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# 1-Benzyl-3′-[(1*H*-indol-3-yl)carbonyl]-1′-methyl-2-oxo-4′-(pyridin-3-yl)spiro[indoline-3,2′-pyrrolidine]-3′-carbonitrile

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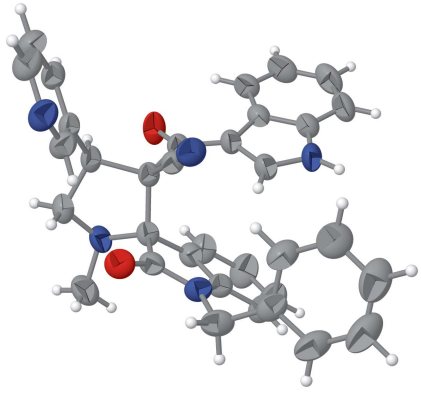
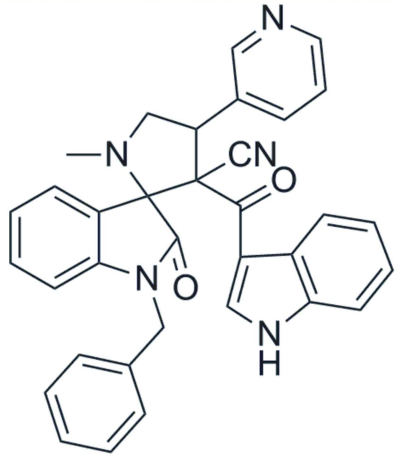
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{34}H_{27}N_5O_2$, the central pyrrolidine ring adopts an envelope conformation, with the N atom as the flap. The mean planes of the two indoline ring systems are inclined to the mean plane of the central pyrrolidine ring by 86.26 (9) and 69.30 (9)°, respectively. The dihedral angle between the benzene and pyridine rings is 75.09 (11)°. In the crystal, molecules are linked by N—H···N and C—H···N hydrogen bonds, forming sheets parallel to the *ab* plane.

3D view



Chemical scheme




## Structure description

Spiro-pyrrolidine derivatives are unique tetracyclic 5-HT(2A) receptor antagonists (Obniska *et al.*, 2003; Peddi *et al.*, 2004). These derivatives possess anticancer (Zapf *et al.*, 2011) and anti-influenza virus (Stylianakis *et al.*, 2003) activities. Highly functionalized pyrrolidines have attracted much interest in recent years as they constitute the main structural element of many natural and synthetic pharmacologically active compounds (Waldmann, 1995). Optically active pyrrolidines have been used as intermediates, chiral ligands or auxiliaries in controlled asymmetric synthesis (Suzuki *et al.*, 1994; Huryn *et al.*, 1991). In view of their importance and in continuation of our work on the crystal structure analysis of spiro-pyrrolidine derivatives, we report herein on the synthesis and crystal structure of a new spiro-pyrrolidine derivative.

The molecular structure of the title compound is illustrated in Fig. 1. The five-membered ring (N2/C6–C9) in the pyrrolidine moiety adopts an envelope conformation, with atom N2 as the flap atom [puckering parameters: $q_2$ = 0.410 (2) Å and $\varphi_2$ = 181.7 (3)°], and the pyridine ring (N1/C1–C5) exhibits a slightly twisted conformation [puckering parameters: $q_2$ = 0.093 (2) Å and $\Phi_2$ = 49.9 (2)°]. The sum of angles at atom

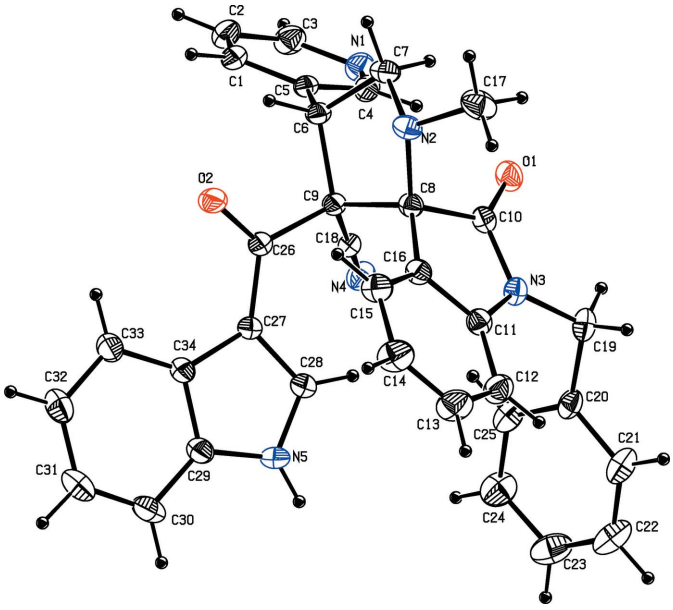



**Figure 1**
The molecular structure of the title compound, showing the atom labelling and 20% probability displacement ellipsoids.

N2 [328.4 (15)°] is in accordance with $sp^2$-hybiridization, and the sum of angles at atom N3 [313.6 (14)°] is in accordance with $sp^3$-hybridization. The dihedral angle between the benzene (C20–C25) and pyridine (N1/C1–C5) rings is 75.09 (11)°.

In the crystal, molecules are linked by N—H···N and C—H···N hydrogen bonds, forming sheets parallel to the *ab* plane (Table 1 and Fig. 2).

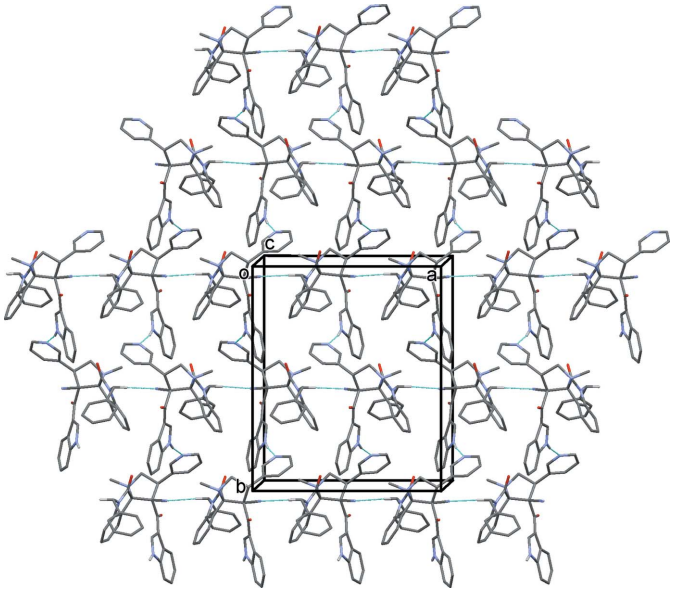



**Figure 2**
The crystal packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only H atoms H5 and H19*A* have been included.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5···N1$^{i}$ | 0.86 | 1.96 | 2.812 (2) | 170 |
| C19—H19$A$···N4$^{ii}$ | 0.97 | 2.46 | 3.370 (3) | 157 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{34}H_{27}N_5O_2$ |
| $M_r$ | 537.60 |
| Crystal system, space group | Orthorhombic, *Pbca* |
| Temperature (K) | 296 |
| *a*, *b*, *c* (Å) | 14.7421 (6), 17.5573 (6), 21.4675 (9) |
| $V$ (Å$^3$) | 5556.5 (4) |
| $Z$ | 8 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.08 |
| Crystal size (mm) | 0.25 × 0.16 × 0.12 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 22838, 4884, 3251 |
| $R_{int}$ | 0.031 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.595 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.040, 0.095, 0.97 |
| No. of reflections | 4884 |
| No. of parameters | 372 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.13, −0.17 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

## Synthesis and crystallization

*N*-Benzylisatin, (1) (0.3 mmol), was mixed with sarcosine, (2) (0.3 mmol), and (*E*)-2-[(1*H*-indol-3-yl)carbonyl]-3-(pyridin-3-yl)acrylonitrile in ethanol (10 ml) in a round-bottomed flask. The reaction mixture was heated at 358 K for 3 h. After cooling to ambient temperature, the reaction mixture was filtered to afford the pure title product as a white solid (yield 92%). The filtrate was left to evaporate slowly and after 48 h yellow crystals of the title compound were obtained.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2016). **1**, x161686 [https://doi.org/10.1107/S2414314616016862]

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*Crystal data*

$C_{34}H_{27}N_5O_2$
$M_r$ = 537.60
Orthorhombic, *Pbca*
$a$ = 14.7421 (6) Å
$b$ = 17.5573 (6) Å
$c$ = 21.4675 (9) Å
$V$ = 5556.5 (4) Å$^3$
$Z$ = 8
$F(000)$ = 2256
$D_x$ = 1.285 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5384 reflections
$\theta$ = 2.3–24.1°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 296 K
Rectangular, yellow
0.25 × 0.16 × 0.12 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
22838 measured reflections
4884 independent reflections
3251 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.9°
$h$ = −14→17
$k$ = −20→20
$l$ = −18→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.095
$S$ = 0.97
4884 reflections
372 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 2.8668P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Extinction correction: SHELXL2014 (Sheldrick 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00063 (9)

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.63234 (14) | −0.06447 (11) | 0.42023 (9) | 0.0517 (5) |
| H1 | 0.6404 | −0.0377 | 0.4572 | 0.062* |
| C2 | 0.70167 (15) | −0.10825 (13) | 0.39656 (11) | 0.0627 (6) |
| H2 | 0.7568 | −0.1116 | 0.4174 | 0.075* |
| C3 | 0.68837 (16) | −0.14676 (12) | 0.34183 (11) | 0.0644 (6) |
| H3 | 0.7358 | −0.1758 | 0.3259 | 0.077* |
| C4 | 0.54388 (15) | −0.10303 (11) | 0.33427 (10) | 0.0524 (5) |
| H4 | 0.4889 | −0.1024 | 0.3131 | 0.063* |
| C5 | 0.55064 (13) | −0.06054 (10) | 0.38871 (9) | 0.0438 (5) |
| C6 | 0.47250 (13) | −0.01328 (10) | 0.41220 (9) | 0.0445 (5) |
| H6 | 0.4907 | 0.0063 | 0.4531 | 0.053* |
| C7 | 0.38438 (14) | −0.05742 (11) | 0.42225 (10) | 0.0537 (5) |
| H7A | 0.3763 | −0.0960 | 0.3904 | 0.064* |
| H7B | 0.3837 | −0.0817 | 0.4628 | 0.064* |
| C8 | 0.33670 (12) | 0.04828 (10) | 0.36441 (9) | 0.0419 (5) |
| C9 | 0.44388 (13) | 0.05810 (10) | 0.37192 (8) | 0.0405 (4) |
| C10 | 0.31830 (13) | 0.01138 (11) | 0.29978 (10) | 0.0458 (5) |
| C11 | 0.24722 (13) | 0.12705 (11) | 0.29981 (9) | 0.0470 (5) |
| C12 | 0.19527 (15) | 0.18821 (12) | 0.28185 (11) | 0.0637 (6) |
| H12 | 0.1732 | 0.1926 | 0.2414 | 0.076* |
| C13 | 0.17724 (17) | 0.24293 (13) | 0.32648 (13) | 0.0788 (8) |
| H13 | 0.1433 | 0.2855 | 0.3155 | 0.095* |
| C14 | 0.20803 (18) | 0.23604 (13) | 0.38641 (12) | 0.0757 (7) |
| H14 | 0.1939 | 0.2734 | 0.4155 | 0.091* |
| C15 | 0.26003 (15) | 0.17389 (11) | 0.40409 (10) | 0.0593 (6) |
| H15 | 0.2804 | 0.1689 | 0.4449 | 0.071* |
| C16 | 0.28089 (13) | 0.11976 (10) | 0.35996 (9) | 0.0455 (5) |
| C17 | 0.22168 (15) | −0.02969 (13) | 0.41757 (12) | 0.0748 (7) |
| H17A | 0.1792 | 0.0112 | 0.4119 | 0.112* |
| H17B | 0.2097 | −0.0547 | 0.4565 | 0.112* |
| H17C | 0.2155 | −0.0656 | 0.3841 | 0.112* |
| C18 | 0.48887 (13) | 0.05771 (10) | 0.31095 (10) | 0.0426 (5) |
| C19 | 0.24710 (15) | 0.04824 (13) | 0.19947 (10) | 0.0622 (6) |
| H19A | 0.1814 | 0.0489 | 0.1969 | 0.075* |
| H19B | 0.2673 | −0.0025 | 0.1883 | 0.075* |
| C20 | 0.28439 (15) | 0.10381 (12) | 0.15286 (9) | 0.0522 (5) |
| C21 | 0.22805 (17) | 0.13774 (15) | 0.10973 (11) | 0.0762 (7) |
| H21 | 0.1660 | 0.1283 | 0.1113 | 0.091* |
| C22 | 0.2618 (2) | 0.18511 (17) | 0.06460 (13) | 0.0908 (9) |
| H22 | 0.2226 | 0.2070 | 0.0357 | 0.109* |
| C23 | 0.3517 (2) | 0.20027 (16) | 0.06171 (13) | 0.0888 (9) |
| H23 | 0.3743 | 0.2321 | 0.0308 | 0.107* |
| C24 | 0.40917 (18) | 0.16848 (16) | 0.10455 (12) | 0.0805 (8) |
| H24 | 0.4708 | 0.1797 | 0.1033 | 0.097* |
| C25 | 0.37569 (15) | 0.11979 (13) | 0.14957 (10) | 0.0620 (6) |

| | | | | |
|---|---|---|---|---|
| H25 | 0.4153 | 0.0975 | 0.1780 | 0.074* |
| C26 | 0.47020 (13) | 0.13396 (10) | 0.40690 (9) | 0.0453 (5) |
| C27 | 0.47548 (13) | 0.20507 (10) | 0.37413 (9) | 0.0455 (5) |
| C28 | 0.44590 (14) | 0.22198 (11) | 0.31459 (10) | 0.0528 (5) |
| H28 | 0.4239 | 0.1863 | 0.2863 | 0.063* |
| C29 | 0.48880 (14) | 0.33263 (11) | 0.35534 (10) | 0.0531 (5) |
| C30 | 0.50841 (16) | 0.40925 (12) | 0.36446 (13) | 0.0700 (7) |
| H30 | 0.4986 | 0.4452 | 0.3334 | 0.084* |
| C31 | 0.54281 (18) | 0.42924 (13) | 0.42120 (14) | 0.0776 (8) |
| H31 | 0.5563 | 0.4801 | 0.4291 | 0.093* |
| C32 | 0.55800 (16) | 0.37571 (13) | 0.46725 (12) | 0.0710 (7) |
| H32 | 0.5813 | 0.3914 | 0.5054 | 0.085* |
| C33 | 0.53938 (14) | 0.29933 (12) | 0.45804 (10) | 0.0565 (6) |
| H33 | 0.5506 | 0.2637 | 0.4892 | 0.068* |
| C34 | 0.50338 (13) | 0.27721 (10) | 0.40092 (9) | 0.0465 (5) |
| N1 | 0.61087 (13) | −0.14454 (9) | 0.31048 (8) | 0.0588 (5) |
| N2 | 0.31418 (11) | 0.00086 (9) | 0.41796 (8) | 0.0509 (4) |
| N3 | 0.27357 (10) | 0.06328 (9) | 0.26387 (7) | 0.0477 (4) |
| N4 | 0.52502 (12) | 0.05610 (10) | 0.26381 (8) | 0.0572 (5) |
| N5 | 0.45319 (12) | 0.29669 (9) | 0.30315 (8) | 0.0587 (5) |
| H5 | 0.4382 | 0.3189 | 0.2690 | 0.070* |
| O1 | 0.34090 (10) | −0.05210 (7) | 0.28292 (7) | 0.0599 (4) |
| O2 | 0.48569 (11) | 0.12999 (7) | 0.46262 (7) | 0.0646 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0643 (14) | 0.0493 (12) | 0.0416 (12) | −0.0037 (11) | −0.0093 (11) | 0.0065 (10) |
| C2 | 0.0557 (14) | 0.0682 (14) | 0.0643 (16) | 0.0042 (12) | −0.0136 (12) | 0.0109 (13) |
| C3 | 0.0679 (16) | 0.0581 (13) | 0.0671 (16) | 0.0158 (12) | −0.0047 (13) | 0.0013 (13) |
| C4 | 0.0580 (13) | 0.0468 (11) | 0.0525 (14) | 0.0043 (10) | −0.0129 (11) | −0.0027 (11) |
| C5 | 0.0566 (13) | 0.0371 (10) | 0.0377 (11) | −0.0020 (9) | −0.0059 (10) | 0.0053 (9) |
| C6 | 0.0592 (13) | 0.0388 (10) | 0.0354 (11) | −0.0025 (9) | −0.0034 (10) | 0.0058 (9) |
| C7 | 0.0684 (14) | 0.0415 (11) | 0.0512 (13) | −0.0009 (10) | 0.0045 (11) | 0.0087 (10) |
| C8 | 0.0483 (11) | 0.0384 (10) | 0.0388 (11) | −0.0013 (8) | 0.0022 (9) | −0.0019 (9) |
| C9 | 0.0496 (11) | 0.0392 (10) | 0.0326 (11) | −0.0036 (9) | −0.0018 (9) | 0.0026 (9) |
| C10 | 0.0423 (11) | 0.0433 (11) | 0.0516 (13) | −0.0045 (9) | −0.0008 (10) | −0.0034 (10) |
| C11 | 0.0439 (11) | 0.0456 (11) | 0.0515 (13) | 0.0002 (9) | 0.0001 (10) | −0.0020 (10) |
| C12 | 0.0667 (15) | 0.0608 (13) | 0.0638 (15) | 0.0106 (12) | −0.0107 (12) | −0.0001 (12) |
| C13 | 0.0919 (19) | 0.0590 (14) | 0.086 (2) | 0.0292 (14) | −0.0058 (16) | −0.0034 (15) |
| C14 | 0.100 (2) | 0.0584 (14) | 0.0689 (18) | 0.0263 (14) | 0.0033 (15) | −0.0124 (13) |
| C15 | 0.0755 (15) | 0.0527 (12) | 0.0495 (13) | 0.0070 (11) | 0.0058 (12) | −0.0051 (11) |
| C16 | 0.0474 (12) | 0.0430 (10) | 0.0460 (12) | −0.0008 (9) | 0.0037 (10) | −0.0013 (10) |
| C17 | 0.0643 (16) | 0.0686 (15) | 0.0914 (19) | −0.0096 (12) | 0.0192 (14) | 0.0141 (14) |
| C18 | 0.0445 (11) | 0.0431 (11) | 0.0401 (12) | −0.0027 (9) | −0.0077 (10) | 0.0038 (10) |
| C19 | 0.0595 (14) | 0.0734 (15) | 0.0535 (14) | −0.0075 (12) | −0.0152 (12) | −0.0114 (12) |
| C20 | 0.0577 (14) | 0.0597 (12) | 0.0393 (12) | 0.0074 (11) | −0.0110 (11) | −0.0101 (11) |
| C21 | 0.0650 (16) | 0.105 (2) | 0.0589 (16) | 0.0134 (15) | −0.0171 (14) | −0.0009 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C22 | 0.099 (2) | 0.113 (2) | 0.0605 (18) | 0.0353 (19) | −0.0144 (17) | 0.0123 (17) |
| C23 | 0.112 (3) | 0.095 (2) | 0.0593 (18) | 0.0244 (19) | 0.0108 (17) | 0.0166 (15) |
| C24 | 0.0728 (17) | 0.103 (2) | 0.0654 (17) | 0.0064 (15) | 0.0134 (15) | 0.0091 (16) |
| C25 | 0.0571 (15) | 0.0769 (15) | 0.0520 (14) | 0.0146 (12) | −0.0048 (12) | 0.0003 (13) |
| C26 | 0.0529 (12) | 0.0434 (11) | 0.0397 (12) | −0.0050 (9) | −0.0050 (10) | 0.0033 (10) |
| C27 | 0.0533 (13) | 0.0407 (10) | 0.0426 (12) | −0.0071 (9) | −0.0053 (10) | 0.0067 (10) |
| C28 | 0.0608 (13) | 0.0461 (11) | 0.0516 (14) | −0.0110 (10) | −0.0063 (11) | 0.0084 (10) |
| C29 | 0.0521 (13) | 0.0463 (11) | 0.0611 (14) | −0.0071 (10) | 0.0001 (11) | 0.0064 (11) |
| C30 | 0.0755 (17) | 0.0464 (13) | 0.0882 (19) | −0.0106 (11) | 0.0065 (15) | 0.0124 (13) |
| C31 | 0.0872 (19) | 0.0482 (13) | 0.097 (2) | −0.0185 (13) | 0.0103 (17) | −0.0056 (15) |
| C32 | 0.0763 (17) | 0.0647 (15) | 0.0719 (17) | −0.0191 (13) | 0.0038 (14) | −0.0151 (14) |
| C33 | 0.0570 (13) | 0.0539 (12) | 0.0585 (14) | −0.0078 (10) | −0.0008 (11) | −0.0026 (11) |
| C34 | 0.0448 (11) | 0.0435 (11) | 0.0512 (13) | −0.0059 (9) | −0.0001 (10) | 0.0024 (10) |
| N1 | 0.0668 (12) | 0.0492 (10) | 0.0603 (12) | 0.0118 (9) | −0.0086 (10) | −0.0058 (9) |
| N2 | 0.0547 (11) | 0.0461 (9) | 0.0518 (11) | −0.0049 (8) | 0.0098 (9) | 0.0080 (8) |
| N3 | 0.0474 (10) | 0.0515 (9) | 0.0440 (10) | −0.0014 (8) | −0.0062 (8) | −0.0062 (8) |
| N4 | 0.0557 (11) | 0.0711 (12) | 0.0447 (11) | 0.0006 (9) | 0.0005 (9) | 0.0045 (10) |
| N5 | 0.0698 (12) | 0.0487 (10) | 0.0575 (12) | −0.0070 (9) | −0.0063 (10) | 0.0211 (9) |
| O1 | 0.0665 (10) | 0.0466 (8) | 0.0666 (10) | 0.0015 (7) | −0.0079 (8) | −0.0144 (7) |
| O2 | 0.1075 (13) | 0.0464 (8) | 0.0399 (9) | −0.0101 (8) | −0.0152 (9) | 0.0022 (7) |

*Geometric parameters (Å, º)*

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| C1—C2 | 1.376 (3) | C17—H17A | 0.9600 |
| C1—C5 | 1.383 (3) | C17—H17B | 0.9600 |
| C1—H1 | 0.9300 | C17—H17C | 0.9600 |
| C2—C3 | 1.370 (3) | C18—N4 | 1.144 (2) |
| C2—H2 | 0.9300 | C19—N3 | 1.460 (2) |
| C3—N1 | 1.327 (3) | C19—C20 | 1.502 (3) |
| C3—H3 | 0.9300 | C19—H19A | 0.9700 |
| C4—N1 | 1.329 (2) | C19—H19B | 0.9700 |
| C4—C5 | 1.390 (3) | C20—C25 | 1.377 (3) |
| C4—H4 | 0.9300 | C20—C21 | 1.379 (3) |
| C5—C6 | 1.507 (3) | C21—C22 | 1.370 (4) |
| C6—C7 | 1.528 (3) | C21—H21 | 0.9300 |
| C6—C9 | 1.580 (2) | C22—C23 | 1.353 (4) |
| C6—H6 | 0.9800 | C22—H22 | 0.9300 |
| C7—N2 | 1.458 (2) | C23—C24 | 1.369 (3) |
| C7—H7A | 0.9700 | C23—H23 | 0.9300 |
| C7—H7B | 0.9700 | C24—C25 | 1.381 (3) |
| C8—N2 | 1.458 (2) | C24—H24 | 0.9300 |
| C8—C16 | 1.504 (2) | C25—H25 | 0.9300 |
| C8—C10 | 1.555 (3) | C26—O2 | 1.220 (2) |
| C8—C9 | 1.598 (3) | C26—C27 | 1.435 (2) |
| C9—C18 | 1.467 (3) | C27—C28 | 1.383 (3) |
| C9—C26 | 1.578 (2) | C27—C34 | 1.451 (2) |
| C10—O1 | 1.218 (2) | C28—N5 | 1.339 (2) |
| C10—N3 | 1.364 (2) | C28—H28 | 0.9300 |

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| C11—C12 | 1.374 (3) | C29—C30 | 1.390 (3) |
| C11—C16 | 1.389 (3) | C29—N5 | 1.389 (3) |
| C11—N3 | 1.414 (2) | C29—C34 | 1.397 (3) |
| C12—C13 | 1.383 (3) | C30—C31 | 1.365 (3) |
| C12—H12 | 0.9300 | C30—H30 | 0.9300 |
| C13—C14 | 1.370 (3) | C31—C32 | 1.382 (3) |
| C13—H13 | 0.9300 | C31—H31 | 0.9300 |
| C14—C15 | 1.387 (3) | C32—C33 | 1.383 (3) |
| C14—H14 | 0.9300 | C32—H32 | 0.9300 |
| C15—C16 | 1.377 (3) | C33—C34 | 1.391 (3) |
| C15—H15 | 0.9300 | C33—H33 | 0.9300 |
| C17—N2 | 1.465 (3) | N5—H5 | 0.8600 |

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| C2—C1—C5 | 119.6 (2) | H17A—C17—H17C | 109.5 |
| C2—C1—H1 | 120.2 | H17B—C17—H17C | 109.5 |
| C5—C1—H1 | 120.2 | N4—C18—C9 | 178.5 (2) |
| C3—C2—C1 | 119.1 (2) | N3—C19—C20 | 114.55 (17) |
| C3—C2—H2 | 120.5 | N3—C19—H19A | 108.6 |
| C1—C2—H2 | 120.5 | C20—C19—H19A | 108.6 |
| N1—C3—C2 | 123.0 (2) | N3—C19—H19B | 108.6 |
| N1—C3—H3 | 118.5 | C20—C19—H19B | 108.6 |
| C2—C3—H3 | 118.5 | H19A—C19—H19B | 107.6 |
| N1—C4—C5 | 124.34 (19) | C25—C20—C21 | 117.8 (2) |
| N1—C4—H4 | 117.8 | C25—C20—C19 | 121.6 (2) |
| C5—C4—H4 | 117.8 | C21—C20—C19 | 120.5 (2) |
| C1—C5—C4 | 116.54 (19) | C22—C21—C20 | 121.2 (3) |
| C1—C5—C6 | 121.97 (18) | C22—C21—H21 | 119.4 |
| C4—C5—C6 | 121.49 (18) | C20—C21—H21 | 119.4 |
| C5—C6—C7 | 114.71 (15) | C23—C22—C21 | 120.5 (3) |
| C5—C6—C9 | 117.24 (15) | C23—C22—H22 | 119.8 |
| C7—C6—C9 | 104.63 (15) | C21—C22—H22 | 119.8 |
| C5—C6—H6 | 106.5 | C22—C23—C24 | 119.7 (3) |
| C7—C6—H6 | 106.5 | C22—C23—H23 | 120.2 |
| C9—C6—H6 | 106.5 | C24—C23—H23 | 120.2 |
| N2—C7—C6 | 103.80 (15) | C23—C24—C25 | 120.1 (3) |
| N2—C7—H7A | 111.0 | C23—C24—H24 | 120.0 |
| C6—C7—H7A | 111.0 | C25—C24—H24 | 120.0 |
| N2—C7—H7B | 111.0 | C20—C25—C24 | 120.8 (2) |
| C6—C7—H7B | 111.0 | C20—C25—H25 | 119.6 |
| H7A—C7—H7B | 109.0 | C24—C25—H25 | 119.6 |
| N2—C8—C16 | 113.72 (15) | O2—C26—C27 | 121.35 (17) |
| N2—C8—C10 | 115.22 (15) | O2—C26—C9 | 117.69 (16) |
| C16—C8—C10 | 101.27 (15) | C27—C26—C9 | 120.97 (17) |
| N2—C8—C9 | 101.96 (14) | C28—C27—C26 | 128.52 (18) |
| C16—C8—C9 | 117.23 (15) | C28—C27—C34 | 105.57 (16) |
| C10—C8—C9 | 107.90 (15) | C26—C27—C34 | 125.49 (18) |
| C18—C9—C26 | 108.50 (15) | N5—C28—C27 | 110.76 (18) |
| C18—C9—C6 | 111.34 (15) | N5—C28—H28 | 124.6 |

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| C26—C9—C6 | 110.09 (14) | C27—C28—H28 | 124.6 |
| C18—C9—C8 | 110.89 (15) | C30—C29—N5 | 129.2 (2) |
| C26—C9—C8 | 112.48 (15) | C30—C29—C34 | 122.9 (2) |
| C6—C9—C8 | 103.51 (14) | N5—C29—C34 | 107.86 (17) |
| O1—C10—N3 | 125.13 (19) | C31—C30—C29 | 116.8 (2) |
| O1—C10—C8 | 126.77 (18) | C31—C30—H30 | 121.6 |
| N3—C10—C8 | 108.09 (16) | C29—C30—H30 | 121.6 |
| C12—C11—C16 | 122.13 (19) | C30—C31—C32 | 121.6 (2) |
| C12—C11—N3 | 128.23 (19) | C30—C31—H31 | 119.2 |
| C16—C11—N3 | 109.63 (16) | C32—C31—H31 | 119.2 |
| C11—C12—C13 | 117.1 (2) | C33—C32—C31 | 121.7 (2) |
| C11—C12—H12 | 121.4 | C33—C32—H32 | 119.2 |
| C13—C12—H12 | 121.4 | C31—C32—H32 | 119.2 |
| C14—C13—C12 | 121.7 (2) | C32—C33—C34 | 118.2 (2) |
| C14—C13—H13 | 119.1 | C32—C33—H33 | 120.9 |
| C12—C13—H13 | 119.1 | C34—C33—H33 | 120.9 |
| C13—C14—C15 | 120.7 (2) | C33—C34—C29 | 118.79 (18) |
| C13—C14—H14 | 119.7 | C33—C34—C27 | 134.53 (18) |
| C15—C14—H14 | 119.7 | C29—C34—C27 | 106.67 (18) |
| C16—C15—C14 | 118.6 (2) | C3—N1—C4 | 117.45 (19) |
| C16—C15—H15 | 120.7 | C8—N2—C7 | 106.80 (15) |
| C14—C15—H15 | 120.7 | C8—N2—C17 | 114.61 (17) |
| C15—C16—C11 | 119.75 (18) | C7—N2—C17 | 113.82 (16) |
| C15—C16—C8 | 130.88 (19) | C10—N3—C11 | 110.69 (16) |
| C11—C16—C8 | 109.36 (16) | C10—N3—C19 | 122.93 (17) |
| N2—C17—H17A | 109.5 | C11—N3—C19 | 125.88 (17) |
| N2—C17—H17B | 109.5 | C28—N5—C29 | 109.12 (17) |
| H17A—C17—H17B | 109.5 | C28—N5—H5 | 125.4 |
| N2—C17—H17C | 109.5 | C29—N5—H5 | 125.4 |

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| C5—C1—C2—C3 | 0.4 (3) | C21—C22—C23—C24 | −0.5 (4) |
| C1—C2—C3—N1 | −0.7 (3) | C22—C23—C24—C25 | 1.5 (4) |
| C2—C1—C5—C4 | 0.8 (3) | C21—C20—C25—C24 | 0.2 (3) |
| C2—C1—C5—C6 | −179.71 (17) | C19—C20—C25—C24 | 177.1 (2) |
| N1—C4—C5—C1 | −1.9 (3) | C23—C24—C25—C20 | −1.4 (4) |
| N1—C4—C5—C6 | 178.56 (18) | C18—C9—C26—O2 | −139.91 (19) |
| C1—C5—C6—C7 | −123.4 (2) | C6—C9—C26—O2 | −17.8 (2) |
| C4—C5—C6—C7 | 56.0 (2) | C8—C9—C26—O2 | 97.0 (2) |
| C1—C5—C6—C9 | 113.2 (2) | C18—C9—C26—C27 | 40.2 (2) |
| C4—C5—C6—C9 | −67.3 (2) | C6—C9—C26—C27 | 162.28 (17) |
| C5—C6—C7—N2 | −156.36 (16) | C8—C9—C26—C27 | −82.8 (2) |
| C9—C6—C7—N2 | −26.51 (19) | O2—C26—C27—C28 | −168.1 (2) |
| C5—C6—C9—C18 | 10.9 (2) | C9—C26—C27—C28 | 11.8 (3) |
| C7—C6—C9—C18 | −117.49 (17) | O2—C26—C27—C34 | 3.4 (3) |
| C5—C6—C9—C26 | −109.52 (18) | C9—C26—C27—C34 | −176.69 (18) |
| C7—C6—C9—C26 | 122.14 (17) | C26—C27—C28—N5 | 172.8 (2) |
| C5—C6—C9—C8 | 130.04 (16) | C34—C27—C28—N5 | −0.1 (2) |
| C7—C6—C9—C8 | 1.70 (18) | N5—C29—C30—C31 | 179.6 (2) |

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| N2—C8—C9—C18 | 142.99 (15) | C34—C29—C30—C31 | −0.4 (3) |
| C16—C8—C9—C18 | −92.16 (19) | C29—C30—C31—C32 | 0.4 (4) |
| C10—C8—C9—C18 | 21.2 (2) | C30—C31—C32—C33 | 0.2 (4) |
| N2—C8—C9—C26 | −95.31 (16) | C31—C32—C33—C34 | −0.8 (4) |
| C16—C8—C9—C26 | 29.5 (2) | C32—C33—C34—C29 | 0.8 (3) |
| C10—C8—C9—C26 | 142.95 (15) | C32—C33—C34—C27 | −179.9 (2) |
| N2—C8—C9—C6 | 23.50 (17) | C30—C29—C34—C33 | −0.2 (3) |
| C16—C8—C9—C6 | 148.35 (16) | N5—C29—C34—C33 | 179.80 (18) |
| C10—C8—C9—C6 | −98.24 (16) | C30—C29—C34—C27 | −179.7 (2) |
| N2—C8—C10—O1 | −48.4 (3) | N5—C29—C34—C27 | 0.3 (2) |
| C16—C8—C10—O1 | −171.61 (19) | C28—C27—C34—C33 | −179.5 (2) |
| C9—C8—C10—O1 | 64.7 (2) | C26—C27—C34—C33 | 7.4 (4) |
| N2—C8—C10—N3 | 132.87 (16) | C28—C27—C34—C29 | −0.2 (2) |
| C16—C8—C10—N3 | 9.69 (19) | C26—C27—C34—C29 | −173.29 (19) |
| C9—C8—C10—N3 | −113.99 (16) | C2—C3—N1—C4 | −0.4 (3) |
| C16—C11—C12—C13 | −0.2 (3) | C5—C4—N1—C3 | 1.7 (3) |
| N3—C11—C12—C13 | 178.6 (2) | C16—C8—N2—C7 | −169.48 (16) |
| C11—C12—C13—C14 | −1.3 (4) | C10—C8—N2—C7 | 74.2 (2) |
| C12—C13—C14—C15 | 1.1 (4) | C9—C8—N2—C7 | −42.32 (18) |
| C13—C14—C15—C16 | 0.7 (4) | C16—C8—N2—C17 | 63.5 (2) |
| C14—C15—C16—C11 | −2.2 (3) | C10—C8—N2—C17 | −52.8 (2) |
| C14—C15—C16—C8 | 178.4 (2) | C9—C8—N2—C17 | −169.36 (16) |
| C12—C11—C16—C15 | 1.9 (3) | C6—C7—N2—C8 | 44.46 (19) |
| N3—C11—C16—C15 | −177.05 (17) | C6—C7—N2—C17 | 171.97 (17) |
| C12—C11—C16—C8 | −178.56 (18) | O1—C10—N3—C11 | 172.32 (19) |
| N3—C11—C16—C8 | 2.4 (2) | C8—C10—N3—C11 | −9.0 (2) |
| N2—C8—C16—C15 | 48.1 (3) | O1—C10—N3—C19 | −0.1 (3) |
| C10—C8—C16—C15 | 172.3 (2) | C8—C10—N3—C19 | 178.67 (16) |
| C9—C8—C16—C15 | −70.7 (3) | C12—C11—N3—C10 | −174.6 (2) |
| N2—C8—C16—C11 | −131.37 (17) | C16—C11—N3—C10 | 4.3 (2) |
| C10—C8—C16—C11 | −7.2 (2) | C12—C11—N3—C19 | −2.5 (3) |
| C9—C8—C16—C11 | 109.90 (19) | C16—C11—N3—C19 | 176.42 (18) |
| N3—C19—C20—C25 | 52.9 (3) | C20—C19—N3—C10 | −122.3 (2) |
| N3—C19—C20—C21 | −130.3 (2) | C20—C19—N3—C11 | 66.5 (3) |
| C25—C20—C21—C22 | 0.7 (3) | C27—C28—N5—C29 | 0.3 (3) |
| C19—C20—C21—C22 | −176.1 (2) | C30—C29—N5—C28 | 179.6 (2) |
| C20—C21—C22—C23 | −0.6 (4) | C34—C29—N5—C28 | −0.4 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N5—H5···N1$^{i}$ | 0.86 | 1.96 | 2.812 (2) | 170 |
| C19—H19*A*···N4$^{ii}$ | 0.97 | 2.46 | 3.370 (3) | 157 |

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