Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 5-Methoxy-3-[(5-methoxy-1*H*-indol-3-yl)(phenyl)methyl]-1*H*-indole

**P. Narayanan,[a] K. Sethusankar,[a]* K. Ramachandiran[b] and P. T. Perumal[b]**

[a]Department of Physics, RKM Vivekananda College (Autonomous), Chennai 600 004, India, and [b]Organic Chemistry Division, Central Leather Research Institute, Adyar, Chennai 600 020, India
Correspondence e-mail: ksethusankar@yahoo.co.in

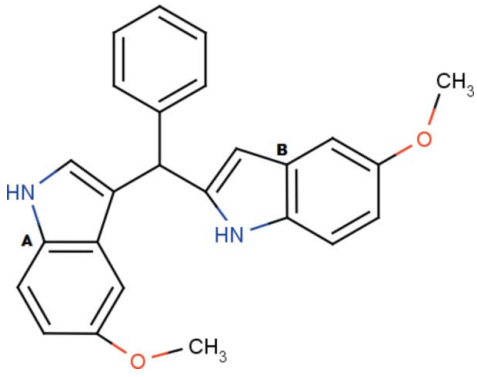
Received 13 October 2011; accepted 29 October 2011

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.041; $wR$ factor = 0.119; data-to-parameter ratio = 11.7.

In the title compound, $C_{25}H_{22}N_2O_2$, the indole rings are individually almost planar [with maximum deviations of 0.0116 (19) and 0.0113 (18) Å] and are almost orthogonal to each other, making a dihedral angle of 84.49 (6)°. The benzene ring is inclined at 72.83 (9) and 80.85 (9)° with respect to the indole rings. In the crystal, molecules are linked by N—H···O interactions into chains running parallel to the $c$ axis. The crystal structure is further stabilized by C—H···$\pi$ interactions.

## Related literature

For the biological activity and uses of indole derivatives, see: Bell *et al.* (1994); Ge *et al.* (1996). For related structures, see: Zhang *et al.* (2006, 2007).




## Experimental

### Crystal data

$C_{25}H_{22}N_2O_2$
$M_r$ = 382.45
Monoclinic, $P2_1/n$
$a$ = 9.1545 (4) Å
$b$ = 10.5954 (6) Å
$c$ = 21.1668 (13) Å
$\beta$ = 93.679 (2)°
$V$ = 2048.86 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 K
0.25 × 0.20 × 0.15 mm

### Data collection

Bruker APEXII KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.981, $T_{max}$ = 0.988
16790 measured reflections
3087 independent reflections
2317 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 23.7°

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.119
$S$ = 1.03
3087 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

*Cg*2, *Cg*3, *Cg*4 and *Cg*5 are the centroids of the N2/C17–C20, C1–C6, C10–C15 and C19–C24 rings, respectively

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*A*···O2$^{i}$ | 0.86 | 2.09 | 2.904 (2) | 158 |
| C25—H25*B*···*Cg*2$^{ii}$ | 0.96 | 2.95 | 3.515 (3) | 119 |
| C16—H16*C*···*Cg*3$^{iii}$ | 0.96 | 2.90 | 3.508 (3) | 122 |
| N2—H2*A*···*Cg*4$^{iv}$ | 0.86 | 2.49 | 3.3149 (19) | 160 |
| C3—H3···*Cg*5$^{v}$ | 0.93 | 2.60 | 3.470 (2) | 157 |

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+1, y, z$; (iv) $-x+2, -y+1, -z+1$; (v) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

PN and KS thank Dr Babu Varghese, Senior Scientific Officer, SAIF, IIT, Chennai, India, for the X-ray intensity data collection and Dr V. Murugan, Head of the Department of Physics, for providing facilities in the department to carry out this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2461).

## References

Bell, R., Carmeli, S. & Sar, N. (1994). *J. Nat. Prod.* **57**, 1587–1590.
Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Ge, X., Yannai, S., Rennert, G., Gruener, N. & Fares, F. A. (1996). *Biochem. Biophys. Res. Commun.* **228**, pp. 153–158.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Zhang, D.-M., Tang, Q.-G., Ji, C.-X. & Guo, C. (2007). *Acta Cryst.* E**63**, o81–o82.
Zhang, D.-M., Tang, S.-G., Wu, W.-Y., Tang, Q.-G. & Guo, C. (2006). *Acta Cryst.* E**62**, o5467–o5468.

# supporting information

*Acta Cryst.* (2011). E**67**, o3196 [https://doi.org/10.1107/S1600536811045491]

## 5-Methoxy-3-[(5-methoxy-1*H*-indol-3-yl)(phenyl)methyl]-1*H*-indole

**P. Narayanan, K. Sethusankar, K. Ramachandiran and P. T. Perumal**

### S1. Comment

The synthesis of bis-indolylalkanes (BIAs) has been of considerable interest because of their occurance in various natural products posessing biological activities and usefulness in drug design (Bell, *et al.* 1994). These compounds also inhibit the proliferation of both estrogen dependent and independent cultured breast tumor cells (Ge, *et al.* 1996). In this paper, we present the synthesis and crystal structure of the title bis-indolylalkane derivative.

The title compound (Fig. 1) comprises a benzene ring and two methoxy indole rings connected through a carbon atom C7. The bicyclic indole rings, are individually planar with maximum deviations of 0.0116 (19)Å for C10 atom, in ring A (N1/C8–C15) and -0.0113 (18)Å for N2 atom, in ring B (N2/C17–C24). The indole rings are almost orthogonal to each other, with a dihedral angle of 84.49 (6)°. The deviations of methoxy group carbon atoms C16 and C25 from the rings A & B, are -0.118 (3)Å and -0.100 (3) Å, respectively.

The benzene ring (C1–C6) is inclined at 72.83 (9)° and 80.85 (9)°, with the indole rings A & B, respectively. The angles around atom C7 [C8–C7–C17 = 113.07 (14)°, C8–C7–C6 = 112.52 (14)° and C17–C7–C6 = 111.53 (15)°] deviate significantly from the ideal tetrahedral values which may be a result of steric interactions between benzene ring and the indole rings.

In the crystal packing, the molecules are linked by N—H···O intermolecular interactions into infinite chains running parallel to the *c* axis (Fig. 2). The crystal structure is further stabilized by C—H···*Cg* interactions where *Cg*2, *Cg*3, *Cg*4 and *Cg*5 are the centers of gravity of rings (N2/C17–C20), (C1–C6), (C10–C15) and (C19–C24), respectively (Table 1).

### S2. Experimental

To benzaldehyde (1 mmol) in $CH_2Cl_2$ (10 ml) was added $KHSO_4$ (30 mol%) and the mixture was stirred for 5 min. Methoxyindole (2 mmol) was added to the mixture and the stirring was continued following the progress of the reaction by TLC. After completion of the reaction, the reaction mixture was extracted with ethyl acetate (3 *x* 10 ml), dried over anhydrous sodium sulfate, filtered, concentrated under reduced pressure and the residue was column chromatographed over silica gel using EtOAc/Petroleum ether (1:19) as eluent to get the pure product, the title compound, which was recrystallized by slow evaporation of its solution in ethyl acetate, resulting in single crystals, suitable for XRD studies.

### S3. Refinement

The hydrogen atoms were placed in calculated positions with C–H = 0.93 to 0.98 and N–H = 0.86 Å and refined in the riding model with fixed isotropic displacement parameters: $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl groups and $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*) for others. The crystal did not diffract beyond $\theta$ =23.7 ° as its mosaicity was quite high and a low temperature facility was not used for intensity data collection.

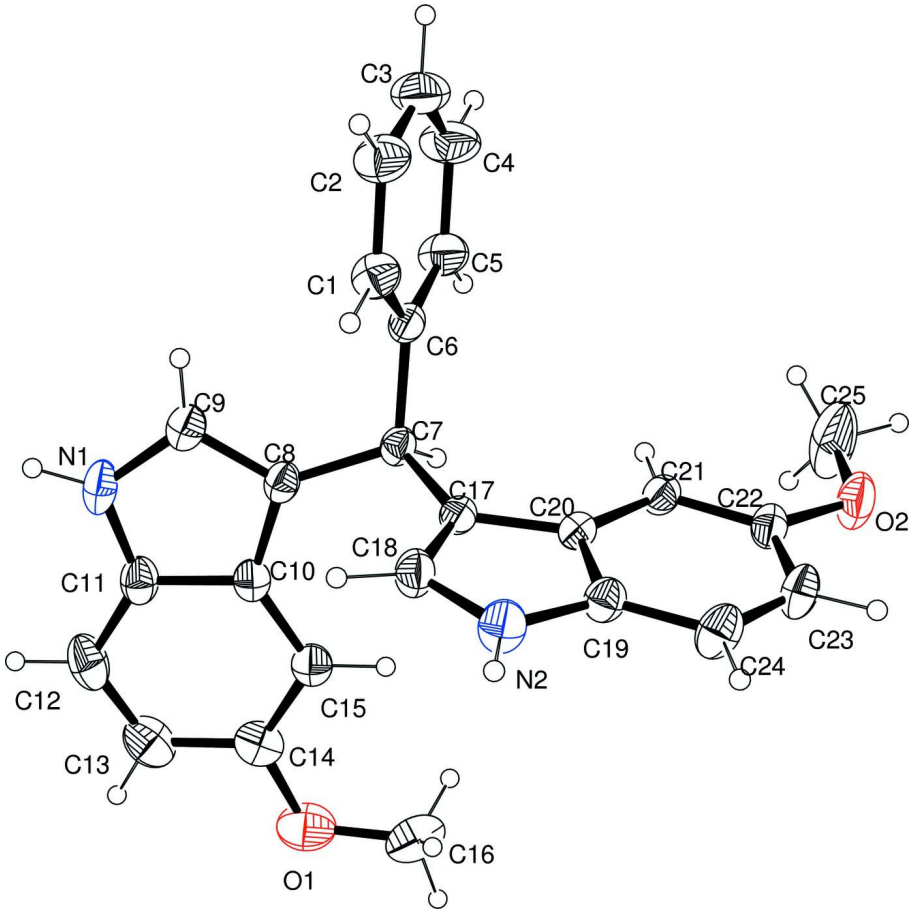



**Figure 1**

The molecular structure of the title compound with the atom numbering scheme; displacement ellipsoids are drawn at 30% probability level.

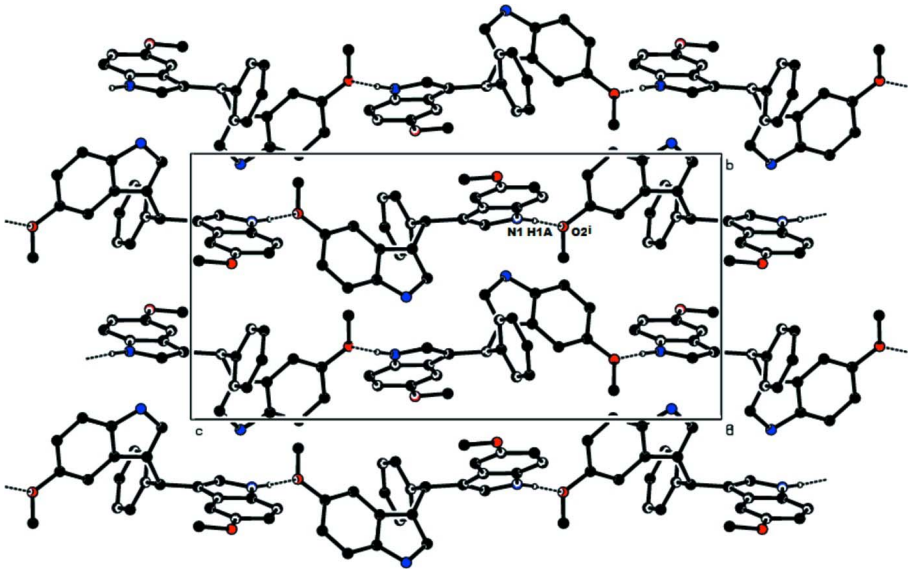



**Figure 2**

The packing arrangement of the title compound viewed down the *a* axis. The dashed lines indicate N—H···O intermolecular interactions resulting in chaims of molecules running parallel to the *c* axis.

## 5-Methoxy-3-[(5-methoxy-1*H*-indol-3-yl)(phenyl)methyl]-1*H*-indole

*Crystal data*

$C_{25}H_{22}N_2O_2$
$M_r = 382.45$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.1545\ (4)$ Å
$b = 10.5954\ (6)$ Å
$c = 21.1668\ (13)$ Å
$\beta = 93.679\ (2)°$
$V = 2048.86\ (19)$ Å$^3$
$Z = 4$
$F(000) = 808$
$D_x = 1.240$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3087 reflections
$\theta = 2.2–23.7°$
$\mu = 0.08$ mm$^{-1}$
$T = 293$ K
Block, brown
0.25 × 0.20 × 0.15 mm

*Data collection*

Bruker APEXII KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.981$, $T_{max} = 0.988$
16790 measured reflections
3087 independent reflections
2317 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 23.7°$, $\theta_{min} = 2.2°$
$h = -7\rightarrow10$
$k = -11\rightarrow11$
$l = -22\rightarrow23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.119$
$S = 1.03$
3087 reflections
264 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

$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 0.4003P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å$^{-3}$
$\Delta\rho_{min} = -0.18$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4797 (2) | 0.37371 (19) | 0.41816 (10) | 0.0532 (5) |
| H1 | 0.5236 | 0.4447 | 0.4370 | 0.064* |
| C2 | 0.3360 (2) | 0.3804 (2) | 0.39415 (11) | 0.0661 (6) |
| H2 | 0.2837 | 0.4552 | 0.3973 | 0.079* |
| C3 | 0.2704 (2) | 0.2767 (3) | 0.36573 (12) | 0.0748 (7) |
| H3 | 0.1739 | 0.2812 | 0.3493 | 0.090* |
| C4 | 0.3477 (2) | 0.1667 (3) | 0.36166 (12) | 0.0776 (8) |
| H4 | 0.3033 | 0.0962 | 0.3426 | 0.093* |
| C5 | 0.4916 (2) | 0.1600 (2) | 0.38590 (10) | 0.0580 (6) |
| H5 | 0.5433 | 0.0850 | 0.3827 | 0.070* |
| C6 | 0.55940 (18) | 0.26319 (17) | 0.41470 (8) | 0.0405 (5) |
| C7 | 0.71658 (18) | 0.25468 (16) | 0.44225 (8) | 0.0374 (4) |
| H7 | 0.7559 | 0.1752 | 0.4268 | 0.045* |
| C8 | 0.72666 (19) | 0.24617 (17) | 0.51335 (8) | 0.0394 (4) |
| C9 | 0.6212 (2) | 0.26862 (18) | 0.55446 (9) | 0.0493 (5) |
| H9 | 0.5270 | 0.2967 | 0.5429 | 0.059* |
| C10 | 0.85246 (19) | 0.20426 (17) | 0.55141 (8) | 0.0402 (4) |
| C11 | 0.8153 (2) | 0.20311 (18) | 0.61463 (9) | 0.0489 (5) |
| C12 | 0.9142 (3) | 0.1637 (2) | 0.66314 (10) | 0.0639 (6) |
| H12 | 0.8885 | 0.1626 | 0.7049 | 0.077* |
| C13 | 1.0503 (3) | 0.1267 (2) | 0.64757 (11) | 0.0681 (6) |
| H13 | 1.1183 | 0.1007 | 0.6795 | 0.082* |
| C14 | 1.0901 (2) | 0.1267 (2) | 0.58488 (11) | 0.0566 (6) |
| C15 | 0.9929 (2) | 0.16574 (17) | 0.53660 (9) | 0.0460 (5) |
| H15 | 1.0197 | 0.1666 | 0.4950 | 0.055* |
| C16 | 1.2814 (2) | 0.0968 (2) | 0.51545 (13) | 0.0767 (7) |
| H16A | 1.2214 | 0.0460 | 0.4866 | 0.115* |
| H16B | 1.3809 | 0.0682 | 0.5160 | 0.115* |
| H16C | 1.2763 | 0.1834 | 0.5020 | 0.115* |
| C17 | 0.80985 (17) | 0.35843 (17) | 0.41750 (8) | 0.0378 (4) |

| | | | | |
|---|---|---|---|---|
| C18 | 0.8511 (2) | 0.46889 (19) | 0.44561 (9) | 0.0502 (5) |
| H18 | 0.8282 | 0.4933 | 0.4860 | 0.060* |
| C19 | 0.94249 (19) | 0.47413 (18) | 0.35062 (9) | 0.0445 (5) |
| C20 | 0.86769 (17) | 0.35972 (16) | 0.35638 (8) | 0.0365 (4) |
| C21 | 0.86324 (18) | 0.27284 (18) | 0.30657 (8) | 0.0422 (5) |
| H21 | 0.8142 | 0.1964 | 0.3095 | 0.051* |
| C22 | 0.9332 (2) | 0.30362 (19) | 0.25334 (9) | 0.0468 (5) |
| C23 | 1.0038 (2) | 0.4195 (2) | 0.24795 (10) | 0.0566 (6) |
| H23 | 1.0473 | 0.4387 | 0.2106 | 0.068* |
| C24 | 1.0106 (2) | 0.5050 (2) | 0.29604 (10) | 0.0571 (6) |
| H24 | 1.0592 | 0.5815 | 0.2924 | 0.069* |
| C25 | 0.8751 (4) | 0.1091 (3) | 0.20263 (14) | 0.1214 (14) |
| H25A | 0.9235 | 0.0574 | 0.2348 | 0.182* |
| H25B | 0.8804 | 0.0692 | 0.1621 | 0.182* |
| H25C | 0.7744 | 0.1199 | 0.2116 | 0.182* |
| N1 | 0.6733 (2) | 0.24406 (16) | 0.61507 (8) | 0.0585 (5) |
| H1A | 0.6248 | 0.2529 | 0.6483 | 0.070* |
| N2 | 0.93115 (18) | 0.53917 (16) | 0.40619 (8) | 0.0568 (5) |
| H2A | 0.9683 | 0.6122 | 0.4148 | 0.068* |
| O1 | 1.23040 (17) | 0.08657 (16) | 0.57707 (8) | 0.0778 (5) |
| O2 | 0.94253 (17) | 0.22539 (15) | 0.20173 (7) | 0.0693 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0506 (12) | 0.0478 (13) | 0.0616 (14) | 0.0015 (10) | 0.0059 (10) | −0.0035 (10) |
| C2 | 0.0535 (13) | 0.0641 (16) | 0.0804 (17) | 0.0134 (11) | 0.0026 (11) | −0.0016 (13) |
| C3 | 0.0444 (12) | 0.092 (2) | 0.0867 (18) | 0.0084 (13) | −0.0066 (11) | −0.0137 (15) |
| C4 | 0.0510 (13) | 0.0825 (19) | 0.097 (2) | −0.0035 (13) | −0.0095 (12) | −0.0342 (15) |
| C5 | 0.0470 (11) | 0.0568 (14) | 0.0701 (15) | 0.0024 (10) | 0.0022 (10) | −0.0191 (11) |
| C6 | 0.0387 (10) | 0.0447 (12) | 0.0390 (11) | −0.0023 (8) | 0.0090 (8) | −0.0032 (8) |
| C7 | 0.0385 (9) | 0.0368 (10) | 0.0376 (11) | −0.0013 (8) | 0.0088 (8) | −0.0050 (8) |
| C8 | 0.0442 (10) | 0.0363 (11) | 0.0390 (11) | −0.0053 (8) | 0.0115 (8) | −0.0025 (8) |
| C9 | 0.0522 (11) | 0.0499 (12) | 0.0472 (13) | −0.0019 (9) | 0.0134 (10) | −0.0004 (9) |
| C10 | 0.0504 (11) | 0.0320 (10) | 0.0387 (11) | −0.0068 (8) | 0.0072 (8) | −0.0012 (8) |
| C11 | 0.0643 (13) | 0.0415 (12) | 0.0419 (12) | −0.0069 (10) | 0.0118 (10) | 0.0000 (9) |
| C12 | 0.0972 (18) | 0.0559 (14) | 0.0384 (12) | −0.0070 (13) | 0.0021 (12) | 0.0074 (10) |
| C13 | 0.0833 (17) | 0.0560 (15) | 0.0626 (16) | 0.0029 (12) | −0.0130 (13) | 0.0122 (12) |
| C14 | 0.0611 (13) | 0.0438 (13) | 0.0641 (15) | −0.0001 (10) | −0.0033 (11) | 0.0032 (10) |
| C15 | 0.0514 (11) | 0.0403 (11) | 0.0464 (12) | −0.0042 (9) | 0.0046 (9) | −0.0017 (9) |
| C16 | 0.0547 (13) | 0.0661 (17) | 0.111 (2) | 0.0008 (11) | 0.0160 (14) | 0.0084 (15) |
| C17 | 0.0364 (9) | 0.0403 (11) | 0.0372 (11) | −0.0024 (8) | 0.0056 (8) | −0.0028 (8) |
| C18 | 0.0574 (12) | 0.0516 (13) | 0.0427 (11) | −0.0084 (10) | 0.0122 (9) | −0.0075 (10) |
| C19 | 0.0474 (10) | 0.0405 (11) | 0.0463 (12) | −0.0032 (9) | 0.0079 (9) | 0.0011 (9) |
| C20 | 0.0341 (9) | 0.0378 (11) | 0.0379 (11) | −0.0009 (8) | 0.0047 (7) | 0.0008 (8) |
| C21 | 0.0402 (10) | 0.0454 (12) | 0.0418 (11) | −0.0063 (8) | 0.0089 (8) | −0.0014 (9) |
| C22 | 0.0490 (11) | 0.0546 (13) | 0.0379 (11) | −0.0024 (9) | 0.0112 (9) | −0.0024 (10) |
| C23 | 0.0662 (13) | 0.0579 (14) | 0.0483 (13) | −0.0051 (11) | 0.0236 (10) | 0.0102 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.0662 (13) | 0.0416 (13) | 0.0659 (15) | −0.0092 (10) | 0.0223 (11) | 0.0068 (11) |
| C25 | 0.167 (3) | 0.118 (3) | 0.086 (2) | −0.081 (2) | 0.067 (2) | −0.0612 (19) |
| N1 | 0.0740 (12) | 0.0639 (12) | 0.0403 (11) | −0.0035 (9) | 0.0243 (9) | −0.0015 (8) |
| N2 | 0.0704 (11) | 0.0422 (10) | 0.0591 (11) | −0.0166 (8) | 0.0140 (9) | −0.0078 (9) |
| O1 | 0.0604 (10) | 0.0750 (12) | 0.0961 (14) | 0.0174 (8) | −0.0089 (9) | 0.0057 (9) |
| O2 | 0.0840 (11) | 0.0779 (11) | 0.0491 (9) | −0.0194 (9) | 0.0296 (8) | −0.0157 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.382 (3) | C14—C15 | 1.374 (3) |
| C1—C6 | 1.384 (3) | C15—H15 | 0.9300 |
| C1—H1 | 0.9300 | C16—O1 | 1.417 (3) |
| C2—C3 | 1.372 (3) | C16—H16A | 0.9600 |
| C2—H2 | 0.9300 | C16—H16B | 0.9600 |
| C3—C4 | 1.369 (3) | C16—H16C | 0.9600 |
| C3—H3 | 0.9300 | C17—C18 | 1.356 (3) |
| C4—C5 | 1.385 (3) | C17—C20 | 1.429 (2) |
| C4—H4 | 0.9300 | C18—N2 | 1.366 (2) |
| C5—C6 | 1.379 (3) | C18—H18 | 0.9300 |
| C5—H5 | 0.9300 | C19—N2 | 1.373 (2) |
| C6—C7 | 1.520 (2) | C19—C24 | 1.386 (3) |
| C7—C8 | 1.505 (2) | C19—C20 | 1.401 (2) |
| C7—C17 | 1.506 (2) | C20—C21 | 1.398 (2) |
| C7—H7 | 0.9800 | C21—C22 | 1.371 (3) |
| C8—C9 | 1.362 (3) | C21—H21 | 0.9300 |
| C8—C10 | 1.433 (3) | C22—O2 | 1.378 (2) |
| C9—N1 | 1.365 (3) | C22—C23 | 1.395 (3) |
| C9—H9 | 0.9300 | C23—C24 | 1.361 (3) |
| C10—C11 | 1.402 (3) | C23—H23 | 0.9300 |
| C10—C15 | 1.404 (3) | C24—H24 | 0.9300 |
| C11—N1 | 1.371 (3) | C25—O2 | 1.379 (3) |
| C11—C12 | 1.389 (3) | C25—H25A | 0.9600 |
| C12—C13 | 1.367 (3) | C25—H25B | 0.9600 |
| C12—H12 | 0.9300 | C25—H25C | 0.9600 |
| C13—C14 | 1.398 (3) | N1—H1A | 0.8600 |
| C13—H13 | 0.9300 | N2—H2A | 0.8600 |
| C14—O1 | 1.373 (2) | | |

| | | | |
|---|---|---|---|
| C2—C1—C6 | 121.1 (2) | C14—C15—H15 | 120.7 |
| C2—C1—H1 | 119.4 | C10—C15—H15 | 120.7 |
| C6—C1—H1 | 119.4 | O1—C16—H16A | 109.5 |
| C3—C2—C1 | 120.0 (2) | O1—C16—H16B | 109.5 |
| C3—C2—H2 | 120.0 | H16A—C16—H16B | 109.5 |
| C1—C2—H2 | 120.0 | O1—C16—H16C | 109.5 |
| C4—C3—C2 | 119.8 (2) | H16A—C16—H16C | 109.5 |
| C4—C3—H3 | 120.1 | H16B—C16—H16C | 109.5 |
| C2—C3—H3 | 120.1 | C18—C17—C20 | 106.26 (15) |
| C3—C4—C5 | 120.2 (2) | C18—C17—C7 | 128.73 (16) |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 119.9 | C20—C17—C7 | 124.96 (15) |
| C5—C4—H4 | 119.9 | C17—C18—N2 | 110.36 (17) |
| C6—C5—C4 | 120.9 (2) | C17—C18—H18 | 124.8 |
| C6—C5—H5 | 119.5 | N2—C18—H18 | 124.8 |
| C4—C5—H5 | 119.5 | N2—C19—C24 | 131.17 (18) |
| C5—C6—C1 | 118.03 (17) | N2—C19—C20 | 107.18 (15) |
| C5—C6—C7 | 120.69 (17) | C24—C19—C20 | 121.65 (18) |
| C1—C6—C7 | 121.27 (17) | C21—C20—C19 | 119.64 (16) |
| C8—C7—C17 | 113.07 (14) | C21—C20—C17 | 132.98 (16) |
| C8—C7—C6 | 112.52 (14) | C19—C20—C17 | 107.37 (15) |
| C17—C7—C6 | 111.53 (15) | C22—C21—C20 | 118.07 (17) |
| C8—C7—H7 | 106.4 | C22—C21—H21 | 121.0 |
| C17—C7—H7 | 106.4 | C20—C21—H21 | 121.0 |
| C6—C7—H7 | 106.4 | C21—C22—O2 | 124.35 (18) |
| C9—C8—C10 | 105.80 (17) | C21—C22—C23 | 121.32 (18) |
| C9—C8—C7 | 128.92 (17) | O2—C22—C23 | 114.32 (17) |
| C10—C8—C7 | 125.19 (15) | C24—C23—C22 | 121.57 (18) |
| C8—C9—N1 | 110.34 (18) | C24—C23—H23 | 119.2 |
| C8—C9—H9 | 124.8 | C22—C23—H23 | 119.2 |
| N1—C9—H9 | 124.8 | C23—C24—C19 | 117.70 (19) |
| C11—C10—C15 | 119.51 (18) | C23—C24—H24 | 121.2 |
| C11—C10—C8 | 107.68 (16) | C19—C24—H24 | 121.2 |
| C15—C10—C8 | 132.80 (17) | O2—C25—H25A | 109.5 |
| N1—C11—C12 | 131.56 (19) | O2—C25—H25B | 109.5 |
| N1—C11—C10 | 106.98 (17) | H25A—C25—H25B | 109.5 |
| C12—C11—C10 | 121.46 (19) | O2—C25—H25C | 109.5 |
| C13—C12—C11 | 118.0 (2) | H25A—C25—H25C | 109.5 |
| C13—C12—H12 | 121.0 | H25B—C25—H25C | 109.5 |
| C11—C12—H12 | 121.0 | C9—N1—C11 | 109.19 (16) |
| C12—C13—C14 | 121.7 (2) | C9—N1—H1A | 125.4 |
| C12—C13—H13 | 119.2 | C11—N1—H1A | 125.4 |
| C14—C13—H13 | 119.2 | C18—N2—C19 | 108.83 (16) |
| O1—C14—C15 | 124.7 (2) | C18—N2—H2A | 125.6 |
| O1—C14—C13 | 114.60 (19) | C19—N2—H2A | 125.6 |
| C15—C14—C13 | 120.7 (2) | C14—O1—C16 | 116.91 (17) |
| C14—C15—C10 | 118.66 (19) | C22—O2—C25 | 118.42 (16) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.7 (3) | C8—C10—C15—C14 | −178.15 (19) |
| C1—C2—C3—C4 | 0.4 (4) | C8—C7—C17—C18 | −28.6 (3) |
| C2—C3—C4—C5 | −0.2 (4) | C6—C7—C17—C18 | 99.3 (2) |
| C3—C4—C5—C6 | 0.3 (4) | C8—C7—C17—C20 | 154.25 (16) |
| C4—C5—C6—C1 | −0.5 (3) | C6—C7—C17—C20 | −77.8 (2) |
| C4—C5—C6—C7 | 178.92 (19) | C20—C17—C18—N2 | −0.1 (2) |
| C2—C1—C6—C5 | 0.7 (3) | C7—C17—C18—N2 | −177.62 (17) |
| C2—C1—C6—C7 | −178.74 (18) | N2—C19—C20—C21 | −179.02 (16) |
| C5—C6—C7—C8 | −104.3 (2) | C24—C19—C20—C21 | 1.2 (3) |
| C1—C6—C7—C8 | 75.1 (2) | N2—C19—C20—C17 | 0.3 (2) |
| C5—C6—C7—C17 | 127.43 (19) | C24—C19—C20—C17 | −179.42 (17) |

| | | | |
|---|---|---|---|
| C1—C6—C7—C17 | −53.1 (2) | C18—C17—C20—C21 | 179.09 (19) |
| C17—C7—C8—C9 | 113.9 (2) | C7—C17—C20—C21 | −3.3 (3) |
| C6—C7—C8—C9 | −13.6 (3) | C18—C17—C20—C19 | −0.2 (2) |
| C17—C7—C8—C10 | −70.0 (2) | C7—C17—C20—C19 | 177.49 (16) |
| C6—C7—C8—C10 | 162.53 (17) | C19—C20—C21—C22 | 0.0 (3) |
| C10—C8—C9—N1 | 0.3 (2) | C17—C20—C21—C22 | −179.20 (18) |
| C7—C8—C9—N1 | 176.99 (16) | C20—C21—C22—O2 | 177.46 (17) |
| C9—C8—C10—C11 | 0.2 (2) | C20—C21—C22—C23 | −1.7 (3) |
| C7—C8—C10—C11 | −176.63 (16) | C21—C22—C23—C24 | 2.3 (3) |
| C9—C8—C10—C15 | 179.1 (2) | O2—C22—C23—C24 | −176.93 (19) |
| C7—C8—C10—C15 | 2.2 (3) | C22—C23—C24—C19 | −1.1 (3) |
| C15—C10—C11—N1 | −179.67 (17) | N2—C19—C24—C23 | 179.6 (2) |
| C8—C10—C11—N1 | −0.7 (2) | C20—C19—C24—C23 | −0.7 (3) |
| C15—C10—C11—C12 | −0.5 (3) | C8—C9—N1—C11 | −0.7 (2) |
| C8—C10—C11—C12 | 178.51 (18) | C12—C11—N1—C9 | −178.2 (2) |
| N1—C11—C12—C13 | 179.5 (2) | C10—C11—N1—C9 | 0.9 (2) |
| C10—C11—C12—C13 | 0.5 (3) | C17—C18—N2—C19 | 0.3 (2) |
| C11—C12—C13—C14 | −0.6 (3) | C24—C19—N2—C18 | 179.3 (2) |
| C12—C13—C14—O1 | −179.8 (2) | C20—C19—N2—C18 | −0.4 (2) |
| C12—C13—C14—C15 | 0.7 (3) | C15—C14—O1—C16 | 5.7 (3) |
| O1—C14—C15—C10 | 179.89 (18) | C13—C14—O1—C16 | −173.79 (19) |
| C13—C14—C15—C10 | −0.7 (3) | C21—C22—O2—C25 | 1.3 (3) |
| C11—C10—C15—C14 | 0.6 (3) | C23—C22—O2—C25 | −179.6 (2) |

*Hydrogen-bond geometry (Å, º)*

*Cg*2, *Cg*3, *Cg*4 and *Cg*5 are the centroids of the N2/C17–C20, C1–C6, C10–C15 and C19–C24 rings, respectively

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O2$^{i}$ | 0.86 | 2.09 | 2.904 (2) | 158 |
| C25—H25*B*···*Cg*2$^{ii}$ | 0.96 | 2.95 | 3.515 (3) | 119 |
| C16—H16*C*···*Cg*3$^{iii}$ | 0.96 | 2.90 | 3.508 (3) | 122 |
| N2—H2*A*···*Cg*4$^{iv}$ | 0.86 | 2.49 | 3.3149 (19) | 160 |
| C3—H3···*Cg*5$^{v}$ | 0.93 | 2.60 | 3.470 (2) | 157 |

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) *x*+1, *y*, *z*; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*−1, *y*, *z*.