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# *t*-3,*t*-5-Dimethyl-*r*-2,*c*-6-diphenylpiperidin-4-one

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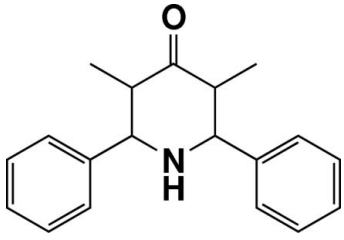
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.043; $wR$ factor = 0.127; data-to-parameter ratio = 18.6.

In the title molecule, $C_{19}H_{21}NO$, the piperidine ring adopts a chair conformation. Two phenyl rings and two methyl groups, attached to the piperidine ring at positions 2, 6, 3 and 5, respectively, occupy equatorial positions. The dihedral angle between the two phenyl rings is 57.1 (1)°. Molecules are linked by N—H···O hydrogen bonds.

## Related literature

For related literature, see: Noller & Baliah (1948); Hasan *et al.* (1985); Balamurugan *et al.* (2006, 2007); Thiruvalluvar, Balamurugan, Jayabharathi, Manimekalai & Rajarajan (2007); Thiruvalluvar, Balamurugan, Jayabharathi & Manimekalai (2007).




## Experimental

### *Crystal data*

$C_{19}H_{21}NO$
$M_r$ = 279.37
Triclinic, $P\overline{1}$
$a$ = 7.1392 (3) Å
$b$ = 10.5811 (5) Å
$c$ = 11.6276 (5) Å
$\alpha$ = 102.320 (2)°
$\beta$ = 107.613 (2)°
$\gamma$ = 101.735 (2)°
$V$ = 783.31 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 298 (2) K
0.30 × 0.22 × 0.18 mm

### *Data collection*

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.854, $T_{max}$ = 0.987
17560 measured reflections
3606 independent reflections
2507 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
$S$ = 1.05
3606 reflections
194 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O4$^{i}$ | 0.90 (2) | 2.43 (2) | 3.3109 (17) | 170.2 (15) |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT-NT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2193).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o3504 [ **doi:10.1107/S1600536807034010** ]

# *t*-3,*t*-5-Dimethyl-*r*-2,*c*-6-diphenylpiperidin-4-one

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## Comment

The conformation of the title compound was established by NMR spectroscopy by Hasan *et al.* (1985). Crystal structures of di-2-furylpiperidin-4-one derivatives have been reported, wherein the piperidine ring adopts a chair (Balamurugan *et al.*, 2006), a twist-boat (Balamurugan *et al.*, 2007) and a chair conformation (Thiruvalluvar, Balamurugan, Jayabharathi & Manimekalai, 2007). Thiruvalluvar, Balamurugan, Jayabharathi, Manimekalai & Rajarajan (2007) have reported the crystal structure of diphenylpiperidin-4-ol derivative, wherein the piperidine ring adopts a chair conformation.

In the title molecule, $C_{19}H_{21}NO$, the piperidine ring adopts a chair conformation (Fig. 1). Two phenyl rings and two methyl groups attached to the piperidine ring at the positions 2, 6, 3 and 5, respectively, have equatorial orientations. The dihedral angle between the two phenyl rings is 57.1 (1)°. Molecules are linked by an N1—H1···O4 (−1 + *x*, *y*, *z*) hydrogen bond (Fig. 2).

## Experimental

The title compound was prepared by the known procedure (Noller & Baliah, 1948) and characterized using NMR techniques (Hasan *et al.*, 1985).

## Refinement

Atom H1 at N1 was located in a difference Fourier map and refined isotropically. Remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.98 Å and with $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C).

## Figures

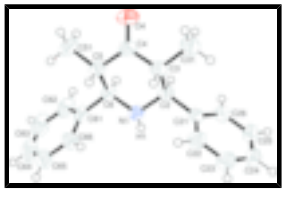

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

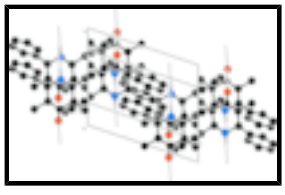

Fig. 2. The molecular packing of the title compound, viewed down the *b* axis, showing the hydrogen bonds (dashed lines).

### t-3,t-5-Dimethyl-r-2,c-6-diphenylpiperidin-4-one

*Crystal data*

| | |
|---|---|
| $C_{19}H_{21}NO$ | $Z = 2$ |
| $M_r = 279.37$ | $F_{000} = 300$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.184$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 405(1) K |
| $a = 7.1392$ (3) Å | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $b = 10.5811$ (5) Å | Cell parameters from 10924 reflections |
| $c = 11.6276$ (5) Å | $\theta = 1.9$–$27.8^\circ$ |
| $\alpha = 102.320$ (2)° | $\mu = 0.07$ mm$^{-1}$ |
| $\beta = 107.613$ (2)° | $T = 298$ (2) K |
| $\gamma = 101.735$ (2)° | Block, yellow |
| $V = 783.31$ (6) Å$^3$ | 0.30 × 0.22 × 0.18 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII diffractometer | 3606 independent reflections |
| Radiation source: fine-focus sealed tube | 2507 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.022$ |
| $T = 298$(2) K | $\theta_{max} = 27.8^\circ$ |
| φ and ω scans | $\theta_{min} = 1.9^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2004) | $h = -9 \rightarrow 9$ |
| $T_{min} = 0.854$, $T_{max} = 0.987$ | $k = -13 \rightarrow 13$ |
| 17560 measured reflections | $l = -15 \rightarrow 15$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.127$ | $w = 1/[\sigma^2(F_o^2) + (0.0551P)^2 + 0.1535P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 3606 reflections | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 194 parameters | $\Delta\rho_{min} = -0.15$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.43830 (15) | 0.75505 (11) | 0.24410 (10) | 0.0382 (3) |
| H1 | 0.331 (3) | 0.7840 (16) | 0.2495 (14) | 0.058 (4)* |
| C2 | 0.49854 (18) | 0.79381 (13) | 0.14409 (12) | 0.0377 (3) |
| H2 | 0.5555 | 0.8923 | 0.1702 | 0.045* |
| C3 | 0.6675 (2) | 0.72851 (15) | 0.12688 (13) | 0.0452 (3) |
| H3 | 0.6095 | 0.6303 | 0.1032 | 0.054* |
| C4 | 0.8407 (2) | 0.77112 (15) | 0.25275 (14) | 0.0478 (3) |
| O4 | 1.01600 (16) | 0.82417 (15) | 0.26561 (12) | 0.0783 (4) |
| C5 | 0.78155 (19) | 0.74549 (15) | 0.36128 (13) | 0.0469 (3) |
| H5 | 0.7275 | 0.6475 | 0.3422 | 0.056* |
| C6 | 0.60440 (18) | 0.80756 (13) | 0.36724 (12) | 0.0390 (3) |
| H6 | 0.6554 | 0.9058 | 0.3869 | 0.047* |
| C21 | 0.31407 (18) | 0.75191 (13) | 0.02317 (12) | 0.0385 (3) |
| C22 | 0.2010 (2) | 0.61779 (15) | −0.03430 (14) | 0.0500 (3) |
| H22 | 0.2367 | 0.5525 | 0.0031 | 0.060* |
| C23 | 0.0361 (2) | 0.57985 (17) | −0.14633 (14) | 0.0590 (4) |
| H23 | −0.0375 | 0.4892 | −0.1845 | 0.071* |
| C24 | −0.0200 (2) | 0.67568 (18) | −0.20191 (14) | 0.0589 (4) |
| H24 | −0.1312 | 0.6500 | −0.2775 | 0.071* |
| C25 | 0.0882 (2) | 0.80852 (17) | −0.14564 (14) | 0.0564 (4) |
| H25 | 0.0501 | 0.8736 | −0.1826 | 0.068* |
| C26 | 0.2547 (2) | 0.84655 (15) | −0.03351 (13) | 0.0464 (3) |
| H26 | 0.3276 | 0.9373 | 0.0042 | 0.056* |
| C31 | 0.7402 (3) | 0.7603 (2) | 0.02373 (16) | 0.0680 (5) |
| H31A | 0.6255 | 0.7314 | −0.0546 | 0.102* |
| H31B | 0.8396 | 0.7138 | 0.0148 | 0.102* |
| H31C | 0.8016 | 0.8559 | 0.0456 | 0.102* |
| C51 | 0.9625 (2) | 0.7943 (2) | 0.48516 (16) | 0.0728 (5) |
| H51A | 0.9169 | 0.7753 | 0.5510 | 0.109* |
| H51B | 1.0219 | 0.8899 | 0.5054 | 0.109* |
| H51C | 1.0634 | 0.7487 | 0.4776 | 0.109* |
| C61 | 0.53009 (19) | 0.77581 (14) | 0.46923 (12) | 0.0425 (3) |
| C62 | 0.5871 (2) | 0.87132 (18) | 0.58451 (14) | 0.0602 (4) |
| H62 | 0.6657 | 0.9587 | 0.5985 | 0.072* |

| | | | | |
|---|---|---|---|---|
| C63 | 0.5270 (3) | 0.8370 (2) | 0.67992 (15) | 0.0767 (6) |
| H63 | 0.5681 | 0.9014 | 0.7578 | 0.092* |
| C64 | 0.4088 (3) | 0.7101 (3) | 0.66034 (17) | 0.0745 (6) |
| H64 | 0.3681 | 0.6882 | 0.7241 | 0.089* |
| C65 | 0.3509 (3) | 0.6158 (2) | 0.54676 (17) | 0.0659 (5) |
| H65 | 0.2700 | 0.5292 | 0.5330 | 0.079* |
| C66 | 0.4113 (2) | 0.64769 (16) | 0.45176 (14) | 0.0511 (4) |
| H66 | 0.3713 | 0.5819 | 0.3749 | 0.061* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O4 | 0.0375 (5) | 0.1211 (11) | 0.0795 (9) | 0.0161 (6) | 0.0247 (5) | 0.0370 (8) |
| N1 | 0.0302 (5) | 0.0506 (7) | 0.0349 (6) | 0.0144 (5) | 0.0118 (4) | 0.0120 (5) |
| C2 | 0.0337 (6) | 0.0413 (7) | 0.0395 (7) | 0.0125 (5) | 0.0138 (5) | 0.0123 (5) |
| C3 | 0.0411 (7) | 0.0547 (8) | 0.0489 (8) | 0.0204 (6) | 0.0228 (6) | 0.0173 (7) |
| C4 | 0.0362 (6) | 0.0569 (8) | 0.0603 (9) | 0.0223 (6) | 0.0215 (6) | 0.0226 (7) |
| C5 | 0.0372 (7) | 0.0601 (9) | 0.0509 (8) | 0.0228 (6) | 0.0156 (6) | 0.0232 (7) |
| C6 | 0.0324 (6) | 0.0427 (7) | 0.0390 (7) | 0.0129 (5) | 0.0089 (5) | 0.0102 (6) |
| C21 | 0.0359 (6) | 0.0476 (8) | 0.0349 (7) | 0.0128 (5) | 0.0163 (5) | 0.0124 (6) |
| C22 | 0.0496 (8) | 0.0481 (8) | 0.0492 (8) | 0.0123 (6) | 0.0152 (6) | 0.0134 (7) |
| C23 | 0.0536 (8) | 0.0592 (9) | 0.0485 (9) | 0.0039 (7) | 0.0130 (7) | 0.0040 (7) |
| C24 | 0.0473 (8) | 0.0830 (12) | 0.0363 (8) | 0.0090 (8) | 0.0094 (6) | 0.0150 (8) |
| C25 | 0.0546 (8) | 0.0723 (11) | 0.0461 (8) | 0.0194 (8) | 0.0144 (7) | 0.0290 (8) |
| C26 | 0.0451 (7) | 0.0510 (8) | 0.0436 (8) | 0.0123 (6) | 0.0153 (6) | 0.0176 (6) |
| C31 | 0.0589 (9) | 0.1070 (14) | 0.0626 (10) | 0.0384 (9) | 0.0378 (8) | 0.0371 (10) |
| C51 | 0.0436 (8) | 0.1164 (15) | 0.0646 (11) | 0.0352 (9) | 0.0114 (7) | 0.0395 (10) |
| C61 | 0.0376 (6) | 0.0565 (9) | 0.0338 (7) | 0.0231 (6) | 0.0090 (5) | 0.0108 (6) |
| C62 | 0.0613 (9) | 0.0684 (10) | 0.0442 (9) | 0.0308 (8) | 0.0101 (7) | 0.0045 (8) |
| C63 | 0.0870 (13) | 0.1156 (17) | 0.0349 (9) | 0.0604 (13) | 0.0194 (8) | 0.0113 (10) |
| C64 | 0.0760 (12) | 0.1259 (18) | 0.0549 (11) | 0.0593 (12) | 0.0361 (9) | 0.0466 (12) |
| C65 | 0.0635 (10) | 0.0901 (13) | 0.0654 (11) | 0.0327 (9) | 0.0328 (8) | 0.0417 (10) |
| C66 | 0.0486 (8) | 0.0627 (9) | 0.0454 (8) | 0.0186 (7) | 0.0189 (6) | 0.0175 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O4—C4 | 1.212 (2) | C64—C65 | 1.360 (3) |
| N1—C2 | 1.4628 (17) | C65—C66 | 1.381 (3) |
| N1—C6 | 1.4595 (17) | C2—H2 | 0.9800 |
| N1—H1 | 0.90 (2) | C3—H3 | 0.9800 |
| C2—C3 | 1.549 (2) | C5—H5 | 0.9800 |
| C2—C21 | 1.5112 (18) | C6—H6 | 0.9800 |
| C3—C31 | 1.516 (2) | C22—H22 | 0.9300 |
| C3—C4 | 1.507 (2) | C23—H23 | 0.9300 |
| C4—C5 | 1.505 (2) | C24—H24 | 0.9300 |
| C5—C51 | 1.515 (2) | C25—H25 | 0.9300 |
| C5—C6 | 1.552 (2) | C26—H26 | 0.9300 |
| C6—C61 | 1.5096 (19) | C31—H31A | 0.9600 |
| C21—C22 | 1.384 (2) | C31—H31B | 0.9600 |

| | | | |
|---|---|---|---|
| C21—C26 | 1.379 (2) | C31—H31C | 0.9600 |
| C22—C23 | 1.379 (2) | C51—H51A | 0.9600 |
| C23—C24 | 1.376 (3) | C51—H51B | 0.9600 |
| C24—C25 | 1.364 (3) | C51—H51C | 0.9600 |
| C25—C26 | 1.385 (2) | C62—H62 | 0.9300 |
| C61—C66 | 1.382 (2) | C63—H63 | 0.9300 |
| C61—C62 | 1.381 (2) | C64—H64 | 0.9300 |
| C62—C63 | 1.394 (3) | C65—H65 | 0.9300 |
| C63—C64 | 1.364 (4) | C66—H66 | 0.9300 |
| O4···H1$^{i}$ | 2.43 (2) | H5···H65$^{iv}$ | 2.6000 |
| O4···H31B | 2.6800 | H6···H2 | 2.3600 |
| O4···H31C | 2.6800 | H6···H62 | 2.3800 |
| O4···H51B | 2.7100 | H6···H51B$^{ii}$ | 2.5700 |
| O4···H51C | 2.7000 | H22···N1 | 2.8700 |
| O4···H62$^{ii}$ | 2.6600 | H22···C3 | 2.9700 |
| N1···H22 | 2.8700 | H22···H3 | 2.4400 |
| N1···H66 | 2.6800 | H23···H66$^{v}$ | 2.5500 |
| C24···C31$^{iii}$ | 3.599 (3) | H24···H66$^{v}$ | 2.4800 |
| C31···C24$^{i}$ | 3.599 (3) | H26···H2 | 2.3300 |
| C51···C62 | 3.398 (3) | H26···H26$^{vii}$ | 2.5900 |
| C62···C51 | 3.398 (3) | H31A···C21 | 2.6700 |
| C65···C66$^{iv}$ | 3.547 (3) | H31A···H64$^{viii}$ | 2.5500 |
| C66···C65$^{iv}$ | 3.547 (3) | H31B···O4 | 2.6800 |
| C3···H22 | 2.9700 | H31B···C23$^{i}$ | 2.9600 |
| C21···H31A | 2.6700 | H31B···C24$^{i}$ | 2.9600 |
| C22···H3 | 2.8300 | H31C···O4 | 2.6800 |
| C23···H31B$^{iii}$ | 2.9600 | H51A···C61 | 2.6400 |
| C24···H66$^{v}$ | 3.1000 | H51A···C62 | 2.8400 |
| C24···H31B$^{iii}$ | 2.9600 | H51B···O4 | 2.7100 |
| C61···H51A | 2.6400 | H51B···H6$^{ii}$ | 2.5700 |
| C62···H51A | 2.8400 | H51B···H51B$^{ii}$ | 2.4400 |
| C64···H51C$^{iii}$ | 2.8900 | H51C···O4 | 2.7000 |
| C65···H51C$^{iii}$ | 2.7400 | H51C···C64$^{i}$ | 2.8900 |
| C66···H5 | 2.9100 | H51C···C65$^{i}$ | 2.7400 |
| C66···H51C$^{iii}$ | 2.9700 | H51C···C66$^{i}$ | 2.9700 |
| C66···H1 | 2.985 (16) | H62···H6 | 2.3800 |
| H1···O4$^{iii}$ | 2.43 (2) | H62···O4$^{ii}$ | 2.6600 |
| H1···C66 | 2.985 (16) | H63···H2$^{vi}$ | 2.5900 |
| H2···H6 | 2.3600 | H64···H31A$^{ix}$ | 2.5500 |
| H2···H26 | 2.3300 | H65···H5$^{iv}$ | 2.6000 |
| H2···H63$^{vi}$ | 2.5900 | H66···N1 | 2.6800 |
| H3···C22 | 2.8300 | H66···C24$^{v}$ | 3.1000 |
| H3···H22 | 2.4400 | H66···H23$^{v}$ | 2.5500 |

| | | | |
|---|---|---|---|
| H5···C66 | 2.9100 | H66···H24$^{v}$ | 2.4800 |
| C2—N1—C6 | 112.91 (11) | C31—C3—H3 | 108.00 |
| C2—N1—H1 | 110.0 (10) | C4—C5—H5 | 107.00 |
| C6—N1—H1 | 109.1 (10) | C6—C5—H5 | 107.00 |
| C3—C2—C21 | 111.82 (11) | C51—C5—H5 | 107.00 |
| N1—C2—C21 | 110.33 (11) | N1—C6—H6 | 109.00 |
| N1—C2—C3 | 108.65 (11) | C5—C6—H6 | 109.00 |
| C2—C3—C31 | 113.35 (14) | C61—C6—H6 | 109.00 |
| C4—C3—C31 | 112.24 (14) | C21—C22—H22 | 120.00 |
| C2—C3—C4 | 108.12 (12) | C23—C22—H22 | 120.00 |
| C3—C4—C5 | 115.81 (13) | C22—C23—H23 | 120.00 |
| O4—C4—C3 | 121.85 (14) | C24—C23—H23 | 120.00 |
| O4—C4—C5 | 122.34 (14) | C23—C24—H24 | 120.00 |
| C6—C5—C51 | 113.06 (12) | C25—C24—H24 | 120.00 |
| C4—C5—C6 | 108.70 (12) | C24—C25—H25 | 120.00 |
| C4—C5—C51 | 112.75 (13) | C26—C25—H25 | 120.00 |
| N1—C6—C5 | 108.99 (11) | C21—C26—H26 | 119.00 |
| N1—C6—C61 | 111.00 (11) | C25—C26—H26 | 119.00 |
| C5—C6—C61 | 110.51 (11) | C3—C31—H31A | 109.00 |
| C2—C21—C22 | 121.10 (13) | C3—C31—H31B | 109.00 |
| C22—C21—C26 | 118.14 (13) | C3—C31—H31C | 109.00 |
| C2—C21—C26 | 120.76 (13) | H31A—C31—H31B | 109.00 |
| C21—C22—C23 | 120.80 (15) | H31A—C31—H31C | 109.00 |
| C22—C23—C24 | 120.21 (16) | H31B—C31—H31C | 109.00 |
| C23—C24—C25 | 119.72 (14) | C5—C51—H51A | 109.00 |
| C24—C25—C26 | 120.07 (16) | C5—C51—H51B | 109.00 |
| C21—C26—C25 | 121.05 (15) | C5—C51—H51C | 109.00 |
| C6—C61—C62 | 121.21 (14) | H51A—C51—H51B | 109.00 |
| C62—C61—C66 | 118.15 (14) | H51A—C51—H51C | 109.00 |
| C6—C61—C66 | 120.56 (12) | H51B—C51—H51C | 109.00 |
| C61—C62—C63 | 120.10 (17) | C61—C62—H62 | 120.00 |
| C62—C63—C64 | 120.74 (16) | C63—C62—H62 | 120.00 |
| C63—C64—C65 | 119.5 (2) | C62—C63—H63 | 120.00 |
| C64—C65—C66 | 120.5 (2) | C64—C63—H63 | 120.00 |
| C61—C66—C65 | 121.02 (15) | C63—C64—H64 | 120.00 |
| N1—C2—H2 | 109.00 | C65—C64—H64 | 120.00 |
| C3—C2—H2 | 109.00 | C64—C65—H65 | 120.00 |
| C21—C2—H2 | 109.00 | C66—C65—H65 | 120.00 |
| C2—C3—H3 | 108.00 | C61—C66—H66 | 120.00 |
| C4—C3—H3 | 108.00 | C65—C66—H66 | 119.00 |
| C6—N1—C2—C3 | 64.29 (14) | C51—C5—C6—N1 | 179.84 (13) |
| C6—N1—C2—C21 | −172.79 (11) | C51—C5—C6—C61 | −57.92 (17) |
| C2—N1—C6—C5 | −63.18 (14) | N1—C6—C61—C62 | −136.85 (15) |
| C2—N1—C6—C61 | 174.88 (11) | N1—C6—C61—C66 | 46.50 (18) |
| N1—C2—C3—C4 | −55.70 (15) | C5—C6—C61—C62 | 102.10 (17) |
| N1—C2—C3—C31 | 179.19 (13) | C5—C6—C61—C66 | −74.55 (17) |
| C21—C2—C3—C4 | −177.71 (12) | C2—C21—C22—C23 | −178.30 (13) |
| C21—C2—C3—C31 | 57.18 (17) | C26—C21—C22—C23 | 1.2 (2) |

| | | | |
|---|---|---|---|
| N1—C2—C21—C22 | −59.92 (17) | C2—C21—C26—C25 | 178.73 (13) |
| N1—C2—C21—C26 | 120.57 (14) | C22—C21—C26—C25 | −0.8 (2) |
| C3—C2—C21—C22 | 61.12 (17) | C21—C22—C23—C24 | −0.8 (2) |
| C3—C2—C21—C26 | −118.38 (15) | C22—C23—C24—C25 | 0.0 (2) |
| C2—C3—C4—O4 | −125.93 (17) | C23—C24—C25—C26 | 0.5 (2) |
| C2—C3—C4—C5 | 53.21 (17) | C24—C25—C26—C21 | 0.0 (2) |
| C31—C3—C4—O4 | −0.2 (2) | C6—C61—C62—C63 | −175.98 (17) |
| C31—C3—C4—C5 | 178.97 (14) | C66—C61—C62—C63 | 0.8 (3) |
| O4—C4—C5—C6 | 126.84 (17) | C6—C61—C66—C65 | 176.81 (16) |
| O4—C4—C5—C51 | 0.7 (2) | C62—C61—C66—C65 | 0.1 (3) |
| C3—C4—C5—C6 | −52.29 (17) | C61—C62—C63—C64 | −1.1 (3) |
| C3—C4—C5—C51 | −178.47 (14) | C62—C63—C64—C65 | 0.7 (3) |
| C4—C5—C6—N1 | 53.83 (15) | C63—C64—C65—C66 | 0.2 (3) |
| C4—C5—C6—C61 | 176.07 (12) | C64—C65—C66—C61 | −0.5 (3) |

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+2, −*y*+2, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*, −*y*+1, −*z*; (vi) −*x*+1, −*y*+2, −*z*+1; (vii) −*x*+1, −*y*+2, −*z*; (viii) *x*, *y*, *z*−1; (ix) *x*, *y*, *z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O4$^{iii}$ | 0.90 (2) | 2.43 (2) | 3.3109 (17) | 170.2 (15) |

Symmetry codes: (iii) *x*−1, *y*, *z*.

**Fig. 1**

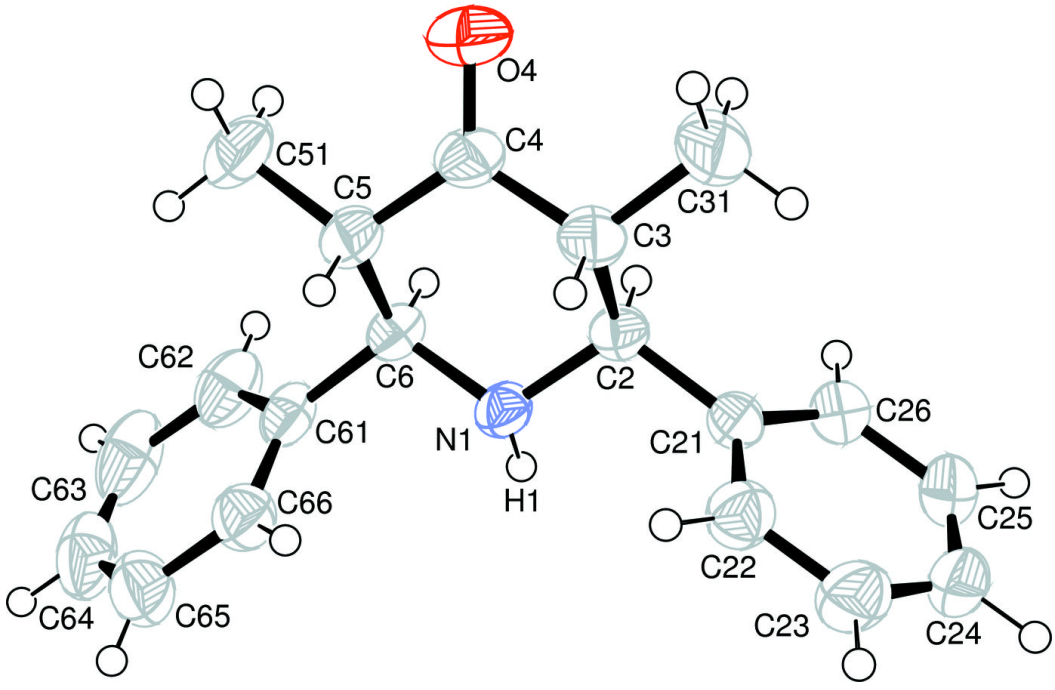
O4
C4
C51
C5
C31
C3
C62
C6
C2
C26
C61
N1
C21
H1
C63
C66
C25
C22
C64
C65
C23
C24

**Fig. 2**