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# 10-Benzyl-9-(4-ethoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8(2*H*,5*H*)-dione

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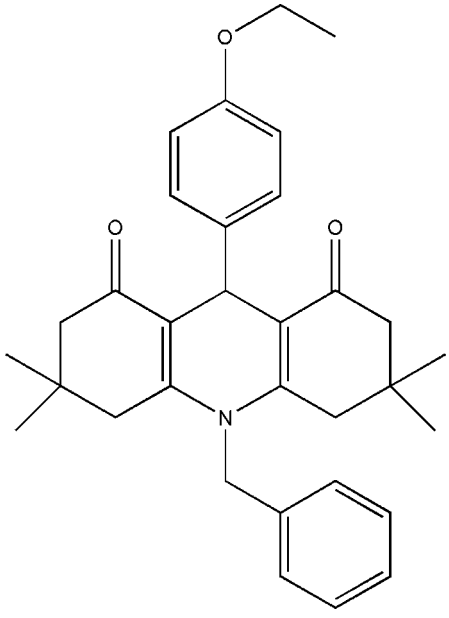
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.044; $wR$ factor = 0.128; data-to-parameter ratio = 19.7.

In the title compound, $C_{32}H_{37}NO_3$, the central dihydropyridine ring adopts a nearly planar flattened-boat conformation, whereas both cyclohexenone rings adopt half-chair conformations. The mean and maximum deviations from the mean plane of the dihydropyridine ring are 0.1252 (9) and 0.188 (1) Å, respectively. The 4-ethoxyphenyl and phenyl rings form dihedral angles of 75.20 (4) and 82.14 (5)° with the dihydropyridine mean plane, respectively.

## Related literature

For general background, see: Wysocka-Skrzela & Ledochowski (1976); Nasim & Brychcy (1979); Thull & Testa (1994); Reil *et al.* (1994); Mandi *et al.* (1994). For related structures, see: Abdelhamid *et al.* (2011); Khalilov *et al.* (2011); Tang *et al.* (2008); Tu *et al.* (2004). For a related synthesis, see: Li *et al.* (2003). For ring-puckering parameters, see: Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

$C_{32}H_{37}NO_3$
$M_r$ = 483.63
Orthorhombic, *Pbca*
$a$ = 16.8172 (7) Å
$b$ = 15.7033 (7) Å
$c$ = 19.908 (1) Å
$V$ = 5257.4 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 296 K
0.30 × 0.20 × 0.20 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.976, $T_{max}$ = 0.986
54483 measured reflections
6422 independent reflections
4439 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.128
$S$ = 1.03
6422 reflections
326 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*/*SAINT* (Bruker, 2004); data reduction: *SAINT*/*XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2066).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o2755 [doi:10.1107/S1600536812036094]

## 10-Benzyl-9-(4-ethoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8(2*H*,5*H*)-dione

**V. Sughanya and N. Sureshbabu**

### Comment

Acridine derivatives with a dihydropyridine unit belong to a special class of compounds, because of their wide range of applications in the pharmaceutical and dye industries. They are also well known as therapeutic agents (Wysocka-Skrzela & Ledochowski, 1976; Nasim & Brychcy,1979; Thull & Testa, 1994; Reil *et al.*, 1994; Mandi *et al.*, 1994).

The central dihydropyridine ring is almost planar with a mean deviation from the mean plane of 0.1252 (9) Å and with a maximum deviation of 0.188 (1) Å for C9. The planar 4-ethoxyphenyl and phenyl rings form dihedral angles of 75.20 (4)° and 82.14 (5)° with the dihydropyridine mean plane. The rings A (C1–C6), B (N1/C3/C4/C9/C10/C11) and C (C10–C15) show total puckering amplitudes Q(T) of 0.506 (2) Å, 0.307 (1) Å and 0.470 (2) Å, respectively. The cyclohexenone rings A and C adopt half chair conformation, whereas the central ring B adopts flattened boat conformation. This can be understood from the Cremer & Pople (1975) puckering parameters: $\varphi$ = = -7.10 (2)° and $\theta$ = 62.2 (2)° (for A); $\varphi$ = 166.5 (2)°, and $\theta$ = 77.4 (2)° (for B) and $\varphi$ = -163.97 (3)°, $\theta$ = 56.9 (2)° (for C), respectively. In the title compound, the bond lengths (Allen *et al.*, 1987) and angles are generally within normal ranges. In the dihydropyridine ring C10=C11 and C4=C3 are double bonds (C10—C11 = 1.3489 (18) Å and C4—C3 = 1.3540 (18) Å), as indicated by the bond distances. The C11—C10—C15 [120.39 (13)°] and C3—C4—C5 [119.51 (13)°] angles are almost the same. In this conformation C1 and C13 may be described as flap atoms being away from the plane of the ring. The observed carbonyl bond lengths (C15—O1 = 1.2232 (17) Å and C5—O2 = 1.2275 (17) Å) are also normal.

### Experimental

The title compound was prepared in two stages. In the first stage, a mixture of 4-ethoxybenzaldehyde (1.2 g, 8 mmol), 5,5-dimethylcyclohexane-1,3-dione (2.24 g, 16 mmol) and 20 ml of ethanol was heated to 70°C for about 10 minutes. The reaction mixture was allowed to cool to room temperature and the resulting solid intermediate, 2,2′-((4-ethoxyphenyl)methylene)bis(3-hydroxy-5,5-dimethylcyclohex-2-enone) was filtered and dried (m.p.: 411 K, yield: 78%). In the second stage about 0.8 g of this intermediate was dissoloved in 25 ml of acetic acid. The solution was refluxed together with benzylamine (0.33 g, 3 mmol) for 8 h with the reaction being monitored by TLC. After completion of the reaction, the reaction mixture was poured into crushed ice and stirred well. The solid that separated was filtered and dried and then recrystallized from ethanol to yield yellow crystals of the title compound (m.p.: 433 K, yield: 82%).

### Refinement

All the hydrogen atoms were fixed in calculated positions and allowed to ride on their parent atom with d(C—H) = 0.96 Å and $U_{iso}$(H) = 1.5 $U_{eq}$(C) for $CH_3$, d(C—H) = 0.97 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C) for $CH_2$, d(C—H) = 0.98 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C) for aliphatic CH and with d(C—H) = 0.93 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C) for aromatic CH.

### Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*/*SAINT* (Bruker, 2004); data reduction: *SAINT*/*XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and Mercury (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

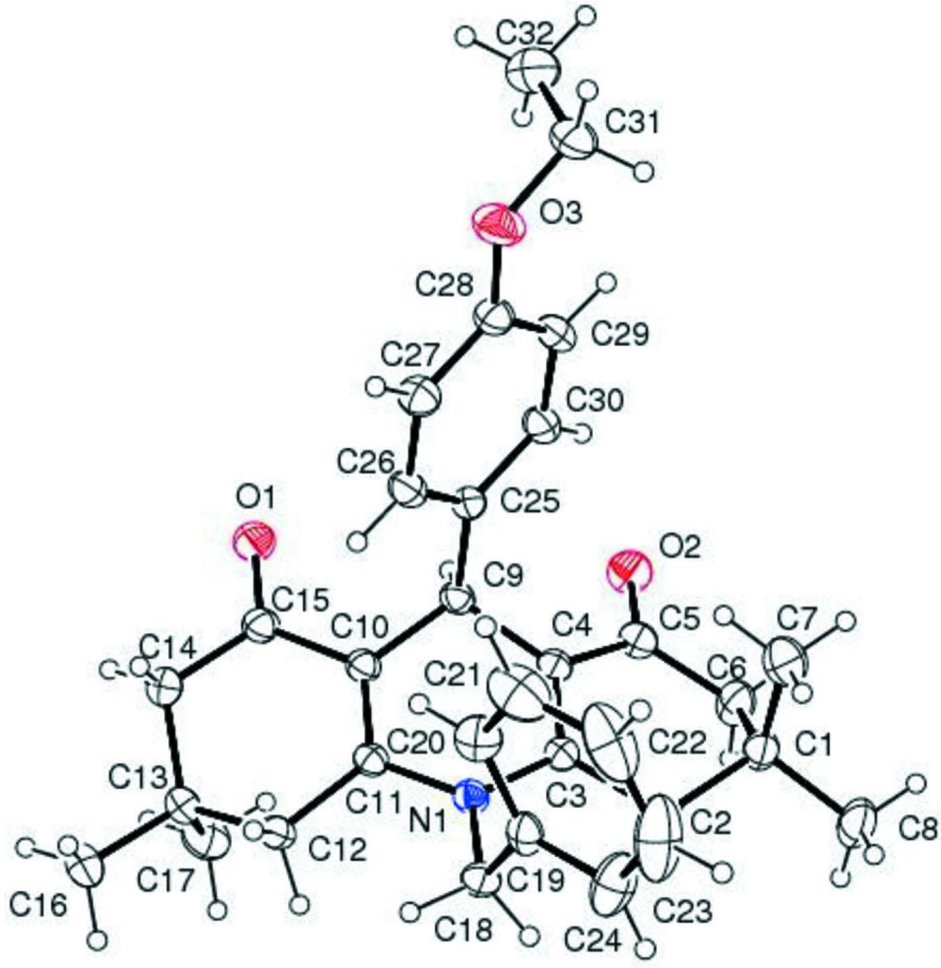


**Figure 1**

A view of the structure of the title compound showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

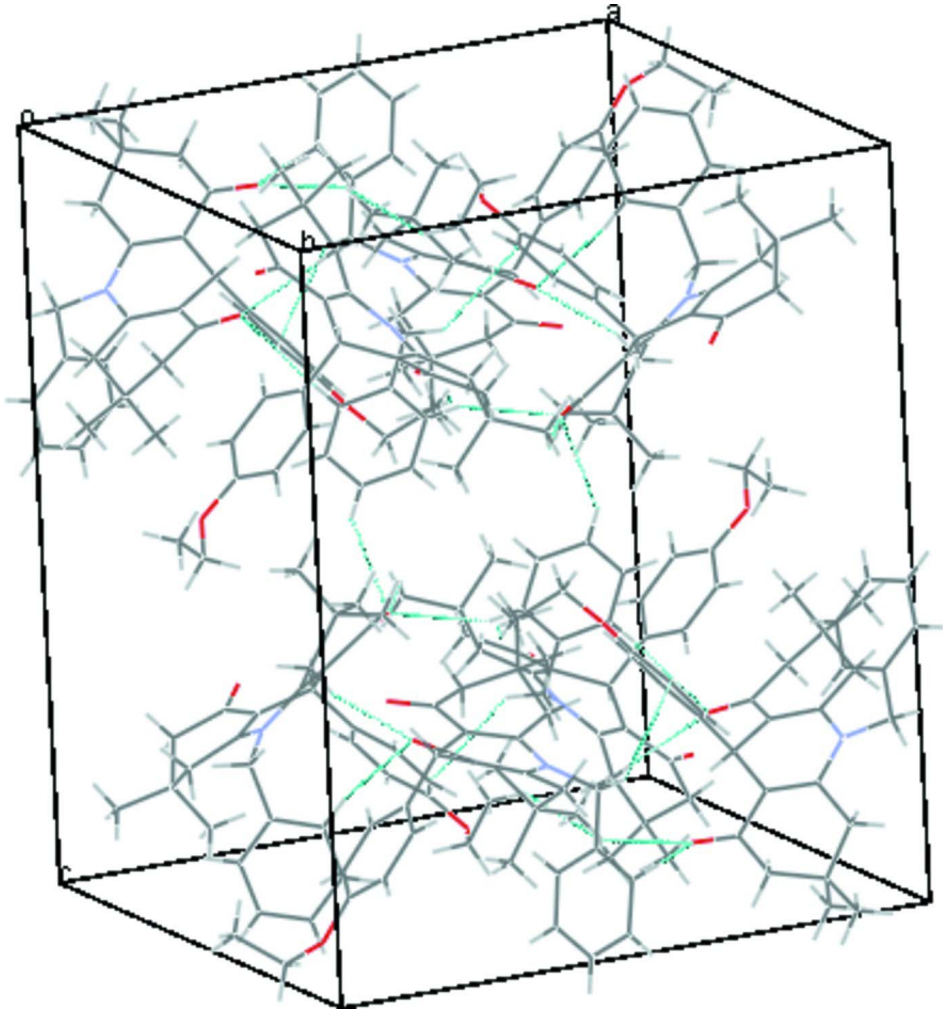

**Figure 2**

Packing diagram for the title compound.

**10-Benzyl-9-(4-ethoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10- hexahydroacridine-1,8(2*H*,5*H*)-dione**

*Crystal data*

$C_{32}H_{37}NO_3$
$M_r = 483.63$
Orthorhombic, *Pbca*
$a = 16.8172$ (7) Å
$b = 15.7033$ (7) Å
$c = 19.908$ (1) Å
$V = 5257.4$ (4) Å$^3$
$Z = 8$
$F(000) = 2080$
$D_x = 1.222$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6423 reflections
$\theta = 2.4$–27.3°
$\mu = 0.08$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.976$, $T_{max} = 0.986$

54483 measured reflections
6422 independent reflections
4439 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 28.1°$, $\theta_{min} = 2.1°$
$h = -22 \rightarrow 22$
$k = -20 \rightarrow 20$
$l = -26 \rightarrow 26$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.128$
$S = 1.03$
6422 reflections
326 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 1.5474P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å$^{-3}$
$\Delta\rho_{min} = -0.16$ e Å$^{-3}$
Extinction correction: *SHELXL97*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0017 (3)

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.43933 (9) | 0.70202 (10) | 0.33199 (8) | 0.0427 (4) |
| C2 | 0.44922 (8) | 0.61875 (9) | 0.29361 (8) | 0.0386 (3) |
| H2A | 0.4920 | 0.6251 | 0.2613 | 0.046* |
| H2B | 0.4644 | 0.5743 | 0.3249 | 0.046* |
| C3 | 0.37519 (8) | 0.59175 (8) | 0.25718 (7) | 0.0308 (3) |
| C4 | 0.31496 (8) | 0.64638 (8) | 0.24372 (7) | 0.0323 (3) |
| C5 | 0.32733 (9) | 0.73706 (9) | 0.25208 (7) | 0.0386 (3) |
| C6 | 0.40380 (10) | 0.76626 (10) | 0.28343 (9) | 0.0512 (4) |
| H6A | 0.3943 | 0.8192 | 0.3072 | 0.061* |
| H6B | 0.4421 | 0.7777 | 0.2481 | 0.061* |
| C7 | 0.38514 (12) | 0.68989 (15) | 0.39259 (9) | 0.0668 (5) |
| H7A | 0.4084 | 0.6491 | 0.4227 | 0.100* |
| H7B | 0.3342 | 0.6696 | 0.3779 | 0.100* |
| H7C | 0.3787 | 0.7433 | 0.4154 | 0.100* |
| C8 | 0.52092 (11) | 0.73258 (12) | 0.35585 (11) | 0.0629 (5) |
| H8A | 0.5430 | 0.6916 | 0.3863 | 0.094* |
| H8B | 0.5154 | 0.7864 | 0.3783 | 0.094* |
| H8C | 0.5556 | 0.7390 | 0.3179 | 0.094* |
| C9 | 0.23605 (8) | 0.61457 (9) | 0.21724 (7) | 0.0325 (3) |
| H9 | 0.2149 | 0.6583 | 0.1870 | 0.039* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.25047 (8) | 0.53568 (9) | 0.17623 (7) | 0.0329 (3) |
| C11 | 0.31540 (8) | 0.48656 (8) | 0.18523 (6) | 0.0307 (3) |
| C12 | 0.33256 (8) | 0.41003 (9) | 0.14247 (7) | 0.0362 (3) |
| H12A | 0.3216 | 0.3592 | 0.1685 | 0.043* |
| H12B | 0.3887 | 0.4097 | 0.1314 | 0.043* |
| C13 | 0.28452 (9) | 0.40604 (10) | 0.07704 (7) | 0.0418 (4) |
| C14 | 0.19796 (9) | 0.42652 (11) | 0.09332 (8) | 0.0462 (4) |
| H14A | 0.1676 | 0.4279 | 0.0519 | 0.055* |
| H14B | 0.1763 | 0.3816 | 0.1213 | 0.055* |
| C15 | 0.18853 (8) | 0.51014 (10) | 0.12889 (7) | 0.0382 (3) |
| C16 | 0.29115 (11) | 0.31582 (12) | 0.04862 (10) | 0.0615 (5) |
| H16A | 0.2715 | 0.2758 | 0.0810 | 0.092* |
| H16B | 0.3458 | 0.3034 | 0.0388 | 0.092* |
| H16C | 0.2603 | 0.3117 | 0.0082 | 0.092* |
| C17 | 0.31637 (12) | 0.46944 (13) | 0.02556 (8) | 0.0594 (5) |
| H17A | 0.3709 | 0.4563 | 0.0156 | 0.089* |
| H17B | 0.3130 | 0.5261 | 0.0435 | 0.089* |
| H17C | 0.2853 | 0.4659 | −0.0148 | 0.089* |
| C18 | 0.42660 (9) | 0.44408 (9) | 0.26170 (8) | 0.0385 (3) |
| H18A | 0.4806 | 0.4657 | 0.2601 | 0.046* |
| H18B | 0.4244 | 0.3932 | 0.2341 | 0.046* |
| C19 | 0.40643 (9) | 0.42094 (9) | 0.33302 (8) | 0.0390 (3) |
| C20 | 0.32955 (11) | 0.39930 (11) | 0.35078 (9) | 0.0523 (4) |
| H20 | 0.2897 | 0.3994 | 0.3184 | 0.063* |
| C21 | 0.31140 (15) | 0.37766 (14) | 0.41603 (11) | 0.0765 (6) |
| H21 | 0.2596 | 0.3626 | 0.4271 | 0.092* |
| C22 | 0.3683 (2) | 0.37810 (14) | 0.46431 (11) | 0.0875 (8) |
| H22 | 0.3555 | 0.3637 | 0.5083 | 0.105* |
| C23 | 0.4439 (2) | 0.39963 (15) | 0.44815 (12) | 0.0943 (9) |
| H23 | 0.4827 | 0.4008 | 0.4814 | 0.113* |
| C24 | 0.46399 (13) | 0.42012 (12) | 0.38220 (11) | 0.0687 (6) |
| H24 | 0.5164 | 0.4333 | 0.3714 | 0.082* |
| C25 | 0.17591 (8) | 0.60221 (9) | 0.27392 (7) | 0.0339 (3) |
| C26 | 0.14725 (9) | 0.52322 (10) | 0.29309 (7) | 0.0396 (3) |
| H26 | 0.1657 | 0.4746 | 0.2715 | 0.048* |
| C27 | 0.09150 (9) | 0.51533 (10) | 0.34395 (8) | 0.0436 (4) |
| H27 | 0.0730 | 0.4616 | 0.3560 | 0.052* |
| C28 | 0.06319 (9) | 0.58640 (11) | 0.37696 (8) | 0.0428 (4) |
| C29 | 0.09195 (9) | 0.66542 (11) | 0.35946 (9) | 0.0500 (4) |
| H29 | 0.0743 | 0.7138 | 0.3819 | 0.060* |
| C30 | 0.14731 (9) | 0.67259 (10) | 0.30830 (8) | 0.0453 (4) |
| H30 | 0.1659 | 0.7264 | 0.2966 | 0.054* |
| C31 | −0.02477 (11) | 0.64092 (14) | 0.46208 (9) | 0.0619 (5) |
| H31A | 0.0179 | 0.6797 | 0.4739 | 0.074* |
| H31B | −0.0482 | 0.6201 | 0.5035 | 0.074* |
| C32 | −0.08674 (12) | 0.68881 (16) | 0.42322 (11) | 0.0756 (6) |
| H32A | −0.1065 | 0.7351 | 0.4500 | 0.113* |
| H32B | −0.1297 | 0.6511 | 0.4121 | 0.113* |
| H32C | −0.0637 | 0.7109 | 0.3827 | 0.113* |

| | | | | |
|---|---|---|---|---|
| N1 | 0.37233 (7) | 0.50849 (7) | 0.23366 (6) | 0.0327 (3) |
| O1 | 0.12873 (7) | 0.55348 (8) | 0.12149 (6) | 0.0547 (3) |
| O2 | 0.27853 (7) | 0.78993 (7) | 0.23301 (6) | 0.0527 (3) |
| O3 | 0.00768 (7) | 0.57079 (9) | 0.42588 (6) | 0.0605 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0415 (8) | 0.0388 (8) | 0.0478 (9) | −0.0022 (6) | −0.0073 (7) | −0.0038 (7) |
| C2 | 0.0337 (7) | 0.0346 (8) | 0.0475 (8) | −0.0009 (6) | −0.0024 (6) | 0.0010 (6) |
| C3 | 0.0325 (7) | 0.0302 (7) | 0.0298 (7) | −0.0012 (5) | 0.0028 (5) | 0.0021 (5) |
| C4 | 0.0338 (7) | 0.0312 (7) | 0.0319 (7) | 0.0020 (5) | 0.0015 (5) | 0.0009 (5) |
| C5 | 0.0428 (8) | 0.0332 (7) | 0.0397 (8) | 0.0031 (6) | 0.0025 (6) | 0.0031 (6) |
| C6 | 0.0535 (9) | 0.0308 (8) | 0.0693 (11) | −0.0031 (7) | −0.0105 (8) | −0.0004 (7) |
| C7 | 0.0682 (12) | 0.0884 (15) | 0.0437 (10) | −0.0004 (11) | −0.0013 (9) | −0.0126 (10) |
| C8 | 0.0554 (10) | 0.0464 (10) | 0.0868 (14) | −0.0040 (8) | −0.0236 (10) | −0.0120 (9) |
| C9 | 0.0330 (7) | 0.0325 (7) | 0.0321 (7) | 0.0061 (5) | −0.0010 (5) | −0.0012 (5) |
| C10 | 0.0329 (6) | 0.0353 (7) | 0.0306 (7) | 0.0019 (6) | 0.0018 (5) | −0.0015 (5) |
| C11 | 0.0329 (6) | 0.0308 (7) | 0.0284 (6) | −0.0001 (5) | 0.0044 (5) | 0.0009 (5) |
| C12 | 0.0344 (7) | 0.0354 (8) | 0.0389 (7) | 0.0024 (6) | 0.0055 (6) | −0.0046 (6) |
| C13 | 0.0422 (8) | 0.0451 (9) | 0.0383 (8) | 0.0018 (7) | 0.0019 (6) | −0.0116 (7) |
| C14 | 0.0397 (8) | 0.0525 (10) | 0.0465 (9) | −0.0004 (7) | −0.0046 (7) | −0.0121 (7) |
| C15 | 0.0353 (7) | 0.0461 (9) | 0.0332 (7) | 0.0029 (6) | 0.0009 (6) | −0.0022 (6) |
| C16 | 0.0597 (11) | 0.0598 (11) | 0.0650 (12) | 0.0051 (9) | −0.0049 (9) | −0.0286 (9) |
| C17 | 0.0684 (12) | 0.0712 (12) | 0.0386 (9) | 0.0050 (10) | 0.0105 (8) | 0.0003 (8) |
| C18 | 0.0363 (7) | 0.0323 (7) | 0.0470 (8) | 0.0082 (6) | −0.0030 (6) | −0.0009 (6) |
| C19 | 0.0482 (8) | 0.0245 (7) | 0.0443 (8) | 0.0033 (6) | −0.0097 (7) | −0.0009 (6) |
| C20 | 0.0543 (10) | 0.0492 (10) | 0.0534 (10) | 0.0019 (8) | −0.0001 (8) | 0.0036 (8) |
| C21 | 0.0986 (17) | 0.0636 (13) | 0.0672 (14) | 0.0018 (12) | 0.0270 (13) | 0.0092 (10) |
| C22 | 0.162 (3) | 0.0540 (13) | 0.0459 (11) | −0.0053 (15) | 0.0005 (15) | 0.0041 (9) |
| C23 | 0.152 (3) | 0.0677 (15) | 0.0630 (14) | −0.0223 (16) | −0.0547 (16) | 0.0181 (11) |
| C24 | 0.0751 (13) | 0.0590 (12) | 0.0719 (13) | −0.0124 (10) | −0.0339 (11) | 0.0174 (10) |
| C25 | 0.0295 (6) | 0.0380 (8) | 0.0343 (7) | 0.0033 (6) | −0.0017 (5) | −0.0050 (6) |
| C26 | 0.0416 (8) | 0.0384 (8) | 0.0390 (8) | 0.0066 (6) | 0.0021 (6) | −0.0044 (6) |
| C27 | 0.0453 (8) | 0.0424 (9) | 0.0430 (8) | 0.0002 (7) | 0.0037 (7) | 0.0017 (7) |
| C28 | 0.0376 (7) | 0.0561 (10) | 0.0347 (8) | 0.0011 (7) | 0.0031 (6) | −0.0045 (7) |
| C29 | 0.0464 (9) | 0.0493 (10) | 0.0541 (10) | 0.0008 (7) | 0.0115 (7) | −0.0199 (8) |
| C30 | 0.0431 (8) | 0.0383 (8) | 0.0545 (9) | −0.0022 (7) | 0.0073 (7) | −0.0115 (7) |
| C31 | 0.0512 (10) | 0.0908 (15) | 0.0437 (9) | 0.0045 (10) | 0.0093 (8) | −0.0171 (9) |
| C32 | 0.0558 (11) | 0.0931 (16) | 0.0777 (14) | 0.0088 (11) | 0.0036 (10) | −0.0102 (12) |
| N1 | 0.0338 (6) | 0.0297 (6) | 0.0347 (6) | 0.0041 (5) | −0.0014 (5) | −0.0003 (5) |
| O1 | 0.0443 (6) | 0.0648 (8) | 0.0551 (7) | 0.0161 (6) | −0.0139 (5) | −0.0119 (6) |
| O2 | 0.0547 (7) | 0.0340 (6) | 0.0693 (8) | 0.0090 (5) | −0.0071 (6) | 0.0060 (5) |
| O3 | 0.0585 (7) | 0.0716 (9) | 0.0515 (7) | 0.0025 (6) | 0.0200 (6) | −0.0040 (6) |

*Geometric parameters (Å, º)*

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| C1—C6 | 1.520 (2) | C16—H16B | 0.9600 |
| C1—C2 | 1.523 (2) | C16—H16C | 0.9600 |
| C1—C7 | 1.524 (2) | C17—H17A | 0.9600 |

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|---|---|---|---|
| C1—C8 | 1.529 (2) | C17—H17B | 0.9600 |
| C2—C3 | 1.5020 (19) | C17—H17C | 0.9600 |
| C2—H2A | 0.9700 | C18—N1 | 1.4723 (17) |
| C2—H2B | 0.9700 | C18—C19 | 1.504 (2) |
| C3—C4 | 1.3540 (18) | C18—H18A | 0.9700 |
| C3—N1 | 1.3896 (17) | C18—H18B | 0.9700 |
| C4—C5 | 1.449 (2) | C19—C24 | 1.377 (2) |
| C4—C9 | 1.5127 (19) | C19—C20 | 1.383 (2) |
| C5—O2 | 1.2275 (17) | C20—C21 | 1.377 (3) |
| C5—C6 | 1.501 (2) | C20—H20 | 0.9300 |
| C6—H6A | 0.9700 | C21—C22 | 1.357 (3) |
| C6—H6B | 0.9700 | C21—H21 | 0.9300 |
| C7—H7A | 0.9600 | C22—C23 | 1.353 (4) |
| C7—H7B | 0.9600 | C22—H22 | 0.9300 |
| C7—H7C | 0.9600 | C23—C24 | 1.394 (3) |
| C8—H8A | 0.9600 | C23—H23 | 0.9300 |
| C8—H8B | 0.9600 | C24—H24 | 0.9300 |
| C8—H8C | 0.9600 | C25—C26 | 1.384 (2) |
| C9—C10 | 1.5033 (19) | C25—C30 | 1.386 (2) |
| C9—C25 | 1.5277 (19) | C26—C27 | 1.385 (2) |
| C9—H9 | 0.9800 | C26—H26 | 0.9300 |
| C10—C11 | 1.3489 (18) | C27—C28 | 1.380 (2) |
| C10—C15 | 1.4609 (19) | C27—H27 | 0.9300 |
| C11—N1 | 1.4017 (17) | C28—O3 | 1.3711 (19) |
| C11—C12 | 1.5007 (18) | C28—C29 | 1.377 (2) |
| C12—C13 | 1.534 (2) | C29—C30 | 1.384 (2) |
| C12—H12A | 0.9700 | C29—H29 | 0.9300 |
| C12—H12B | 0.9700 | C30—H30 | 0.9300 |
| C13—C14 | 1.526 (2) | C31—O3 | 1.425 (2) |
| C13—C17 | 1.526 (2) | C31—C32 | 1.500 (3) |
| C13—C16 | 1.530 (2) | C31—H31A | 0.9700 |
| C14—C15 | 1.500 (2) | C31—H31B | 0.9700 |
| C14—H14A | 0.9700 | C32—H32A | 0.9600 |
| C14—H14B | 0.9700 | C32—H32B | 0.9600 |
| C15—O1 | 1.2232 (17) | C32—H32C | 0.9600 |
| C16—H16A | 0.9600 | | |

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| C6—C1—C2 | 107.08 (13) | C10—C15—C14 | 118.00 (12) |
| C6—C1—C7 | 110.58 (15) | C13—C16—H16A | 109.5 |
| C2—C1—C7 | 110.80 (14) | C13—C16—H16B | 109.5 |
| C6—C1—C8 | 110.00 (14) | H16A—C16—H16B | 109.5 |
| C2—C1—C8 | 109.09 (13) | C13—C16—H16C | 109.5 |
| C7—C1—C8 | 109.26 (15) | H16A—C16—H16C | 109.5 |
| C3—C2—C1 | 113.20 (12) | H16B—C16—H16C | 109.5 |
| C3—C2—H2A | 108.9 | C13—C17—H17A | 109.5 |
| C1—C2—H2A | 108.9 | C13—C17—H17B | 109.5 |
| C3—C2—H2B | 108.9 | H17A—C17—H17B | 109.5 |
| C1—C2—H2B | 108.9 | C13—C17—H17C | 109.5 |
| H2A—C2—H2B | 107.8 | H17A—C17—H17C | 109.5 |

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| C4—C3—N1 | 120.23 (12) | H17B—C17—H17C | 109.5 |
| C4—C3—C2 | 122.47 (12) | N1—C18—C19 | 112.58 (12) |
| N1—C3—C2 | 117.19 (11) | N1—C18—H18A | 109.1 |
| C3—C4—C5 | 119.51 (13) | C19—C18—H18A | 109.1 |
| C3—C4—C9 | 121.07 (12) | N1—C18—H18B | 109.1 |
| C5—C4—C9 | 119.37 (12) | C19—C18—H18B | 109.1 |
| O2—C5—C4 | 122.23 (14) | H18A—C18—H18B | 107.8 |
| O2—C5—C6 | 119.65 (13) | C24—C19—C20 | 118.25 (17) |
| C4—C5—C6 | 118.10 (13) | C24—C19—C18 | 120.99 (16) |
| C5—C6—C1 | 113.49 (13) | C20—C19—C18 | 120.76 (14) |
| C5—C6—H6A | 108.9 | C21—C20—C19 | 120.61 (19) |
| C1—C6—H6A | 108.9 | C21—C20—H20 | 119.7 |
| C5—C6—H6B | 108.9 | C19—C20—H20 | 119.7 |
| C1—C6—H6B | 108.9 | C22—C21—C20 | 120.7 (2) |
| H6A—C6—H6B | 107.7 | C22—C21—H21 | 119.7 |
| C1—C7—H7A | 109.5 | C20—C21—H21 | 119.7 |
| C1—C7—H7B | 109.5 | C23—C22—C21 | 119.7 (2) |
| H7A—C7—H7B | 109.5 | C23—C22—H22 | 120.1 |
| C1—C7—H7C | 109.5 | C21—C22—H22 | 120.1 |
| H7A—C7—H7C | 109.5 | C22—C23—C24 | 120.6 (2) |
| H7B—C7—H7C | 109.5 | C22—C23—H23 | 119.7 |
| C1—C8—H8A | 109.5 | C24—C23—H23 | 119.7 |
| C1—C8—H8B | 109.5 | C19—C24—C23 | 120.1 (2) |
| H8A—C8—H8B | 109.5 | C19—C24—H24 | 120.0 |
| C1—C8—H8C | 109.5 | C23—C24—H24 | 120.0 |
| H8A—C8—H8C | 109.5 | C26—C25—C30 | 117.22 (13) |
| H8B—C8—H8C | 109.5 | C26—C25—C9 | 123.23 (12) |
| C10—C9—C4 | 108.65 (11) | C30—C25—C9 | 119.55 (13) |
| C10—C9—C25 | 113.78 (12) | C25—C26—C27 | 121.14 (14) |
| C4—C9—C25 | 111.43 (11) | C25—C26—H26 | 119.4 |
| C10—C9—H9 | 107.6 | C27—C26—H26 | 119.4 |
| C4—C9—H9 | 107.6 | C28—C27—C26 | 120.61 (15) |
| C25—C9—H9 | 107.6 | C28—C27—H27 | 119.7 |
| C11—C10—C15 | 120.39 (13) | C26—C27—H27 | 119.7 |
| C11—C10—C9 | 121.99 (12) | O3—C28—C29 | 125.46 (14) |
| C15—C10—C9 | 117.48 (12) | O3—C28—C27 | 115.37 (15) |
| C10—C11—N1 | 120.24 (12) | C29—C28—C27 | 119.16 (14) |
| C10—C11—C12 | 122.57 (12) | C28—C29—C30 | 119.72 (14) |
| N1—C11—C12 | 117.11 (11) | C28—C29—H29 | 120.1 |
| C11—C12—C13 | 114.40 (12) | C30—C29—H29 | 120.1 |
| C11—C12—H12A | 108.7 | C29—C30—C25 | 122.12 (15) |
| C13—C12—H12A | 108.7 | C29—C30—H30 | 118.9 |
| C11—C12—H12B | 108.7 | C25—C30—H30 | 118.9 |
| C13—C12—H12B | 108.7 | O3—C31—C32 | 113.12 (16) |
| H12A—C12—H12B | 107.6 | O3—C31—H31A | 109.0 |
| C14—C13—C17 | 109.87 (14) | C32—C31—H31A | 109.0 |
| C14—C13—C16 | 110.08 (13) | O3—C31—H31B | 109.0 |
| C17—C13—C16 | 109.29 (14) | C32—C31—H31B | 109.0 |
| C14—C13—C12 | 108.27 (12) | H31A—C31—H31B | 107.8 |

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| C17—C13—C12 | 111.03 (13) | C31—C32—H32A | 109.5 |
| C16—C13—C12 | 108.28 (13) | C31—C32—H32B | 109.5 |
| C15—C14—C13 | 112.68 (13) | H32A—C32—H32B | 109.5 |
| C15—C14—H14A | 109.1 | C31—C32—H32C | 109.5 |
| C13—C14—H14A | 109.1 | H32A—C32—H32C | 109.5 |
| C15—C14—H14B | 109.1 | H32B—C32—H32C | 109.5 |
| C13—C14—H14B | 109.1 | C3—N1—C11 | 119.12 (11) |
| H14A—C14—H14B | 107.8 | C3—N1—C18 | 119.81 (11) |
| O1—C15—C10 | 120.74 (13) | C11—N1—C18 | 121.02 (11) |
| O1—C15—C14 | 121.13 (13) | C28—O3—C31 | 118.81 (15) |

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| C6—C1—C2—C3 | −50.29 (17) | C9—C10—C15—C14 | −173.31 (13) |
| C7—C1—C2—C3 | 70.38 (17) | C13—C14—C15—O1 | 148.98 (15) |
| C8—C1—C2—C3 | −169.30 (14) | C13—C14—C15—C10 | −35.1 (2) |
| C1—C2—C3—C4 | 18.00 (19) | N1—C18—C19—C24 | −130.50 (16) |
| C1—C2—C3—N1 | −165.83 (12) | N1—C18—C19—C20 | 49.97 (19) |
| N1—C3—C4—C5 | −163.38 (12) | C24—C19—C20—C21 | 0.1 (3) |
| C2—C3—C4—C5 | 12.7 (2) | C18—C19—C20—C21 | 179.61 (16) |
| N1—C3—C4—C9 | 13.97 (19) | C19—C20—C21—C22 | 0.8 (3) |
| C2—C3—C4—C9 | −169.97 (12) | C20—C21—C22—C23 | −0.3 (4) |
| C3—C4—C5—O2 | 170.96 (14) | C21—C22—C23—C24 | −1.0 (4) |
| C9—C4—C5—O2 | −6.4 (2) | C20—C19—C24—C23 | −1.3 (3) |
| C3—C4—C5—C6 | −7.3 (2) | C18—C19—C24—C23 | 179.12 (18) |
| C9—C4—C5—C6 | 175.34 (13) | C22—C23—C24—C19 | 1.8 (4) |
| O2—C5—C6—C1 | 153.19 (15) | C10—C9—C25—C26 | 10.19 (19) |
| C4—C5—C6—C1 | −28.5 (2) | C4—C9—C25—C26 | −113.05 (15) |
| C2—C1—C6—C5 | 55.69 (18) | C10—C9—C25—C30 | −169.34 (13) |
| C7—C1—C6—C5 | −65.12 (19) | C4—C9—C25—C30 | 67.41 (17) |
| C8—C1—C6—C5 | 174.12 (15) | C30—C25—C26—C27 | 0.8 (2) |
| C3—C4—C9—C10 | −30.37 (17) | C9—C25—C26—C27 | −178.69 (13) |
| C5—C4—C9—C10 | 146.99 (13) | C25—C26—C27—C28 | −0.1 (2) |
| C3—C4—C9—C25 | 95.76 (15) | C26—C27—C28—O3 | 179.40 (14) |
| C5—C4—C9—C25 | −86.89 (15) | C26—C27—C28—C29 | −1.0 (2) |
| C4—C9—C10—C11 | 23.49 (18) | O3—C28—C29—C30 | −179.07 (15) |
| C25—C9—C10—C11 | −101.26 (15) | C27—C28—C29—C30 | 1.4 (2) |
| C4—C9—C10—C15 | −160.71 (12) | C28—C29—C30—C25 | −0.7 (3) |
| C25—C9—C10—C15 | 74.54 (15) | C26—C25—C30—C29 | −0.5 (2) |
| C15—C10—C11—N1 | −176.05 (12) | C9—C25—C30—C29 | 179.10 (14) |
| C9—C10—C11—N1 | −0.4 (2) | C4—C3—N1—C11 | 12.70 (18) |
| C15—C10—C11—C12 | 7.3 (2) | C2—C3—N1—C11 | −163.56 (12) |
| C9—C10—C11—C12 | −176.98 (12) | C4—C3—N1—C18 | −164.86 (12) |
| C10—C11—C12—C13 | 15.91 (19) | C2—C3—N1—C18 | 18.88 (18) |
| N1—C11—C12—C13 | −160.80 (12) | C10—C11—N1—C3 | −19.72 (18) |
| C11—C12—C13—C14 | −45.85 (17) | C12—C11—N1—C3 | 157.07 (12) |
| C11—C12—C13—C17 | 74.84 (16) | C10—C11—N1—C18 | 157.81 (13) |
| C11—C12—C13—C16 | −165.18 (13) | C12—C11—N1—C18 | −25.40 (18) |
| C17—C13—C14—C15 | −66.36 (17) | C19—C18—N1—C3 | 70.01 (16) |
| C16—C13—C14—C15 | 173.24 (14) | C19—C18—N1—C11 | −107.50 (14) |
| C12—C13—C14—C15 | 55.05 (18) | C29—C28—O3—C31 | 0.7 (2) |

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| C11—C10—C15—O1 | 178.49 (14) | C27—C28—O3—C31 | −179.71 (14) |
| C9—C10—C15—O1 | 2.6 (2) | C32—C31—O3—C28 | 77.7 (2) |
| C11—C10—C15—C14 | 2.6 (2) | | |