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

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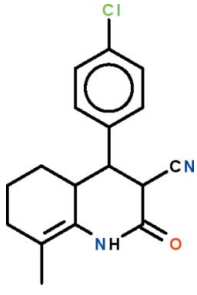
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.079; wR factor = 0.273; data-to-parameter ratio = 30.9.

The six-membered *N*-heterocyclic ring of title compound, $C_{17}H_{17}ClN_2O$, is fused with a methyl-substituted cyclohexene ring. The nitrogen-bearing ring has an envelope conformation with the benzene ring-bearing C atom lying 0.432 (6) Å out of the plane defined by the other five atoms (r.m.s. deviation 0.011 Å); its benzene substituent is aligned at 84.7 (1)° to the latter plane. The cyclohexene ring adopts a half-chair conformation. In the crystal, two molecules are linked about a center of inversion by pairs of N–H···O hydrogen bonds, generating dimers. An ethylene portion is disordered over two orientations in a 1:1 ratio. The crystal studied was a non-merohedral twin with a 15.3 (1)% minor component.

Related literature

For a similar compound that has two more H atoms, see: Asiri *et al.* (2011).



Experimental

Crystal data

$C_{17}H_{17}ClN_2O$
M_r = 300.78
Monoclinic, $P2_1/c$
a = 11.0699 (7) Å
b = 7.6018 (3) Å
c = 18.2247 (9) Å
β = 100.505 (6)°
V = 1507.92 (13) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.24 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.554, T_{max} = 0.896
25955 measured reflections
6143 independent reflections
3143 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.273
S = 1.10
6140 reflections
199 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 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}	0.88	2.07	2.923 (3)	162

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: XU5321).

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