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## Structure Reports

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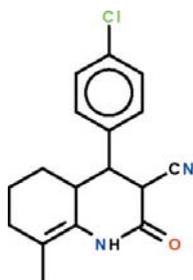
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å; disorder in main residue;  $R$  factor = 0.079;  $wR$  factor = 0.273; data-to-parameter ratio = 30.9.

The six-membered  $N$ -heterocyclic ring of title compound,  $\text{C}_{17}\text{H}_{17}\text{ClN}_2\text{O}$ , 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  $\text{N}-\text{H}\cdots\text{O}$  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

$\text{C}_{17}\text{H}_{17}\text{ClN}_2\text{O}$   
 $M_r = 300.78$   
Monoclinic,  $P2_1/c$   
 $a = 11.0699$  (7) Å  
 $b = 7.6018$  (3) Å  
 $c = 18.2247$  (9) Å  
 $\beta = 100.505$  (6)°  
 $V = 1507.92$  (13) Å<sup>3</sup>  
 $Z = 4$   
Cu  $K\alpha$  radiation  
 $\mu = 2.24$  mm<sup>-1</sup>  
 $T = 100$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$

## 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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.46$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	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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