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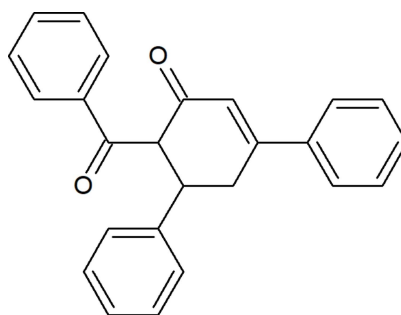
# Crystal structure and Hirshfeld surface analysis of 6-benzoyl-3,5-diphenylcyclohex-2-en-1-one

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In the title compound, C<sub>25</sub>H<sub>20</sub>O<sub>2</sub>, the central cyclohexenone ring adopts an envelope conformation. The mean plane of the cyclohexenone ring makes dihedral angles of 87.66 (11) and 23.76 (12)°, respectively, with the two attached phenyl rings, while it is inclined by 69.55 (11)° to the phenyl ring of the benzoyl group. In the crystal, the molecules are linked by C—H···O and C—H···π interactions, forming a three-dimensional network.

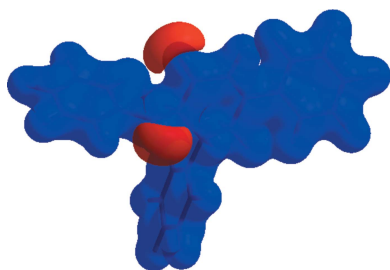
## 1. Chemical context

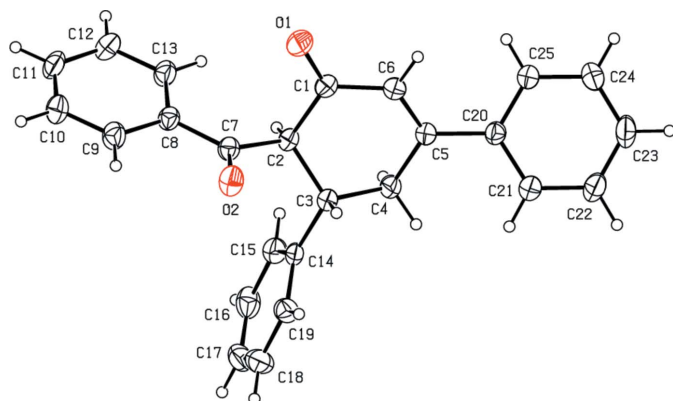
There have been a series of significant examples of enone derivatives used as target products as well as synthetic intermediates (Abdelhamid *et al.*, 2011; Asgarova *et al.*, 2019; Khalilov *et al.*, 2018*a,b*; Thomas, 2007). Moreover, a number of useful compounds containing enone moieties have been found in nature, such as cyanthiwigin U, (+)-cepharamine, phorbol and grandisine G, which were the object of a total synthesis (Pfeiffer *et al.*, 2005; Schultz & Wang, 1998; Kawamura *et al.*, 2016; Cuthbertson & Taylor, 2013). As part of a further study on the chemistry of  $\alpha,\beta$ -unsaturated ketones (Naghiyev *et al.*, 2016), we report herein the crystal structure and Hirshfeld surface analysis of the title compound.



## 2. Structural commentary

In the title compound (Fig. 1), the central cyclohexenone ring adopts an envelope conformation with puckering parameters  $Q_T = 0.470$  (2) Å,  $\theta = 125.3$  (2)° and  $\varphi = 300.8$  (3)°. The mean plane of the cyclohexenone ring [maximum deviation = 0.335 (2) Å] makes dihedral angles of 87.66 (11) and 23.76 (12)°, respectively, with the C14–C18 and C20–C25





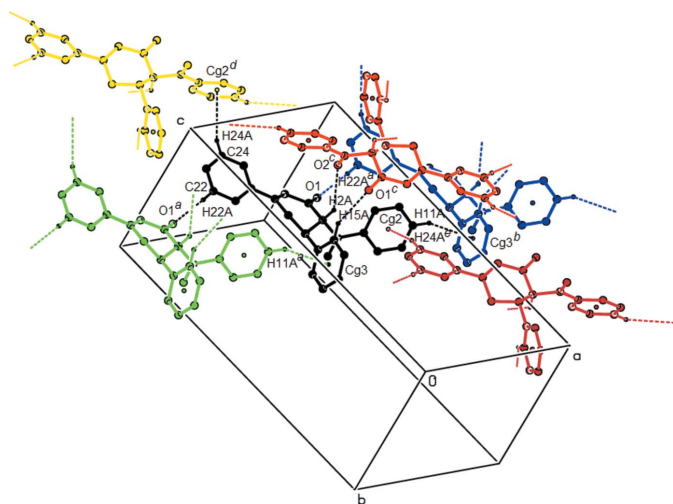
**Figure 1**  
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius.

phenyl rings, whereas it is inclined by  $69.55(11)^\circ$  to the C8–C13 phenyl ring of the benzoyl group.

### 3. Supramolecular features and Hirshfeld surface analysis

In the crystal, the molecules are linked by C–H $\cdots$ O and C–H $\cdots\pi$  interactions (C2–H2A $\cdots$ O2<sup>i</sup>, C15–H15A $\cdots$ O1<sup>i</sup>, C22–H22A $\cdots$ O1<sup>ii</sup> and C11–H11A $\cdots$ Cg3<sup>iii</sup>, symmetry codes as given in Table 1; Cg3 is the centroid of the C14–C19 ring), forming layers parallel to the *ab* plane. The layers are further connected by another C–H $\cdots\pi$  interaction (C24–H24A $\cdots$ Cg2<sup>iv</sup>; Table 1; Cg2 is the centroid of the C8–C13 ring), forming a three-dimensional network (Fig. 2).

The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) was performed using *CrystalExplorer* 3.1 (Wolff *et al.*, 2012). The surface of the title compound mapped over  $d_{\text{norm}}$  is



**Figure 2**  
A packing view of the title compound, formed by C–H $\cdots$ O and C–H $\cdots\pi$  interactions (dashed lines). [Symmetry codes: (a)  $x - 1, y, z$ ; (b)  $x + 1, y, z$ ; (c)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (d)  $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (e)  $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$ .]

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

Cg2 and Cg3 are the centroids of the C8–C13 and C14–C19 phenyl rings, respectively.

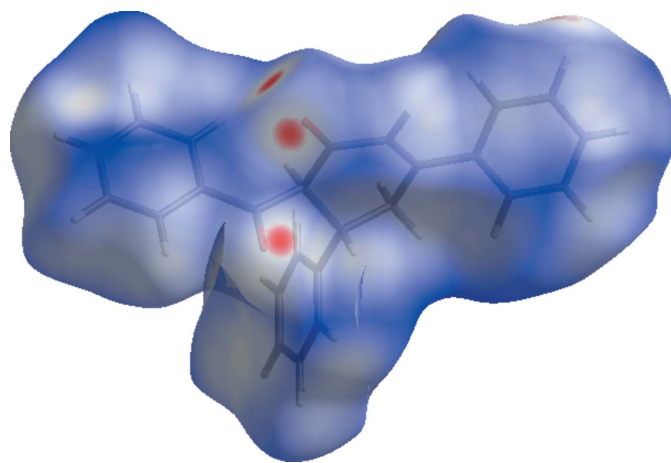
<i>D</i> –H $\cdots$ <i>A</i>	<i>D</i> –H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> –H $\cdots$ <i>A</i>
C2–H2A $\cdots$ O2 <sup>i</sup>	0.98	2.50	3.251 (3)	133
C15–H15A $\cdots$ O1 <sup>i</sup>	0.93	2.55	3.369 (3)	148
C22–H22A $\cdots$ O1 <sup>ii</sup>	0.93	2.54	3.472 (3)	175
C11–H11A $\cdots$ Cg3 <sup>iii</sup>	0.93	2.88	3.717 (2)	150
C24–H24A $\cdots$ Cg2 <sup>iv</sup>	0.93	2.78	3.667 (3)	159

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

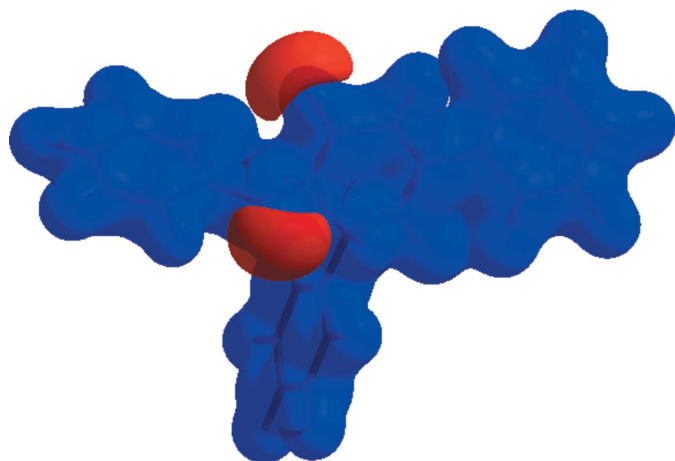
shown in Fig. 3. The dark-red spots on the  $d_{\text{norm}}$  surface arise as a result of short interatomic contacts, while the other weaker intermolecular interactions appear as light-red spots. The Hirshfeld surface mapped over electrostatic potential (Spackman *et al.*, 2008; Jayatilaka *et al.*, 2005) is shown in Fig. 4. The blue regions indicate positive electrostatic potential (hydrogen-bond donors), while the red regions indicate negative electrostatic potential (hydrogen-bond acceptors). The overall two-dimensional fingerprint plot (Spackman & McKinnon, 2002), and those delineated into H $\cdots$ H (48.8%), C $\cdots$ H/H $\cdots$ C (34.9%) and O $\cdots$ H/H $\cdots$ O (15%) contacts are illustrated in Fig. 5*a–d*, respectively. The most significant intermolecular contribution is from the H $\cdots$ H contact (48.8%) (Fig. 5*b*). The other minor contributions to the Hirshfeld surface are by C $\cdots$ C (0.9%), O $\cdots$ C/C $\cdots$ O (0.5%) and O $\cdots$ O (0.1%) contacts. The large number of H $\cdots$ H, C $\cdots$ H/H $\cdots$ C and O $\cdots$ H/H $\cdots$ O interactions suggest that van der Waals interactions and hydrogen bonding play the major roles in the crystal packing (Hathwar *et al.*, 2015).

### 4. Database survey

Although a search of the Cambridge Structural Database (CSD, Version 5.41, November 2019; Groom *et al.*, 2016) for 3,5-diphenylcyclohex-2-en-1-one derivatives gave 44 hits, no

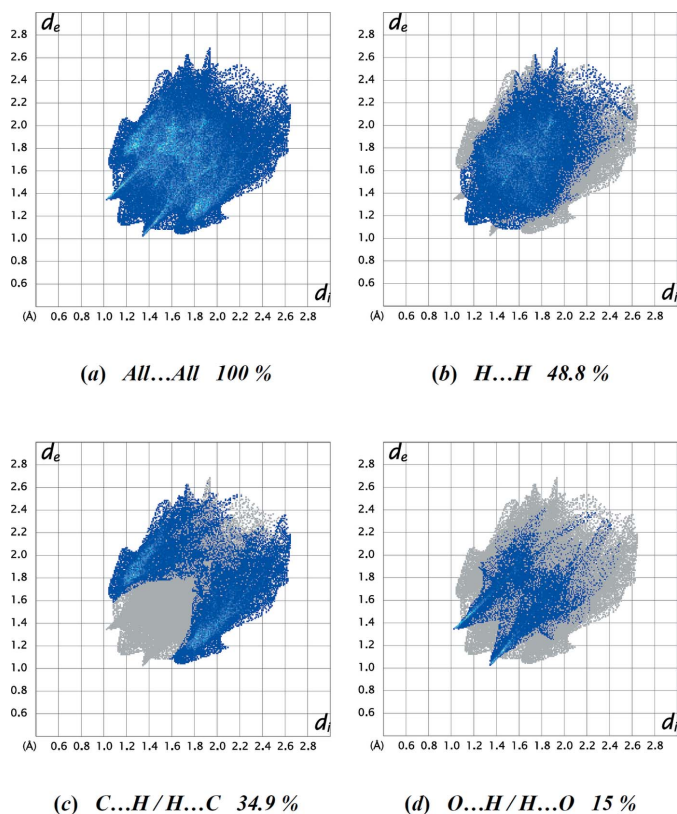


**Figure 3**  
The Hirshfeld surface of the title compound plotted over  $d_{\text{norm}}$  using a standard surface resolution with a fixed colour scale of  $-0.1582$  (red) to  $1.4399$  a.u. (blue).



**Figure 4**  
The Hirshfeld surface of the title compound plotted over electrostatic potential energy in the range from  $-0.0500$  to  $0.0500$  a.u. using the STO-3 G basis set at the Hartree–Fock level of theory. Hydrogen-bond donors and acceptors are shown as blue and red regions around the atoms, corresponding to positive and negative potentials, respectively.

compound having a skeleton of 6-acetyl-3,5-diphenylcyclohex-2-en-1-one was found. As related compounds, nine derivatives of ethyl 2-oxo-4,6-diphenylcyclohex-3-ene carboxylate were reported.



**Figure 5**  
The two-dimensional fingerprint plots for the title compound, showing (a) all interactions, and delineated into (b) H...H, (c) C...H/H...C, (d) O...H/H...O interactions. The  $d_i$  and  $d_e$  values are the closest internal and external distances ( $\text{\AA}$ ) from given points on the Hirshfeld surface.

**Table 2**  
Experimental details.

<b>Crystal data</b>	
Chemical formula	$\text{C}_{25}\text{H}_{20}\text{O}_2$
$M_r$	352.41
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
$a, b, c$ ( $\text{\AA}$ )	10.2365 (4), 9.7989 (4), 19.3759 (8)
$\beta$ ( $^\circ$ )	103.333 (2)
$V$ ( $\text{\AA}^3$ )	1891.14 (13)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.08
Crystal size (mm)	$0.23 \times 0.20 \times 0.12$
<b>Data collection</b>	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2003)
$T_{\min}$ , $T_{\max}$	0.660, 0.746
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	23764, 4102, 2471
$R_{\text{int}}$	0.073
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.639
<b>Refinement</b>	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.059, 0.149, 1.01
No. of reflections	4102
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	0.19, $-0.19$

Computer programs: APEX2 and SAINT (Bruker, 2003), SHELXT (Sheldrick, 2015a) and SHELXL2018 (Sheldrick, 2015b).

## 5. Synthesis and crystallization

To a solution of 1,3-diphenyl-2-propen-1-one (1.90 mmol) in benzene (15 ml), 1-phenylbutane-1,3-dione (1.90 mmol) and 0.05 ml of dry piperidine were added in this order, and the mixture was stirred at room temperature for 24 h. After completion of the reaction (as monitored by TLC), the solvent was removed under reduced pressure, and the residue was washed with hot water. Then, the products were recrystallized from ethanol (yield 72%, m.p. 446 K). IR (KBr): 2926, 2966, 3006 and 3062  $\nu(\text{CH})$ , 1610, 1650 and 1676  $\nu(\text{C}=\text{O})$   $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300.130 MHz, DMSO- $d_6$ ):  $\delta$  3.12 (*dd*, 2H,  $\text{CH}_2$ ,  $^2J_{\text{H-H}} = 16.3$  Hz,  $^3J_{\text{H-H}} = 8.2$  Hz), 3.91 (*t*, 1H, CH,  $^3J_{\text{H-H}} = 12.4$  Hz), 5.52 (*d*, 1H, CH,  $^3J_{\text{H-H}} = 12.4$  Hz), 6.56 (*s*, 1H, CH=), 7.1–7.92 (*m*, 15H, arom, 3Ar);  $^{13}\text{C}$  NMR (75.468 MHz, DMSO- $d_6$ ):  $\delta$  199.4, 197.5, 159.6, 142.7, 138.3, 137.8, 133.7, 130.9, 129.3, 129.1, 128.8, 128.0, 127.2, 126.9, 124.2, 58.2, 43.9, 36.4; MS (ESI):  $m/z$ : 353.15 [ $M + \text{H}$ ] $^+$ .

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed at calculated positions using a riding model, with C–H = 0.93–0.98  $\text{\AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . Owing to poor agreement between observed and calculated intensities, eighteen outliers ( $\bar{2}25$ ), ( $322$ ), ( $\bar{1}22$ ), ( $503$ ), ( $011$ ), ( $513$ ), ( $\bar{4}04$ ), ( $\bar{2}17$ ), ( $\bar{5}23$ ), ( $\bar{5}35$ ), ( $\bar{2}112$ ), ( $243$ ), ( $487$ ), ( $\bar{3}07$ ), ( $\bar{2}105$ ), ( $255$ ), ( $\bar{3}215$ ) and ( $012$ ) were omitted in the final cycle of refinement.

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## supporting information

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## Crystal structure and Hirshfeld surface analysis of 6-benzoyl-3,5-diphenylcyclohex-2-en-1-one

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### Computing details

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINTE* (Bruker, 2003); data reduction: *SAINTE* (Bruker, 2003); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b).

### 6-Benzoyl-3,5-diphenylcyclohex-2-en-1-one

#### Crystal data

C<sub>25</sub>H<sub>20</sub>O<sub>2</sub>

$M_r = 352.41$

Monoclinic,  $P2_1/n$

$a = 10.2365$  (4) Å

$b = 9.7989$  (4) Å

$c = 19.3759$  (8) Å

$\beta = 103.333$  (2)°

$V = 1891.14$  (13) Å<sup>3</sup>

$Z = 4$

$F(000) = 744$

$D_x = 1.238$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3243 reflections

$\theta = 2.5$ – $25.0$ °

$\mu = 0.08$  mm<sup>-1</sup>

$T = 296$  K

Prism, colourless

$0.23 \times 0.20 \times 0.12$  mm

#### Data collection

Bruker APEXII CCD  
diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2003)

$T_{\min} = 0.660$ ,  $T_{\max} = 0.746$

23764 measured reflections

4102 independent reflections

2471 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.073$

$\theta_{\max} = 27.0$ °,  $\theta_{\min} = 2.1$ °

$h = -13 \rightarrow 13$

$k = -12 \rightarrow 12$

$l = -24 \rightarrow 24$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.149$

$S = 1.00$

4102 reflections

244 parameters

0 restraints

Primary atom site location: difference Fourier  
map

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.020P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.19$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.19$  e Å<sup>-3</sup>



*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.84873 (15)	0.4571 (2)	0.84508 (9)	0.0662 (5)
O2	0.73311 (16)	0.59881 (16)	0.68577 (9)	0.0556 (4)
C1	0.7327 (2)	0.4250 (2)	0.81963 (11)	0.0432 (5)
C2	0.68555 (19)	0.3941 (2)	0.74035 (11)	0.0377 (5)
H2A	0.703396	0.297799	0.732533	0.045*
C3	0.53461 (19)	0.4203 (2)	0.71377 (10)	0.0380 (5)
H3A	0.519851	0.518223	0.718969	0.046*
C4	0.4572 (2)	0.3451 (3)	0.76099 (11)	0.0471 (6)
H4A	0.362962	0.369151	0.746260	0.056*
H4B	0.464862	0.247638	0.754221	0.056*
C5	0.5064 (2)	0.3775 (2)	0.83834 (10)	0.0388 (5)
C6	0.6339 (2)	0.4151 (2)	0.86315 (11)	0.0442 (5)
H6A	0.661662	0.436354	0.911083	0.053*
C7	0.7682 (2)	0.4818 (2)	0.70074 (11)	0.0401 (5)
C8	0.89014 (19)	0.4261 (2)	0.68142 (11)	0.0403 (5)
C9	0.9499 (2)	0.5025 (3)	0.63619 (12)	0.0532 (6)
H9A	0.912888	0.586024	0.619070	0.064*
C10	1.0629 (2)	0.4558 (3)	0.61664 (13)	0.0612 (7)
H10A	1.101409	0.507482	0.586302	0.073*
C11	1.1189 (2)	0.3329 (3)	0.64180 (13)	0.0580 (7)
H11A	1.194874	0.301126	0.628243	0.070*
C12	1.0623 (2)	0.2568 (3)	0.68717 (13)	0.0570 (6)
H12A	1.101121	0.174324	0.704782	0.068*
C13	0.9480 (2)	0.3026 (2)	0.70664 (12)	0.0486 (6)
H13A	0.909822	0.250122	0.736835	0.058*
C14	0.47921 (18)	0.3846 (2)	0.63661 (10)	0.0375 (5)
C15	0.4852 (2)	0.2530 (3)	0.61136 (12)	0.0515 (6)
H15A	0.529328	0.185343	0.641574	0.062*
C16	0.4257 (2)	0.2214 (3)	0.54103 (13)	0.0604 (7)
H16A	0.429682	0.132362	0.525007	0.073*
C17	0.3615 (2)	0.3190 (3)	0.49526 (13)	0.0620 (7)
H17A	0.322732	0.297407	0.448269	0.074*
C18	0.3552 (3)	0.4496 (3)	0.51981 (13)	0.0625 (7)
H18A	0.311330	0.516816	0.489171	0.075*
C19	0.4131 (2)	0.4825 (2)	0.58944 (12)	0.0491 (6)
H19A	0.407775	0.571668	0.604998	0.059*
C20	0.4106 (2)	0.3634 (2)	0.88513 (11)	0.0398 (5)
C21	0.2742 (2)	0.3877 (3)	0.86040 (13)	0.0550 (6)
H21A	0.241528	0.412364	0.813221	0.066*

C22	0.1862 (2)	0.3760 (3)	0.90421 (15)	0.0667 (8)
H22A	0.095277	0.393434	0.886588	0.080*
C23	0.2324 (3)	0.3389 (3)	0.97356 (15)	0.0662 (7)
H23A	0.173169	0.331066	1.003253	0.079*
C24	0.3663 (3)	0.3132 (3)	0.99904 (14)	0.0625 (7)
H24A	0.397718	0.287297	1.046135	0.075*
C25	0.4553 (2)	0.3253 (3)	0.95566 (12)	0.0516 (6)
H25A	0.545976	0.307812	0.973826	0.062*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0359 (9)	0.1016 (15)	0.0586 (10)	−0.0170 (9)	0.0056 (8)	−0.0036 (9)
O2	0.0606 (10)	0.0407 (10)	0.0728 (11)	0.0030 (8)	0.0305 (9)	0.0069 (8)
C1	0.0342 (11)	0.0494 (13)	0.0456 (13)	−0.0024 (10)	0.0084 (9)	0.0009 (10)
C2	0.0310 (10)	0.0410 (12)	0.0426 (12)	−0.0015 (9)	0.0115 (9)	0.0000 (9)
C3	0.0340 (10)	0.0434 (12)	0.0379 (11)	0.0018 (9)	0.0107 (9)	−0.0001 (9)
C4	0.0342 (11)	0.0680 (16)	0.0398 (12)	−0.0073 (10)	0.0101 (9)	0.0004 (11)
C5	0.0367 (11)	0.0434 (13)	0.0376 (12)	0.0024 (9)	0.0112 (9)	0.0001 (9)
C6	0.0398 (12)	0.0545 (14)	0.0378 (12)	0.0003 (10)	0.0074 (9)	−0.0019 (10)
C7	0.0383 (11)	0.0404 (13)	0.0428 (12)	−0.0034 (10)	0.0118 (9)	−0.0003 (9)
C8	0.0354 (11)	0.0432 (12)	0.0434 (12)	−0.0054 (9)	0.0111 (9)	−0.0038 (10)
C9	0.0485 (13)	0.0566 (15)	0.0587 (15)	−0.0081 (11)	0.0211 (11)	0.0045 (12)
C10	0.0459 (14)	0.0793 (19)	0.0643 (17)	−0.0090 (13)	0.0248 (12)	0.0062 (14)
C11	0.0313 (11)	0.082 (2)	0.0644 (16)	−0.0024 (12)	0.0176 (11)	−0.0128 (14)
C12	0.0389 (12)	0.0618 (16)	0.0717 (16)	0.0052 (11)	0.0159 (12)	0.0005 (13)
C13	0.0407 (12)	0.0528 (15)	0.0557 (14)	−0.0018 (10)	0.0183 (10)	0.0054 (11)
C14	0.0298 (10)	0.0491 (13)	0.0365 (11)	−0.0019 (9)	0.0136 (8)	−0.0015 (9)
C15	0.0490 (13)	0.0568 (15)	0.0501 (14)	0.0037 (11)	0.0141 (11)	−0.0028 (12)
C16	0.0615 (16)	0.0654 (17)	0.0603 (16)	−0.0112 (13)	0.0261 (13)	−0.0215 (13)
C17	0.0562 (15)	0.092 (2)	0.0387 (13)	−0.0195 (15)	0.0123 (11)	−0.0051 (14)
C18	0.0600 (16)	0.0763 (19)	0.0468 (14)	−0.0068 (13)	0.0035 (12)	0.0123 (13)
C19	0.0496 (13)	0.0522 (14)	0.0455 (13)	−0.0026 (11)	0.0110 (10)	0.0046 (11)
C20	0.0369 (11)	0.0449 (12)	0.0393 (12)	0.0016 (9)	0.0122 (9)	−0.0039 (9)
C21	0.0421 (12)	0.0775 (18)	0.0470 (14)	0.0041 (12)	0.0137 (11)	−0.0002 (12)
C22	0.0405 (13)	0.099 (2)	0.0657 (18)	0.0000 (13)	0.0214 (12)	−0.0073 (15)
C23	0.0624 (16)	0.083 (2)	0.0653 (18)	0.0023 (14)	0.0404 (14)	−0.0014 (14)
C24	0.0645 (16)	0.0813 (19)	0.0476 (14)	0.0096 (14)	0.0254 (12)	0.0091 (13)
C25	0.0429 (12)	0.0707 (17)	0.0434 (13)	0.0104 (11)	0.0146 (10)	0.0034 (11)

*Geometric parameters (Å, °)*

O1—C1	1.218 (2)	C12—C13	1.384 (3)
O2—C7	1.217 (2)	C12—H12A	0.9300
C1—C6	1.461 (3)	C13—H13A	0.9300
C1—C2	1.530 (3)	C14—C15	1.385 (3)
C2—C7	1.530 (3)	C14—C19	1.389 (3)
C2—C3	1.533 (3)	C15—C16	1.393 (3)

C2—H2A	0.9800	C15—H15A	0.9300
C3—C14	1.513 (3)	C16—C17	1.366 (4)
C3—C4	1.530 (3)	C16—H16A	0.9300
C3—H3A	0.9800	C17—C18	1.371 (4)
C4—C5	1.501 (3)	C17—H17A	0.9300
C4—H4A	0.9700	C18—C19	1.381 (3)
C4—H4B	0.9700	C18—H18A	0.9300
C5—C6	1.335 (3)	C19—H19A	0.9300
C5—C20	1.487 (3)	C20—C25	1.388 (3)
C6—H6A	0.9300	C20—C21	1.388 (3)
C7—C8	1.487 (3)	C21—C22	1.378 (3)
C8—C13	1.387 (3)	C21—H21A	0.9300
C8—C9	1.396 (3)	C22—C23	1.367 (4)
C9—C10	1.376 (3)	C22—H22A	0.9300
C9—H9A	0.9300	C23—C24	1.370 (3)
C10—C11	1.374 (4)	C23—H23A	0.9300
C10—H10A	0.9300	C24—C25	1.379 (3)
C11—C12	1.378 (3)	C24—H24A	0.9300
C11—H11A	0.9300	C25—H25A	0.9300
O1—C1—C6	121.6 (2)	C11—C12—C13	120.3 (2)
O1—C1—C2	120.64 (19)	C11—C12—H12A	119.8
C6—C1—C2	117.80 (17)	C13—C12—H12A	119.8
C1—C2—C7	108.05 (16)	C12—C13—C8	120.4 (2)
C1—C2—C3	111.34 (16)	C12—C13—H13A	119.8
C7—C2—C3	111.64 (17)	C8—C13—H13A	119.8
C1—C2—H2A	108.6	C15—C14—C19	117.7 (2)
C7—C2—H2A	108.6	C15—C14—C3	121.83 (19)
C3—C2—H2A	108.6	C19—C14—C3	120.35 (19)
C14—C3—C4	110.59 (16)	C14—C15—C16	120.5 (2)
C14—C3—C2	114.35 (16)	C14—C15—H15A	119.7
C4—C3—C2	109.83 (16)	C16—C15—H15A	119.7
C14—C3—H3A	107.2	C17—C16—C15	121.0 (2)
C4—C3—H3A	107.2	C17—C16—H16A	119.5
C2—C3—H3A	107.2	C15—C16—H16A	119.5
C5—C4—C3	113.23 (17)	C16—C17—C18	118.8 (2)
C5—C4—H4A	108.9	C16—C17—H17A	120.6
C3—C4—H4A	108.9	C18—C17—H17A	120.6
C5—C4—H4B	108.9	C17—C18—C19	120.8 (2)
C3—C4—H4B	108.9	C17—C18—H18A	119.6
H4A—C4—H4B	107.7	C19—C18—H18A	119.6
C6—C5—C20	122.24 (19)	C18—C19—C14	121.1 (2)
C6—C5—C4	119.54 (18)	C18—C19—H19A	119.5
C20—C5—C4	118.20 (17)	C14—C19—H19A	119.5
C5—C6—C1	124.03 (19)	C25—C20—C21	117.5 (2)
C5—C6—H6A	118.0	C25—C20—C5	120.77 (18)
C1—C6—H6A	118.0	C21—C20—C5	121.71 (19)
O2—C7—C8	120.30 (19)	C22—C21—C20	121.5 (2)



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O2—C7—C2	118.76 (18)	C22—C21—H21A	119.3
C8—C7—C2	120.94 (19)	C20—C21—H21A	119.3
C13—C8—C9	118.4 (2)	C23—C22—C21	120.0 (2)
C13—C8—C7	123.14 (19)	C23—C22—H22A	120.0
C9—C8—C7	118.4 (2)	C21—C22—H22A	120.0
C10—C9—C8	120.8 (2)	C22—C23—C24	119.6 (2)
C10—C9—H9A	119.6	C22—C23—H23A	120.2
C8—C9—H9A	119.6	C24—C23—H23A	120.2
C11—C10—C9	120.2 (2)	C23—C24—C25	120.7 (2)
C11—C10—H10A	119.9	C23—C24—H24A	119.6
C9—C10—H10A	119.9	C25—C24—H24A	119.6
C10—C11—C12	119.9 (2)	C24—C25—C20	120.6 (2)
C10—C11—H11A	120.1	C24—C25—H25A	119.7
C12—C11—H11A	120.1	C20—C25—H25A	119.7
O1—C1—C2—C7	-31.1 (3)	C10—C11—C12—C13	1.0 (4)
C6—C1—C2—C7	148.64 (19)	C11—C12—C13—C8	-0.8 (4)
O1—C1—C2—C3	-154.1 (2)	C9—C8—C13—C12	0.0 (3)
C6—C1—C2—C3	25.7 (3)	C7—C8—C13—C12	-179.4 (2)
C1—C2—C3—C14	-176.81 (17)	C4—C3—C14—C15	-63.8 (2)
C7—C2—C3—C14	62.3 (2)	C2—C3—C14—C15	60.8 (3)
C1—C2—C3—C4	-51.8 (2)	C4—C3—C14—C19	112.4 (2)
C7—C2—C3—C4	-172.67 (17)	C2—C3—C14—C19	-123.0 (2)
C14—C3—C4—C5	-179.34 (18)	C19—C14—C15—C16	-0.4 (3)
C2—C3—C4—C5	53.5 (2)	C3—C14—C15—C16	175.84 (19)
C3—C4—C5—C6	-27.3 (3)	C14—C15—C16—C17	0.7 (3)
C3—C4—C5—C20	153.97 (19)	C15—C16—C17—C18	-0.6 (4)
C20—C5—C6—C1	177.5 (2)	C16—C17—C18—C19	0.3 (4)
C4—C5—C6—C1	-1.2 (3)	C17—C18—C19—C14	-0.1 (4)
O1—C1—C6—C5	-178.4 (2)	C15—C14—C19—C18	0.1 (3)
C2—C1—C6—C5	1.8 (3)	C3—C14—C19—C18	-176.2 (2)
C1—C2—C7—O2	-83.9 (2)	C6—C5—C20—C25	-30.6 (3)
C3—C2—C7—O2	38.9 (3)	C4—C5—C20—C25	148.1 (2)
C1—C2—C7—C8	95.4 (2)	C6—C5—C20—C21	149.3 (2)
C3—C2—C7—C8	-141.80 (19)	C4—C5—C20—C21	-32.0 (3)
O2—C7—C8—C13	169.2 (2)	C25—C20—C21—C22	0.7 (4)
C2—C7—C8—C13	-10.2 (3)	C5—C20—C21—C22	-179.2 (2)
O2—C7—C8—C9	-10.3 (3)	C20—C21—C22—C23	-0.5 (4)
C2—C7—C8—C9	170.39 (19)	C21—C22—C23—C24	-0.1 (4)
C13—C8—C9—C10	0.5 (3)	C22—C23—C24—C25	0.4 (4)
C7—C8—C9—C10	180.0 (2)	C23—C24—C25—C20	-0.2 (4)
C8—C9—C10—C11	-0.3 (4)	C21—C20—C25—C24	-0.4 (4)
C9—C10—C11—C12	-0.5 (4)	C5—C20—C25—C24	179.6 (2)

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*Hydrogen-bond geometry (Å, °)*

*Cg*2 and *Cg*3 are the centroids of the C8–C13 and C14–C19 phenyl rings, respectively.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H2 <i>A</i> ···O2 <sup>i</sup>	0.98	2.50	3.251 (3)	133
C15—H15 <i>A</i> ···O1 <sup>i</sup>	0.93	2.55	3.369 (3)	148
C22—H22 <i>A</i> ···O1 <sup>ii</sup>	0.93	2.54	3.472 (3)	175
C11—H11 <i>A</i> ··· <i>Cg</i> 3 <sup>iii</sup>	0.93	2.88	3.717 (2)	150
C24—H24 <i>A</i> ··· <i>Cg</i> 2 <sup>iv</sup>	0.93	2.78	3.667 (3)	159

Symmetry codes: (i)  $-x+3/2, y-1/2, -z+3/2$ ; (ii)  $x-1, y, z$ ; (iii)  $x+1, y, z$ ; (iv)  $x-3/2, -y-1/2, z-1/2$ .