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# 4-Benzyloxy-1,1′-biphenyl

Farook Adam,[a]* Nadiah Ameram,[a] Shevgoor Dhiraj Kamath,[b] Pallavi[c] and Seranthimata Samshuddin[c]

[a]School of Chemical Sciences, Universiti Sains Malaysia, 11800 Pulau Pinang, Malaysia, [b]Department of P.G. Studies in Analytical Chemistry, Alva's College, Moodbidri, Karnataka 574 227, India, and [c]Department of P.G. Studies in Chemistry, Alva's College, Moodbidri, Karnataka 574 227, India. *Correspondence e-mail: farook@usm.my

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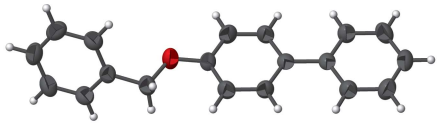
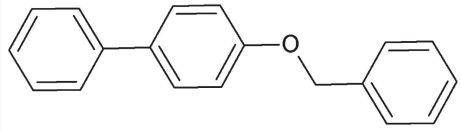
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{19}H_{16}O$, the dihedral angle between the benzene rings of the biphenyl unit is 1.54 (13)° and the C—O—C—C torsion angle is 174.4 (2)°. In the crystal, very weak C—H···$\pi$ interactions link the molecules into a three-dimensional network.

**3D view**



**Chemical scheme**




## Structure description

Many diaryl ethers exhibit various pharmacological properties including anti-bacterial, anti-inflammatory, antifungal and herbicidal activities (Ley & Thomas, 2003; Frlan & Kikelj, 2006). The crystal structures of some aryl ethers *viz*., 2,4-dichloro-1-[1-(2,4 dichlorobenzyloxy)ethyl]benzene (Jasinski *et al.*, 2010) and 2,6-bis[2-(4-benzyloxyphenyl)ethyl]biphenyl (Moratti *et al.*, 2007) have been reported. As part of our studies in this area, the synthesis and structure of the title compound are reported.

The title molecule (Fig. 1) consists of three benzene rings, C1–C6 (*A*), C7–C12 (*B*) and C14–C19 (*C*). The dihedral angles *A*/*B*, *A*/*C* and *B*/*C* are 1.54 (13), 61.50 (14) and 62.80 (14)°, respectively. Five weak C—H···$\pi$ interactions are observed in the crystal structure (Table 1). The crystal packing is illustrated in Fig. 2.

## Synthesis and crystallization

A mixture of (1,1′-biphenyl)-4-ol (1.70 g, 0.01 mol) and benzyl chloride (5 ml) was refluxed for 30 min. The reaction mixture was cooled and poured into 25 ml hexane. The precipitate was collected by filtration and purified by recrystallization from ethanol. Single crystals were grown from 1,4-dioxane solution by the slow evaporation method; m.p. 421–425 K, yield 85%.

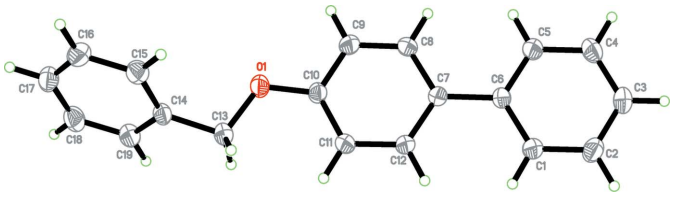



**Figure 1**
The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

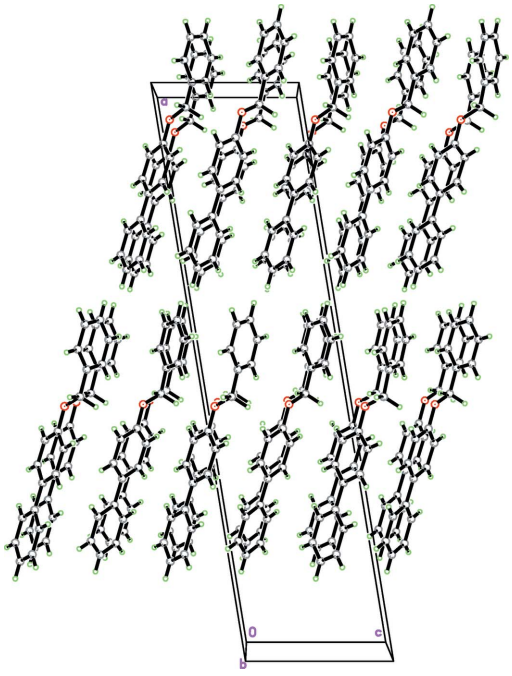



**Figure 2**
The crystal packing, viewed along the *b* axis.

## Refinement

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

## Acknowledgements

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C7–C12 and C14–C19 benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1*A*···*Cg*1$^{i}$ | 0.93 | 2.99 | 3.700 (3) | 134 |
| C4—H4*A*···*Cg*1$^{ii}$ | 0.93 | 2.97 | 3.700 (3) | 134 |
| C8—H8*A*···*Cg*2$^{ii}$ | 0.93 | 2.96 | 3.687 (3) | 137 |
| C11—H11*A*···*Cg*2$^{i}$ | 0.93 | 2.93 | 3.650 (3) | 135 |
| C19—H19*A*···*Cg*3$^{iii}$ | 0.93 | 2.90 | 3.591 (3) | 133 |

Symmetry codes: (i) $x, -y+1, z+\frac{1}{2}$; (ii) $x, -y, z-\frac{1}{2}$; (iii) $x, -y+1, z-\frac{1}{2}$.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{19}H_{16}O$ |
| $M_r$ | 260.32 |
| Crystal system, space group | Monoclinic, *Cc* |
| Temperature (K) | 296 |
| *a*, *b*, *c* (Å) | 31.270 (2), 5.6720 (4), 7.8812 (5) |
| $\beta$ (°) | 99.271 (3) |
| *V* (Å$^3$) | 1379.58 (16) |
| *Z* | 4 |
| Radiation type | Mo *K*$\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.08 |
| Crystal size (mm) | 0.39 × 0.31 × 0.09 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2010) |
| $T_{min}$, $T_{max}$ | 0.891, 0.969 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 18200, 2435, 2218 |
| $R_{int}$ | 0.027 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.595 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.034, 0.104, 0.87 |
| No. of reflections | 2435 |
| No. of parameters | 181 |
| No. of restraints | 2 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.12, −0.12 |

Computer programs: *APEX2* (Bruker, 2010), *SAINT* (Bruker, 2010), *SHELXS97* (Sheldrick 2008), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick 2008).

# full crystallographic data

*IUCrData* (2016). **1**, x160398 [doi:10.1107/S2414314616003989]

## 4-Benzyloxy-1,1′-biphenyl

**Farook Adam, Nadiah Ameram, Shevgoor Dhiraj Kamath, Pallavi and Seranthimata Samshuddin**

### 4-Benzyloxy-1,1′-biphenyl

*Crystal data*

$C_{19}H_{16}O$
$M_r$ = 260.32
Monoclinic, *Cc*
*a* = 31.270 (2) Å
*b* = 5.6720 (4) Å
*c* = 7.8812 (5) Å
*β* = 99.271 (3)°
*V* = 1379.58 (16) Å$^3$
*Z* = 4
*F*(000) = 552
$D_x$ = 1.253 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 7054 reflections
*θ* = 2.6–31.7°
*μ* = 0.08 mm$^{-1}$
*T* = 296 K
Plate, colourless
0.39 × 0.31 × 0.09 mm

*Data collection*

Bruker APEXII CCD diffractometer
*φ* and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2010)
$T_{min}$ = 0.891, $T_{max}$ = 0.969
18200 measured reflections
2435 independent reflections
2218 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.6°
*h* = −36→36
*k* = −6→6
*l* = −9→9

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.104
*S* = 0.87
2435 reflections
181 parameters
2 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2 + 0.3664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.12 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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.44220 (6) | 0.2333 (3) | 1.0798 (2) | 0.0538 (5) |

| | | | | |
|---|---|---|---|---|
| C1 | 0.23730 (9) | 0.4280 (5) | 0.7983 (4) | 0.0517 (7) |
| H1A | 0.2475 | 0.5521 | 0.8709 | 0.062* |
| C2 | 0.19447 (9) | 0.4248 (5) | 0.7236 (4) | 0.0579 (8) |
| H2A | 0.1761 | 0.5458 | 0.7463 | 0.069* |
| C3 | 0.17851 (9) | 0.2446 (5) | 0.6158 (4) | 0.0538 (7) |
| H3A | 0.1495 | 0.2416 | 0.5659 | 0.065* |
| C4 | 0.20609 (9) | 0.0691 (5) | 0.5831 (4) | 0.0588 (8) |
| H4A | 0.1958 | −0.0529 | 0.5088 | 0.071* |
| C5 | 0.24892 (9) | 0.0712 (5) | 0.6590 (4) | 0.0515 (7) |
| H5A | 0.2670 | −0.0512 | 0.6362 | 0.062* |
| C6 | 0.26585 (8) | 0.2510 (4) | 0.7683 (3) | 0.0377 (6) |
| C7 | 0.31216 (8) | 0.2517 (4) | 0.8516 (3) | 0.0366 (6) |
| C8 | 0.34084 (9) | 0.0771 (5) | 0.8203 (4) | 0.0523 (8) |
| H8A | 0.3309 | −0.0435 | 0.7442 | 0.063* |
| C9 | 0.38322 (9) | 0.0756 (5) | 0.8973 (4) | 0.0553 (8) |
| H9A | 0.4013 | −0.0461 | 0.8738 | 0.066* |
| C10 | 0.39943 (8) | 0.2524 (4) | 1.0094 (3) | 0.0408 (6) |
| C11 | 0.37210 (8) | 0.4295 (5) | 1.0437 (3) | 0.0491 (7) |
| H11A | 0.3823 | 0.5502 | 1.1194 | 0.059* |
| C12 | 0.32920 (8) | 0.4267 (5) | 0.9646 (3) | 0.0476 (7) |
| H12A | 0.3111 | 0.5479 | 0.9886 | 0.057* |
| C13 | 0.45998 (9) | 0.4022 (5) | 1.2055 (4) | 0.0512 (7) |
| H13A | 0.4429 | 0.4080 | 1.2977 | 0.061* |
| H13B | 0.4598 | 0.5575 | 1.1539 | 0.061* |
| C14 | 0.50538 (8) | 0.3302 (5) | 1.2746 (3) | 0.0434 (6) |
| C15 | 0.51377 (9) | 0.1223 (5) | 1.3677 (4) | 0.0527 (7) |
| H15A | 0.4909 | 0.0250 | 1.3852 | 0.063* |
| C16 | 0.55562 (10) | 0.0597 (5) | 1.4339 (4) | 0.0595 (8) |
| H16A | 0.5611 | −0.0792 | 1.4963 | 0.071* |
| C17 | 0.58958 (10) | 0.2035 (6) | 1.4075 (4) | 0.0612 (8) |
| H17A | 0.6179 | 0.1610 | 1.4516 | 0.073* |
| C18 | 0.58158 (9) | 0.4071 (6) | 1.3169 (4) | 0.0587 (7) |
| H18A | 0.6045 | 0.5045 | 1.3004 | 0.070* |
| C19 | 0.53974 (9) | 0.4697 (5) | 1.2493 (4) | 0.0503 (7) |
| H19A | 0.5347 | 0.6079 | 1.1858 | 0.060* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0395 (10) | 0.0632 (12) | 0.0561 (11) | 0.0062 (8) | −0.0001 (8) | −0.0172 (9) |
| C1 | 0.0494 (17) | 0.0478 (16) | 0.0544 (17) | 0.0041 (11) | −0.0016 (13) | −0.0105 (12) |
| C2 | 0.0472 (16) | 0.0626 (18) | 0.0615 (19) | 0.0129 (13) | 0.0016 (14) | −0.0039 (14) |
| C3 | 0.0393 (14) | 0.0658 (19) | 0.0537 (16) | −0.0012 (12) | −0.0006 (12) | 0.0044 (13) |
| C4 | 0.0514 (18) | 0.0628 (18) | 0.0591 (19) | −0.0092 (14) | −0.0009 (14) | −0.0135 (14) |
| C5 | 0.0452 (16) | 0.0525 (16) | 0.0556 (17) | 0.0035 (12) | 0.0049 (13) | −0.0130 (12) |
| C6 | 0.0388 (14) | 0.0411 (13) | 0.0338 (13) | −0.0009 (9) | 0.0077 (10) | 0.0044 (9) |
| C7 | 0.0416 (14) | 0.0372 (13) | 0.0317 (12) | −0.0009 (9) | 0.0081 (10) | 0.0024 (9) |
| C8 | 0.0480 (17) | 0.0464 (15) | 0.0590 (18) | 0.0032 (11) | −0.0024 (14) | −0.0199 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0491 (17) | 0.0514 (16) | 0.0630 (19) | 0.0128 (12) | 0.0019 (14) | −0.0180 (13) |
| C10 | 0.0373 (14) | 0.0476 (14) | 0.0369 (14) | 0.0018 (10) | 0.0043 (11) | −0.0021 (10) |
| C11 | 0.0476 (18) | 0.0465 (16) | 0.0510 (17) | 0.0005 (11) | 0.0015 (13) | −0.0140 (12) |
| C12 | 0.0429 (16) | 0.0441 (14) | 0.0547 (17) | 0.0073 (11) | 0.0041 (13) | −0.0124 (12) |
| C13 | 0.0446 (15) | 0.0550 (16) | 0.0513 (16) | −0.0010 (12) | 0.0000 (12) | −0.0087 (12) |
| C14 | 0.0415 (14) | 0.0481 (13) | 0.0384 (13) | 0.0008 (11) | −0.0002 (11) | −0.0059 (11) |
| C15 | 0.0520 (16) | 0.0490 (14) | 0.0557 (17) | −0.0058 (12) | 0.0045 (13) | 0.0000 (13) |
| C16 | 0.067 (2) | 0.0510 (16) | 0.0568 (17) | 0.0114 (14) | −0.0022 (15) | 0.0046 (13) |
| C17 | 0.0471 (16) | 0.071 (2) | 0.0611 (18) | 0.0112 (14) | −0.0058 (13) | −0.0100 (16) |
| C18 | 0.0443 (16) | 0.0687 (19) | 0.0619 (17) | −0.0106 (14) | 0.0052 (13) | −0.0074 (15) |
| C19 | 0.0522 (17) | 0.0509 (14) | 0.0464 (14) | −0.0053 (12) | 0.0041 (12) | 0.0033 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C10 | 1.367 (3) | C9—H9A | 0.9300 |
| O1—C13 | 1.425 (3) | C10—C11 | 1.374 (4) |
| C1—C2 | 1.374 (4) | C11—C12 | 1.386 (4) |
| C1—C6 | 1.389 (4) | C11—H11A | 0.9300 |
| C1—H1A | 0.9300 | C12—H12A | 0.9300 |
| C2—C3 | 1.370 (4) | C13—C14 | 1.493 (4) |
| C2—H2A | 0.9300 | C13—H13A | 0.9700 |
| C3—C4 | 1.369 (4) | C13—H13B | 0.9700 |
| C3—H3A | 0.9300 | C14—C19 | 1.374 (4) |
| C4—C5 | 1.376 (4) | C14—C15 | 1.391 (4) |
| C4—H4A | 0.9300 | C15—C16 | 1.375 (4) |
| C5—C6 | 1.384 (4) | C15—H15A | 0.9300 |
| C5—H5A | 0.9300 | C16—C17 | 1.381 (5) |
| C6—C7 | 1.491 (3) | C16—H16A | 0.9300 |
| C7—C12 | 1.382 (4) | C17—C18 | 1.359 (4) |
| C7—C8 | 1.384 (4) | C17—H17A | 0.9300 |
| C8—C9 | 1.366 (4) | C18—C19 | 1.378 (4) |
| C8—H8A | 0.9300 | C18—H18A | 0.9300 |
| C9—C10 | 1.378 (4) | C19—H19A | 0.9300 |
| | | | |
| C10—O1—C13 | 118.39 (19) | C10—C11—C12 | 119.4 (2) |
| C2—C1—C6 | 121.7 (3) | C10—C11—H11A | 120.3 |
| C2—C1—H1A | 119.1 | C12—C11—H11A | 120.3 |
| C6—C1—H1A | 119.1 | C7—C12—C11 | 122.9 (2) |
| C3—C2—C1 | 120.6 (3) | C7—C12—H12A | 118.6 |
| C3—C2—H2A | 119.7 | C11—C12—H12A | 118.6 |
| C1—C2—H2A | 119.7 | O1—C13—C14 | 108.1 (2) |
| C4—C3—C2 | 118.8 (3) | O1—C13—H13A | 110.1 |
| C4—C3—H3A | 120.6 | C14—C13—H13A | 110.1 |
| C2—C3—H3A | 120.6 | O1—C13—H13B | 110.1 |
| C3—C4—C5 | 120.7 (3) | C14—C13—H13B | 110.1 |
| C3—C4—H4A | 119.7 | H13A—C13—H13B | 108.4 |
| C5—C4—H4A | 119.7 | C19—C14—C15 | 118.6 (2) |
| C4—C5—C6 | 121.7 (2) | C19—C14—C13 | 120.6 (2) |

| | | | |
|---|---|---|---|
| C4—C5—H5A | 119.2 | C15—C14—C13 | 120.8 (2) |
| C6—C5—H5A | 119.2 | C16—C15—C14 | 120.4 (3) |
| C5—C6—C1 | 116.5 (2) | C16—C15—H15A | 119.8 |
| C5—C6—C7 | 121.5 (2) | C14—C15—H15A | 119.8 |
| C1—C6—C7 | 121.9 (2) | C15—C16—C17 | 119.9 (3) |
| C12—C7—C8 | 115.8 (2) | C15—C16—H16A | 120.1 |
| C12—C7—C6 | 122.1 (2) | C17—C16—H16A | 120.1 |
| C8—C7—C6 | 122.1 (2) | C18—C17—C16 | 120.0 (3) |
| C9—C8—C7 | 122.4 (2) | C18—C17—H17A | 120.0 |
| C9—C8—H8A | 118.8 | C16—C17—H17A | 120.0 |
| C7—C8—H8A | 118.8 | C17—C18—C19 | 120.3 (3) |
| C8—C9—C10 | 120.7 (2) | C17—C18—H18A | 119.8 |
| C8—C9—H9A | 119.7 | C19—C18—H18A | 119.8 |
| C10—C9—H9A | 119.7 | C14—C19—C18 | 120.8 (3) |
| O1—C10—C11 | 125.2 (2) | C14—C19—H19A | 119.6 |
| O1—C10—C9 | 115.9 (2) | C18—C19—H19A | 119.6 |
| C11—C10—C9 | 118.8 (2) | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.1 (5) | C8—C9—C10—C11 | 0.6 (4) |
| C1—C2—C3—C4 | −0.5 (5) | O1—C10—C11—C12 | −179.4 (2) |
| C2—C3—C4—C5 | 1.0 (5) | C9—C10—C11—C12 | −0.3 (4) |
| C3—C4—C5—C6 | −1.0 (5) | C8—C7—C12—C11 | −0.4 (4) |
| C4—C5—C6—C1 | 0.4 (4) | C6—C7—C12—C11 | 179.7 (2) |
| C4—C5—C6—C7 | 179.4 (2) | C10—C11—C12—C7 | 0.2 (4) |
| C2—C1—C6—C5 | 0.1 (4) | C10—O1—C13—C14 | 174.4 (2) |
| C2—C1—C6—C7 | −178.9 (2) | O1—C13—C14—C19 | 115.6 (3) |
| C5—C6—C7—C12 | −178.2 (3) | O1—C13—C14—C15 | −65.1 (3) |
| C1—C6—C7—C12 | 0.7 (3) | C19—C14—C15—C16 | 0.6 (4) |
| C5—C6—C7—C8 | 1.9 (3) | C13—C14—C15—C16 | −178.7 (2) |
| C1—C6—C7—C8 | −179.2 (3) | C14—C15—C16—C17 | −0.2 (4) |
| C12—C7—C8—C9 | 0.7 (4) | C15—C16—C17—C18 | 0.3 (4) |
| C6—C7—C8—C9 | −179.4 (3) | C16—C17—C18—C19 | −0.8 (5) |
| C7—C8—C9—C10 | −0.8 (5) | C15—C14—C19—C18 | −1.0 (4) |
| C13—O1—C10—C11 | 3.3 (4) | C13—C14—C19—C18 | 178.2 (3) |
| C13—O1—C10—C9 | −175.8 (3) | C17—C18—C19—C14 | 1.1 (4) |
| C8—C9—C10—O1 | 179.7 (3) | | |

*Hydrogen-bond geometry (Å, º)*

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C7–C12 and C14–C19 benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1*A*···*Cg*1$^{i}$ | 0.93 | 2.99 | 3.700 (3) | 134 |
| C4—H4*A*···*Cg*1$^{ii}$ | 0.93 | 2.97 | 3.700 (3) | 134 |
| C8—H8*A*···*Cg*2$^{ii}$ | 0.93 | 2.96 | 3.687 (3) | 137 |
| C11—H11*A*···*Cg*2$^{i}$ | 0.93 | 2.93 | 3.650 (3) | 135 |
| C19—H19*A*···*Cg*3$^{iii}$ | 0.93 | 2.90 | 3.591 (3) | 133 |

Symmetry codes: (i) *x*, −*y*+1, *z*+1/2; (ii) *x*, −*y*, *z*−1/2; (iii) *x*, −*y*+1, *z*−1/2.