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8-Ethoxy-3-(4-isopropylbenzylidene)-6-methylchroman-4-one

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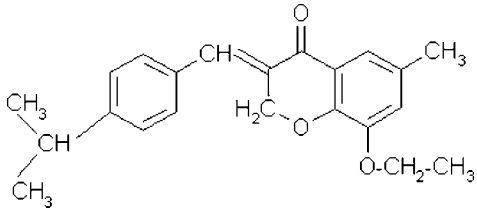
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.054; wR factor = 0.158; data-to-parameter ratio = 17.1.

In the title compound, $C_{22}H_{24}O_3$, the non-fused benzene ring makes a dihedral angle of 52.56 (7)° with the benzene ring of the chromanone unit. The molecular structure is stabilized by a weak intramolecular C—H···O interaction and the crystal packing is stabilized by weak intermolecular C—H···O interactions. The isopropyl group is disordered over two positions, with site occupancies of 0.48/0.52.

Related literature

For related literature, see: Kang *et al.* (2004); Marx *et al.* (2007); Puviarasan *et al.* (1998); Tillekeratne *et al.* (2001); Nissa *et al.* (2001); Schollmeyer *et al.* (2005). A related compound has been reported by Marx *et al.* (2007).



Experimental

Crystal data

$C_{22}H_{24}O_3$
M_r = 336.41
Monoclinic, $P2_1/n$
a = 10.3568 (9) Å
b = 16.8154 (15) Å
c = 10.8962 (10) Å
β = 99.873 (1)°
V = 1869.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.983, T_{max} = 0.988
21105 measured reflections
4385 independent reflections
3220 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.158
S = 1.02
4385 reflections
256 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O2^{i}	0.97	2.60	3.407 (2)	141
C10—H10···O2	0.93	2.47	2.823 (2)	103

Symmetry code: (i) $-x+2, -y, -z+2$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2050).

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supporting information

Acta Cryst. (2008). E**64**, o328 [https://doi.org/10.1107/S1600536807066925]

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S1. Comment

The Chromanone moiety present in the title compound consisting of the pyrone ring and benzene ring plays an important role in many areas of medicines such as inhibition of HIV replication (Tillekeratne *et al.*, 2001).

The geometric parameters in (I) agree with the reported values of similar structure (Puviarasan *et al.*, 1998; Schollmeyer *et al.*, 2005; Nissa *et al.*, 2001). The chromanone moiety consists of one benzene ring fused with a six membered heterocyclic ring which adopts a half-chair conformation. The C11—C16 benzene ring makes a dihedral angle of 52.56 (7)° with the benzene ring of chromanone unit.

The molecular structure is stabilized by weak intramolecular C—H···O interaction and the crystal packing is stabilized by weak intermolecular C—H···O interaction (Table 1.).

The methyl and aromatic C atoms in the ligand are disordered over two positions each with the site occupancy factors of 0.520 (10) [for C17, C18, C19] and 0.480 (10) for [C171, C181, C191].

S2. Experimental

Baylis-Hillman reaction of *p*-isopropyl benzaldehyde with methyl acrylate afforded methyl-3-hydroxy-3-(*p*-isopropyl phenyl-)-2-methylene propanoate. This ester was converted to methyl-(2-*Z*)-2-bromomethyl-3-(*p*-isopropyl phenyl)-prop-2-enoate on treatment with hydrobromic acid in presence of concentrated sulfuric acid. The resulting propenoate was treated with 2-ethoxy-4-methyl phenol in presence of potassium carbonate and acetone to get methyl-3-(*p*-isopropyl phenyl)-2-(2-ethoxy-4-methyl)-phenoxy methyl-prop-2-enoate. The phenoxy propenoate was hydrolysed by alkali solution to get the prop-2-enoic acid. Cyclization of the acid on treatment with trifluoro acetic anhydride in dichloro-methane resulted in 3-(4-isopropyl) benzylidine-8-ethoxy-6-methyl chroman-4-one.

S3. Refinement

The site occupancy factors for disordered C atoms were refined as 0.520 (10) [for C17, C18, C19] and 0.480 (10) for [C171, C181, C191]. during anisotropic refinement. C17—C19, C17—C18, C171–181 C171–191 distances were restrained to 1.55 (1). H atoms were positioned geometrically and refined using riding model with C—H = 0.93Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C—H, C—H = 0.97Å and U_{iso}(H) = 1.2Ueq(C) for CH2, C—H = 0.96Å and U_{iso}(H) = 1.5Ueq(C) for CH3.

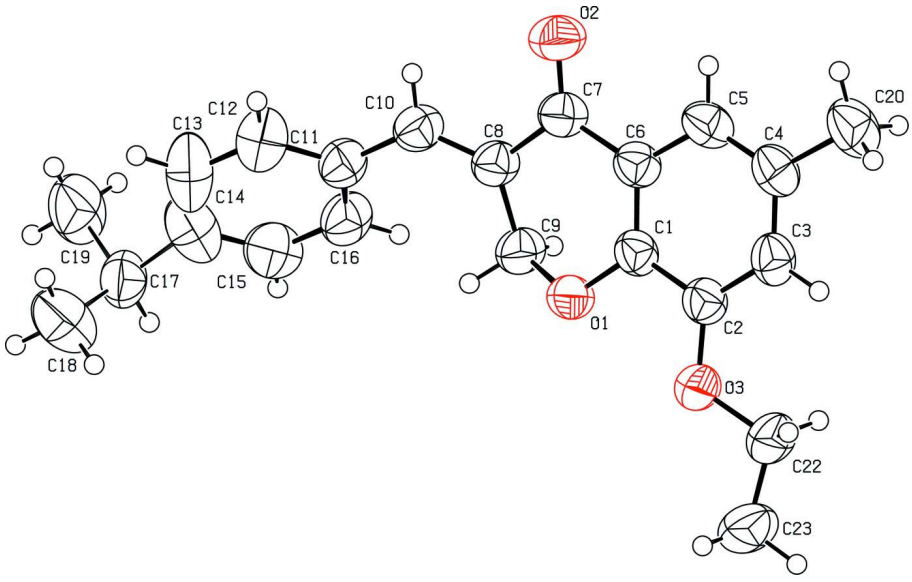

Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

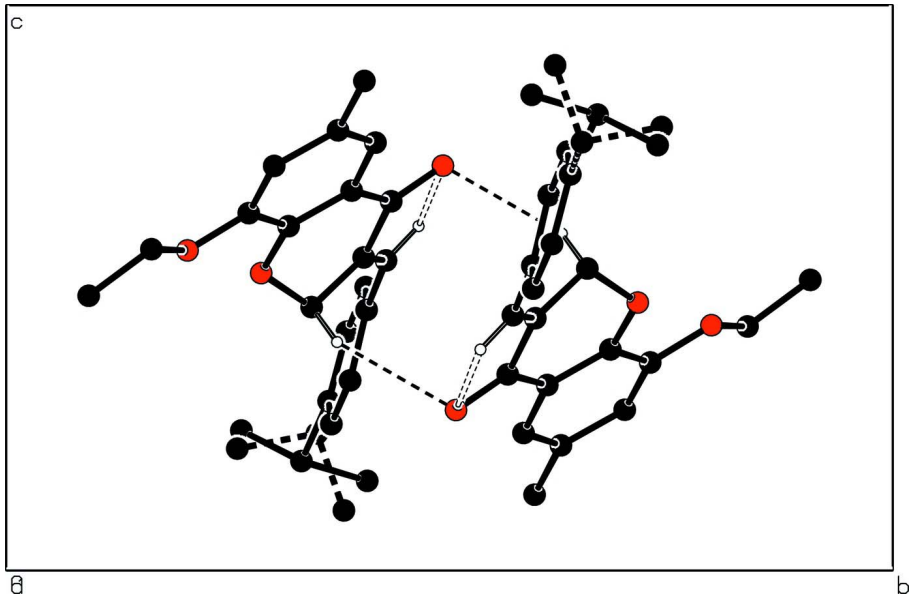

Figure 2

The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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Crystal data

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Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
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c = 10.8962 (10) Å
β = 99.873 (1)°
V = 1869.5 (3) Å^3
Z = 4

$F(000) = 720$
$D_x = 1.195$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 1.9$–$27.2°$
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Block, colourless
0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.983$, $T_{max} = 0.988$
21105 measured reflections
4385 independent reflections
3220 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.3°$
$h = -13 \rightarrow 13$
$k = -21 \rightarrow 21$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.158$
$S = 1.02$
4385 reflections
256 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2 + 0.3281P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	1.16222 (14)	0.18147 (9)	1.10909 (13)	0.0528 (3)	
C2	1.27835 (14)	0.22634 (9)	1.13210 (14)	0.0554 (4)	
C3	1.38353 (15)	0.19764 (10)	1.21563 (14)	0.0607 (4)	
H3	1.4607	0.2270	1.2304	0.073*	
C4	1.37726 (16)	0.12575 (10)	1.27856 (15)	0.0630 (4)	
C5	1.26264 (17)	0.08359 (10)	1.25682 (15)	0.0636 (4)	
H5	1.2568	0.0361	1.2992	0.076*	
C6	1.15337 (15)	0.11036 (9)	1.17194 (14)	0.0555 (4)	
C7	1.02883 (16)	0.06564 (9)	1.15305 (14)	0.0587 (4)	
C8	0.92415 (15)	0.09672 (9)	1.05370 (14)	0.0568 (4)	
C9	0.96801 (16)	0.15548 (10)	0.96569 (15)	0.0631 (4)	
H9A	1.0068	0.1268	0.9039	0.076*	
H9B	0.8919	0.1837	0.9224	0.076*	
C10	0.80031 (16)	0.07161 (10)	1.04848 (15)	0.0621 (4)	
H10	0.7877	0.0351	1.1094	0.075*	
C11	0.68243 (16)	0.09345 (10)	0.96090 (16)	0.0621 (4)	
C12	0.56167 (19)	0.09445 (13)	1.0015 (2)	0.0835 (6)	
H12	0.5574	0.0804	1.0833	0.100*	
C13	0.4489 (2)	0.11585 (16)	0.9224 (3)	0.1030 (8)	
H13	0.3702	0.1166	0.9525	0.124*	
C14	0.4489 (2)	0.13620 (13)	0.7997 (2)	0.0946 (7)	

C15	0.5682 (2)	0.13326 (12)	0.7588 (2)	0.0844 (6)	
H15	0.5714	0.1461	0.6763	0.101*	
C16	0.68203 (18)	0.11198 (11)	0.83633 (17)	0.0713 (5)	
H16	0.7601	0.1099	0.8050	0.086*	
C17	0.3423 (5)	0.1672 (3)	0.6930 (5)	0.0724 (14)	0.520 (10)
H17	0.3805	0.1842	0.6209	0.087*	0.520 (10)
C18	0.2693 (9)	0.2337 (4)	0.7420 (8)	0.091 (2)	0.520 (10)
H18A	0.3260	0.2789	0.7596	0.136*	0.520 (10)
H18B	0.2403	0.2168	0.8169	0.136*	0.520 (10)
H18C	0.1948	0.2480	0.6807	0.136*	0.520 (10)
C19	0.2513 (8)	0.0950 (5)	0.6613 (10)	0.107 (3)	0.520 (10)
H19A	0.2994	0.0521	0.6323	0.160*	0.520 (10)
H19B	0.1792	0.1094	0.5974	0.160*	0.520 (10)
H19C	0.2184	0.0784	0.7345	0.160*	0.520 (10)
C171	0.3016 (5)	0.1501 (3)	0.7409 (6)	0.0780 (16)	0.480 (10)
H171	0.2387	0.1293	0.7905	0.094*	0.480 (10)
C181	0.2898 (16)	0.2399 (6)	0.7148 (16)	0.176 (7)	0.480 (10)
H18D	0.3035	0.2684	0.7922	0.263*	0.480 (10)
H18E	0.2039	0.2515	0.6696	0.263*	0.480 (10)
H18F	0.3545	0.2557	0.6662	0.263*	0.480 (10)
C191	0.2836 (11)	0.1179 (9)	0.6070 (8)	0.150 (5)	0.480 (10)
H19D	0.2892	0.0609	0.6090	0.225*	0.480 (10)
H19E	0.3510	0.1390	0.5658	0.225*	0.480 (10)
H19F	0.1993	0.1337	0.5626	0.225*	0.480 (10)
C20	1.4972 (2)	0.09598 (14)	1.36590 (19)	0.0858 (6)	
H20A	1.4713	0.0568	1.4210	0.129*	
H20B	1.5390	0.1397	1.4138	0.129*	
H20C	1.5573	0.0726	1.3183	0.129*	
C22	1.39808 (17)	0.33615 (11)	1.06840 (18)	0.0725 (5)	
H22A	1.4609	0.3015	1.0385	0.087*	
H22B	1.4340	0.3525	1.1527	0.087*	
C23	1.3708 (2)	0.40699 (12)	0.9860 (2)	0.0940 (7)	
H23A	1.3325	0.3902	0.9036	0.141*	
H23B	1.4512	0.4348	0.9830	0.141*	
H23C	1.3111	0.4417	1.0183	0.141*	
O1	1.06117 (10)	0.21232 (6)	1.02605 (10)	0.0640 (3)	
O2	1.01289 (13)	0.00744 (8)	1.21616 (12)	0.0782 (4)	
O3	1.27649 (10)	0.29549 (7)	1.06605 (11)	0.0669 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0486 (8)	0.0529 (8)	0.0538 (8)	0.0013 (6)	−0.0002 (6)	−0.0003 (6)
C2	0.0514 (8)	0.0528 (8)	0.0596 (8)	−0.0002 (6)	0.0030 (6)	−0.0019 (6)
C3	0.0490 (8)	0.0660 (9)	0.0636 (9)	−0.0004 (7)	−0.0003 (7)	−0.0083 (7)
C4	0.0599 (9)	0.0664 (9)	0.0580 (9)	0.0099 (7)	−0.0029 (7)	−0.0024 (7)
C5	0.0696 (10)	0.0583 (9)	0.0588 (9)	0.0072 (7)	−0.0005 (7)	0.0059 (7)
C6	0.0576 (8)	0.0535 (8)	0.0535 (8)	0.0008 (6)	0.0037 (6)	0.0002 (6)

C7	0.0636 (9)	0.0543 (8)	0.0570 (8)	−0.0022 (7)	0.0067 (7)	0.0036 (7)
C8	0.0577 (9)	0.0546 (8)	0.0557 (8)	−0.0063 (6)	0.0028 (6)	−0.0002 (6)
C9	0.0585 (9)	0.0649 (9)	0.0605 (9)	−0.0138 (7)	−0.0053 (7)	0.0080 (7)
C10	0.0630 (9)	0.0598 (9)	0.0626 (9)	−0.0092 (7)	0.0081 (7)	0.0016 (7)
C11	0.0571 (9)	0.0582 (9)	0.0687 (10)	−0.0089 (7)	0.0041 (7)	−0.0073 (7)
C12	0.0677 (11)	0.1012 (15)	0.0823 (12)	−0.0061 (10)	0.0152 (9)	−0.0173 (11)
C13	0.0573 (11)	0.1235 (19)	0.125 (2)	0.0081 (11)	0.0063 (12)	−0.0504 (16)
C14	0.0822 (14)	0.0752 (13)	0.1122 (17)	0.0145 (10)	−0.0234 (12)	−0.0352 (12)
C15	0.0834 (14)	0.0780 (12)	0.0816 (12)	−0.0117 (10)	−0.0150 (10)	−0.0032 (10)
C16	0.0630 (10)	0.0764 (11)	0.0705 (10)	−0.0161 (8)	0.0004 (8)	−0.0039 (8)
C17	0.050 (2)	0.086 (3)	0.079 (3)	−0.0014 (19)	0.0047 (18)	0.002 (2)
C18	0.088 (4)	0.084 (4)	0.091 (3)	0.033 (3)	−0.011 (3)	−0.017 (3)
C19	0.069 (3)	0.087 (3)	0.150 (8)	−0.011 (2)	−0.024 (4)	−0.006 (4)
C171	0.052 (2)	0.082 (3)	0.103 (4)	−0.003 (2)	0.020 (2)	0.000 (3)
C181	0.164 (10)	0.089 (6)	0.253 (16)	−0.004 (6)	−0.023 (9)	0.054 (7)
C191	0.100 (7)	0.194 (13)	0.133 (7)	0.046 (7)	−0.045 (5)	−0.088 (8)
C20	0.0715 (12)	0.0963 (14)	0.0802 (12)	0.0151 (10)	−0.0134 (9)	0.0089 (10)
C22	0.0577 (9)	0.0707 (11)	0.0840 (11)	−0.0181 (8)	−0.0025 (8)	0.0016 (9)
C23	0.0835 (14)	0.0758 (12)	0.1151 (17)	−0.0291 (10)	−0.0043 (12)	0.0166 (11)
O1	0.0531 (6)	0.0561 (6)	0.0748 (7)	−0.0085 (4)	−0.0115 (5)	0.0130 (5)
O2	0.0812 (8)	0.0705 (8)	0.0798 (8)	−0.0099 (6)	0.0050 (6)	0.0233 (6)
O3	0.0513 (6)	0.0614 (6)	0.0832 (8)	−0.0095 (5)	−0.0023 (5)	0.0121 (5)

Geometric parameters (Å, º)

C1—O1	1.3632 (17)	C15—H15	0.9300
C1—C6	1.389 (2)	C16—H16	0.9300
C1—C2	1.405 (2)	C17—C18	1.499 (6)
C2—O3	1.3659 (18)	C17—C19	1.540 (6)
C2—C3	1.381 (2)	C17—H17	0.9800
C3—C4	1.397 (2)	C18—H18A	0.9600
C3—H3	0.9300	C18—H18B	0.9600
C4—C5	1.368 (2)	C18—H18C	0.9600
C4—C20	1.514 (2)	C19—H19A	0.9600
C5—C6	1.407 (2)	C19—H19B	0.9600
C5—H5	0.9300	C19—H19C	0.9600
C6—C7	1.477 (2)	C171—C181	1.536 (9)
C7—O2	1.2234 (19)	C171—C191	1.538 (8)
C7—C8	1.489 (2)	C171—H171	0.9800
C8—C10	1.342 (2)	C181—H18D	0.9600
C8—C9	1.501 (2)	C181—H18E	0.9600
C9—O1	1.4351 (18)	C181—H18F	0.9600
C9—H9A	0.9700	C191—H19D	0.9600
C9—H9B	0.9700	C191—H19E	0.9600
C10—C11	1.462 (2)	C191—H19F	0.9600
C10—H10	0.9300	C20—H20A	0.9600
C11—C16	1.392 (2)	C20—H20B	0.9600
C11—C12	1.396 (3)	C20—H20C	0.9600

C12—C13	1.375 (3)	C22—O3	1.4294 (19)
C12—H12	0.9300	C22—C23	1.489 (3)
C13—C14	1.379 (4)	C22—H22A	0.9700
C13—H13	0.9300	C22—H22B	0.9700
C14—C15	1.384 (3)	C23—H23A	0.9600
C14—C17	1.550 (5)	C23—H23B	0.9600
C14—C171	1.568 (5)	C23—H23C	0.9600
C15—C16	1.375 (3)		

O1—C1—C6	123.15 (13)	C19—C17—C14	103.5 (5)
O1—C1—C2	116.76 (13)	C18—C17—H17	111.5
C6—C1—C2	120.07 (13)	C19—C17—H17	111.5
O3—C2—C3	125.65 (14)	C14—C17—H17	111.5
O3—C2—C1	115.38 (13)	C17—C18—H18A	109.5
C3—C2—C1	118.96 (14)	C17—C18—H18B	109.5
C2—C3—C4	121.87 (15)	H18A—C18—H18B	109.5
C2—C3—H3	119.1	C17—C18—H18C	109.5
C4—C3—H3	119.1	H18A—C18—H18C	109.5
C5—C4—C3	118.40 (14)	H18B—C18—H18C	109.5
C5—C4—C20	122.08 (17)	C17—C19—H19A	109.5
C3—C4—C20	119.50 (16)	C17—C19—H19B	109.5
C4—C5—C6	121.61 (15)	H19A—C19—H19B	109.5
C4—C5—H5	119.2	C17—C19—H19C	109.5
C6—C5—H5	119.2	H19A—C19—H19C	109.5
C1—C6—C5	119.07 (14)	H19B—C19—H19C	109.5
C1—C6—C7	119.98 (13)	C181—C171—C191	100.2 (12)
C5—C6—C7	120.90 (14)	C181—C171—C14	105.3 (7)
O2—C7—C6	121.86 (15)	C191—C171—C14	106.7 (6)
O2—C7—C8	122.52 (15)	C181—C171—H171	114.4
C6—C7—C8	115.61 (13)	C191—C171—H171	114.4
C10—C8—C7	119.45 (14)	C14—C171—H171	114.4
C10—C8—C9	124.88 (14)	C171—C181—H18D	109.5
C7—C8—C9	115.66 (13)	C171—C181—H18E	109.5
O1—C9—C8	113.53 (12)	H18D—C181—H18E	109.5
O1—C9—H9A	108.9	C171—C181—H18F	109.5
C8—C9—H9A	108.9	H18D—C181—H18F	109.5
O1—C9—H9B	108.9	H18E—C181—H18F	109.5
C8—C9—H9B	108.9	C171—C191—H19D	109.5
H9A—C9—H9B	107.7	C171—C191—H19E	109.5
C8—C10—C11	129.32 (15)	H19D—C191—H19E	109.5
C8—C10—H10	115.3	C171—C191—H19F	109.5
C11—C10—H10	115.3	H19D—C191—H19F	109.5
C16—C11—C12	116.94 (17)	H19E—C191—H19F	109.5
C16—C11—C10	123.74 (15)	C4—C20—H20A	109.5
C12—C11—C10	119.30 (16)	C4—C20—H20B	109.5
C13—C12—C11	121.0 (2)	H20A—C20—H20B	109.5
C13—C12—H12	119.5	C4—C20—H20C	109.5
C11—C12—H12	119.5	H20A—C20—H20C	109.5

C12—C13—C14	122.1 (2)	H20B—C20—H20C	109.5
C12—C13—H13	119.0	O3—C22—C23	107.23 (15)
C14—C13—H13	119.0	O3—C22—H22A	110.3
C13—C14—C15	116.85 (19)	C23—C22—H22A	110.3
C13—C14—C17	133.8 (3)	O3—C22—H22B	110.3
C15—C14—C17	109.3 (3)	C23—C22—H22B	110.3
C13—C14—C171	105.8 (4)	H22A—C22—H22B	108.5
C15—C14—C171	137.1 (4)	C22—C23—H23A	109.5
C16—C15—C14	122.0 (2)	C22—C23—H23B	109.5
C16—C15—H15	119.0	H23A—C23—H23B	109.5
C14—C15—H15	119.0	C22—C23—H23C	109.5
C15—C16—C11	121.08 (18)	H23A—C23—H23C	109.5
C15—C16—H16	119.5	H23B—C23—H23C	109.5
C11—C16—H16	119.5	C1—O1—C9	115.47 (12)
C18—C17—C19	109.9 (8)	C2—O3—C22	117.71 (12)
C18—C17—C14	108.7 (5)		

O1—C1—C2—O3	−1.1 (2)	C16—C11—C12—C13	−2.4 (3)
C6—C1—C2—O3	−179.60 (13)	C10—C11—C12—C13	179.00 (19)
O1—C1—C2—C3	179.92 (13)	C11—C12—C13—C14	0.9 (3)
C6—C1—C2—C3	1.4 (2)	C12—C13—C14—C15	0.7 (3)
O3—C2—C3—C4	−179.43 (15)	C12—C13—C14—C17	−175.5 (3)
C1—C2—C3—C4	−0.6 (2)	C12—C13—C14—C171	175.9 (3)
C2—C3—C4—C5	−0.6 (2)	C13—C14—C15—C16	−0.7 (3)
C2—C3—C4—C20	178.01 (16)	C17—C14—C15—C16	176.4 (2)
C3—C4—C5—C6	1.0 (3)	C171—C14—C15—C16	−173.9 (3)
C20—C4—C5—C6	−177.59 (16)	C14—C15—C16—C11	−0.9 (3)
O1—C1—C6—C5	−179.45 (14)	C12—C11—C16—C15	2.5 (3)
C2—C1—C6—C5	−1.1 (2)	C10—C11—C16—C15	−179.04 (17)
O1—C1—C6—C7	−1.9 (2)	C13—C14—C17—C18	47.0 (8)
C2—C1—C6—C7	176.48 (14)	C15—C14—C17—C18	−129.5 (6)
C4—C5—C6—C1	−0.2 (2)	C171—C14—C17—C18	64.2 (8)
C4—C5—C6—C7	−177.71 (15)	C13—C14—C17—C19	−69.9 (7)
C1—C6—C7—O2	−172.15 (15)	C15—C14—C17—C19	113.7 (7)
C5—C6—C7—O2	5.3 (3)	C171—C14—C17—C19	−52.7 (8)
C1—C6—C7—C8	7.1 (2)	C13—C14—C171—C181	111.4 (9)
C5—C6—C7—C8	−175.42 (14)	C15—C14—C171—C181	−74.9 (9)
O2—C7—C8—C10	14.1 (2)	C17—C14—C171—C181	−55.8 (9)
C6—C7—C8—C10	−165.17 (15)	C13—C14—C171—C191	−142.7 (9)
O2—C7—C8—C9	−166.14 (16)	C15—C14—C171—C191	31.0 (10)
C6—C7—C8—C9	14.6 (2)	C17—C14—C171—C191	50.1 (9)
C10—C8—C9—O1	138.48 (17)	C6—C1—O1—C9	−26.1 (2)
C7—C8—C9—O1	−41.3 (2)	C2—C1—O1—C9	155.44 (14)
C7—C8—C10—C11	179.85 (15)	C8—C9—O1—C1	47.03 (19)
C9—C8—C10—C11	0.1 (3)	C3—C2—O3—C22	9.9 (2)
C8—C10—C11—C16	33.2 (3)	C1—C2—O3—C22	−168.97 (14)
C8—C10—C11—C12	−148.30 (19)	C23—C22—O3—C2	177.70 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O2^{i}	0.97	2.60	3.407 (2)	141
C10—H10···O2	0.93	2.47	2.823 (2)	103

Symmetry code: (i) −*x*+2, −*y*, −*z*+2.