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

In the title compound, C₁₇H₁₆ClNO, the tetrahydroindole ring system is nearly planar, except for the dimethyl-substituted C atom. Molecules are linked via C—H⋯O and C—H⋯π interactions, forming chains along the b axis.

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⋯π (Nishio et al., 1995; Umezawa et al., 1999; Takahashi et al., 2000), π stacking (Hunter, 1993, 1994) and C—H⋯O (Steiner, 2002) interactions have been found to generate different crystalline motifs. Organohalo compounds have also been found to generate motifs via C—H⋯X, X⋯X and C⋯X⋯π 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).

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
puckering parameters as \( Q(2) = 0.367 (2) \) \( \text{Å} \), \( \phi(2) = 294.0 (3) ^\circ \), \( Q(3) = -0.267 (2) \) \( \text{Å} \), \( Q = 0.454 (2) \) \( \text{Å} \) and \( \theta = 126.0 (3)^\circ \). The molecules pack via the involvement of \( C-H \cdots \pi \) and \( C-H \cdots O \) interactions (Table 2), \( C-H \cdots O \) interactions involving atom H14 form molecular dimers (Fig. 2), which are further stabilized by \( C-H \cdots \pi \) interactions, where \( Cg1 \) in Table 2 is the centroid of the five-membered indole ring. Such dimers [Etter's graph set symbol \( R_2^1(16); \) Bernstein et al., 1995] are held further by \( C-H \cdots O \) interactions involving atom H13, forming zigzag double chains along the \( b \) axis along with a tetrameric molecular motif \( [R_2^1(10)] \). 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**

\[
\begin{align*}
C_{14}H_{14}ClNO & ; \quad D = 2.153 \text{ Mg m}^{-3} \\
M_r & = 287.77 \\
\sigma & = 0.236 (5) \text{ Å} \\
b & = 9.003 (6) \text{ Å} \\
c & = 10.781 (7) \text{ Å} \\
\beta & = 82.203 (10) \\
\gamma & = 7.584 (11) \\
V & = 762.6 (8) \text{ Å}^3
\end{align*}
\]

**Data collection**

Bruker SMART CCD area-detector diffractometer

2955 independent reflections

2511 reflections with \( I > 2 \sigma(I) \)

\( R_{	ext{int}} = 0.015 \)

Absorption correction: multi-scan

\( h = -9 \rightarrow +9 \)

\( k = -11 \rightarrow +11 \)

6193 measured reflections

\( l = -13 \rightarrow +13 \)

**Refinement**

Refinement on \( F^2 \)

\( wR(F^2) = 0.042 \)

\( S = 1.04 \)

2955 reflections

233 parameters

All H-atoms parameters refined

**Table 1**

Selected geometric parameters (Å, °).

<p>| | | | | |</p>
<table>
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<tr>
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<tbody>
<tr>
<td>C1–C12</td>
<td>1.7372 (18)</td>
<td>N1–C1</td>
<td>1.397 (2)</td>
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<tr>
<td>O1–C3</td>
<td>1.2244 (19)</td>
<td>N1–C9</td>
<td>1.4316 (19)</td>
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<tr>
<td>C9–N1–C7–C8</td>
<td>178.09 (13)</td>
<td>C4–C5–C6–C7</td>
<td>-47.34 (18)</td>
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<tr>
<td>C7–N1–C9–C14</td>
<td>-70.9 (2)</td>
<td>C7–N1–C1–C15</td>
<td>177.81 (16)</td>
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<tr>
<td>C1–N1–C9–C10</td>
<td>-71.2 (2)</td>
<td>C7–O1–C1–C4</td>
<td>1.79 (19)</td>
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<tr>
<td>O6–C7–C8–C3</td>
<td>1.5 (2)</td>
<td>C5–O4–C3–C1–O1</td>
<td>151.94 (14)</td>
<td></td>
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<tr>
<td>C3–C4–C5–C6</td>
<td>53.77 (18)</td>
<td>C5–C4–C3–C8</td>
<td>-30.52 (18)</td>
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<tr>
<td>C8–C7–C6–C5</td>
<td>22.9 (2)</td>
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**Table 2**

Hydrogen-bond geometry (Å, °).

<table>
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<th>D–H–A</th>
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<th>H–A</th>
<th>D–A</th>
<th>D–H–A</th>
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</thead>
<tbody>
<tr>
<td>C14–H14–O11'</td>
<td>0.92 (2)</td>
<td>2.47 (2)</td>
<td>3.379 (3)</td>
<td>170 (2)</td>
</tr>
<tr>
<td>C13–H13–O1'</td>
<td>0.94 (2)</td>
<td>2.38 (2)</td>
<td>3.04 (2)</td>
<td>171 (2)</td>
</tr>
<tr>
<td>C4–H4A–C111'</td>
<td>0.97 (2)</td>
<td>2.65 (2)</td>
<td>3.589 (3)</td>
<td>163 (1)</td>
</tr>
</tbody>
</table>

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

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: SHEL97 (Altomare et al., 1993); program(s) used to refine structure: SHELX97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin et al., 2001).
We thank the Department of Science and Technology, India, for data collection on the CCD facility at IISc, Bangalore, under the IRHPA-DST program. DC acknowledges CSIR, India, for a junior research fellowship.

References
