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# Ethyl 3-benzoylindolizine-1-carboxylate

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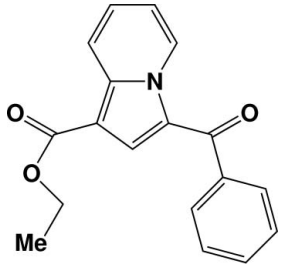
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.048; $wR$ factor = 0.129; data-to-parameter ratio = 13.0.

The title compound, $C_{18}H_{15}NO_3$, consists of an indolizine ring system and an aromatic ring. The two ring systems are not coplanar, the dihedral angle between the two being 54.26 (7)°. In the crystal, inversion dimers are formed by weak C—H···O interactions. These dimeric groups are further extended to form a regular two-dimensional structure by additional weak C—H···O interactions.

## Related literature

For background information on indolizine and its derivatives, see: Tukulula *et al.* (2010); James *et al.* (2008); Teklu *et al.* (2005); Shen *et al.* (2008, 2006). For the synthesis of the title compound, see: Wang *et al.* (2000).




## Experimental

### Crystal data

$C_{18}H_{15}NO_3$
$M_r$ = 293.31
Monoclinic, $P2_1/c$
$a$ = 10.030 (2) Å
$b$ = 19.223 (3) Å
$c$ = 7.9652 (17) Å
$\beta$ = 103.073 (3)°
$V$ = 1495.9 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 291 K
0.24 × 0.20 × 0.18 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.979, $T_{max}$ = 0.984
8910 measured reflections
2604 independent reflections
1604 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.129
$S$ = 1.00
2604 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O1$^{i}$ | 0.93 | 2.45 | 3.163 (3) | 134 |
| C14—H14···O3$^{ii}$ | 0.93 | 2.58 | 3.455 (3) | 157 |

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2326).

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# supporting information

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## Ethyl 3-benzoylindolizine-1-carboxylate

**Wei-Jin Gu, Jin Zhuang, Yu-Liang Jiang and Bing-Xiang Wang**

### S1. Comment

Indolizine and it's derivatives have been comprehensively applied in biology and medicine due to their particular structures (Tukulula *et al.*, 2010; James *et al.*, 2008; Teklu *et al.*, 2005). They can also be used as organic fluorescence probes (Shen *et al.*, 2008; Shen *et al.*, 2006). In our continuing studies in organic fluorescence probes, we synthesized the ethyl-3-benzoylindolizine-1-carboxylate (I).

The crystal structure of the title compound, $C_{18}H_{15}NO_3$, reveals that all bond lengths and angles have normal values (Table 1 and 2). In the asymmetric unit there is one title compound molecule. The molecular structure consists of one indolizine ring A (C1—C8/N) and an aromatic ring B(C10—C15) (Fig. 1). Rings A and ring B are not coplanar with the dihedral angle between them being 54.26 (7) °.

In the crystal packing there are weak C1—H1···O1$^{i}$ (i: 1 - *x*,-*y*,2 - *z*) interactions between neighbouring molecules forming dimeric groups (Fig. 2). These dimeric groups are further extended into a tegular 2-D structure *via* weak C14—H14···O3$^{ii}$ (ii: -*x*,-1/2 + *y*,0.5 - *z*) interactions (Fig. 2).

### S2. Experimental

Ethyl-3-benzoylindolizine-1-carboxylate was prepared by 1,3-dipolar cycloaddition according to a procedure described in the literature (Wang, *et al.*, 2000). A suspension of *N*-(benzoylmethyl)pyridinium bromide ($C_5H_5N^+$–$CH_2COC_6H_5$ $Br^-$) (10 mmol), ethyl acrylate (40 mmol), $Et_3N$ (20 ml) and $CrO_3$ (20 mmol) in DMF (40 ml) was stirred at 90°C for 2 h (monitored by TLC). The mixture was then cooled to room temperature and poured into 5% aqueous HCl (200 mL). The mixture was extracted with $CH_2Cl_2$ (2 times 50 mL) and the combined extracts were washed with water (2 times 50 mL) and dried over $Na_2SO_4$. The solvent was removed to give a solid, which was purified by chromatography [silica gel, 20% ethyl acetate in light petroleum (b.p. 60–90°C)] to yield 1.90 g (68%) (I). Yellow crystals were obtained by recrystallization from ethyl acetate at room temperature.

H-NMR ($CDCl_3$, 400 MHz) $\delta$: 1.41 (t, 3H, $CH_3$), 4.38 (q, 2H, $CH_2$), 7.10 (t, 1H, H6), 7.44–7.84 (m, 7H, H7, H2 and PhH), 8.39 (d, 1H, H8), 9.98 (d, 1H, H5).

### S3. Refinement

The H atoms were placed in calculated positions and included as part of a riding model, with C—H = 0.93–0.97 Å, and with $U_{equiv}$ values set at 1.2–1.5 $U_{equiv}$ of the parent atoms.

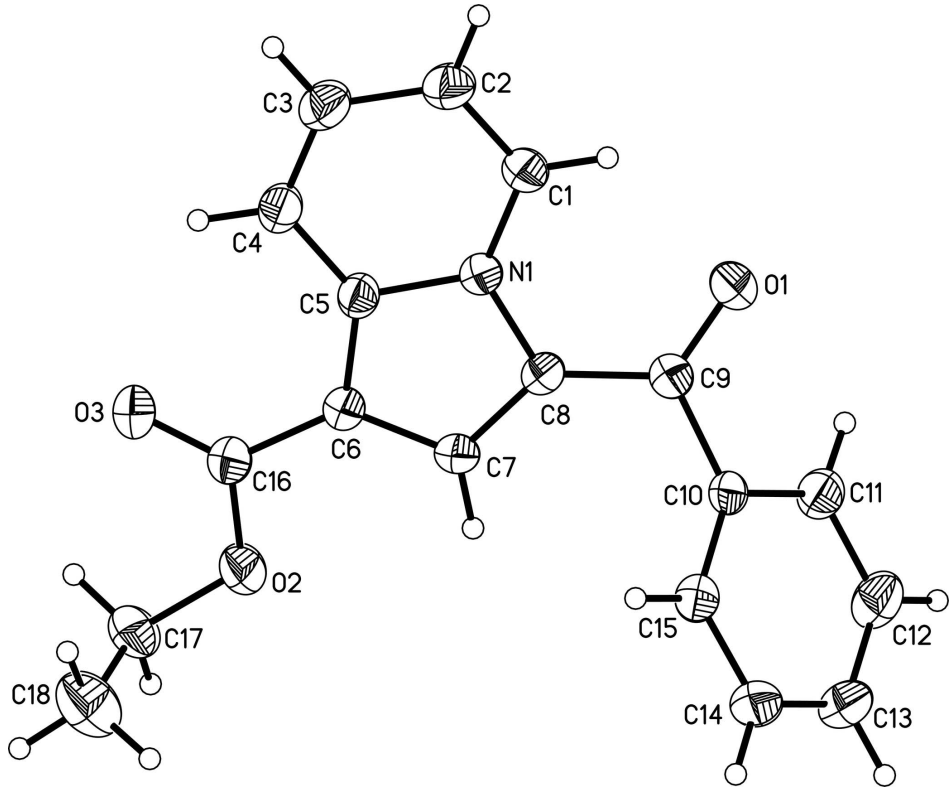


**Figure 1**

A view of the title compound showing the atom-numbering scheme and displacement ellipsoids drawn at 30% probability level.

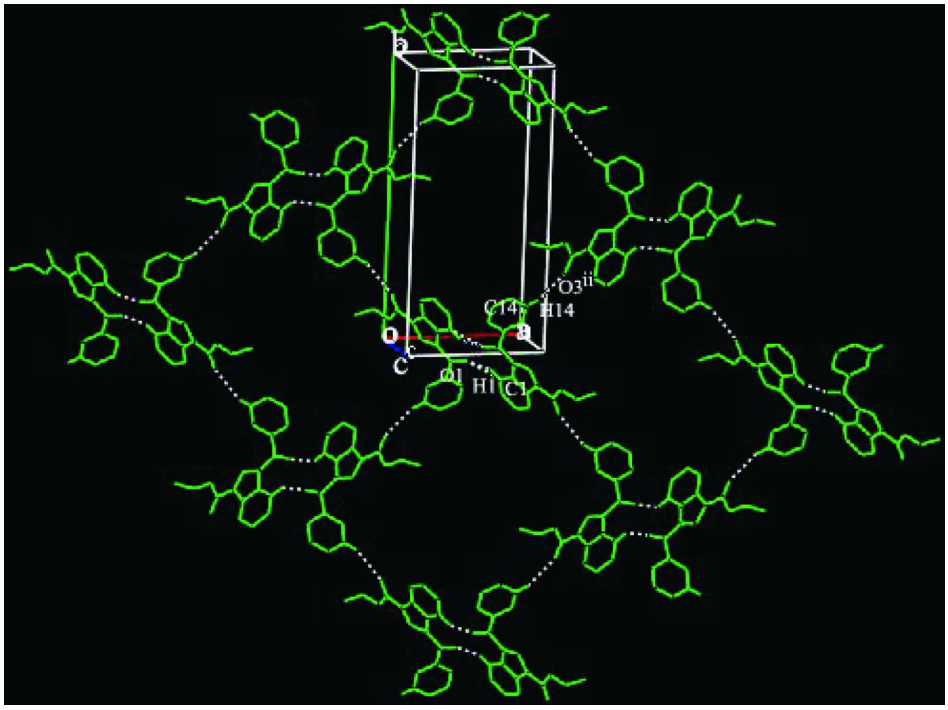


**Figure 2**

A view of the 2-D structure down *c* axis (i: 1 - *x*,-*y*,2 - *z*; ii: -*x*,-1/2 + *y*,0.5 - *z*).

### Ethyl 3-benzoylindolizine-1-carboxylate

*Crystal data*

$C_{18}H_{15}NO_3$
$M_r$ = 293.31
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 10.030 (2) Å
$b$ = 19.223 (3) Å
$c$ = 7.9652 (17) Å
$\beta$ = 103.073 (3)°
$V$ = 1495.9 (5) Å$^3$
$Z$ = 4
$F(000)$ = 616
$D_x$ = 1.302 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1073 reflections
$\theta$ = 2.3–19.4°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 291 K
Block, yellow
0.24 × 0.20 × 0.18 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.979, $T_{max}$ = 0.984
8910 measured reflections
2604 independent reflections
1604 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.1°
$h$ = −11→11
$k$ = −22→20
$l$ = −9→9

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.129$
$S = 1.00$
2604 reflections
201 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
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ e Å$^{-3}$
Extinction correction: *SHELXL97*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.015 (2)

*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.
Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
8.2801 (0.0047) *x* + 9.1394 (0.0112) *y* - 3.8457 (0.0039) *z* = 0.2003 (0.0031)
* 0.0099 (0.0018) C1 * 0.0019 (0.0019) C2 * -0.0097 (0.0019) C3 * -0.0087 (0.0017) C4 * 0.0066 (0.0018) C5 * 0.0165 (0.0017) C6 * -0.0108 (0.0017) C7 * -0.0130 (0.0017) C8 * 0.0072 (0.0016) N1
Rms deviation of fitted atoms = 0.0101
- 0.9358 (0.0101) *x* - 10.1188 (0.0159) *y* + 6.7251 (0.0044) *z* = 4.3984 (0.0037)
Angle to previous plane (with approximate e.s.d.) = 54.26 (0.07)
* -0.0091 (0.0016) C10 * 0.0153 (0.0017) C11 * -0.0081 (0.0018) C12 * -0.0053 (0.0019) C13 * 0.0114 (0.0018) C14 * -0.0042 (0.0016) C15
Rms deviation of fitted atoms = 0.0097

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.3367 (2) | 0.08044 (12) | 0.8614 (3) | 0.0535 (7) |
| H1 | 0.4005 | 0.0494 | 0.9231 | 0.064* |
| C2 | 0.3057 (3) | 0.13943 (12) | 0.9370 (3) | 0.0620 (7) |
| H2 | 0.3483 | 0.1490 | 1.0509 | 0.074* |
| C3 | 0.2092 (3) | 0.18631 (13) | 0.8436 (3) | 0.0613 (7) |
| H3 | 0.1880 | 0.2267 | 0.8963 | 0.074* |
| C4 | 0.1464 (2) | 0.17291 (11) | 0.6764 (3) | 0.0501 (6) |
| H4 | 0.0825 | 0.2041 | 0.6154 | 0.060* |
| C5 | 0.1782 (2) | 0.11209 (10) | 0.5963 (3) | 0.0426 (6) |
| C6 | 0.1348 (2) | 0.08293 (10) | 0.4309 (3) | 0.0445 (6) |
| C7 | 0.2020 (2) | 0.02004 (11) | 0.4333 (3) | 0.0477 (6) |
| H7 | 0.1906 | −0.0104 | 0.3403 | 0.057* |
| C8 | 0.2880 (2) | 0.00854 (10) | 0.5917 (3) | 0.0449 (6) |
| C9 | 0.3887 (2) | −0.04547 (11) | 0.6464 (3) | 0.0473 (6) |
| C10 | 0.3774 (2) | −0.10994 (10) | 0.5398 (3) | 0.0411 (6) |

| | | | | |
|---|---|---|---|---|
| C11 | 0.4968 (3) | −0.13982 (12) | 0.5151 (3) | 0.0536 (7) |
| H11 | 0.5808 | −0.1192 | 0.5626 | 0.064* |
| C12 | 0.4918 (3) | −0.20014 (12) | 0.4201 (4) | 0.0670 (8) |
| H12 | 0.5722 | −0.2191 | 0.4002 | 0.080* |
| C13 | 0.3690 (3) | −0.23235 (13) | 0.3550 (3) | 0.0674 (8) |
| H13 | 0.3662 | −0.2732 | 0.2917 | 0.081* |
| C14 | 0.2502 (3) | −0.20418 (12) | 0.3833 (3) | 0.0611 (7) |
| H14 | 0.1671 | −0.2265 | 0.3414 | 0.073* |
| C15 | 0.2542 (2) | −0.14261 (11) | 0.4742 (3) | 0.0497 (6) |
| H15 | 0.1734 | −0.1231 | 0.4912 | 0.060* |
| C16 | 0.0427 (2) | 0.11668 (12) | 0.2879 (3) | 0.0496 (6) |
| C17 | −0.0756 (3) | 0.10378 (13) | −0.0047 (3) | 0.0640 (7) |
| H17A | −0.0512 | 0.0856 | −0.1073 | 0.077* |
| H17B | −0.0680 | 0.1541 | −0.0066 | 0.077* |
| C18 | −0.2186 (3) | 0.08400 (16) | −0.0048 (4) | 0.0880 (10) |
| H18A | −0.2252 | 0.0343 | 0.0015 | 0.132* |
| H18B | −0.2785 | 0.1003 | −0.1089 | 0.132* |
| H18C | −0.2446 | 0.1046 | 0.0928 | 0.132* |
| N1 | 0.27358 (18) | 0.06663 (9) | 0.6934 (2) | 0.0438 (5) |
| O1 | 0.48475 (18) | −0.03908 (9) | 0.7719 (2) | 0.0698 (5) |
| O2 | 0.01794 (18) | 0.07657 (8) | 0.1471 (2) | 0.0672 (5) |
| O3 | −0.00443 (17) | 0.17415 (8) | 0.2920 (2) | 0.0662 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0636 (17) | 0.0482 (14) | 0.0423 (14) | 0.0019 (12) | −0.0016 (12) | −0.0008 (11) |
| C2 | 0.080 (2) | 0.0534 (15) | 0.0490 (16) | 0.0019 (14) | 0.0082 (14) | −0.0108 (13) |
| C3 | 0.0735 (19) | 0.0484 (15) | 0.0631 (18) | 0.0056 (13) | 0.0175 (15) | −0.0091 (13) |
| C4 | 0.0506 (15) | 0.0421 (13) | 0.0576 (17) | 0.0043 (11) | 0.0123 (13) | 0.0015 (12) |
| C5 | 0.0403 (14) | 0.0374 (12) | 0.0488 (14) | 0.0011 (10) | 0.0075 (12) | 0.0033 (11) |
| C6 | 0.0471 (15) | 0.0389 (12) | 0.0440 (14) | 0.0024 (11) | 0.0033 (11) | −0.0009 (11) |
| C7 | 0.0532 (16) | 0.0408 (13) | 0.0445 (15) | −0.0015 (11) | 0.0015 (12) | −0.0058 (10) |
| C8 | 0.0510 (15) | 0.0372 (12) | 0.0431 (14) | 0.0017 (11) | 0.0035 (12) | −0.0031 (10) |
| C9 | 0.0464 (15) | 0.0434 (13) | 0.0485 (15) | 0.0003 (11) | 0.0028 (13) | 0.0015 (11) |
| C10 | 0.0458 (15) | 0.0342 (12) | 0.0406 (13) | 0.0014 (11) | 0.0040 (11) | 0.0066 (10) |
| C11 | 0.0483 (16) | 0.0473 (14) | 0.0643 (17) | 0.0002 (12) | 0.0109 (13) | 0.0001 (12) |
| C12 | 0.0695 (19) | 0.0521 (16) | 0.084 (2) | 0.0083 (14) | 0.0271 (16) | −0.0052 (15) |
| C13 | 0.084 (2) | 0.0468 (15) | 0.0695 (19) | −0.0001 (16) | 0.0127 (17) | −0.0128 (13) |
| C14 | 0.0613 (18) | 0.0481 (15) | 0.0678 (18) | −0.0107 (13) | 0.0020 (14) | −0.0026 (13) |
| C15 | 0.0471 (16) | 0.0444 (13) | 0.0550 (16) | 0.0025 (11) | 0.0061 (13) | 0.0017 (12) |
| C16 | 0.0505 (16) | 0.0441 (14) | 0.0505 (16) | 0.0011 (12) | 0.0037 (12) | 0.0040 (12) |
| C17 | 0.069 (2) | 0.0711 (17) | 0.0429 (15) | 0.0018 (15) | −0.0064 (14) | 0.0072 (13) |
| C18 | 0.072 (2) | 0.113 (2) | 0.074 (2) | −0.0102 (18) | 0.0051 (17) | 0.0196 (18) |
| N1 | 0.0485 (12) | 0.0381 (10) | 0.0412 (11) | −0.0003 (9) | 0.0027 (9) | −0.0013 (8) |
| O1 | 0.0645 (12) | 0.0669 (12) | 0.0635 (12) | 0.0164 (9) | −0.0162 (10) | −0.0144 (9) |
| O2 | 0.0783 (13) | 0.0639 (11) | 0.0487 (11) | 0.0165 (9) | −0.0083 (9) | −0.0023 (9) |
| O3 | 0.0722 (13) | 0.0488 (10) | 0.0679 (13) | 0.0143 (9) | −0.0041 (10) | 0.0056 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.353 (3) | C10—C11 | 1.382 (3) |
| C1—N1 | 1.370 (3) | C11—C12 | 1.379 (3) |
| C1—H1 | 0.9300 | C11—H11 | 0.9300 |
| C2—C3 | 1.406 (3) | C12—C13 | 1.372 (3) |
| C2—H2 | 0.9300 | C12—H12 | 0.9300 |
| C3—C4 | 1.363 (3) | C13—C14 | 1.373 (3) |
| C3—H3 | 0.9300 | C13—H13 | 0.9300 |
| C4—C5 | 1.403 (3) | C14—C15 | 1.383 (3) |
| C4—H4 | 0.9300 | C14—H14 | 0.9300 |
| C5—N1 | 1.393 (3) | C15—H15 | 0.9300 |
| C5—C6 | 1.407 (3) | C16—O3 | 1.205 (3) |
| C6—C7 | 1.382 (3) | C16—O2 | 1.337 (3) |
| C6—C16 | 1.448 (3) | C17—O2 | 1.450 (3) |
| C7—C8 | 1.376 (3) | C17—C18 | 1.484 (3) |
| C7—H7 | 0.9300 | C17—H17A | 0.9700 |
| C8—N1 | 1.406 (2) | C17—H17B | 0.9700 |
| C8—C9 | 1.445 (3) | C18—H18A | 0.9600 |
| C9—O1 | 1.228 (3) | C18—H18B | 0.9600 |
| C9—C10 | 1.492 (3) | C18—H18C | 0.9600 |
| C10—C15 | 1.379 (3) | | |
| | | | |
| C2—C1—N1 | 119.7 (2) | C10—C11—H11 | 119.9 |
| C2—C1—H1 | 120.2 | C13—C12—C11 | 120.4 (2) |
| N1—C1—H1 | 120.2 | C13—C12—H12 | 119.8 |
| C1—C2—C3 | 120.1 (2) | C11—C12—H12 | 119.8 |
| C1—C2—H2 | 119.9 | C12—C13—C14 | 119.9 (2) |
| C3—C2—H2 | 119.9 | C12—C13—H13 | 120.1 |
| C4—C3—C2 | 120.4 (2) | C14—C13—H13 | 120.1 |
| C4—C3—H3 | 119.8 | C13—C14—C15 | 120.0 (2) |
| C2—C3—H3 | 119.8 | C13—C14—H14 | 120.0 |
| C3—C4—C5 | 120.0 (2) | C15—C14—H14 | 120.0 |
| C3—C4—H4 | 120.0 | C10—C15—C14 | 120.3 (2) |
| C5—C4—H4 | 120.0 | C10—C15—H15 | 119.8 |
| N1—C5—C4 | 117.9 (2) | C14—C15—H15 | 119.8 |
| N1—C5—C6 | 107.35 (18) | O3—C16—O2 | 123.5 (2) |
| C4—C5—C6 | 134.7 (2) | O3—C16—C6 | 125.0 (2) |
| C7—C6—C5 | 106.80 (19) | O2—C16—C6 | 111.5 (2) |
| C7—C6—C16 | 128.7 (2) | O2—C17—C18 | 110.6 (2) |
| C5—C6—C16 | 124.45 (19) | O2—C17—H17A | 109.5 |
| C8—C7—C6 | 110.83 (19) | C18—C17—H17A | 109.5 |
| C8—C7—H7 | 124.6 | O2—C17—H17B | 109.5 |
| C6—C7—H7 | 124.6 | C18—C17—H17B | 109.5 |
| C7—C8—N1 | 106.01 (18) | H17A—C17—H17B | 108.1 |
| C7—C8—C9 | 129.9 (2) | C17—C18—H18A | 109.5 |
| N1—C8—C9 | 123.6 (2) | C17—C18—H18B | 109.5 |
| O1—C9—C8 | 122.7 (2) | H18A—C18—H18B | 109.5 |

| | | | |
|---|---|---|---|
| O1—C9—C10 | 119.4 (2) | C17—C18—H18C | 109.5 |
| C8—C9—C10 | 117.9 (2) | H18A—C18—H18C | 109.5 |
| C15—C10—C11 | 119.2 (2) | H18B—C18—H18C | 109.5 |
| C15—C10—C9 | 122.7 (2) | C1—N1—C5 | 121.86 (18) |
| C11—C10—C9 | 118.0 (2) | C1—N1—C8 | 129.14 (19) |
| C12—C11—C10 | 120.2 (2) | C5—N1—C8 | 109.00 (18) |
| C12—C11—H11 | 119.9 | C16—O2—C17 | 116.98 (18) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C3 | 0.0 (4) | C10—C11—C12—C13 | −2.4 (4) |
| C1—C2—C3—C4 | −0.2 (4) | C11—C12—C13—C14 | 0.5 (4) |
| C2—C3—C4—C5 | −0.1 (4) | C12—C13—C14—C15 | 1.4 (4) |
| C3—C4—C5—N1 | 0.6 (3) | C11—C10—C15—C14 | −0.6 (3) |
| C3—C4—C5—C6 | −179.7 (2) | C9—C10—C15—C14 | −176.8 (2) |
| N1—C5—C6—C7 | 1.5 (2) | C13—C14—C15—C10 | −1.3 (4) |
| C4—C5—C6—C7 | −178.2 (2) | C7—C6—C16—O3 | −174.1 (2) |
| N1—C5—C6—C16 | −175.5 (2) | C5—C6—C16—O3 | 2.2 (4) |
| C4—C5—C6—C16 | 4.8 (4) | C7—C6—C16—O2 | 4.5 (3) |
| C5—C6—C7—C8 | −1.1 (3) | C5—C6—C16—O2 | −179.2 (2) |
| C16—C6—C7—C8 | 175.7 (2) | C2—C1—N1—C5 | 0.5 (3) |
| C6—C7—C8—N1 | 0.3 (3) | C2—C1—N1—C8 | −178.6 (2) |
| C6—C7—C8—C9 | −172.0 (2) | C4—C5—N1—C1 | −0.8 (3) |
| C7—C8—C9—O1 | 157.9 (2) | C6—C5—N1—C1 | 179.45 (18) |
| N1—C8—C9—O1 | −13.2 (4) | C4—C5—N1—C8 | 178.43 (18) |
| C7—C8—C9—C10 | −19.2 (4) | C6—C5—N1—C8 | −1.3 (2) |
| N1—C8—C9—C10 | 169.63 (18) | C7—C8—N1—C1 | 179.8 (2) |
| O1—C9—C10—C15 | 139.8 (2) | C9—C8—N1—C1 | −7.3 (3) |
| C8—C9—C10—C15 | −43.0 (3) | C7—C8—N1—C5 | 0.6 (2) |
| O1—C9—C10—C11 | −36.4 (3) | C9—C8—N1—C5 | 173.6 (2) |
| C8—C9—C10—C11 | 140.8 (2) | O3—C16—O2—C17 | −2.7 (3) |
| C15—C10—C11—C12 | 2.5 (3) | C6—C16—O2—C17 | 178.65 (19) |
| C9—C10—C11—C12 | 178.8 (2) | C18—C17—O2—C16 | −89.0 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O1$^{i}$ | 0.93 | 2.45 | 3.163 (3) | 134 |
| C14—H14···O3$^{ii}$ | 0.93 | 2.58 | 3.455 (3) | 157 |

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