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Crystal structure of dimethyl 1-oxo-2,4-diphenyl-1,2-dihydronaphthalene-2,3-dicarboxylate

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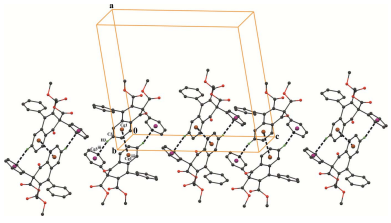
In the title compound, $C_{26}H_{20}O_5$, a 1,2-dihydronaphthalene derivative, the cyclohexa-1,3-diene ring of the 1,2-dihydronaphthalene ring system adopts a half-chair conformation. The mean plane of the 1,2-dihydronapthalene ring system makes dihedral angles of 86.23 (6) and 64.80 (7)° with two phenyl rings. The carbonyl O atom attached to the dihydronaphthalene ring system deviates from the mean plane of the 1,2-dihydronaphthalene ring system by 0.618 (1) Å. In the crystal, the molecules are linked into layers parallel to the *bc* plane *via* two kinds of C—H···O interactions, one of which forms a $C(10)$ chain motif running along the *c*-axis direction and the other forms an $R_2^2(6)$ ring motif. Adjacent layers are further connected by C—H···π and offset π–π interactions [centroid–centroid distance = 3.6318 (9) Å].

1. Chemical context

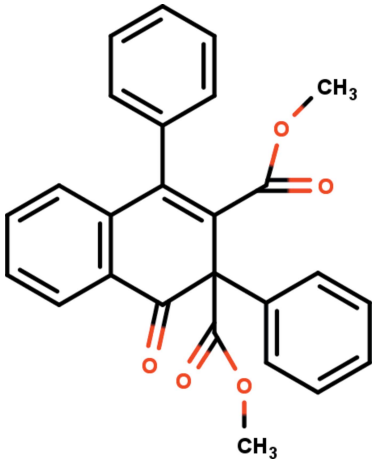
Naphthalene derivatives have manifested applications in many fields, for example, as colorants, explosives, disinfectants, insecticides and the plant hormone auxin. Naphthalene is believed to play a role in the chemical defence against biological enemies (Wiltz *et al.*, 1998; Wright *et al.*, 2000). Naphthalene derivatives have been identified as a new range of potent anti-microbials that are effective against a wide range of human pathogens and have diverse and interesting antibiotic properties with minimum toxicity (Rokade & Sayyed, 2009; Upadhayaya *et al.*, 2010). Compounds with non-coplanarly accumulated aromatic rings have received attention from organic chemists and materials chemists as unique structural building blocks, because they provide characteristic optical and electronic properties originating from their structural features. For example, biphenyl and binaphthyl are applied to optically active molecular catalysts and polymer materials on the basis of their axial chiralities (Deria *et al.*, 2013). The structures of similar 1-oxo-1,2-dihydronaphtalene derivatives, namely, dimethyl 4-(4-methoxyphenyl)-2-(4-methylphenyl)-1-oxo-1,2-dihydronaphthalene-2,3-dicarboxylate, dimethyl 1-oxo-2-(pyren-4-yl)-4-(thiophen-2-yl)-1,2-dihydronaphthalene-2,3-dicarboxylate and ethyl 1-oxo-2-phenyl-2,4-bis(thiophen-2-yl)-1,2-dihydronaphthalene-3-carboxylate, have been reported by Gopinath *et al.* (2017).



2. Structural commentary

In the title compound (Fig. 1), the 1,2-dihydronaphthalene C1–C10 ring system is not strictly planar and the cyclohexa-

1,3-diene C5–C10 ring adopts a half-chair conformation with puckering and smallest displacement parameters q_2 = 0.3091 (14) Å, q_3 = 0.1461 (14) Å, φ_2 = 155.9 (3)° and θ = 64.7 (2)° and ΔC_s = 4.41 (19). The dihedral angle between the C1–C6 and C5–C10 rings is 10.15 (6)°. The C11–C16 phenyl ring is almost perpendicular to the 1,2-dihydronaphthalene C1–C10 ring system with a dihedral angle of 83.83 (7)° between them. The other phenyl ring (C21–C26) makes dihedral angles of 64.80 (7) and 29.06 (8)° with the mean plane of C1–C10 ring system and the C11–C16 phenyl ring, respectively. Atom O1 of the carbonyl group deviates from the mean plane of the 1,2-dihydronaphthalene ring system by 0.647 (1) Å.



3. Supramolecular features

In the crystal, the molecules are linked *via* C—H···O hydrogen bonds (C24—H24···O2^{i}; symmetry code as in Table 1), which generates $C(10)$ zigzag chains running along the *c*-axis direction (Fig. 2). In addition, the chains are linked *via* pairs of C—H···O interactions (C20—H20*B*···O5^{ii}; Table 2) with an $R_2^2(6)$ ring motif (Fig. 3), forming layers

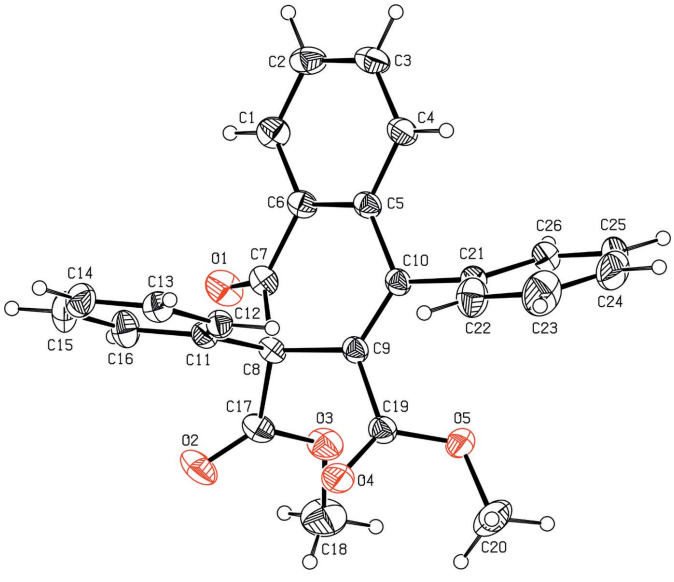


Figure 1
The molecular structure of the title compound with the atom-numbering scheme. The displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radii.

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

*Cg*3 is the centroid of the phenyl C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C24—H24···O2^{i}	0.93	2.59	3.449 (3)	155
C20—H20*B*···O5^{ii}	0.96	2.59	3.430 (2)	146
C3—H3···*Cg*3^{iii}	0.93	2.77	3.6338 (16)	154

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+1, -z$; (iii) $-x, -y+1, -z$.

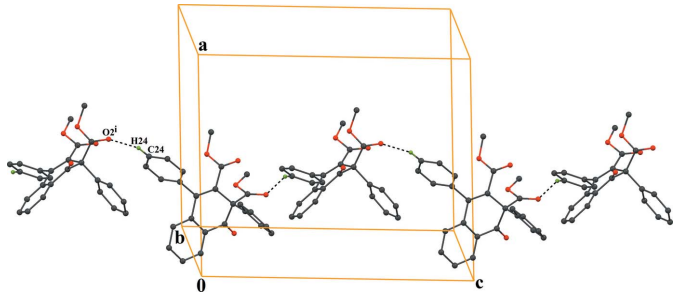


Figure 2
A packing diagram of the title compound, showing a $C(10)$ zigzag chain along to the *c* axis formed *via* C—H···O hydrogen bonds (dashed lines). The H atoms not involved in the hydrogen bonding have been excluded for clarity. [Symmetry code: (i) $x, \frac{3}{2}-y, -\frac{1}{2}+z$.]

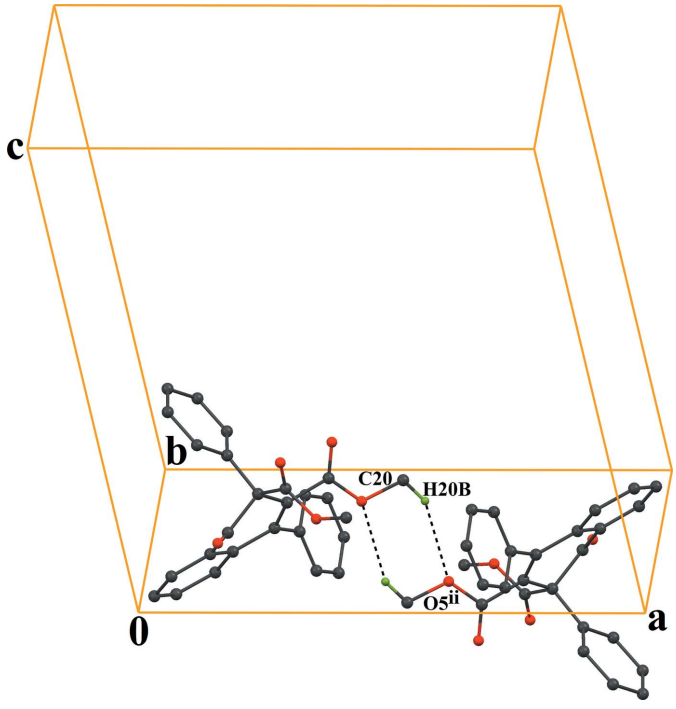


Figure 3
A part of the crystal packing of the title compound, showing an $R^2_2(6)$ inversion dimer formed *via* a pair of C—H···O hydrogen bonds (dashed lines). The H atoms not involved in the hydrogen bonding have been excluded for clarity. [Symmetry code: (ii) $1-x, 1-y, -z$.]

parallel to the *bc* plane. Between the layers there are also C—H···π (C3—H3···*Cg*3^{iii}; Table 1) and π–π stacking interactions (Fig. 4) [*Cg*1···*Cg*1^{iii} = 3.6318 (9) Å, interplanar distance = 3.343 (1) Å and offset distance = 1.419 (1) Å; symmetry code: (iii) $-x$, $1-y$, $-z$; *Cg*1 and *Cg*3 are the centroids of the C1–C6 and C11–C16 rings, respectively].

4. Synthesis and crystallization

To a solution of 1,3-diphenylisobenzofuran (1 g, 3.70 mmol) in dry dichloromethane, dimethyl acetylenedicarboxylate (0.58 g, 4.07 mmol) was added and the reaction mixture was stirred at room temperature for 1 h. Removal of solvent followed by column chromatographic purification (silica gel; 15% ethyl acetate in hexane) afforded isobenzofurandimethyl acetylenedicarboxylate adduct as a colourless solid (1.10 g, 72%). To a solution of the adduct (0.50 g, 1.21 mmol) in dry dichloromethane, $BF_3{\cdot}OEt_2$ (0.075 g, 0.52 mmol) was added and the reaction mixture was stirred at room temperature for 5 min. Removal of solvent followed by column chromatographic purification (silica gel; 15% ethyl acetate in hexane) gave the title compound as a colourless solid (0.45 g, 94%). Single crystals suitable for X-ray diffraction were prepared by slow evaporation of an ethyl acetate solution of the title compound at room temperature (m.p. = 454–456 K).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were localized in a difference-Fourier map and then were treated as riding atoms, with C—H = 0.93 and 0.96 Å for aryl and methyl groups, respectively, and with U_{iso}(H) = 1.2U_{eq}(aryl C) and 1.5U_{eq}(methyl C), allowing for free rotation of the methyl groups.

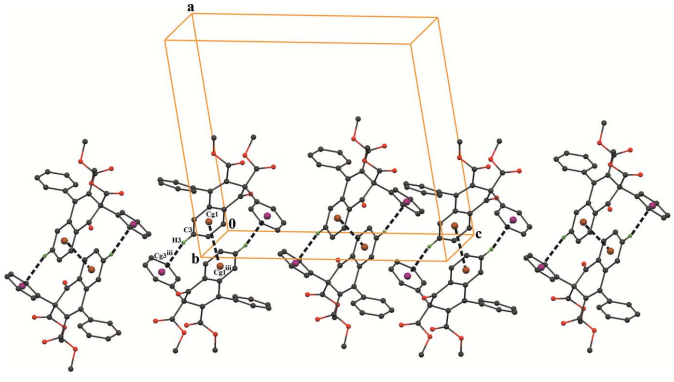


Figure 4
A packing diagram of the title compound, showing C—H···π and π–π interactions (dashed lines), where *Cg*1 and *Cg*3 are the centroids of the phenyl C1–C6 and C11–C16 rings, respectively. [Symmetry code: (iii) $-x$, $1-y$, $-z$.]

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{20}O_5$
M_r	412.42
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	15.8021 (8), 7.4706 (4), 17.8599 (9)
β (°)	96.581 (2)
V (Å^3)	2094.49 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.30 × 0.25
Data collection	
Diffractometer	Bruker Kappa APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.969, 0.978
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21819, 4614, 3375
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.108, 1.03
No. of reflections	4614
No. of parameters	283
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.15

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

Acknowledgements

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Crystal structure of dimethyl 1-oxo-2,4-diphenyl-1,2-dihydronaphthalene-2,3-dicarboxylate

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Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); 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, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Dimethyl 1-oxo-2,4-diphenyl-1,2-dihydronaphthalene-2,3-dicarboxylate

Crystal data

$C_{26}H_{20}O_5$
$M_r = 412.42$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.8021$ (8) Å
$b = 7.4706$ (4) Å
$c = 17.8599$ (9) Å
$\beta = 96.581$ (2)°
$V = 2094.49$ (19) Å^3
$Z = 4$
$F(000) = 864$
$D_x = 1.308$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3375 reflections
$\theta = 2.3$–$27.1°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Block, colourless
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω & φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.969$, $T_{max} = 0.978$
21819 measured reflections
4614 independent reflections
3375 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.1°$, $\theta_{min} = 2.3°$
$h = -20 \rightarrow 13$
$k = -9 \rightarrow 8$
$l = -22 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.108$
$S = 1.03$
4614 reflections
283 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

$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.4036P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.017$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0033 (8)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.05662 (10)	0.2111 (2)	0.01264 (8)	0.0463 (4)
H1	0.0388	0.1135	0.0391	0.056*
C2	0.00596 (10)	0.2750 (2)	−0.04963 (8)	0.0512 (4)
H2	−0.0464	0.2217	−0.0648	0.061*
C3	0.03304 (10)	0.4172 (2)	−0.08905 (8)	0.0488 (4)
H3	−0.0011	0.4600	−0.1311	0.059*
C4	0.11058 (9)	0.4978 (2)	−0.06695 (7)	0.0433 (3)
H4	0.1284	0.5932	−0.0947	0.052*
C5	0.16244 (8)	0.43761 (18)	−0.00354 (7)	0.0354 (3)
C6	0.13411 (8)	0.29249 (18)	0.03586 (7)	0.0368 (3)
C7	0.18723 (9)	0.22355 (19)	0.10317 (7)	0.0384 (3)
C8	0.24887 (8)	0.35947 (17)	0.14498 (6)	0.0338 (3)
C9	0.28722 (8)	0.48058 (18)	0.08927 (7)	0.0336 (3)
C10	0.24565 (8)	0.52183 (18)	0.02146 (7)	0.0338 (3)
C11	0.19360 (8)	0.46192 (18)	0.19635 (6)	0.0344 (3)
C12	0.18236 (8)	0.64551 (18)	0.19151 (7)	0.0368 (3)
H12	0.2110	0.7110	0.1580	0.044*
C13	0.12938 (9)	0.7325 (2)	0.23568 (8)	0.0447 (3)
H13	0.1228	0.8560	0.2319	0.054*
C14	0.08630 (10)	0.6384 (2)	0.28520 (8)	0.0530 (4)
H14	0.0499	0.6971	0.3145	0.064*
C15	0.09745 (11)	0.4569 (3)	0.29111 (9)	0.0595 (5)
H15	0.0691	0.3926	0.3252	0.071*
C16	0.15022 (10)	0.3687 (2)	0.24720 (8)	0.0505 (4)
H16	0.1568	0.2453	0.2517	0.061*
C17	0.31896 (9)	0.24874 (19)	0.19065 (8)	0.0430 (3)
C18	0.44438 (13)	0.0867 (3)	0.17834 (12)	0.0857 (7)
H18A	0.4743	0.1552	0.2185	0.129*
H18B	0.4820	0.0603	0.1412	0.129*
H18C	0.4246	−0.0231	0.1982	0.129*
C19	0.37168 (9)	0.55771 (19)	0.11799 (7)	0.0387 (3)

C20	0.50781 (11)	0.6419 (3)	0.08805 (11)	0.0783 (6)
H20A	0.5019	0.7671	0.0983	0.117*
H20B	0.5429	0.6268	0.0480	0.117*
H20C	0.5338	0.5825	0.1325	0.117*
C21	0.27693 (8)	0.6601 (2)	−0.02840 (7)	0.0398 (3)
C22	0.28407 (11)	0.8357 (2)	−0.00451 (10)	0.0593 (4)
H22	0.2708	0.8659	0.0433	0.071*
C23	0.31073 (13)	0.9673 (3)	−0.05105 (14)	0.0824 (6)
H23	0.3156	1.0851	−0.0344	0.099*
C24	0.33002 (12)	0.9242 (4)	−0.12164 (13)	0.0846 (7)
H24	0.3474	1.0127	−0.1531	0.102*
C25	0.32355 (11)	0.7507 (4)	−0.14553 (9)	0.0723 (6)
H25	0.3375	0.7214	−0.1932	0.087*
C26	0.29671 (9)	0.6184 (3)	−0.10003 (8)	0.0531 (4)
H26	0.2918	0.5010	−0.1173	0.064*
O1	0.18036 (7)	0.07330 (14)	0.12689 (6)	0.0561 (3)
O2	0.32467 (8)	0.21704 (16)	0.25637 (6)	0.0629 (3)
O3	0.37245 (7)	0.18860 (15)	0.14387 (6)	0.0548 (3)
O4	0.38995 (7)	0.60087 (17)	0.18244 (5)	0.0600 (3)
O5	0.42502 (6)	0.56566 (15)	0.06595 (5)	0.0508 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0517 (8)	0.0388 (8)	0.0475 (8)	−0.0064 (7)	0.0016 (6)	−0.0088 (6)
C2	0.0441 (8)	0.0553 (10)	0.0514 (8)	−0.0034 (7)	−0.0068 (7)	−0.0165 (7)
C3	0.0473 (8)	0.0566 (10)	0.0394 (7)	0.0071 (7)	−0.0084 (6)	−0.0076 (7)
C4	0.0447 (8)	0.0500 (9)	0.0340 (7)	0.0043 (7)	−0.0011 (6)	0.0003 (6)
C5	0.0384 (7)	0.0373 (8)	0.0300 (6)	0.0046 (6)	0.0016 (5)	−0.0049 (5)
C6	0.0422 (7)	0.0334 (7)	0.0338 (6)	0.0010 (6)	0.0006 (5)	−0.0076 (5)
C7	0.0466 (8)	0.0326 (8)	0.0359 (7)	0.0017 (6)	0.0044 (6)	−0.0022 (6)
C8	0.0398 (7)	0.0326 (7)	0.0281 (6)	0.0019 (5)	−0.0006 (5)	0.0004 (5)
C9	0.0361 (6)	0.0361 (7)	0.0288 (6)	0.0026 (5)	0.0041 (5)	−0.0029 (5)
C10	0.0362 (6)	0.0370 (7)	0.0285 (6)	0.0045 (6)	0.0052 (5)	−0.0026 (5)
C11	0.0385 (7)	0.0366 (8)	0.0275 (6)	−0.0022 (6)	0.0013 (5)	−0.0001 (5)
C12	0.0380 (7)	0.0380 (8)	0.0342 (6)	−0.0032 (6)	0.0041 (5)	0.0007 (5)
C13	0.0464 (8)	0.0421 (9)	0.0454 (8)	0.0010 (6)	0.0047 (6)	−0.0078 (6)
C14	0.0490 (9)	0.0658 (12)	0.0463 (8)	−0.0050 (8)	0.0146 (7)	−0.0155 (8)
C15	0.0701 (11)	0.0657 (12)	0.0475 (9)	−0.0119 (9)	0.0272 (8)	0.0014 (8)
C16	0.0668 (10)	0.0416 (9)	0.0452 (8)	−0.0066 (7)	0.0155 (7)	0.0035 (7)
C17	0.0506 (8)	0.0381 (8)	0.0383 (7)	0.0050 (6)	−0.0036 (6)	0.0008 (6)
C18	0.0694 (13)	0.0904 (16)	0.0951 (15)	0.0431 (11)	0.0000 (11)	0.0129 (12)
C19	0.0384 (7)	0.0431 (8)	0.0344 (7)	0.0035 (6)	0.0030 (5)	−0.0026 (6)
C20	0.0424 (9)	0.1093 (17)	0.0855 (13)	−0.0188 (10)	0.0176 (9)	−0.0311 (12)
C21	0.0363 (7)	0.0489 (9)	0.0343 (7)	0.0033 (6)	0.0039 (5)	0.0079 (6)
C22	0.0679 (11)	0.0505 (11)	0.0622 (10)	0.0009 (8)	0.0191 (8)	0.0096 (8)
C23	0.0831 (14)	0.0603 (13)	0.1064 (17)	−0.0032 (10)	0.0224 (12)	0.0306 (12)
C24	0.0596 (12)	0.1074 (19)	0.0883 (15)	−0.0008 (12)	0.0150 (10)	0.0621 (14)

C25	0.0470 (9)	0.128 (2)	0.0429 (9)	0.0034 (11)	0.0090 (7)	0.0312 (11)
C26	0.0438 (8)	0.0809 (12)	0.0347 (7)	0.0026 (8)	0.0045 (6)	0.0059 (7)
O1	0.0767 (8)	0.0338 (6)	0.0554 (6)	−0.0059 (5)	−0.0029 (5)	0.0052 (5)
O2	0.0806 (8)	0.0670 (8)	0.0383 (6)	0.0193 (6)	−0.0058 (5)	0.0116 (5)
O3	0.0531 (6)	0.0581 (7)	0.0521 (6)	0.0213 (5)	0.0011 (5)	−0.0005 (5)
O4	0.0472 (6)	0.0932 (9)	0.0387 (5)	−0.0121 (6)	0.0013 (4)	−0.0186 (6)
O5	0.0362 (5)	0.0741 (8)	0.0430 (5)	−0.0041 (5)	0.0081 (4)	−0.0076 (5)

Geometric parameters (Å, º)

C1—C2	1.379 (2)	C14—H14	0.9300
C1—C6	1.3873 (19)	C15—C16	1.376 (2)
C1—H1	0.9300	C15—H15	0.9300
C2—C3	1.370 (2)	C16—H16	0.9300
C2—H2	0.9300	C17—O2	1.1905 (16)
C3—C4	1.381 (2)	C17—O3	1.3328 (18)
C3—H3	0.9300	C18—O3	1.4456 (19)
C4—C5	1.3942 (17)	C18—H18A	0.9600
C4—H4	0.9300	C18—H18B	0.9600
C5—C6	1.3940 (19)	C18—H18C	0.9600
C5—C10	1.4796 (18)	C19—O4	1.1985 (15)
C6—C7	1.4777 (18)	C19—O5	1.3256 (17)
C7—O1	1.2090 (17)	C20—O5	1.4399 (19)
C7—C8	1.5397 (18)	C20—H20A	0.9600
C8—C9	1.5212 (18)	C20—H20B	0.9600
C8—C17	1.5392 (17)	C20—H20C	0.9600
C8—C11	1.5408 (18)	C21—C22	1.380 (2)
C9—C10	1.3457 (16)	C21—C26	1.3867 (19)
C9—C19	1.4897 (18)	C22—C23	1.384 (2)
C10—C21	1.4852 (18)	C22—H22	0.9300
C11—C12	1.3844 (19)	C23—C24	1.369 (3)
C11—C16	1.3866 (19)	C23—H23	0.9300
C12—C13	1.3774 (19)	C24—C25	1.365 (3)
C12—H12	0.9300	C24—H24	0.9300
C13—C14	1.371 (2)	C25—C26	1.377 (3)
C13—H13	0.9300	C25—H25	0.9300
C14—C15	1.369 (2)	C26—H26	0.9300
C2—C1—C6	120.04 (15)	C14—C15—C16	120.74 (15)
C2—C1—H1	120.0	C14—C15—H15	119.6
C6—C1—H1	120.0	C16—C15—H15	119.6
C3—C2—C1	119.74 (14)	C15—C16—C11	120.65 (15)
C3—C2—H2	120.1	C15—C16—H16	119.7
C1—C2—H2	120.1	C11—C16—H16	119.7
C2—C3—C4	120.68 (13)	O2—C17—O3	124.69 (13)
C2—C3—H3	119.7	O2—C17—C8	126.72 (14)
C4—C3—H3	119.7	O3—C17—C8	108.57 (11)
C3—C4—C5	120.74 (14)	O3—C18—H18A	109.5

C3—C4—H4	119.6	O3—C18—H18B	109.5
C5—C4—H4	119.6	H18A—C18—H18B	109.5
C6—C5—C4	117.90 (12)	O3—C18—H18C	109.5
C6—C5—C10	120.27 (11)	H18A—C18—H18C	109.5
C4—C5—C10	121.82 (12)	H18B—C18—H18C	109.5
C1—C6—C5	120.89 (12)	O4—C19—O5	123.97 (13)
C1—C6—C7	119.35 (13)	O4—C19—C9	122.85 (13)
C5—C6—C7	119.76 (12)	O5—C19—C9	113.11 (11)
O1—C7—C6	122.90 (12)	O5—C20—H20A	109.5
O1—C7—C8	121.30 (11)	O5—C20—H20B	109.5
C6—C7—C8	115.69 (11)	H20A—C20—H20B	109.5
C9—C8—C17	110.48 (11)	O5—C20—H20C	109.5
C9—C8—C7	110.63 (10)	H20A—C20—H20C	109.5
C17—C8—C7	106.22 (10)	H20B—C20—H20C	109.5
C9—C8—C11	112.92 (10)	C22—C21—C26	118.68 (14)
C17—C8—C11	111.96 (10)	C22—C21—C10	119.79 (12)
C7—C8—C11	104.24 (10)	C26—C21—C10	121.49 (14)
C10—C9—C19	123.16 (12)	C21—C22—C23	120.60 (17)
C10—C9—C8	122.34 (11)	C21—C22—H22	119.7
C19—C9—C8	114.40 (10)	C23—C22—H22	119.7
C9—C10—C5	119.96 (12)	C24—C23—C22	120.1 (2)
C9—C10—C21	122.49 (12)	C24—C23—H23	119.9
C5—C10—C21	117.40 (10)	C22—C23—H23	119.9
C12—C11—C16	117.97 (13)	C25—C24—C23	119.64 (18)
C12—C11—C8	122.16 (11)	C25—C24—H24	120.2
C16—C11—C8	119.81 (12)	C23—C24—H24	120.2
C13—C12—C11	120.92 (13)	C24—C25—C26	120.94 (18)
C13—C12—H12	119.5	C24—C25—H25	119.5
C11—C12—H12	119.5	C26—C25—H25	119.5
C14—C13—C12	120.45 (14)	C25—C26—C21	120.02 (18)
C14—C13—H13	119.8	C25—C26—H26	120.0
C12—C13—H13	119.8	C21—C26—H26	120.0
C15—C14—C13	119.25 (14)	C17—O3—C18	115.77 (13)
C15—C14—H14	120.4	C19—O5—C20	117.16 (12)
C13—C14—H14	120.4		

C6—C1—C2—C3	1.0 (2)	C9—C8—C11—C16	176.27 (12)
C1—C2—C3—C4	−0.1 (2)	C17—C8—C11—C16	−58.27 (16)
C2—C3—C4—C5	−0.8 (2)	C7—C8—C11—C16	56.13 (14)
C3—C4—C5—C6	1.0 (2)	C16—C11—C12—C13	−0.28 (18)
C3—C4—C5—C10	−179.82 (13)	C8—C11—C12—C13	176.90 (12)
C2—C1—C6—C5	−0.8 (2)	C11—C12—C13—C14	−0.3 (2)
C2—C1—C6—C7	179.38 (13)	C12—C13—C14—C15	1.0 (2)
C4—C5—C6—C1	−0.2 (2)	C13—C14—C15—C16	−1.0 (2)
C10—C5—C6—C1	−179.37 (12)	C14—C15—C16—C11	0.4 (2)
C4—C5—C6—C7	179.65 (12)	C12—C11—C16—C15	0.2 (2)
C10—C5—C6—C7	0.44 (18)	C8—C11—C16—C15	−177.00 (13)
C1—C6—C7—O1	21.7 (2)	C9—C8—C17—O2	138.57 (16)

C5—C6—C7—O1	−158.09 (14)	C7—C8—C17—O2	−101.40 (17)
C1—C6—C7—C8	−154.54 (12)	C11—C8—C17—O2	11.8 (2)
C5—C6—C7—C8	25.65 (18)	C9—C8—C17—O3	−42.97 (14)
O1—C7—C8—C9	145.22 (13)	C7—C8—C17—O3	77.06 (14)
C6—C7—C8—C9	−38.46 (15)	C11—C8—C17—O3	−169.76 (11)
O1—C7—C8—C17	25.29 (17)	C10—C9—C19—O4	140.82 (15)
C6—C7—C8—C17	−158.39 (11)	C8—C9—C19—O4	−35.58 (19)
O1—C7—C8—C11	−93.12 (15)	C10—C9—C19—O5	−42.04 (18)
C6—C7—C8—C11	83.21 (13)	C8—C9—C19—O5	141.56 (12)
C17—C8—C9—C10	146.53 (12)	C9—C10—C21—C22	−62.17 (19)
C7—C8—C9—C10	29.18 (17)	C5—C10—C21—C22	113.49 (15)
C11—C8—C9—C10	−87.22 (15)	C9—C10—C21—C26	120.02 (15)
C17—C8—C9—C19	−37.04 (15)	C5—C10—C21—C26	−64.33 (17)
C7—C8—C9—C19	−154.38 (11)	C26—C21—C22—C23	−0.2 (2)
C11—C8—C9—C19	89.22 (13)	C10—C21—C22—C23	−178.11 (15)
C19—C9—C10—C5	179.15 (12)	C21—C22—C23—C24	0.3 (3)
C8—C9—C10—C5	−4.73 (19)	C22—C23—C24—C25	−0.6 (3)
C19—C9—C10—C21	−5.3 (2)	C23—C24—C25—C26	0.9 (3)
C8—C9—C10—C21	170.82 (12)	C24—C25—C26—C21	−0.9 (2)
C6—C5—C10—C9	−11.87 (19)	C22—C21—C26—C25	0.6 (2)
C4—C5—C10—C9	168.95 (13)	C10—C21—C26—C25	178.39 (13)
C6—C5—C10—C21	172.36 (12)	O2—C17—O3—C18	−3.7 (2)
C4—C5—C10—C21	−6.82 (18)	C8—C17—O3—C18	177.83 (14)
C9—C8—C11—C12	−0.86 (16)	O4—C19—O5—C20	−4.2 (2)
C17—C8—C11—C12	124.60 (13)	C9—C19—O5—C20	178.73 (14)
C7—C8—C11—C12	−121.00 (12)		

Hydrogen-bond geometry (Å, º)

*Cg*3 is the centroid of the phenyl C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C24—H24···O2^{i}	0.93	2.59	3.449 (3)	155
C20—H20*B*···O5^{ii}	0.96	2.59	3.430 (2)	146
C3—H3···*Cg*3^{iii}	0.93	2.77	3.6338 (16)	154

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*, −*y*+1, −*z*.