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Indomethacin methyl ester

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.117
Data-to-parameter ratio = 13.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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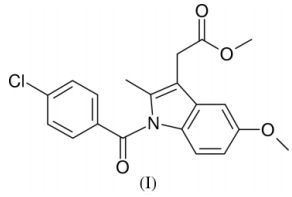
The cystal structure of the title compound [systematic name: methyl 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indole-3-acetate], $C_{20}H_{18}ClNO_4$, exhibits a short axis similar to another indomethacin analogue. Also observed in the structure is a packing of molecules influenced by weak C—H···O hydrogen bonds.

Comment

As part of an investigation into the crystallization of pharmaceutical compounds, the crystal structures of indomethacin derivatives are of interest. Numerous studies have been reported on various crystal structures of the drug indomethacin (γ-form: Kistenmacher & Marsh, 1972; α-form: Chen *et al.*, 2002; *t*-butanol and methanol solvates: Joshi *et al.*, 1998). In contrast, the structure of its methyl ester, (I), has not been reported to date. We report here its crystal structure and describe the intermolecular interactions involved.



(I)

The asymmetric unit of (I) comprises one molecule (Fig. 1). Although the crystal structure of the indomethacin methyl ester differs significantly from that of the parent carboxylic acid, it bears some similarity to the structure of another indomethacin derivative, iodoindomethacin (Loll *et al.*, 1996). Both crystal structures exhibit a relatively short axis [4.8326 (1) Å for the methyl ester derivative *versus* 4.7250 (10) Å for the iodo derivative]. In addition, both crystal structures show a halogen contact to a carbonyl O atom [Cl1···O4 = 3.575 (2) Å *versus* I1···O4 = 3.162 (5) Å].

In the absence of the carboxylic acid group of indomethacin, no strong O—H···O hydrogen bonding can be expected in the crystal structure of the methyl ester. Instead, C—H···O hydrogen bonds form a three-dimensional supramolecular network, as shown in Fig. 2. Hydrogen-bond distances and angles are provided in Table 1.

Experimental

Indomethacin and anhydrous benzenesulfonic acid were obtained from Sigma–Aldrich and were used as received. Indomethacin (130 mg, 0.364 mmol) and benzensulfonic acid (115 mg, 0.727 mmol) were dissolved in methanol with heating. Crystals precipitated as the

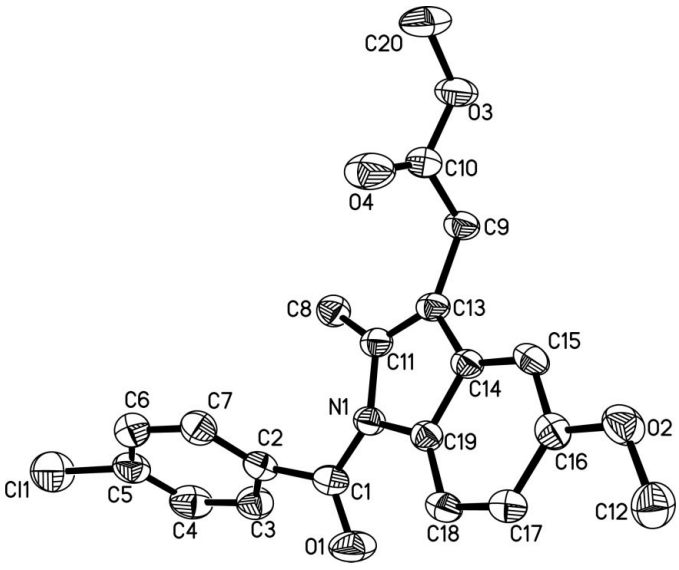


Figure 1
Molecular unit showing displacement ellipsoids at the 50% probability level.

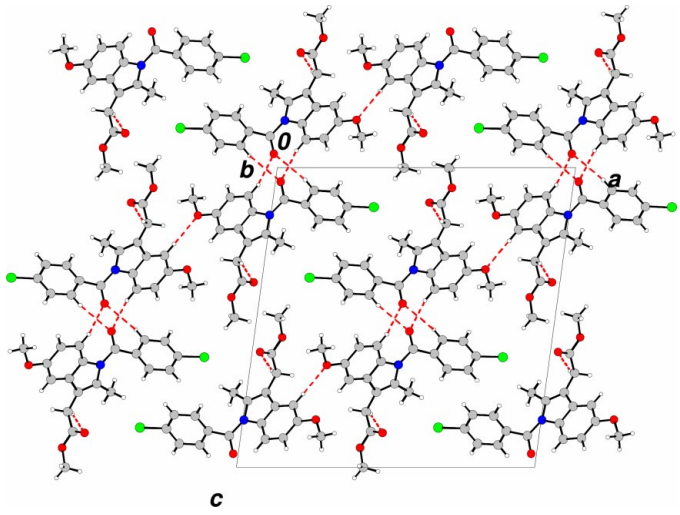


Figure 2
Projection on to (010), showing the packing involving C—H···O interactions. The intermolecular C9—H9*A*···O4(x, $y-1$, z) hydrogen bond projects parallel to the b axis.

solution cooled to room temperature and were immediately isolated and dried.

Crystal data

$C_{20}H_{18}ClNO_4$
M_r = 371.82
Monoclinic, $P2_1/n$
a = 19.0206 (5) Å
b = 4.8326 (1) Å
c = 19.3092 (8) Å
β = 97.739 (1)°
V = 1758.72 (9) Å^3
Z = 4
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6724 reflections
θ = 1.0–25.0°
μ = 0.24 mm^{-1}
T = 180 (2) K
Needle, yellow
0.46 × 0.07 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.946, T_{max} = 0.985
10 009 measured reflections
3086 independent reflections
2410 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.0°
$h = -22 \rightarrow 22$
$k = -5 \rightarrow 5$
$l = -22 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.117
S = 1.04
3086 reflections
238 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 1.0445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···O1^{i}	0.95	2.34	3.260 (3)	162
C3—H3···O1^{ii}	0.95	2.59	3.480 (3)	156
C9—H9*A*···O4^{iii}	0.99	2.62	3.565 (3)	160
C15—H15···O2^{iv}	0.95	2.48	3.419 (2)	170

Symmetry codes: (i) $2-x, 1-y, 2-z$; (ii) $2-x, -y, 2-z$; (iii) $x, y-1, z$; (iv) $\frac{5}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$.

All H atoms were placed geometrically and treated using a riding model. The U_{iso} values for methyl H atoms were fixed at $1.5U_{eq}$ of the carrier atom. For all other H atoms, U_{iso}(H) = $1.2U_{eq}$(carrier atom). The C—H distances of methyl groups were fixed at 0.98 Å; all other C—H distances were fixed at 0.95 Å.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL*97.

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supporting information

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Methyl [1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-ylmethyl]acetate

Crystal data

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$\beta = 97.739$ (1)°
$V = 1758.72$ (9) Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.404$ Mg m^{-3}
Melting point: not measured K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6724 reflections
$\theta = 1.0$–$25.0°$
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$T = 180$ K
Needle, yellow
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Data collection

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Radiation source: fine-focus sealed tube
Graphite monochromator
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Absorption correction: multi-scan Sortav (Blessing, 1995)
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2410 reflections with $I > 2\sigma(I)$
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$h = -22 \rightarrow 22$
$k = -5 \rightarrow 5$
$l = -22 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.117$
$S = 1.04$
3086 reflections
238 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
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 1.0445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-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	0.65787 (4)	−0.17803 (18)	0.86754 (4)	0.0706 (3)
O1	0.98228 (10)	0.2360 (4)	0.95373 (9)	0.0550 (5)
O2	1.24396 (8)	0.8532 (3)	0.84051 (8)	0.0436 (4)
O3	1.09430 (9)	0.0986 (3)	0.56653 (8)	0.0458 (4)
O4	1.02616 (11)	0.3946 (4)	0.61588 (9)	0.0613 (5)
N1	1.00383 (9)	0.2127 (3)	0.84188 (9)	0.0299 (4)
C1	0.96165 (12)	0.1665 (5)	0.89405 (11)	0.0355 (5)
C2	0.88813 (12)	0.0526 (5)	0.87820 (11)	0.0354 (5)
C3	0.86722 (13)	−0.1409 (5)	0.92464 (12)	0.0431 (6)
H3	0.9013	−0.2196	0.9596	0.052*
C4	0.79675 (14)	−0.2190 (5)	0.92002 (13)	0.0498 (7)
H4	0.7824	−0.3554	0.9507	0.060*
C5	0.74766 (13)	−0.0969 (5)	0.87051 (13)	0.0451 (6)
C6	0.76742 (13)	0.0955 (5)	0.82406 (13)	0.0451 (6)
H6	0.7329	0.1779	0.7901	0.054*
C7	0.83837 (12)	0.1670 (5)	0.82758 (12)	0.0404 (6)
H7	0.8529	0.2953	0.7950	0.049*
C8	0.95660 (12)	−0.1570 (5)	0.75198 (12)	0.0377 (5)
H8A	0.9761	−0.2628	0.7156	0.057*
H8B	0.9113	−0.0739	0.7323	0.057*
H8C	0.9491	−0.2806	0.7905	0.057*
C9	1.09125 (12)	0.0424 (4)	0.68596 (10)	0.0335 (5)
H9A	1.0756	−0.1523	0.6792	0.040*
H9B	1.1438	0.0434	0.6931	0.040*
C10	1.06587 (12)	0.2015 (4)	0.62062 (11)	0.0339 (5)
C11	1.00736 (11)	0.0656 (4)	0.77853 (10)	0.0307 (5)
C12	1.26800 (13)	1.0394 (5)	0.89591 (13)	0.0465 (6)
H12A	1.3122	1.1275	0.8866	0.070*
H12B	1.2765	0.9371	0.9401	0.070*
H12C	1.2318	1.1815	0.8991	0.070*
C13	1.06544 (11)	0.1519 (4)	0.75071 (10)	0.0302 (5)
C14	1.10167 (11)	0.3605 (4)	0.79639 (10)	0.0286 (5)
C15	1.16259 (11)	0.5171 (4)	0.79317 (11)	0.0321 (5)
H15	1.1895	0.4955	0.7555	0.039*
C16	1.18318 (11)	0.7055 (4)	0.84620 (11)	0.0325 (5)
C17	1.14376 (11)	0.7377 (4)	0.90166 (11)	0.0332 (5)
H17	1.1586	0.8689	0.9373	0.040*
C18	1.08335 (11)	0.5814 (4)	0.90559 (11)	0.0332 (5)
H18	1.0564	0.6038	0.9432	0.040*
C19	1.06351 (11)	0.3918 (4)	0.85293 (10)	0.0289 (5)

C20	1.07509 (17)	0.2359 (7)	0.50019 (13)	0.0614 (8)
H20A	1.0996	0.1470	0.4646	0.092*
H20B	1.0890	0.4311	0.5045	0.092*
H20C	1.0237	0.2227	0.4865	0.092*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0484 (4)	0.0997 (6)	0.0658 (5)	−0.0277 (4)	0.0158 (3)	−0.0150 (4)
O1	0.0611 (11)	0.0762 (13)	0.0302 (10)	−0.0255 (10)	0.0156 (8)	−0.0075 (9)
O2	0.0426 (10)	0.0463 (10)	0.0448 (10)	−0.0091 (7)	0.0166 (8)	−0.0041 (7)
O3	0.0578 (11)	0.0550 (10)	0.0263 (8)	0.0105 (8)	0.0117 (7)	−0.0011 (7)
O4	0.0880 (14)	0.0593 (12)	0.0367 (10)	0.0352 (11)	0.0081 (9)	0.0053 (8)
N1	0.0325 (10)	0.0326 (10)	0.0253 (9)	0.0025 (7)	0.0065 (7)	0.0004 (7)
C1	0.0416 (13)	0.0373 (12)	0.0291 (12)	−0.0008 (10)	0.0097 (10)	0.0004 (9)
C2	0.0394 (13)	0.0363 (12)	0.0324 (12)	−0.0015 (10)	0.0124 (10)	−0.0048 (10)
C3	0.0472 (14)	0.0451 (14)	0.0381 (13)	−0.0045 (11)	0.0096 (11)	0.0023 (11)
C4	0.0604 (17)	0.0491 (15)	0.0429 (15)	−0.0159 (12)	0.0181 (13)	−0.0009 (12)
C5	0.0420 (14)	0.0543 (15)	0.0408 (14)	−0.0127 (11)	0.0123 (11)	−0.0147 (12)
C6	0.0422 (14)	0.0513 (15)	0.0414 (14)	0.0002 (11)	0.0043 (11)	−0.0049 (11)
C7	0.0424 (14)	0.0411 (13)	0.0392 (14)	−0.0013 (10)	0.0109 (11)	0.0019 (10)
C8	0.0403 (13)	0.0369 (12)	0.0358 (13)	0.0031 (10)	0.0046 (10)	−0.0046 (10)
C9	0.0419 (13)	0.0329 (12)	0.0265 (11)	0.0082 (9)	0.0075 (9)	−0.0016 (9)
C10	0.0385 (12)	0.0353 (13)	0.0286 (12)	0.0004 (10)	0.0067 (10)	−0.0044 (9)
C11	0.0369 (12)	0.0286 (11)	0.0261 (11)	0.0074 (9)	0.0028 (9)	0.0009 (8)
C12	0.0437 (14)	0.0465 (14)	0.0492 (15)	−0.0077 (11)	0.0063 (12)	−0.0006 (12)
C13	0.0385 (12)	0.0286 (11)	0.0234 (11)	0.0089 (9)	0.0035 (9)	0.0019 (8)
C14	0.0335 (12)	0.0297 (11)	0.0231 (11)	0.0083 (9)	0.0054 (9)	0.0042 (8)
C15	0.0363 (12)	0.0338 (12)	0.0284 (12)	0.0093 (9)	0.0124 (9)	0.0041 (9)
C16	0.0340 (12)	0.0313 (12)	0.0332 (12)	0.0033 (9)	0.0078 (9)	0.0065 (9)
C17	0.0394 (12)	0.0317 (11)	0.0291 (12)	0.0008 (9)	0.0063 (10)	−0.0016 (9)
C18	0.0380 (12)	0.0361 (12)	0.0272 (11)	0.0026 (9)	0.0104 (9)	−0.0012 (9)
C19	0.0318 (11)	0.0293 (11)	0.0260 (11)	0.0039 (8)	0.0054 (9)	0.0028 (9)
C20	0.078 (2)	0.081 (2)	0.0256 (13)	0.0024 (16)	0.0099 (13)	0.0064 (13)

Geometric parameters (Å, º)

Cl1—C5	1.746 (2)	C8—H8B	0.9800
O1—C1	1.214 (3)	C8—H8C	0.9800
O2—C16	1.376 (3)	C9—C13	1.500 (3)
O2—C12	1.425 (3)	C9—C10	1.501 (3)
O3—C10	1.335 (3)	C9—H9A	0.9900
O3—C20	1.445 (3)	C9—H9B	0.9900
O4—C10	1.196 (3)	C11—C13	1.357 (3)
N1—C1	1.388 (3)	C12—H12A	0.9800
N1—C19	1.420 (3)	C12—H12B	0.9800
N1—C11	1.424 (3)	C12—H12C	0.9800
C1—C2	1.496 (3)	C13—C14	1.451 (3)

C2—C7	1.381 (3)	C14—C15	1.393 (3)
C2—C3	1.390 (3)	C14—C19	1.398 (3)
C3—C4	1.384 (3)	C15—C16	1.386 (3)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.376 (4)	C16—C17	1.396 (3)
C4—H4	0.9500	C17—C18	1.386 (3)
C5—C6	1.379 (4)	C17—H17	0.9500
C6—C7	1.386 (3)	C18—C19	1.383 (3)
C6—H6	0.9500	C18—H18	0.9500
C7—H7	0.9500	C20—H20A	0.9800
C8—C11	1.490 (3)	C20—H20B	0.9800
C8—H8A	0.9800	C20—H20C	0.9800

C16—O2—C12	117.11 (17)	O4—C10—C9	126.3 (2)
C10—O3—C20	116.21 (19)	O3—C10—C9	110.39 (18)
C1—N1—C19	121.17 (17)	C13—C11—N1	108.76 (18)
C1—N1—C11	129.92 (18)	C13—C11—C8	127.59 (19)
C19—N1—C11	107.69 (16)	N1—C11—C8	123.55 (18)
O1—C1—N1	120.0 (2)	O2—C12—H12A	109.5
O1—C1—C2	118.03 (19)	O2—C12—H12B	109.5
N1—C1—C2	121.79 (19)	H12A—C12—H12B	109.5
C7—C2—C3	119.8 (2)	O2—C12—H12C	109.5
C7—C2—C1	122.0 (2)	H12A—C12—H12C	109.5
C3—C2—C1	117.2 (2)	H12B—C12—H12C	109.5
C4—C3—C2	120.0 (2)	C11—C13—C14	108.55 (18)
C4—C3—H3	120.0	C11—C13—C9	126.6 (2)
C2—C3—H3	120.0	C14—C13—C9	124.73 (19)
C5—C4—C3	119.2 (2)	C15—C14—C19	119.89 (19)
C5—C4—H4	120.4	C15—C14—C13	132.90 (19)
C3—C4—H4	120.4	C19—C14—C13	107.21 (18)
C4—C5—C6	121.5 (2)	C16—C15—C14	118.56 (18)
C4—C5—Cl1	119.7 (2)	C16—C15—H15	120.7
C6—C5—Cl1	118.8 (2)	C14—C15—H15	120.7
C5—C6—C7	119.0 (2)	O2—C16—C15	116.01 (18)
C5—C6—H6	120.5	O2—C16—C17	123.2 (2)
C7—C6—H6	120.5	C15—C16—C17	120.8 (2)
C2—C7—C6	120.3 (2)	C18—C17—C16	121.1 (2)
C2—C7—H7	119.8	C18—C17—H17	119.5
C6—C7—H7	119.8	C16—C17—H17	119.5
C11—C8—H8A	109.5	C19—C18—C17	117.84 (19)
C11—C8—H8B	109.5	C19—C18—H18	121.1
H8A—C8—H8B	109.5	C17—C18—H18	121.1
C11—C8—H8C	109.5	C18—C19—C14	121.80 (19)
H8A—C8—H8C	109.5	C18—C19—N1	130.35 (19)
H8B—C8—H8C	109.5	C14—C19—N1	107.77 (17)
C13—C9—C10	114.56 (17)	O3—C20—H20A	109.5
C13—C9—H9A	108.6	O3—C20—H20B	109.5
C10—C9—H9A	108.6	H20A—C20—H20B	109.5

C13—C9—H9B	108.6	O3—C20—H20C	109.5
C10—C9—H9B	108.6	H20A—C20—H20C	109.5
H9A—C9—H9B	107.6	H20B—C20—H20C	109.5
O4—C10—O3	123.3 (2)		

C19—N1—C1—O1	−13.8 (3)	N1—C11—C13—C9	176.99 (18)
C11—N1—C1—O1	152.0 (2)	C8—C11—C13—C9	0.6 (3)
C19—N1—C1—C2	161.21 (19)	C10—C9—C13—C11	94.3 (3)
C11—N1—C1—C2	−33.0 (3)	C10—C9—C13—C14	−89.3 (2)
O1—C1—C2—C7	123.7 (2)	C11—C13—C14—C15	−179.5 (2)
N1—C1—C2—C7	−51.4 (3)	C9—C13—C14—C15	3.5 (3)
O1—C1—C2—C3	−44.9 (3)	C11—C13—C14—C19	0.9 (2)
N1—C1—C2—C3	140.0 (2)	C9—C13—C14—C19	−176.05 (18)
C7—C2—C3—C4	0.1 (3)	C19—C14—C15—C16	−1.1 (3)
C1—C2—C3—C4	169.0 (2)	C13—C14—C15—C16	179.3 (2)
C2—C3—C4—C5	−2.0 (4)	C12—O2—C16—C15	−177.32 (19)
C3—C4—C5—C6	1.9 (4)	C12—O2—C16—C17	2.3 (3)
C3—C4—C5—Cl1	−176.15 (19)	C14—C15—C16—O2	179.62 (18)
C4—C5—C6—C7	0.0 (4)	C14—C15—C16—C17	0.0 (3)
Cl1—C5—C6—C7	178.05 (18)	O2—C16—C17—C18	−179.13 (19)
C3—C2—C7—C6	1.8 (3)	C15—C16—C17—C18	0.5 (3)
C1—C2—C7—C6	−166.5 (2)	C16—C17—C18—C19	0.2 (3)
C5—C6—C7—C2	−1.8 (4)	C17—C18—C19—C14	−1.4 (3)
C20—O3—C10—O4	0.6 (3)	C17—C18—C19—N1	−177.6 (2)
C20—O3—C10—C9	−179.1 (2)	C15—C14—C19—C18	1.9 (3)
C13—C9—C10—O4	−2.9 (3)	C13—C14—C19—C18	−178.48 (19)
C13—C9—C10—O3	176.79 (19)	C15—C14—C19—N1	178.81 (17)
C1—N1—C11—C13	−168.3 (2)	C13—C14—C19—N1	−1.5 (2)
C19—N1—C11—C13	−1.1 (2)	C1—N1—C19—C18	−13.2 (3)
C1—N1—C11—C8	8.3 (3)	C11—N1—C19—C18	178.2 (2)
C19—N1—C11—C8	175.50 (19)	C1—N1—C19—C14	170.21 (18)
N1—C11—C13—C14	0.1 (2)	C11—N1—C19—C14	1.6 (2)
C8—C11—C13—C14	−176.28 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···O1^{i}	0.95	2.34	3.260 (3)	162
C3—H3···O1^{ii}	0.95	2.59	3.480 (3)	156
C9—H9*A*···O4^{iii}	0.99	2.62	3.565 (3)	160
C15—H15···O2^{iv}	0.95	2.48	3.419 (2)	170

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+2; (ii) −*x*+2, −*y*, −*z*+2; (iii) *x*, *y*−1, *z*; (iv) −*x*+5/2, *y*−1/2, −*z*+3/2.