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1,*t*-3-Dimethyl-*r*-2,*c*-6-diphenylpiperidin-*c*-4-yl acetate

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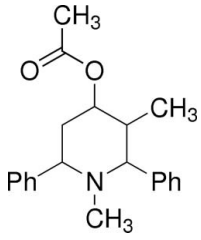
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.066; wR factor = 0.244; data-to-parameter ratio = 27.8.

The piperidine ring of the title molecule, $C_{21}H_{25}NO_2$, is in the chair form. The dihedral angle between the two phenyl rings is 46.1 (1)°. All the substituents of the central ring have equatorial orientations. The crystal packing is stabilized by C—H···O intermolecular interactions.

Related literature

For related crystal structure, see: Balamurugan *et al.* (2007). For application of piperidines, see: Jayabharathi *et al.* (2007). For the NMR characterization of the title compound, see: Nanjappan *et al.* (1983).



Experimental

Crystal data

$C_{21}H_{25}NO_2$
M_r = 323.42
Monoclinic, $P2_1/c$
a = 14.4091 (5) Å
b = 12.8347 (4) Å
c = 10.1715 (4) Å
β = 99.584 (4)°
V = 1854.83 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 200 (2) K
0.46 × 0.41 × 0.33 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.887, T_{max} = 1.000 (expected range = 0.866–0.976)
17595 measured reflections
6096 independent reflections
2679 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.244
S = 1.16
6096 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15D···O14^{i}	0.98	2.58	3.546 (3)	170
C65—H65···O14^{ii}	0.95	2.59	3.460 (3)	152

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer. AT thanks the UGC, India, for the award of a Minor Research Project [File No. MRP-2355/06(UGC-SERO), Link No. 2355, 10/01/2007].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2640).

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supplementary materials

Acta Cryst. (2007). E**63**, o4826 [**doi:10.1107/S1600536807058849**]

1,*t*-3-Dimethyl-*r*-2,*c*-6-diphenylpiperidin-*c*-4-yl acetate

S. Balamurugan, A. Thiruvalluvar, R. J. Butcher, A. Manimekalai and J. Jayabharathi

Comment

Jayabharathi *et al.* (2007) have reported the synthesis, stereochemistry and antimicrobial evaluation of t3-benzyl-r2,c6-diarylpiperidin- 4-one and its derivatives. Balamurugan *et al.* (2007) have reported a crystal structure of t3,t5-Dimethyl-r2,c-6-diphenylpiperidin-4-one in which the piperidine ring is in chair form. Nanjappan *et al.*, 1983, have reported the NMR characterization of the title compound, (I).

The piperidine ring of (I) (Fig. 1), is in chair form. The dihedral angle between the two phenyl rings is 46.1 (1)°. The methyl groups at 1 and 3, the phenyl rings at 2 and 6 and the methyl acetate group at the 4 position all have equatorial orientations. The packing is stabilized by C—H···O intermolecular interactions (Table 1).

Experimental

A mixture of piperidin-4-ol (10 mmol, 2.64 g), acetic anhydride (30 mmol, 2.84 ml) and triethylamine (30 mmol, 4.18 ml) in dry benzene (50 ml) was refluxed for 6–8 h to afford the corresponding acetate. The reaction mixture was washed with sodium bicarbonate (10%) followed by water and then solvent was removed at low temperature. The residue was recrystallized from distilled ethanol to yield colourless prisms of (I). The yield of the isolated product was 2.50 g.

Refinement

The H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.95–1.00 Å and U_{iso} = 1.2 to 1.5U_{eq}(C). The H atoms of the acetoxy methyl group are disordered over two positions.

Figures

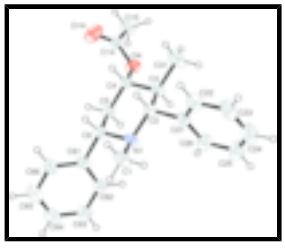

Fig. 1. The molecular structure of (I) with 30% probability displacement ellipsoids. H atoms are shown shown as spheres of arbitrary radius.

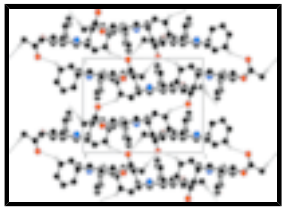

Fig. 2. The molecular packing of (I), viewed down the *a* axis showing the C—H···O (dashed lines) hydrogen bonds.

1,t-3-Dimethyl-r-2,c-6-diphenylpiperidin-c-4-yl acetate

Crystal data

$C_{21}H_{25}NO_2$	F_{000} = 696
M_r = 323.42	D_x = 1.158 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 417.5 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.4091 (5) Å	Cell parameters from 4918 reflections
b = 12.8347 (4) Å	θ = 4.7–32.4º
c = 10.1715 (4) Å	μ = 0.07 mm^{-1}
β = 99.584 (4)º	T = 200 (2) K
V = 1854.83 (12) Å^3	Prism, colourless
Z = 4	0.46 × 0.41 × 0.33 mm

Data collection

Oxford Diffraction Gemini diffractometer	6096 independent reflections
Radiation source: fine-focus sealed tube	2679 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 200(2) K	θ_{max} = 32.4º
φ and ω scans	θ_{min} = 4.7º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	h = −21→21
T_{min} = 0.887, T_{max} = 1.000	k = −18→18
17595 measured reflections	l = −14→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.066	H-atom parameters constrained
$wR(F^2)$ = 0.244	$w = 1/[\sigma^2(F_o^2) + (0.1131P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.16	$(\Delta/\sigma)_{max}$ = <0.001
6096 reflections	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
219 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O4	0.32202 (9)	0.16159 (9)	0.28687 (11)	0.0581 (4)	
O14	0.40523 (13)	0.12506 (13)	0.48554 (14)	0.0921 (7)	
N1	0.17919 (9)	0.44697 (10)	0.30565 (13)	0.0475 (4)	
C1	0.13618 (14)	0.53586 (15)	0.3646 (2)	0.0755 (8)	
C2	0.13055 (11)	0.34956 (12)	0.33244 (15)	0.0455 (5)	
C3	0.17600 (12)	0.25368 (12)	0.27927 (17)	0.0497 (5)	
C4	0.27921 (12)	0.25084 (12)	0.34094 (16)	0.0481 (5)	
C5	0.32762 (12)	0.34910 (13)	0.30930 (17)	0.0507 (5)	
C6	0.28042 (11)	0.44450 (12)	0.35972 (15)	0.0460 (5)	
C14	0.38088 (12)	0.10260 (13)	0.37059 (18)	0.0547 (6)	
C15	0.41314 (15)	0.00998 (15)	0.3039 (2)	0.0700 (7)	
C21	0.02718 (12)	0.35535 (13)	0.27306 (17)	0.0514 (5)	
C22	−0.04151 (14)	0.33077 (16)	0.3474 (2)	0.0657 (7)	
C23	−0.13596 (15)	0.33014 (19)	0.2895 (3)	0.0831 (9)	
C24	−0.16096 (16)	0.3535 (2)	0.1571 (3)	0.0887 (10)	
C25	−0.09400 (16)	0.3800 (2)	0.0813 (2)	0.0833 (9)	
C26	−0.00075 (14)	0.38055 (17)	0.13943 (19)	0.0679 (7)	
C31	0.12658 (17)	0.15319 (16)	0.3069 (3)	0.0859 (9)	
C61	0.32906 (11)	0.54246 (13)	0.32239 (16)	0.0495 (5)	
C62	0.31558 (13)	0.57689 (16)	0.19171 (18)	0.0635 (6)	
C63	0.36139 (16)	0.66412 (17)	0.1563 (2)	0.0755 (8)	
C64	0.42193 (15)	0.71767 (16)	0.2499 (3)	0.0725 (8)	
C65	0.43677 (16)	0.68523 (18)	0.3786 (2)	0.0793 (8)	
C66	0.39077 (14)	0.59724 (16)	0.41530 (19)	0.0675 (7)	
H1A	0.16658	0.60060	0.34337	0.1132*	
H1B	0.14449	0.52725	0.46159	0.1132*	
H1C	0.06887	0.53888	0.32809	0.1132*	
H2	0.13573	0.34185	0.43122	0.0546*	
H3	0.17142	0.26135	0.18056	0.0596*	
H4	0.28518	0.24319	0.43983	0.0576*	
H5A	0.32507	0.35465	0.21169	0.0608*	
H5B	0.39460	0.34670	0.35176	0.0608*	
H6	0.28822	0.44051	0.45914	0.0552*	
H15A	0.38309	0.00912	0.21010	0.1049*	0.500

H15B	0.39605	−0.05334	0.34812	0.1049*	0.500
H15C	0.48164	0.01289	0.30937	0.1049*	0.500
H15D	0.45743	−0.03001	0.36829	0.1049*	0.500
H15E	0.44447	0.03245	0.23027	0.1049*	0.500
H15F	0.35887	−0.03378	0.26903	0.1049*	0.500
H22	−0.02411	0.31409	0.43924	0.0788*	
H23	−0.18290	0.31359	0.34162	0.0998*	
H24	−0.22538	0.35132	0.11704	0.1062*	
H25	−0.11192	0.39779	−0.01007	0.1000*	
H26	0.04565	0.39854	0.08706	0.0815*	
H31A	0.15747	0.09400	0.27127	0.1290*	
H31B	0.06051	0.15625	0.26391	0.1290*	
H31C	0.12993	0.14462	0.40332	0.1290*	
H62	0.27415	0.53987	0.12545	0.0762*	
H63	0.35079	0.68712	0.06627	0.0906*	
H64	0.45362	0.77756	0.22498	0.0869*	
H65	0.47866	0.72268	0.44389	0.0951*	
H66	0.40206	0.57466	0.50550	0.0810*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0702 (8)	0.0458 (7)	0.0578 (7)	0.0185 (6)	0.0092 (6)	−0.0004 (5)
O14	0.1109 (13)	0.0877 (12)	0.0712 (9)	0.0419 (10)	−0.0041 (9)	−0.0010 (8)
N1	0.0431 (7)	0.0340 (7)	0.0665 (8)	0.0016 (5)	0.0124 (6)	−0.0016 (6)
C1	0.0684 (12)	0.0419 (10)	0.1217 (17)	0.0023 (9)	0.0322 (12)	−0.0159 (11)
C2	0.0490 (9)	0.0385 (9)	0.0506 (8)	−0.0008 (7)	0.0130 (7)	0.0000 (6)
C3	0.0556 (9)	0.0350 (8)	0.0597 (9)	0.0037 (7)	0.0130 (8)	−0.0015 (7)
C4	0.0567 (9)	0.0356 (8)	0.0523 (9)	0.0093 (7)	0.0102 (7)	0.0011 (6)
C5	0.0454 (8)	0.0442 (9)	0.0614 (10)	0.0057 (7)	0.0059 (7)	−0.0011 (7)
C6	0.0469 (8)	0.0402 (9)	0.0507 (8)	0.0033 (7)	0.0077 (7)	−0.0025 (7)
C14	0.0588 (10)	0.0396 (9)	0.0656 (11)	0.0075 (8)	0.0103 (8)	0.0050 (8)
C15	0.0735 (12)	0.0412 (10)	0.0952 (13)	0.0082 (9)	0.0142 (10)	−0.0011 (10)
C21	0.0490 (9)	0.0444 (9)	0.0619 (10)	0.0005 (7)	0.0124 (8)	−0.0050 (7)
C22	0.0600 (11)	0.0612 (12)	0.0799 (12)	0.0008 (9)	0.0231 (10)	−0.0045 (9)
C23	0.0538 (11)	0.0769 (15)	0.124 (2)	−0.0102 (10)	0.0305 (13)	−0.0149 (14)
C24	0.0553 (12)	0.0796 (17)	0.125 (2)	0.0042 (11)	−0.0028 (14)	−0.0324 (14)
C25	0.0707 (14)	0.0895 (17)	0.0851 (14)	0.0139 (12)	−0.0008 (12)	−0.0152 (12)
C26	0.0603 (11)	0.0718 (13)	0.0720 (12)	0.0079 (10)	0.0123 (9)	−0.0036 (10)
C31	0.0740 (14)	0.0439 (12)	0.145 (2)	−0.0015 (10)	0.0337 (14)	−0.0047 (12)
C61	0.0481 (8)	0.0397 (9)	0.0624 (9)	0.0016 (7)	0.0140 (7)	−0.0032 (7)
C62	0.0582 (10)	0.0624 (12)	0.0654 (10)	−0.0073 (9)	−0.0029 (9)	0.0090 (9)
C63	0.0738 (13)	0.0670 (14)	0.0855 (14)	−0.0088 (11)	0.0125 (11)	0.0197 (11)
C64	0.0672 (12)	0.0449 (11)	0.1109 (17)	−0.0047 (9)	0.0312 (12)	−0.0009 (11)
C65	0.0797 (14)	0.0655 (14)	0.0944 (15)	−0.0220 (11)	0.0197 (12)	−0.0245 (12)
C66	0.0762 (13)	0.0608 (12)	0.0650 (11)	−0.0137 (10)	0.0101 (10)	−0.0140 (9)

Geometric parameters (Å, °)

O4—C4	1.452 (2)	C1—H1B	0.9800
O4—C14	1.333 (2)	C1—H1C	0.9800
O14—C14	1.199 (2)	C2—H2	1.0000
N1—C1	1.473 (2)	C3—H3	1.0000
N1—C2	1.481 (2)	C4—H4	1.0000
N1—C6	1.471 (2)	C5—H5A	0.9900
C2—C3	1.534 (2)	C5—H5B	0.9900
C2—C21	1.513 (2)	C6—H6	1.0000
C3—C4	1.515 (2)	C15—H15A	0.9800
C3—C31	1.522 (3)	C15—H15B	0.9800
C4—C5	1.502 (2)	C15—H15C	0.9800
C5—C6	1.530 (2)	C15—H15D	0.9800
C6—C61	1.518 (2)	C15—H15E	0.9800
C14—C15	1.481 (3)	C15—H15F	0.9800
C21—C22	1.379 (3)	C22—H22	0.9500
C21—C26	1.390 (3)	C23—H23	0.9500
C22—C23	1.390 (3)	C24—H24	0.9500
C23—C24	1.368 (4)	C25—H25	0.9500
C24—C25	1.374 (3)	C26—H26	0.9500
C25—C26	1.375 (3)	C31—H31A	0.9800
C61—C62	1.383 (2)	C31—H31B	0.9800
C61—C66	1.378 (3)	C31—H31C	0.9800
C62—C63	1.378 (3)	C62—H62	0.9500
C63—C64	1.365 (3)	C63—H63	0.9500
C64—C65	1.356 (4)	C64—H64	0.9500
C65—C66	1.392 (3)	C65—H65	0.9500
C1—H1A	0.9800	C66—H66	0.9500
C4—O4—C14	118.12 (13)	C6—C5—H5A	110.00
C1—N1—C2	109.57 (13)	C6—C5—H5B	110.00
C1—N1—C6	108.83 (13)	H5A—C5—H5B	108.00
C2—N1—C6	112.54 (12)	N1—C6—H6	108.00
N1—C2—C3	111.69 (13)	C5—C6—H6	108.00
N1—C2—C21	110.47 (13)	C61—C6—H6	108.00
C3—C2—C21	110.38 (13)	C14—C15—H15A	109.00
C2—C3—C4	108.69 (13)	C14—C15—H15B	109.00
C2—C3—C31	111.99 (16)	C14—C15—H15C	109.00
C4—C3—C31	111.12 (15)	C14—C15—H15D	109.00
O4—C4—C3	108.17 (13)	C14—C15—H15E	109.00
O4—C4—C5	109.85 (14)	C14—C15—H15F	109.00
C3—C4—C5	110.49 (13)	H15A—C15—H15B	109.00
C4—C5—C6	110.61 (14)	H15A—C15—H15C	109.00
N1—C6—C5	111.12 (13)	H15A—C15—H15D	141.00
N1—C6—C61	111.04 (13)	H15A—C15—H15E	56.00
C5—C6—C61	109.24 (13)	H15A—C15—H15F	56.00
O4—C14—O14	122.57 (17)	H15B—C15—H15C	109.00
O4—C14—C15	112.21 (15)	H15B—C15—H15D	56.00

O14—C14—C15	125.20 (18)	H15B—C15—H15E	141.00
C2—C21—C22	121.25 (16)	H15B—C15—H15F	56.00
C2—C21—C26	120.49 (16)	H15C—C15—H15D	56.00
C22—C21—C26	118.18 (17)	H15C—C15—H15E	56.00
C21—C22—C23	120.7 (2)	H15C—C15—H15F	141.00
C22—C23—C24	119.6 (2)	H15D—C15—H15E	109.00
C23—C24—C25	120.8 (2)	H15D—C15—H15F	109.00
C24—C25—C26	119.2 (2)	H15E—C15—H15F	109.00
C21—C26—C25	121.50 (18)	C21—C22—H22	120.00
C6—C61—C62	120.53 (15)	C23—C22—H22	120.00
C6—C61—C66	121.55 (15)	C22—C23—H23	120.00
C62—C61—C66	117.86 (16)	C24—C23—H23	120.00
C61—C62—C63	120.93 (17)	C23—C24—H24	120.00
C62—C63—C64	120.4 (2)	C25—C24—H24	120.00
C63—C64—C65	119.9 (2)	C24—C25—H25	120.00
C64—C65—C66	120.2 (2)	C26—C25—H25	120.00
C61—C66—C65	120.80 (18)	C21—C26—H26	119.00
N1—C1—H1A	109.00	C25—C26—H26	119.00
N1—C1—H1B	109.00	C3—C31—H31A	109.00
N1—C1—H1C	109.00	C3—C31—H31B	109.00
H1A—C1—H1B	109.00	C3—C31—H31C	109.00
H1A—C1—H1C	109.00	H31A—C31—H31B	109.00
H1B—C1—H1C	109.00	H31A—C31—H31C	109.00
N1—C2—H2	108.00	H31B—C31—H31C	109.00
C3—C2—H2	108.00	C61—C62—H62	120.00
C21—C2—H2	108.00	C63—C62—H62	120.00
C2—C3—H3	108.00	C62—C63—H63	120.00
C4—C3—H3	108.00	C64—C63—H63	120.00
C31—C3—H3	108.00	C63—C64—H64	120.00
O4—C4—H4	109.00	C65—C64—H64	120.00
C3—C4—H4	109.00	C64—C65—H65	120.00
C5—C4—H4	109.00	C66—C65—H65	120.00
C4—C5—H5A	110.00	C61—C66—H66	120.00
C4—C5—H5B	110.00	C65—C66—H66	120.00
C14—O4—C4—C3	−136.45 (15)	O4—C4—C5—C6	177.30 (13)
C14—O4—C4—C5	102.88 (16)	C3—C4—C5—C6	58.04 (17)
C4—O4—C14—O14	−6.1 (3)	C4—C5—C6—N1	−55.41 (17)
C4—O4—C14—C15	175.42 (15)	C4—C5—C6—C61	−178.26 (13)
C1—N1—C2—C3	−177.06 (14)	N1—C6—C61—C62	−49.7 (2)
C1—N1—C2—C21	59.67 (17)	N1—C6—C61—C66	133.17 (17)
C6—N1—C2—C3	−55.83 (16)	C5—C6—C61—C62	73.23 (19)
C6—N1—C2—C21	−179.10 (12)	C5—C6—C61—C66	−103.94 (18)
C1—N1—C6—C5	176.04 (13)	C2—C21—C22—C23	−175.99 (18)
C1—N1—C6—C61	−62.16 (16)	C26—C21—C22—C23	0.7 (3)
C2—N1—C6—C5	54.38 (16)	C2—C21—C26—C25	175.93 (19)
C2—N1—C6—C61	176.19 (12)	C22—C21—C26—C25	−0.8 (3)
N1—C2—C3—C4	56.64 (17)	C21—C22—C23—C24	0.4 (3)
N1—C2—C3—C31	179.79 (16)	C22—C23—C24—C25	−1.6 (4)
C21—C2—C3—C4	179.96 (12)	C23—C24—C25—C26	1.5 (4)

C21—C2—C3—C31	−56.9 (2)	C24—C25—C26—C21	−0.3 (4)
N1—C2—C21—C22	−130.29 (17)	C6—C61—C62—C63	−178.25 (18)
N1—C2—C21—C26	53.1 (2)	C66—C61—C62—C63	−1.0 (3)
C3—C2—C21—C22	105.69 (18)	C6—C61—C66—C65	178.18 (18)
C3—C2—C21—C26	−71.0 (2)	C62—C61—C66—C65	0.9 (3)
C2—C3—C4—O4	−178.33 (12)	C61—C62—C63—C64	0.7 (3)
C2—C3—C4—C5	−58.06 (17)	C62—C63—C64—C65	−0.3 (3)
C31—C3—C4—O4	58.00 (19)	C63—C64—C65—C66	0.3 (3)
C31—C3—C4—C5	178.27 (16)	C64—C65—C66—C61	−0.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15D···O14^{i}	0.98	2.58	3.546 (3)	170
C65—H65···O14^{ii}	0.95	2.59	3.460 (3)	152

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.

Fig. 1

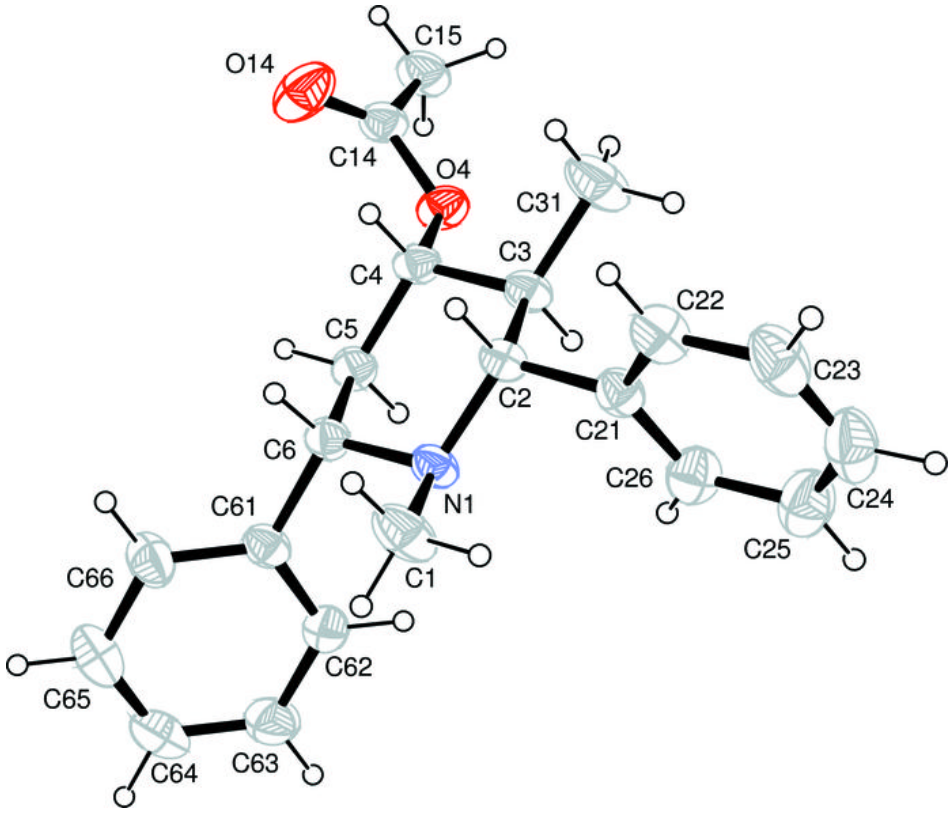
C15
O14
C14
O4
C31
C3
C4
C22
C5
C23
C2
C21
C6
C26
N1
C24
C61
C25
C1
C66
C62
C65
C64
C63

Fig. 2