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Crystal structure and Hirshfeld surface analysis of (*E*)-2-(2,4,6-trimethylbenzylidene)-3,4-dihydronaphthalen-1(2*H*)-one

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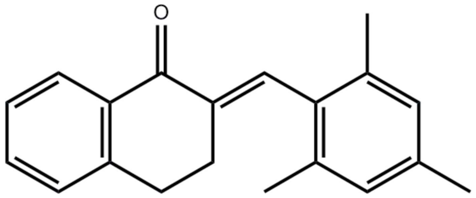
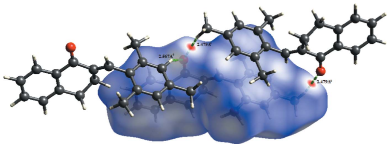
A novel chalcone, $C_{20}H_{20}O$, derived from benzylidenetetralone, was synthesized *via* Claissen–Schmidt condensation between tetralone and 2,4,6-trimethylbenzaldehyde. In the crystal, molecules are linked by C—H⋯O hydrogen bonds, producing $R_2^2(20)$ and $R_2^4(12)$ ring motifs. In addition, weak C—H⋯π and π-stacking interactions are observed. The intermolecular interactions were investigated using Hirshfeld surface analysis and two-dimensional fingerprint plots, revealing that the most important contributions for the crystal packing are from H⋯H (66.0%), H⋯C/ C⋯H (22.3%), H⋯O/O⋯H (9.3%), and C⋯C (2.4%) interactions. Shape-index plots show π–π stacking interactions and the curvedness plots show flat surface patches characteristic of planar stacking.

1. Chemical context

Chalcone (systematic name 1,3-diphenyl-2-propene-1-one) is an aromatic ketone that represents the central core for various derivatives with interesting properties, known as chalcones (Kostanecki & Tambor, 1899). For example, chalcones are found in fruits, vegetables, spices, tea or soy, and find applications as pharmaceuticals (Di Carlo *et al.*, 1999). Chalcones are also major intermediates in the synthesis of natural products and are widely used in synthetic and pharmaceutical chemistry (Dhar, 1981; Ansari *et al.*, 2005) because they have antitumor (Modzelewska *et al.*, 2006), antifungal (López *et al.*, 2001), anti-inflammatory (Lee *et al.*, 2006), anti-bacterial (Batovska *et al.*, 2009) or antitubercular properties (Lin *et al.*, 2002). In general, chalcones consist of two aromatic rings that are linked by a three-carbon α,β-unsaturated carbonyl system, leading to a completely delocalized π-electron system. Recently, chalcones have also been used in the field of materials science as non-linear optical devices (Raghavendra *et al.*, 2017). As part of our studies in this area, we report herein the synthesis, crystal structure and Hirshfeld surface analysis of a new chalcone.





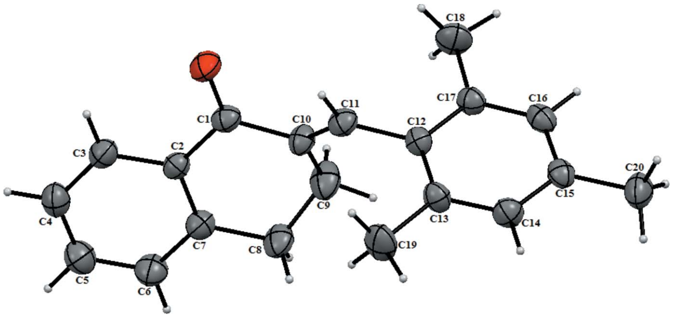


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

In the title molecule (Fig. 1), the cyclohexanone ring (C1/C2,C7/C8,C9/C10) has an envelope conformation with the flap atom C9 deviating by 0.280 (3) Å from the least-squares plane through the ring. The cyclohexanone ring is nearly co-planar with the benzene ring (C2–C7) being fused at a dihedral angle of 4.70 (18)°, but is inclined to the other benzene ring (C12–C17) by 74.95 (13)°. Torsion angles involving the methylene group C10═C11 are 83.3 (5)° (C17—C12—C11—C10), 129.8 (4)° (C11—C10—C9—C8) and 27.7 (6)° (O1—C1—C10—C11).

3. Supramolecular features

The main intermolecular interactions in the crystal structure of the title compound are of type C—H⋯O, C—H⋯π (Table 1) and π–π. Interactions between a methyl group and the carbonyl O atom (C20—H20*C*⋯O1^{ii}) as well as between an aromatic H atom and the carbonyl atom (C16—H16⋯O1^{i}) lead to $R_2^2(20)$ and $R_2^4(12)$ motifs (Fig. 2), linking adjacent molecules parallel to (001) (Table 2, Fig. 2). A weak C9—H9*A*⋯*Cg*2^{iii} (*Cg*2 is the centroid of the C2–C7 benzene ring) interaction is also present (Fig. 2), along with weak aromatic π-stacking interactions [*Cg*2⋯*Cg*2(−2 − *x*, −*y*, −1 − *z*) = 3.887 (3) Å] that consolidate the three-dimensional packing.

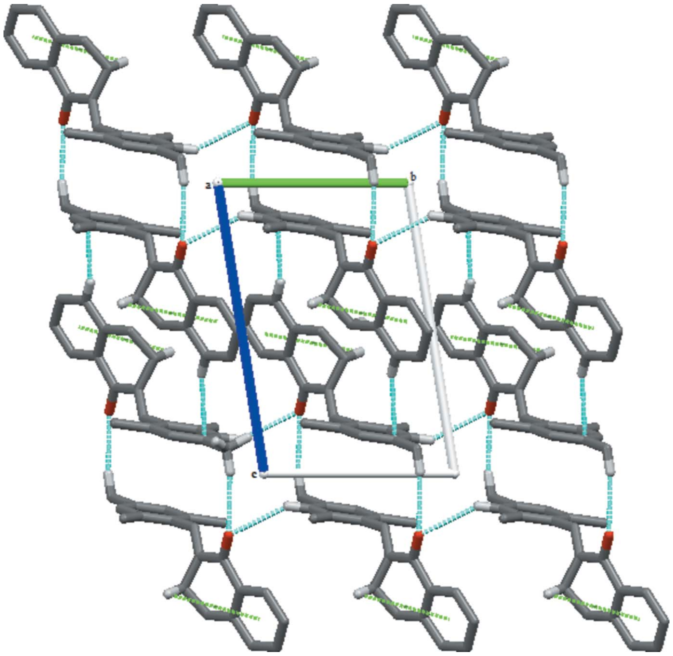


Figure 2
A view along the *a* axis of the title structure. Blue dashed lines denote the C—H⋯O hydrogen bonds which form $R_2^2(20)$ and $R_2^4(12)$ ring motifs. C—H⋯π interactions are shown as green dashes lines.

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

*Cg*2 is the centroid of the C2–C7 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C16—H16⋯O1^{i}	0.93	2.69	3.493 (5)	145
C20—H20*C*⋯O1^{ii}	0.96	2.60	3.535 (5)	165
C9—H9*A*⋯*Cg*2^{iii}	0.97	2.90	3.865 (6)	175

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

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update November 2018; Groom *et al.*, 2016) using (*E*)-2-(4-methylbenzylidene)-3,4-dihydronaphthalen-1(2*H*)-one as the main skeleton revealed the presence of four structures containing the chalcone moiety with different substituents that are similar to the title compound: (*E*)-4-[(1-oxo-3,4-dihydronaphthalen-2(1*H*)-ylidene)methyl]benzonitrile (QEVMAI; Baddeley *et al.*, 2017); (*E*)-4-[(5-methoxy-1-oxo-3,4-dihydronaphthalen-2(1*H*)-ylidene)methyl]benzonitrile (QEVMEM; Baddeley *et al.*, 2017); (*E*)-4-[(6-methoxy-1-oxo-3,4-dihydronaphthalen-2(1*H*)-ylidene)methyl]benzonitrile (QEVMIQ; Baddeley *et al.*, 2017); 1′-(4-bromophenyl)-4′-{4-[(1-oxo-3,4-dihydronaphthalen-2(1*H*)-ylidene) methyl]phenyl}-3″,4″-dihydro-1″*H*,2*H*-dispiro(acenaphthylene-1,2′-pyrrolidine-3′,2″-naphthalene)-1″,2-dione (VUZXOE; Saravanan *et al.*, 2010). QEVMAI and VUZXOE both crystallize in space group $P\overline{1}$, while QEVMEM and QEVMIQ crystallize in space group $P2_1/c$. In the structures of QEVMAI, QEVMEM and QEVMIQ, the dihedral angles between the phenyl groups are 45.66 (5), 55.06 (7) and 69.78 (5)°, respectively. In the structure of VUZXOE, the central benzene ring makes a dihedral angle of 42.71 (7)° with the bromophenyl ring.

5. Hirshfeld surface analysis

A Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were performed with *CrystalExplorer17* (Turner *et al.*, 2017), using standard surface resolution with the three-dimensional $d_{\rm norm}$ surfaces plotted over a fixed colour scale of −0.0870 (red) to 1.2944 (blue) a.u.. The three-dimensional $d_{\rm norm}$ surface of the title molecule is illustrated in Fig. 3*a* and 4. The pale-red spots symbolize short contacts and negative $d_{\rm norm}$ values on the surface correspond

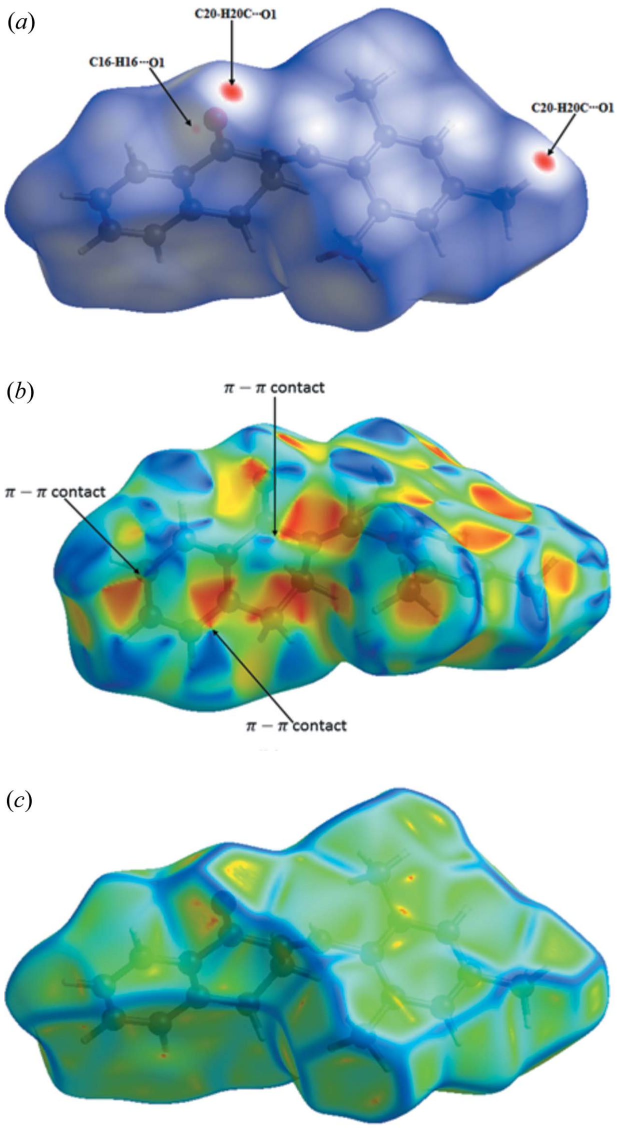


Figure 3
(*a*) d_{norm} mapped on Hirshfeld surfaces for visualizing the intermolecular interactions; (*b*) shape-index map and (*c*) curvedness map of the title compound.

to the C—H···O interactions described above (Table 1). The overall two-dimensional fingerprint plot is illustrated in Fig. 5*a*. The Hirshfeld surfaces mapped over $d_{\rm norm}$ are shown for the H···H, H···C/ C···H, H···O/O···H, C···C contacts (McKinnon *et al.*, 2007), and the two-dimensional fingerprint plots are shown in Fig. 5*b* and 5*c*, respectively, associated with their relative contributions to the Hirshfeld surface. The largest contribution to the overall crystal packing is from H···H interactions (66.0%); H···H contacts are shown in the middle region 1.10 Å < $(d_{\rm i} + d_{\rm e})$ < 1.18 Å. H···C/C···H contacts contribute 22.3% to the Hirshfeld surface, resulting in two pairs of characteristic wings in the fingerprint plot. The pair of tips appears at 1.10 Å < $(d_{\rm i} + d_{\rm e})$ < 1.65 Å. H···O/O···H contacts make a 9.3% contribution to the Hirshfeld surface. The contacts are represented by a pair of sharp spikes in the region 1.05 Å < $(d_{\rm i} + d_{\rm e})$ < 1.4 Å in the fingerprint plot. The C···C contacts are a measure of π–π stacking interactions and contribute 2.4% to the Hirshfeld surface. They appear as an arrow-shaped distribution at 1.80 Å < $(d_{\rm i} + d_{\rm e})$ < 2.0 Å.

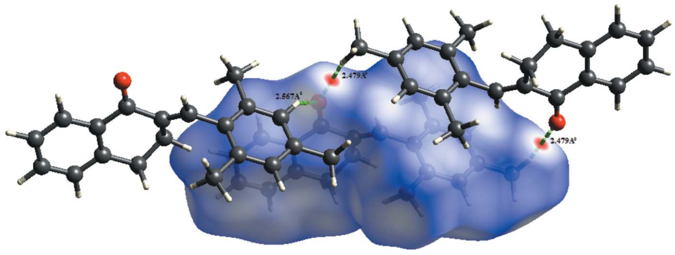


Figure 4
d_{norm} mapped on Hirshfeld surfaces for visualizing the intermolecular interactions.

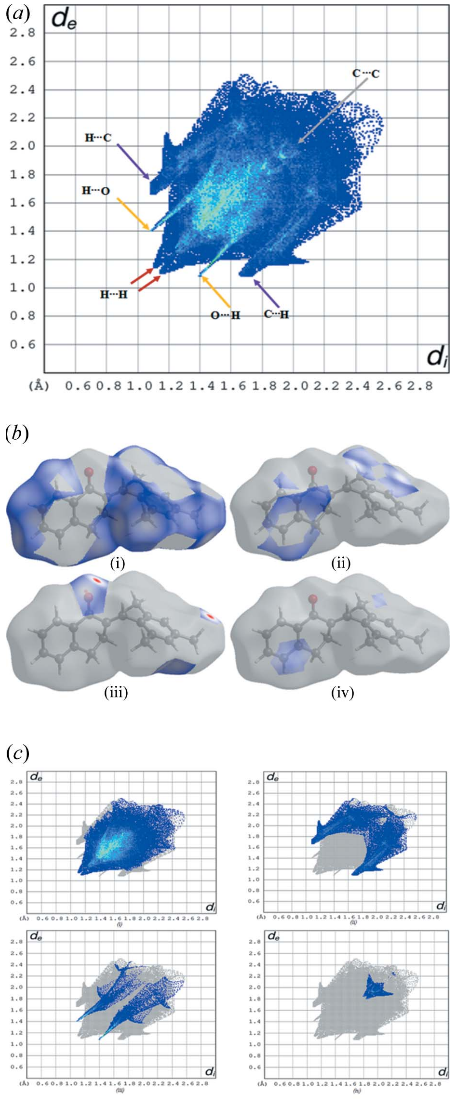


Figure 5
(*a*) The overall two-dimensional fingerprint plot and (*b*) Hirshfeld surface representations with the function $d_{\rm norm}$ plotted onto the surface for (i) H···H, (ii) H···C/C···H, (iii) H···O/O···H and (iv) C···C interactions. (*c*) The two-dimensional fingerprint plots for the title compound, delineated into (i) H···H, (ii) H···C/ C···H, (iii) H···O/O···H, (iv) C···C interactions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{20}O$
M_r	276.36
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, b, c (Å)	8.728 (2), 8.757 (2), 12.094 (3)
α, β, γ (°)	77.768 (19), 80.822 (19), 61.929 (18)
V (Å^3)	795.2 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.64 × 0.51 × 0.33
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.956, 0.982
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8143, 2726, 1102
R_{int}	0.088
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.061, 0.155, 0.91
No. of reflections	2726
No. of parameters	194
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.14

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2002), *SHELXT2017* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

The shape-index map of the title molecule (Fig. 3*b*) was generated in the ranges −1 to 1 Å. The convex blue regions symbolize hydrogen-donor groups and concave red regions symbolize hydrogen-acceptor groups. π–π interactions on the shape-index map are indicated by adjacent red and blue triangles. As can be seen in Fig. 3*b*, there are π–π interactions present between adjacent molecules in the title complex.

The curvedness map of the title compound (Fig. 3*c*) was generated in the range −4 to 0.4 Å. The large green regions represent a relatively flat (*i.e.* planar) surface area, while the blue regions demonstrate areas of curvature. The presence of π–π stacking interactions is also evident as flat regions around the rings on the Hirshfeld surface plotted over curvedness.

6. Synthesis and crystallization

2,4,6-Trimethylbenzylidenetetralone was prepared according to a literature protocol (Kumar *et al.*, 2017). 10 ml of a NaOH solution (40%$_{wt}$) was slowly added to a mixture of tetralone (1 mmol) and 2,4,6-trimethylbenzaldehyde (1 mmol) in ethanol (10 ml) at room temperature and stirred overnight. Then ice-cold water was added to the reaction mixture. The resulting precipitate was filtered off and dried *in vacuo*. The compound was purified by crystallization from ethanol, resulting in colourless prismatic crystals.

Yield 85%, m.p. 358 K; IR (ν, cm^{-1}): 3060 (C—H, aromatic), 2920 (C—H, aliphatic), 1670 (C=O), 1620 (C=C, aromatic); ^{1}H NMR (300 MHz, DMSO-d_6, δ, ppm): 7.9 (1H, *d*, =C—H), 7.58 (1H, *s*, =C—H), 7.50 (1H, *t*, =C—H), 7.38 (1H,t, =C—H), 7.30 (1H, d, =C—H), 6.82 (2H, s, =C—H), 2.8 (2H, t, $-CH_2$), 2.4 (2H, t, $-CH_2$), 2.2 (3H, s,$-CH_3$), 2.02 (6H, s, 2 CH_3); ^{13}C NMR (75 MHz, DMSO-d_6, δ, ppm): 186.9, 144.5, 138.0, 137.2, 135.9, 135.6, 134.2, 133.5, 132.4, 129.3, 128.6, 128.0, 127.6, 28.9, 27.4, 21.3, 20.5. Analysis calculated for $C_{20}H_{20}O$: C, 86.92%; H, 7.29%; O, 5.79%. Found: C, 86.99%; H, 7.35%; O, 5.90%.

7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were fixed geometrically and treated as riding, with C—H = 0.97 Å for methyl groups, 0.96 Å for methylene groups, 0.93 Å for aromatic hydrogen atoms and 0.98 Å for methine groups, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(C-methyl).

Funding information

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: SHELXT2017 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *SHELXL2018* (Sheldrick, 2015b), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

(*E*)-2-(2,4,6-Trimethylbenzylidene)-3,4-dihydronaphthalen-1(2*H*)-one

Crystal data

$C_{20}H_{20}O$
$M_r = 276.36$
Triclinic, $P\bar{1}$
$a = 8.728$ (2) Å
$b = 8.757$ (2) Å
$c = 12.094$ (3) Å
$\alpha = 77.768$ (19)°
$\beta = 80.822$ (19)°
$\gamma = 61.929$ (18)°
$V = 795.2$ (4) Å^3

$Z = 2$
$F(000) = 296$
$D_x = 1.154$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 12610 reflections
$\theta = 2.7$–30.2°
$\mu = 0.07$ mm^{-1}
$T = 293$ K
Prism, colorless
0.64 × 0.51 × 0.33 mm

Data collection

Stoe IPDS 2 diffractometer
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{\min} = 0.956$, $T_{\max} = 0.982$
8143 measured reflections

2726 independent reflections
1102 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.088$
$\theta_{\max} = 25.0$°, $\theta_{\min} = 2.7$°
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.155$
$S = 0.91$
2726 reflections
194 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.25$ e Å^{-3}
$\Delta\rho_{\min} = -0.14$ e Å^{-3}

Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.016 (4)

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 (Å²)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
O1	−1.0524 (3)	−0.2385 (4)	−0.7862 (2)	0.0977 (9)
C12	−0.4930 (4)	−0.5186 (5)	−0.8354 (3)	0.0635 (9)
C2	−1.0387 (4)	−0.2214 (4)	−0.5971 (3)	0.0639 (9)
C17	−0.4278 (4)	−0.6907 (5)	−0.8516 (3)	0.0705 (10)
C1	−0.9638 (4)	−0.2867 (5)	−0.7056 (3)	0.0715 (10)
C10	−0.7746 (4)	−0.4083 (4)	−0.7133 (3)	0.0695 (10)
C13	−0.3805 (5)	−0.4437 (5)	−0.8456 (3)	0.0744 (10)
C11	−0.6837 (4)	−0.4120 (4)	−0.8119 (3)	0.0736 (11)
H11	−0.745928	−0.339613	−0.873942	0.088*
C15	−0.1364 (4)	−0.7151 (5)	−0.8870 (3)	0.0711 (10)
C7	−0.9379 (4)	−0.2800 (5)	−0.5040 (3)	0.0743 (10)
C16	−0.2502 (5)	−0.7860 (5)	−0.8766 (3)	0.0762 (11)
H16	−0.206551	−0.902035	−0.886559	0.091*
C14	−0.2038 (5)	−0.5443 (5)	−0.8704 (3)	0.0798 (11)
H14	−0.128920	−0.494447	−0.875919	0.096*
C3	−1.2113 (4)	−0.0905 (5)	−0.5883 (3)	0.0792 (11)
H3	−1.280000	−0.051417	−0.649452	0.095*
C9	−0.7027 (5)	−0.5193 (6)	−0.6044 (3)	0.1051 (15)
H9A	−0.745452	−0.606334	−0.583241	0.126*
H9B	−0.576855	−0.580756	−0.615353	0.126*
C8	−0.7503 (4)	−0.4167 (5)	−0.5111 (3)	0.0951 (13)
H8A	−0.676588	−0.358974	−0.520287	0.114*
H8B	−0.726257	−0.496759	−0.439895	0.114*
C4	−1.2801 (5)	−0.0192 (5)	−0.4895 (4)	0.0909 (13)
H4	−1.394381	0.067973	−0.484398	0.109*
C6	−1.0115 (5)	−0.2062 (6)	−0.4058 (3)	0.0942 (13)
H6	−0.945571	−0.244732	−0.343260	0.113*
C5	−1.1799 (6)	−0.0771 (6)	−0.4000 (4)	0.0988 (14)
H5	−1.226312	−0.028553	−0.333787	0.119*
C20	0.0576 (4)	−0.8225 (6)	−0.9157 (3)	0.1039 (15)
H20A	0.094884	−0.940932	−0.877619	0.156*
H20B	0.121224	−0.772547	−0.891430	0.156*
H20C	0.078722	−0.821651	−0.996162	0.156*
C18	−0.5449 (5)	−0.7765 (5)	−0.8436 (4)	0.1077 (15)
H18A	−0.589023	−0.792507	−0.766309	0.162*

H18B	−0.479794	−0.888378	−0.868695	0.162*
H18C	−0.640231	−0.703345	−0.890605	0.162*
C19	−0.4477 (5)	−0.2554 (5)	−0.8281 (4)	0.1150 (16)
H19A	−0.531484	−0.178397	−0.882365	0.173*
H19B	−0.352349	−0.226633	−0.838182	0.173*
H19C	−0.501571	−0.241994	−0.752796	0.173*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0782 (16)	0.112 (2)	0.088 (2)	−0.0233 (15)	−0.0269 (14)	−0.0175 (16)
C12	0.069 (2)	0.057 (2)	0.060 (2)	−0.0271 (19)	−0.0034 (16)	−0.0044 (18)
C2	0.061 (2)	0.066 (2)	0.066 (2)	−0.0311 (19)	−0.0055 (18)	−0.0045 (19)
C17	0.079 (2)	0.061 (3)	0.073 (3)	−0.032 (2)	−0.0094 (18)	−0.0086 (19)
C1	0.073 (2)	0.071 (3)	0.069 (3)	−0.031 (2)	−0.019 (2)	−0.001 (2)
C10	0.062 (2)	0.070 (3)	0.062 (2)	−0.0218 (19)	−0.0091 (18)	0.0017 (19)
C13	0.082 (3)	0.058 (3)	0.081 (3)	−0.032 (2)	0.0010 (19)	−0.014 (2)
C11	0.072 (2)	0.072 (3)	0.072 (3)	−0.029 (2)	−0.0174 (19)	−0.001 (2)
C15	0.077 (2)	0.070 (3)	0.058 (2)	−0.026 (2)	−0.0030 (18)	−0.012 (2)
C7	0.071 (2)	0.084 (3)	0.067 (2)	−0.037 (2)	−0.005 (2)	−0.006 (2)
C16	0.095 (3)	0.059 (3)	0.069 (2)	−0.028 (2)	−0.010 (2)	−0.0122 (19)
C14	0.082 (3)	0.081 (3)	0.085 (3)	−0.045 (2)	0.0018 (19)	−0.015 (2)
C3	0.069 (2)	0.077 (3)	0.091 (3)	−0.032 (2)	−0.013 (2)	−0.008 (2)
C9	0.092 (3)	0.101 (3)	0.079 (3)	−0.013 (2)	−0.015 (2)	0.003 (3)
C8	0.080 (3)	0.099 (3)	0.081 (3)	−0.018 (2)	−0.024 (2)	−0.003 (3)
C4	0.076 (3)	0.085 (3)	0.102 (3)	−0.030 (2)	0.008 (3)	−0.022 (3)
C6	0.095 (3)	0.109 (3)	0.072 (3)	−0.040 (3)	−0.010 (2)	−0.012 (3)
C5	0.101 (3)	0.107 (4)	0.085 (3)	−0.045 (3)	0.008 (3)	−0.025 (3)
C20	0.076 (3)	0.113 (4)	0.098 (3)	−0.020 (2)	0.003 (2)	−0.030 (3)
C18	0.114 (3)	0.093 (3)	0.141 (4)	−0.065 (3)	−0.010 (3)	−0.023 (3)
C19	0.107 (3)	0.073 (3)	0.172 (5)	−0.044 (2)	0.007 (3)	−0.038 (3)

Geometric parameters (Å, º)

O1—C1	1.218 (4)	C3—C4	1.383 (5)
C12—C17	1.384 (4)	C3—H3	0.9300
C12—C13	1.393 (4)	C9—C8	1.477 (5)
C12—C11	1.491 (4)	C9—H9A	0.9700
C2—C7	1.396 (5)	C9—H9B	0.9700
C2—C3	1.404 (4)	C8—H8A	0.9700
C2—C1	1.473 (4)	C8—H8B	0.9700
C17—C16	1.390 (4)	C4—C5	1.359 (5)
C17—C18	1.510 (5)	C4—H4	0.9300
C1—C10	1.486 (4)	C6—C5	1.371 (5)
C10—C11	1.319 (4)	C6—H6	0.9300
C10—C9	1.490 (5)	C5—H5	0.9300
C13—C14	1.389 (4)	C20—H20A	0.9600
C13—C19	1.519 (5)	C20—H20B	0.9600

C11—H11	0.9300	C20—H20C	0.9600
C15—C14	1.373 (5)	C18—H18A	0.9600
C15—C16	1.377 (5)	C18—H18B	0.9600
C15—C20	1.524 (4)	C18—H18C	0.9600
C7—C6	1.390 (5)	C19—H19A	0.9600
C7—C8	1.508 (5)	C19—H19B	0.9600
C16—H16	0.9300	C19—H19C	0.9600
C14—H14	0.9300		

C17—C12—C13	119.7 (3)	C10—C9—H9A	109.0
C17—C12—C11	120.0 (3)	C8—C9—H9B	109.0
C13—C12—C11	120.3 (3)	C10—C9—H9B	109.0
C7—C2—C3	119.0 (3)	H9A—C9—H9B	107.8
C7—C2—C1	121.2 (3)	C9—C8—C7	114.6 (4)
C3—C2—C1	119.8 (4)	C9—C8—H8A	108.6
C12—C17—C16	119.0 (3)	C7—C8—H8A	108.6
C12—C17—C18	121.7 (3)	C9—C8—H8B	108.6
C16—C17—C18	119.3 (4)	C7—C8—H8B	108.6
O1—C1—C2	121.3 (3)	H8A—C8—H8B	107.6
O1—C1—C10	121.8 (3)	C5—C4—C3	119.6 (4)
C2—C1—C10	116.9 (4)	C5—C4—H4	120.2
C11—C10—C1	119.9 (3)	C3—C4—H4	120.2
C11—C10—C9	125.0 (3)	C5—C6—C7	120.9 (4)
C1—C10—C9	115.1 (3)	C5—C6—H6	119.6
C14—C13—C12	119.3 (3)	C7—C6—H6	119.6
C14—C13—C19	119.7 (4)	C4—C5—C6	121.0 (4)
C12—C13—C19	121.1 (3)	C4—C5—H5	119.5
C10—C11—C12	127.7 (3)	C6—C5—H5	119.5
C10—C11—H11	116.2	C15—C20—H20A	109.5
C12—C11—H11	116.2	C15—C20—H20B	109.5
C14—C15—C16	117.6 (3)	H20A—C20—H20B	109.5
C14—C15—C20	121.2 (4)	C15—C20—H20C	109.5
C16—C15—C20	121.2 (4)	H20A—C20—H20C	109.5
C6—C7—C2	118.9 (3)	H20B—C20—H20C	109.5
C6—C7—C8	120.4 (4)	C17—C18—H18A	109.5
C2—C7—C8	120.6 (3)	C17—C18—H18B	109.5
C15—C16—C17	122.4 (4)	H18A—C18—H18B	109.5
C15—C16—H16	118.8	C17—C18—H18C	109.5
C17—C16—H16	118.8	H18A—C18—H18C	109.5
C15—C14—C13	122.0 (4)	H18B—C18—H18C	109.5
C15—C14—H14	119.0	C13—C19—H19A	109.5
C13—C14—H14	119.0	C13—C19—H19B	109.5
C4—C3—C2	120.6 (4)	H19A—C19—H19B	109.5
C4—C3—H3	119.7	C13—C19—H19C	109.5
C2—C3—H3	119.7	H19A—C19—H19C	109.5
C8—C9—C10	112.8 (4)	H19B—C19—H19C	109.5
C8—C9—H9A	109.0		

C13—C12—C17—C16	0.7 (5)	C3—C2—C7—C8	−178.2 (3)
C11—C12—C17—C16	178.2 (3)	C1—C2—C7—C8	−2.0 (5)
C13—C12—C17—C18	−178.9 (3)	C14—C15—C16—C17	0.8 (5)
C11—C12—C17—C18	−1.3 (5)	C20—C15—C16—C17	−179.4 (3)
C7—C2—C1—O1	178.4 (4)	C12—C17—C16—C15	−0.7 (5)
C3—C2—C1—O1	−5.3 (5)	C18—C17—C16—C15	178.9 (3)
C7—C2—C1—C10	−3.8 (5)	C16—C15—C14—C13	−1.0 (5)
C3—C2—C1—C10	172.5 (3)	C20—C15—C14—C13	179.2 (3)
O1—C1—C10—C11	27.7 (6)	C12—C13—C14—C15	1.0 (5)
C2—C1—C10—C11	−150.1 (3)	C19—C13—C14—C15	−179.9 (4)
O1—C1—C10—C9	−152.2 (4)	C7—C2—C3—C4	0.7 (5)
C2—C1—C10—C9	30.0 (5)	C1—C2—C3—C4	−175.6 (3)
C17—C12—C13—C14	−0.8 (5)	C11—C10—C9—C8	129.8 (4)
C11—C12—C13—C14	−178.4 (3)	C1—C10—C9—C8	−50.3 (5)
C17—C12—C13—C19	−179.9 (4)	C10—C9—C8—C7	43.9 (5)
C11—C12—C13—C19	2.6 (5)	C6—C7—C8—C9	163.5 (4)
C1—C10—C11—C12	177.2 (3)	C2—C7—C8—C9	−18.7 (6)
C9—C10—C11—C12	−2.9 (7)	C2—C3—C4—C5	−0.4 (6)
C17—C12—C11—C10	83.3 (5)	C2—C7—C6—C5	−0.3 (6)
C13—C12—C11—C10	−99.2 (5)	C8—C7—C6—C5	177.5 (4)
C3—C2—C7—C6	−0.4 (5)	C3—C4—C5—C6	−0.3 (7)
C1—C2—C7—C6	175.9 (3)	C7—C6—C5—C4	0.7 (7)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O1^{i}	0.93	2.69	3.493 (5)	145
C20—H20*C*···O1^{ii}	0.96	2.60	3.535 (5)	165
C9—H9*A*···*Cg*2^{iii}	0.97	2.90	3.865 (6)	175

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