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4-(3,4-Dichlorophenyl)-3,4-dihydronaphthalen-1(2*H*)-one

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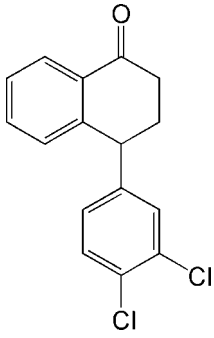
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 18.3.

The title compound, $C_{16}H_{12}Cl_2O$, was synthesized from 1-naphthol and 1,2-dichlorobenzene with anhydrous aluminium chloride as a cataylst. In the molecule, the two ring systems are approximately perpendicular to one other with a dihedral angle of 82.06 (4)°. There are two CH-type hydrogen bonds.

Related literature

Synthesis: Taber *et al.* (2004); Vukics *et al.* (2002); Quallich (2005).



Experimental

Crystal data

$C_{16}H_{12}Cl_2O$
M_r = 291.16
Monoclinic, $P2_1/n$
a = 10.7705 (14) Å
b = 10.7317 (14) Å
c = 12.3765 (16) Å
β = 111.359 (6)°
V = 1332.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 113 (2) K
0.22 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.903, T_{max} = 0.920
16212 measured reflections
3172 independent reflections
2676 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.11
3172 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O1^{i}	0.95	2.40	3.3469 (17)	172
C9—H9···Cl1^{ii}	0.95	2.91	3.6984 (16)	142
C16—H16···Cl1^{iii}	0.95	2.91	3.7705 (15)	151

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CHEMDRAW* (Cambridgesoft, 2003); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2151).

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supporting information

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4-(3,4-Dichlorophenyl)-3,4-dihydronaphthalen-1(2*H*)-one

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S1. Comment

The title compound (I) is an intermediate for the synthesis of sertraline hydrochloride. Sertraline hydrochloride is an inhibitor of synaptosomal serotonin uptake makng it an important pharmaceutical agent for the treatment of depression and other anxiety-related disorders.

The molecular structure of the title compound is illustrated in Fig. 1. In the molecule, the angle between the two benzene ring planes is 82.06(0.04). In the molecule, the two ring systems are approximately perpendicular to one other with a dihedral angle of 82.06 (4). There are two CH type hydrogen bonds (Cl···H at 2.9Å and O..H of 2.4 Å).

S2. Experimental

To a stirred solution of 1-naphthol(21.62 g, 0.15 mol) in 1,2-dichlorobenzene(160 ml) anhydrous AlCl3(53.3 g, 0.4 mol)was added. The reaction mixture was heated to 110¡ae and stirred at this temperature for 3 h. The mixture was then cooled to room temperature and poured into ice(300 g) and concentrated hydrochloric acid(80 ml), followed by addition of CH2Cl2(300 ml). The organic layer was separated, and washed with water(300 ml). The solvents were evaporated in vacuum. To the oily residue methanol(50 ml) was added. The product was crystallized, filtered,and then washed twice with methanol(50 ml). Yield:32.0 g(73.4%). (Taber *et al.*, 2004; Vukics *et al.*, 2002; Quallich, 2005). Crystals suitable for X-ray analysis were white by slow evaporation of an absolute methanol and acetone solution at room temperature over 15 days.

S3. Refinement

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2 U_{eq}(C).

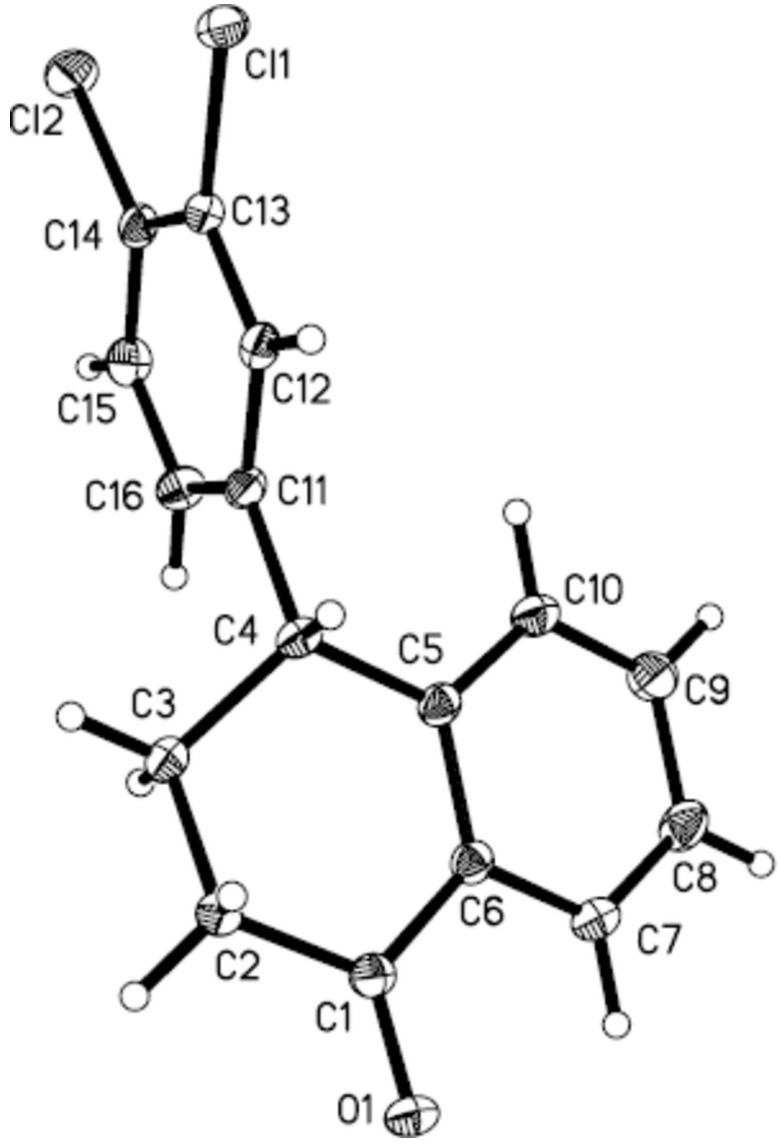

Figure 1

The molecular structure of (I), drawn with 30% probability ellipsoids.

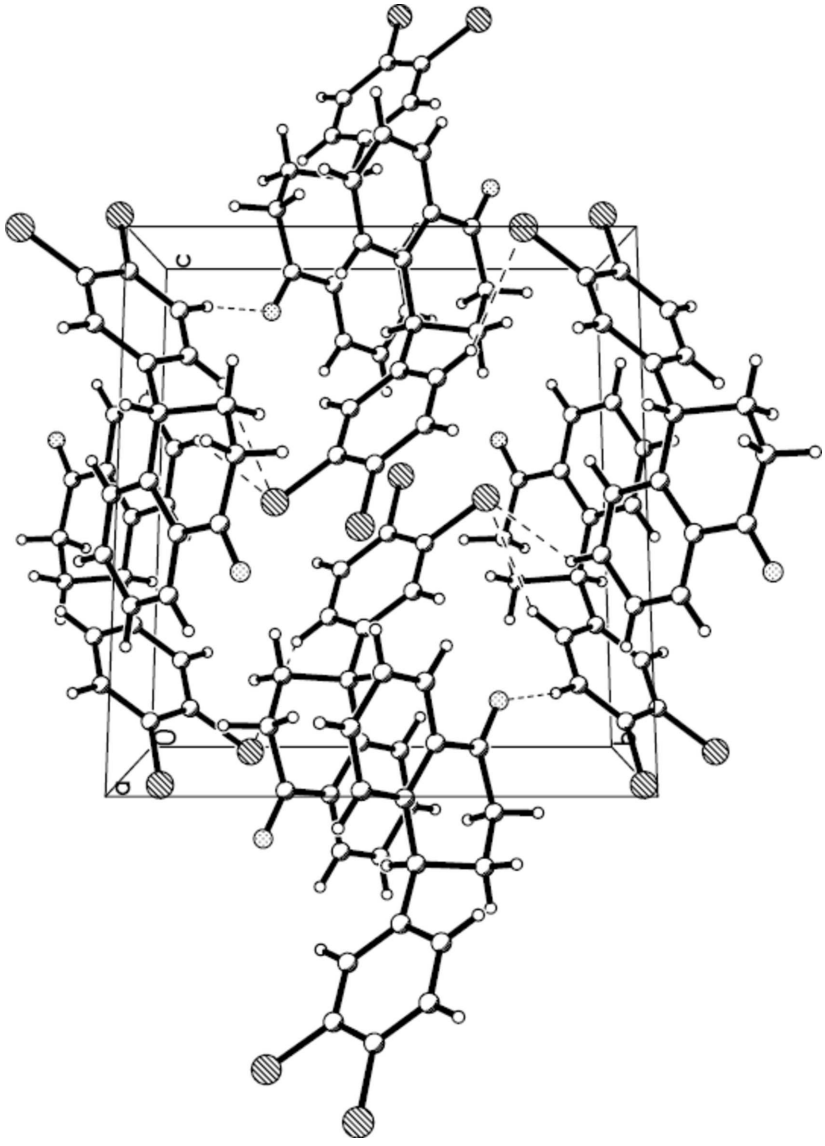

Figure 2

The crystal structure of (I), viewed along *a* axis

4-(3,4-Dichlorophenyl)-3,4-dihydronaphthalen-1(2*H*)-one

Crystal data

$C_{16}H_{12}Cl_2O$
$M_r = 291.16$
Monoclinic, $P2_1/n$
$a = 10.7705\ (14)$ Å
$b = 10.7317\ (14)$ Å
$c = 12.3765\ (16)$ Å
$\beta = 111.359\ (6)°$
$V = 1332.3\ (3)$ Å^3
$Z = 4$
$F(000) = 600$
$D_x = 1.452$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 3625 reflections
$\theta = 2.6–25.0°$
$\mu = 0.47$ mm^{-1}
$T = 113$ K
Prism, colorless
0.22 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.903, T_{max} = 0.920
16212 measured reflections
3172 independent reflections
2676 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.9°, θ_{min} = 2.2°
h = −14→14
k = −14→14
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.11
3172 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.1288P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.43486 (4)	0.71805 (3)	0.50411 (3)	0.01997 (10)
Cl2	0.22276 (4)	0.54210 (3)	0.54838 (3)	0.02382 (11)
O1	0.47445 (10)	0.26530 (10)	−0.12559 (9)	0.0211 (2)
C1	0.45158 (13)	0.30731 (13)	−0.04246 (12)	0.0154 (3)
C2	0.53907 (14)	0.27547 (13)	0.08047 (11)	0.0180 (3)
H2A	0.6217	0.3257	0.1024	0.022*
H2B	0.5647	0.1866	0.0838	0.022*
C3	0.47278 (14)	0.29863 (13)	0.16876 (12)	0.0180 (3)
H3A	0.5383	0.2851	0.2482	0.022*
H3B	0.3985	0.2391	0.1555	0.022*
C4	0.41922 (14)	0.43295 (13)	0.15738 (11)	0.0155 (3)
H4	0.4967	0.4897	0.1693	0.019*
C5	0.32019 (13)	0.45560 (12)	0.03435 (11)	0.0150 (3)
C6	0.33808 (13)	0.39489 (12)	−0.05995 (11)	0.0148 (3)
C7	0.24896 (14)	0.41618 (13)	−0.17352 (12)	0.0177 (3)
H7	0.2617	0.3743	−0.2363	0.021*

C8	0.14277 (15)	0.49738 (15)	−0.19542 (13)	0.0223 (3)
H8	0.0826	0.5114	−0.2725	0.027*
C9	0.12560 (15)	0.55839 (15)	−0.10222 (13)	0.0234 (3)
H9	0.0531	0.6144	−0.1162	0.028*
C10	0.21314 (15)	0.53833 (14)	0.01059 (13)	0.0201 (3)
H10	0.2002	0.5815	0.0727	0.024*
C11	0.36440 (14)	0.46337 (13)	0.25172 (11)	0.0154 (3)
C12	0.41425 (13)	0.56497 (13)	0.32404 (11)	0.0153 (3)
H12	0.4787	0.6176	0.3116	0.018*
C13	0.37027 (14)	0.59043 (13)	0.41504 (11)	0.0151 (3)
C14	0.27583 (14)	0.51357 (13)	0.43366 (12)	0.0167 (3)
C15	0.22341 (14)	0.41266 (14)	0.36055 (12)	0.0187 (3)
H15	0.1581	0.3607	0.3724	0.022*
C16	0.26752 (14)	0.38851 (14)	0.26993 (12)	0.0186 (3)
H16	0.2312	0.3201	0.2196	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0274 (2)	0.01779 (18)	0.01560 (17)	−0.00214 (14)	0.00882 (14)	−0.00271 (13)
Cl2	0.0328 (2)	0.0250 (2)	0.02175 (19)	0.00121 (15)	0.01954 (16)	0.00068 (14)
O1	0.0258 (6)	0.0237 (5)	0.0172 (5)	0.0048 (4)	0.0119 (4)	−0.0016 (4)
C1	0.0169 (7)	0.0145 (7)	0.0163 (7)	−0.0020 (5)	0.0076 (6)	−0.0007 (5)
C2	0.0203 (7)	0.0187 (7)	0.0160 (7)	0.0050 (6)	0.0079 (6)	0.0009 (5)
C3	0.0217 (7)	0.0196 (7)	0.0136 (6)	0.0034 (6)	0.0074 (6)	0.0020 (5)
C4	0.0175 (7)	0.0178 (7)	0.0125 (6)	−0.0002 (5)	0.0072 (5)	−0.0010 (5)
C5	0.0166 (7)	0.0155 (7)	0.0141 (6)	−0.0021 (5)	0.0069 (5)	0.0002 (5)
C6	0.0159 (7)	0.0148 (7)	0.0144 (6)	−0.0018 (5)	0.0064 (5)	0.0004 (5)
C7	0.0190 (7)	0.0204 (7)	0.0150 (7)	−0.0016 (6)	0.0077 (6)	−0.0022 (5)
C8	0.0199 (7)	0.0300 (8)	0.0147 (7)	0.0035 (6)	0.0034 (6)	0.0018 (6)
C9	0.0213 (7)	0.0267 (8)	0.0222 (7)	0.0091 (6)	0.0079 (6)	0.0019 (6)
C10	0.0231 (7)	0.0225 (8)	0.0167 (7)	0.0040 (6)	0.0097 (6)	−0.0007 (6)
C11	0.0162 (6)	0.0178 (7)	0.0118 (6)	0.0028 (5)	0.0048 (5)	0.0005 (5)
C12	0.0162 (7)	0.0168 (7)	0.0132 (6)	0.0007 (5)	0.0058 (5)	0.0027 (5)
C13	0.0177 (7)	0.0141 (6)	0.0123 (6)	0.0020 (5)	0.0041 (5)	0.0004 (5)
C14	0.0196 (7)	0.0189 (7)	0.0142 (7)	0.0047 (6)	0.0094 (6)	0.0038 (5)
C15	0.0176 (7)	0.0197 (7)	0.0202 (7)	−0.0017 (6)	0.0084 (6)	0.0020 (6)
C16	0.0184 (7)	0.0204 (7)	0.0162 (7)	−0.0018 (6)	0.0055 (6)	−0.0024 (6)

Geometric parameters (Å, º)

Cl1—C13	1.7367 (14)	C7—C8	1.384 (2)
Cl2—C14	1.7400 (14)	C7—H7	0.9500
O1—C1	1.2276 (16)	C8—C9	1.396 (2)
C1—C6	1.4939 (19)	C8—H8	0.9500
C1—C2	1.5083 (19)	C9—C10	1.388 (2)
C2—C3	1.5278 (18)	C9—H9	0.9500
C2—H2A	0.9900	C10—H10	0.9500

C2—H2B	0.9900	C11—C12	1.3886 (19)
C3—C4	1.5399 (19)	C11—C16	1.399 (2)
C3—H3A	0.9900	C12—C13	1.3985 (18)
C3—H3B	0.9900	C12—H12	0.9500
C4—C11	1.5234 (18)	C13—C14	1.392 (2)
C4—C5	1.5272 (18)	C14—C15	1.392 (2)
C4—H4	1.0000	C15—C16	1.3924 (19)
C5—C10	1.399 (2)	C15—H15	0.9500
C5—C6	1.4098 (18)	C16—H16	0.9500
C6—C7	1.4024 (19)		

O1—C1—C6	120.86 (12)	C6—C7—H7	119.5
O1—C1—C2	121.32 (12)	C7—C8—C9	118.83 (13)
C6—C1—C2	117.79 (11)	C7—C8—H8	120.6
C1—C2—C3	113.68 (11)	C9—C8—H8	120.6
C1—C2—H2A	108.8	C10—C9—C8	120.84 (14)
C3—C2—H2A	108.8	C10—C9—H9	119.6
C1—C2—H2B	108.8	C8—C9—H9	119.6
C3—C2—H2B	108.8	C9—C10—C5	121.05 (13)
H2A—C2—H2B	107.7	C9—C10—H10	119.5
C2—C3—C4	110.11 (11)	C5—C10—H10	119.5
C2—C3—H3A	109.6	C12—C11—C16	118.89 (12)
C4—C3—H3A	109.6	C12—C11—C4	119.70 (12)
C2—C3—H3B	109.6	C16—C11—C4	121.37 (12)
C4—C3—H3B	109.6	C11—C12—C13	120.51 (13)
H3A—C3—H3B	108.2	C11—C12—H12	119.7
C11—C4—C5	113.90 (11)	C13—C12—H12	119.7
C11—C4—C3	111.55 (11)	C14—C13—C12	119.97 (13)
C5—C4—C3	110.03 (11)	C14—C13—Cl1	120.66 (11)
C11—C4—H4	107.0	C12—C13—Cl1	119.36 (11)
C5—C4—H4	107.0	C15—C14—C13	120.07 (13)
C3—C4—H4	107.0	C15—C14—Cl2	119.42 (11)
C10—C5—C6	118.03 (12)	C13—C14—Cl2	120.51 (11)
C10—C5—C4	122.23 (12)	C14—C15—C16	119.45 (13)
C6—C5—C4	119.70 (12)	C14—C15—H15	120.3
C7—C6—C5	120.29 (12)	C16—C15—H15	120.3
C7—C6—C1	118.23 (12)	C15—C16—C11	121.08 (13)
C5—C6—C1	121.48 (12)	C15—C16—H16	119.5
C8—C7—C6	120.93 (13)	C11—C16—H16	119.5
C8—C7—H7	119.5		

O1—C1—C2—C3	−160.86 (13)	C8—C9—C10—C5	−0.6 (2)
C6—C1—C2—C3	20.89 (17)	C6—C5—C10—C9	1.2 (2)
C1—C2—C3—C4	−52.96 (16)	C4—C5—C10—C9	179.15 (14)
C2—C3—C4—C11	−174.50 (11)	C5—C4—C11—C12	−110.85 (14)
C2—C3—C4—C5	58.08 (15)	C3—C4—C11—C12	123.85 (14)
C11—C4—C5—C10	23.18 (19)	C5—C4—C11—C16	71.33 (17)
C3—C4—C5—C10	149.28 (13)	C3—C4—C11—C16	−53.97 (17)

C11—C4—C5—C6	−158.88 (12)	C16—C11—C12—C13	1.3 (2)
C3—C4—C5—C6	−32.78 (16)	C4—C11—C12—C13	−176.57 (12)
C10—C5—C6—C7	−1.1 (2)	C11—C12—C13—C14	0.0 (2)
C4—C5—C6—C7	−179.11 (12)	C11—C12—C13—Cl1	179.87 (11)
C10—C5—C6—C1	178.62 (13)	C12—C13—C14—C15	−1.1 (2)
C4—C5—C6—C1	0.60 (19)	Cl1—C13—C14—C15	179.05 (11)
O1—C1—C6—C7	7.5 (2)	C12—C13—C14—Cl2	178.62 (10)
C2—C1—C6—C7	−174.23 (12)	Cl1—C13—C14—Cl2	−1.21 (17)
O1—C1—C6—C5	−172.20 (13)	C13—C14—C15—C16	0.8 (2)
C2—C1—C6—C5	6.05 (19)	Cl2—C14—C15—C16	−178.90 (11)
C5—C6—C7—C8	0.5 (2)	C14—C15—C16—C11	0.5 (2)
C1—C6—C7—C8	−179.25 (13)	C12—C11—C16—C15	−1.6 (2)
C6—C7—C8—C9	0.1 (2)	C4—C11—C16—C15	176.25 (13)
C7—C8—C9—C10	0.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O1^{i}	0.95	2.40	3.3469 (17)	172
C9—H9···Cl1^{ii}	0.95	2.91	3.6984 (16)	142
C16—H16···Cl1^{iii}	0.95	2.91	3.7705 (15)	151

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