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# [2-(1*H*-Indol-4-yl)ethyl]dipropylamine

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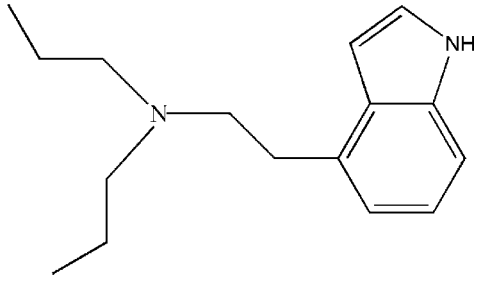
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.060; $wR$ factor = 0.122; data-to-parameter ratio = 16.9.

In the title compound, $C_{16}H_{24}N_2$, the aliphatic amine substituent is rotated almost orthogonally [C—C—C—C torsion angle = 75.7 (3)°] out of the plane of the indole unit. The amine N atom has a pyramidal configuration deviating by 0.380 (3) Å from the plane of the adjacent C atoms. All of the aliphatic groups are in extended transoid conformations. In the crystal, molecules form chains along the *a* axis *via* N—H···N hydrogen bonds.

## Related literature

For the synthesis and applications of the title compound, see: Srivastava *et al.* (1999).




## Experimental

### Crystal data

$C_{16}H_{24}N_2$ $M_r$ = 244.37
Orthorhombic, *Pbca*
$a$ = 12.1100 (9) Å
$b$ = 15.5996 (12) Å
$c$ = 16.0253 (12) Å
$V$ = 3027.4 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.06 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.981, $T_{max}$ = 0.994
2757 measured reflections
2757 independent reflections
1294 reflections with $I > 2\sigma(I)$
3 standard reflections every 200 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.122
$S$ = 1.00
2757 reflections
163 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.12 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···N2$^{i}$ | 0.86 | 2.10 | 2.945 (3) | 166 |

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; 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*.

The work was supported by the center of Testing and Analysis, Nanjing University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2053).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1502 [doi:10.1107/S1600536812015474]

## [2-(1*H*-Indol-4-yl)ethyl]dipropylamine

**De-Cai Wang, Hua-Yang Pan, Jun-Song Song, Ping Wei and Ping-Kai Ou-yang**

### Comment

The title compound is an important organic intermediate for the synthesis of 4-[2-(dipropylamino)ethyl]indol-2-one, an important compound for stimulating presynaptic dopamine autoreceptors in mammals (Srivastava *et al.*, 1999). In the process of synthesis, we obtained the crystal of the intermediate and we report its crystal structure.

### Experimental

The title compound was synthesized according to the published procedure (Srivastava *et al.*, 1999). A mixture of 4-[(2-amino)ethyl]indole (3.0 g, 18.72 mmol), 1-bromopropane (4.61 g, 37.44 mmol), $K_2CO_3$ (1 g, 7.25 mmol) in toluene (40 ml) was stirred at reflux temperature until the reaction completion is checked by thin layer silica gel (60–80 mesh) plates. When the mixture reached room temperature, it was filtered and the filtrate was poured in water and extracted with chloroform. The combined extract is washed with 10% brine solution, dried over $Na_2S0_4$ and concentrated to afford the crude product, which was filtered through column. The obtained material was distilled to afford the pure product 3.62 g with a 79% yield. The product (0.3 g) was crystallized from methanol (15 ml) at room temperature to give colorless crystals that were used for data collection.

### Refinement

Carbon- and nitrogen-bound H atoms were placed in calculated positions and were treated as riding on the parent C and N atoms with C—H = 0.96 (methyl), 0.97 (methylene) and N—H = 0.86 Å, $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C,*N*). The hydrogen atoms for methyl groups were placed in staggered positions. Rigid body restrains were applied to atoms N2, C11, C12 and C13 because of their excessive thermal motion

### Computing details

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); 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* (Sheldrick, 2008).

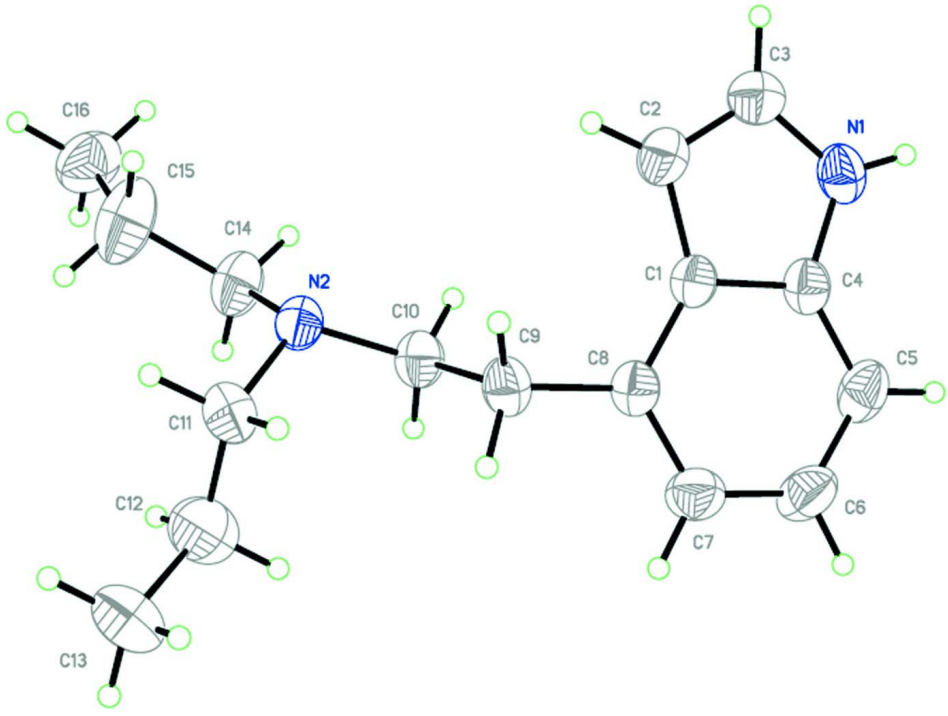


**Figure 1**

The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids.

### [2-(1*H*-Indol-4-yl)ethyl]dipropylamine

*Crystal data*

$C_{16}H_{24}N_2$
$M_r = 244.37$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.1100\ (9)$ Å
$b = 15.5996\ (12)$ Å
$c = 16.0253\ (12)$ Å
$V = 3027.4\ (4)$ Å$^3$
$Z = 8$
$F(000) = 1072$
$D_x = 1.072$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–$13°$
$\mu = 0.06$ mm$^{-1}$
$T = 293$ K
Block, white
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North et al., 1968)
$T_{min} = 0.981$, $T_{max} = 0.994$
2757 measured reflections
2757 independent reflections
1294 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 25.4°$, $\theta_{min} = 2.5°$
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 19$
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.122$
$S = 1.00$
2757 reflections
163 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{min} = -0.12$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.69898 (17) | 0.17493 (14) | 0.51171 (13) | 0.0529 (6) |
| N1 | 0.80610 (17) | 0.26448 (12) | 0.58576 (12) | 0.0672 (6) |
| H1A | 0.8600 | 0.2852 | 0.6144 | 0.081* |
| N2 | 0.46143 (14) | 0.14524 (11) | 0.30351 (11) | 0.0570 (5) |
| C2 | 0.64447 (19) | 0.25584 (16) | 0.51942 (15) | 0.0661 (7) |
| H2A | 0.5756 | 0.2705 | 0.4981 | 0.079* |
| C3 | 0.7130 (2) | 0.30703 (15) | 0.56402 (16) | 0.0719 (7) |
| H3A | 0.6980 | 0.3638 | 0.5778 | 0.086* |
| C4 | 0.79988 (18) | 0.18272 (15) | 0.55438 (14) | 0.0572 (6) |
| C5 | 0.87487 (19) | 0.11580 (17) | 0.55988 (17) | 0.0738 (8) |
| H5A | 0.9418 | 0.1220 | 0.5877 | 0.089* |
| C6 | 0.8458 (2) | 0.04041 (16) | 0.52256 (17) | 0.0809 (8) |
| H6A | 0.8942 | −0.0058 | 0.5252 | 0.097* |
| C7 | 0.7459 (2) | 0.03062 (15) | 0.48071 (16) | 0.0736 (7) |
| H7A | 0.7294 | −0.0219 | 0.4563 | 0.088* |
| C8 | 0.67057 (17) | 0.09681 (14) | 0.47445 (13) | 0.0562 (6) |
| C9 | 0.56340 (17) | 0.08773 (14) | 0.42753 (14) | 0.0611 (6) |
| H9A | 0.5043 | 0.1133 | 0.4599 | 0.073* |
| H9B | 0.5467 | 0.0274 | 0.4204 | 0.073* |
| C10 | 0.56870 (18) | 0.13063 (14) | 0.34234 (13) | 0.0608 (6) |
| H10A | 0.6061 | 0.1853 | 0.3482 | 0.073* |
| H10B | 0.6128 | 0.0952 | 0.3054 | 0.073* |
| C11 | 0.3925 (2) | 0.06598 (15) | 0.29295 (17) | 0.0822 (8) |
| H11A | 0.3830 | 0.0401 | 0.3475 | 0.099* |
| H11B | 0.3200 | 0.0835 | 0.2737 | 0.099* |
| C12 | 0.4330 (2) | 0.00010 (17) | 0.2365 (2) | 0.1074 (10) |

| | | | | |
|---|---|---|---|---|
| H12A | 0.5053 | −0.0195 | 0.2543 | 0.129* |
| H12B | 0.4396 | 0.0231 | 0.1804 | 0.129* |
| C13 | 0.3492 (3) | −0.07629 (16) | 0.2374 (2) | 0.1313 (13) |
| H13A | 0.3739 | −0.1201 | 0.1996 | 0.197* |
| H13B | 0.2777 | −0.0562 | 0.2203 | 0.197* |
| H13C | 0.3445 | −0.0994 | 0.2928 | 0.197* |
| C14 | 0.4724 (2) | 0.19861 (16) | 0.22911 (15) | 0.0805 (8) |
| H14A | 0.5079 | 0.1647 | 0.1860 | 0.097* |
| H14B | 0.5215 | 0.2459 | 0.2423 | 0.097* |
| C15 | 0.3695 (2) | 0.2346 (2) | 0.1942 (2) | 0.1199 (11) |
| H15A | 0.3244 | 0.2555 | 0.2398 | 0.144* |
| H15B | 0.3289 | 0.1888 | 0.1670 | 0.144* |
| C16 | 0.3850 (2) | 0.30558 (17) | 0.13303 (18) | 0.1030 (10) |
| H16A | 0.3141 | 0.3258 | 0.1146 | 0.155* |
| H16B | 0.4262 | 0.2850 | 0.0860 | 0.155* |
| H16C | 0.4245 | 0.3517 | 0.1591 | 0.155* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0514 (12) | 0.0586 (14) | 0.0488 (14) | −0.0011 (12) | −0.0021 (12) | 0.0050 (12) |
| N1 | 0.0656 (13) | 0.0724 (14) | 0.0634 (14) | −0.0148 (11) | −0.0121 (11) | 0.0002 (11) |
| N2 | 0.0528 (11) | 0.0663 (11) | 0.0520 (12) | 0.0045 (9) | −0.0036 (10) | 0.0009 (10) |
| C2 | 0.0560 (14) | 0.0747 (16) | 0.0675 (18) | 0.0034 (13) | −0.0038 (14) | 0.0044 (15) |
| C3 | 0.0754 (17) | 0.0649 (16) | 0.0755 (19) | 0.0011 (15) | −0.0004 (15) | −0.0017 (15) |
| C4 | 0.0540 (14) | 0.0626 (16) | 0.0549 (15) | −0.0124 (13) | −0.0051 (13) | 0.0077 (13) |
| C5 | 0.0543 (15) | 0.0775 (18) | 0.090 (2) | −0.0078 (14) | −0.0185 (14) | 0.0184 (16) |
| C6 | 0.0620 (17) | 0.0649 (17) | 0.116 (2) | 0.0074 (13) | −0.0148 (17) | 0.0109 (17) |
| C7 | 0.0730 (17) | 0.0570 (15) | 0.091 (2) | −0.0010 (14) | −0.0053 (16) | −0.0016 (14) |
| C8 | 0.0528 (14) | 0.0616 (15) | 0.0542 (15) | −0.0063 (12) | −0.0022 (12) | 0.0056 (13) |
| C9 | 0.0570 (14) | 0.0686 (15) | 0.0575 (15) | −0.0113 (12) | −0.0067 (13) | 0.0029 (13) |
| C10 | 0.0523 (14) | 0.0735 (16) | 0.0567 (16) | −0.0031 (12) | 0.0003 (13) | 0.0031 (13) |
| C11 | 0.0859 (19) | 0.0750 (16) | 0.086 (2) | −0.0045 (12) | −0.0250 (16) | −0.0099 (16) |
| C12 | 0.110 (2) | 0.098 (2) | 0.115 (3) | −0.0031 (16) | −0.004 (2) | −0.015 (2) |
| C13 | 0.142 (3) | 0.086 (2) | 0.166 (3) | −0.0158 (17) | −0.045 (2) | −0.032 (2) |
| C14 | 0.0766 (18) | 0.099 (2) | 0.065 (2) | 0.0077 (15) | −0.0086 (15) | 0.0167 (16) |
| C15 | 0.090 (2) | 0.170 (3) | 0.100 (3) | 0.013 (2) | −0.010 (2) | 0.046 (2) |
| C16 | 0.125 (2) | 0.101 (2) | 0.083 (2) | 0.0286 (19) | −0.0048 (19) | 0.0154 (19) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C8 | 1.400 (3) | C9—H9B | 0.9700 |
| C1—C4 | 1.405 (3) | C10—H10A | 0.9700 |
| C1—C2 | 1.430 (3) | C10—H10B | 0.9700 |
| N1—C3 | 1.354 (3) | C11—C12 | 1.455 (3) |
| N1—C4 | 1.373 (2) | C11—H11A | 0.9700 |
| N1—H1A | 0.8600 | C11—H11B | 0.9700 |
| N2—C10 | 1.458 (2) | C12—C13 | 1.566 (3) |
| N2—C14 | 1.460 (3) | C12—H12A | 0.9700 |
| N2—C11 | 1.501 (2) | C12—H12B | 0.9700 |

| | | | |
|---|---|---|---|
| C2—C3 | 1.355 (3) | C13—H13A | 0.9600 |
| C2—H2A | 0.9300 | C13—H13B | 0.9600 |
| C3—H3A | 0.9300 | C13—H13C | 0.9600 |
| C4—C5 | 1.386 (3) | C14—C15 | 1.477 (3) |
| C5—C6 | 1.366 (3) | C14—H14A | 0.9700 |
| C5—H5A | 0.9300 | C14—H14B | 0.9700 |
| C6—C7 | 1.391 (3) | C15—C16 | 1.490 (3) |
| C6—H6A | 0.9300 | C15—H15A | 0.9700 |
| C7—C8 | 1.381 (3) | C15—H15B | 0.9700 |
| C7—H7A | 0.9300 | C16—H16A | 0.9600 |
| C8—C9 | 1.507 (3) | C16—H16B | 0.9600 |
| C9—C10 | 1.522 (3) | C16—H16C | 0.9600 |
| C9—H9A | 0.9700 | | |

| | | | |
|---|---|---|---|
| C8—C1—C4 | 119.8 (2) | N2—C10—H10B | 108.6 |
| C8—C1—C2 | 133.8 (2) | C9—C10—H10B | 108.6 |
| C4—C1—C2 | 106.4 (2) | H10A—C10—H10B | 107.6 |
| C3—N1—C4 | 108.38 (19) | C12—C11—N2 | 117.7 (2) |
| C3—N1—H1A | 125.8 | C12—C11—H11A | 107.9 |
| C4—N1—H1A | 125.8 | N2—C11—H11A | 107.9 |
| C10—N2—C14 | 110.90 (17) | C12—C11—H11B | 107.9 |
| C10—N2—C11 | 114.50 (17) | N2—C11—H11B | 107.9 |
| C14—N2—C11 | 115.34 (19) | H11A—C11—H11B | 107.2 |
| C3—C2—C1 | 106.4 (2) | C11—C12—C13 | 108.2 (2) |
| C3—C2—H2A | 126.8 | C11—C12—H12A | 110.0 |
| C1—C2—H2A | 126.8 | C13—C12—H12A | 110.0 |
| N1—C3—C2 | 110.9 (2) | C11—C12—H12B | 110.0 |
| N1—C3—H3A | 124.6 | C13—C12—H12B | 110.0 |
| C2—C3—H3A | 124.6 | H12A—C12—H12B | 108.4 |
| N1—C4—C5 | 129.8 (2) | C12—C13—H13A | 109.5 |
| N1—C4—C1 | 107.8 (2) | C12—C13—H13B | 109.5 |
| C5—C4—C1 | 122.4 (2) | H13A—C13—H13B | 109.5 |
| C6—C5—C4 | 116.8 (2) | C12—C13—H13C | 109.5 |
| C6—C5—H5A | 121.6 | H13A—C13—H13C | 109.5 |
| C4—C5—H5A | 121.6 | H13B—C13—H13C | 109.5 |
| C5—C6—C7 | 122.0 (2) | N2—C14—C15 | 116.7 (2) |
| C5—C6—H6A | 119.0 | N2—C14—H14A | 108.1 |
| C7—C6—H6A | 119.0 | C15—C14—H14A | 108.1 |
| C8—C7—C6 | 121.8 (2) | N2—C14—H14B | 108.1 |
| C8—C7—H7A | 119.1 | C15—C14—H14B | 108.1 |
| C6—C7—H7A | 119.1 | H14A—C14—H14B | 107.3 |
| C7—C8—C1 | 117.2 (2) | C14—C15—C16 | 115.2 (3) |
| C7—C8—C9 | 122.3 (2) | C14—C15—H15A | 108.5 |
| C1—C8—C9 | 120.4 (2) | C16—C15—H15A | 108.5 |
| C8—C9—C10 | 111.72 (17) | C14—C15—H15B | 108.5 |
| C8—C9—H9A | 109.3 | C16—C15—H15B | 108.5 |
| C10—C9—H9A | 109.3 | H15A—C15—H15B | 107.5 |
| C8—C9—H9B | 109.3 | C15—C16—H16A | 109.5 |
| C10—C9—H9B | 109.3 | C15—C16—H16B | 109.5 |

| | | | |
|---|---|---|---|
| H9A—C9—H9B | 107.9 | H16A—C16—H16B | 109.5 |
| N2—C10—C9 | 114.46 (18) | C15—C16—H16C | 109.5 |
| N2—C10—H10A | 108.6 | H16A—C16—H16C | 109.5 |
| C9—C10—H10A | 108.6 | H16B—C16—H16C | 109.5 |
| | | | |
| C8—C1—C2—C3 | 178.9 (2) | C4—C1—C8—C7 | −1.0 (3) |
| C4—C1—C2—C3 | 0.6 (2) | C2—C1—C8—C7 | −179.2 (2) |
| C4—N1—C3—C2 | 0.4 (3) | C4—C1—C8—C9 | −179.20 (19) |
| C1—C2—C3—N1 | −0.6 (3) | C2—C1—C8—C9 | 2.7 (4) |
| C3—N1—C4—C5 | 179.7 (2) | C7—C8—C9—C10 | −102.4 (2) |
| C3—N1—C4—C1 | 0.0 (2) | C1—C8—C9—C10 | 75.7 (3) |
| C8—C1—C4—N1 | −178.98 (19) | C14—N2—C10—C9 | 170.78 (18) |
| C2—C1—C4—N1 | −0.4 (2) | C11—N2—C10—C9 | −56.6 (3) |
| C8—C1—C4—C5 | 1.4 (3) | C8—C9—C10—N2 | −163.88 (18) |
| C2—C1—C4—C5 | 180.0 (2) | C10—N2—C11—C12 | −65.2 (3) |
| N1—C4—C5—C6 | 179.5 (2) | C14—N2—C11—C12 | 65.3 (3) |
| C1—C4—C5—C6 | −0.9 (4) | N2—C11—C12—C13 | 178.8 (2) |
| C4—C5—C6—C7 | 0.1 (4) | C10—N2—C14—C15 | −166.8 (2) |
| C5—C6—C7—C8 | 0.1 (4) | C11—N2—C14—C15 | 61.0 (3) |
| C6—C7—C8—C1 | 0.3 (4) | N2—C14—C15—C16 | 164.9 (2) |
| C6—C7—C8—C9 | 178.5 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···N2$^{i}$ | 0.86 | 2.10 | 2.945 (3) | 166 |

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