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# Crystal structure of 3-(morpholin-4-yl)-1-phenyl-3-(pyridin-2-yl)propan-1-one

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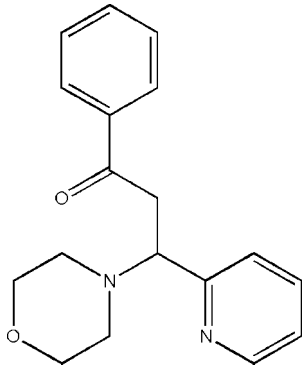
In the title compound $C_{18}H_{20}N_2O_2$, the morpholine ring adopts a chair conformation with the exocyclic N—C bond in an equatorial orientation. The N atom of the morpholine ring and the C atom of the carbonyl group are in an *anti* conformation about the central C—C bond [torsion angle = −162.92 (11)°] and the dihedral angle between the planes of the benzene ring and the pyridine ring is 83.30 (5)°. In the crystal, pairs of very weak C—H$\cdots\pi$ interactions link the molecules into inversion dimers.

**Keywords:** crystal structure; morpholin-4-yl; pyridin-2-yl; propan-1-one; biological activity.

**CCDC reference**: 1036843

## 1. Related literature

For background to the biological activity of morpholine derivatives, see: Panneerselvam *et al.* (2009); Subhashini *et al.* (2013); Sawant *et al.* (2013); Dave & Sasaki (2006); For related structures, see: Chen *et al.* (2011); Meti *et al.* (2013);




## 2. Experimental

### 2.1. Crystal data

$C_{18}H_{20}N_2O_2$
$M_r$ = 296.36
Orthorhombic, *Pbca*
$a$ = 12.4554 (6) Å
$b$ = 8.2204 (4) Å
$c$ = 30.6681 (17) Å
$V$ = 3140.1 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 295 K
0.20 × 0.15 × 0.10 mm

### 2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.954, $T_{max}$ = 0.975
16093 measured reflections
3812 independent reflections
2547 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
$S$ = 1.03
3812 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

*Cg*2 is the centroid of the C10–C14/N1 ring.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C2—H2$\cdots$*Cg*2$^{i}$ | 0.93 | 2.90 | 3.780 (6) | 159 |

Symmetry code: (i) $-x, -y+1, -z$.

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: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7328).

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# supporting information

*Acta Cryst.* (2015). E**71**, o24–o25 [doi:10.1107/S2056989014026292]

## Crystal structure of 3-(morpholin-4-yl)-1-phenyl-3-(pyridin-2-yl)propan-1-one

**F. M. Mashood Ahamed, M. Syed Ali Padusha and B. Gunasekaran**

### S1. Comment

Morpholines are six-membered heterocycles featuring both cyclic amine and ether functional group. These compounds possess important applications in pharmaceuticals and in industries (Panneerselvam *et al.*, 2009; Subhashini *et al.*, 2013). Chiral morpholine derivatives have found numerous applications in asymmetric synthesis as chiral auxiliaries as well as chiral ligands (Sawant *et al.*, 2013; Dave & Sasaki 2006).

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structure (Chen *et al.*, 2011; Meti *et al.*, 2013). The morpholine (N2/O2/C15—C18)ring adopts a chair conformation [Q = 0.5756 (3) Å, Θ = 179.09 (3)°, $\varphi$ = 332.57 (5)°]. The phenyl ring makes a dihedral angles of 83.30 (5) ° with the pyridine ring. In the crystal, a weak C—H···$\pi$ interaction is observed.

### S2. Experimental

To an ethanolic solution of acetophenone (3.0 ml, 0.025 mol) taken in a round bottom flask, morpholine (2.1 ml, 0.025 mol) and pyridine-2-carboldehyde (2.6 ml, 0.025 mol) were added. The reaction mixture was kept over a magnetic stirrer and stirred well in an ice cold condition for 3 hr. The colourless solid formed was filtered and washed several times with petroleum ether (40–60%). The crude solid obtained was dried and recrystallized using absolute alcohol. The recrystallized product was dried over vacuum. The yield is 78% and MP is 445 K.

### S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and $U_{iso}$(H) = 1.2Ueq(C) for aromatic C—H, C—H = 0.98 Å and $U_{iso}$(H) = 1.2Ueq(C) for C—H, C—H = 0.97 Å and $U_{iso}$(H) = 1.2Ueq(C) for C—H2,

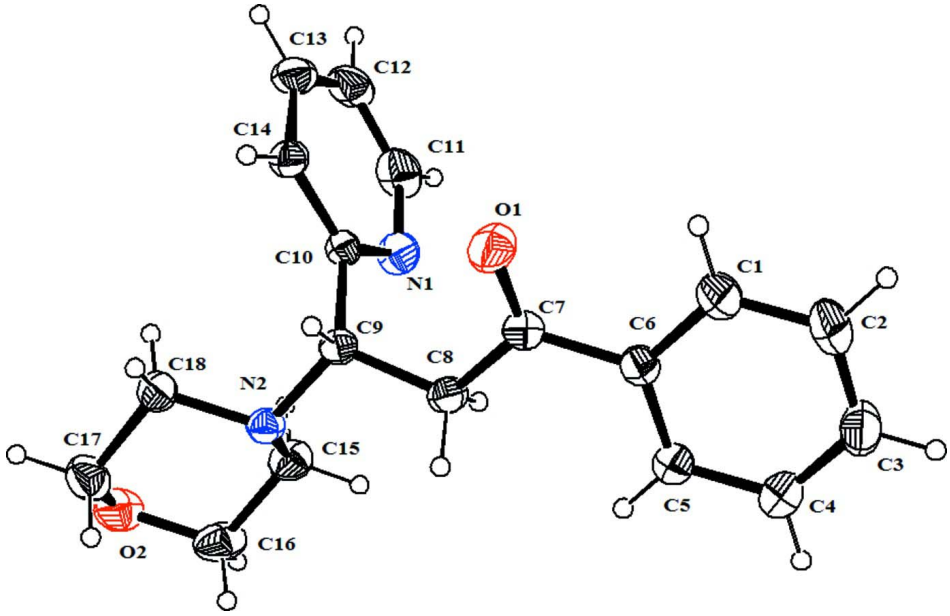


**Figure 1**

The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

### 3-(Morpholin-4-yl)-1-phenyl-3-(pyridin-2-yl)propan-1-one

*Crystal data*

$C_{18}H_{20}N_2O_2$
$M_r = 296.36$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.4554\ (6)$ Å
$b = 8.2204\ (4)$ Å
$c = 30.6681\ (17)$ Å
$V = 3140.1\ (3)$ Å$^3$
$Z = 8$
$F(000) = 1264$
$D_x = 1.254$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3812 reflections
$\theta = 1.3–28.4°$
$\mu = 0.08$ mm$^{-1}$
$T = 295$ K
Block, colourless
0.20 × 0.15 × 0.10 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.954$, $T_{max} = 0.975$
16093 measured reflections
3812 independent reflections
2547 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.3°$
$h = -15\rightarrow15$
$k = -10\rightarrow10$
$l = -35\rightarrow40$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.111$
$S = 1.03$
3812 reflections
199 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

$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 0.6298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å$^{-3}$
$\Delta\rho_{min} = -0.16$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.42802 (13) | −0.1732 (2) | 0.02138 (5) | 0.0604 (4) |
| H1 | 0.5020 | −0.1642 | 0.0182 | 0.073* |
| C2 | 0.36782 (16) | −0.2413 (2) | −0.01152 (6) | 0.0746 (5) |
| H2 | 0.4013 | −0.2768 | −0.0369 | 0.089* |
| C3 | 0.25900 (16) | −0.2571 (2) | −0.00707 (5) | 0.0680 (5) |
| H3 | 0.2186 | −0.3050 | −0.0291 | 0.082* |
| C4 | 0.21022 (13) | −0.2020 (2) | 0.02998 (6) | 0.0653 (5) |
| H4 | 0.1362 | −0.2121 | 0.0330 | 0.078* |
| C5 | 0.26935 (12) | −0.13170 (19) | 0.06292 (5) | 0.0529 (4) |
| H5 | 0.2350 | −0.0932 | 0.0878 | 0.063* |
| C6 | 0.37980 (11) | −0.11808 (15) | 0.05909 (4) | 0.0412 (3) |
| C7 | 0.44770 (10) | −0.04735 (16) | 0.09421 (4) | 0.0417 (3) |
| C8 | 0.39381 (10) | 0.03707 (17) | 0.13181 (4) | 0.0429 (3) |
| H8A | 0.3510 | −0.0418 | 0.1477 | 0.051* |
| H8B | 0.3453 | 0.1190 | 0.1204 | 0.051* |
| C9 | 0.47105 (9) | 0.11758 (15) | 0.16326 (4) | 0.0364 (3) |
| H9 | 0.5269 | 0.0372 | 0.1697 | 0.044* |
| C10 | 0.52724 (10) | 0.26260 (15) | 0.14299 (4) | 0.0368 (3) |
| C11 | 0.51464 (16) | 0.4990 (2) | 0.10454 (6) | 0.0666 (5) |
| H11 | 0.4726 | 0.5746 | 0.0898 | 0.080* |
| C12 | 0.62216 (16) | 0.5287 (2) | 0.10752 (6) | 0.0678 (5) |
| H12 | 0.6520 | 0.6215 | 0.0951 | 0.081* |
| C13 | 0.68473 (13) | 0.4190 (2) | 0.12904 (5) | 0.0610 (5) |
| H13 | 0.7585 | 0.4344 | 0.1313 | 0.073* |
| C14 | 0.63651 (11) | 0.28526 (18) | 0.14735 (5) | 0.0452 (3) |
| H14 | 0.6775 | 0.2099 | 0.1627 | 0.054* |
| C15 | 0.33073 (11) | 0.2736 (2) | 0.20287 (5) | 0.0532 (4) |
| H15A | 0.2787 | 0.2424 | 0.1809 | 0.064* |
| H15B | 0.3602 | 0.3787 | 0.1949 | 0.064* |
| C16 | 0.27665 (12) | 0.2851 (2) | 0.24674 (6) | 0.0662 (5) |
| H16A | 0.2195 | 0.3651 | 0.2453 | 0.079* |
| H16B | 0.2447 | 0.1808 | 0.2539 | 0.079* |
| C17 | 0.43388 (14) | 0.2128 (2) | 0.28202 (5) | 0.0632 (4) |
| H17A | 0.4040 | 0.1078 | 0.2898 | 0.076* |
| H17B | 0.4846 | 0.2440 | 0.3045 | 0.076* |
| C18 | 0.49150 (11) | 0.19882 (18) | 0.23921 (4) | 0.0462 (3) |
| H18A | 0.5247 | 0.3021 | 0.2320 | 0.055* |
| H18B | 0.5477 | 0.1176 | 0.2415 | 0.055* |
| N1 | 0.46563 (10) | 0.36867 (15) | 0.12143 (4) | 0.0526 (3) |

| | | | | |
|---|---|---|---|---|
| N2 | 0.41661 (8) | 0.15290 (13) | 0.20488 (4) | 0.0394 (3) |
| O1 | 0.54495 (8) | −0.05833 (15) | 0.09246 (4) | 0.0655 (3) |
| O2 | 0.35010 (10) | 0.32957 (14) | 0.27995 (4) | 0.0678 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0564 (9) | 0.0742 (11) | 0.0506 (9) | −0.0007 (8) | 0.0083 (8) | −0.0126 (8) |
| C2 | 0.0842 (13) | 0.0925 (14) | 0.0470 (10) | −0.0019 (11) | 0.0067 (9) | −0.0220 (9) |
| C3 | 0.0815 (12) | 0.0728 (11) | 0.0497 (9) | −0.0123 (10) | −0.0134 (9) | −0.0073 (9) |
| C4 | 0.0567 (9) | 0.0784 (12) | 0.0607 (10) | −0.0166 (9) | −0.0049 (8) | −0.0085 (9) |
| C5 | 0.0495 (9) | 0.0615 (9) | 0.0477 (8) | −0.0098 (7) | 0.0030 (7) | −0.0074 (7) |
| C6 | 0.0473 (7) | 0.0366 (7) | 0.0399 (7) | −0.0009 (6) | 0.0012 (6) | 0.0008 (6) |
| C7 | 0.0410 (7) | 0.0392 (7) | 0.0449 (8) | 0.0005 (6) | 0.0027 (6) | 0.0003 (6) |
| C8 | 0.0379 (7) | 0.0446 (7) | 0.0461 (8) | −0.0049 (6) | 0.0040 (6) | −0.0039 (6) |
| C9 | 0.0328 (6) | 0.0363 (7) | 0.0402 (7) | 0.0024 (5) | 0.0011 (5) | 0.0002 (6) |
| C10 | 0.0376 (7) | 0.0382 (7) | 0.0346 (6) | −0.0004 (5) | 0.0020 (5) | −0.0025 (5) |
| C11 | 0.0910 (13) | 0.0498 (9) | 0.0589 (10) | −0.0004 (9) | −0.0032 (9) | 0.0166 (8) |
| C12 | 0.0926 (13) | 0.0549 (10) | 0.0559 (10) | −0.0279 (10) | 0.0183 (9) | 0.0017 (8) |
| C13 | 0.0555 (9) | 0.0663 (10) | 0.0613 (10) | −0.0229 (8) | 0.0155 (8) | −0.0162 (9) |
| C14 | 0.0389 (7) | 0.0512 (8) | 0.0456 (8) | −0.0027 (6) | 0.0030 (6) | −0.0067 (7) |
| C15 | 0.0404 (7) | 0.0569 (9) | 0.0624 (10) | 0.0062 (7) | 0.0048 (7) | −0.0090 (8) |
| C16 | 0.0500 (9) | 0.0641 (10) | 0.0844 (12) | −0.0057 (8) | 0.0237 (9) | −0.0198 (9) |
| C17 | 0.0810 (11) | 0.0612 (10) | 0.0473 (9) | −0.0109 (9) | 0.0080 (8) | −0.0065 (8) |
| C18 | 0.0483 (8) | 0.0451 (8) | 0.0453 (8) | −0.0029 (7) | −0.0002 (6) | −0.0014 (6) |
| N1 | 0.0530 (7) | 0.0496 (7) | 0.0553 (7) | 0.0018 (6) | −0.0067 (6) | 0.0125 (6) |
| N2 | 0.0355 (5) | 0.0409 (6) | 0.0419 (6) | −0.0012 (5) | 0.0040 (5) | −0.0024 (5) |
| O1 | 0.0412 (6) | 0.0847 (9) | 0.0707 (8) | 0.0064 (5) | 0.0016 (5) | −0.0247 (6) |
| O2 | 0.0733 (7) | 0.0648 (7) | 0.0654 (7) | −0.0114 (6) | 0.0215 (6) | −0.0235 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.376 (2) | C11—N1 | 1.338 (2) |
| C1—C6 | 1.380 (2) | C11—C12 | 1.364 (3) |
| C1—H1 | 0.9300 | C11—H11 | 0.9300 |
| C2—C3 | 1.368 (3) | C12—C13 | 1.362 (2) |
| C2—H2 | 0.9300 | C12—H12 | 0.9300 |
| C3—C4 | 1.366 (2) | C13—C14 | 1.373 (2) |
| C3—H3 | 0.9300 | C13—H13 | 0.9300 |
| C4—C5 | 1.377 (2) | C14—H14 | 0.9300 |
| C4—H4 | 0.9300 | C15—N2 | 1.4604 (17) |
| C5—C6 | 1.3852 (19) | C15—C16 | 1.508 (2) |
| C5—H5 | 0.9300 | C15—H15A | 0.9700 |
| C6—C7 | 1.4878 (19) | C15—H15B | 0.9700 |
| C7—O1 | 1.2159 (15) | C16—O2 | 1.417 (2) |
| C7—C8 | 1.5039 (19) | C16—H16A | 0.9700 |
| C8—C9 | 1.5146 (18) | C16—H16B | 0.9700 |
| C8—H8A | 0.9700 | C17—O2 | 1.419 (2) |

| | | | |
|---|---|---|---|
| C8—H8B | 0.9700 | C17—C18 | 1.500 (2) |
| C9—N2 | 1.4741 (16) | C17—H17A | 0.9700 |
| C9—C10 | 1.5157 (18) | C17—H17B | 0.9700 |
| C9—H9 | 0.9800 | C18—N2 | 1.4565 (17) |
| C10—N1 | 1.3365 (17) | C18—H18A | 0.9700 |
| C10—C14 | 1.3803 (17) | C18—H18B | 0.9700 |
| | | | |
| C2—C1—C6 | 120.73 (15) | C13—C12—C11 | 118.42 (15) |
| C2—C1—H1 | 119.6 | C13—C12—H12 | 120.8 |
| C6—C1—H1 | 119.6 | C11—C12—H12 | 120.8 |
| C3—C2—C1 | 120.36 (16) | C12—C13—C14 | 118.55 (15) |
| C3—C2—H2 | 119.8 | C12—C13—H13 | 120.7 |
| C1—C2—H2 | 119.8 | C14—C13—H13 | 120.7 |
| C4—C3—C2 | 119.47 (16) | C13—C14—C10 | 119.99 (15) |
| C4—C3—H3 | 120.3 | C13—C14—H14 | 120.0 |
| C2—C3—H3 | 120.3 | C10—C14—H14 | 120.0 |
| C3—C4—C5 | 120.76 (15) | N2—C15—C16 | 109.39 (13) |
| C3—C4—H4 | 119.6 | N2—C15—H15A | 109.8 |
| C5—C4—H4 | 119.6 | C16—C15—H15A | 109.8 |
| C4—C5—C6 | 120.18 (14) | N2—C15—H15B | 109.8 |
| C4—C5—H5 | 119.9 | C16—C15—H15B | 109.8 |
| C6—C5—H5 | 119.9 | H15A—C15—H15B | 108.2 |
| C1—C6—C5 | 118.48 (13) | O2—C16—C15 | 111.65 (12) |
| C1—C6—C7 | 119.19 (12) | O2—C16—H16A | 109.3 |
| C5—C6—C7 | 122.33 (12) | C15—C16—H16A | 109.3 |
| O1—C7—C6 | 120.35 (13) | O2—C16—H16B | 109.3 |
| O1—C7—C8 | 120.85 (12) | C15—C16—H16B | 109.3 |
| C6—C7—C8 | 118.80 (11) | H16A—C16—H16B | 108.0 |
| C7—C8—C9 | 113.98 (10) | O2—C17—C18 | 111.37 (13) |
| C7—C8—H8A | 108.8 | O2—C17—H17A | 109.4 |
| C9—C8—H8A | 108.8 | C18—C17—H17A | 109.4 |
| C7—C8—H8B | 108.8 | O2—C17—H17B | 109.4 |
| C9—C8—H8B | 108.8 | C18—C17—H17B | 109.4 |
| H8A—C8—H8B | 107.7 | H17A—C17—H17B | 108.0 |
| N2—C9—C8 | 110.20 (10) | N2—C18—C17 | 110.24 (12) |
| N2—C9—C10 | 114.37 (10) | N2—C18—H18A | 109.6 |
| C8—C9—C10 | 112.07 (11) | C17—C18—H18A | 109.6 |
| N2—C9—H9 | 106.6 | N2—C18—H18B | 109.6 |
| C8—C9—H9 | 106.6 | C17—C18—H18B | 109.6 |
| C10—C9—H9 | 106.6 | H18A—C18—H18B | 108.1 |
| N1—C10—C14 | 121.74 (13) | C10—N1—C11 | 116.89 (13) |
| N1—C10—C9 | 116.80 (11) | C18—N2—C15 | 108.87 (11) |
| C14—C10—C9 | 121.45 (12) | C18—N2—C9 | 112.48 (10) |
| N1—C11—C12 | 124.40 (17) | C15—N2—C9 | 115.74 (11) |
| N1—C11—H11 | 117.8 | C16—O2—C17 | 109.40 (12) |
| C12—C11—H11 | 117.8 | | |
| | | | |
| C6—C1—C2—C3 | −0.8 (3) | N1—C11—C12—C13 | 0.0 (3) |

| | | | |
|---|---|---|---|
| C1—C2—C3—C4 | 1.2 (3) | C11—C12—C13—C14 | −1.1 (2) |
| C2—C3—C4—C5 | −0.3 (3) | C12—C13—C14—C10 | 1.3 (2) |
| C3—C4—C5—C6 | −0.9 (3) | N1—C10—C14—C13 | −0.4 (2) |
| C2—C1—C6—C5 | −0.5 (2) | C9—C10—C14—C13 | −179.19 (13) |
| C2—C1—C6—C7 | 179.11 (16) | N2—C15—C16—O2 | 59.10 (17) |
| C4—C5—C6—C1 | 1.3 (2) | O2—C17—C18—N2 | −58.71 (16) |
| C4—C5—C6—C7 | −178.26 (14) | C14—C10—N1—C11 | −0.6 (2) |
| C1—C6—C7—O1 | −10.1 (2) | C9—C10—N1—C11 | 178.23 (13) |
| C5—C6—C7—O1 | 169.48 (15) | C12—C11—N1—C10 | 0.8 (3) |
| C1—C6—C7—C8 | 170.08 (13) | C17—C18—N2—C15 | 57.48 (15) |
| C5—C6—C7—C8 | −10.3 (2) | C17—C18—N2—C9 | −172.87 (12) |
| O1—C7—C8—C9 | 5.6 (2) | C16—C15—N2—C18 | −57.27 (15) |
| C6—C7—C8—C9 | −174.59 (11) | C16—C15—N2—C9 | 174.89 (11) |
| C7—C8—C9—N2 | −162.92 (11) | C8—C9—N2—C18 | 168.06 (11) |
| C7—C8—C9—C10 | 68.50 (15) | C10—C9—N2—C18 | −64.62 (14) |
| N2—C9—C10—N1 | −79.35 (15) | C8—C9—N2—C15 | −65.92 (14) |
| C8—C9—C10—N1 | 47.00 (15) | C10—C9—N2—C15 | 61.40 (14) |
| N2—C9—C10—C14 | 99.47 (14) | C15—C16—O2—C17 | −58.86 (18) |
| C8—C9—C10—C14 | −134.18 (13) | C18—C17—O2—C16 | 58.37 (16) |

*Hydrogen-bond geometry (Å, º)*

Cg2 is the centroid of the C10–C14/N1 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···*Cg*2$^{i}$ | 0.93 | 2.90 | 3.780 (6) | 159 |

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