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# 2-Benzyl-6-nitro-2*H*-indazole

Mohamed Mokhtar Mohamed Abdelahi,[a] Youness El Bakri,[a] Mohammed Benchidmi,[a]* El Mokhtar Essassi[a] and Joel T. Mague[b]

[a]Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche des Sciences des médicaments, URAC 21, Pôle de Compétence Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Université Mohammed V, Rabat, Morocco, and [b]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: jalilmostafa202@gmail.com

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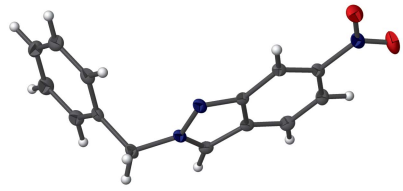
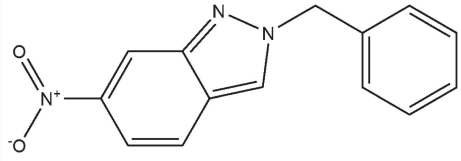
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{14}H_{11}N_3O_2$, the indazole portion is planar to within 0.022 (2) Å and subtends a dihedral angle of 65.87 (7)° with the pendant benzene ring. In the crystal, oblique stacks of molecules extending along the *a*-axis direction are generated by $\pi$–$\pi$ stacking interactions between the five- and six-membered rings [centroid–centroid separation = 3.6743 (19) Å] and the stacks are cross-linked by C—H···O hydrogen bonds.

**3D view**



**Chemical scheme**




## Structure description

Although rare in nature (Liu *et al.*, 2004; Ali *et al.*, 2008), indazoles exhibit a variety of biological activities such as HIV protease inhibition (Patel *et al.*, 1999), antiarrhythmic and analgesic activities (Mosti *et al.*, 2000). As a continuation of our studies of indazole derivatives (Mohamed Abdelahi *et al.*, 2017), we report the synthesis and structure of the title compound (Fig. 1).

The indazole portion is almost planar (r.m.s. deviation 0.017 Å) with the atoms farthest from the mean plane being C6 (0.018 (2) Å) and C5 (−0.022 (2) Å). The dihedral angle between the mean plane of the indazole unit and the benzene ring of the benzyl side chain is 65.87 (7)°. The crystal packing involves oblique stacks of molecules extending along the *a*-axis direction formed by $\pi$–$\pi$-stacking interactions between the five- and six-membered rings of the indazole units with a centroid–centroid distance of 3.6744 (19) Å and a dihedral angle of 1.63 (8)° (Fig. 2). The stacks are associated through C7—H7···O1, C8—H8*B*···O2 and C10—H10···O2 hydrogen bonds (Table 1 and Figs. 2 and 3).

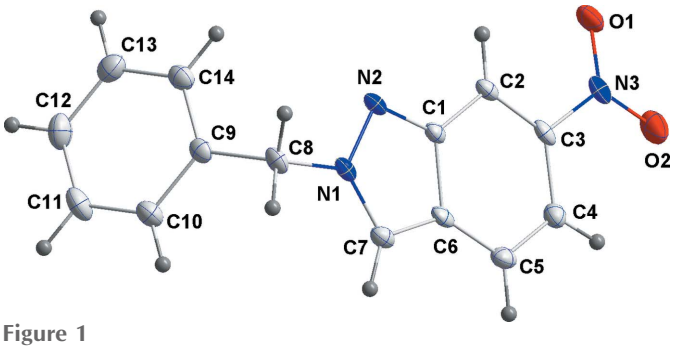



**Figure 1**
The title molecule, with the atom-labeling scheme and 50% probability displacement ellipsoids.

## Synthesis and crystallization

To a solution of 6-nitro-1*H*-indazole (1 g, 5 mmol) in tetrahydrofuran (30 ml) was added benzylchloride (0.8 g, 5 mmol), potassium carbonate (1.24 g, 9 mmol) and a catalytic quantity of tetra-*n*-butylammonium iodide. The mixture was stirred at room temperature for 48 h. The solution was filtered and the solvent removed under reduced pressure. The residue was recrystallized from ethanol solution to afford the title compound as colourless crystals (yield: 86%)

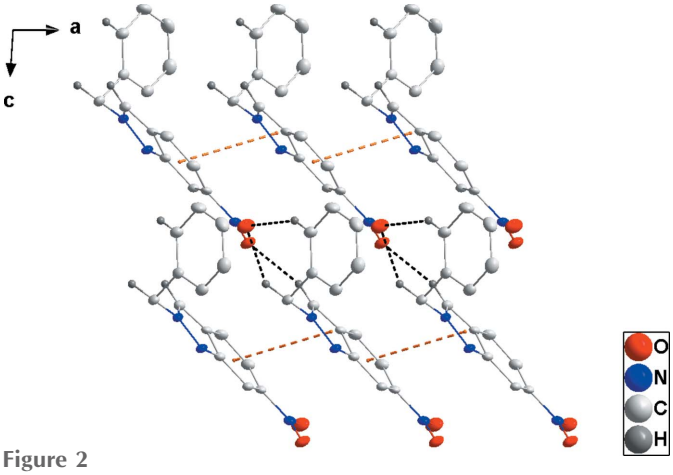



**Figure 2**
Detail of the intermolecular interactions, viewed along the *b*-axis direction. C—H···O hydrogen bonds are shown as black dashed lines, while $\pi$–$\pi$ stacking interactions are shown as orange dashed lines.

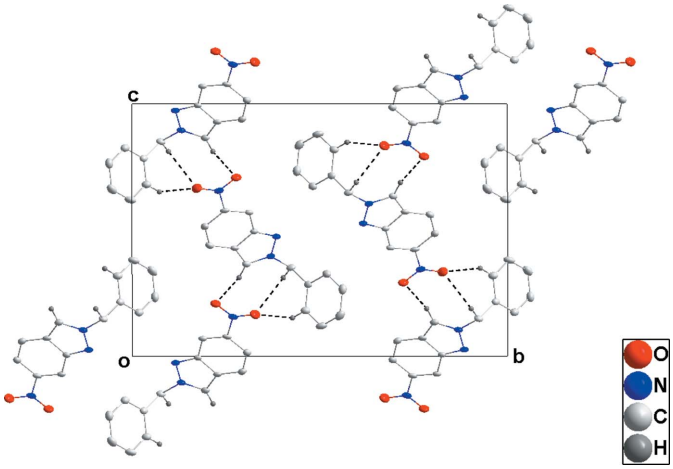



**Figure 3**
Packing, viewed along the *a*-axis direction, with C—H···O hydrogen bonds shown as black dashed lines.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C7—H7···O1$^{i}$ | 0.95 | 2.51 | 3.437 (2) | 164 |
| C8—H8$B$···O2$^{i}$ | 0.99 | 2.53 | 3.407 (2) | 147 |
| C10—H10···O2$^{i}$ | 0.95 | 2.56 | 3.431 (3) | 152 |

Symmetry code: (i) $x-\frac{3}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{14}H_{11}N_3O_2$ |
| $M_r$ | 253.26 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 100 |
| $a$, $b$, $c$ (Å) | 4.4890 (19), 19.770 (8), 13.308 (6) |
| $\beta$ (°) | 93.608 (6) |
| $V$ (Å$^3$) | 1178.6 (9) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.10 |
| Crystal size (mm) | 0.40 × 0.20 × 0.17 |
| | |
| Data collection | |
| Diffractometer | Bruker SMART APEX CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2016) |
| $T_{min}$, $T_{max}$ | 0.96, 0.98 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 22904, 3223, 2210 |
| $R_{int}$ | 0.056 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.693 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.059, 0.150, 0.96 |
| No. of reflections | 3223 |
| No. of parameters | 172 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.54, −0.27 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008*b*).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal used contained a minor twin component (*CELL_NOW;* Sheldrick, 2008*a*), which was considered sufficiently small to be ignored in the final refinement.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2018). **3**, x180151 [https://doi.org/10.1107/S2414314618001517]

## 2-Benzyl-6-nitro-2*H*-indazole

**Mohamed Mokhtar Mohamed Abdelahi, Youness El Bakri, Mohammed Benchidmi, El Mokhtar Essassi and Joel T. Mague**

### 2-Benzyl-6-nitro-2*H*-indazole

*Crystal data*

$C_{14}H_{11}N_3O_2$
$M_r$ = 253.26
Monoclinic, $P2_1/n$
$a$ = 4.4890 (19) Å
$b$ = 19.770 (8) Å
$c$ = 13.308 (6) Å
$\beta$ = 93.608 (6)°
$V$ = 1178.6 (9) Å$^3$
$Z$ = 4
$F(000)$ = 528
$D_x$ = 1.427 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9894 reflections
$\theta$ = 2.6–28.9°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 100 K
Column, colourless
0.40 × 0.20 × 0.17 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
$T_{min}$ = 0.96, $T_{max}$ = 0.98
22904 measured reflections
3223 independent reflections
2210 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056
$\theta_{max}$ = 29.5°, $\theta_{min}$ = 1.9°
$h$ = −6→6
$k$ = 0→27
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.150
$S$ = 0.96
3223 reflections
172 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
$w = 1/[\sigma^2(F_o^2) + (0.0959P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

*Special details*

**Experimental**. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in $\omega$, colllected at $\varphi$ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in $\varphi$, collected at $\omega$ = –30.00 and 210.00°. The scan time was 20 sec/frame.

**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.

**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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å). All were included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 1.1690 (3) | 0.27750 (6) | 0.70851 (9) | 0.0254 (3) |
| O2 | 1.1457 (3) | 0.17253 (6) | 0.66604 (9) | 0.0314 (3) |
| N1 | 0.1797 (3) | 0.36929 (6) | 0.39590 (9) | 0.0156 (3) |
| N2 | 0.3722 (3) | 0.38443 (6) | 0.47413 (9) | 0.0164 (3) |
| N3 | 1.0647 (3) | 0.23134 (6) | 0.65597 (10) | 0.0193 (3) |
| C1 | 0.5118 (3) | 0.32514 (7) | 0.49448 (11) | 0.0143 (3) |
| C2 | 0.7354 (3) | 0.31196 (7) | 0.57032 (11) | 0.0152 (3) |
| H2 | 0.813941 | 0.346431 | 0.614108 | 0.018* |
| C3 | 0.8331 (4) | 0.24708 (8) | 0.57749 (11) | 0.0163 (3) |
| C4 | 0.7253 (4) | 0.19377 (8) | 0.51450 (11) | 0.0189 (3) |
| H4 | 0.800949 | 0.149231 | 0.524440 | 0.023* |
| C5 | 0.5123 (4) | 0.20657 (8) | 0.43946 (11) | 0.0194 (3) |
| H5 | 0.440036 | 0.171504 | 0.395606 | 0.023* |
| C6 | 0.4017 (4) | 0.27289 (7) | 0.42839 (11) | 0.0153 (3) |
| C7 | 0.1870 (3) | 0.30481 (7) | 0.36564 (11) | 0.0171 (3) |
| H7 | 0.068645 | 0.284850 | 0.311847 | 0.020* |
| C8 | −0.0081 (3) | 0.42330 (8) | 0.35141 (11) | 0.0179 (3) |
| H8A | −0.088342 | 0.450603 | 0.405911 | 0.021* |
| H8B | −0.179168 | 0.402997 | 0.311612 | 0.021* |
| C9 | 0.1609 (3) | 0.46872 (7) | 0.28450 (11) | 0.0164 (3) |
| C10 | 0.1313 (4) | 0.46162 (8) | 0.18117 (12) | 0.0216 (4) |
| H10 | 0.006152 | 0.427191 | 0.151969 | 0.026* |
| C11 | 0.2830 (4) | 0.50439 (9) | 0.11997 (13) | 0.0275 (4) |
| H11 | 0.259724 | 0.499660 | 0.048866 | 0.033* |
| C12 | 0.4678 (4) | 0.55385 (8) | 0.16192 (13) | 0.0269 (4) |
| H12 | 0.572625 | 0.583060 | 0.119773 | 0.032* |
| C13 | 0.5007 (4) | 0.56093 (8) | 0.26501 (13) | 0.0247 (4) |
| H13 | 0.628790 | 0.594894 | 0.293986 | 0.030* |
| C14 | 0.3475 (4) | 0.51870 (7) | 0.32611 (12) | 0.0201 (3) |
| H14 | 0.369781 | 0.523851 | 0.397166 | 0.024* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0261 (7) | 0.0325 (7) | 0.0165 (6) | −0.0024 (5) | −0.0068 (5) | 0.0013 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.0377 (8) | 0.0312 (7) | 0.0244 (7) | 0.0144 (5) | −0.0048 (6) | 0.0036 (5) |
| N1 | 0.0136 (7) | 0.0232 (7) | 0.0099 (6) | −0.0006 (5) | −0.0010 (5) | 0.0022 (5) |
| N2 | 0.0166 (7) | 0.0223 (6) | 0.0099 (6) | 0.0001 (5) | −0.0024 (5) | −0.0003 (5) |
| N3 | 0.0193 (8) | 0.0280 (7) | 0.0107 (6) | 0.0029 (5) | 0.0019 (5) | 0.0034 (5) |
| C1 | 0.0155 (8) | 0.0184 (7) | 0.0091 (7) | −0.0018 (6) | 0.0014 (5) | 0.0005 (5) |
| C2 | 0.0150 (8) | 0.0220 (7) | 0.0086 (7) | −0.0019 (6) | 0.0005 (5) | −0.0002 (5) |
| C3 | 0.0153 (8) | 0.0257 (8) | 0.0079 (7) | 0.0010 (6) | 0.0017 (6) | 0.0026 (5) |
| C4 | 0.0234 (9) | 0.0193 (7) | 0.0141 (7) | 0.0026 (6) | 0.0026 (6) | 0.0010 (5) |
| C5 | 0.0232 (9) | 0.0216 (8) | 0.0135 (7) | −0.0023 (6) | 0.0023 (6) | −0.0035 (6) |
| C6 | 0.0158 (8) | 0.0222 (8) | 0.0081 (7) | −0.0023 (6) | 0.0024 (5) | −0.0005 (5) |
| C7 | 0.0168 (8) | 0.0220 (7) | 0.0124 (7) | −0.0034 (6) | 0.0011 (6) | −0.0010 (5) |
| C8 | 0.0157 (8) | 0.0246 (8) | 0.0129 (7) | 0.0030 (6) | −0.0018 (6) | 0.0027 (5) |
| C9 | 0.0154 (8) | 0.0191 (7) | 0.0146 (7) | 0.0049 (6) | −0.0006 (6) | 0.0007 (5) |
| C10 | 0.0224 (9) | 0.0268 (8) | 0.0154 (8) | 0.0000 (6) | −0.0010 (6) | −0.0006 (6) |
| C11 | 0.0294 (11) | 0.0384 (9) | 0.0148 (8) | 0.0023 (7) | 0.0029 (7) | 0.0054 (7) |
| C12 | 0.0246 (10) | 0.0288 (9) | 0.0280 (10) | 0.0016 (7) | 0.0072 (7) | 0.0101 (7) |
| C13 | 0.0240 (10) | 0.0188 (8) | 0.0312 (10) | 0.0001 (6) | −0.0004 (7) | 0.0008 (6) |
| C14 | 0.0203 (9) | 0.0225 (8) | 0.0172 (8) | 0.0037 (6) | −0.0014 (6) | −0.0006 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—N3 | 1.2245 (17) | C6—C7 | 1.387 (2) |
| O2—N3 | 1.2230 (17) | C7—H7 | 0.9500 |
| N1—C7 | 1.3379 (19) | C8—C9 | 1.503 (2) |
| N1—N2 | 1.3441 (17) | C8—H8A | 0.9900 |
| N1—C8 | 1.4623 (19) | C8—H8B | 0.9900 |
| N2—C1 | 1.3487 (19) | C9—C10 | 1.380 (2) |
| N3—C3 | 1.460 (2) | C9—C14 | 1.388 (2) |
| C1—C2 | 1.402 (2) | C10—C11 | 1.383 (2) |
| C1—C6 | 1.425 (2) | C10—H10 | 0.9500 |
| C2—C3 | 1.357 (2) | C11—C12 | 1.378 (3) |
| C2—H2 | 0.9500 | C11—H11 | 0.9500 |
| C3—C4 | 1.413 (2) | C12—C13 | 1.378 (2) |
| C4—C5 | 1.362 (2) | C12—H12 | 0.9500 |
| C4—H4 | 0.9500 | C13—C14 | 1.379 (2) |
| C5—C6 | 1.406 (2) | C13—H13 | 0.9500 |
| C5—H5 | 0.9500 | C14—H14 | 0.9500 |
| | | | |
| C7—N1—N2 | 114.75 (12) | N1—C7—H7 | 126.8 |
| C7—N1—C8 | 126.75 (13) | C6—C7—H7 | 126.8 |
| N2—N1—C8 | 118.49 (12) | N1—C8—C9 | 112.12 (13) |
| N1—N2—C1 | 103.29 (12) | N1—C8—H8A | 109.2 |
| O2—N3—O1 | 123.07 (14) | C9—C8—H8A | 109.2 |
| O2—N3—C3 | 118.31 (13) | N1—C8—H8B | 109.2 |
| O1—N3—C3 | 118.61 (13) | C9—C8—H8B | 109.2 |
| N2—C1—C2 | 127.49 (13) | H8A—C8—H8B | 107.9 |
| N2—C1—C6 | 111.56 (14) | C10—C9—C14 | 119.19 (15) |
| C2—C1—C6 | 120.95 (13) | C10—C9—C8 | 120.59 (14) |

| | | | |
|---|---|---|---|
| C3—C2—C1 | 116.09 (13) | C14—C9—C8 | 120.22 (14) |
| C3—C2—H2 | 122.0 | C9—C10—C11 | 120.31 (15) |
| C1—C2—H2 | 122.0 | C9—C10—H10 | 119.8 |
| C2—C3—C4 | 124.50 (14) | C11—C10—H10 | 119.8 |
| C2—C3—N3 | 117.65 (13) | C12—C11—C10 | 120.11 (16) |
| C4—C3—N3 | 117.85 (14) | C12—C11—H11 | 119.9 |
| C5—C4—C3 | 119.65 (14) | C10—C11—H11 | 119.9 |
| C5—C4—H4 | 120.2 | C13—C12—C11 | 119.97 (16) |
| C3—C4—H4 | 120.2 | C13—C12—H12 | 120.0 |
| C4—C5—C6 | 118.48 (14) | C11—C12—H12 | 120.0 |
| C4—C5—H5 | 120.8 | C12—C13—C14 | 119.98 (16) |
| C6—C5—H5 | 120.8 | C12—C13—H13 | 120.0 |
| C7—C6—C5 | 135.61 (14) | C14—C13—H13 | 120.0 |
| C7—C6—C1 | 104.05 (13) | C13—C14—C9 | 120.44 (15) |
| C5—C6—C1 | 120.32 (14) | C13—C14—H14 | 119.8 |
| N1—C7—C6 | 106.36 (13) | C9—C14—H14 | 119.8 |

| | | | |
|---|---|---|---|
| C7—N1—N2—C1 | 0.19 (16) | N2—C1—C6—C5 | −177.95 (14) |
| C8—N1—N2—C1 | −178.47 (12) | C2—C1—C6—C5 | 1.2 (2) |
| N1—N2—C1—C2 | −179.58 (14) | N2—N1—C7—C6 | 0.16 (17) |
| N1—N2—C1—C6 | −0.48 (16) | C8—N1—C7—C6 | 178.70 (14) |
| N2—C1—C2—C3 | 177.76 (15) | C5—C6—C7—N1 | 177.76 (17) |
| C6—C1—C2—C3 | −1.3 (2) | C1—C6—C7—N1 | −0.43 (16) |
| C1—C2—C3—C4 | 0.1 (2) | C7—N1—C8—C9 | −101.09 (17) |
| C1—C2—C3—N3 | −179.67 (13) | N2—N1—C8—C9 | 77.40 (16) |
| O2—N3—C3—C2 | 176.93 (14) | N1—C8—C9—C10 | 101.16 (16) |
| O1—N3—C3—C2 | −3.1 (2) | N1—C8—C9—C14 | −79.25 (17) |
| O2—N3—C3—C4 | −2.9 (2) | C14—C9—C10—C11 | −0.8 (2) |
| O1—N3—C3—C4 | 177.09 (14) | C8—C9—C10—C11 | 178.78 (15) |
| C2—C3—C4—C5 | 1.2 (2) | C9—C10—C11—C12 | 0.8 (3) |
| N3—C3—C4—C5 | −179.05 (14) | C10—C11—C12—C13 | −0.3 (3) |
| C3—C4—C5—C6 | −1.2 (2) | C11—C12—C13—C14 | −0.3 (3) |
| C4—C5—C6—C7 | −177.89 (17) | C12—C13—C14—C9 | 0.3 (2) |
| C4—C5—C6—C1 | 0.1 (2) | C10—C9—C14—C13 | 0.2 (2) |
| N2—C1—C6—C7 | 0.58 (17) | C8—C9—C14—C13 | −179.36 (14) |
| C2—C1—C6—C7 | 179.75 (14) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···O1$^{i}$ | 0.95 | 2.51 | 3.437 (2) | 164 |
| C8—H8*B*···O2$^{i}$ | 0.99 | 2.53 | 3.407 (2) | 147 |
| C10—H10···O2$^{i}$ | 0.95 | 2.56 | 3.431 (3) | 152 |

Symmetry code: (i) *x*−3/2, −*y*+1/2, *z*−1/2.