Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4′-(Morpholinomethyl)biphenyl-2-carbonitrile

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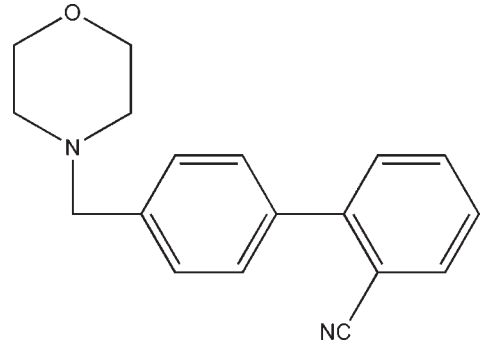
Received 24 June 2010; accepted 26 June 2010

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.053; $wR$ factor = 0.138; data-to-parameter ratio = 18.4.

In the title compound, $C_{18}H_{18}N_2O$, the morpholine ring adopts a chair conformation and the dihedral angle between the aromatic rings is 49.16 (7)°. In the crystal, weak C—H$\cdots\pi$ interactions may help to establish the packing.

## Related literature

For background to ligands related to the title compound, see: Li *et al.* (2008); Zhang *et al.* (2009).




## Experimental

### Crystal data

$C_{18}H_{18}N_2O$
$M_r$ = 278.34
Monoclinic, $P2_1/n$
$a$ = 10.924 (6) Å
$b$ = 10.891 (5) Å
$c$ = 12.943 (7) Å
$\beta$ = 93.269 (7)°
$V$ = 1537.4 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 K
0.20 × 0.20 × 0.20 mm

### Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.985, $T_{max}$ = 0.985
16364 measured reflections
3493 independent reflections
2757 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.138
$S$ = 1.10
3493 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

*Cg*2 is the centroid of the C6–C11 ring.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C1—H1$A\cdots Cg2^{i}$ | 0.96 | 2.76 | 3.638 (3) | 151 |
| C16—H16$A\cdots Cg2^{ii}$ | 0.93 | 2.87 | 3.746 (3) | 157 |

Symmetry codes: (i) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *SHELXL97*.

The author is grateful to the starter fund of Southeast University for financial support to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5523).

## References

Li, X. Z., Qu, Z. R. & Xiong, R. G. (2008). *Chin. J. Chem.* **11**, 1959–1962.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, W., Chen, L. Z., Xiong, R. G., Nakamura, T. & Huang, S. D. (2009). *J. Am. Chem. Soc.* **131**, 12544–12545.

# supporting information

*Acta Cryst.* (2010). E**66**, o1884 [https://doi.org/10.1107/S1600536810025109]

## 4′-(Morpholinomethyl)biphenyl-2-carbonitrile

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### S1. Experimental

A solution of 4′-bromomethylbiphenyl-2-carbonitrile (10 mmol) in acetone was added dropwise to a mixture of morpholine (10 mmol) and potassium carbonate anhydrous (10 mmol) at 331 K with stirring for 6 h; the reaction solution was then filted. Colourless prisms of (I) were formed after several weeks by slow evaporation of the solvent at room temperature. The compound shows no dielectric irregularity in the temperature range of 93–352 K.

### S2. Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C, N atoms to which they are bonded, with C—H =0.93 to 0.97 Å, $U_{iso}$(H) = 1.2 $U_{eq}$(C), N—H = 0.89 Å, $U_{iso}$(H)= 1.5 $U_{eq}$(N).

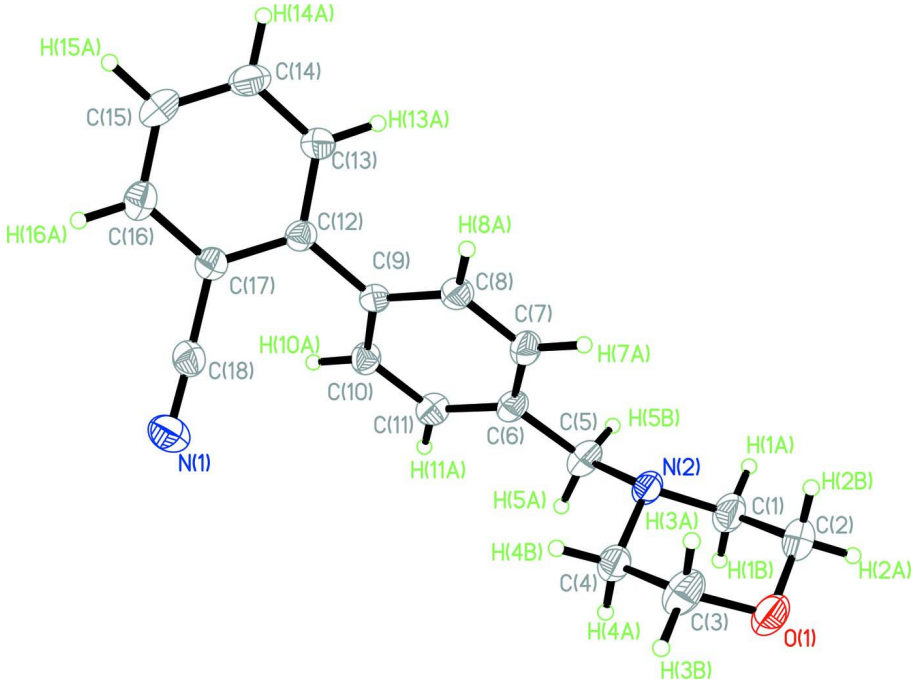


**Figure 1**

The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level, and all H atoms have been omitted for clarity.

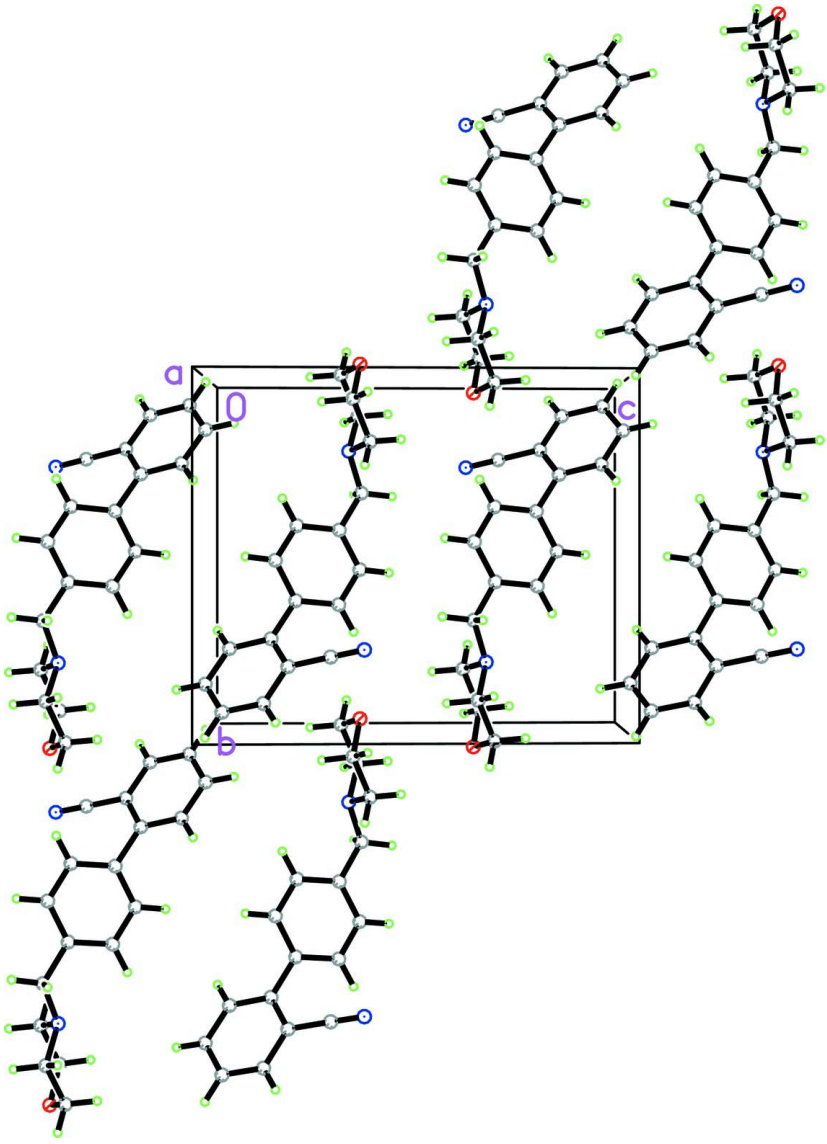


**Figure 2**

A view of the packing of the title compound, stacking along the *a* axis. Dashed lines indicate hydrogen bonds.

## 4′-(Morpholinomethyl)biphenyl-2-carbonitrile

*Crystal data*

$C_{18}H_{18}N_2O$
$M_r = 278.34$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.924\ (6)$ Å
$b = 10.891\ (5)$ Å
$c = 12.943\ (7)$ Å
$\beta = 93.269\ (7)°$
$V = 1537.4\ (13)$ Å$^3$
$Z = 4$

$F(000) = 592$
$D_x = 1.203$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3548 reflections
$\theta = 2.4–27.4°$
$\mu = 0.08$ mm$^{-1}$
$T = 293$ K
Prism, colourless
0.20 × 0.20 × 0.20 mm

*Data collection*

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.985, $T_{max}$ = 0.985
16364 measured reflections
3493 independent reflections
2757 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.4°
$h$ = −14→14
$k$ = −14→14
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.138
$S$ = 1.10
3493 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.152P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C5 | 1.14259 (16) | 0.82069 (14) | 0.13367 (14) | 0.0528 (4) |
| H5A | 1.1325 | 0.8304 | 0.0600 | 0.063* |
| H5B | 1.2288 | 0.8226 | 0.1527 | 0.063* |
| C9 | 0.97335 (13) | 1.12626 (12) | 0.28571 (10) | 0.0365 (3) |
| N2 | 1.09293 (12) | 0.70241 (11) | 0.16311 (10) | 0.0448 (3) |
| C12 | 0.92172 (13) | 1.23165 (12) | 0.34199 (11) | 0.0380 (3) |
| C17 | 0.82704 (13) | 1.30573 (13) | 0.29907 (11) | 0.0395 (3) |
| C7 | 1.04111 (15) | 0.91490 (13) | 0.28539 (12) | 0.0459 (4) |
| H7A | 1.0501 | 0.8374 | 0.3203 | 0.055* |
| C10 | 1.01117 (14) | 1.13799 (13) | 0.18511 (11) | 0.0420 (3) |
| H10A | 1.0006 | 1.2150 | 0.1497 | 0.050* |
| C6 | 1.08033 (14) | 0.92683 (13) | 0.18531 (12) | 0.0421 (4) |
| O1 | 1.00038 (13) | 0.45991 (10) | 0.13465 (10) | 0.0654 (4) |
| C16 | 0.78280 (14) | 1.40534 (14) | 0.35368 (13) | 0.0484 (4) |
| H16A | 0.7205 | 1.4542 | 0.3238 | 0.058* |
| C18 | 0.76939 (14) | 1.27795 (14) | 0.19868 (13) | 0.0471 (4) |

| | | | | |
|---|---|---|---|---|
| C11 | 1.06370 (14) | 1.03952 (14) | 0.13615 (12) | 0.0452 (4) |
| H11A | 1.0885 | 1.0491 | 0.0666 | 0.054* |
| C8 | 0.98879 (15) | 1.01272 (13) | 0.33456 (12) | 0.0439 (4) |
| H8A | 0.9631 | 1.0025 | 0.4038 | 0.053* |
| C13 | 0.96826 (16) | 1.26019 (14) | 0.44174 (12) | 0.0493 (4) |
| H13A | 1.0335 | 1.2114 | 0.4731 | 0.059* |
| C4 | 0.97391 (15) | 0.67913 (14) | 0.11041 (14) | 0.0505 (4) |
| H4A | 0.9831 | 0.6723 | 0.0373 | 0.061* |
| H4B | 0.9195 | 0.7463 | 0.1219 | 0.061* |
| C14 | 0.92365 (18) | 1.35790 (16) | 0.49598 (13) | 0.0576 (5) |
| H14A | 0.9561 | 1.3749 | 0.5650 | 0.069* |
| C15 | 0.83137 (17) | 1.43118 (15) | 0.45173 (14) | 0.0556 (4) |
| H15A | 0.8015 | 1.4998 | 0.4894 | 0.067* |
| N1 | 0.71962 (15) | 1.25687 (16) | 0.12030 (12) | 0.0694 (5) |
| C1 | 1.17405 (17) | 0.59987 (15) | 0.14313 (16) | 0.0639 (5) |
| H1A | 1.2532 | 0.6137 | 0.1773 | 0.077* |
| H1B | 1.1843 | 0.5923 | 0.0702 | 0.077* |
| C3 | 0.92168 (18) | 0.56140 (15) | 0.14975 (17) | 0.0666 (5) |
| H3A | 0.9090 | 0.5703 | 0.2222 | 0.080* |
| H3B | 0.8435 | 0.5460 | 0.1144 | 0.080* |
| C2 | 1.1182 (2) | 0.48294 (16) | 0.18227 (17) | 0.0732 (6) |
| H2A | 1.1716 | 0.4151 | 0.1701 | 0.088* |
| H2B | 1.1113 | 0.4901 | 0.2556 | 0.088* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C5 | 0.0498 (10) | 0.0402 (8) | 0.0696 (11) | −0.0040 (7) | 0.0130 (8) | −0.0107 (7) |
| C9 | 0.0376 (8) | 0.0340 (7) | 0.0373 (7) | −0.0013 (6) | −0.0025 (6) | −0.0027 (6) |
| N2 | 0.0462 (7) | 0.0338 (6) | 0.0542 (8) | 0.0031 (5) | 0.0015 (6) | −0.0064 (5) |
| C12 | 0.0419 (8) | 0.0338 (7) | 0.0384 (7) | −0.0034 (6) | 0.0017 (6) | −0.0004 (6) |
| C17 | 0.0372 (8) | 0.0379 (8) | 0.0434 (8) | −0.0038 (6) | 0.0033 (6) | −0.0002 (6) |
| C7 | 0.0559 (10) | 0.0331 (8) | 0.0487 (9) | −0.0002 (6) | 0.0027 (7) | 0.0025 (6) |
| C10 | 0.0462 (9) | 0.0363 (7) | 0.0437 (8) | 0.0003 (6) | 0.0034 (6) | 0.0035 (6) |
| C6 | 0.0402 (8) | 0.0353 (8) | 0.0511 (9) | −0.0045 (6) | 0.0041 (6) | −0.0060 (6) |
| O1 | 0.0846 (10) | 0.0374 (6) | 0.0742 (9) | −0.0038 (6) | 0.0041 (7) | −0.0066 (5) |
| C16 | 0.0425 (9) | 0.0417 (8) | 0.0617 (10) | 0.0020 (6) | 0.0078 (7) | −0.0027 (7) |
| C18 | 0.0405 (9) | 0.0480 (9) | 0.0525 (9) | 0.0043 (7) | −0.0011 (7) | −0.0003 (7) |
| C11 | 0.0488 (9) | 0.0445 (9) | 0.0431 (8) | −0.0032 (7) | 0.0101 (7) | 0.0000 (6) |
| C8 | 0.0540 (9) | 0.0395 (8) | 0.0381 (8) | −0.0013 (7) | 0.0018 (6) | 0.0007 (6) |
| C13 | 0.0590 (10) | 0.0444 (9) | 0.0433 (8) | 0.0013 (7) | −0.0068 (7) | −0.0042 (7) |
| C4 | 0.0464 (9) | 0.0406 (8) | 0.0644 (10) | 0.0029 (7) | 0.0015 (7) | −0.0049 (7) |
| C14 | 0.0777 (13) | 0.0520 (10) | 0.0428 (9) | −0.0052 (9) | 0.0003 (8) | −0.0113 (7) |
| C15 | 0.0628 (11) | 0.0451 (9) | 0.0603 (11) | −0.0028 (8) | 0.0164 (8) | −0.0150 (8) |
| N1 | 0.0603 (10) | 0.0852 (12) | 0.0608 (10) | 0.0075 (8) | −0.0139 (8) | −0.0089 (8) |
| C1 | 0.0558 (11) | 0.0444 (10) | 0.0903 (14) | 0.0115 (8) | −0.0053 (10) | −0.0108 (9) |
| C3 | 0.0625 (12) | 0.0464 (10) | 0.0923 (15) | −0.0088 (8) | 0.0161 (10) | −0.0087 (9) |
| C2 | 0.0919 (16) | 0.0431 (10) | 0.0824 (14) | 0.0137 (10) | −0.0138 (12) | −0.0018 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C5—N2 | 1.457 (2) | C16—C15 | 1.376 (2) |
| C5—C6 | 1.516 (2) | C16—H16A | 0.9300 |
| C5—H5A | 0.9600 | C18—N1 | 1.146 (2) |
| C5—H5B | 0.9601 | C11—H11A | 0.9601 |
| C9—C10 | 1.394 (2) | C8—H8A | 0.9599 |
| C9—C8 | 1.395 (2) | C13—C14 | 1.379 (2) |
| C9—C12 | 1.4877 (19) | C13—H13A | 0.9600 |
| N2—C4 | 1.456 (2) | C4—C3 | 1.504 (2) |
| N2—C1 | 1.458 (2) | C4—H4A | 0.9600 |
| C12—C13 | 1.395 (2) | C4—H4B | 0.9600 |
| C12—C17 | 1.401 (2) | C14—C15 | 1.384 (3) |
| C17—C16 | 1.396 (2) | C14—H14A | 0.9600 |
| C17—C18 | 1.443 (2) | C15—H15A | 0.9600 |
| C7—C8 | 1.381 (2) | C1—C2 | 1.512 (3) |
| C7—C6 | 1.393 (2) | C1—H1A | 0.9600 |
| C7—H7A | 0.9601 | C1—H1B | 0.9599 |
| C10—C11 | 1.387 (2) | C3—H3A | 0.9601 |
| C10—H10A | 0.9600 | C3—H3B | 0.9599 |
| C6—C11 | 1.390 (2) | C2—H2A | 0.9600 |
| O1—C2 | 1.417 (3) | C2—H2B | 0.9599 |
| O1—C3 | 1.421 (2) | | |
| | | | |
| N2—C5—C6 | 112.08 (13) | C7—C8—H8A | 119.4 |
| N2—C5—H5A | 109.5 | C9—C8—H8A | 119.4 |
| C6—C5—H5A | 109.0 | C14—C13—C12 | 121.48 (15) |
| N2—C5—H5B | 109.0 | C14—C13—H13A | 119.2 |
| C6—C5—H5B | 109.2 | C12—C13—H13A | 119.3 |
| H5A—C5—H5B | 108.0 | N2—C4—C3 | 109.62 (14) |
| C10—C9—C8 | 118.04 (13) | N2—C4—H4A | 109.6 |
| C10—C9—C12 | 121.83 (12) | C3—C4—H4A | 109.3 |
| C8—C9—C12 | 120.10 (13) | N2—C4—H4B | 109.8 |
| C4—N2—C5 | 111.55 (13) | C3—C4—H4B | 110.3 |
| C4—N2—C1 | 108.61 (12) | H4A—C4—H4B | 108.2 |
| C5—N2—C1 | 113.06 (14) | C13—C14—C15 | 120.30 (15) |
| C13—C12—C17 | 117.41 (13) | C13—C14—H14A | 120.0 |
| C13—C12—C9 | 119.78 (13) | C15—C14—H14A | 119.7 |
| C17—C12—C9 | 122.81 (13) | C16—C15—C14 | 119.81 (15) |
| C16—C17—C12 | 121.04 (14) | C16—C15—H15A | 120.2 |
| C16—C17—C18 | 118.22 (14) | C14—C15—H15A | 120.0 |
| C12—C17—C18 | 120.70 (13) | N2—C1—C2 | 108.95 (16) |
| C8—C7—C6 | 120.91 (14) | N2—C1—H1A | 109.8 |
| C8—C7—H7A | 119.7 | C2—C1—H1A | 110.3 |
| C6—C7—H7A | 119.4 | N2—C1—H1B | 110.3 |
| C11—C10—C9 | 120.56 (13) | C2—C1—H1B | 109.2 |
| C11—C10—H10A | 120.0 | H1A—C1—H1B | 108.3 |
| C9—C10—H10A | 119.5 | O1—C3—C4 | 111.87 (15) |

| | | | |
|---|---|---|---|
| C11—C6—C7 | 117.96 (14) | O1—C3—H3A | 109.6 |
| C11—C6—C5 | 121.46 (14) | C4—C3—H3A | 108.8 |
| C7—C6—C5 | 120.55 (14) | O1—C3—H3B | 109.1 |
| C2—O1—C3 | 110.13 (13) | C4—C3—H3B | 109.4 |
| C15—C16—C17 | 119.96 (15) | H3A—C3—H3B | 108.0 |
| C15—C16—H16A | 120.0 | O1—C2—C1 | 112.15 (15) |
| C17—C16—H16A | 120.0 | O1—C2—H2A | 109.7 |
| N1—C18—C17 | 177.55 (18) | C1—C2—H2A | 109.5 |
| C10—C11—C6 | 121.37 (14) | O1—C2—H2B | 108.9 |
| C10—C11—H11A | 119.4 | C1—C2—H2B | 108.6 |
| C6—C11—H11A | 119.3 | H2A—C2—H2B | 107.9 |
| C7—C8—C9 | 121.16 (14) | | |

| | | | |
|---|---|---|---|
| C6—C5—N2—C4 | 75.91 (17) | C9—C10—C11—C6 | 0.0 (2) |
| C6—C5—N2—C1 | −161.33 (14) | C7—C6—C11—C10 | 0.8 (2) |
| C10—C9—C12—C13 | −129.59 (16) | C5—C6—C11—C10 | −177.38 (14) |
| C8—C9—C12—C13 | 48.3 (2) | C6—C7—C8—C9 | 0.1 (2) |
| C10—C9—C12—C17 | 50.1 (2) | C10—C9—C8—C7 | 0.6 (2) |
| C8—C9—C12—C17 | −131.94 (15) | C12—C9—C8—C7 | −177.35 (13) |
| C13—C12—C17—C16 | 1.0 (2) | C17—C12—C13—C14 | −0.4 (2) |
| C9—C12—C17—C16 | −178.70 (13) | C9—C12—C13—C14 | 179.34 (15) |
| C13—C12—C17—C18 | −176.48 (14) | C5—N2—C4—C3 | −175.30 (13) |
| C9—C12—C17—C18 | 3.8 (2) | C1—N2—C4—C3 | 59.43 (18) |
| C8—C9—C10—C11 | −0.7 (2) | C12—C13—C14—C15 | −0.5 (3) |
| C12—C9—C10—C11 | 177.28 (13) | C17—C16—C15—C14 | −0.3 (2) |
| C8—C7—C6—C11 | −0.8 (2) | C13—C14—C15—C16 | 0.9 (3) |
| C8—C7—C6—C5 | 177.36 (14) | C4—N2—C1—C2 | −59.12 (19) |
| N2—C5—C6—C11 | −147.09 (15) | C5—N2—C1—C2 | 176.50 (14) |
| N2—C5—C6—C7 | 34.8 (2) | C2—O1—C3—C4 | 56.2 (2) |
| C12—C17—C16—C15 | −0.7 (2) | N2—C4—C3—O1 | −58.5 (2) |
| C18—C17—C16—C15 | 176.86 (15) | C3—O1—C2—C1 | −56.5 (2) |
| C16—C17—C18—N1 | −39 (4) | N2—C1—C2—O1 | 58.6 (2) |
| C12—C17—C18—N1 | 138 (4) | | |

*Hydrogen-bond geometry (Å, º)*

Cg2 is the centroid of the C6–C11 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1*A*···*Cg*2$^{i}$ | 0.96 | 2.76 | 3.638 (3) | 151 |
| C16—H16*A*···*Cg*2$^{ii}$ | 0.93 | 2.87 | 3.746 (3) | 157 |

Symmetry codes: (i) −*x*+5/2, *y*−1/2, −*z*+1/2; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2.