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# *N*′-(1-Allyl-2-oxoindolin-3-ylidene)-benzohydrazide

**Abdulsalam Alsubari,[a] Ahmed Moussaif,[a] Hafid Zouihri,[b] El Mokhtar Essassi[a] and Seik Weng Ng[c]***

[a]Laboratoire de Chimie Organique Hétérocyclique, Pôle de Compétences Pharmacochimie, Université Mohammed V-Agdal, BP 1014 Avenue Ibn Batout, Rabat, Morocco, [b]CNRST Division UATRS, Angle Allal Fassi/FAR, BP 8027 Hay Riad, Rabat, Morocco, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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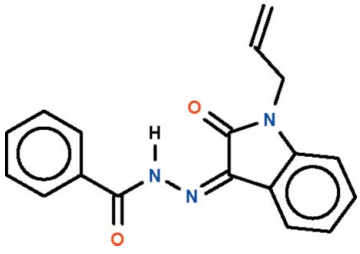
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.041; $wR$ factor = 0.108; data-to-parameter ratio = 15.5.

In the title compound, $C_{18}H_{15}N_3O_2$, the dihedral angle between the ring systems is 15.1 (1)°. The amino H atom is hydrogen bonded to the exocyclic O atom of the five-membered ring, forming an $S$(6) motif.

## Related literature

For the use of the title compound as the starting reactant for the synthesis of other heterocyclic systems, see: Alsubari *et al.* (2009). For a related structure, see: Ali *et al.* (2005*a*,*b*).



## Experimental

### *Crystal data*

$C_{18}H_{15}N_3O_2$ $M_r$ = 305.33
Monoclinic, $P2_1/c$
$a$ = 7.5921 (2) Å
$b$ = 15.1968 (4) Å
$c$ = 12.8716 (3) Å
$\beta$ = 94.481 (2)°
$V$ = 1480.53 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.35 × 0.30 × 0.20 mm

### *Data collection*

Bruker X8 APEXII diffractometer
17477 measured reflections
3286 independent reflections
2343 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.059

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
$S$ = 1.00
3286 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···O1 | 0.88 (2) | 1.98 (2) | 2.721 (2) | 141 (2) |

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Université Mohammed V-Agdal and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2174).

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# supporting information

*Acta Cryst.* (2010). E**66**, o1905 [https://doi.org/10.1107/S1600536810024918]

## *N*′-(1-Allyl-2-oxoindolin-3-ylidene)benzohydrazide

**Abdulsalam Alsubari, Ahmed Moussaif, Hafid Zouihri, El Mokhtar Essassi and Seik Weng Ng**

### S1. Comment

An earlier study reports the synthesis of oxindole derivatives bearing an oxazolidin-2-one sub-unit. The title Sciff base (Scheme I) is the starting reactant for the synthesis of other heterocyclic systems (Alsubari *et al.*, 2009). We have previously determined the crystal structure of two modifications of the Schiff base derived by condensing isatin and benzoylhydrazine. In both, the amino unit of the five-membered ring functions as a hydrogen bond donor to carbonyl group of an adjacent molecule to generate a chain structure. Meanwhile, the amino –NH– unit forms an intramolecular hydrogen bond to the –C(═O)– unit of the five-membered ring (Ali *et al.*, 2005*a*, 2005*b*). The molecule of $C_{18}H_{15}N_3O_2$ (Fig, 1) has a phenyl ring connected to a nine-membered fused-ring through the three-atom –C(═O)–N(H)–N═unit, whose amino H-atom is hydrogen bonded to the carbonyl group of the fused-ring. The two ring systems are aligned at 15.1 (1) °.

### S2. Experimental

1-Allylindoline-2,3-dione (0.5 g, 2.7 mmol) and benzoyl hydrazine (0.36 g, 2.7 mmol) were heated in ethanol (20 ml) for 2 h. The solvent was evaporated and the yellow solid was recrystallized from ethanol in 90% yield.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with $U$(H) set to 1.2$U_{eq}$(C).

The amino H-atom was located in a difference Fourier map; the N–H distance was restrained to 0.86±0.01 Å; the temperature factor of this hydrogen atom was freely refined.

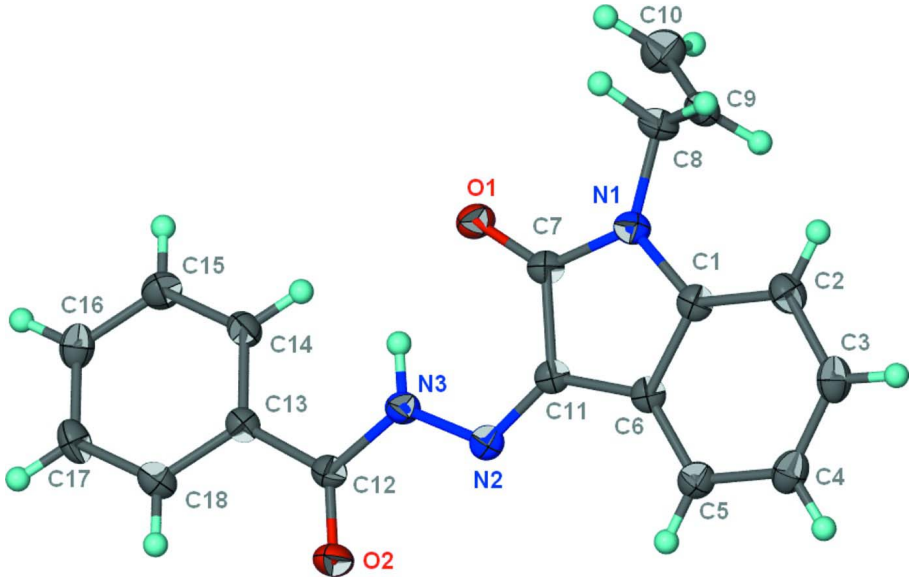


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of the molecule of $C_{18}H_{15}N_3O_2$ at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii.

### *N*′-(1-Allyl-2-oxoindolin-3-ylidene)benzohydrazide

*Crystal data*

$C_{18}H_{15}N_3O_2$
$M_r = 305.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.5921\ (2)$ Å
$b = 15.1968\ (4)$ Å
$c = 12.8716\ (3)$ Å
$\beta = 94.481\ (2)°$
$V = 1480.53\ (7)$ Å$^3$
$Z = 4$
$F(000) = 640$
$D_x = 1.370$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3004 reflections
$\theta = 2.7–25.0°$
$\mu = 0.09$ mm$^{-1}$
$T = 293$ K
Prism, yellow
0.35 × 0.30 × 0.20 mm

*Data collection*

Bruker X8 APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
17477 measured reflections
3286 independent reflections
2343 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 27.1°$, $\theta_{min} = 2.7°$
$h = -9\rightarrow9$
$k = -19\rightarrow19$
$l = -16\rightarrow16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.108$
$S = 1.00$
3286 reflections
212 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.3757P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.63773 (15) | 0.55475 (7) | 0.60381 (8) | 0.0315 (3) |
| O2 | 0.68617 (16) | 0.66838 (8) | 0.24350 (8) | 0.0353 (3) |
| N1 | 0.76855 (17) | 0.41763 (9) | 0.62121 (10) | 0.0271 (3) |
| N2 | 0.75597 (16) | 0.53877 (8) | 0.38503 (9) | 0.0248 (3) |
| N3 | 0.67263 (17) | 0.61477 (9) | 0.40734 (10) | 0.0259 (3) |
| H3 | 0.638 (2) | 0.6205 (11) | 0.4710 (14) | 0.034 (5)* |
| C1 | 0.8544 (2) | 0.35920 (10) | 0.55565 (12) | 0.0261 (3) |
| C2 | 0.9222 (2) | 0.27683 (11) | 0.57850 (13) | 0.0318 (4) |
| H2 | 0.9162 | 0.2518 | 0.6441 | 0.038* |
| C3 | 1.0002 (2) | 0.23266 (11) | 0.49925 (14) | 0.0342 (4) |
| H3A | 1.0454 | 0.1765 | 0.5120 | 0.041* |
| C4 | 1.0126 (2) | 0.27008 (11) | 0.40166 (14) | 0.0338 (4) |
| H4 | 1.0683 | 0.2395 | 0.3509 | 0.041* |
| C5 | 0.9423 (2) | 0.35293 (11) | 0.37944 (12) | 0.0292 (4) |
| H5 | 0.9496 | 0.3781 | 0.3141 | 0.035* |
| C6 | 0.86100 (19) | 0.39725 (10) | 0.45682 (12) | 0.0248 (3) |
| C7 | 0.7178 (2) | 0.49230 (11) | 0.56872 (12) | 0.0258 (3) |
| C8 | 0.7558 (2) | 0.40781 (12) | 0.73353 (12) | 0.0306 (4) |
| H8A | 0.7490 | 0.3458 | 0.7505 | 0.037* |
| H8B | 0.6484 | 0.4359 | 0.7529 | 0.037* |
| C9 | 0.9114 (2) | 0.44791 (11) | 0.79466 (12) | 0.0302 (4) |
| H9 | 1.0233 | 0.4259 | 0.7850 | 0.036* |
| C10 | 0.8980 (3) | 0.51229 (13) | 0.86094 (14) | 0.0418 (5) |
| H10A | 0.7876 | 0.5354 | 0.8720 | 0.050* |
| H10B | 0.9988 | 0.5350 | 0.8971 | 0.050* |
| C11 | 0.77560 (19) | 0.48267 (10) | 0.46041 (11) | 0.0238 (3) |
| C12 | 0.6459 (2) | 0.67879 (11) | 0.33277 (11) | 0.0255 (3) |
| C13 | 0.5594 (2) | 0.76046 (10) | 0.36850 (11) | 0.0254 (3) |
| C14 | 0.5437 (2) | 0.78064 (11) | 0.47319 (12) | 0.0300 (4) |
| H14 | 0.5883 | 0.7420 | 0.5248 | 0.036* |
| C15 | 0.4623 (2) | 0.85771 (12) | 0.50059 (13) | 0.0351 (4) |
| H15 | 0.4523 | 0.8708 | 0.5705 | 0.042* |
| C16 | 0.3957 (2) | 0.91536 (11) | 0.42413 (14) | 0.0339 (4) |
| H16 | 0.3399 | 0.9669 | 0.4427 | 0.041* |
| C17 | 0.4119 (2) | 0.89656 (11) | 0.32019 (13) | 0.0338 (4) |
| H17 | 0.3677 | 0.9356 | 0.2689 | 0.041* |
| C18 | 0.4937 (2) | 0.81987 (11) | 0.29260 (13) | 0.0313 (4) |
| H18 | 0.5051 | 0.8077 | 0.2226 | 0.038* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0376 (6) | 0.0279 (6) | 0.0296 (6) | 0.0016 (5) | 0.0074 (5) | −0.0031 (5) |
| O2 | 0.0445 (7) | 0.0378 (7) | 0.0243 (6) | 0.0041 (6) | 0.0065 (5) | 0.0008 (5) |
| N1 | 0.0309 (7) | 0.0272 (7) | 0.0234 (6) | −0.0021 (6) | 0.0028 (5) | −0.0006 (5) |
| N2 | 0.0254 (7) | 0.0229 (7) | 0.0258 (6) | −0.0022 (5) | 0.0005 (5) | −0.0037 (5) |
| N3 | 0.0325 (7) | 0.0226 (7) | 0.0230 (7) | 0.0006 (6) | 0.0036 (5) | −0.0020 (6) |
| C1 | 0.0244 (8) | 0.0247 (8) | 0.0286 (8) | −0.0056 (7) | −0.0011 (6) | −0.0035 (6) |
| C2 | 0.0336 (9) | 0.0272 (9) | 0.0338 (9) | −0.0038 (7) | −0.0015 (7) | 0.0037 (7) |
| C3 | 0.0342 (9) | 0.0223 (9) | 0.0452 (10) | 0.0013 (7) | −0.0030 (8) | −0.0014 (7) |
| C4 | 0.0323 (9) | 0.0284 (9) | 0.0402 (10) | 0.0022 (7) | 0.0003 (7) | −0.0094 (7) |
| C5 | 0.0292 (8) | 0.0296 (9) | 0.0283 (8) | −0.0014 (7) | 0.0000 (7) | −0.0052 (7) |
| C6 | 0.0239 (7) | 0.0231 (8) | 0.0267 (8) | −0.0042 (6) | −0.0013 (6) | −0.0028 (6) |
| C7 | 0.0260 (8) | 0.0260 (9) | 0.0254 (8) | −0.0051 (7) | 0.0023 (6) | −0.0018 (6) |
| C8 | 0.0366 (9) | 0.0315 (9) | 0.0241 (8) | −0.0049 (7) | 0.0048 (7) | 0.0037 (7) |
| C9 | 0.0319 (9) | 0.0327 (10) | 0.0259 (8) | 0.0010 (7) | 0.0017 (7) | 0.0056 (7) |
| C10 | 0.0400 (10) | 0.0462 (12) | 0.0386 (10) | −0.0019 (9) | −0.0007 (8) | −0.0081 (9) |
| C11 | 0.0237 (7) | 0.0225 (8) | 0.0249 (8) | −0.0048 (6) | 0.0007 (6) | −0.0036 (6) |
| C12 | 0.0251 (8) | 0.0273 (9) | 0.0237 (8) | −0.0033 (7) | 0.0001 (6) | −0.0002 (6) |
| C13 | 0.0258 (8) | 0.0239 (8) | 0.0262 (8) | −0.0030 (6) | 0.0000 (6) | 0.0003 (6) |
| C14 | 0.0339 (9) | 0.0300 (9) | 0.0255 (8) | 0.0023 (7) | −0.0005 (7) | 0.0028 (7) |
| C15 | 0.0401 (10) | 0.0343 (10) | 0.0309 (9) | 0.0022 (8) | 0.0034 (7) | −0.0056 (7) |
| C16 | 0.0319 (9) | 0.0248 (9) | 0.0441 (10) | 0.0013 (7) | −0.0018 (7) | −0.0034 (7) |
| C17 | 0.0361 (9) | 0.0258 (9) | 0.0380 (9) | −0.0011 (7) | −0.0066 (7) | 0.0070 (7) |
| C18 | 0.0378 (9) | 0.0292 (9) | 0.0265 (8) | −0.0036 (7) | −0.0006 (7) | 0.0021 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.2318 (18) | C7—C11 | 1.501 (2) |
| O2—C12 | 1.2223 (18) | C8—C9 | 1.497 (2) |
| N1—C7 | 1.361 (2) | C8—H8A | 0.9700 |
| N1—C1 | 1.418 (2) | C8—H8B | 0.9700 |
| N1—C8 | 1.4641 (19) | C9—C10 | 1.307 (2) |
| N2—C11 | 1.2915 (19) | C9—H9 | 0.9300 |
| N2—N3 | 1.3584 (18) | C10—H10A | 0.9300 |
| N3—C12 | 1.371 (2) | C10—H10B | 0.9300 |
| N3—H3 | 0.883 (18) | C12—C13 | 1.493 (2) |
| C1—C2 | 1.377 (2) | C13—C18 | 1.394 (2) |
| C1—C6 | 1.402 (2) | C13—C14 | 1.396 (2) |
| C2—C3 | 1.392 (2) | C14—C15 | 1.383 (2) |
| C2—H2 | 0.9300 | C14—H14 | 0.9300 |
| C3—C4 | 1.389 (2) | C15—C16 | 1.383 (2) |
| C3—H3A | 0.9300 | C15—H15 | 0.9300 |
| C4—C5 | 1.388 (2) | C16—C17 | 1.383 (2) |
| C4—H4 | 0.9300 | C16—H16 | 0.9300 |
| C5—C6 | 1.387 (2) | C17—C18 | 1.380 (2) |
| C5—H5 | 0.9300 | C17—H17 | 0.9300 |

| | | | |
|---|---|---|---|
| C6—C11 | 1.453 (2) | C18—H18 | 0.9300 |
| | | | |
| C7—N1—C1 | 110.61 (12) | C9—C8—H8B | 109.3 |
| C7—N1—C8 | 122.50 (13) | H8A—C8—H8B | 108.0 |
| C1—N1—C8 | 126.35 (14) | C10—C9—C8 | 123.28 (16) |
| C11—N2—N3 | 115.52 (13) | C10—C9—H9 | 118.4 |
| N2—N3—C12 | 120.10 (13) | C8—C9—H9 | 118.4 |
| N2—N3—H3 | 117.1 (11) | C9—C10—H10A | 120.0 |
| C12—N3—H3 | 122.8 (11) | C9—C10—H10B | 120.0 |
| C2—C1—C6 | 121.98 (15) | H10A—C10—H10B | 120.0 |
| C2—C1—N1 | 128.60 (15) | N2—C11—C6 | 126.25 (14) |
| C6—C1—N1 | 109.42 (14) | N2—C11—C7 | 127.48 (14) |
| C1—C2—C3 | 117.11 (15) | C6—C11—C7 | 106.27 (13) |
| C1—C2—H2 | 121.4 | O2—C12—N3 | 122.15 (15) |
| C3—C2—H2 | 121.4 | O2—C12—C13 | 123.06 (14) |
| C4—C3—C2 | 121.89 (16) | N3—C12—C13 | 114.77 (13) |
| C4—C3—H3A | 119.1 | C18—C13—C14 | 118.77 (15) |
| C2—C3—H3A | 119.1 | C18—C13—C12 | 117.67 (14) |
| C5—C4—C3 | 120.37 (16) | C14—C13—C12 | 123.55 (14) |
| C5—C4—H4 | 119.8 | C15—C14—C13 | 120.38 (15) |
| C3—C4—H4 | 119.8 | C15—C14—H14 | 119.8 |
| C6—C5—C4 | 118.56 (15) | C13—C14—H14 | 119.8 |
| C6—C5—H5 | 120.7 | C14—C15—C16 | 120.05 (16) |
| C4—C5—H5 | 120.7 | C14—C15—H15 | 120.0 |
| C5—C6—C1 | 120.06 (15) | C16—C15—H15 | 120.0 |
| C5—C6—C11 | 132.96 (15) | C17—C16—C15 | 120.14 (16) |
| C1—C6—C11 | 106.97 (13) | C17—C16—H16 | 119.9 |
| O1—C7—N1 | 126.09 (14) | C15—C16—H16 | 119.9 |
| O1—C7—C11 | 127.17 (14) | C18—C17—C16 | 119.95 (16) |
| N1—C7—C11 | 106.74 (13) | C18—C17—H17 | 120.0 |
| N1—C8—C9 | 111.54 (13) | C16—C17—H17 | 120.0 |
| N1—C8—H8A | 109.3 | C17—C18—C13 | 120.69 (15) |
| C9—C8—H8A | 109.3 | C17—C18—H18 | 119.7 |
| N1—C8—H8B | 109.3 | C13—C18—H18 | 119.7 |
| | | | |
| C11—N2—N3—C12 | 179.73 (14) | N3—N2—C11—C7 | −0.3 (2) |
| C7—N1—C1—C2 | −178.87 (15) | C5—C6—C11—N2 | 0.6 (3) |
| C8—N1—C1—C2 | 9.5 (3) | C1—C6—C11—N2 | 179.33 (14) |
| C7—N1—C1—C6 | 0.38 (17) | C5—C6—C11—C7 | −178.78 (16) |
| C8—N1—C1—C6 | −171.30 (14) | C1—C6—C11—C7 | −0.03 (16) |
| C6—C1—C2—C3 | 0.7 (2) | O1—C7—C11—N2 | 1.9 (3) |
| N1—C1—C2—C3 | 179.84 (15) | N1—C7—C11—N2 | −179.10 (14) |
| C1—C2—C3—C4 | 1.1 (2) | O1—C7—C11—C6 | −178.79 (15) |
| C2—C3—C4—C5 | −1.7 (3) | N1—C7—C11—C6 | 0.26 (16) |
| C3—C4—C5—C6 | 0.4 (2) | N2—N3—C12—O2 | 4.0 (2) |
| C4—C5—C6—C1 | 1.4 (2) | N2—N3—C12—C13 | −177.63 (12) |
| C4—C5—C6—C11 | 179.98 (16) | O2—C12—C13—C18 | 11.9 (2) |
| C2—C1—C6—C5 | −1.9 (2) | N3—C12—C13—C18 | −166.38 (14) |

| | | | |
|---|---|---|---|
| N1—C1—C6—C5 | 178.75 (13) | O2—C12—C13—C14 | −167.09 (15) |
| C2—C1—C6—C11 | 179.12 (14) | N3—C12—C13—C14 | 14.6 (2) |
| N1—C1—C6—C11 | −0.19 (16) | C18—C13—C14—C15 | 0.8 (2) |
| C1—N1—C7—O1 | 178.68 (15) | C12—C13—C14—C15 | 179.84 (15) |
| C8—N1—C7—O1 | −9.3 (2) | C13—C14—C15—C16 | 0.0 (3) |
| C1—N1—C7—C11 | −0.38 (16) | C14—C15—C16—C17 | −0.6 (3) |
| C8—N1—C7—C11 | 171.67 (13) | C15—C16—C17—C18 | 0.4 (3) |
| C7—N1—C8—C9 | −83.08 (19) | C16—C17—C18—C13 | 0.5 (3) |
| C1—N1—C8—C9 | 87.67 (19) | C14—C13—C18—C17 | −1.1 (2) |
| N1—C8—C9—C10 | 119.36 (18) | C12—C13—C18—C17 | 179.85 (14) |
| N3—N2—C11—C6 | −179.51 (13) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···O1 | 0.88 (2) | 1.98 (2) | 2.721 (2) | 141 (2) |