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1-(4-Chlorophenyl)-2,6,6-trimethyl-1,5,6,7-tetrahydro-4*H*-indol-4-one

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In the title compound, $C_{17}H_{18}ClNO$, the tetrahydroindole ring system is nearly planar, except for the dimethyl-substituted C atom. Molecules are linked *via* C—H$\cdots$O and C—H$\cdots\pi$ interactions, forming chains along the *b* axis.

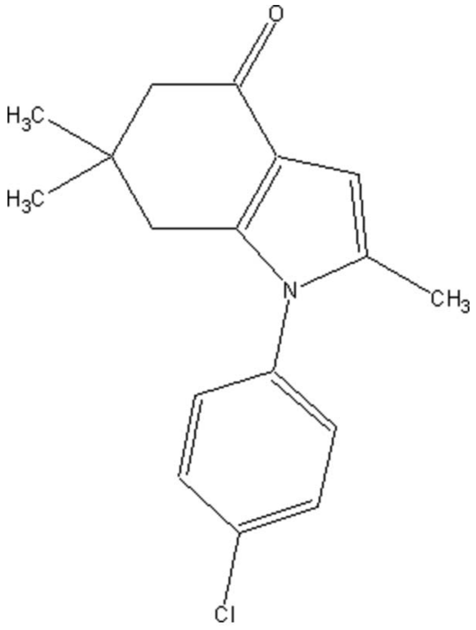
Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.118
Data-to-parameter ratio = 11.7

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

Comment

Crystal engineering *via* manipulation of hydrogen bonding has attracted much interest in recent literature (Aakeröy, 1997; Guru Row, 1999; Desiraju, 2000, 2002; Hunter *et al.*, 2001). Weak C—H$\cdots\pi$ (Nishio *et al.*, 1995; Umezawa *et al.*, 1999; Takahashi *et al.*, 2000), π stacking (Hunter, 1993, 1994) and C—H$\cdots$O (Steiner, 2002) interactions have been found to generate different crystalline motifs. Organohalo compounds have also been found to generate motifs *via* C—H$\cdots X$, $X\cdots X$ and C—$X\cdots\pi$ interactions (Thalladi *et al.*, 1998). It has been shown that fluorine does not readily accept hydrogen bonding and hence behaves differently from Cl and Br (Shimoni & Glusker, 1994; Howard *et al.*, 1996; Dunitz & Taylor, 1997; Desiraju & Parthasarathi, 1989). We have been interested in the study of the role that chlorine plays in the packing of organic molecules that exhibit biological activity and report here the structure of the title compound, (I).



(I)

In the tetrahydroindole ring system, atom C5 deviates 0.633 (2) Å from the C6–C8/C3/C4 plane (Fig. 1). Cremer & Pople (1975) analysis for this six-membered ring reveals the

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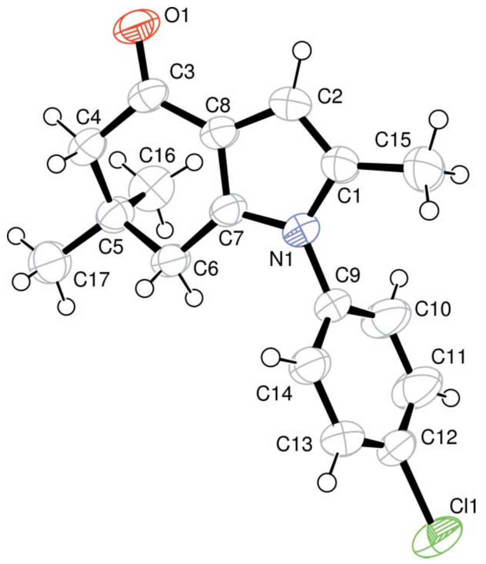

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids.

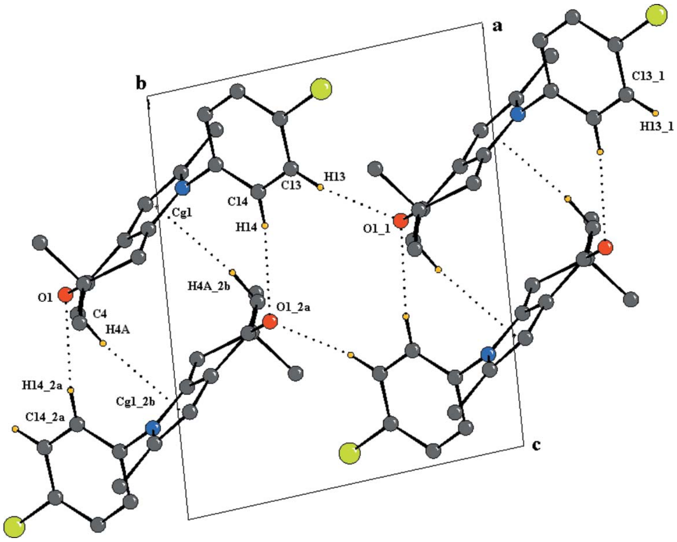

Figure 2
Packing diagram of (I) viewed down the *a* axis. The dotted lines indicate C—H⋯π and C—H⋯O interactions. H atoms have been omitted unless they are involved in hydrogen bonding. The symmetry-related positions have been labelled '1', '2a' and '2b', where the symmetry codes refer to $(x-1, y+1, z)$, $(-x+2, -y, -z+1)$ and $(-x, -y, -z+1)$, respectively.

puckering parameters as $Q(2) = 0.367$ (2) Å, $\varphi(2) = 294.0$ (3)°, $Q(3) = -0.267$ (2) Å, $Q = 0.454$ (2) Å and $\theta = 126.0$ (3)°. The molecules pack *via* the involvement of C—H⋯O and C—H⋯π interactions (Table 2). C—H⋯O interactions involving atom H14 form molecular dimers (Fig. 2), which are further stabilized by C—H⋯π interactions, where *Cg*1 in Table 2 is the centroid of the five-membered indole ring. Such dimers [Etter's graph set symbol $R_2^2(16)$; Bernstein *et al.*, 1995] are held further by C—H⋯O interactions involving atom H13, forming zigzag double chains along the *b* axis along with a tetrameric molecular motif [$R_2^4(10)$]. The Cl atom does not participate in any significant intermolecular interactions.

Experimental

Compound (I) was synthesized according to the procedure reported in the literature (Nagarajan *et al.*, 1985) and was crystallized from acetone by slow evaporation at 278 K.

Crystal data

$C_{17}H_{18}ClNO$
$M_r = 287.77$
Triclinic, $P\overline{1}$
$a = 8.236$ (5) Å
$b = 9.003$ (6) Å
$c = 10.781$ (7) Å
$\alpha = 82.203$ (10)°
$\beta = 85.384$ (11)°
$\gamma = 74.530$ (10)°
$V = 762.6$ (8) Å^3

$Z = 2$
$D_x = 1.253$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 835 reflections
$\theta = 1.6$–25.4°
$\mu = 0.25$ mm^{-1}
$T = 290$ (2) K
Block, colourless
0.35 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.905$, $T_{max} = 0.953$
6193 measured reflections

2955 independent reflections
2551 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 26.4$°
$h = -9 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.118$
$S = 1.04$
2955 reflections
253 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 0.1529P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C12	1.7372 (18)	N1—C1	1.397 (2)
O1—C3	1.2244 (19)	N1—C9	1.4318 (19)
N1—C7	1.3676 (19)		
C9—N1—C7—C8	179.09 (13)	C4—C5—C6—C7	−47.34 (18)
C7—N1—C9—C14	−70.9 (2)	C7—N1—C1—C15	177.81 (16)
C1—N1—C9—C10	−71.2 (2)	C7—C8—C3—C4	1.79 (19)
C6—C7—C8—C3	1.5 (2)	C5—C4—C3—O1	151.94 (14)
C3—C4—C5—C6	53.77 (18)	C5—C4—C3—C8	−30.52 (18)
C8—C7—C6—C5	22.9 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C14—H14⋯O1^{i}	0.92 (2)	2.47 (2)	3.379 (3)	170 (2)
C13—H13⋯O1^{ii}	0.94 (2)	2.38 (2)	3.304 (2)	171 (2)
C4—H4*A*⋯*Cg*1^{iii}	0.97 (2)	2.65 (2)	3.589 (3)	163 (1)

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $x-1, y+1, z$; (iii) $-x, -y, -z+1$.

All H atoms were located from difference Fourier maps and refined isotropically. The C—H distances are 0.92 (2)–1.02 (2) Å.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et* *al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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