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# (3*E*)-11,16-Dioxatricyclo[15.4.0.0$^{5,10}$]-henicosa-1(21),3,5,7,9,17,19-heptaen-2-one

**Gnanavelu Ganesh,[a] Santhanagopalan Purushothaman,[b] Piskala Subburaman Kannan,[a] Raghavachary Raghunathan[b] and Arunachalathevar SubbiahPandi[c]***

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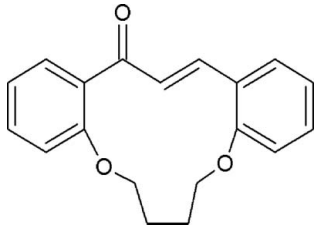
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.045; $wR$ factor = 0.143; data-to-parameter ratio = 15.8.

The title compound, $C_{19}H_{18}O_3$, crystallizes with three molecules (*A*, *B* and *C*) in the asymmetric unit. The carbonyl O atom shows positional disorder over two sites in molecules *A* and *B*; the site-occupancy ratios are 0.76 (3):0.24 (3) and 0.86 (3):0.14 (3), respectively. The ethylene fragments in each molecule have an *E* conformation, while the C—O—C—C torsion angles indicate near planarity. The dihedral angles formed by the aromatic rings are 20.0 (1), 23.7 (1) and 16.1 (1)° for molecules *A*, *B* and *C*, respectively. Intramolecular C—H···O hydrogen bonds occur in each molecule.

## Related literature

For the biological activities of chalcones, see: Xue *et al.* (2004); Lee *et al.* (2006); Bhat *et al.* (2005); Satyanarayana *et al.* (2004). For a related crown ether structure, see: Anh *et al.* (2011).



## Experimental

### Crystal data

$C_{19}H_{18}O_3$
$M_r$ = 294.34
Triclinic, $P\overline{1}$
$a$ = 9.0976 (6) Å
$b$ = 16.9797 (11) Å
$c$ = 17.2713 (9) Å
$\alpha$ = 62.590 (2)°
$\beta$ = 88.440 (2)°
$\gamma$ = 78.092 (2)°
$V$ = 2310.4 (2) Å$^3$
$Z$ = 6
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.40 × 0.30 × 0.25 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.967, $T_{max}$ = 0.979
44770 measured reflections
9919 independent reflections
5862 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.143
$S$ = 1.04
9919 reflections
629 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C18—H18···O2 | 0.93 | 2.15 | 2.746 (2) | 121 |
| C18—H18···O3 | 0.93 | 2.12 | 2.763 (2) | 126 |
| C38—H38···O5 | 0.93 | 2.24 | 2.753 (2) | 114 |
| C38—H38···O6 | 0.93 | 2.13 | 2.753 (3) | 123 |
| C56—H56···O8 | 0.93 | 2.23 | 2.766 (2) | 116 |
| C56—H56···O9 | 0.93 | 2.15 | 2.764 (2) | 122 |

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors thank Dr Babu Varghese and SAIF, IIT, Chennai, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2434).

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# supporting information

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# (3*E*)-11,16-Dioxatricyclo[15.4.0.0$^{5,10}$]henicosa-1(21),3,5,7,9,17,19-heptaen-2-one

**Gnanavelu Ganesh, Santhanagopalan Purushothaman, Piskala Subburaman Kannan, Raghavachary Raghunathan and Arunachalathevar SubbiahPandi**

## S1. Comment

Chalcone derivatives possess a wide range of biological properties such as antimalarial (Xue *et al.*, 2004), antiangiogenic and antitumour (Lee *et al.*, 2006), anticancer (Bhat *et al.*, 2005) and antihyperglycemic (Satyanarayana *et al.*, 2004) activities. Chalcones have been widely studied and developed as one of the pharmaceutically important molecules. Herein we report the crystal structure of the title compound.

The macomolecular structure of the title compound, $C_{57}H_{52}O_9$, includes 14-crown-2-ether skeletal moiety (Fig. 1). The bond lengths and bond angles are comparable with the related crown ether structure (Anh *et al.*, 2011). The compound crystallizes with three independent molecules (A, B and C) per asymmetric unit. Out of three molecules, two molecules are disordered with two alternate positions for the O atoms [atom O1/O1′ in molecule A, and O4/O4′ in molecule B] with site occupancies are 0.76/0.24 and 0.86/0.14. The ethylene fragments in all the three molecules have E configuration, while the C—O—C—C torsion angles indicate planarity of the segments. The dihedral angles between the aromatic rings are 20.0 (1), 23.7 (1) and 16.1 (1)° for molecules A, B and C, respectively.

Each molecule of the asymmetric unit exhibits intramolecular C—H···O hydrogen bonds [Table 1].

## S2. Experimental

To a solution of 2 g (5.08 mmol) of 2-(4-(4-((2-acetylphenoxy) methyl)-1*H*-1,2,3-triazol-1-yl) butoxy)benzaldehyde in 30 ml of methanol, 0.30 g (7.63 mmol) of NaOH in 30 ml of methanol was added drop wise and the mixture was stirred vigorously at room temperature for about 8 h. After the completion of the reaction, as evidenced by TLC analysis, the solvent was removed under vacuum. The crude product was then subjected to column chromatography using petroleum ether/ethylacetate (1:1) as eluent. The single crystal suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in methanol at room temperature.

## S3. Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C—H distances fixed in the range 0.93–0.97 Å with $U_{iso}$(H) = 1.2$U_{eq}$(C) for other H atoms. The carbonyl group O atoms of two molecules shows positional disorder and were refined split into two positions with occupancies of 0.76 (3)/0.24 (3) and 0.86 (3)/0.14 (3).

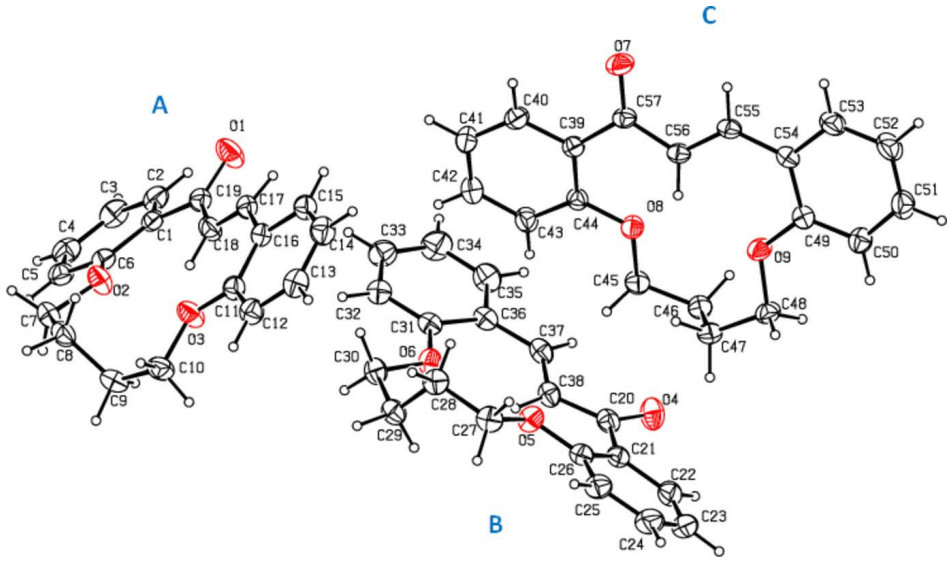


**Figure 1**

The structure of the title compound, showing the atom-numbering scheme. The displacement ellipsoids are drawn at the 30% probability level.

### (3*E*)-11,16-Dioxatricyclo[15.4.0.0$^{5,10}$]henicosa-1(21),3,5,7,9,17,19- heptaen-2-one

*Crystal data*

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$M_r$ = 294.34
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 9.0976 (6) Å
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$\alpha$ = 62.590 (2)°
$\beta$ = 88.440 (2)°
$\gamma$ = 78.092 (2)°
$V$ = 2310.4 (2) Å$^3$
$Z$ = 6
$F(000)$ = 936
$D_x$ = 1.269 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9919 reflections
$\theta$ = 2.0–26.9°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
Block, white crystalline
0.40 × 0.30 × 0.25 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.967, $T_{max}$ = 0.979
44770 measured reflections
9919 independent reflections
5862 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
$\theta_{max}$ = 26.9°, $\theta_{min}$ = 1.4°
$h$ = −11→11
$k$ = −21→21
$l$ = −21→21

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.143
$S$ = 1.04
9919 reflections
629 parameters
15 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.2901P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å$^{-3}$
$\Delta\rho_{min} = -0.16$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.2486 (2) | 0.55742 (11) | 0.08728 (12) | 0.0588 (5) | |
| C2 | 0.3295 (3) | 0.56983 (13) | 0.01475 (14) | 0.0739 (6) | |
| H2 | 0.4339 | 0.5592 | 0.0212 | 0.089* | |
| C3 | 0.2613 (3) | 0.59712 (15) | −0.06609 (15) | 0.0862 (7) | |
| H3 | 0.3189 | 0.6037 | −0.1132 | 0.103* | |
| C4 | 0.1071 (3) | 0.61454 (15) | −0.07661 (15) | 0.0819 (6) | |
| H4 | 0.0599 | 0.6341 | −0.1314 | 0.098* | |
| C5 | 0.0222 (3) | 0.60341 (13) | −0.00704 (13) | 0.0705 (5) | |
| H5 | −0.0822 | 0.6151 | −0.0149 | 0.085* | |
| C6 | 0.0908 (2) | 0.57491 (12) | 0.07496 (12) | 0.0604 (5) | |
| C7 | −0.1490 (2) | 0.58850 (16) | 0.13795 (14) | 0.0746 (6) | |
| H7A | −0.1910 | 0.5576 | 0.1115 | 0.089* | |
| H7B | −0.1840 | 0.6536 | 0.1023 | 0.089* | |
| C8 | −0.1943 (2) | 0.55946 (15) | 0.22954 (14) | 0.0751 (6) | |
| H8A | −0.3007 | 0.5853 | 0.2272 | 0.090* | |
| H8B | −0.1389 | 0.5840 | 0.2573 | 0.090* | |
| C9 | −0.1666 (2) | 0.45690 (16) | 0.28566 (15) | 0.0799 (6) | |
| H9A | −0.2619 | 0.4386 | 0.2900 | 0.096* | |
| H9B | −0.1012 | 0.4281 | 0.2563 | 0.096* | |
| C10 | −0.0971 (2) | 0.42235 (16) | 0.37628 (14) | 0.0788 (6) | |
| H10A | −0.1556 | 0.4536 | 0.4057 | 0.095* | |
| H10B | −0.0919 | 0.3577 | 0.4105 | 0.095* | |
| C11 | 0.1433 (2) | 0.42178 (13) | 0.43431 (13) | 0.0630 (5) | |
| C12 | 0.1029 (2) | 0.38431 (14) | 0.51991 (13) | 0.0713 (5) | |
| H12 | 0.0078 | 0.3714 | 0.5316 | 0.086* | |
| C13 | 0.2019 (3) | 0.36627 (15) | 0.58727 (14) | 0.0776 (6) | |
| H13 | 0.1743 | 0.3402 | 0.6445 | 0.093* | |
| C14 | 0.3413 (3) | 0.38636 (16) | 0.57095 (15) | 0.0823 (6) | |
| H14 | 0.4080 | 0.3749 | 0.6167 | 0.099* | |
| C15 | 0.3817 (2) | 0.42369 (13) | 0.48619 (14) | 0.0720 (5) | |

| | | | | |
|---|---|---|---|---|
| H15 | 0.4765 | 0.4372 | 0.4757 | 0.086* |
| C16 | 0.2861 (2) | 0.44200 (12) | 0.41563 (12) | 0.0601 (5) |
| C17 | 0.3411 (2) | 0.47976 (13) | 0.32785 (14) | 0.0654 (5) |
| C18 | 0.2732 (2) | 0.49489 (13) | 0.25304 (13) | 0.0716 (6) |
| H18 | 0.1781 | 0.4823 | 0.2549 | 0.086* |
| C19 | 0.3368 (2) | 0.52898 (12) | 0.17062 (13) | 0.0663 (5) |
| C20 | 0.7253 (2) | −0.13378 (14) | 0.66919 (13) | 0.0646 (5) |
| C21 | 0.6521 (2) | −0.17445 (13) | 0.75325 (13) | 0.0626 (5) |
| C22 | 0.6970 (3) | −0.26840 (16) | 0.80557 (16) | 0.0811 (6) |
| H22 | 0.7659 | −0.3022 | 0.7855 | 0.097* |
| C23 | 0.6422 (3) | −0.31261 (17) | 0.88618 (18) | 0.0928 (7) |
| H23 | 0.6719 | −0.3754 | 0.9190 | 0.111* |
| C24 | 0.5441 (3) | −0.26358 (19) | 0.91737 (18) | 0.0963 (7) |
| H24 | 0.5100 | −0.2930 | 0.9726 | 0.116* |
| C25 | 0.4957 (3) | −0.17205 (16) | 0.86847 (15) | 0.0809 (6) |
| H25 | 0.4280 | −0.1395 | 0.8903 | 0.097* |
| C26 | 0.5470 (2) | −0.12669 (14) | 0.78589 (13) | 0.0644 (5) |
| C27 | 0.3856 (2) | 0.01519 (14) | 0.76303 (13) | 0.0705 (5) |
| H27A | 0.4206 | 0.0144 | 0.8160 | 0.085* |
| H27B | 0.2971 | −0.0108 | 0.7746 | 0.085* |
| C28 | 0.3489 (2) | 0.11039 (14) | 0.69007 (12) | 0.0674 (5) |
| H28A | 0.4423 | 0.1304 | 0.6721 | 0.081* |
| H28B | 0.2909 | 0.1495 | 0.7121 | 0.081* |
| C29 | 0.2608 (2) | 0.12287 (15) | 0.60977 (13) | 0.0698 (5) |
| H29A | 0.2617 | 0.0635 | 0.6148 | 0.084* |
| H29B | 0.1569 | 0.1520 | 0.6090 | 0.084* |
| C30 | 0.3217 (2) | 0.17845 (14) | 0.52471 (12) | 0.0666 (5) |
| H30A | 0.2539 | 0.1920 | 0.4757 | 0.080* |
| H30B | 0.3349 | 0.2352 | 0.5213 | 0.080* |
| C31 | 0.5525 (2) | 0.15677 (13) | 0.45736 (12) | 0.0564 (4) |
| C32 | 0.5141 (2) | 0.24309 (14) | 0.38767 (12) | 0.0672 (5) |
| H32 | 0.4224 | 0.2812 | 0.3844 | 0.081* |
| C33 | 0.6110 (3) | 0.27270 (17) | 0.32327 (15) | 0.0850 (6) |
| H33 | 0.5843 | 0.3307 | 0.2763 | 0.102* |
| C34 | 0.7463 (3) | 0.2176 (2) | 0.32775 (18) | 0.1040 (8) |
| H34 | 0.8125 | 0.2382 | 0.2845 | 0.125* |
| C35 | 0.7843 (3) | 0.13101 (18) | 0.39687 (16) | 0.0888 (7) |
| H35 | 0.8769 | 0.0940 | 0.3994 | 0.107* |
| C36 | 0.6886 (2) | 0.09715 (14) | 0.46310 (12) | 0.0611 (5) |
| C37 | 0.7366 (2) | 0.00422 (16) | 0.53391 (14) | 0.0654 (5) |
| C38 | 0.6604 (2) | −0.04329 (13) | 0.60039 (12) | 0.0615 (5) |
| H38 | 0.5610 | −0.0171 | 0.6027 | 0.074* |
| C39 | 0.93750 (19) | 0.19043 (12) | 0.74456 (11) | 0.0533 (4) |
| C40 | 0.8673 (2) | 0.28237 (13) | 0.69700 (13) | 0.0678 (5) |
| H40 | 0.8908 | 0.3236 | 0.7134 | 0.081* |
| C41 | 0.7645 (2) | 0.31371 (15) | 0.62675 (15) | 0.0797 (6) |
| H41 | 0.7184 | 0.3751 | 0.5969 | 0.096* |
| C42 | 0.7305 (2) | 0.25418 (16) | 0.60102 (15) | 0.0810 (6) |

| | | | | | |
|---|---|---|---|---|---|
| H42 | 0.6623 | 0.2754 | 0.5529 | 0.097* | |
| C43 | 0.7958 (2) | 0.16383 (14) | 0.64527 (13) | 0.0697 (5) | |
| H43 | 0.7717 | 0.1240 | 0.6270 | 0.084* | |
| C44 | 0.89803 (19) | 0.13060 (12) | 0.71742 (11) | 0.0546 (4) | |
| C45 | 0.9246 (2) | −0.02235 (13) | 0.73831 (13) | 0.0680 (5) | |
| H45A | 0.9565 | −0.0116 | 0.6809 | 0.082* | |
| H45B | 0.8162 | −0.0159 | 0.7369 | 0.082* | |
| C46 | 1.0010 (2) | −0.11563 (13) | 0.80595 (13) | 0.0671 (5) | |
| H46A | 1.1071 | −0.1172 | 0.8130 | 0.081* | |
| H46B | 0.9933 | −0.1587 | 0.7848 | 0.081* | |
| C47 | 0.9366 (2) | −0.14613 (13) | 0.89507 (13) | 0.0699 (5) | |
| H47A | 0.8698 | −0.0941 | 0.8960 | 0.084* | |
| H47B | 0.8769 | −0.1901 | 0.9030 | 0.084* | |
| C48 | 1.0545 (2) | −0.18769 (13) | 0.97021 (13) | 0.0692 (5) | |
| H48A | 1.0096 | −0.2139 | 1.0256 | 0.083* | |
| H48B | 1.1307 | −0.2349 | 0.9666 | 0.083* | |
| C49 | 1.2255 (2) | −0.12862 (13) | 1.02307 (11) | 0.0564 (4) | |
| C50 | 1.2922 (2) | −0.21385 (14) | 1.08800 (13) | 0.0709 (5) | |
| H50 | 1.2628 | −0.2649 | 1.0921 | 0.085* | |
| C51 | 1.4023 (3) | −0.22336 (17) | 1.14669 (14) | 0.0836 (6) | |
| H51 | 1.4475 | −0.2810 | 1.1902 | 0.100* | |
| C52 | 1.4454 (3) | −0.14910 (19) | 1.14138 (15) | 0.0945 (7) | |
| H52 | 1.5192 | −0.1558 | 1.1814 | 0.113* | |
| C53 | 1.3792 (2) | −0.06407 (17) | 1.07647 (14) | 0.0808 (6) | |
| H53 | 1.4099 | −0.0139 | 1.0735 | 0.097* | |
| C54 | 1.26825 (19) | −0.05043 (13) | 1.01523 (11) | 0.0557 (4) | |
| C55 | 1.2065 (2) | 0.04182 (13) | 0.94696 (12) | 0.0569 (4) | |
| H55 | 1.2542 | 0.0861 | 0.9449 | 0.068* | |
| C56 | 1.09217 (19) | 0.07140 (12) | 0.88751 (11) | 0.0534 (4) | |
| H56 | 1.0363 | 0.0303 | 0.8898 | 0.064* | |
| C57 | 1.0495 (2) | 0.16541 (12) | 0.81842 (12) | 0.0554 (4) | |
| O1 | 0.4695 (2) | 0.54064 (15) | 0.16521 (13) | 0.1011 (9) | 0.797 (4) |
| O1′ | 0.4746 (8) | 0.4998 (7) | 0.3293 (9) | 0.100 (3) | 0.204 (4) |
| O2 | 0.01235 (14) | 0.56378 (11) | 0.14559 (9) | 0.0789 (4) | |
| O3 | 0.05022 (15) | 0.44048 (11) | 0.36520 (9) | 0.0831 (4) | |
| O4 | 0.84438 (19) | −0.17918 (15) | 0.66161 (14) | 0.0896 (7) | 0.907 (4) |
| O4′ | 0.8606 (10) | −0.036 (2) | 0.519 (2) | 0.121 (9) | 0.095 (4) |
| O5 | 0.50151 (15) | −0.03546 (9) | 0.73550 (8) | 0.0712 (4) | |
| O6 | 0.46332 (14) | 0.12368 (9) | 0.52412 (8) | 0.0669 (4) | |
| O7 | 1.10487 (18) | 0.22515 (9) | 0.81922 (10) | 0.0826 (4) | |
| O8 | 0.96687 (14) | 0.04133 (8) | 0.76207 (8) | 0.0635 (3) | |
| O9 | 1.11850 (16) | −0.11450 (8) | 0.96222 (8) | 0.0692 (4) | |
| H17 | 0.4431 (7) | 0.4810 (13) | 0.327 (3) | 0.083* | 0.797 (4) |
| H19 | 0.4298 (5) | 0.5422 (5) | 0.1523 (6) | 0.083* | 0.204 (4) |
| H37 | 0.8275 (6) | −0.024 (3) | 0.522 (3) | 0.083* | 0.907 (4) |
| H20 | 0.815 (2) | −0.166 (11) | 0.662 (11) | 0.083* | 0.095 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0621 (12) | 0.0419 (10) | 0.0679 (12) | −0.0111 (8) | 0.0108 (9) | −0.0222 (9) |
| C2 | 0.0787 (14) | 0.0573 (12) | 0.0780 (14) | −0.0147 (10) | 0.0209 (12) | −0.0257 (11) |
| C3 | 0.108 (2) | 0.0759 (15) | 0.0725 (15) | −0.0216 (13) | 0.0268 (14) | −0.0332 (12) |
| C4 | 0.114 (2) | 0.0695 (14) | 0.0671 (14) | −0.0258 (13) | 0.0062 (13) | −0.0332 (11) |
| C5 | 0.0821 (14) | 0.0606 (12) | 0.0723 (13) | −0.0221 (10) | 0.0007 (11) | −0.0308 (11) |
| C6 | 0.0680 (13) | 0.0512 (11) | 0.0638 (12) | −0.0162 (9) | 0.0098 (10) | −0.0271 (9) |
| C7 | 0.0511 (11) | 0.0862 (15) | 0.0838 (14) | −0.0082 (10) | −0.0030 (10) | −0.0397 (12) |
| C8 | 0.0482 (11) | 0.0897 (16) | 0.0924 (15) | −0.0108 (10) | 0.0067 (10) | −0.0482 (13) |
| C9 | 0.0614 (13) | 0.0990 (18) | 0.0937 (16) | −0.0342 (12) | 0.0097 (11) | −0.0503 (14) |
| C10 | 0.0625 (13) | 0.0915 (16) | 0.0852 (15) | −0.0322 (11) | 0.0170 (11) | −0.0378 (13) |
| C11 | 0.0589 (12) | 0.0605 (12) | 0.0649 (12) | −0.0069 (9) | 0.0030 (9) | −0.0277 (10) |
| C12 | 0.0671 (13) | 0.0722 (14) | 0.0730 (13) | −0.0095 (10) | 0.0118 (11) | −0.0352 (11) |
| C13 | 0.0893 (17) | 0.0758 (15) | 0.0682 (13) | −0.0053 (12) | 0.0098 (12) | −0.0394 (11) |
| C14 | 0.0887 (17) | 0.0839 (16) | 0.0762 (15) | −0.0056 (13) | −0.0079 (12) | −0.0434 (13) |
| C15 | 0.0661 (13) | 0.0657 (13) | 0.0821 (15) | −0.0076 (10) | −0.0037 (11) | −0.0349 (11) |
| C16 | 0.0546 (11) | 0.0507 (11) | 0.0690 (12) | −0.0038 (8) | −0.0004 (9) | −0.0257 (9) |
| C17 | 0.0504 (11) | 0.0567 (12) | 0.0773 (14) | −0.0054 (9) | 0.0035 (11) | −0.0239 (10) |
| C18 | 0.0493 (11) | 0.0829 (15) | 0.0690 (13) | −0.0173 (10) | 0.0036 (10) | −0.0227 (11) |
| C19 | 0.0566 (12) | 0.0562 (12) | 0.0761 (13) | −0.0092 (9) | 0.0065 (10) | −0.0239 (10) |
| C20 | 0.0573 (12) | 0.0747 (14) | 0.0786 (13) | −0.0071 (10) | −0.0052 (10) | −0.0521 (12) |
| C21 | 0.0588 (11) | 0.0622 (12) | 0.0732 (12) | −0.0139 (9) | −0.0088 (9) | −0.0358 (10) |
| C22 | 0.0760 (14) | 0.0733 (15) | 0.0978 (17) | −0.0102 (12) | −0.0179 (13) | −0.0440 (14) |
| C23 | 0.0973 (19) | 0.0671 (15) | 0.0985 (19) | −0.0282 (14) | −0.0157 (15) | −0.0203 (14) |
| C24 | 0.0984 (19) | 0.0875 (19) | 0.0934 (18) | −0.0382 (15) | 0.0097 (15) | −0.0268 (16) |
| C25 | 0.0810 (15) | 0.0785 (16) | 0.0796 (15) | −0.0282 (12) | 0.0141 (12) | −0.0299 (13) |
| C26 | 0.0610 (12) | 0.0670 (13) | 0.0699 (12) | −0.0207 (10) | 0.0024 (10) | −0.0328 (11) |
| C27 | 0.0714 (13) | 0.0829 (15) | 0.0701 (12) | −0.0177 (11) | 0.0212 (10) | −0.0469 (12) |
| C28 | 0.0715 (13) | 0.0739 (14) | 0.0701 (12) | −0.0128 (10) | 0.0194 (10) | −0.0466 (11) |
| C29 | 0.0526 (11) | 0.0845 (14) | 0.0787 (13) | −0.0106 (10) | 0.0152 (10) | −0.0457 (12) |
| C30 | 0.0570 (11) | 0.0759 (13) | 0.0704 (12) | −0.0012 (10) | 0.0084 (9) | −0.0426 (11) |
| C31 | 0.0556 (11) | 0.0716 (13) | 0.0587 (11) | −0.0166 (9) | 0.0090 (8) | −0.0433 (10) |
| C32 | 0.0712 (13) | 0.0709 (14) | 0.0661 (12) | −0.0156 (10) | 0.0090 (10) | −0.0375 (11) |
| C33 | 0.0911 (17) | 0.0847 (16) | 0.0788 (15) | −0.0267 (14) | 0.0202 (13) | −0.0353 (13) |
| C34 | 0.100 (2) | 0.105 (2) | 0.0972 (19) | −0.0329 (17) | 0.0438 (15) | −0.0366 (17) |
| C35 | 0.0691 (14) | 0.1033 (19) | 0.0983 (17) | −0.0151 (13) | 0.0281 (13) | −0.0532 (16) |
| C36 | 0.0560 (11) | 0.0763 (14) | 0.0653 (12) | −0.0148 (10) | 0.0089 (9) | −0.0450 (11) |
| C37 | 0.0502 (11) | 0.0862 (15) | 0.0769 (13) | −0.0054 (11) | 0.0042 (11) | −0.0561 (12) |
| C38 | 0.0540 (11) | 0.0717 (13) | 0.0677 (12) | −0.0020 (10) | 0.0015 (9) | −0.0445 (11) |
| C39 | 0.0499 (10) | 0.0532 (11) | 0.0595 (10) | −0.0126 (8) | 0.0129 (8) | −0.0282 (9) |
| C40 | 0.0667 (12) | 0.0571 (12) | 0.0801 (13) | −0.0163 (10) | 0.0156 (11) | −0.0317 (11) |
| C41 | 0.0701 (14) | 0.0611 (13) | 0.0848 (15) | −0.0014 (11) | −0.0053 (12) | −0.0192 (12) |
| C42 | 0.0704 (14) | 0.0776 (16) | 0.0792 (14) | −0.0040 (12) | −0.0134 (11) | −0.0272 (13) |
| C43 | 0.0657 (12) | 0.0718 (14) | 0.0712 (13) | −0.0082 (10) | −0.0069 (10) | −0.0351 (11) |
| C44 | 0.0491 (10) | 0.0569 (11) | 0.0592 (11) | −0.0095 (8) | 0.0053 (8) | −0.0290 (9) |
| C45 | 0.0749 (13) | 0.0705 (13) | 0.0748 (13) | −0.0138 (10) | −0.0067 (10) | −0.0474 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C46 | 0.0723 (13) | 0.0632 (12) | 0.0829 (14) | −0.0085 (10) | −0.0070 (10) | −0.0501 (11) |
| C47 | 0.0722 (13) | 0.0606 (12) | 0.0876 (14) | −0.0209 (10) | 0.0005 (11) | −0.0406 (11) |
| C48 | 0.0858 (14) | 0.0536 (12) | 0.0744 (13) | −0.0209 (10) | −0.0016 (11) | −0.0321 (10) |
| C49 | 0.0562 (11) | 0.0631 (12) | 0.0539 (10) | −0.0095 (9) | 0.0047 (8) | −0.0321 (9) |
| C50 | 0.0760 (14) | 0.0668 (13) | 0.0653 (12) | −0.0101 (11) | 0.0009 (11) | −0.0289 (11) |
| C51 | 0.0762 (15) | 0.0821 (16) | 0.0709 (14) | −0.0058 (12) | −0.0059 (11) | −0.0218 (12) |
| C52 | 0.0787 (16) | 0.112 (2) | 0.0822 (16) | −0.0230 (15) | −0.0214 (13) | −0.0337 (16) |
| C53 | 0.0742 (14) | 0.0912 (17) | 0.0804 (14) | −0.0287 (12) | −0.0087 (12) | −0.0376 (13) |
| C54 | 0.0499 (10) | 0.0691 (12) | 0.0569 (10) | −0.0167 (9) | 0.0062 (8) | −0.0352 (10) |
| C55 | 0.0574 (11) | 0.0632 (12) | 0.0663 (11) | −0.0226 (9) | 0.0090 (9) | −0.0399 (10) |
| C56 | 0.0574 (11) | 0.0568 (11) | 0.0588 (10) | −0.0195 (8) | 0.0089 (9) | −0.0349 (9) |
| C57 | 0.0579 (11) | 0.0554 (11) | 0.0649 (11) | −0.0177 (9) | 0.0146 (9) | −0.0362 (10) |
| O1 | 0.0545 (12) | 0.139 (2) | 0.0884 (14) | −0.0309 (12) | 0.0096 (10) | −0.0315 (13) |
| O1′ | 0.079 (6) | 0.142 (8) | 0.090 (6) | −0.063 (5) | 0.018 (4) | −0.047 (6) |
| O2 | 0.0511 (8) | 0.1105 (12) | 0.0688 (9) | −0.0109 (7) | 0.0041 (6) | −0.0391 (8) |
| O3 | 0.0572 (8) | 0.1169 (12) | 0.0693 (9) | −0.0312 (8) | 0.0090 (7) | −0.0337 (8) |
| O4 | 0.0751 (12) | 0.0944 (13) | 0.0961 (13) | 0.0129 (9) | 0.0005 (9) | −0.0541 (10) |
| O4′ | 0.052 (10) | 0.097 (15) | 0.162 (19) | 0.027 (10) | 0.005 (12) | −0.034 (13) |
| O5 | 0.0779 (9) | 0.0655 (9) | 0.0703 (8) | −0.0123 (7) | 0.0215 (7) | −0.0338 (7) |
| O6 | 0.0605 (8) | 0.0707 (9) | 0.0639 (8) | −0.0012 (6) | 0.0161 (6) | −0.0324 (7) |
| O7 | 0.1009 (11) | 0.0641 (9) | 0.0927 (10) | −0.0327 (8) | −0.0031 (8) | −0.0382 (8) |
| O8 | 0.0721 (8) | 0.0557 (8) | 0.0694 (8) | −0.0076 (6) | −0.0115 (6) | −0.0363 (7) |
| O9 | 0.0904 (10) | 0.0537 (8) | 0.0676 (8) | −0.0195 (7) | −0.0140 (7) | −0.0289 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.388 (3) | C29—H29A | 0.9700 |
| C1—C6 | 1.406 (3) | C29—H29B | 0.9700 |
| C1—C19 | 1.487 (3) | C30—O6 | 1.428 (2) |
| C2—C3 | 1.372 (3) | C30—H30A | 0.9700 |
| C2—H2 | 0.9300 | C30—H30B | 0.9700 |
| C3—C4 | 1.371 (3) | C31—O6 | 1.358 (2) |
| C3—H3 | 0.9300 | C31—C32 | 1.381 (3) |
| C4—C5 | 1.370 (3) | C31—C36 | 1.402 (2) |
| C4—H4 | 0.9300 | C32—C33 | 1.372 (3) |
| C5—C6 | 1.386 (3) | C32—H32 | 0.9300 |
| C5—H5 | 0.9300 | C33—C34 | 1.364 (3) |
| C6—O2 | 1.353 (2) | C33—H33 | 0.9300 |
| C7—O2 | 1.433 (2) | C34—C35 | 1.379 (3) |
| C7—C8 | 1.499 (3) | C34—H34 | 0.9300 |
| C7—H7A | 0.9700 | C35—C36 | 1.394 (3) |
| C7—H7B | 0.9700 | C35—H35 | 0.9300 |
| C8—C9 | 1.521 (3) | C36—C37 | 1.464 (3) |
| C8—H8A | 0.9700 | C37—O4′ | 1.276 (9) |
| C8—H8B | 0.9700 | C37—C38 | 1.336 (3) |
| C9—C10 | 1.500 (3) | C37—H37 | 0.935 (5) |
| C9—H9A | 0.9700 | C38—H38 | 0.9300 |
| C9—H9B | 0.9700 | C39—C40 | 1.399 (3) |

| | | | |
|---|---|---|---|
| C10—O3 | 1.425 (2) | C39—C44 | 1.407 (2) |
| C10—H10A | 0.9700 | C39—C57 | 1.496 (2) |
| C10—H10B | 0.9700 | C40—C41 | 1.375 (3) |
| C11—O3 | 1.355 (2) | C40—H40 | 0.9300 |
| C11—C12 | 1.388 (3) | C41—C42 | 1.366 (3) |
| C11—C16 | 1.404 (3) | C41—H41 | 0.9300 |
| C12—C13 | 1.369 (3) | C42—C43 | 1.364 (3) |
| C12—H12 | 0.9300 | C42—H42 | 0.9300 |
| C13—C14 | 1.370 (3) | C43—C44 | 1.391 (3) |
| C13—H13 | 0.9300 | C43—H43 | 0.9300 |
| C14—C15 | 1.376 (3) | C44—O8 | 1.358 (2) |
| C14—H14 | 0.9300 | C45—O8 | 1.440 (2) |
| C15—C16 | 1.391 (3) | C45—C46 | 1.497 (3) |
| C15—H15 | 0.9300 | C45—H45A | 0.9700 |
| C16—C17 | 1.468 (3) | C45—H45B | 0.9700 |
| C17—O1′ | 1.331 (6) | C46—C47 | 1.524 (3) |
| C17—C18 | 1.337 (3) | C46—H46A | 0.9700 |
| C17—H17 | 0.933 (5) | C46—H46B | 0.9700 |
| C18—C19 | 1.425 (3) | C47—C48 | 1.501 (3) |
| C18—H18 | 0.9300 | C47—H47A | 0.9700 |
| C19—O1 | 1.258 (2) | C47—H47B | 0.9700 |
| C19—H19 | 0.930 (5) | C48—O9 | 1.428 (2) |
| C20—O4 | 1.235 (2) | C48—H48A | 0.9700 |
| C20—C38 | 1.451 (3) | C48—H48B | 0.9700 |
| C20—C21 | 1.497 (3) | C49—O9 | 1.355 (2) |
| C20—H20 | 0.930 (5) | C49—C50 | 1.379 (3) |
| C21—C22 | 1.397 (3) | C49—C54 | 1.406 (2) |
| C21—C26 | 1.400 (3) | C50—C51 | 1.377 (3) |
| C22—C23 | 1.380 (3) | C50—H50 | 0.9300 |
| C22—H22 | 0.9300 | C51—C52 | 1.359 (3) |
| C23—C24 | 1.364 (4) | C51—H51 | 0.9300 |
| C23—H23 | 0.9300 | C52—C53 | 1.375 (3) |
| C24—C25 | 1.361 (3) | C52—H52 | 0.9300 |
| C24—H24 | 0.9300 | C53—C54 | 1.388 (3) |
| C25—C26 | 1.395 (3) | C53—H53 | 0.9300 |
| C25—H25 | 0.9300 | C54—C55 | 1.460 (3) |
| C26—O5 | 1.357 (2) | C55—C56 | 1.325 (2) |
| C27—O5 | 1.433 (2) | C55—H55 | 0.9300 |
| C27—C28 | 1.496 (3) | C56—C57 | 1.462 (2) |
| C27—H27A | 0.9700 | C56—H56 | 0.9300 |
| C27—H27B | 0.9700 | C57—O7 | 1.228 (2) |
| C28—C29 | 1.527 (3) | O1—H19 | 0.420 (5) |
| C28—H28A | 0.9700 | O1′—H17 | 0.484 (15) |
| C28—H28B | 0.9700 | O4—H20 | 0.31 (3) |
| C29—C30 | 1.500 (3) | O4′—H37 | 0.342 (12) |
| | | | |
| C2—C1—C6 | 117.19 (18) | C28—C29—H29B | 108.8 |
| C2—C1—C19 | 116.88 (18) | H29A—C29—H29B | 107.7 |

| | | | |
|---|---|---|---|
| C6—C1—C19 | 125.91 (17) | O6—C30—C29 | 105.39 (16) |
| C3—C2—C1 | 122.5 (2) | O6—C30—H30A | 110.7 |
| C3—C2—H2 | 118.7 | C29—C30—H30A | 110.7 |
| C1—C2—H2 | 118.7 | O6—C30—H30B | 110.7 |
| C4—C3—C2 | 119.1 (2) | C29—C30—H30B | 110.7 |
| C4—C3—H3 | 120.4 | H30A—C30—H30B | 108.8 |
| C2—C3—H3 | 120.4 | O6—C31—C32 | 123.27 (17) |
| C5—C4—C3 | 120.5 (2) | O6—C31—C36 | 115.58 (17) |
| C5—C4—H4 | 119.7 | C32—C31—C36 | 121.15 (17) |
| C3—C4—H4 | 119.7 | C33—C32—C31 | 120.1 (2) |
| C4—C5—C6 | 120.5 (2) | C33—C32—H32 | 119.9 |
| C4—C5—H5 | 119.8 | C31—C32—H32 | 119.9 |
| C6—C5—H5 | 119.8 | C34—C33—C32 | 120.4 (2) |
| O2—C6—C5 | 122.91 (18) | C34—C33—H33 | 119.8 |
| O2—C6—C1 | 116.99 (17) | C32—C33—H33 | 119.8 |
| C5—C6—C1 | 120.09 (18) | C33—C34—C35 | 119.5 (2) |
| O2—C7—C8 | 105.59 (16) | C33—C34—H34 | 120.2 |
| O2—C7—H7A | 110.6 | C35—C34—H34 | 120.2 |
| C8—C7—H7A | 110.6 | C34—C35—C36 | 122.2 (2) |
| O2—C7—H7B | 110.6 | C34—C35—H35 | 118.9 |
| C8—C7—H7B | 110.6 | C36—C35—H35 | 118.9 |
| H7A—C7—H7B | 108.8 | C35—C36—C31 | 116.46 (19) |
| C7—C8—C9 | 113.87 (18) | C35—C36—C37 | 118.94 (18) |
| C7—C8—H8A | 108.8 | C31—C36—C37 | 124.58 (17) |
| C9—C8—H8A | 108.8 | O4′—C37—C38 | 119.5 (18) |
| C7—C8—H8B | 108.8 | O4′—C37—C36 | 110.8 (18) |
| C9—C8—H8B | 108.8 | C38—C37—C36 | 128.95 (17) |
| H8A—C8—H8B | 107.7 | O4′—C37—H37 | 1 (5) |
| C10—C9—C8 | 114.65 (18) | C38—C37—H37 | 121 (3) |
| C10—C9—H9A | 108.6 | C36—C37—H37 | 109 (3) |
| C8—C9—H9A | 108.6 | C37—C38—C20 | 123.12 (18) |
| C10—C9—H9B | 108.6 | C37—C38—H38 | 118.4 |
| C8—C9—H9B | 108.6 | C20—C38—H38 | 118.4 |
| H9A—C9—H9B | 107.6 | C40—C39—C44 | 116.89 (17) |
| O3—C10—C9 | 105.56 (16) | C40—C39—C57 | 116.85 (16) |
| O3—C10—H10A | 110.6 | C44—C39—C57 | 126.25 (16) |
| C9—C10—H10A | 110.6 | C41—C40—C39 | 122.10 (19) |
| O3—C10—H10B | 110.6 | C41—C40—H40 | 119.0 |
| C9—C10—H10B | 110.6 | C39—C40—H40 | 119.0 |
| H10A—C10—H10B | 108.8 | C42—C41—C40 | 119.6 (2) |
| O3—C11—C12 | 123.02 (18) | C42—C41—H41 | 120.2 |
| O3—C11—C16 | 116.58 (17) | C40—C41—H41 | 120.2 |
| C12—C11—C16 | 120.39 (19) | C43—C42—C41 | 120.6 (2) |
| C13—C12—C11 | 120.5 (2) | C43—C42—H42 | 119.7 |
| C13—C12—H12 | 119.7 | C41—C42—H42 | 119.7 |
| C11—C12—H12 | 119.7 | C42—C43—C44 | 120.7 (2) |
| C12—C13—C14 | 120.4 (2) | C42—C43—H43 | 119.7 |
| C12—C13—H13 | 119.8 | C44—C43—H43 | 119.7 |

| | | | |
|---|---|---|---|
| C14—C13—H13 | 119.8 | O8—C44—C43 | 122.17 (16) |
| C13—C14—C15 | 119.3 (2) | O8—C44—C39 | 117.63 (15) |
| C13—C14—H14 | 120.4 | C43—C44—C39 | 120.16 (17) |
| C15—C14—H14 | 120.4 | O8—C45—C46 | 107.12 (14) |
| C14—C15—C16 | 122.5 (2) | O8—C45—H45A | 110.3 |
| C14—C15—H15 | 118.7 | C46—C45—H45A | 110.3 |
| C16—C15—H15 | 118.7 | O8—C45—H45B | 110.3 |
| C15—C16—C11 | 116.87 (18) | C46—C45—H45B | 110.3 |
| C15—C16—C17 | 118.42 (18) | H45A—C45—H45B | 108.5 |
| C11—C16—C17 | 124.71 (18) | C45—C46—C47 | 114.28 (16) |
| O1′—C17—C18 | 121.0 (6) | C45—C46—H46A | 108.7 |
| O1′—C17—C16 | 111.1 (6) | C47—C46—H46A | 108.7 |
| C18—C17—C16 | 127.94 (18) | C45—C46—H46B | 108.7 |
| O1′—C17—H17 | 14.2 (12) | C47—C46—H46B | 108.7 |
| C18—C17—H17 | 116 (3) | H46A—C46—H46B | 107.6 |
| C16—C17—H17 | 114 (3) | C48—C47—C46 | 113.72 (17) |
| C17—C18—C19 | 124.49 (19) | C48—C47—H47A | 108.8 |
| C17—C18—H18 | 117.8 | C46—C47—H47A | 108.8 |
| C19—C18—H18 | 117.8 | C48—C47—H47B | 108.8 |
| O1—C19—C18 | 120.5 (2) | C46—C47—H47B | 108.8 |
| O1—C19—C1 | 116.98 (19) | H47A—C47—H47B | 107.7 |
| C18—C19—C1 | 122.37 (18) | O9—C48—C47 | 105.23 (15) |
| O1—C19—H19 | 13.9 (6) | O9—C48—H48A | 110.7 |
| C18—C19—H19 | 134.5 (6) | C47—C48—H48A | 110.7 |
| C1—C19—H19 | 103.1 (6) | O9—C48—H48B | 110.7 |
| O4—C20—C38 | 121.5 (2) | C47—C48—H48B | 110.7 |
| O4—C20—C21 | 117.6 (2) | H48A—C48—H48B | 108.8 |
| C38—C20—C21 | 120.96 (17) | O9—C49—C50 | 123.04 (17) |
| O4—C20—H20 | 2 (10) | O9—C49—C54 | 115.83 (16) |
| C38—C20—H20 | 120 (10) | C50—C49—C54 | 121.12 (17) |
| C21—C20—H20 | 119 (10) | C51—C50—C49 | 120.0 (2) |
| C22—C21—C26 | 116.9 (2) | C51—C50—H50 | 120.0 |
| C22—C21—C20 | 116.97 (19) | C49—C50—H50 | 120.0 |
| C26—C21—C20 | 126.07 (18) | C52—C51—C50 | 120.4 (2) |
| C23—C22—C21 | 122.0 (2) | C52—C51—H51 | 119.8 |
| C23—C22—H22 | 119.0 | C50—C51—H51 | 119.8 |
| C21—C22—H22 | 119.0 | C51—C52—C53 | 119.7 (2) |
| C24—C23—C22 | 119.6 (2) | C51—C52—H52 | 120.2 |
| C24—C23—H23 | 120.2 | C53—C52—H52 | 120.2 |
| C22—C23—H23 | 120.2 | C52—C53—C54 | 122.4 (2) |
| C25—C24—C23 | 120.6 (2) | C52—C53—H53 | 118.8 |
| C25—C24—H24 | 119.7 | C54—C53—H53 | 118.8 |
| C23—C24—H24 | 119.7 | C53—C54—C49 | 116.41 (18) |
| C24—C25—C26 | 120.5 (2) | C53—C54—C55 | 119.04 (17) |
| C24—C25—H25 | 119.8 | C49—C54—C55 | 124.54 (16) |
| C26—C25—H25 | 119.8 | C56—C55—C54 | 129.21 (17) |
| O5—C26—C25 | 122.03 (19) | C56—C55—H55 | 115.4 |
| O5—C26—C21 | 117.57 (17) | C54—C55—H55 | 115.4 |

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| C25—C26—C21 | 120.4 (2) | C55—C56—C57 | 123.24 (16) |
| O5—C27—C28 | 106.78 (15) | C55—C56—H56 | 118.4 |
| O5—C27—H27A | 110.4 | C57—C56—H56 | 118.4 |
| C28—C27—H27A | 110.4 | O7—C57—C56 | 121.13 (17) |
| O5—C27—H27B | 110.4 | O7—C57—C39 | 118.62 (16) |
| C28—C27—H27B | 110.4 | C56—C57—C39 | 120.25 (15) |
| H27A—C27—H27B | 108.6 | C19—O1—H19 | 32.3 (13) |
| C27—C28—C29 | 114.89 (17) | C17—O1′—H17 | 28.3 (18) |
| C27—C28—H28A | 108.5 | C6—O2—C7 | 121.20 (15) |
| C29—C28—H28A | 108.5 | C11—O3—C10 | 121.56 (16) |
| C27—C28—H28B | 108.5 | C20—O4—H20 | 5 (10) |
| C29—C28—H28B | 108.5 | C37—O4′—H37 | 4 (10) |
| H28A—C28—H28B | 107.5 | C26—O5—C27 | 119.54 (15) |
| C30—C29—C28 | 113.87 (17) | C31—O6—C30 | 120.30 (15) |
| C30—C29—H29A | 108.8 | C44—O8—C45 | 119.07 (14) |
| C28—C29—H29A | 108.8 | C49—O9—C48 | 120.23 (14) |
| C30—C29—H29B | 108.8 | | |

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| C6—C1—C2—C3 | −0.6 (3) | C32—C31—C36—C35 | 2.4 (3) |
| C19—C1—C2—C3 | −179.13 (19) | O6—C31—C36—C37 | 1.0 (3) |
| C1—C2—C3—C4 | 1.2 (3) | C32—C31—C36—C37 | −178.98 (17) |
| C2—C3—C4—C5 | −1.1 (3) | C35—C36—C37—O4′ | −5.5 (3) |
| C3—C4—C5—C6 | 0.4 (3) | C31—C36—C37—O4′ | 175.9 (3) |
| C4—C5—C6—O2 | 179.27 (18) | C35—C36—C37—C38 | −175.71 (19) |
| C4—C5—C6—C1 | 0.2 (3) | C31—C36—C37—C38 | 5.7 (3) |
| C2—C1—C6—O2 | −179.23 (16) | O4′—C37—C38—C20 | 14.1 (4) |
| C19—C1—C6—O2 | −0.9 (3) | C36—C37—C38—C20 | −176.43 (17) |
| C2—C1—C6—C5 | −0.1 (3) | O4—C20—C38—C37 | −14.3 (3) |
| C19—C1—C6—C5 | 178.27 (17) | C21—C20—C38—C37 | 163.96 (17) |
| O2—C7—C8—C9 | −69.8 (2) | C44—C39—C40—C41 | −0.1 (3) |
| C7—C8—C9—C10 | 135.73 (19) | C57—C39—C40—C41 | 178.80 (17) |
| C8—C9—C10—O3 | −66.2 (2) | C39—C40—C41—C42 | −1.0 (3) |
| O3—C11—C12—C13 | 179.56 (19) | C40—C41—C42—C43 | 1.1 (3) |
| C16—C11—C12—C13 | −0.2 (3) | C41—C42—C43—C44 | 0.0 (3) |
| C11—C12—C13—C14 | 1.1 (3) | C42—C43—C44—O8 | −178.90 (18) |
| C12—C13—C14—C15 | −0.9 (3) | C42—C43—C44—C39 | −1.2 (3) |
| C13—C14—C15—C16 | −0.1 (3) | C40—C39—C44—O8 | 179.03 (15) |
| C14—C15—C16—C11 | 0.9 (3) | C57—C39—C44—O8 | 0.2 (3) |
| C14—C15—C16—C17 | −178.48 (18) | C40—C39—C44—C43 | 1.2 (2) |
| O3—C11—C16—C15 | 179.47 (17) | C57—C39—C44—C43 | −177.58 (17) |
| C12—C11—C16—C15 | −0.7 (3) | O8—C45—C46—C47 | 71.1 (2) |
| O3—C11—C16—C17 | −1.2 (3) | C45—C46—C47—C48 | −133.37 (17) |
| C12—C11—C16—C17 | 178.60 (18) | C46—C47—C48—O9 | 68.7 (2) |
| C15—C16—C17—O1′ | −6.6 (5) | O9—C49—C50—C51 | 178.75 (18) |
| C11—C16—C17—O1′ | 174.1 (5) | C54—C49—C50—C51 | 0.2 (3) |
| C15—C16—C17—C18 | 173.84 (18) | C49—C50—C51—C52 | 0.3 (3) |
| C11—C16—C17—C18 | −5.5 (3) | C50—C51—C52—C53 | −0.5 (4) |
| O1′—C17—C18—C19 | 2.8 (5) | C51—C52—C53—C54 | 0.2 (4) |

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| C16—C17—C18—C19 | −177.69 (17) | C52—C53—C54—C49 | 0.3 (3) |
| C17—C18—C19—O1 | 5.5 (2) | C52—C53—C54—C55 | −178.4 (2) |
| C17—C18—C19—C1 | −170.82 (18) | O9—C49—C54—C53 | −179.17 (16) |
| C2—C1—C19—O1 | 17.7 (3) | C50—C49—C54—C53 | −0.5 (3) |
| C6—C1—C19—O1 | −160.68 (19) | O9—C49—C54—C55 | −0.5 (2) |
| C2—C1—C19—C18 | −165.91 (16) | C50—C49—C54—C55 | 178.11 (17) |
| C6—C1—C19—C18 | 15.7 (3) | C53—C54—C55—C56 | −173.20 (19) |
| O4—C20—C21—C22 | −18.2 (3) | C49—C54—C55—C56 | 8.2 (3) |
| C38—C20—C21—C22 | 163.50 (17) | C54—C55—C56—C57 | −175.25 (16) |
| O4—C20—C21—C26 | 159.25 (18) | C55—C56—C57—O7 | −10.3 (3) |
| C38—C20—C21—C26 | −19.0 (3) | C55—C56—C57—C39 | 169.22 (16) |
| C26—C21—C22—C23 | −0.7 (3) | C40—C39—C57—O7 | −19.8 (2) |
| C20—C21—C22—C23 | 177.04 (18) | C44—C39—C57—O7 | 159.01 (17) |
| C21—C22—C23—C24 | −1.7 (3) | C40—C39—C57—C56 | 160.68 (15) |
| C22—C23—C24—C25 | 2.4 (4) | C44—C39—C57—C56 | −20.5 (3) |
| C23—C24—C25—C26 | −0.7 (4) | C5—C6—O2—C7 | −5.4 (3) |
| C24—C25—C26—O5 | −179.8 (2) | C1—C6—O2—C7 | 173.73 (17) |
| C24—C25—C26—C21 | −1.7 (3) | C8—C7—O2—C6 | 175.49 (17) |
| C22—C21—C26—O5 | −179.53 (17) | C12—C11—O3—C10 | −0.2 (3) |
| C20—C21—C26—O5 | 3.0 (3) | C16—C11—O3—C10 | 179.64 (18) |
| C22—C21—C26—C25 | 2.3 (3) | C9—C10—O3—C11 | 176.79 (18) |
| C20—C21—C26—C25 | −175.11 (18) | C25—C26—O5—C27 | −6.7 (3) |
| O5—C27—C28—C29 | 72.9 (2) | C21—C26—O5—C27 | 175.18 (16) |
| C27—C28—C29—C30 | −133.58 (18) | C28—C27—O5—C26 | −173.76 (16) |
| C28—C29—C30—O6 | 68.8 (2) | C32—C31—O6—C30 | 0.3 (3) |
| O6—C31—C32—C33 | 178.75 (17) | C36—C31—O6—C30 | −179.69 (16) |
| C36—C31—C32—C33 | −1.3 (3) | C29—C30—O6—C31 | −176.31 (15) |
| C31—C32—C33—C34 | −0.5 (3) | C43—C44—O8—C45 | −4.8 (3) |
| C32—C33—C34—C35 | 1.1 (4) | C39—C44—O8—C45 | 177.49 (16) |
| C33—C34—C35—C36 | 0.1 (4) | C46—C45—O8—C44 | −171.89 (15) |
| C34—C35—C36—C31 | −1.8 (3) | C50—C49—O9—C48 | 8.7 (3) |
| C34—C35—C36—C37 | 179.5 (2) | C54—C49—O9—C48 | −172.64 (16) |
| O6—C31—C36—C35 | −177.69 (17) | C47—C48—O9—C49 | 177.11 (15) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O1 | 0.93 | 2.37 | 2.712 (3) | 101 |
| C18—H18···O2 | 0.93 | 2.15 | 2.746 (2) | 121 |
| C18—H18···O3 | 0.93 | 2.12 | 2.763 (2) | 126 |
| C38—H38···O5 | 0.93 | 2.24 | 2.753 (2) | 114 |
| C38—H38···O6 | 0.93 | 2.13 | 2.753 (3) | 123 |
| C55—H55···O7 | 0.93 | 2.50 | 2.829 (2) | 101 |
| C56—H56···O8 | 0.93 | 2.23 | 2.766 (2) | 116 |
| C56—H56···O9 | 0.93 | 2.15 | 2.764 (2) | 122 |