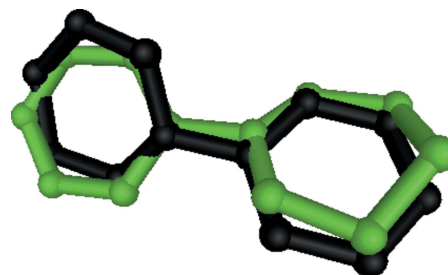


Figure 2
A superimposed fit of (I) (green) and related literature (black).

crystal structure [–42.0 (3) and –43.3 (3)°] and the optimized structure (–51.06 and –50.41°). Whereas the C1—C6—C7—C11 and C5—C6—C7—O1 torsion angles are (+)anticlinal in both the crystal structure [138.6 (2) and 136.1 (2)°] and the optimized structure (129.70 and 128.83°).

A geometry optimization of (I) with a Parameterized Model 7 computation was performed using MOPAC2012. Hartree–Fock closed-shell (restricted) wavefunctions were used for calculations. The HOMO and LUMO energy levels were found to be –9.734 and –0.800 eV, respectively. The total energy and dipole moment of the title molecules are –3389.77227 eV and 5.358 Debye, respectively. In the geometry-optimized structure of (I), it was observed that the O1—C8 bond length decreased to 1.456 Å (1.476 Å in the crystal structure). Also, the C6—C7 bond length in the geometry-optimized structure increased to 1.468 Å (1.483 Å in the crystal structure). The O1—C7—C6 bond angle decreased from 110.42 to 109.81° and the O1—C8—C9 bond angle increased from 108.85 to 110.75°. A superimposed fit of (I) with its energy-minimized molecule gives an r.m.s deviation of 0.452 Å (Fig. 3).

The interaction between C9—O2 and C15—O2 *via* atoms H9B and H15A, Table 1, enclosing an $R_2^2(6)$ ring motif, form a chain of molecules along the *c* axis (Fig. 4). A short intramolecular contact is also found between the atoms O2 and O4 [2.942 (3) Å], giving rise to an $S(5)$ motif.

When compared with a similar pyran derivative, *i.e.* 4-(4-fluorophenyl)-6-methylamino-5-nitro-2-phenyl-4*H*-pyran-3-carbonitrile (Vishnupriya *et al.*, 2013), the six-membered central

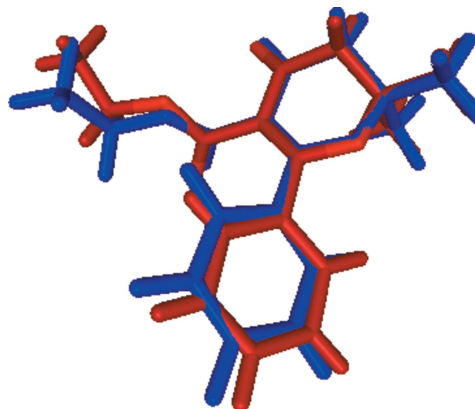


Figure 3
A superimposed fit of (I) (red) and its energy-minimized counterpart (blue).

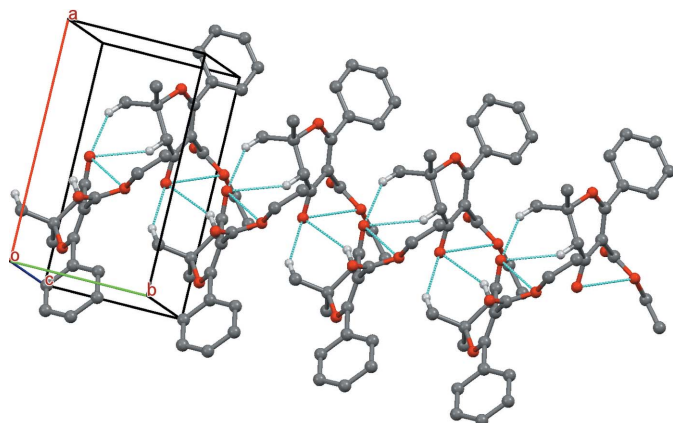


Figure 4
The crystal packing of (I), showing the C–H...O interactions in the $R_2^1(6)$ motif along the c axis as dashed lines. Other H atoms have been omitted for clarity.

pyran ring adopts a boat conformation in the related structure, whereas it is in a half-chair conformation in (I). The variation in conformation between the two structures is also reflected in the dihedral angle between the central pyran ring and the phenyl ring at atom C7 [49.22 (2)° in the related structure and 39.39 (10)° in (I)].

Synthesis and crystallization

To a solution of ethyl benzoylacetate (192 mg, 1.0 mmol), CaCl_2 (11 mg, 0.1 mmol), triethylamine (278 μl , 2.0 mmol) in dichloromethane (4 ml) was added senecioid chloride (systematic name: 3-methylbut-2-enoyl chloride) (112 μl , 1.0 mmol) dropwise at 283 K. After completion of the addition, the reaction mixture was stirred at room temperature for 6 h. The progress of the reaction was monitored by thin-layer chromatography (TLC). The reaction mixture was quenched with water, neutralized with dilute HCl, extracted with CH_2Cl_2 (2 \times 8 ml) and washed with brine. The organic layer was separated, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography (EtOAc/hexane = 2:8 v/v as eluent). The title compound was obtained as a colourless solid (yield 80%, 219 mg) which was crystallized from hexane/EtOAc (m.p. 351–353 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{16}\text{H}_{18}\text{O}_4$
M_r	274.30
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	296
a, b, c (Å)	10.4566 (2), 5.9821 (1), 12.2040 (3)
β (°)	97.460 (1)
V (Å ³)	756.93 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.18 \times 0.16 \times 0.10
Data collection	
Diffractometer	Bruker SMART CCD area detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9344, 4067, 2956
R_{int}	0.022
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.730
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.122, 1.05
No. of reflections	4067
No. of parameters	181
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.17, -0.18
Absolute structure	Flack x determined using 1007 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.3 (4)

Computer programs: SMART and SAINT (Bruker, 2008), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), QMOL (Gans & Shalloway, 2001), Mercury (Macrae *et al.*, 2008), MOPAC (Stewart, 2012), ORTEPIII (Burnett & Johnson, 1996), WinGX (Farrugia, 2012) and PLATON (Spek, 2009).

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full crystallographic data

IUCrData (2016). **1**, x161924 [https://doi.org/10.1107/S2414314616019246]

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Ethyl 2,2-dimethyl-4-oxo-6-phenyl-3,4-dihydro-2H-pyran-5-carboxylate

Crystal data

$C_{16}H_{18}O_4$	$D_x = 1.204 \text{ Mg m}^{-3}$
$M_r = 274.30$	Melting point: 353 K
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 10.4566 (2) \text{ \AA}$	Cell parameters from 4503 reflections
$b = 5.9821 (1) \text{ \AA}$	$\theta = 2.8\text{--}27.1^\circ$
$c = 12.2040 (3) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$\beta = 97.460 (1)^\circ$	$T = 296 \text{ K}$
$V = 756.93 (3) \text{ \AA}^3$	Prism, colourless
$Z = 2$	$0.18 \times 0.16 \times 0.10 \text{ mm}$
$F(000) = 292$	

Data collection

Bruker SMART CCD area detector diffractometer	2956 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.022$
Graphite monochromator	$\theta_{\text{max}} = 31.3^\circ$, $\theta_{\text{min}} = 1.7^\circ$
φ and ω scans	$h = -14 \rightarrow 13$
9344 measured reflections	$k = -8 \rightarrow 8$
4067 independent reflections	$l = -17 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.0653P]$
$wR(F^2) = 0.122$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\text{max}} < 0.001$
4067 reflections	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
181 parameters	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
1 restraint	Absolute structure: Flack x determined using 1007 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons <i>et al.</i> , 2013)
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.3 (4)
Secondary atom site location: difference Fourier map	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.12555 (13)	0.2273 (3)	0.39523 (11)	0.0489 (4)
O2	0.50752 (14)	0.2713 (4)	0.37581 (15)	0.0755 (6)
O3	0.3243 (2)	0.3359 (4)	0.10399 (14)	0.0881 (8)
O4	0.40770 (18)	0.6100 (4)	0.21193 (13)	0.0752 (6)
C1	-0.0461 (2)	0.2348 (5)	0.20244 (19)	0.0561 (5)
H1	-0.0462	0.1011	0.2413	0.067*
C2	-0.1503 (2)	0.2900 (6)	0.1253 (2)	0.0729 (8)
H2	-0.2191	0.1912	0.1111	0.087*
C3	-0.1528 (3)	0.4892 (5)	0.0698 (2)	0.0674 (7)
H3	-0.2235	0.5261	0.0187	0.081*
C4	-0.0512 (3)	0.6335 (5)	0.08947 (19)	0.0627 (6)
H4	-0.0532	0.7691	0.0520	0.075*
C5	0.0551 (2)	0.5787 (4)	0.16510 (18)	0.0541 (5)
H5	0.1244	0.6769	0.1777	0.065*
C6	0.05799 (18)	0.3777 (4)	0.22179 (15)	0.0424 (4)
C7	0.16819 (18)	0.3149 (4)	0.30515 (15)	0.0423 (4)
C8	0.2174 (2)	0.1069 (4)	0.47652 (17)	0.0530 (5)
C9	0.3435 (2)	0.2362 (4)	0.49400 (17)	0.0528 (5)
H9A	0.3300	0.3770	0.5302	0.063*
H9B	0.4070	0.1512	0.5420	0.063*
C10	0.3938 (2)	0.2810 (4)	0.38704 (18)	0.0521 (5)
C11	0.29465 (19)	0.3414 (4)	0.29526 (16)	0.0459 (5)
C12	0.3405 (2)	0.4251 (5)	0.19222 (17)	0.0547 (6)
C13	0.4738 (3)	0.6981 (8)	0.1238 (2)	0.0963 (13)
H13A	0.5113	0.5760	0.0865	0.116*
H13B	0.4125	0.7746	0.0701	0.116*
C14	0.5723 (3)	0.8489 (8)	0.1667 (3)	0.1034 (13)
H14A	0.6150	0.9056	0.1075	0.155*
H14B	0.5349	0.9707	0.2027	0.155*
H14C	0.6336	0.7725	0.2191	0.155*
C15	0.2348 (3)	-0.1253 (5)	0.4300 (3)	0.0783 (9)
H15A	0.2942	-0.2090	0.4808	0.117*
H15B	0.1531	-0.2007	0.4192	0.117*
H15C	0.2681	-0.1128	0.3605	0.117*
C16	0.1518 (3)	0.1011 (8)	0.5791 (2)	0.0875 (10)
H16A	0.2058	0.0246	0.6369	0.131*
H16B	0.1367	0.2511	0.6023	0.131*
H16C	0.0710	0.0239	0.5638	0.131*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0441 (7)	0.0547 (9)	0.0467 (7)	0.0023 (7)	0.0011 (6)	0.0116 (7)
O2	0.0423 (8)	0.1023 (16)	0.0785 (11)	-0.0052 (10)	-0.0048 (7)	-0.0141 (11)
O3	0.0995 (14)	0.115 (2)	0.0519 (9)	-0.0407 (14)	0.0162 (9)	-0.0276 (11)

O4	0.0920 (13)	0.0859 (14)	0.0504 (8)	-0.0423 (12)	0.0197 (8)	-0.0099 (9)
C1	0.0504 (11)	0.0567 (14)	0.0589 (12)	-0.0055 (11)	-0.0020 (9)	0.0120 (11)
C2	0.0513 (12)	0.080 (2)	0.0815 (17)	-0.0104 (13)	-0.0140 (11)	0.0144 (16)
C3	0.0580 (13)	0.0758 (19)	0.0637 (14)	0.0122 (13)	-0.0104 (11)	0.0126 (13)
C4	0.0772 (16)	0.0557 (15)	0.0529 (12)	0.0123 (13)	-0.0002 (11)	0.0138 (11)
C5	0.0625 (12)	0.0468 (13)	0.0516 (11)	-0.0038 (11)	0.0021 (9)	0.0065 (10)
C6	0.0434 (10)	0.0437 (11)	0.0397 (9)	0.0029 (9)	0.0035 (7)	0.0003 (8)
C7	0.0465 (10)	0.0401 (11)	0.0396 (9)	-0.0008 (9)	0.0027 (7)	-0.0020 (8)
C8	0.0549 (11)	0.0503 (13)	0.0498 (10)	-0.0030 (11)	-0.0086 (9)	0.0126 (10)
C9	0.0562 (11)	0.0478 (12)	0.0495 (11)	-0.0008 (11)	-0.0115 (9)	-0.0011 (10)
C10	0.0460 (10)	0.0511 (14)	0.0565 (11)	-0.0084 (10)	-0.0042 (9)	-0.0112 (11)
C11	0.0448 (10)	0.0484 (13)	0.0437 (9)	-0.0061 (9)	0.0024 (8)	-0.0055 (9)
C12	0.0472 (11)	0.0685 (17)	0.0479 (11)	-0.0093 (11)	0.0042 (9)	-0.0089 (11)
C13	0.097 (2)	0.142 (4)	0.0517 (13)	-0.052 (2)	0.0141 (13)	0.0076 (17)
C14	0.106 (2)	0.127 (3)	0.0813 (19)	-0.042 (2)	0.0285 (18)	0.006 (2)
C15	0.0798 (17)	0.0445 (14)	0.100 (2)	-0.0041 (13)	-0.0282 (16)	0.0054 (14)
C16	0.0816 (17)	0.122 (3)	0.0569 (14)	-0.016 (2)	0.0003 (12)	0.0320 (17)

Geometric parameters (Å, °)

O1—C7	1.345 (2)	C8—C9	1.519 (3)
O1—C8	1.476 (2)	C8—C15	1.521 (4)
O2—C10	1.216 (2)	C9—C10	1.493 (3)
O3—C12	1.194 (3)	C9—H9A	0.9700
O4—C12	1.316 (3)	C9—H9B	0.9700
O4—C13	1.452 (3)	C10—C11	1.469 (3)
C1—C6	1.380 (3)	C11—C12	1.489 (3)
C1—C2	1.384 (3)	C13—C14	1.417 (5)
C1—H1	0.9300	C13—H13A	0.9700
C2—C3	1.369 (4)	C13—H13B	0.9700
C2—H2	0.9300	C14—H14A	0.9600
C3—C4	1.366 (4)	C14—H14B	0.9600
C3—H3	0.9300	C14—H14C	0.9600
C4—C5	1.389 (3)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.386 (3)	C15—H15C	0.9600
C5—H5	0.9300	C16—H16A	0.9600
C6—C7	1.483 (3)	C16—H16B	0.9600
C7—C11	1.353 (3)	C16—H16C	0.9600
C8—C16	1.505 (3)		
C7—O1—C8	118.91 (15)	H9A—C9—H9B	108.0
C12—O4—C13	117.7 (2)	O2—C10—C11	122.0 (2)
C6—C1—C2	120.2 (2)	O2—C10—C9	123.4 (2)
C6—C1—H1	119.9	C11—C10—C9	114.65 (17)
C2—C1—H1	119.9	C7—C11—C10	120.29 (18)
C3—C2—C1	120.4 (3)	C7—C11—C12	122.69 (18)
C3—C2—H2	119.8	C10—C11—C12	117.00 (17)

C1—C2—H2	119.8	O3—C12—O4	123.4 (2)
C4—C3—C2	119.9 (2)	O3—C12—C11	126.0 (2)
C4—C3—H3	120.0	O4—C12—C11	110.56 (18)
C2—C3—H3	120.0	C14—C13—O4	110.5 (2)
C3—C4—C5	120.3 (2)	C14—C13—H13A	109.6
C3—C4—H4	119.8	O4—C13—H13A	109.6
C5—C4—H4	119.8	C14—C13—H13B	109.6
C6—C5—C4	120.0 (2)	O4—C13—H13B	109.6
C6—C5—H5	120.0	H13A—C13—H13B	108.1
C4—C5—H5	120.0	C13—C14—H14A	109.5
C1—C6—C5	119.12 (19)	C13—C14—H14B	109.5
C1—C6—C7	119.06 (19)	H14A—C14—H14B	109.5
C5—C6—C7	121.8 (2)	C13—C14—H14C	109.5
O1—C7—C11	123.38 (17)	H14A—C14—H14C	109.5
O1—C7—C6	110.42 (15)	H14B—C14—H14C	109.5
C11—C7—C6	126.20 (17)	C8—C15—H15A	109.5
O1—C8—C16	104.07 (19)	C8—C15—H15B	109.5
O1—C8—C9	108.85 (18)	H15A—C15—H15B	109.5
C16—C8—C9	112.1 (2)	C8—C15—H15C	109.5
O1—C8—C15	107.07 (18)	H15A—C15—H15C	109.5
C16—C8—C15	112.3 (3)	H15B—C15—H15C	109.5
C9—C8—C15	112.0 (2)	C8—C16—H16A	109.5
C10—C9—C8	111.47 (17)	C8—C16—H16B	109.5
C10—C9—H9A	109.3	H16A—C16—H16B	109.5
C8—C9—H9A	109.3	C8—C16—H16C	109.5
C10—C9—H9B	109.3	H16A—C16—H16C	109.5
C8—C9—H9B	109.3	H16B—C16—H16C	109.5
C6—C1—C2—C3	-1.8 (4)	C15—C8—C9—C10	64.4 (3)
C1—C2—C3—C4	0.8 (4)	C8—C9—C10—O2	-140.8 (3)
C2—C3—C4—C5	0.4 (4)	C8—C9—C10—C11	40.0 (3)
C3—C4—C5—C6	-0.6 (4)	O1—C7—C11—C10	-2.2 (3)
C2—C1—C6—C5	1.6 (4)	C6—C7—C11—C10	177.1 (2)
C2—C1—C6—C7	179.8 (2)	O1—C7—C11—C12	176.0 (2)
C4—C5—C6—C1	-0.4 (3)	C6—C7—C11—C12	-4.7 (3)
C4—C5—C6—C7	-178.6 (2)	O2—C10—C11—C7	169.0 (2)
C8—O1—C7—C11	-14.6 (3)	C9—C10—C11—C7	-11.7 (3)
C8—O1—C7—C6	165.99 (18)	O2—C10—C11—C12	-9.3 (4)
C1—C6—C7—O1	-42.0 (3)	C9—C10—C11—C12	169.9 (2)
C5—C6—C7—O1	136.1 (2)	C13—O4—C12—O3	-5.2 (4)
C1—C6—C7—C11	138.6 (2)	C13—O4—C12—C11	172.1 (3)
C5—C6—C7—C11	-43.3 (3)	C7—C11—C12—O3	-62.4 (4)
C7—O1—C8—C16	161.9 (2)	C10—C11—C12—O3	115.9 (3)
C7—O1—C8—C9	42.2 (3)	C7—C11—C12—O4	120.3 (2)
C7—O1—C8—C15	-79.0 (2)	C10—C11—C12—O4	-61.4 (3)
O1—C8—C9—C10	-53.7 (3)	C12—O4—C13—C14	-161.2 (3)
C16—C8—C9—C10	-168.3 (3)		

Hydrogen-bond geometry (Å, °)

<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
C9—H9B···O2 ⁱ	0.97	2.60	3.470 (3)	150
C15—H15A···O2 ⁱ	0.96	2.54	3.406 (3)	151

Symmetry code: (i) $-x+1, y-1/2, -z+1$.