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(4-Chlorobenzoyl)(2-ethoxy-7-methoxynaphthalen-1-yl)methanone

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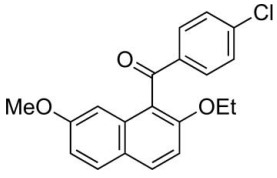
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 14.2.

In the title compound, $C_{20}H_{17}ClO_3$, the naphthalene and benzene rings form an interplanar angle of 83.30 (8)°. The conformation around the central C=O group is such that the C=O bond vector forms a larger angle to the plane of the naphthalene ring than to the plane of the benzene ring, *viz*. 55.8 (2)° *versus* 15.8 (2)°. The 4-chlorophenyl groups form a centrosymmetric π–π interaction, with a centroid–centroid distance of 3.829 (1) Å and a lateral offset of 1.758 Å. An intermolecular C—H···O interaction is formed between the 4-chlorophenyl group and the O atom of a neighbouring methoxy group, and two very weak C—H···π contacts are present.

Related literature

For structures of closely related compounds, see: Mitsui, Nakaema, Noguchi, Okamoto & Yonezawa (2008); Mitsui, Nakaema, Noguchi & Yonezawa (2008).



Experimental

Crystal data

$C_{20}H_{17}ClO_3$ M_r = 340.79
Monoclinic, $P2_1/c$
a = 7.26434 (13) Å
b = 20.8849 (4) Å
c = 12.2094 (2) Å
β = 113.201 (1)°
V = 1702.55 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.11 mm^{-1}
T = 193 K
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.542, T_{max} = 0.656
30947 measured reflections
3104 independent reflections
2544 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.10
3104 reflections
218 parameters
23 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20B···$Cg1^{i}$	0.98	3.02	3.821 (3)	140
C20—H20C···$Cg1^{ii}$	0.98	3.01	3.477 (3)	110
C13—H13···O3^{iii}	0.95	2.44	3.213 (2)	138

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$. $Cg1$ is the centroid of the C1–C5/C10 ring.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2344).

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supporting information

Acta Cryst. (2009). E**65**, o543 [doi:10.1107/S1600536809004796]

(4-Chlorobenzoyl)(2-ethoxy-7-methoxynaphthalen-1-yl)methanone

Ryosuke Mitsui, Keiichi Noguchi and Noriyuki Yonezawa

S1. Comment

Recently, we have reported the crystal structures of 1-(4-chlorobenzoyl)-2,7-dimethoxynaphthalene and (4-chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone (Mitsui, Nakaema, Noguchi, Okamoto & Yonezawa, 2008; Mitsui, Nakaema, Noguchi & Yonezawa, 2008). As a part of our ongoing studies on the synthesis and crystal structure analyses of aroylated naphthalene derivatives, this paper reports the crystal structure of the title compound, prepared by ethylation of (4-chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone with ethyl iodide.

In the molecule (Fig. 1), the interplanar angle between the benzene ring [C12–C17] and the naphthalene ring [C1–C10] is 83.30 (8)°. The C=O bond vector lies close to the mean plane of the benzene ring (angle 15.8 (2)°), but forms an angle of 55.77 (15)° to the plane of the naphthalene ring. The conformation of these groups is similar to 1-(4-chlorobenzoyl)-2,7-dimethoxynaphthalene. On the other hand, the methoxy group is arranged toward the aroyl group [C20—O3—C8—C7 torsion angle = 177.7 (2)°] while that of the aforementioned related compound is arranged toward the naphthalene ring [-7.1 (3)°]. In both compounds, the C—O bond vector of the methoxy group lies approximately in the plane of the naphthalene ring [angle 4.2 (1)° in the title compound, 5.05 (9)° in the related compound].

In the crystal structure, the naphthalene rings interact with ethyl groups [C7···H18A = 2.87 Å, C7···H18B = 2.88 Å] and methyl groups [C5···H20B = 2.75 Å] of the adjacent molecule along the *a* axis (Fig. 2). The neighboring inversion-related ethyl groups interact with each other [H19C···H19C = 2.39 Å] along the *c* axis. The C=O groups interact with benzene rings [O1···H17 = 2.66 Å] along the *b* axis (Fig. 3). Adjacent 4-chlorophenyl groups related by crystallographic inversion centers are exactly antiparallel and the perpendicular distance between the mean planes of these groups is 3.402 (1) Å (Fig. 4). The centroid–centroid distance between the two antiparallel phenyl rings is 3.829 (1) Å and the lateral offset is 1.758 Å, indicating the presence of a π–π interaction. Moreover, molecules are linked by C—H···π interactions. The methyl group acts as a hydrogen-bond donor and the π system of the naphthalene ring [C1/C2/C3/C4/C5/C10 ring (with centroid *Cg1*)] of an adjacent molecule acts as an acceptor, *viz.* C20—H20B···π, C20—H20C···π (Fig. 2 and Table 1). Intermolecular C—H···O hydrogen bonds between the methoxy O and an H atom of the 4-chlorophenyl group of the adjacent molecule are also found along the *c* axis (C13—H13···O3^{i}; Fig. 2 and Table 1).

S2. Experimental

(4-Chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone (0.13 g, 0.40 mmol) was dissolved in acetone (1.0 ml) and aqueous 0.8M NaOH (1.0 ml). EtI (0.31 g, 2.0 mmol) was added and the reaction mixture was heated at reflux for 6 h. Upon cooling to ambient temperature, the mixture was poured into H_2O (5 ml) and $CHCl_3$ (5 ml), and the aqueous layer was extracted with $CHCl_3$ (3 × 5 ml). The combined organic layers were washed with brine (3 × 20 ml), and dried over $MgSO_4$ overnight. The solvent was removed *in vacuo* and the crude material was purified by recrystallization from hexanes to give the title compound as colorless blocks (m.p. 365.5–366.0 K, yield 95 mg, 70%).

Spectroscopic Data: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, 1H), 7.77 (d, 2H), 7.70 (d, 1H), 7.38 (d, 2H), 7.11 (d, 1H), 7.02 (dd, 1H), 6.86 (d, 1H), 4.05 (q, 2H), 3.74 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.8, 159.1, 154.8, 139.4, 137.1, 133.2, 131.3, 130.7, 129.7, 128.7, 124.5, 121.7, 117.2, 111.5, 102.3, 65.0, 55.2, 14.6; IR (KBr): 1671, 1624, 1582, 1511, 1464, 1249, 1227, 1046; HRMS (*m*/*z*): $[M + H]^+$ calcd for $C_{20}H_{18}ClO_3$, 341.0945; found, 341.0903.

S3. Refinement

Rigid bond restraints were applied to the U_{ij} values of the naphthalene ring (C4—C7) (5 restraints with the DELU command in *SHELXL97*). Further restraints were used to generate similar U_{ij} values for the atoms of naphthalene ring (18 restraints with the SIMU command in *SHELXL97*). All H atoms were visible in difference maps but were subsequently placed in calculated positions and refined as riding, with C—H = 0.95 (aromatic), 0.98 (methyl) and 0.99 (methylene) Å, and with U_{iso}(H) = 1.2U_{eq}(C).

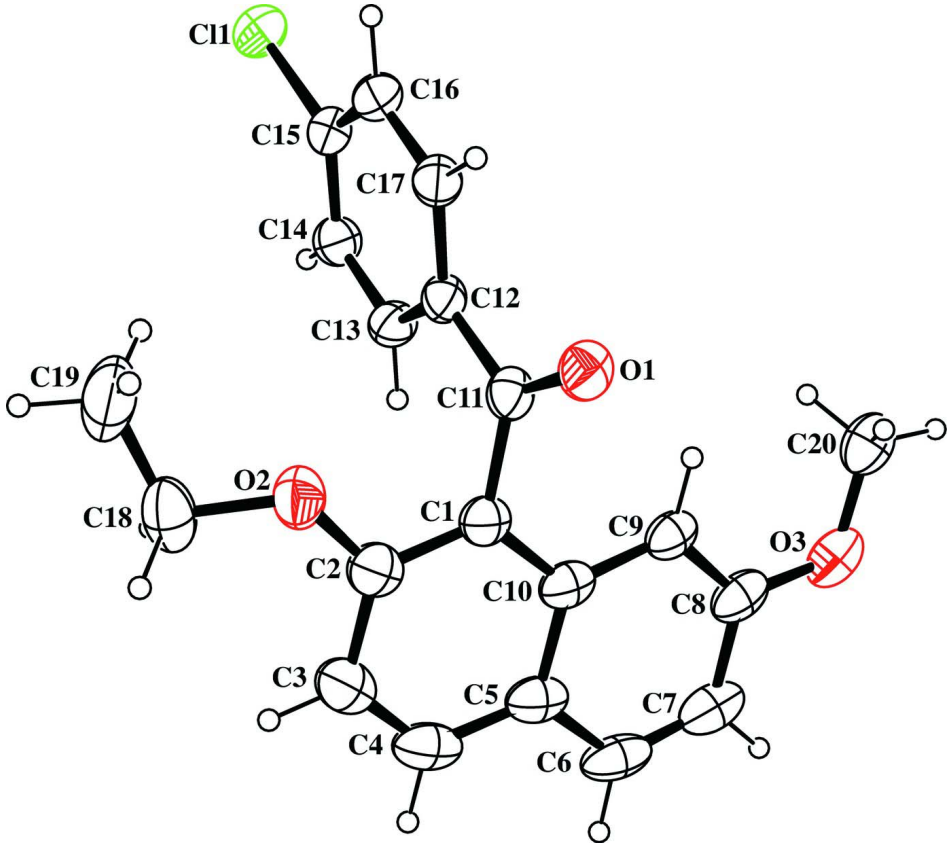

Figure 1

Molecular structure with displacement ellipsoids at 30% probability for non-H atoms.

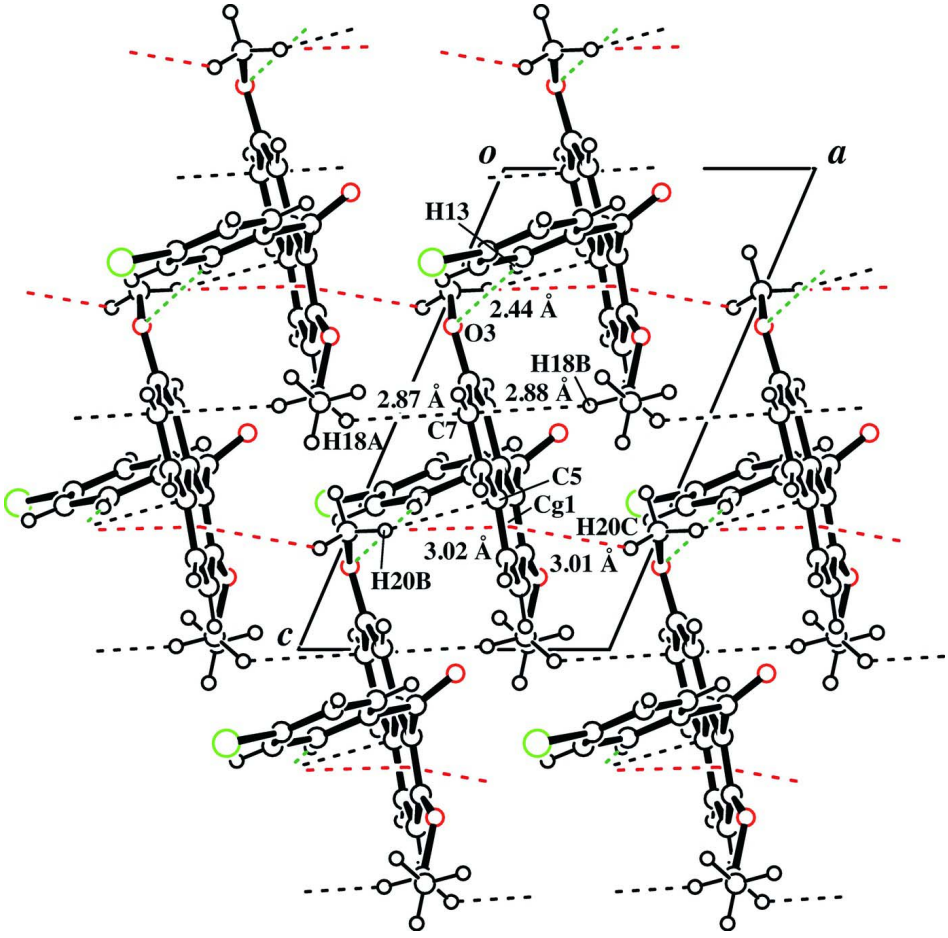

Figure 2

Packing diagram viewed down the *b* axis. Van der Waals, C—H···π and C—H···O interactions are shown as black, red and green dashed lines, respectively.

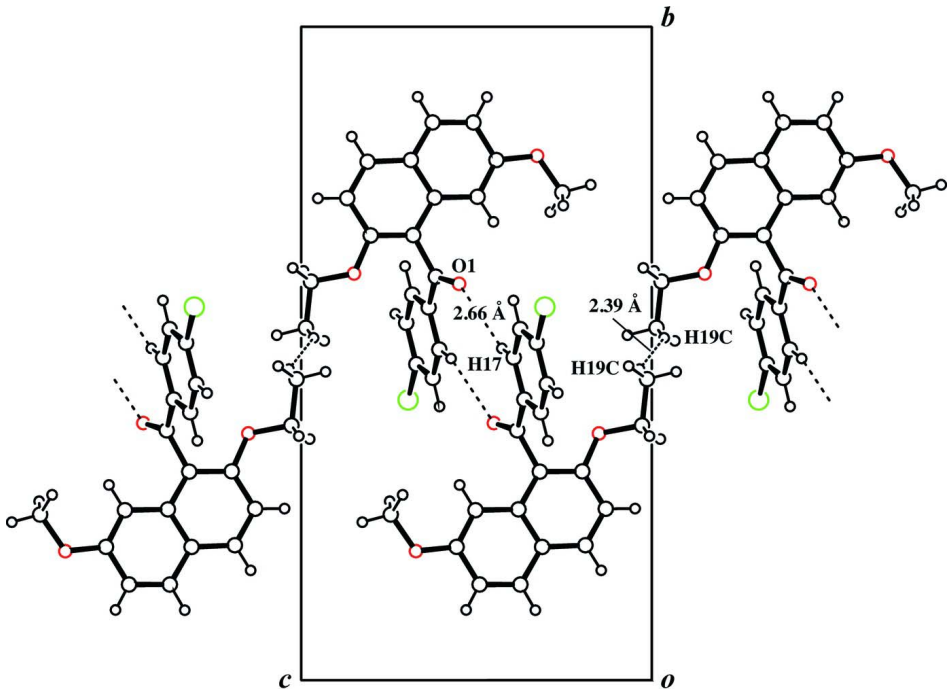

Figure 3

Partial packing diagram viewed down the *a* axis. Van der Waals interactions are shown as dashed lines.

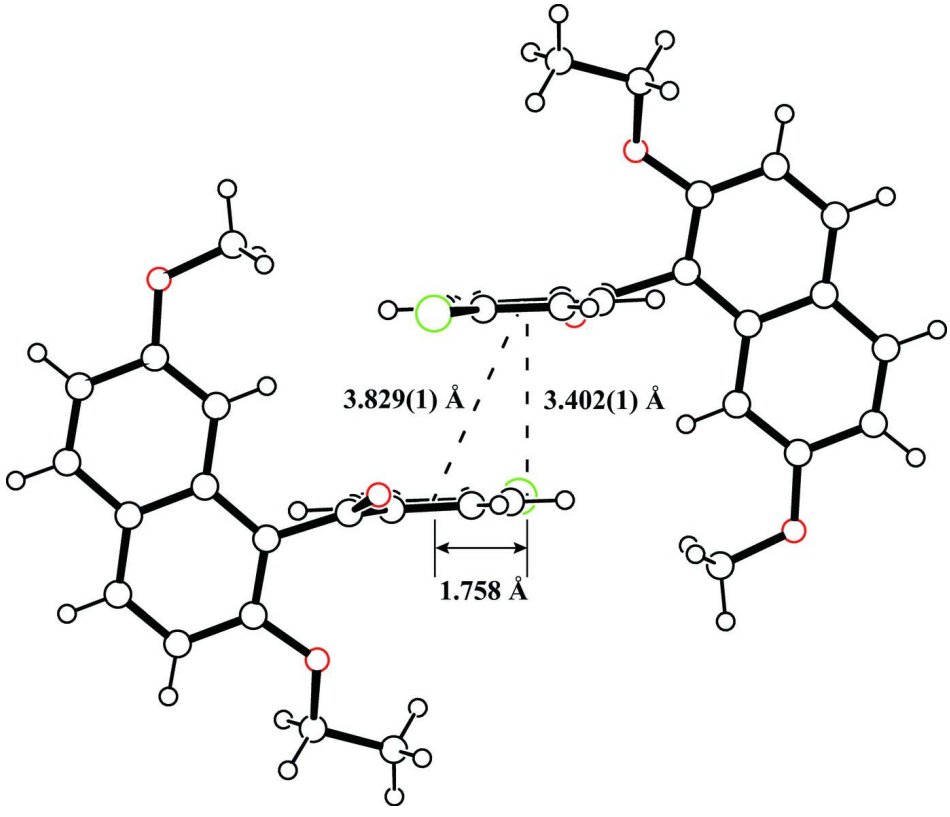

Figure 4

Side-on view of the π–π interaction.

(4-Chlorobenzoyl)(2-ethoxy-7-methoxynaphthalen-1-yl)methanone

Crystal data

$C_{20}H_{17}ClO_3$
M_r = 340.79
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.26434 (13) Å
b = 20.8849 (4) Å
c = 12.2094 (2) Å
β = 113.201 (1)°
V = 1702.55 (5) Å^3
Z = 4
$F(000)$ = 712
D_x = 1.330 Mg m^{-3}
Melting point = 365.5–366.0 K
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 26200 reflections
θ = 3.9–68.1°
μ = 2.11 mm^{-1}
T = 193 K
Block, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotating anode
Graphite monochromator
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.542, T_{max} = 0.656
30947 measured reflections
3104 independent reflections
2544 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 68.1°, θ_{min} = 4.2°
h = −8→8
k = −25→25
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.10
3104 reflections
218 parameters
23 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
$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.3688P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0020 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.10278 (9)	0.57118 (2)	0.30495 (5)	0.0781 (2)
O1	0.4618 (2)	0.39338 (6)	0.45026 (12)	0.0659 (4)
O2	0.3297 (2)	0.37751 (7)	0.15066 (12)	0.0756 (4)
O3	0.9489 (2)	0.19765 (7)	0.67286 (15)	0.0765 (4)
C1	0.5171 (3)	0.31905 (9)	0.31945 (17)	0.0566 (4)
C2	0.4068 (3)	0.31950 (10)	0.19824 (18)	0.0656 (5)
C3	0.3762 (3)	0.26240 (12)	0.1314 (2)	0.0767 (6)
H3	0.3019	0.2628	0.0476	0.092*
C4	0.4553 (3)	0.20662 (11)	0.1892 (2)	0.0784 (7)
H4	0.4326	0.1681	0.1443	0.094*
C5	0.5692 (3)	0.20400 (9)	0.3128 (2)	0.0671 (5)
C6	0.6600 (4)	0.14645 (10)	0.3747 (3)	0.0794 (7)
H6	0.6349	0.1072	0.3321	0.095*
C7	0.7796 (4)	0.14653 (10)	0.4912 (3)	0.0785 (6)
H7	0.8367	0.1075	0.5296	0.094*
C8	0.8208 (3)	0.20409 (9)	0.5568 (2)	0.0665 (5)
C9	0.7332 (3)	0.26027 (8)	0.50295 (18)	0.0572 (4)
H9	0.7589	0.2987	0.5482	0.069*
C10	0.6044 (3)	0.26155 (8)	0.38026 (18)	0.0579 (5)
C11	0.5461 (3)	0.38232 (8)	0.38384 (15)	0.0536 (4)
C12	0.6830 (3)	0.42954 (8)	0.36347 (15)	0.0505 (4)
C13	0.8197 (3)	0.40999 (8)	0.31679 (16)	0.0547 (4)
H13	0.8235	0.3663	0.2963	0.066*
C14	0.9509 (3)	0.45307 (9)	0.29947 (16)	0.0587 (4)
H14	1.0453	0.4393	0.2684	0.070*
C15	0.9411 (3)	0.51637 (8)	0.32839 (15)	0.0569 (4)
C16	0.8073 (3)	0.53732 (9)	0.37524 (16)	0.0599 (5)
H16	0.8032	0.5812	0.3945	0.072*
C17	0.6795 (3)	0.49384 (8)	0.39383 (16)	0.0569 (4)
H17	0.5887	0.5077	0.4275	0.068*
C18	0.2883 (4)	0.38987 (15)	0.0278 (2)	0.0872 (7)
H18A	0.1616	0.3689	−0.0242	0.105*
H18B	0.3980	0.3735	0.0067	0.105*
C19	0.2714 (5)	0.46071 (17)	0.0136 (3)	0.1199 (11)
H19A	0.2428	0.4720	−0.0695	0.144*
H19B	0.3976	0.4806	0.0658	0.144*
H19C	0.1626	0.4761	0.0350	0.144*
C20	1.0050 (3)	0.25362 (11)	0.7447 (2)	0.0754 (6)
H20A	1.0970	0.2420	0.8256	0.090*
H20B	0.8853	0.2738	0.7476	0.090*
H20C	1.0715	0.2837	0.7105	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0934 (4)	0.0670 (3)	0.0780 (4)	−0.0205 (3)	0.0382 (3)	0.0047 (2)
O1	0.0784 (9)	0.0658 (8)	0.0721 (8)	0.0068 (7)	0.0496 (7)	0.0002 (6)
O2	0.0841 (10)	0.0855 (10)	0.0595 (8)	−0.0073 (8)	0.0306 (7)	0.0064 (7)
O3	0.0712 (9)	0.0656 (9)	0.1016 (11)	0.0101 (7)	0.0435 (9)	0.0261 (8)
C1	0.0633 (11)	0.0567 (10)	0.0629 (11)	−0.0068 (8)	0.0390 (9)	−0.0048 (8)
C2	0.0665 (12)	0.0731 (13)	0.0699 (12)	−0.0139 (10)	0.0406 (10)	−0.0083 (10)
C3	0.0749 (14)	0.0969 (17)	0.0735 (13)	−0.0280 (12)	0.0457 (11)	−0.0229 (12)
C4	0.0799 (14)	0.0744 (14)	0.1077 (17)	−0.0300 (12)	0.0658 (14)	−0.0359 (13)
C5	0.0698 (12)	0.0585 (11)	0.0970 (15)	−0.0162 (9)	0.0586 (12)	−0.0188 (10)
C6	0.0850 (15)	0.0482 (11)	0.138 (2)	−0.0128 (10)	0.0796 (16)	−0.0187 (12)
C7	0.0798 (15)	0.0507 (11)	0.128 (2)	0.0019 (10)	0.0655 (15)	0.0056 (12)
C8	0.0659 (12)	0.0546 (11)	0.1001 (16)	0.0007 (9)	0.0554 (12)	0.0089 (10)
C9	0.0637 (11)	0.0479 (9)	0.0766 (12)	0.0002 (8)	0.0453 (10)	0.0028 (8)
C10	0.0628 (11)	0.0496 (9)	0.0820 (12)	−0.0056 (8)	0.0507 (10)	−0.0057 (8)
C11	0.0607 (10)	0.0541 (10)	0.0527 (9)	0.0091 (8)	0.0295 (8)	0.0040 (7)
C12	0.0617 (10)	0.0464 (9)	0.0483 (9)	0.0066 (7)	0.0270 (8)	0.0026 (7)
C13	0.0677 (11)	0.0456 (9)	0.0600 (10)	0.0003 (8)	0.0351 (9)	−0.0031 (7)
C14	0.0658 (11)	0.0593 (10)	0.0589 (10)	−0.0008 (8)	0.0332 (9)	−0.0021 (8)
C15	0.0676 (11)	0.0525 (9)	0.0491 (9)	−0.0038 (8)	0.0213 (8)	0.0060 (7)
C16	0.0758 (12)	0.0439 (9)	0.0585 (10)	0.0067 (8)	0.0247 (9)	0.0043 (7)
C17	0.0691 (11)	0.0508 (9)	0.0550 (9)	0.0120 (8)	0.0290 (9)	0.0019 (7)
C18	0.0657 (13)	0.134 (2)	0.0608 (12)	−0.0117 (13)	0.0243 (10)	0.0111 (13)
C19	0.119 (2)	0.142 (3)	0.0847 (18)	−0.014 (2)	0.0247 (16)	0.0474 (18)
C20	0.0702 (13)	0.0782 (14)	0.0890 (15)	0.0106 (11)	0.0434 (12)	0.0189 (12)

Geometric parameters (Å, º)

Cl1—C15	1.7426 (19)	C9—H9	0.950
O1—C11	1.215 (2)	C11—C12	1.490 (3)
O2—C2	1.365 (3)	C12—C13	1.387 (2)
O2—C18	1.432 (3)	C12—C17	1.396 (2)
O3—C8	1.361 (3)	C13—C14	1.386 (3)
O3—C20	1.421 (3)	C13—H13	0.950
C1—C2	1.378 (3)	C14—C15	1.377 (3)
C1—C10	1.423 (3)	C14—H14	0.950
C1—C11	1.509 (2)	C15—C16	1.379 (3)
C2—C3	1.413 (3)	C16—C17	1.380 (3)
C3—C4	1.366 (4)	C16—H16	0.950
C3—H3	0.950	C17—H17	0.950
C4—C5	1.408 (3)	C18—C19	1.489 (4)
C4—H4	0.950	C18—H18A	0.990
C5—C10	1.422 (3)	C18—H18B	0.990
C5—C6	1.435 (3)	C19—H19A	0.980
C6—C7	1.343 (3)	C19—H19B	0.980
C6—H6	0.950	C19—H19C	0.980

C7—C8	1.410 (3)	C20—H20A	0.980
C7—H7	0.950	C20—H20B	0.980
C8—C9	1.373 (3)	C20—H20C	0.980
C9—C10	1.420 (3)		

C2—O2—C18	119.19 (18)	C13—C12—C11	120.47 (15)
C8—O3—C20	118.27 (16)	C17—C12—C11	120.62 (16)
C2—C1—C10	121.15 (17)	C14—C13—C12	121.21 (16)
C2—C1—C11	117.15 (17)	C14—C13—H13	119.4
C10—C1—C11	121.68 (16)	C12—C13—H13	119.4
O2—C2—C1	115.52 (17)	C15—C14—C13	118.40 (17)
O2—C2—C3	124.0 (2)	C15—C14—H14	120.8
C1—C2—C3	120.5 (2)	C13—C14—H14	120.8
C4—C3—C2	118.9 (2)	C14—C15—C16	121.81 (17)
C4—C3—H3	120.6	C14—C15—Cl1	118.81 (15)
C2—C3—H3	120.6	C16—C15—Cl1	119.38 (14)
C3—C4—C5	122.49 (19)	C15—C16—C17	119.29 (17)
C3—C4—H4	118.8	C15—C16—H16	120.4
C5—C4—H4	118.8	C17—C16—H16	120.4
C4—C5—C10	118.9 (2)	C16—C17—C12	120.37 (17)
C4—C5—C6	123.5 (2)	C16—C17—H17	119.8
C10—C5—C6	117.6 (2)	C12—C17—H17	119.8
C7—C6—C5	121.9 (2)	O2—C18—C19	106.0 (2)
C7—C6—H6	119.1	O2—C18—H18A	110.5
C5—C6—H6	119.1	C19—C18—H18A	110.5
C6—C7—C8	120.4 (2)	O2—C18—H18B	110.5
C6—C7—H7	119.8	C19—C18—H18B	110.5
C8—C7—H7	119.8	H18A—C18—H18B	108.7
O3—C8—C9	125.51 (19)	C18—C19—H19A	109.5
O3—C8—C7	114.35 (19)	C18—C19—H19B	109.5
C9—C8—C7	120.1 (2)	H19A—C19—H19B	109.5
C8—C9—C10	120.65 (18)	C18—C19—H19C	109.5
C8—C9—H9	119.7	H19A—C19—H19C	109.5
C10—C9—H9	119.7	H19B—C19—H19C	109.5
C9—C10—C5	119.24 (18)	O3—C20—H20A	109.5
C9—C10—C1	122.64 (16)	O3—C20—H20B	109.5
C5—C10—C1	118.02 (19)	H20A—C20—H20B	109.5
O1—C11—C12	122.05 (16)	O3—C20—H20C	109.5
O1—C11—C1	120.71 (16)	H20A—C20—H20C	109.5
C12—C11—C1	117.24 (14)	H20B—C20—H20C	109.5
C13—C12—C17	118.90 (16)		

C18—O2—C2—C1	154.21 (17)	C6—C5—C10—C1	179.21 (16)
C18—O2—C2—C3	−26.8 (3)	C2—C1—C10—C9	174.41 (16)
C10—C1—C2—O2	179.52 (15)	C11—C1—C10—C9	−3.8 (3)
C11—C1—C2—O2	−2.2 (2)	C2—C1—C10—C5	−2.0 (3)
C10—C1—C2—C3	0.5 (3)	C11—C1—C10—C5	179.83 (16)
C11—C1—C2—C3	178.82 (16)	C2—C1—C11—O1	109.0 (2)

O2—C2—C3—C4	−177.90 (18)	C10—C1—C11—O1	−72.7 (2)
C1—C2—C3—C4	1.0 (3)	C2—C1—C11—C12	−71.7 (2)
C2—C3—C4—C5	−1.1 (3)	C10—C1—C11—C12	106.57 (18)
C3—C4—C5—C10	−0.4 (3)	O1—C11—C12—C13	161.18 (18)
C3—C4—C5—C6	−177.56 (19)	C1—C11—C12—C13	−18.1 (2)
C4—C5—C6—C7	175.11 (19)	O1—C11—C12—C17	−17.2 (3)
C10—C5—C6—C7	−2.1 (3)	C1—C11—C12—C17	163.60 (16)
C5—C6—C7—C8	−0.4 (3)	C17—C12—C13—C14	−0.3 (3)
C20—O3—C8—C9	−2.8 (3)	C11—C12—C13—C14	−178.72 (16)
C20—O3—C8—C7	177.68 (16)	C12—C13—C14—C15	−0.8 (3)
C6—C7—C8—O3	−178.08 (17)	C13—C14—C15—C16	1.0 (3)
C6—C7—C8—C9	2.3 (3)	C13—C14—C15—Cl1	−179.07 (14)
O3—C8—C9—C10	178.81 (16)	C14—C15—C16—C17	0.0 (3)
C7—C8—C9—C10	−1.7 (3)	Cl1—C15—C16—C17	−179.94 (14)
C8—C9—C10—C5	−0.9 (3)	C15—C16—C17—C12	−1.2 (3)
C8—C9—C10—C1	−177.22 (16)	C13—C12—C17—C16	1.4 (3)
C4—C5—C10—C9	−174.63 (16)	C11—C12—C17—C16	179.72 (16)
C6—C5—C10—C9	2.7 (2)	C2—O2—C18—C19	−162.1 (2)
C4—C5—C10—C1	1.9 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20*B*···*Cg*1^{i}	0.98	3.02	3.821 (3)	140
C20—H20*C*···*Cg*1^{ii}	0.98	3.01	3.477 (3)	110
C13—H13···O3^{iii}	0.95	2.44	3.213 (2)	138

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