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4-(4-Chlorophenyl)-8-methyl-2-oxo-1,2,5,6,7,8-hexahydroquinoline-3-carbonitrile

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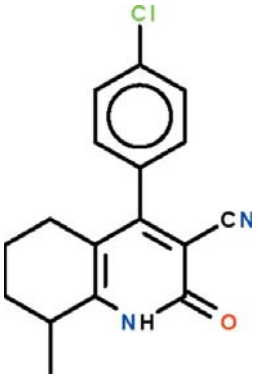
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.065; wR factor = 0.187; data-to-parameter ratio = 15.5.

The six-membered *N*-heterocyclic ring of the title compound, $C_{17}H_{15}ClN_2O$, is fused with a methyl-substituted cyclohexene ring. The approximately planar nitrogen-bearing ring (r.m.s. deviation 0.019 Å) is aromatic, and the N atom shows a trigonal–planar coordination; its benzene substituent is aligned at 77.1 (1) °. The cyclohexene ring adopts a half-chair conformation. In the crystal, inversion-related molecules are linked by pairs of N—H···O hydrogen bonds, generating dimers.

Related literature

For a related compound, see: Asiri *et al.* (2011).



Experimental

Crystal data

$C_{17}H_{15}ClN_2O$
M_r = 298.76
Monoclinic, $C2/c$
a = 18.6304 (4) Å
b = 18.7399 (4) Å
c = 8.5209 (2) Å
β = 90.229 (2)°
V = 2974.89 (11) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 2.27 mm^{-1}
T = 100 K
0.30 × 0.03 × 0.03 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.550, T_{max} = 0.935
10387 measured reflections
3014 independent reflections
2682 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.187
S = 1.03
3014 reflections
194 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.91 (4)	1.84 (4)	2.744 (3)	174 (4)

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5320).

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