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# Crystal structure of 3-(3,4-dimethylanilino)-2-benzofuran-1(3*H*)-one

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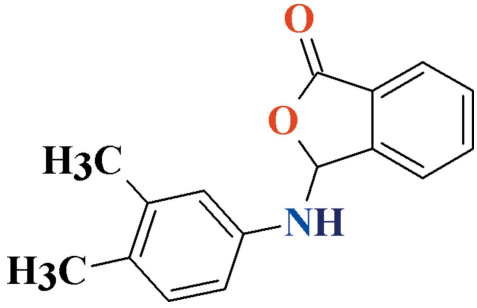
In the title compound, $C_{16}H_{15}NO_2$, the 2-benzofuran-1(3*H*)-one and 3,4-dimethylaniline fragments are oriented with a dihedral angle of 89.12 (5)°. N—H···O hydrogen-bond interactions join molecules into *C*(6) chains propagating along the *a* axis. In addition, there are $\pi$–$\pi$ stacking interactions between the 2-benzofuranone benzene rings [centroid–centroid distance = 3.7870 (13) Å] and C—H···$\pi$ interactions between one of the methyl groups and the 3,4-dimethylaniline benzene ring.

**Keywords:** crystal structure; 2-benzofuranone; hydrogen bonding.

**CCDC reference**: 1401225

## 1. Related literature

For related crystal structures, see: Li *et al.* (2009); Odabaşoğlu & Büyükgüngör (2006*a*,*b*, 2007*a*,*b*). For graph-set notation, see: Bernstein *et al.* (1995).




## 2. Experimental

### 2.1. Crystal data

$C_{16}H_{15}NO_2$ $M_r$ = 253.29

Orthorhombic, *Pbca*
*a* = 7.3386 (7) Å
*b* = 14.9133 (11) Å
*c* = 24.3322 (18) Å
*V* = 2663.0 (4) Å$^3$
*Z* = 8
Mo *K*$\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
*T* = 296 K
0.38 × 0.23 × 0.16 mm

### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.970, $T_{max}$ = 0.988
20839 measured reflections
2906 independent reflections
1660 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.144
*S* = 1.02
2906 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

*Cg*3 is the centroid of the C9—C14

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.86 | 2.31 | 3.025 (2) | 141 |
| C15—H15*B*···*Cg*3$^{ii}$ | 0.96 | 2.88 | 3.661 (3) | 139 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: GK2634).

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# supporting information

*Acta Cryst.* (2015). E**71**, o413 [doi:10.1107/S2056989015009299]

## Crystal structure of 3-(3,4-dimethylanilino)-2-benzofuran-1(3*H*)-one

**Muhammad Salim, Muhammad Nawaz Tahir, Muhammad Shahid and Munawar Ali Munawar**

### S1. Comment

The crystal structures of 3-anilinoisobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2006*a*), 3-(2,6-dimethylanilino)isobenzofuran-1(3*H*) -one (Odabaşoğlu & Büyükgüngör, 2006*b*), 3-(4-methylanilino)isobenzo furan-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2007*a*), 3-(2- (hydroxymethyl)anilino)isobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2007*b*), and 3-((3-oxo-1,3-dihydroisobenzofuran-1-yl)amino) benzoic acid Li *et al.*, 2009) have been published which are related to the title compound (I, Fig. 1). The title compound was synthesized for the biological studies and for the preparation of further derivitives.

The benzofuran ring A (C1–C8/O1/O2) and the 3,4-dmethylaniline group B (C9–C16/N1) are planar with r. m. s. deviation of 0.0209 and 0.0101 Å, respectively. The dihedral angle between A/B fragments is 89.12 (5)°. Intermolecular hydrogen bond of N—H···O type generates *C* (6) chains (Bernstein *et al.*, 1995) along the crystallographic *a* axis (Table 1, Fig. 2). The $\pi$–$\pi$ interactions are observed between the 2-benzofuranone fragments [ *Cg*1—*Cg*2$^{i}$ 3.6204 (12) Å; *Cg*1—*Cg*1$^{i}$ 3.8138 (13) Å; *Cg*2—*Cg*2$^{i}$ 3.7870 (13) Å, *Cg*1 - centroid of C1/C2/C7/C8/O1, *Cg*2 - centroid of C2–C7); i = - 1/2 + *x*, *y*, 1/2 - *z* ]. In addition there are also C—H···$\pi$ interactions (Table 1).

### S2. Experimental

Equimolar quantities of 3,4-dimethylaniline (0.605 g. 5 mmol) and 2-formylbenzoic acid (0.751 g, 5 mmol) were stirred in methanol for 2 h. The solution was kept at room temperature for crystallization which afforded light brown needles after 48 h.

### S3. Refinement

The H atoms were positioned geometrically (C–H = 0.93–0.96 Å, N—H= 0.86 Å) and refined as riding on their carriers with $U_{iso}$(H) = $xU_{eq}$(C, N), where *x* = 1.5 for methyl and *x* =1.2 for other H-atoms.

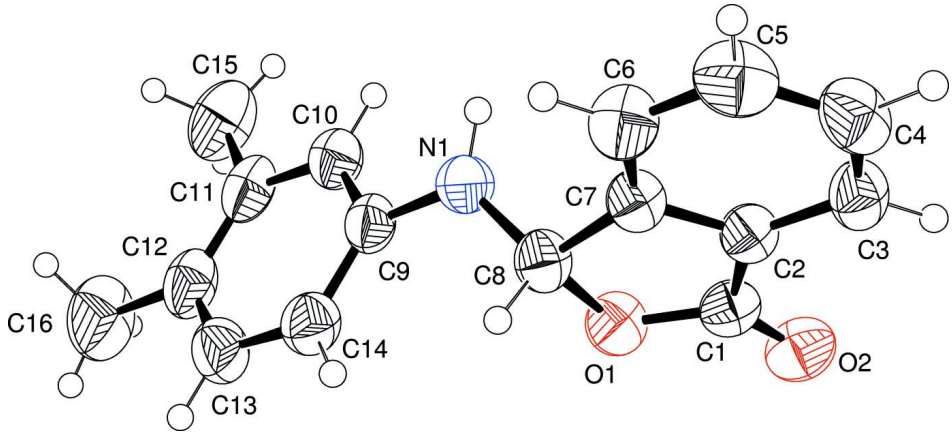


**Figure 1**

Molecular structure with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii.

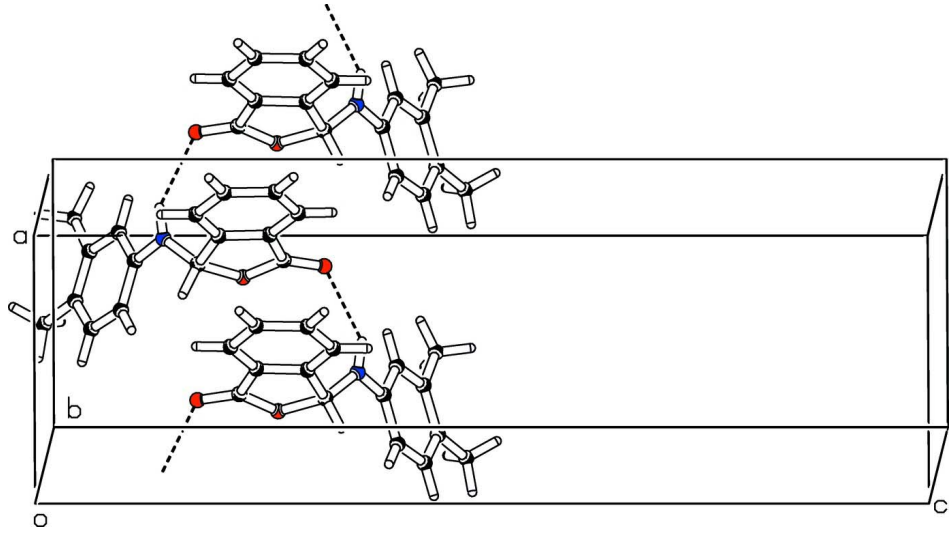


**Figure 2**

The chains of molecules along the *a* axis *via* N—H···O hydrogen bond (*PLATON*; Spek, 2009).

### 3-(3,4-Dimethylanilino)-2-benzofuran-1(3*H*)-one

*Crystal data*

$C_{16}H_{15}NO_2$
$M_r$ = 253.29
Orthorhombic, *Pbca*
*a* = 7.3386 (7) Å
*b* = 14.9133 (11) Å
*c* = 24.3322 (18) Å
*V* = 2663.0 (4) Å$^3$
*Z* = 8
*F*(000) = 1072

$D_x$ = 1.264 Mg m$^{-3}$
Mo *Kα* radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4689 reflections
$\theta$ = 1.4–27.0°
$\mu$ = 0.08 mm$^{-1}$
*T* = 296 K
Needle, light brown
0.38 × 0.23 × 0.16 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.80 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.970, $T_{max}$ = 0.988
20839 measured reflections
2906 independent reflections
1660 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.7°
$h$ = −5→9
$k$ = −19→18
$l$ = −31→31

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.144
$S$ = 1.02
2906 reflections
174 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
$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 0.3907P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.80336 (19) | 0.14473 (8) | 0.23068 (5) | 0.0528 (4) |
| O2 | 0.8396 (2) | 0.16231 (9) | 0.32129 (5) | 0.0614 (4) |
| N1 | 0.9466 (2) | 0.15132 (10) | 0.14175 (6) | 0.0533 (5) |
| H1 | 1.0572 | 0.1688 | 0.1371 | 0.064* |
| C1 | 0.8541 (3) | 0.19202 (12) | 0.27513 (7) | 0.0457 (5) |
| C2 | 0.9241 (3) | 0.27938 (11) | 0.25746 (7) | 0.0424 (5) |
| C3 | 0.9848 (3) | 0.35141 (12) | 0.28845 (8) | 0.0523 (5) |
| H3 | 0.9871 | 0.3488 | 0.3266 | 0.063* |
| C4 | 1.0416 (3) | 0.42698 (13) | 0.26083 (9) | 0.0610 (6) |
| H4 | 1.0827 | 0.4765 | 0.2805 | 0.073* |
| C5 | 1.0381 (3) | 0.42990 (13) | 0.20393 (10) | 0.0651 (6) |
| H5 | 1.0775 | 0.4815 | 0.1860 | 0.078* |
| C6 | 0.9774 (3) | 0.35782 (12) | 0.17306 (8) | 0.0575 (6) |
| H6 | 0.9761 | 0.3602 | 0.1349 | 0.069* |
| C7 | 0.9189 (3) | 0.28247 (11) | 0.20076 (7) | 0.0443 (5) |
| C8 | 0.8370 (3) | 0.19769 (12) | 0.17912 (7) | 0.0472 (5) |

| | | | | |
|---|---|---|---|---|
| H8 | 0.7199 | 0.2115 | 0.1617 | 0.057* |
| C9 | 0.8834 (3) | 0.07697 (11) | 0.11132 (7) | 0.0463 (5) |
| C10 | 1.0086 (3) | 0.01250 (12) | 0.09499 (7) | 0.0521 (5) |
| H10 | 1.1299 | 0.0189 | 0.1054 | 0.062* |
| C11 | 0.9584 (4) | −0.06119 (12) | 0.06359 (7) | 0.0572 (6) |
| C12 | 0.7769 (4) | −0.07110 (13) | 0.04754 (7) | 0.0618 (6) |
| C13 | 0.6529 (3) | −0.00635 (14) | 0.06404 (8) | 0.0632 (6) |
| H13 | 0.5317 | −0.0124 | 0.0535 | 0.076* |
| C14 | 0.7027 (3) | 0.06721 (13) | 0.09569 (7) | 0.0553 (6) |
| H14 | 0.6161 | 0.1093 | 0.1063 | 0.066* |
| C15 | 1.1015 (4) | −0.12910 (15) | 0.04791 (10) | 0.0846 (8) |
| H15A | 1.2147 | −0.1140 | 0.0654 | 0.127* |
| H15B | 1.1175 | −0.1289 | 0.0087 | 0.127* |
| H15C | 1.0635 | −0.1877 | 0.0596 | 0.127* |
| C16 | 0.7133 (4) | −0.15104 (15) | 0.01424 (10) | 0.0953 (9) |
| H16A | 0.5847 | −0.1462 | 0.0076 | 0.143* |
| H16B | 0.7378 | −0.2052 | 0.0342 | 0.143* |
| H16C | 0.7769 | −0.1524 | −0.0202 | 0.143* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0623 (10) | 0.0370 (7) | 0.0592 (8) | −0.0047 (6) | 0.0027 (7) | −0.0033 (6) |
| O2 | 0.0646 (11) | 0.0614 (9) | 0.0581 (8) | 0.0045 (7) | 0.0074 (7) | 0.0143 (7) |
| N1 | 0.0515 (11) | 0.0518 (9) | 0.0566 (9) | −0.0076 (8) | 0.0071 (8) | −0.0179 (7) |
| C1 | 0.0457 (12) | 0.0391 (10) | 0.0524 (11) | 0.0075 (9) | 0.0045 (9) | 0.0000 (9) |
| C2 | 0.0434 (12) | 0.0356 (9) | 0.0481 (10) | 0.0067 (9) | −0.0002 (9) | −0.0037 (8) |
| C3 | 0.0577 (14) | 0.0450 (11) | 0.0542 (10) | 0.0084 (10) | −0.0029 (10) | −0.0122 (9) |
| C4 | 0.0638 (16) | 0.0385 (11) | 0.0809 (15) | −0.0005 (10) | −0.0047 (12) | −0.0147 (10) |
| C5 | 0.0725 (17) | 0.0377 (11) | 0.0851 (15) | −0.0050 (11) | 0.0028 (13) | 0.0061 (10) |
| C6 | 0.0714 (16) | 0.0458 (11) | 0.0552 (11) | −0.0007 (11) | 0.0001 (11) | 0.0060 (9) |
| C7 | 0.0481 (12) | 0.0355 (9) | 0.0493 (10) | 0.0038 (9) | −0.0016 (9) | −0.0025 (8) |
| C8 | 0.0524 (13) | 0.0405 (9) | 0.0487 (10) | 0.0021 (9) | −0.0026 (9) | −0.0040 (8) |
| C9 | 0.0561 (14) | 0.0444 (10) | 0.0385 (9) | −0.0047 (10) | 0.0014 (9) | −0.0042 (8) |
| C10 | 0.0591 (14) | 0.0495 (11) | 0.0476 (10) | 0.0010 (11) | 0.0013 (10) | −0.0049 (9) |
| C11 | 0.0845 (18) | 0.0456 (11) | 0.0417 (10) | 0.0002 (12) | 0.0104 (11) | −0.0029 (8) |
| C12 | 0.0906 (19) | 0.0489 (12) | 0.0460 (10) | −0.0145 (13) | 0.0064 (12) | −0.0084 (9) |
| C13 | 0.0706 (17) | 0.0646 (13) | 0.0543 (11) | −0.0185 (13) | −0.0032 (11) | −0.0076 (10) |
| C14 | 0.0604 (15) | 0.0512 (11) | 0.0542 (11) | −0.0034 (11) | 0.0041 (10) | −0.0084 (9) |
| C15 | 0.119 (2) | 0.0601 (13) | 0.0749 (14) | 0.0175 (14) | 0.0172 (16) | −0.0143 (12) |
| C16 | 0.135 (3) | 0.0685 (15) | 0.0821 (15) | −0.0301 (16) | 0.0022 (17) | −0.0282 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.344 (2) | C8—H8 | 0.9800 |
| O1—C8 | 1.503 (2) | C9—C14 | 1.387 (3) |
| O2—C1 | 1.212 (2) | C9—C10 | 1.388 (3) |
| N1—C8 | 1.397 (2) | C10—C11 | 1.388 (3) |

| | | | |
|---|---|---|---|
| N1—C9 | 1.412 (2) | C10—H10 | 0.9300 |
| N1—H1 | 0.8600 | C11—C12 | 1.395 (3) |
| C1—C2 | 1.465 (3) | C11—C15 | 1.509 (3) |
| C2—C7 | 1.381 (2) | C12—C13 | 1.386 (3) |
| C2—C3 | 1.386 (2) | C12—C16 | 1.515 (3) |
| C3—C4 | 1.377 (3) | C13—C14 | 1.389 (3) |
| C3—H3 | 0.9300 | C13—H13 | 0.9300 |
| C4—C5 | 1.385 (3) | C14—H14 | 0.9300 |
| C4—H4 | 0.9300 | C15—H15A | 0.9600 |
| C5—C6 | 1.385 (3) | C15—H15B | 0.9600 |
| C5—H5 | 0.9300 | C15—H15C | 0.9600 |
| C6—C7 | 1.379 (2) | C16—H16A | 0.9600 |
| C6—H6 | 0.9300 | C16—H16B | 0.9600 |
| C7—C8 | 1.496 (2) | C16—H16C | 0.9600 |
| | | | |
| C1—O1—C8 | 110.53 (13) | C14—C9—C10 | 118.79 (17) |
| C8—N1—C9 | 122.76 (17) | C14—C9—N1 | 122.70 (17) |
| C8—N1—H1 | 118.6 | C10—C9—N1 | 118.48 (19) |
| C9—N1—H1 | 118.6 | C9—C10—C11 | 122.0 (2) |
| O2—C1—O1 | 121.98 (17) | C9—C10—H10 | 119.0 |
| O2—C1—C2 | 128.89 (17) | C11—C10—H10 | 119.0 |
| O1—C1—C2 | 109.12 (15) | C10—C11—C12 | 119.4 (2) |
| C7—C2—C3 | 121.78 (16) | C10—C11—C15 | 119.1 (2) |
| C7—C2—C1 | 108.25 (15) | C12—C11—C15 | 121.5 (2) |
| C3—C2—C1 | 129.96 (17) | C13—C12—C11 | 118.15 (18) |
| C4—C3—C2 | 117.78 (18) | C13—C12—C16 | 120.0 (2) |
| C4—C3—H3 | 121.1 | C11—C12—C16 | 121.8 (2) |
| C2—C3—H3 | 121.1 | C12—C13—C14 | 122.5 (2) |
| C3—C4—C5 | 120.53 (18) | C12—C13—H13 | 118.7 |
| C3—C4—H4 | 119.7 | C14—C13—H13 | 118.7 |
| C5—C4—H4 | 119.7 | C9—C14—C13 | 119.1 (2) |
| C6—C5—C4 | 121.57 (19) | C9—C14—H14 | 120.4 |
| C6—C5—H5 | 119.2 | C13—C14—H14 | 120.4 |
| C4—C5—H5 | 119.2 | C11—C15—H15A | 109.5 |
| C7—C6—C5 | 117.87 (18) | C11—C15—H15B | 109.5 |
| C7—C6—H6 | 121.1 | H15A—C15—H15B | 109.5 |
| C5—C6—H6 | 121.1 | C11—C15—H15C | 109.5 |
| C6—C7—C2 | 120.46 (16) | H15A—C15—H15C | 109.5 |
| C6—C7—C8 | 129.93 (16) | H15B—C15—H15C | 109.5 |
| C2—C7—C8 | 109.55 (15) | C12—C16—H16A | 109.5 |
| N1—C8—C7 | 114.58 (17) | C12—C16—H16B | 109.5 |
| N1—C8—O1 | 112.19 (14) | H16A—C16—H16B | 109.5 |
| C7—C8—O1 | 102.49 (13) | C12—C16—H16C | 109.5 |
| N1—C8—H8 | 109.1 | H16A—C16—H16C | 109.5 |
| C7—C8—H8 | 109.1 | H16B—C16—H16C | 109.5 |
| O1—C8—H8 | 109.1 | | |
| | | | |
| C8—O1—C1—O2 | −179.85 (17) | C2—C7—C8—N1 | −123.94 (17) |

| | | | |
|---|---|---|---|
| C8—O1—C1—C2 | 0.2 (2) | C6—C7—C8—O1 | −179.40 (19) |
| O2—C1—C2—C7 | 178.4 (2) | C2—C7—C8—O1 | −2.2 (2) |
| O1—C1—C2—C7 | −1.6 (2) | C1—O1—C8—N1 | 124.55 (17) |
| O2—C1—C2—C3 | −2.8 (4) | C1—O1—C8—C7 | 1.1 (2) |
| O1—C1—C2—C3 | 177.13 (18) | C8—N1—C9—C14 | 30.1 (3) |
| C7—C2—C3—C4 | −0.4 (3) | C8—N1—C9—C10 | −151.93 (17) |
| C1—C2—C3—C4 | −179.03 (19) | C14—C9—C10—C11 | 0.0 (3) |
| C2—C3—C4—C5 | −0.2 (3) | N1—C9—C10—C11 | −178.05 (16) |
| C3—C4—C5—C6 | 0.2 (3) | C9—C10—C11—C12 | 0.3 (3) |
| C4—C5—C6—C7 | 0.4 (3) | C9—C10—C11—C15 | −179.31 (18) |
| C5—C6—C7—C2 | −1.0 (3) | C10—C11—C12—C13 | −0.3 (3) |
| C5—C6—C7—C8 | 176.0 (2) | C15—C11—C12—C13 | 179.33 (18) |
| C3—C2—C7—C6 | 1.0 (3) | C10—C11—C12—C16 | −178.75 (18) |
| C1—C2—C7—C6 | 179.92 (18) | C15—C11—C12—C16 | 0.9 (3) |
| C3—C2—C7—C8 | −176.51 (17) | C11—C12—C13—C14 | 0.0 (3) |
| C1—C2—C7—C8 | 2.4 (2) | C16—C12—C13—C14 | 178.46 (19) |
| C9—N1—C8—C7 | −171.10 (16) | C10—C9—C14—C13 | −0.3 (3) |
| C9—N1—C8—O1 | 72.6 (2) | N1—C9—C14—C13 | 177.65 (16) |
| C6—C7—C8—N1 | 58.8 (3) | C12—C13—C14—C9 | 0.3 (3) |

*Hydrogen-bond geometry (Å, º)*

Cg3 is the centroid of the C9—C14

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.86 | 2.31 | 3.025 (2) | 141 |
| C15—H15*B*···*Cg*3$^{ii}$ | 0.96 | 2.88 | 3.661 (3) | 139 |

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