# 9-Ethyl-3-(2-methylbenzoyl)-9*H*-carbazole

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In the title compound, $C_{22}H_{19}NO$, the dihedral angle between the benzene ring and the carbazole ring system 77.1 (1)°.. The crystal structure is stabilized by intermolecular aromatic $\pi$–$\pi$ interactions between the benzene ring and the pyrrole ring of the carbazole system of neighbouring molecules [centroid–centroid distance = 3.617 (4) Å]. In addition, the crystal structure exhibits a weak intermolecular C—H$\cdots\pi$ interaction.

## Related literature

For the synthesis, see Feng *et al.* (2007); For bond-length data, see: Allen *et al.* (1987). For background, see: Bai *et al.* (2007); Promarak *et al.* (2007); Liu *et al.* (2009).
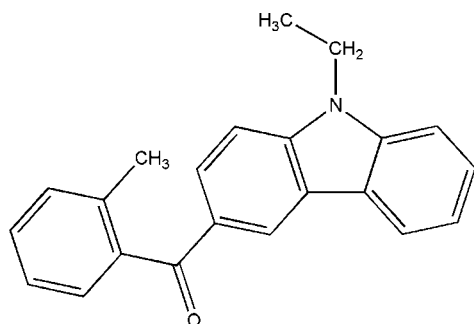
## Experimental

### Crystal data

| | |
|---|---|
| $C_{22}H_{19}NO$ | Monoclinic, $P2_1/c$ |
| $M_r$ = 313.38 | $a$ = 11.676 (2) Å |
| $b$ = 10.569 (2) Å | Mo $K\alpha$ radiation |
| $c$ = 13.756 (3) Å | $\mu$ = 0.08 mm$^{-1}$ |
| $\beta$ = 96.48 (3)° | $T$ = 298 (2) K |
| $V$ = 1686.7 (6) Å$^3$ | $0.30 \times 0.20 \times 0.10$ mm |
| $Z$ = 4 | |

### Data collection

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | 3053 independent reflections |
| Absorption correction: $\psi$ scan (North *et al.*, 1968) | 2046 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.978, $T_{max}$ = 0.993 | 3 standard reflections every 200 reflections intensity decay: 1% |
| 3053 measured reflections | |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.066 | 217 parameters |
| $wR(F^2)$ = 0.173 | H-atom parameters constrained |
| $S$ = 1.08 | $\Delta\rho_{max}$ = 0.37 e Å$^{-3}$ |
| 3053 reflections | $\Delta\rho_{min}$ = −0.32 e Å$^{-3}$ |

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C22—H22B$\cdots$Cg3$^i$ | 0.96 | 2.71 | 3.501 (4) | 140 |

Symmetry codes: (i) $-x, -y + 1, -z$. Cg3 is the centroids of the C16–C21 benzene ring.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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# supporting information

## 9-Ethyl-3-(2-methylbenzoyl)-9*H*-carbazole

### Ye-Chao Hang, Min-Dong Chen and Yong Wang

**S1. Comment**

The title compound is one of important intermediates in synthesis of carbazole-containing compounds used as organic optoelectronic materials which have the characteristic of large $\pi$—$\pi$ conjugation bones (Bai *et al.* 2007; Promarak *et al.* 2007; Liu *et al.* 2009). Here we report the crystal structure of the title compound, 9-ethyl-3-(2-methylbenzoyl)carbazole (Fig. 1).

   In the title compound, the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings of A (C3–8), B (C3/C8/C9/C14/N), C (C9–14) and D (C16–21) are approximately plane, and dihedral angles of the four rings are: A/B = 1.1 (1)°, B/C = 2.6 (1)°, C/D = 76.0 (2)°. The crystals structure is stabilized by intermolecular aromatic $\pi$—$\pi$ interactions between the benzene ring and the pyrrole ring of the carbazole system of neighbouring molecules. The Cg1···Cg2[iii] distance is 3.617 (4) Å (Fig. 2; Cg1 and Cg2 are the centroids of the C3–C8 benzene ring and the C3/C8/C9/C14/N pyrrole ring, respectively, symmetry code as in Fig. 2). The molecular packing is further stabilized by intermolecular C—H···$\pi$ interactions ; one between the hydrogen on the benzene ring and the benzene ring of neighbouring molecules (C12—H12A···Cg1[i]), a second the hydrogen on the benzene ring and the pyrrole ring of neighbouring molecules (C13—H13A···Cg2[i]), a third between the hydrogen of C–22 methyl group and the benzene ring of neighbouring molecules (C22—H22B···Cg3[ii]) (Fig. 2 and Table 1; Cg3 is the centroids of the C16–C21 benzene ring, symmetry code as in Fig. 2).

**S2. Experimental**

The title compound, (I) was prepared by a silimar method reported in literature (Feng *et al.*, 2007) with some modification. The crystals were obtained by dissolving I (0.15 g) in a mixture solvent of methanol (30 ml) and dichloromethane (20 ml) and evaporating the solvent slowly at room temperature for about 2 d.

**S3. Refinement**

H atoms were positioned geometrically, with O—H = 0.82 and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}$(H) = $xU_{eq}$(C/O), where $x$ = 1.2 for aromatic H and $x$ = 1.5 for other H.
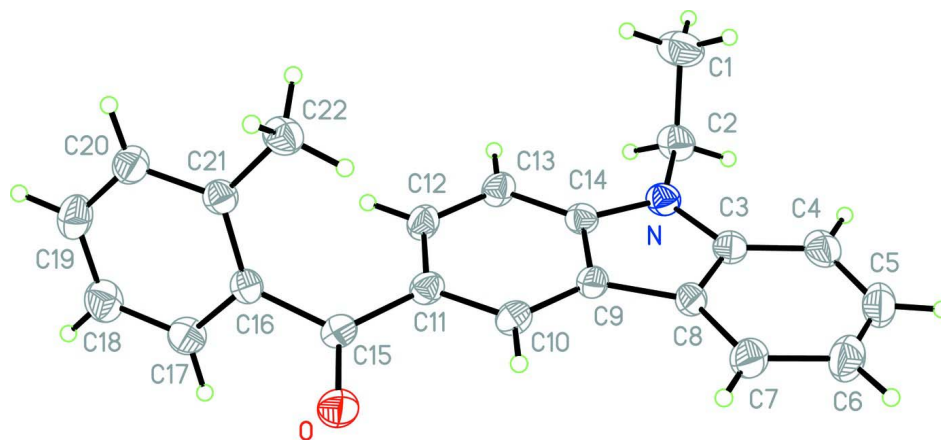
**Figure 1**

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.
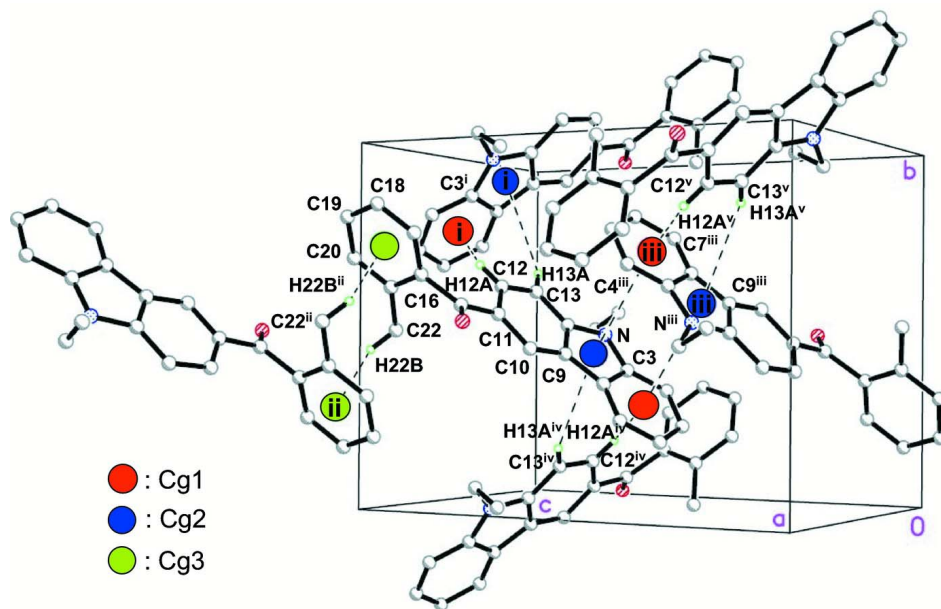


**Figure 2**

$\pi$—$\pi$ and C—H$\cdots\pi$ interactions (dotted lines) in the title compound. Cg denotes ring centroid. [Symmetry code: (i) -x+1, y-1/2, -z+1/2; (ii) -x, -y+1, -z (iii) -x+1, -y+1, -z+1; (iv) -x+1, y+1/2, -z+1/2; (v) x, -y+1/2, z+1/2.]

**9-Ethyl-3-(2-methylbenzoyl)-9H-carbazole**

*Crystal data*

| | |
|---|---|
| $C_{22}H_{19}NO$ | $F(000) = 664$ |
| $M_r = 313.38$ | $D_x = 1.234$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 25 reflections |
| $a = 11.676$ (2) Å | $\theta = 9$–$13°$ |
| $b = 10.569$ (2) Å | $\mu = 0.08$ mm$^{-1}$ |
| $c = 13.756$ (3) Å | $T = 298$ K |
| $\beta = 96.48$ (3)° | Plate, colorless |
| $V = 1686.7$ (6) Å$^3$ | $0.30 \times 0.20 \times 0.10$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | 3053 independent reflections |
| Radiation source: fine-focus sealed tube | 2046 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.000$ |
| $\omega/2\theta$ scans | $\theta_{max} = 25.3°$, $\theta_{min} = 1.8°$ |
| Absorption correction: $\psi$ scan (North *et al.*, 1968) | $h = -14 \rightarrow 13$ |
| | $k = 0 \rightarrow 12$ |
| $T_{min} = 0.978$, $T_{max} = 0.993$ | $l = 0 \rightarrow 16$ |
| 3053 measured reflections | 3 standard reflections every 200 reflections |
| | intensity decay: 1% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.066$ | Hydrogen site location: difference Fourier map |
| $wR(F^2) = 0.173$ | H-atom parameters constrained |
| $S = 1.08$ | $w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 1.9857P]$ |
| 3053 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 217 parameters | $(\Delta/\sigma)_{max} < 0.001$ |
| 0 restraints | $\Delta\rho_{max} = 0.37$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -0.32$ e Å$^{-3}$ |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| O | 0.04033 (19) | 0.4866 (2) | 0.24020 (17) | 0.0606 (7) |
| N | 0.5747 (2) | 0.5162 (3) | 0.36517 (18) | 0.0451 (6) |
| C1 | 0.7412 (3) | 0.4981 (4) | 0.2716 (3) | 0.0768 (12) |
| H1A | 0.8113 | 0.4515 | 0.2686 | 0.115* |
| H1B | 0.7588 | 0.5864 | 0.2808 | 0.115* |
| H1C | 0.6917 | 0.4868 | 0.2116 | 0.115* |
| C2 | 0.6818 (3) | 0.4509 (4) | 0.3554 (2) | 0.0554 (9) |
| H2A | 0.6661 | 0.3613 | 0.3465 | 0.066* |
| H2B | 0.7330 | 0.4610 | 0.4155 | 0.066* |
| C3 | 0.5588 (3) | 0.6168 (3) | 0.4282 (2) | 0.0456 (8) |
| C4 | 0.6411 (3) | 0.6748 (4) | 0.4954 (2) | 0.0576 (9) |
| H4A | 0.7177 | 0.6492 | 0.5033 | 0.069* |
| C5 | 0.6016 (4) | 0.7725 (4) | 0.5493 (3) | 0.0660 (11) |
| H5A | 0.6532 | 0.8118 | 0.5963 | 0.079* |
| C6 | 0.4896 (4) | 0.8141 (3) | 0.5365 (3) | 0.0640 (10) |

| | | | | |
|---|---|---|---|---|
| H6A | 0.4681 | 0.8827 | 0.5727 | 0.077* |
| C7 | 0.4076 (3) | 0.7551 (3) | 0.4703 (2) | 0.0549 (9) |
| H7A | 0.3311 | 0.7817 | 0.4630 | 0.066* |
| C8 | 0.4436 (3) | 0.6549 (3) | 0.4150 (2) | 0.0402 (7) |
| C9 | 0.3850 (2) | 0.5716 (3) | 0.3427 (2) | 0.0393 (7) |
| C10 | 0.2712 (3) | 0.5577 (3) | 0.3037 (2) | 0.0414 (7) |
| H10A | 0.2149 | 0.6117 | 0.3228 | 0.050* |
| C11 | 0.2415 (2) | 0.4626 (3) | 0.2359 (2) | 0.0414 (7) |
| C12 | 0.3274 (3) | 0.3846 (3) | 0.2051 (2) | 0.0458 (8) |
| H12A | 0.3070 | 0.3236 | 0.1575 | 0.055* |
| C13 | 0.4413 (3) | 0.3958 (3) | 0.2433 (2) | 0.0451 (7) |
| H13A | 0.4976 | 0.3423 | 0.2235 | 0.054* |
| C14 | 0.4691 (2) | 0.4903 (3) | 0.3127 (2) | 0.0395 (7) |
| C15 | 0.1190 (3) | 0.4411 (3) | 0.1988 (2) | 0.0433 (7) |
| C16 | 0.0876 (2) | 0.3582 (3) | 0.1113 (2) | 0.0380 (7) |
| C17 | 0.0254 (3) | 0.2480 (3) | 0.1238 (2) | 0.0511 (8) |
| H17A | 0.0064 | 0.2274 | 0.1857 | 0.061* |
| C18 | −0.0088 (3) | 0.1689 (3) | 0.0462 (3) | 0.0604 (9) |
| H18A | −0.0489 | 0.0948 | 0.0560 | 0.072* |
| C19 | 0.0167 (3) | 0.2000 (3) | −0.0451 (3) | 0.0588 (9) |
| H19A | −0.0060 | 0.1474 | −0.0979 | 0.071* |
| C20 | 0.0767 (3) | 0.3106 (3) | −0.0587 (2) | 0.0524 (8) |
| H20A | 0.0914 | 0.3322 | −0.1216 | 0.063* |
| C21 | 0.1159 (2) | 0.3909 (3) | 0.0190 (2) | 0.0421 (7) |
| C22 | 0.1797 (3) | 0.5092 (3) | 0.0004 (2) | 0.0508 (8) |
| H22A | 0.2030 | 0.5510 | 0.0613 | 0.076* |
| H22B | 0.1305 | 0.5642 | −0.0412 | 0.076* |
| H22C | 0.2466 | 0.4884 | −0.0310 | 0.076* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O | 0.0475 (13) | 0.0765 (18) | 0.0590 (14) | 0.0061 (12) | 0.0109 (11) | −0.0164 (13) |
| N | 0.0360 (13) | 0.0548 (17) | 0.0444 (14) | 0.0025 (12) | 0.0042 (11) | 0.0022 (13) |
| C1 | 0.055 (2) | 0.101 (3) | 0.079 (3) | 0.000 (2) | 0.022 (2) | 0.010 (2) |
| C2 | 0.0350 (17) | 0.073 (2) | 0.057 (2) | 0.0078 (16) | −0.0005 (14) | 0.0077 (18) |
| C3 | 0.0535 (19) | 0.0459 (18) | 0.0378 (16) | −0.0090 (15) | 0.0062 (14) | 0.0069 (14) |
| C4 | 0.061 (2) | 0.066 (2) | 0.0453 (18) | −0.0179 (19) | 0.0015 (16) | 0.0135 (18) |
| C5 | 0.082 (3) | 0.065 (3) | 0.048 (2) | −0.029 (2) | −0.0035 (19) | −0.0012 (19) |
| C6 | 0.086 (3) | 0.047 (2) | 0.058 (2) | −0.012 (2) | 0.004 (2) | −0.0085 (18) |
| C7 | 0.069 (2) | 0.0419 (19) | 0.055 (2) | −0.0072 (17) | 0.0134 (17) | −0.0039 (16) |
| C8 | 0.0474 (17) | 0.0347 (16) | 0.0390 (15) | −0.0078 (13) | 0.0067 (13) | 0.0000 (13) |
| C9 | 0.0436 (16) | 0.0357 (16) | 0.0392 (15) | −0.0034 (13) | 0.0080 (13) | −0.0042 (13) |
| C10 | 0.0467 (17) | 0.0364 (16) | 0.0417 (16) | 0.0084 (14) | 0.0076 (13) | −0.0028 (13) |
| C11 | 0.0424 (17) | 0.0423 (18) | 0.0400 (16) | 0.0050 (14) | 0.0070 (13) | −0.0048 (14) |
| C12 | 0.0475 (18) | 0.0461 (18) | 0.0438 (17) | 0.0018 (15) | 0.0047 (14) | −0.0114 (15) |
| C13 | 0.0447 (17) | 0.0450 (18) | 0.0459 (17) | 0.0078 (14) | 0.0061 (14) | −0.0102 (15) |
| C14 | 0.0365 (15) | 0.0432 (17) | 0.0393 (15) | 0.0024 (13) | 0.0060 (12) | 0.0016 (13) |

| C15 | 0.0465 (17) | 0.0463 (18) | 0.0375 (15) | 0.0032 (15) | 0.0071 (14) | −0.0018 (14) |
|-----|-------------|-------------|-------------|-------------|-------------|--------------|
| C16 | 0.0338 (14) | 0.0382 (16) | 0.0411 (15) | 0.0042 (13) | 0.0006 (12) | 0.0021 (13) |
| C17 | 0.058 (2) | 0.0434 (19) | 0.0521 (18) | −0.0050 (16) | 0.0080 (16) | 0.0064 (16) |
| C18 | 0.065 (2) | 0.046 (2) | 0.070 (2) | −0.0097 (17) | 0.0068 (19) | −0.0054 (18) |
| C19 | 0.063 (2) | 0.053 (2) | 0.058 (2) | −0.0001 (18) | −0.0026 (18) | −0.0151 (18) |
| C20 | 0.0509 (19) | 0.061 (2) | 0.0444 (17) | 0.0020 (17) | 0.0023 (15) | −0.0029 (16) |
| C21 | 0.0371 (16) | 0.0461 (18) | 0.0432 (16) | 0.0034 (13) | 0.0043 (13) | 0.0011 (14) |
| C22 | 0.0528 (19) | 0.0474 (19) | 0.0525 (19) | −0.0042 (15) | 0.0066 (15) | 0.0100 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O—C15 | 1.231 (3) | C10—C11 | 1.388 (4) |
| N—C14 | 1.384 (4) | C10—H10A | 0.9300 |
| N—C3 | 1.397 (4) | C11—C12 | 1.400 (4) |
| N—C2 | 1.448 (4) | C11—C15 | 1.481 (4) |
| C1—C2 | 1.497 (5) | C12—C13 | 1.380 (4) |
| C1—H1A | 0.9600 | C12—H12A | 0.9300 |
| C1—H1B | 0.9600 | C13—C14 | 1.394 (4) |
| C1—H1C | 0.9600 | C13—H13A | 0.9300 |
| C2—H2A | 0.9700 | C15—C16 | 1.501 (4) |
| C2—H2B | 0.9700 | C16—C17 | 1.392 (4) |
| C3—C4 | 1.397 (4) | C16—C21 | 1.392 (4) |
| C3—C8 | 1.397 (4) | C17—C18 | 1.379 (5) |
| C4—C5 | 1.380 (5) | C17—H17A | 0.9300 |
| C4—H4A | 0.9300 | C18—C19 | 1.363 (5) |
| C5—C6 | 1.373 (5) | C18—H18A | 0.9300 |
| C5—H5A | 0.9300 | C19—C20 | 1.385 (5) |
| C6—C7 | 1.393 (5) | C19—H19A | 0.9300 |
| C6—H6A | 0.9300 | C20—C21 | 1.401 (4) |
| C7—C8 | 1.396 (4) | C20—H20A | 0.9300 |
| C7—H7A | 0.9300 | C21—C22 | 1.492 (4) |
| C8—C9 | 1.441 (4) | C22—H22A | 0.9600 |
| C9—C10 | 1.385 (4) | C22—H22B | 0.9600 |
| C9—C14 | 1.401 (4) | C22—H22C | 0.9600 |
| | | | |
| C14—N—C3 | 107.6 (2) | C10—C11—C12 | 119.8 (3) |
| C14—N—C2 | 125.8 (3) | C10—C11—C15 | 120.0 (3) |
| C3—N—C2 | 126.6 (3) | C12—C11—C15 | 120.2 (3) |
| C2—C1—H1A | 109.5 | C13—C12—C11 | 121.8 (3) |
| C2—C1—H1B | 109.5 | C13—C12—H12A | 119.1 |
| H1A—C1—H1B | 109.5 | C11—C12—H12A | 119.1 |
| C2—C1—H1C | 109.5 | C12—C13—C14 | 117.5 (3) |
| H1A—C1—H1C | 109.5 | C12—C13—H13A | 121.2 |
| H1B—C1—H1C | 109.5 | C14—C13—H13A | 121.2 |
| N—C2—C1 | 113.1 (3) | N—C14—C13 | 128.6 (3) |
| N—C2—H2A | 109.0 | N—C14—C9 | 109.7 (3) |
| C1—C2—H2A | 109.0 | C13—C14—C9 | 121.7 (3) |
| N—C2—H2B | 109.0 | O—C15—C11 | 121.5 (3) |

| | | | |
|---|---|---|---|
| C1—C2—H2B | 109.0 | O—C15—C16 | 118.1 (3) |
| H2A—C2—H2B | 107.8 | C11—C15—C16 | 120.3 (3) |
| N—C3—C4 | 128.0 (3) | C17—C16—C21 | 120.0 (3) |
| N—C3—C8 | 109.4 (3) | C17—C16—C15 | 118.3 (3) |
| C4—C3—C8 | 122.6 (3) | C21—C16—C15 | 121.7 (3) |
| C5—C4—C3 | 116.0 (3) | C18—C17—C16 | 121.4 (3) |
| C5—C4—H4A | 122.0 | C18—C17—H17A | 119.3 |
| C3—C4—H4A | 122.0 | C16—C17—H17A | 119.3 |
| C6—C5—C4 | 122.8 (3) | C19—C18—C17 | 119.5 (3) |
| C6—C5—H5A | 118.6 | C19—C18—H18A | 120.2 |
| C4—C5—H5A | 118.6 | C17—C18—H18A | 120.2 |
| C5—C6—C7 | 121.0 (4) | C18—C19—C20 | 119.6 (3) |
| C5—C6—H6A | 119.5 | C18—C19—H19A | 120.2 |
| C7—C6—H6A | 119.5 | C20—C19—H19A | 120.2 |
| C6—C7—C8 | 118.0 (3) | C19—C20—C21 | 122.3 (3) |
| C6—C7—H7A | 121.0 | C19—C20—H20A | 118.8 |
| C8—C7—H7A | 121.0 | C21—C20—H20A | 118.8 |
| C7—C8—C3 | 119.6 (3) | C16—C21—C20 | 117.0 (3) |
| C7—C8—C9 | 133.7 (3) | C16—C21—C22 | 122.7 (3) |
| C3—C8—C9 | 106.7 (3) | C20—C21—C22 | 120.2 (3) |
| C10—C9—C14 | 119.6 (3) | C21—C22—H22A | 109.5 |
| C10—C9—C8 | 133.8 (3) | C21—C22—H22B | 109.5 |
| C14—C9—C8 | 106.6 (3) | H22A—C22—H22B | 109.5 |
| C9—C10—C11 | 119.6 (3) | C21—C22—H22C | 109.5 |
| C9—C10—H10A | 120.2 | H22A—C22—H22C | 109.5 |
| C11—C10—H10A | 120.2 | H22B—C22—H22C | 109.5 |
| | | | |
| C14—N—C2—C1 | 82.1 (4) | C2—N—C14—C13 | 2.5 (5) |
| C3—N—C2—C1 | −97.4 (4) | C3—N—C14—C9 | −1.2 (3) |
| C14—N—C3—C4 | 179.7 (3) | C2—N—C14—C9 | 179.2 (3) |
| C2—N—C3—C4 | −0.7 (5) | C12—C13—C14—N | 176.2 (3) |
| C14—N—C3—C8 | −0.4 (3) | C12—C13—C14—C9 | −0.2 (5) |
| C2—N—C3—C8 | 179.2 (3) | C10—C9—C14—N | −176.4 (3) |
| N—C3—C4—C5 | −179.6 (3) | C8—C9—C14—N | 2.2 (3) |
| C8—C3—C4—C5 | 0.5 (5) | C10—C9—C14—C13 | 0.6 (4) |
| C3—C4—C5—C6 | −2.0 (5) | C8—C9—C14—C13 | 179.2 (3) |
| C4—C5—C6—C7 | 2.8 (6) | C10—C11—C15—O | −15.2 (5) |
| C5—C6—C7—C8 | −2.0 (5) | C12—C11—C15—O | 162.8 (3) |
| C6—C7—C8—C3 | 0.5 (5) | C10—C11—C15—C16 | 167.3 (3) |
| C6—C7—C8—C9 | 178.6 (3) | C12—C11—C15—C16 | −14.7 (4) |
| N—C3—C8—C7 | −179.7 (3) | O—C15—C16—C17 | −60.7 (4) |
| C4—C3—C8—C7 | 0.2 (5) | C11—C15—C16—C17 | 116.9 (3) |
| N—C3—C8—C9 | 1.8 (3) | O—C15—C16—C21 | 117.3 (3) |
| C4—C3—C8—C9 | −178.3 (3) | C11—C15—C16—C21 | −65.2 (4) |
| C7—C8—C9—C10 | −2.4 (6) | C21—C16—C17—C18 | 0.5 (5) |
| C3—C8—C9—C10 | 175.9 (3) | C15—C16—C17—C18 | 178.5 (3) |
| C7—C8—C9—C14 | 179.3 (3) | C16—C17—C18—C19 | −1.3 (5) |
| C3—C8—C9—C14 | −2.4 (3) | C17—C18—C19—C20 | 0.1 (5) |

| | | | |
|---|---|---|---|
| C14—C9—C10—C11 | 0.6 (4) | C18—C19—C20—C21 | 2.1 (5) |
| C8—C9—C10—C11 | −177.5 (3) | C17—C16—C21—C20 | 1.5 (4) |
| C9—C10—C11—C12 | −2.2 (4) | C15—C16—C21—C20 | −176.4 (3) |
| C9—C10—C11—C15 | 175.7 (3) | C17—C16—C21—C22 | 178.4 (3) |
| C10—C11—C12—C13 | 2.8 (5) | C15—C16—C21—C22 | 0.5 (4) |
| C15—C11—C12—C13 | −175.2 (3) | C19—C20—C21—C16 | −2.8 (5) |
| C11—C12—C13—C14 | −1.5 (5) | C19—C20—C21—C22 | −179.8 (3) |
| C3—N—C14—C13 | −177.9 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| $D$—H$\cdots$$A$ | $D$—H | H$\cdots$$A$ | $D$$\cdots$$A$ | $D$—H$\cdots$$A$ |
|---|---|---|---|---|
| C12—H12$A$$\cdots$$Cg$1[i] | 0.93 | 3.13 | 3.730 (4) | 124 |
| C13—H13$A$$\cdots$$Cg$2[i] | 0.93 | 3.18 | 3.928 (4) | 138 |
| C22—H22$B$$\cdots$$Cg$3[ii] | 0.96 | 2.71 | 3.501 (4) | 140 |

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*, −*y*+1, −*z*.