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1-(12-Bromododecyl)-5-chloroindoline-2,3-dione

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Keywords: crystal structure; chloroindoline-2,3-dione; chains; hydrogen bonds.

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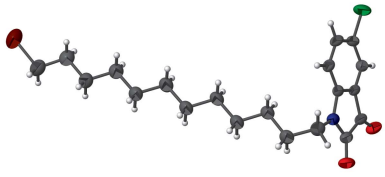
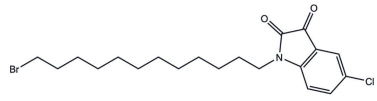
Structural data: full structural data are available from iucrdata.iucr.org

In the structure of the title compound, $C_{20}H_{27}BrClNO_2$, the 5-chloroindoline-2,3-dione ring system is approximately planar, the largest deviation from the mean plane being 0.0237 (10) Å. The mean plane through the fused-ring system makes a dihedral angle of 61.00 (18)° with the mean plane passing through the 1-dodecyl chain. All C atoms of the dodecyl group adopt the planar zigzag arrangement normally observed in *n*-alkane compounds. In the crystal, molecules are linked by C—H···O hydrogen bonds, forming chains parallel to the *b* axis.

3D view



Chemical scheme



Structure description

5-Chloroisatin is a versatile chemical, able to participate in a wide variety of synthetic reactions and form a large number of heterocyclic molecules (Abele *et al.*, 2003) and has an indoline ring structure (Adibi *et al.*,2010). 5-Chloroisatin derivatives possess a wide range of biological activities (Bhrigu *et al.*, 2010; Cerchiaro *et al.*, 2006; Chaluvaraju *et al.*, 2011; Chen *et al.*, 2011; Chibale *et al.*, 2005). The title compound (Fig. 1) was obtained by the reaction of 1,12-dibromododecane with 5-chloroisatin under phase-transfer catalysis conditions.

The 5-chloroindoline-2,3-dione ring system is approximately planar, the largest deviation from the mean plane being 0.0237 (10) A°. The mean plane through the fused-ring system makes a dihedral angle of 61.00 (18)° with the mean plane passing through the 1-dodecyl chain. All C atoms of the dodecyl group adopt the planar zigzag arrangement normally observed in *n*-alkane compounds. In the crystal, molecules are

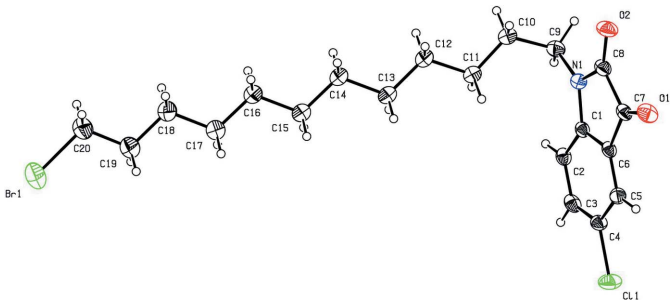


Figure 1
The molecular structure of the title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

linked by C—H···O hydrogen bonds (Table 1, Fig. 2), forming chains parallel to the *b* axis.

Synthesis and crystallization

To a solution of 5-chloro-1*H*-indole-2,3-dione (0.4 g, 2.20 mmol) in *N*,*N*-dimethylformamide (25 ml) was added potassium carbonate (0.5 g, 3.3 mmol), *n*-butylammoium bromide (0.1 g, 0.3 mmol) and 1,12-dibromododecane (0.79 g, 2.42 mmol). The reaction mixture was stirred at 25°C for 48 h. The reaction was monitored by TLC and the resulting mixture was filtered. The title compound was recrystallized from ethanol to afford orange crystals (m.p. 348 K, yield 83%)

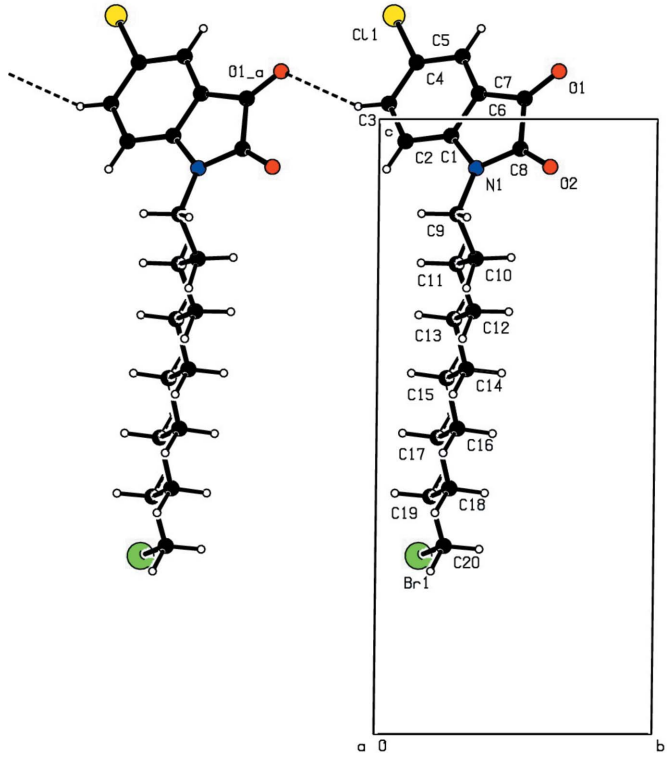


Figure 2
The crystal structure of the title compound, viewed along the *a* axis, showing chains parallel to the *b* axis linked by C— H···O hydrogen bonds (dashed lines).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.93	2.55	3.406 (3)	153

Symmetry code: (i) $x, y-1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{27}BrClNO_2$
M_r	428.78
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.0353 (4), 8.3496 (5), 17.1096 (11)
α, β, γ (°)	84.491 (3), 78.086 (3), 65.126 (2)
V (Å^3)	1018.94 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.16
Crystal size (mm)	0.43 × 0.42 × 0.06
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.616, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27898, 4137, 3048
R_{int}	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.121, 1.04
No. of reflections	4137
No. of parameters	226
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.80, −0.75

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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Crystal data

$C_{20}H_{27}BrClNO_2$
M_r = 428.78
Triclinic, $P\overline{1}$
a = 8.0353 (4) Å
b = 8.3496 (5) Å
c = 17.1096 (11) Å
α = 84.491 (3)°
β = 78.086 (3)°
γ = 65.126 (2)°
V = 1018.94 (10) Å^3
Z = 2
$F(000)$ = 444
D_x = 1.398 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8944 reflections
θ = 2.4–26.1°
μ = 2.16 mm^{-1}
T = 296 K
Plate, orange
0.43 × 0.42 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.616, T_{max} = 0.745
27898 measured reflections
4137 independent reflections
3048 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.4°, θ_{min} = 2.4°
h = −10→9
k = −10→10
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.121
S = 1.04
4137 reflections
226 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.8854P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

Special details

Experimental. SADABS-2014/5 (Bruker,2014/5) was used for absorption correction. wR2(int) was 0.0808 before and 0.0473 after correction. The Ratio of minimum to maximum transmission is 0.8269. The $\lambda/2$ correction factor is 0.00150.

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_{iso}*/U_{eq}
Br1	−0.24071 (6)	0.15532 (6)	0.28981 (3)	0.08347 (19)
Cl1	0.46586 (13)	0.04747 (11)	1.16822 (5)	0.0638 (2)
O1	0.6524 (3)	0.6434 (3)	1.07775 (13)	0.0531 (5)
O2	0.9025 (3)	0.6153 (3)	0.92241 (14)	0.0551 (5)
N1	0.8799 (3)	0.3488 (3)	0.92033 (13)	0.0392 (5)
C1	0.7886 (3)	0.2574 (3)	0.97305 (15)	0.0337 (6)
C6	0.6863 (3)	0.3557 (3)	1.04153 (15)	0.0335 (6)
C7	0.7132 (4)	0.5205 (3)	1.03357 (17)	0.0374 (6)
C2	0.7910 (4)	0.0933 (3)	0.96406 (16)	0.0377 (6)
H2	0.8583	0.0266	0.9186	0.045*
C8	0.8440 (4)	0.5069 (4)	0.95180 (17)	0.0411 (6)
C5	0.5856 (4)	0.2953 (3)	1.10186 (16)	0.0377 (6)
H5	0.5179	0.3617	1.1474	0.045*
C3	0.6898 (4)	0.0324 (3)	1.02514 (18)	0.0432 (7)
H3	0.6900	−0.0779	1.0207	0.052*
C4	0.5887 (4)	0.1309 (4)	1.09226 (17)	0.0399 (6)
C11	0.7731 (4)	0.2822 (4)	0.76445 (17)	0.0452 (7)
H11A	0.6701	0.3224	0.8094	0.054*
H11B	0.8299	0.1542	0.7662	0.054*
C9	1.0082 (4)	0.2821 (4)	0.84536 (18)	0.0486 (7)
H9A	1.0593	0.1541	0.8464	0.058*
H9B	1.1110	0.3168	0.8405	0.058*
C12	0.6981 (5)	0.3432 (4)	0.68750 (18)	0.0525 (7)
H12A	0.6394	0.4712	0.6868	0.063*
H12B	0.8024	0.3062	0.6430	0.063*
C10	0.9151 (4)	0.3500 (4)	0.77284 (18)	0.0512 (7)
H10A	0.8544	0.4778	0.7750	0.061*
H10B	1.0114	0.3187	0.7252	0.061*
C13	0.5587 (5)	0.2750 (4)	0.67480 (18)	0.0530 (8)
H13A	0.4476	0.3236	0.7155	0.064*
H13B	0.6117	0.1476	0.6816	0.064*
C14	0.5031 (5)	0.3204 (5)	0.59322 (18)	0.0543 (8)
H14A	0.4482	0.4478	0.5870	0.065*
H14B	0.6149	0.2740	0.5526	0.065*
C16	0.3166 (5)	0.2901 (5)	0.49670 (19)	0.0567 (8)
H16A	0.2639	0.4170	0.4886	0.068*
H16B	0.4301	0.2402	0.4573	0.068*

C15	0.3668 (5)	0.2501 (5)	0.57882 (19)	0.0575 (8)
H15A	0.4199	0.1231	0.5869	0.069*
H15B	0.2533	0.2998	0.6183	0.069*
C17	0.1805 (5)	0.2208 (5)	0.4821 (2)	0.0601 (8)
H17A	0.0674	0.2696	0.5218	0.072*
H17B	0.2337	0.0936	0.4894	0.072*
C18	0.1295 (5)	0.2636 (5)	0.3997 (2)	0.0609 (9)
H18A	0.0780	0.3907	0.3919	0.073*
H18B	0.2422	0.2130	0.3599	0.073*
C19	−0.0096 (5)	0.1958 (5)	0.3862 (2)	0.0625 (9)
H19A	0.0436	0.0682	0.3917	0.075*
H19B	−0.1209	0.2429	0.4271	0.075*
C20	−0.0632 (6)	0.2455 (5)	0.3059 (2)	0.0700 (10)
H20A	0.0479	0.1991	0.2649	0.084*
H20B	−0.1177	0.3731	0.3005	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0751 (3)	0.0929 (3)	0.0933 (3)	−0.0366 (2)	−0.0263 (2)	−0.0176 (2)
Cl1	0.0758 (6)	0.0589 (5)	0.0656 (5)	−0.0440 (4)	−0.0036 (4)	0.0151 (4)
O1	0.0619 (13)	0.0357 (11)	0.0673 (14)	−0.0256 (10)	−0.0081 (11)	−0.0090 (10)
O2	0.0585 (13)	0.0484 (12)	0.0700 (15)	−0.0354 (11)	−0.0134 (11)	0.0139 (10)
N1	0.0433 (13)	0.0407 (13)	0.0392 (13)	−0.0229 (10)	−0.0080 (10)	0.0020 (10)
C1	0.0341 (13)	0.0316 (13)	0.0392 (15)	−0.0144 (11)	−0.0154 (11)	0.0056 (11)
C6	0.0374 (13)	0.0272 (13)	0.0409 (15)	−0.0152 (11)	−0.0142 (11)	0.0012 (11)
C7	0.0382 (14)	0.0310 (14)	0.0489 (16)	−0.0170 (11)	−0.0158 (12)	0.0022 (12)
C2	0.0430 (15)	0.0310 (14)	0.0421 (15)	−0.0154 (12)	−0.0124 (12)	−0.0034 (11)
C8	0.0418 (15)	0.0376 (15)	0.0513 (17)	−0.0209 (12)	−0.0177 (13)	0.0079 (12)
C5	0.0411 (14)	0.0346 (14)	0.0388 (15)	−0.0164 (11)	−0.0096 (11)	0.0025 (11)
C3	0.0506 (16)	0.0286 (14)	0.0595 (18)	−0.0209 (12)	−0.0218 (14)	0.0046 (12)
C4	0.0445 (15)	0.0361 (15)	0.0457 (16)	−0.0226 (12)	−0.0142 (12)	0.0104 (12)
C11	0.0473 (16)	0.0474 (17)	0.0399 (16)	−0.0205 (13)	−0.0051 (12)	0.0023 (13)
C9	0.0397 (15)	0.0605 (19)	0.0482 (17)	−0.0255 (14)	−0.0020 (13)	−0.0023 (14)
C12	0.0617 (19)	0.060 (2)	0.0405 (17)	−0.0309 (16)	−0.0104 (14)	0.0073 (14)
C10	0.0535 (18)	0.062 (2)	0.0417 (17)	−0.0306 (16)	−0.0037 (14)	0.0031 (14)
C13	0.0595 (19)	0.061 (2)	0.0427 (17)	−0.0304 (16)	−0.0110 (14)	0.0101 (14)
C14	0.065 (2)	0.066 (2)	0.0404 (17)	−0.0354 (17)	−0.0099 (14)	0.0066 (15)
C16	0.067 (2)	0.067 (2)	0.0449 (18)	−0.0368 (18)	−0.0095 (15)	0.0025 (15)
C15	0.062 (2)	0.071 (2)	0.0458 (18)	−0.0358 (18)	−0.0109 (15)	0.0077 (16)
C17	0.063 (2)	0.069 (2)	0.055 (2)	−0.0340 (18)	−0.0134 (16)	0.0025 (16)
C18	0.070 (2)	0.068 (2)	0.053 (2)	−0.0356 (18)	−0.0121 (16)	−0.0028 (16)
C19	0.064 (2)	0.064 (2)	0.065 (2)	−0.0295 (18)	−0.0144 (17)	−0.0034 (17)
C20	0.076 (2)	0.078 (3)	0.069 (2)	−0.042 (2)	−0.0148 (19)	−0.0072 (19)

Geometric parameters (Å, º)

Br1—C20	1.945 (4)	C12—C13	1.512 (4)
Cl1—C4	1.738 (3)	C10—H10A	0.9700
O1—C7	1.199 (3)	C10—H10B	0.9700
O2—C8	1.210 (3)	C13—H13A	0.9700
N1—C1	1.415 (3)	C13—H13B	0.9700
N1—C8	1.367 (4)	C13—C14	1.518 (4)
N1—C9	1.458 (4)	C14—H14A	0.9700
C1—C6	1.394 (4)	C14—H14B	0.9700
C1—C2	1.385 (3)	C14—C15	1.512 (4)
C6—C7	1.470 (3)	C16—H16A	0.9700
C6—C5	1.369 (4)	C16—H16B	0.9700
C7—C8	1.549 (4)	C16—C15	1.510 (4)
C2—H2	0.9300	C16—C17	1.505 (5)
C2—C3	1.381 (4)	C15—H15A	0.9700
C5—H5	0.9300	C15—H15B	0.9700
C5—C4	1.388 (4)	C17—H17A	0.9700
C3—H3	0.9300	C17—H17B	0.9700
C3—C4	1.375 (4)	C17—C18	1.517 (5)
C11—H11A	0.9700	C18—H18A	0.9700
C11—H11B	0.9700	C18—H18B	0.9700
C11—C12	1.515 (4)	C18—C19	1.512 (5)
C11—C10	1.507 (4)	C19—H19A	0.9700
C9—H9A	0.9700	C19—H19B	0.9700
C9—H9B	0.9700	C19—C20	1.494 (5)
C9—C10	1.520 (4)	C20—H20A	0.9700
C12—H12A	0.9700	C20—H20B	0.9700
C12—H12B	0.9700		
C1—N1—C9	126.1 (2)	H10A—C10—H10B	107.4
C8—N1—C1	110.8 (2)	C12—C13—H13A	108.8
C8—N1—C9	123.0 (2)	C12—C13—H13B	108.8
C6—C1—N1	110.7 (2)	C12—C13—C14	113.8 (3)
C2—C1—N1	128.9 (2)	H13A—C13—H13B	107.7
C2—C1—C6	120.4 (2)	C14—C13—H13A	108.8
C1—C6—C7	107.4 (2)	C14—C13—H13B	108.8
C5—C6—C1	121.9 (2)	C13—C14—H14A	108.6
C5—C6—C7	130.7 (2)	C13—C14—H14B	108.6
O1—C7—C6	130.6 (3)	H14A—C14—H14B	107.6
O1—C7—C8	124.5 (2)	C15—C14—C13	114.6 (3)
C6—C7—C8	104.9 (2)	C15—C14—H14A	108.6
C1—C2—H2	121.2	C15—C14—H14B	108.6
C3—C2—C1	117.6 (3)	H16A—C16—H16B	107.5
C3—C2—H2	121.2	C15—C16—H16A	108.6
O2—C8—N1	127.4 (3)	C15—C16—H16B	108.6
O2—C8—C7	126.4 (3)	C17—C16—H16A	108.6
N1—C8—C7	106.2 (2)	C17—C16—H16B	108.6

C6—C5—H5	121.4	C17—C16—C15	114.8 (3)
C6—C5—C4	117.3 (3)	C14—C15—H15A	108.6
C4—C5—H5	121.4	C14—C15—H15B	108.6
C2—C3—H3	119.2	C16—C15—C14	114.5 (3)
C4—C3—C2	121.5 (2)	C16—C15—H15A	108.6
C4—C3—H3	119.2	C16—C15—H15B	108.6
C5—C4—Cl1	118.8 (2)	H15A—C15—H15B	107.6
C3—C4—Cl1	119.9 (2)	C16—C17—H17A	108.7
C3—C4—C5	121.3 (3)	C16—C17—H17B	108.7
H11A—C11—H11B	107.8	C16—C17—C18	114.3 (3)
C12—C11—H11A	109.1	H17A—C17—H17B	107.6
C12—C11—H11B	109.1	C18—C17—H17A	108.7
C10—C11—H11A	109.1	C18—C17—H17B	108.7
C10—C11—H11B	109.1	C17—C18—H18A	108.8
C10—C11—C12	112.7 (2)	C17—C18—H18B	108.8
N1—C9—H9A	109.0	H18A—C18—H18B	107.7
N1—C9—H9B	109.0	C19—C18—C17	113.7 (3)
N1—C9—C10	112.7 (2)	C19—C18—H18A	108.8
H9A—C9—H9B	107.8	C19—C18—H18B	108.8
C10—C9—H9A	109.0	C18—C19—H19A	109.0
C10—C9—H9B	109.0	C18—C19—H19B	109.0
C11—C12—H12A	108.5	H19A—C19—H19B	107.8
C11—C12—H12B	108.5	C20—C19—C18	112.7 (3)
H12A—C12—H12B	107.5	C20—C19—H19A	109.0
C13—C12—C11	115.0 (2)	C20—C19—H19B	109.0
C13—C12—H12A	108.5	Br1—C20—H20A	109.2
C13—C12—H12B	108.5	Br1—C20—H20B	109.2
C11—C10—C9	115.6 (2)	C19—C20—Br1	111.9 (3)
C11—C10—H10A	108.4	C19—C20—H20A	109.2
C11—C10—H10B	108.4	C19—C20—H20B	109.2
C9—C10—H10A	108.4	H20A—C20—H20B	107.9
C9—C10—H10B	108.4		

O1—C7—C8—O2	0.6 (4)	C2—C3—C4—Cl1	−179.1 (2)
O1—C7—C8—N1	−179.6 (3)	C2—C3—C4—C5	−0.7 (4)
N1—C1—C6—C7	−0.4 (3)	C8—N1—C1—C6	0.7 (3)
N1—C1—C6—C5	−179.9 (2)	C8—N1—C1—C2	−179.1 (3)
N1—C1—C2—C3	179.6 (2)	C8—N1—C9—C10	−86.0 (3)
N1—C9—C10—C11	−68.4 (4)	C5—C6—C7—O1	−0.6 (5)
C1—N1—C8—O2	179.1 (3)	C5—C6—C7—C8	179.4 (3)
C1—N1—C8—C7	−0.7 (3)	C11—C12—C13—C14	−173.3 (3)
C1—N1—C9—C10	99.3 (3)	C9—N1—C1—C6	175.9 (2)
C1—C6—C7—O1	−179.9 (3)	C9—N1—C1—C2	−3.9 (4)
C1—C6—C7—C8	0.0 (3)	C9—N1—C8—O2	3.7 (4)
C1—C6—C5—C4	−0.1 (4)	C9—N1—C8—C7	−176.1 (2)
C1—C2—C3—C4	0.5 (4)	C12—C11—C10—C9	−175.2 (3)
C6—C1—C2—C3	−0.2 (4)	C12—C13—C14—C15	178.8 (3)
C6—C7—C8—O2	−179.3 (3)	C10—C11—C12—C13	178.4 (3)

C6—C7—C8—N1	0.4 (3)	C13—C14—C15—C16	−178.0 (3)
C6—C5—C4—Cl1	178.9 (2)	C16—C17—C18—C19	−179.1 (3)
C6—C5—C4—C3	0.4 (4)	C15—C16—C17—C18	179.3 (3)
C7—C6—C5—C4	−179.4 (3)	C17—C16—C15—C14	−179.9 (3)
C2—C1—C6—C7	179.4 (2)	C17—C18—C19—C20	177.8 (3)
C2—C1—C6—C5	0.0 (4)	C18—C19—C20—Br1	179.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.93	2.55	3.406 (3)	153

Symmetry code: (i) *x*, *y*−1, *z*.