

## 1-Acetyl-2-phenylperhydroquinolin-4-yl acetate

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The piperidine and cyclohexane rings in the title compound, C<sub>19</sub>H<sub>25</sub>NO<sub>3</sub>, are *trans*-fused and adopt boat and chair conformations, respectively. The phenyl and ester substituents are oriented axially with respect to the decahydroquinoline moiety. The N atom of the piperidine ring exists in a planar configuration. The keto O atom of the ester group exhibits positional disorder, with an 80:20 population ratio. The crystal structure is stabilized by C—H···O hydrogen bonds.

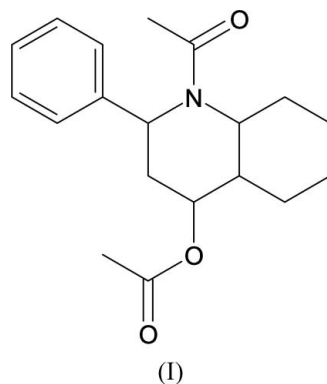
## Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma$ (C—C) = 0.002 Å  
Disorder in main residue  
R factor = 0.049  
wR factor = 0.154  
Data-to-parameter ratio = 18.4

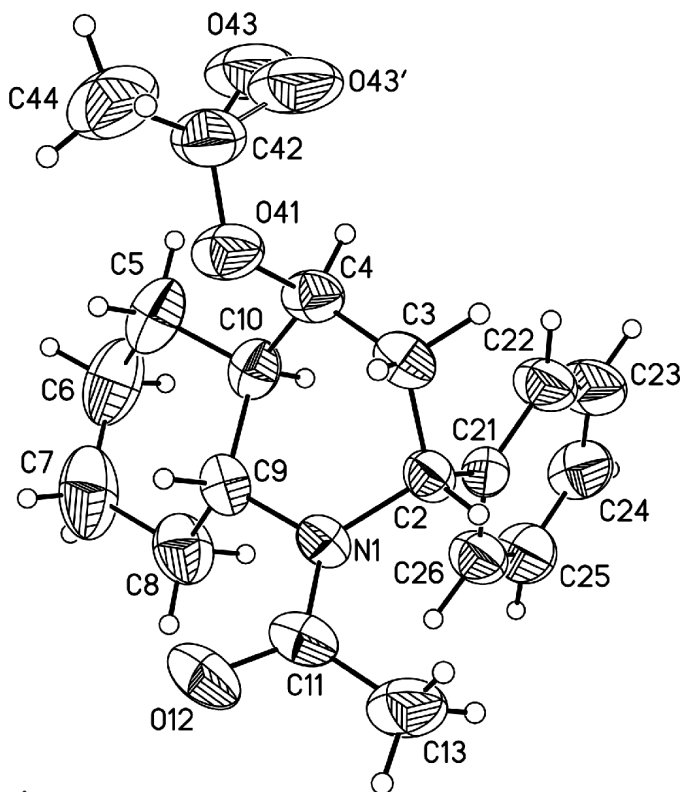
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Comment

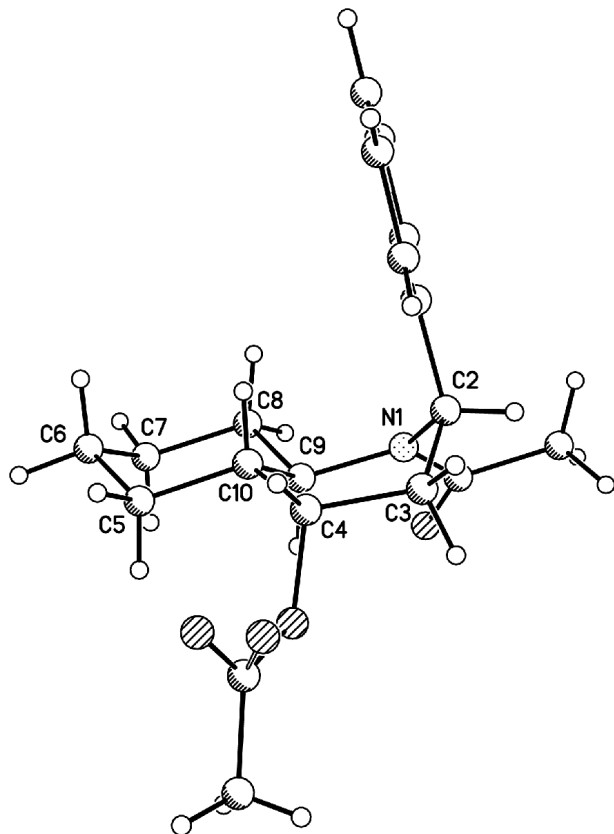
Decahydroquinolines are bicyclic systems consisting of a piperidine ring fused to a cyclohexane ring. The stereochemistry of decahydroquinolines is of interest as they occur in many alkaloids, such as lupinine, reserpine and yohimbine (Nasipuri, 1992). In decahydroquinolines, the cyclohexane ring has a preferred chair conformation, whereas the piperidine ring adopts a range of conformations, such as chair, twist or boat, depending upon the size and position of the substituents attached to the ring. The substitution of a methyl or nitroso group at the N-atom position has a large influence on the conformation of the ring (Vierhapper, 1980; Baliah & Natarajan, 1989). Literature references show that decahydroquinoline derivatives exist with both *cis*- and *trans*-fused ring systems (Le Coz *et al.*, 1990; Nierlich *et al.*, 1991; Nogue *et al.*, 1996; Ganesh *et al.*, 1996; Thiruvalluvar *et al.*, 1997; Paugam *et al.*, 2000). Our study aims to investigate the nature of the ring fusion, the orientation of the substituents and their influence on the conformation of the piperidine ring. We present here the crystal structure of the title compound, (I) (Fig. 1).



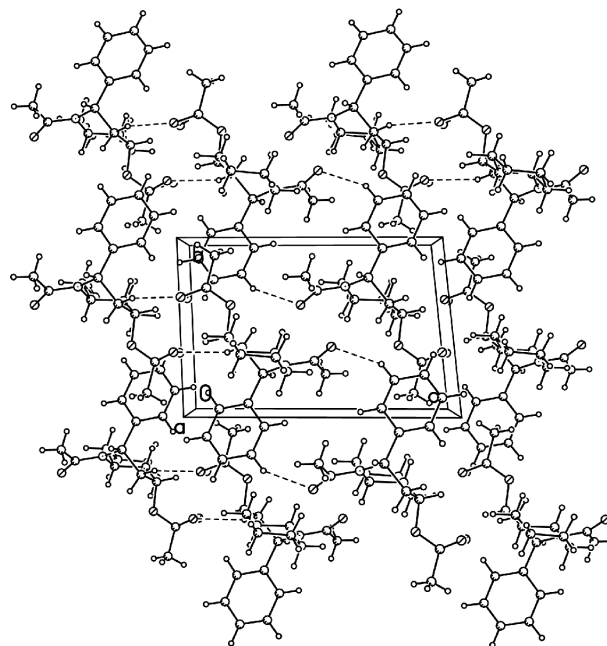
One of the O atoms present in the ester group, O43, shows positional disorder, with an 80:20 population ratio. All the bond lengths and angles in this compound have values in agreement with other decahydroquinoline derivative structures.



**Figure 1**  
A plot of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Both disorder components of O43 are shown.



**Figure 2**  
A perspective view of the molecule of (I), showing the chair and boat conformations of the fused rings.



**Figure 3**  
The packing of the molecules of (I), viewed down the *b* axis. Dashed lines indicate C—H...O hydrogen bonds.

The piperidine and cyclohexane rings of the decahydroquinoline moiety of (I) adopt a *trans*-fused geometry, with an H9—C9—C10—H10 torsion angle of 173 (1)°. The substituents at the N atom of the piperidine ring can yield either planar or pyramidal configurations (Ganesh *et al.*, 1996; Thiruvalluvar *et al.*, 1997; Paugam *et al.*, 2000). The N atom of (I) has a planar configuration; relevant bond lengths and angles are given in Table 1.

Both the phenyl and the ester substituents at C2 and C4 are axial, with the relevant torsion angles listed in Table 1. While the cyclohexane ring exists in a chair conformation, the piperidine ring adopts a boat conformation. Fig. 2 gives a clear picture of the conformations of both rings.

The crystal structure of (I) is stabilized by C—H...O hydrogen bonds involving both keto O atoms, O12 and O43 (Table 2), and by van der Waals interactions

### Experimental

The title compound was prepared according to the procedure of Baliah *et al.* (1978). The white precipitate which was obtained was filtered and recrystallized from ethanol.

#### Crystal data

C<sub>19</sub>H<sub>25</sub>NO<sub>3</sub>  
*M<sub>r</sub>* = 315.40  
 Triclinic, *P* $\bar{1}$   
*a* = 8.856 (1) Å  
*b* = 9.050 (2) Å  
*c* = 12.343 (1) Å  
 $\alpha$  = 85.35 (1)°  
 $\beta$  = 87.82 (1)°  
 $\gamma$  = 64.82 (1)°  
*V* = 892.3 (2) Å<sup>3</sup>

*Z* = 2  
*D<sub>x</sub>* = 1.174 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 25 reflections  
 $\theta$  = 10–20°  
 $\mu$  = 0.08 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Prism, colourless  
 0.42 × 0.38 × 0.30 mm

## Data collection

Enraf-Nonius CAD-4 diffractometer	$\theta_{\max} = 27.5^\circ$
$\omega/2\theta$ scans	$h = -1 \rightarrow 11$
Absorption correction: none	$k = -11 \rightarrow 11$
4839 measured reflections	$l = -16 \rightarrow 16$
4056 independent reflections	2 standard reflections
2925 reflections with $I > 2\sigma(I)$	every 100 reflections
$R_{\text{int}} = 0.013$	intensity decay: 1%

## Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 0.0334P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.154$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.11$	$\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$
4056 reflections	$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$
221 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

N1—C11	1.3565 (17)	N1—C9	1.4827 (18)
N1—C2	1.4707 (16)		
C11—N1—C2	122.98 (12)	C2—N1—C9	117.65 (10)
C11—N1—C9	116.86 (11)		
C9—N1—C2—C3	50.78 (14)	C2—C3—C4—C10	11.68 (15)
C9—N1—C2—C21	-79.08 (14)	C2—N1—C9—C10	1.57 (15)
N1—C2—C3—C4	-57.53 (13)	O41—C4—C10—C9	-76.41 (14)
C21—C2—C3—C4	70.23 (15)	C3—C4—C10—C9	42.14 (15)
C2—C3—C4—O41	131.39 (12)	C8—C9—C10—C4	-173.21 (12)

Table 2

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C3—H3B $\cdots$ O43 <sup>i</sup>	0.97	2.59	3.521 (3)	161
C3—H3B $\cdots$ O43 <sup>i</sup>	0.97	2.56	3.403 (11)	146
C25—H25 $\cdots$ O12 <sup>ii</sup>	0.93	2.50	3.322 (2)	148
C3—H3A $\cdots$ O12 <sup>iii</sup>	0.97	2.63	3.5340 (18)	155
C13—H13C $\cdots$ O12 <sup>iii</sup>	0.96	2.78	3.475 (2)	130

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

The disorder in atom O43 was observed during refinement as a very large displacement ellipsoid. The position was split into two, and their occupancies were initially refined and later fixed at 80:20. The disordered atoms were given the same displacement parameters. The H atoms were located in difference Fourier maps. The positions of atoms H9 and H10, which are attached to atoms C9 and C10, were refined. All other H atoms were made to ride on their respective C atoms, with C—H distances in the range 0.93–0.98  $\text{\AA}$  and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ , or  $1.5U_{\text{eq}}(\text{C})$  for methyl atoms.

Data collection: *CAD-4 EXPRESS* (Enraf-Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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