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# 3-Benzylisochroman-1-one

**Tariq Mahmood Babar,[a] Ghulam Qadeer,[a]* Nasim Hasan Rama,[a]‡ Muhammad Khawar Rauf[a] and Wai-Yeung Wong[b]§**

[a]Department of Chemistry, Quaid-i-azam University, Islamabad 45320, Pakistan, and [b]Department of Chemistry, Hong Kong Baptist University, Waterloo Road, Kowloon Tong, Hong Kong, People's Republic of China
Correspondence e-mail: qadeerqau@yahoo.com

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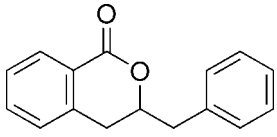
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.042; $wR$ factor = 0.136; data-to-parameter ratio = 18.4.

In the molecule of the title compound, $C_{16}H_{14}O_2$, the aromatic rings are oriented at a dihedral angle of 78.49 (3)°. The heterocyclic ring adopts a twist conformation. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules into chains along the $c$ axis.

## Related literature

For related structures, see: Schmalle *et al.* (1982); Schnebel *et al.* (2003). For a description of the Cambridge Structural Database, see: Allen (2002). For bond-length data, see: Allen *et al.* (1987). For puckering parameters, see: Cremer & Pople (1975).



## Experimental

### Crystal data

$C_{16}H_{14}O_2$
$M_r$ = 238.27
Monoclinic, $P2_1/c$
$a$ = 12.503 (5) Å
$b$ = 8.0200 (9) Å
$c$ = 12.892 (5) Å
$\beta$ = 102.43 (2)°
$V$ = 1262.4 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 294 (2) K
0.32 × 0.26 × 0.21 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.820, $T_{max}$ = 0.983
7148 measured reflections
3024 independent reflections
2546 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.136
$S$ = 1.03
3024 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9$B$···O1$^{i}$ | 0.97 | 2.53 | 3.2922 (18) | 135 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; 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, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2615).

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‡ Additional correspondence author, e-mail nasimhrama@yahoo.com.
§ Additional correspondence author, e-mail rwywong@hkbu.edu.hk.

# supporting information

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## 3-Benzylisochroman-1-one

**Tariq Mahmood Babar, Ghulam Qadeer, Nasim Hasan Rama, Muhammad Khawar Rauf and Wai-Yeung Wong**

### S1. Comment

The title compound was prepared in order to evalute its potential as antibacterial and antifungal agents. The CCDC search (Allen, 2002) showed that the crystal structures of rac-*exo*-tricarbonyl-(h6-3-phenyl isochromanone) -chromium (Schnebel *et al.*, 2003) and 3,4-dihydro-8-hydroxy-3-(4-hydroxy- phenyl)-isocoumarin (Schmalle *et al.*, 1982) have been reported, which have close resemblance as far as isochromane and attached phenyl ring is considered. We report herein the synthesis and crystal structure of the title compound.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C1-C6) and C (C11-C16) are, of course, planar, and they are oriented at a dihedral angle of 78.49 (3)°. Ring B (O2/C5-C9) is not planar, having total puckering amplitude, $Q_T$, of 2.420 (3) Å and twisted conformation [$\varphi$ = 151.98 (3)° and $\theta$ = 88.50 (3)°] (Cremer & Pople, 1975).

In the crystal structure, intermolecular C-H···O hydrogen bonds (Table 1) link the molecules into chains along the c axis, in which they may be effective in the stabilization of the structure.

### S2. Experimental

As shown in Scheme 2, a mixture of homophthalic acid (1.98 g, 11.0 mmol) and 2-phenylacetyl chloride (7.08 g, 46 mmol) was heated under reflux for 6 h at 473 K. After concentration, the residue was chromatographed on silica gel column using petroleum ether (333–353 K) to give 3-benzyl-1*H*-isochromen-1-one. 2-(2-oxo-3-phenylpropyl) benzoic acid was obtained by refluxing a solution of 3-benzyl-1*H*-isochromen-1-one (4 g, 15.9 mmol) in ethanol (200 ml) and potassium hydroxide (5%,200 ml) for 6 h. NaBH4 (1.6 g) was added to a solution of 2-(2-oxo-3-phenylpropyl) benzoic acid (4.81 g, 17.8 mmol) in sodium hydroxide (1%, 180 ml) and the resulting solution was stirred overnight at room temperature. After being acidified with HCl, the whole mixture was extracted with dichloromethane (2 \ times 15 ml). Usual work-up gave crude racemic hydroxy-acid, 2-(2-hydroxy-3-phenylpropyl)benzoic acid, which was dissolved in acetic anhydride (5 ml) and heated under reflux for 2 h to get the title compound (yield; 73%, m.p. 605-606 K). The crude compound was purified by column chromatography on silica gel with petroleum ether and recrystallized in ethanol.

### S3. Refinement

H atoms were positioned geometrically, with C-H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

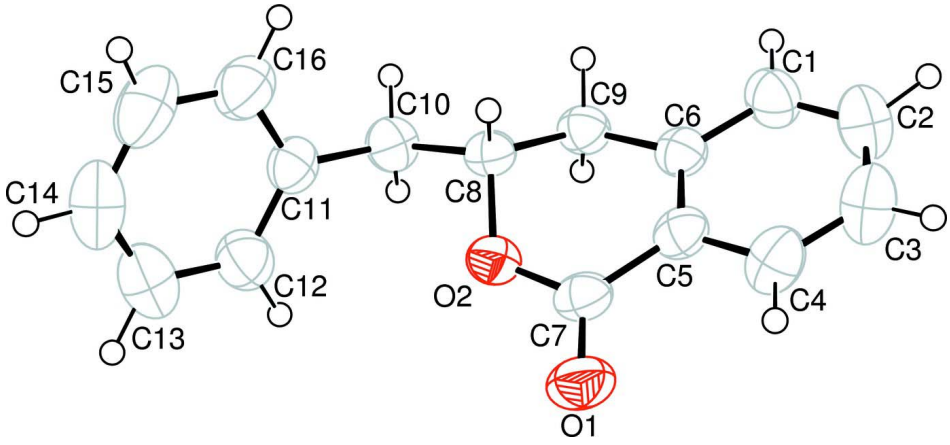


**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

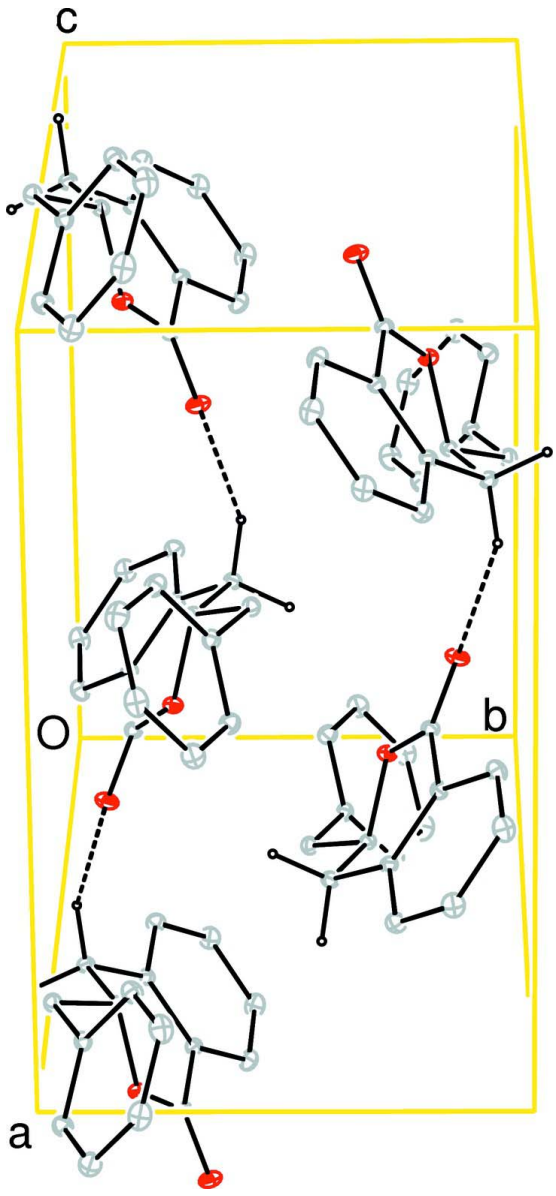


**Figure 2**

A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

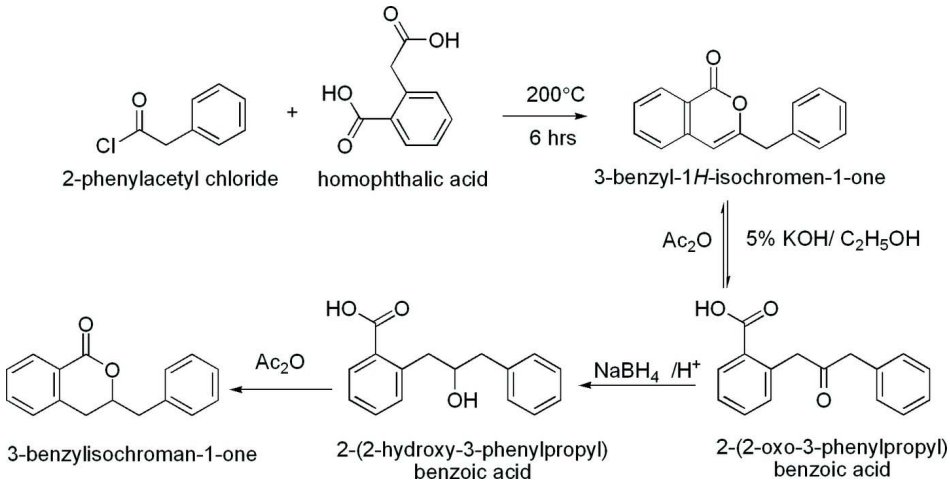


**Figure 3**

The formation of the title compound.

### 3-Benzylisochroman-1-one

*Crystal data*

$C_{16}H_{14}O_2$
$M_r$ = 238.27
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 12.503 (5) Å
$b$ = 8.0200 (9) Å
$c$ = 12.892 (5) Å
$\beta$ = 102.43 (2)°
$V$ = 1262.4 (7) Å$^3$
$Z$ = 4
$F(000)$ = 504
$D_x$ = 1.254 Mg m$^{-3}$
Melting point: 332(1) K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1316 reflections
$\theta$ = 5.3–25.2°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 294 K
Block, colorless
0.32 × 0.26 × 0.21 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.820, $T_{max}$ = 0.983
7148 measured reflections
3024 independent reflections
2546 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021
$\theta_{max}$ = 28.5°, $\theta_{min}$ = 3.0°
$h$ = −16→16
$k$ = −10→10
$l$ = −10→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.136
$S$ = 1.03
3024 reflections
164 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
$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.1131P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.058 (7)

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.00370 (8) | 0.34647 (13) | −0.09298 (6) | 0.0694 (3) |
| O2 | 0.04862 (6) | 0.20854 (10) | 0.05531 (6) | 0.0513 (2) |
| C1 | −0.27750 (10) | 0.22424 (17) | 0.10333 (11) | 0.0614 (3) |
| H1A | −0.2984 | 0.1604 | 0.1558 | 0.074* |
| C2 | −0.35219 (11) | 0.3310 (2) | 0.04219 (14) | 0.0770 (4) |
| H2A | −0.4230 | 0.3383 | 0.0536 | 0.092* |
| C3 | −0.32221 (12) | 0.4264 (2) | −0.03548 (14) | 0.0793 (4) |
| H3A | −0.3728 | 0.4978 | −0.0766 | 0.095* |
| C4 | −0.21631 (11) | 0.41640 (17) | −0.05268 (11) | 0.0653 (3) |
| H4A | −0.1961 | 0.4815 | −0.1050 | 0.078* |
| C5 | −0.14040 (9) | 0.30857 (13) | 0.00867 (8) | 0.0481 (3) |
| C6 | −0.17032 (8) | 0.21122 (13) | 0.08690 (8) | 0.0461 (2) |
| C7 | −0.02835 (9) | 0.29314 (14) | −0.01389 (8) | 0.0495 (3) |
| C8 | 0.02859 (8) | 0.16880 (12) | 0.15967 (7) | 0.0439 (2) |
| H8A | 0.0341 | 0.2713 | 0.2019 | 0.053* |
| C9 | −0.08557 (9) | 0.09595 (13) | 0.14927 (8) | 0.0484 (3) |
| H9A | −0.0896 | −0.0113 | 0.1138 | 0.058* |
| H9B | −0.1002 | 0.0786 | 0.2194 | 0.058* |
| C10 | 0.11974 (9) | 0.05047 (14) | 0.21118 (9) | 0.0528 (3) |
| H10A | 0.1079 | 0.0185 | 0.2804 | 0.063* |
| H10B | 0.1147 | −0.0498 | 0.1683 | 0.063* |
| C11 | 0.23470 (9) | 0.12051 (13) | 0.22511 (9) | 0.0506 (3) |
| C12 | 0.30019 (11) | 0.08497 (17) | 0.15378 (11) | 0.0647 (3) |
| H12A | 0.2725 | 0.0181 | 0.0952 | 0.078* |
| C13 | 0.40664 (12) | 0.1470 (2) | 0.16750 (15) | 0.0809 (4) |
| H13A | 0.4488 | 0.1209 | 0.1185 | 0.097* |
| C14 | 0.44906 (13) | 0.2457 (2) | 0.25261 (17) | 0.0870 (5) |
| H14A | 0.5200 | 0.2870 | 0.2622 | 0.104* |
| C15 | 0.38502 (15) | 0.2832 (2) | 0.32398 (15) | 0.0894 (5) |
| H15A | 0.4131 | 0.3509 | 0.3820 | 0.107* |
| C16 | 0.27839 (13) | 0.22086 (18) | 0.31051 (11) | 0.0708 (4) |
| H16A | 0.2365 | 0.2475 | 0.3597 | 0.085* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0738 (6) | 0.0907 (7) | 0.0453 (4) | −0.0159 (5) | 0.0161 (4) | 0.0086 (4) |
| O2 | 0.0496 (4) | 0.0622 (5) | 0.0443 (4) | −0.0036 (3) | 0.0148 (3) | 0.0004 (3) |
| C1 | 0.0497 (6) | 0.0677 (7) | 0.0686 (7) | −0.0063 (5) | 0.0169 (5) | −0.0006 (6) |
| C2 | 0.0477 (6) | 0.0826 (9) | 0.0997 (11) | 0.0023 (6) | 0.0136 (7) | 0.0030 (8) |
| C3 | 0.0588 (7) | 0.0751 (9) | 0.0955 (10) | 0.0062 (6) | −0.0020 (7) | 0.0134 (8) |
| C4 | 0.0631 (7) | 0.0630 (7) | 0.0640 (7) | −0.0052 (6) | 0.0008 (5) | 0.0107 (6) |
| C5 | 0.0504 (6) | 0.0486 (5) | 0.0430 (5) | −0.0087 (4) | 0.0045 (4) | −0.0041 (4) |
| C6 | 0.0464 (5) | 0.0478 (5) | 0.0438 (5) | −0.0073 (4) | 0.0086 (4) | −0.0074 (4) |
| C7 | 0.0566 (6) | 0.0529 (6) | 0.0387 (5) | −0.0123 (4) | 0.0098 (4) | −0.0043 (4) |
| C8 | 0.0483 (5) | 0.0457 (5) | 0.0380 (5) | −0.0015 (4) | 0.0100 (4) | −0.0036 (4) |
| C9 | 0.0506 (5) | 0.0508 (5) | 0.0453 (5) | −0.0044 (4) | 0.0138 (4) | 0.0014 (4) |
| C10 | 0.0533 (6) | 0.0488 (6) | 0.0564 (6) | 0.0023 (4) | 0.0121 (4) | 0.0014 (5) |
| C11 | 0.0500 (5) | 0.0460 (5) | 0.0527 (6) | 0.0073 (4) | 0.0047 (4) | 0.0031 (4) |
| C12 | 0.0598 (7) | 0.0671 (7) | 0.0680 (7) | 0.0025 (6) | 0.0152 (6) | −0.0048 (6) |
| C13 | 0.0600 (8) | 0.0819 (9) | 0.1042 (11) | 0.0051 (7) | 0.0252 (8) | 0.0072 (9) |
| C14 | 0.0520 (7) | 0.0795 (10) | 0.1203 (14) | −0.0013 (7) | −0.0019 (8) | 0.0093 (10) |
| C15 | 0.0777 (10) | 0.0835 (10) | 0.0908 (11) | −0.0065 (8) | −0.0181 (8) | −0.0153 (8) |
| C16 | 0.0699 (8) | 0.0730 (8) | 0.0633 (8) | 0.0056 (6) | 0.0009 (6) | −0.0116 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.382 (2) | C8—H8A | 0.9800 |
| C1—C6 | 1.405 (2) | C9—H9A | 0.9700 |
| C1—H1A | 0.9300 | C9—H9B | 0.9700 |
| C2—C3 | 1.375 (3) | C10—C11 | 1.517 (2) |
| C2—H2A | 0.9300 | C10—H10A | 0.9700 |
| C3—C4 | 1.391 (3) | C10—H10B | 0.9700 |
| C3—H3A | 0.9300 | C11—C16 | 1.378 (2) |
| C4—C5 | 1.3968 (19) | C11—C12 | 1.386 (2) |
| C4—H4A | 0.9300 | C12—C13 | 1.396 (2) |
| C5—C6 | 1.3889 (18) | C12—H12A | 0.9300 |
| C5—C7 | 1.496 (2) | C13—C14 | 1.365 (3) |
| C6—C9 | 1.5023 (19) | C13—H13A | 0.9300 |
| C7—O1 | 1.2054 (17) | C14—C15 | 1.377 (3) |
| C7—O2 | 1.3463 (17) | C14—H14A | 0.9300 |
| C8—O2 | 1.4559 (19) | C15—C16 | 1.399 (3) |
| C8—C9 | 1.521 (2) | C15—H15A | 0.9300 |
| C8—C10 | 1.5214 (19) | C16—H16A | 0.9300 |
| | | | |
| C2—C1—C6 | 120.63 (13) | C8—C9—H9A | 109.5 |
| C2—C1—H1A | 119.7 | C6—C9—H9B | 109.5 |
| C6—C1—H1A | 119.7 | C8—C9—H9B | 109.5 |
| C3—C2—C1 | 120.23 (14) | H9A—C9—H9B | 108.1 |
| C3—C2—H2A | 119.9 | C11—C10—C8 | 114.97 (12) |
| C1—C2—H2A | 119.9 | C11—C10—H10A | 108.5 |

| | | | |
|---|---|---|---|
| C2—C3—C4 | 120.14 (13) | C8—C10—H10A | 108.5 |
| C2—C3—H3A | 119.9 | C11—C10—H10B | 108.5 |
| C4—C3—H3A | 119.9 | C8—C10—H10B | 108.5 |
| C3—C4—C5 | 119.97 (13) | H10A—C10—H10B | 107.5 |
| C3—C4—H4A | 120.0 | C16—C11—C12 | 117.44 (14) |
| C5—C4—H4A | 120.0 | C16—C11—C10 | 120.88 (11) |
| C6—C5—C4 | 120.18 (13) | C12—C11—C10 | 121.68 (12) |
| C6—C5—C7 | 120.30 (10) | C11—C12—C13 | 121.74 (15) |
| C4—C5—C7 | 119.46 (12) | C11—C12—H12A | 119.1 |
| C5—C6—C1 | 118.84 (11) | C13—C12—H12A | 119.1 |
| C5—C6—C9 | 117.73 (11) | C14—C13—C12 | 120.23 (15) |
| C1—C6—C9 | 123.42 (11) | C14—C13—H13A | 119.9 |
| O1—C7—O2 | 117.57 (12) | C12—C13—H13A | 119.9 |
| O1—C7—C5 | 123.76 (11) | C13—C14—C15 | 118.86 (16) |
| O2—C7—C5 | 118.59 (11) | C13—C14—H14A | 120.6 |
| O2—C8—C9 | 110.33 (8) | C15—C14—H14A | 120.6 |
| O2—C8—C10 | 106.16 (9) | C14—C15—C16 | 120.99 (16) |
| C9—C8—C10 | 113.54 (11) | C14—C15—H15A | 119.5 |
| O2—C8—H8A | 108.9 | C16—C15—H15A | 119.5 |
| C9—C8—H8A | 108.9 | C11—C16—C15 | 120.73 (15) |
| C10—C8—H8A | 108.9 | C11—C16—H16A | 119.6 |
| C6—C9—C8 | 110.56 (11) | C15—C16—H16A | 119.6 |
| C6—C9—H9A | 109.5 | C7—O2—C8 | 118.82 (10) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9*B*···O1$^{i}$ | 0.97 | 2.53 | 3.2922 (18) | 135 |

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