Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diphenylmethyl benzoate

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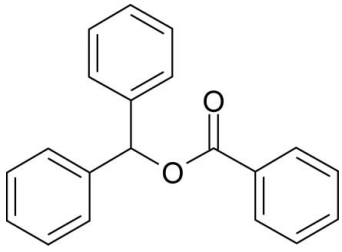
Received 30 November 2012; accepted 6 December 2012

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.094; data-to-parameter ratio = 13.3.

In the title molecule, $C_{20}H_{16}O_2$, the dihedral angle between the phenyl rings of the diphenylmethyl group is 68.3 (2)°. The benzoate group is essentially planar, with a maximum deviation of 0.017 (2) Å for the carbonyl O atom, and the two phenyl rings are twisted by 27.5 (4) and 85.6 (9)° from this plane. In the crystal, weak C—H···O hydrogen bonds link molecules along [100].

Related literature

For related structures, see: Baidya *et al.* (2009*a*,*b*); Gowda *et al.* (2007, 2009). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{16}O_2$
M_r = 288.33
Monoclinic, $P2_1$
a = 5.75357 (19) Å
b = 16.0368 (5) Å
c = 8.3114 (3) Å
β = 95.340 (3)°
V = 763.55 (4) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 173 K
0.38 × 0.26 × 0.24 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.912, T_{max} = 1.000
4414 measured reflections
2659 independent reflections
2528 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.06
2659 reflections
200 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack (1983) 1120 Friedel pairs
Flack parameter: 0.0 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O2^{i}	0.93	2.44	3.334 (2)	160

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); 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*.

MK thanks the UOM for research facilities. JPJ acknowledges the NSF–MRI program (grant No. CHE-1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5566).

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supporting information

Acta Cryst. (2013). E**69**, o81 [https://doi.org/10.1107/S1600536812050064]

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S1. Comment

Benzyl Benzoate is widely used in the perfume and pharmaceutical industries. The crystal structures of some related compounds, viz., 4,4′-bis(dimethylamino)benzhydryl phenyl sulfone (Baidya *et al.*, 2009*a*), benzhydryl phenyl sulfone (Baidya *et al.*, 2009*b*), 4-methylphenyl benzoate (Gowda *et al.*, 2007), 2,4-dimethylphenyl 4-methylbenzoate (Gowda *et al.*, 2009) have been reported. In view of the importance of benzoates, the paper reports the crystal structure of the title compound, (I).

The molecular structure of the title compound is shown in Fig. 1. The dihedral angle between the two phenyl rings (C9-C14 and C15-C20) is 68.3 (2)°. The mean plane of the benzoate group (C1–C7/O1/O2, with a maximum deviation of 0.017 (2)Å for O2) is twisted by 27.5 (4)° (C9–C14) and 85.6 (9)° (C15–C20), respectively, from that of the phenyl rings. In the crystal, weak C—H···O hydrogen bonds (Table 1) link molecules along [100] (Fig. 2).

S2. Experimental

The title compound was obtained as a gift sample from R. L. Fine Chem, Bengaluru, India. X-ray quality crystals were obtained by slow evaporation of acetone and acetone solution (m.p.: 353–355 K).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.93Å (CH). Isotropic displacement parameters for these atoms were set to 1.19-1.20 (CH) times U_{eq} of the parent atom.

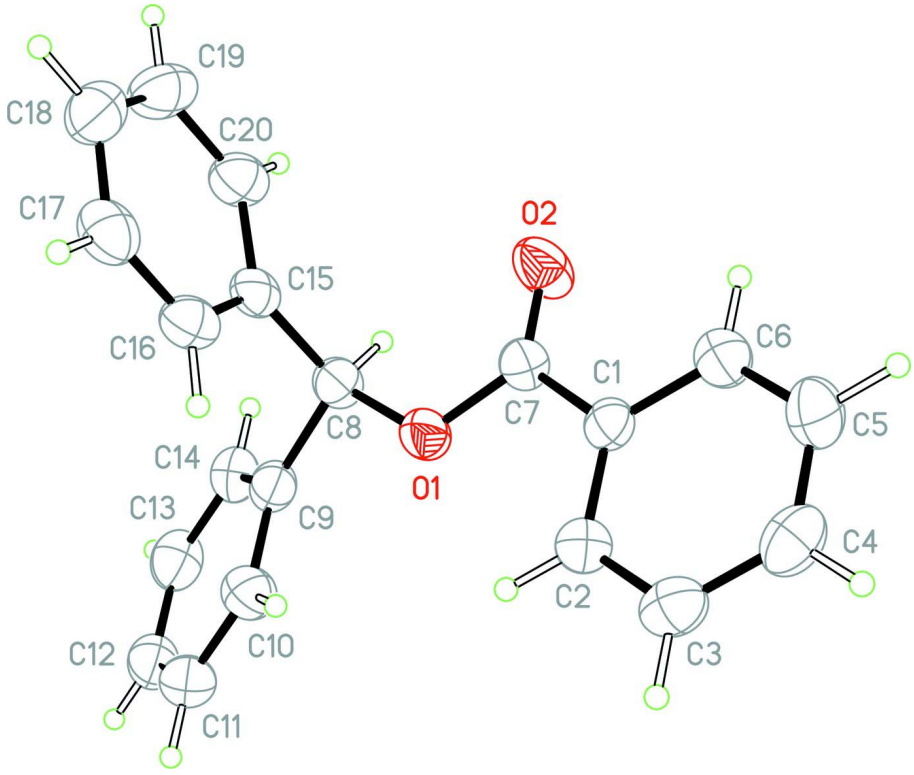

Figure 1

Molecular structure of the title compound showing 50% probability displacement ellipsoids.

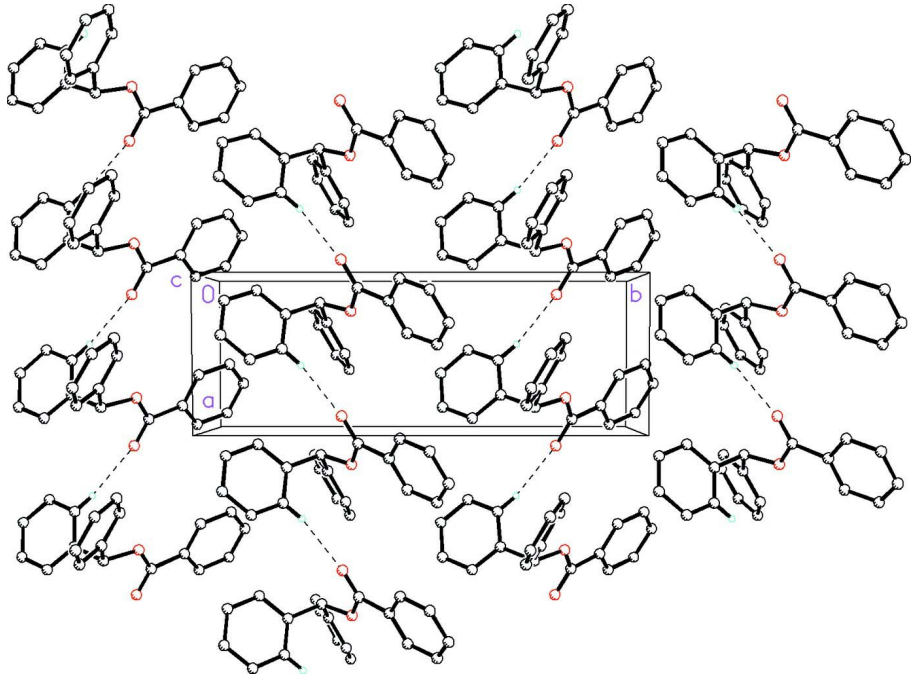

Figure 2

Packing diagram of the title compound viewed along the *c* axis showing weak C—H···O intermolecular interactions (dashed lines) linking the molecules into columns along [100]

Diphenylmethyl benzoate

Crystal data

$C_{20}H_{16}O_2$
$M_r = 288.33$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 5.75357\ (19)$ Å
$b = 16.0368\ (5)$ Å
$c = 8.3114\ (3)$ Å
$\beta = 95.340\ (3)°$
$V = 763.55\ (4)$ Å^3
$Z = 2$
$F(000) = 304$
$D_x = 1.254$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2446 reflections
$\theta = 5.3–72.4°$
$\mu = 0.63$ mm^{-1}
$T = 173$ K
Block, colorless
0.38 × 0.26 × 0.24 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
$T_{min} = 0.912$, $T_{max} = 1.000$
4414 measured reflections
2659 independent reflections
2528 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 72.5°$, $\theta_{min} = 5.4°$
$h = -7\rightarrow5$
$k = -17\rightarrow19$
$l = -6\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.094$
$S = 1.06$
2659 reflections
200 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 0.052P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0104 (11)
Absolute structure: Flack (1983) 1120 Friedel pairs
Absolute structure parameter: 0.0 (2)

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 $F^2 > \sigma(F^2)$ 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}
O1	0.2173 (2)	0.33454 (8)	0.50213 (15)	0.0376 (3)

O2	−0.1042 (2)	0.31628 (10)	0.63104 (18)	0.0495 (4)
C1	0.1598 (3)	0.42599 (10)	0.7144 (2)	0.0312 (4)
C2	0.3646 (3)	0.46769 (11)	0.6891 (2)	0.0364 (4)
H2	0.4547	0.4498	0.6085	0.044*
C3	0.4349 (4)	0.53567 (12)	0.7833 (2)	0.0434 (4)
H3	0.5709	0.5640	0.7648	0.052*
C4	0.3036 (4)	0.56172 (13)	0.9049 (2)	0.0465 (5)
H4	0.3514	0.6074	0.9685	0.056*
C5	0.1008 (4)	0.51969 (13)	0.9320 (2)	0.0491 (5)
H5	0.0133	0.5370	1.0145	0.059*
C6	0.0279 (3)	0.45254 (12)	0.8375 (2)	0.0407 (4)
H6	−0.1092	0.4248	0.8556	0.049*
C7	0.0735 (3)	0.35370 (11)	0.6150 (2)	0.0329 (4)
C8	0.1615 (3)	0.26034 (11)	0.4044 (2)	0.0339 (4)
H8	−0.0074	0.2579	0.3758	0.041*
C9	0.2833 (3)	0.27104 (10)	0.2523 (2)	0.0350 (4)
C10	0.4936 (3)	0.31388 (13)	0.2513 (2)	0.0408 (4)
H10	0.5615	0.3381	0.3459	0.049*
C11	0.6021 (4)	0.32051 (14)	0.1099 (3)	0.0459 (5)
H11	0.7420	0.3495	0.1101	0.055*
C12	0.5040 (4)	0.28435 (12)	−0.0315 (2)	0.0452 (5)
H12	0.5776	0.2890	−0.1261	0.054*
C13	0.2964 (4)	0.24132 (14)	−0.0317 (2)	0.0459 (5)
H13	0.2304	0.2166	−0.1264	0.055*
C14	0.1859 (3)	0.23482 (12)	0.1092 (2)	0.0400 (4)
H14	0.0455	0.2060	0.1081	0.048*
C15	0.2380 (3)	0.18357 (11)	0.50053 (19)	0.0327 (4)
C16	0.4629 (3)	0.17795 (12)	0.5773 (2)	0.0381 (4)
H16	0.5683	0.2212	0.5672	0.046*
C17	0.5304 (4)	0.10861 (14)	0.6684 (2)	0.0456 (5)
H17	0.6804	0.1056	0.7204	0.055*
C18	0.3756 (4)	0.04356 (13)	0.6827 (2)	0.0494 (5)
H18	0.4206	−0.0028	0.7452	0.059*
C19	0.1538 (4)	0.04782 (13)	0.6037 (3)	0.0514 (5)
H19	0.0504	0.0038	0.6115	0.062*
C20	0.0851 (4)	0.11732 (13)	0.5130 (2)	0.0421 (4)
H20	−0.0644	0.1197	0.4601	0.051*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0385 (7)	0.0341 (7)	0.0422 (7)	−0.0057 (5)	0.0136 (5)	−0.0087 (5)
O2	0.0401 (7)	0.0565 (9)	0.0543 (8)	−0.0152 (6)	0.0172 (6)	−0.0205 (7)
C1	0.0333 (8)	0.0287 (8)	0.0316 (8)	0.0040 (6)	0.0032 (6)	0.0031 (6)
C2	0.0354 (9)	0.0348 (9)	0.0396 (9)	−0.0008 (7)	0.0058 (7)	0.0002 (7)
C3	0.0415 (10)	0.0386 (10)	0.0494 (11)	−0.0062 (8)	0.0002 (8)	0.0021 (9)
C4	0.0569 (12)	0.0358 (10)	0.0451 (10)	−0.0034 (9)	−0.0047 (9)	−0.0076 (8)
C5	0.0602 (13)	0.0475 (12)	0.0410 (11)	0.0031 (10)	0.0129 (9)	−0.0103 (9)

C6	0.0410 (10)	0.0402 (10)	0.0419 (10)	−0.0016 (8)	0.0082 (8)	−0.0030 (8)
C7	0.0318 (8)	0.0333 (9)	0.0340 (8)	0.0016 (7)	0.0047 (7)	−0.0001 (7)
C8	0.0327 (8)	0.0345 (9)	0.0349 (8)	−0.0039 (7)	0.0050 (7)	−0.0062 (7)
C9	0.0395 (9)	0.0303 (9)	0.0354 (8)	0.0045 (7)	0.0056 (7)	0.0010 (7)
C10	0.0428 (10)	0.0413 (10)	0.0393 (9)	−0.0018 (8)	0.0088 (8)	−0.0016 (8)
C11	0.0495 (11)	0.0415 (11)	0.0487 (10)	0.0004 (9)	0.0152 (8)	0.0058 (9)
C12	0.0589 (12)	0.0427 (11)	0.0363 (9)	0.0099 (9)	0.0172 (9)	0.0070 (8)
C13	0.0609 (12)	0.0443 (11)	0.0324 (9)	0.0086 (9)	0.0032 (8)	−0.0021 (8)
C14	0.0420 (9)	0.0379 (10)	0.0401 (9)	0.0039 (8)	0.0035 (8)	−0.0035 (8)
C15	0.0374 (9)	0.0340 (9)	0.0282 (8)	−0.0040 (7)	0.0108 (7)	−0.0075 (6)
C16	0.0391 (10)	0.0423 (10)	0.0338 (9)	−0.0060 (8)	0.0076 (7)	−0.0023 (7)
C17	0.0448 (11)	0.0580 (13)	0.0349 (9)	0.0062 (9)	0.0083 (8)	0.0008 (9)
C18	0.0722 (15)	0.0392 (11)	0.0382 (10)	0.0059 (10)	0.0123 (9)	0.0006 (8)
C19	0.0683 (14)	0.0364 (11)	0.0504 (11)	−0.0152 (10)	0.0108 (10)	−0.0032 (9)
C20	0.0421 (10)	0.0423 (10)	0.0427 (10)	−0.0100 (8)	0.0073 (8)	−0.0065 (8)

Geometric parameters (Å, º)

O1—C7	1.343 (2)	C10—C11	1.385 (3)
O1—C8	1.460 (2)	C10—H10	0.9300
O2—C7	1.203 (2)	C11—C12	1.383 (3)
C1—C2	1.388 (2)	C11—H11	0.9300
C1—C6	1.396 (2)	C12—C13	1.379 (3)
C1—C7	1.482 (2)	C12—H12	0.9300
C2—C3	1.381 (3)	C13—C14	1.387 (3)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.382 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—C20	1.390 (2)
C4—C5	1.384 (3)	C15—C16	1.392 (2)
C4—H4	0.9300	C16—C17	1.380 (3)
C5—C6	1.375 (3)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.384 (3)
C6—H6	0.9300	C17—H17	0.9300
C8—C15	1.511 (3)	C18—C19	1.381 (3)
C8—C9	1.511 (2)	C18—H18	0.9300
C8—H8	0.9800	C19—C20	1.382 (3)
C9—C10	1.392 (3)	C19—H19	0.9300
C9—C14	1.394 (3)	C20—H20	0.9300
C7—O1—C8	117.21 (13)	C11—C10—H10	119.9
C2—C1—C6	119.42 (17)	C9—C10—H10	119.9
C2—C1—C7	122.53 (15)	C12—C11—C10	120.54 (19)
C6—C1—C7	118.05 (16)	C12—C11—H11	119.7
C3—C2—C1	120.18 (18)	C10—C11—H11	119.7
C3—C2—H2	119.9	C13—C12—C11	119.72 (17)
C1—C2—H2	119.9	C13—C12—H12	120.1
C2—C3—C4	120.15 (18)	C11—C12—H12	120.1
C2—C3—H3	119.9	C12—C13—C14	120.08 (18)

C4—C3—H3	119.9	C12—C13—H13	120.0
C3—C4—C5	119.89 (18)	C14—C13—H13	120.0
C3—C4—H4	120.1	C13—C14—C9	120.65 (18)
C5—C4—H4	120.1	C13—C14—H14	119.7
C6—C5—C4	120.37 (19)	C9—C14—H14	119.7
C6—C5—H5	119.8	C20—C15—C16	118.97 (17)
C4—C5—H5	119.8	C20—C15—C8	120.50 (16)
C5—C6—C1	119.98 (18)	C16—C15—C8	120.53 (16)
C5—C6—H6	120.0	C17—C16—C15	120.40 (18)
C1—C6—H6	120.0	C17—C16—H16	119.8
O2—C7—O1	123.26 (16)	C15—C16—H16	119.8
O2—C7—C1	124.91 (16)	C16—C17—C18	120.2 (2)
O1—C7—C1	111.83 (14)	C16—C17—H17	119.9
O1—C8—C15	109.39 (13)	C18—C17—H17	119.9
O1—C8—C9	106.13 (14)	C19—C18—C17	119.7 (2)
C15—C8—C9	113.59 (14)	C19—C18—H18	120.1
O1—C8—H8	109.2	C17—C18—H18	120.1
C15—C8—H8	109.2	C18—C19—C20	120.2 (2)
C9—C8—H8	109.2	C18—C19—H19	119.9
C10—C9—C14	118.75 (16)	C20—C19—H19	119.9
C10—C9—C8	122.17 (15)	C19—C20—C15	120.42 (19)
C14—C9—C8	119.06 (16)	C19—C20—H20	119.8
C11—C10—C9	120.26 (18)	C15—C20—H20	119.8

C6—C1—C2—C3	−1.1 (3)	C14—C9—C10—C11	0.4 (3)
C7—C1—C2—C3	178.80 (17)	C8—C9—C10—C11	178.47 (18)
C1—C2—C3—C4	1.0 (3)	C9—C10—C11—C12	−0.4 (3)
C2—C3—C4—C5	−0.2 (3)	C10—C11—C12—C13	0.0 (3)
C3—C4—C5—C6	−0.6 (3)	C11—C12—C13—C14	0.4 (3)
C4—C5—C6—C1	0.5 (3)	C12—C13—C14—C9	−0.4 (3)
C2—C1—C6—C5	0.3 (3)	C10—C9—C14—C13	0.0 (3)
C7—C1—C6—C5	−179.60 (17)	C8—C9—C14—C13	−178.14 (17)
C8—O1—C7—O2	−5.1 (3)	O1—C8—C15—C20	129.89 (16)
C8—O1—C7—C1	175.31 (13)	C9—C8—C15—C20	−111.75 (18)
C2—C1—C7—O2	−179.04 (19)	O1—C8—C15—C16	−50.40 (19)
C6—C1—C7—O2	0.8 (3)	C9—C8—C15—C16	68.0 (2)
C2—C1—C7—O1	0.5 (2)	C20—C15—C16—C17	−1.9 (3)
C6—C1—C7—O1	−179.61 (16)	C8—C15—C16—C17	178.38 (15)
C7—O1—C8—C15	−78.53 (17)	C15—C16—C17—C18	0.7 (3)
C7—O1—C8—C9	158.56 (14)	C16—C17—C18—C19	0.8 (3)
O1—C8—C9—C10	31.5 (2)	C17—C18—C19—C20	−1.1 (3)
C15—C8—C9—C10	−88.7 (2)	C18—C19—C20—C15	−0.1 (3)
O1—C8—C9—C14	−150.37 (15)	C16—C15—C20—C19	1.6 (3)
C15—C8—C9—C14	89.40 (19)	C8—C15—C20—C19	−178.71 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O2^{i}	0.93	2.44	3.334 (2)	160

Symmetry code: (i) *x*+1, *y*, *z*.