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# (2*E*)-1-(2,5-Dimethoxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one

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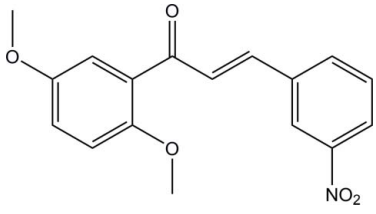
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.048; $wR$ factor = 0.179; data-to-parameter ratio = 20.9.

In the title compound, $C_{17}H_{15}NO_5$, an intramolecular C—H···O hydrogen bond generates an $S(6)$ ring motif. The benzene rings form a dihedral angle of 6.45 (7)° with each other. In the crystal, inversion dimers linked by pairs of C—H···O hydrogen bonds generate $R_2^2(8)$ loops. Adjacent dimers are further connected by C—H···O hydrogen bonds into an infinite chain along the [011] direction.

## Related literature

For biological activities of chalcones, see: Dimmock *et al.* (1999). For the structures of chalcone derivatives, see: Samshuddin *et al.* (2010); Fun *et al.* (2010*a*,*b*); Jasinski *et al.* (2010); Baktır *et al.* (2011*a*,*b*). For related crystal structures, see: Jasinski *et al.* (2008); Sarojini *et al.* (2007); Ma (2007). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For standard bond lengths, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{17}H_{15}NO_5$
$M_r$ = 313.30
Triclinic, $P\overline{1}$
$a$ = 7.5015 (5) Å
$b$ = 7.9962 (5) Å
$c$ = 13.2468 (8) Å
$\alpha$ = 86.507 (1)°
$\beta$ = 80.342 (1)°
$\gamma$ = 76.332 (1)°
$V$ = 760.96 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 296 K
0.41 × 0.38 × 0.13 mm

### Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.960, $T_{max}$ = 0.987
16631 measured reflections
4381 independent reflections
3195 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.179
$S$ = 1.02
4381 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3*A*···O2$^{i}$ | 0.93 | 2.55 | 3.4773 (18) | 172 |
| C8—H8*A*···O1 | 0.93 | 2.12 | 2.7727 (16) | 126 |
| C17—H17*A*···O5$^{ii}$ | 0.96 | 2.50 | 3.309 (2) | 142 |

Symmetry codes: (i) $-x, -y, -z$; (ii) $x, y-1, z-1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2794).

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# supporting information

*Acta Cryst.* (2011). E**67**, o3058–o3059 [doi:10.1107/S1600536811043224]

## (2*E*)-1-(2,5-Dimethoxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one

**Hoong-Kun Fun, Tze Shyang Chia, B. Narayana, Prakash S. Nayak and B. K. Sarojini**

### S1. Comment

Chalcones can be easily obtained from the Claisen–Schmidt reaction of aromatic aldehydes and aromatic ketones. Chalcones have been reported to possess many useful properties including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumour and anticancer activities (Dimmock *et al.*, 1999). The basic skeleton of chalcones which possess the *α*,*β*-unsaturated carbonyl group is a useful synthone for the synthesis of various biodynamic cyclic derivatives such as pyrazoline, benzodiazepine and cyclohexenone derivatives (Samshuddin *et al.*, 2010; Fun *et al.*, 2010*a*,*b*; Jasinski *et al.*, 2010; Baktır *et al.*, 2011*a*,*b*). The crystal structures of some related chalcones which contain the nitro and methoxy groups *viz*: (2*E*)-3-(4-methylphenyl)-1-(3-nitrophenyl)prop-2-en-1-one (Jasinski *et al.*, 2008), (2*E*)-3-(2-chlorophenyl)-1-(3-nitrophenyl)prop-2-en-1-one (Sarojini *et al.*, 2007) and (*E*)-3-(4-methoxyphenyl)-1-(3-nitrophenyl)prop-2-en-1-one (Ma, 2007) have been reported. In view of the importance of chalcones, the crystal structure of the title compound is reported here.

The molecular structure of the title compound is shown in Fig. 1. The benzene rings (C1–C6 and C10–C15) make a dihedral angle of 6.45 (7)° with each other. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to related structures (Jasinski *et al.*, 2008; Sarojini *et al.*, 2007; Ma, 2007). The molecular structure is stabilized by an intramolecular C8—H8A···O1 hydrogen bond (Table 1) which generates an S(6) ring motif (Fig. 1; Bernstein *et al.*, 1995).

In the crystal structure (Fig. 2), the molecules are interconnected by C3—H3A···O2 hydrogen bonds (Table 1), forming a dimer with an $R_2^2(8)$ ring motif. These dimers are further linked by intermolecular C17—H17A···O5 hydrogen bonds into an infinite chains along the [011] direction.

### S2. Experimental

To a mixture of 2,5-dimethoxy acetophenone (1.5 ml, 0.01 mol) and 3-nitrobenzaldehyde (1.51 g, 0.01 mol) in ethanol (50 ml), 10 ml of 10% sodium hydroxide solution was added and stirred at 5–10 °C for 3 h. The precipitate formed was collected by filtration and then purified by recrystallization from ethanol. The single crystals were grown from a DMF solution by slow evaporation method (m.p. 377–379 K).

### S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93 or 0.96 Å) and refined using a riding model with $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(C). A rotating group model was applied to the methyl group.

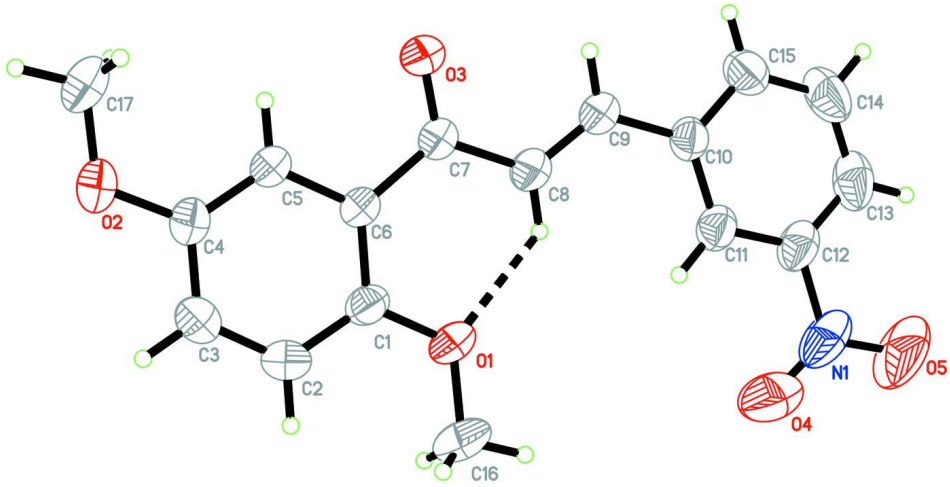


**Figure 1**

The molecular structure of the title compound with atom labels with 50% probability displacement ellipsoids. The intramolecular hydrogen bond is shown by a dashed line.

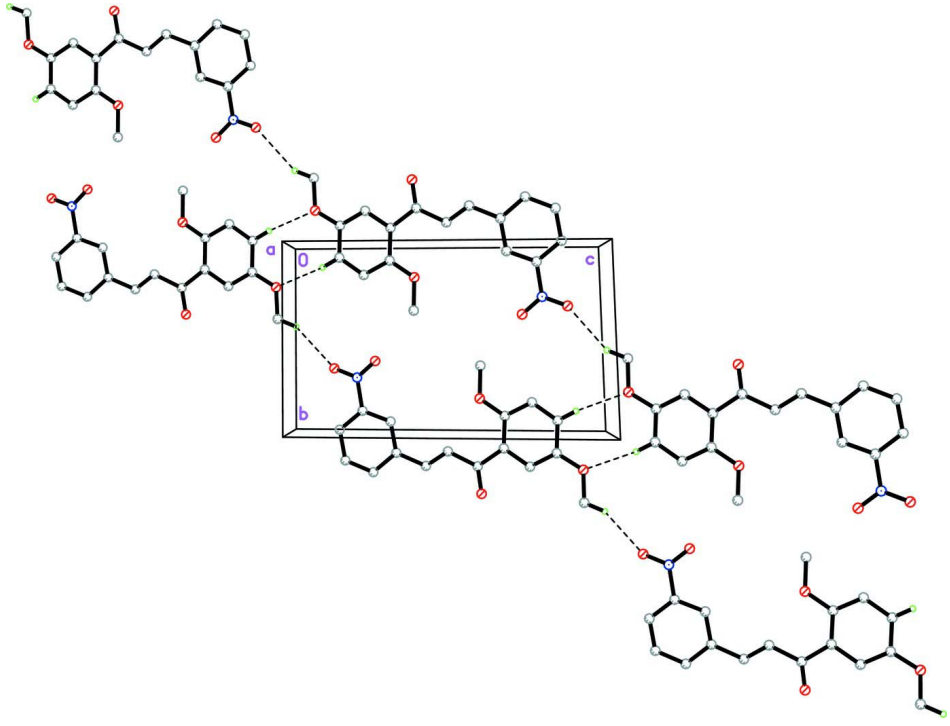


**Figure 2**

A packing diagram of the title compound viewed along the *a* axis. The dashed lines represent the hydrogen bonds.

**(2*E*)-1-(2,5-Dimethoxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one**

*Crystal data*

$C_{17}H_{15}NO_5$
$M_r$ = 313.30
Triclinic, $P\overline{1}$
Hall symbol: -P 1

$a$ = 7.5015 (5) Å
$b$ = 7.9962 (5) Å
$c$ = 13.2468 (8) Å
$\alpha$ = 86.507 (1)°

$\beta$ = 80.342 (1)°
$\gamma$ = 76.332 (1)°
$V$ = 760.96 (8) Å$^3$
$Z$ = 2
$F$(000) = 328
$D_x$ = 1.367 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 5160 reflections
$\theta$ = 2.6–32.3°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 296 K
Block, yellow
0.41 × 0.38 × 0.13 mm

*Data collection*

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.960, $T_{max}$ = 0.987

16631 measured reflections
4381 independent reflections
3195 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021
$\theta_{max}$ = 30.0°, $\theta_{min}$ = 1.6°
$h$ = −10→10
$k$ = −11→11
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.179
$S$ = 1.02
4381 reflections
210 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
$w = 1/[\sigma^2(F_o^2) + (0.1091P)^2 + 0.0754P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 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 | 0.15506 (16) | 0.16718 (11) | 0.39750 (8) | 0.0591 (3) |
| O2 | 0.11277 (18) | −0.21224 (13) | 0.07147 (7) | 0.0671 (3) |
| O3 | 0.3565 (2) | −0.36287 (12) | 0.39765 (9) | 0.0802 (4) |
| O4 | 0.2174 (3) | 0.37169 (16) | 0.74170 (13) | 0.0989 (5) |
| O5 | 0.3301 (3) | 0.3286 (2) | 0.88284 (13) | 0.1121 (6) |
| N1 | 0.2941 (2) | 0.2780 (2) | 0.80490 (12) | 0.0729 (4) |
| C1 | 0.14468 (17) | 0.07338 (14) | 0.31743 (9) | 0.0409 (3) |
| C2 | 0.07436 (19) | 0.15014 (15) | 0.23001 (10) | 0.0487 (3) |
| H2A | 0.0312 | 0.2690 | 0.2265 | 0.058* |
| C3 | 0.0682 (2) | 0.05257 (17) | 0.14937 (10) | 0.0502 (3) |

| | | | | |
|---|---|---|---|---|
| H3A | 0.0228 | 0.1057 | 0.0914 | 0.060* |
| C4 | 0.12955 (19) | −0.12516 (16) | 0.15424 (9) | 0.0458 (3) |
| C5 | 0.19828 (17) | −0.20273 (14) | 0.23995 (9) | 0.0419 (3) |
| H5A | 0.2391 | −0.3219 | 0.2429 | 0.050* |
| C6 | 0.20797 (16) | −0.10584 (13) | 0.32289 (8) | 0.0381 (2) |
| C7 | 0.29087 (19) | −0.20926 (14) | 0.40881 (9) | 0.0452 (3) |
| C8 | 0.2943 (2) | −0.12935 (16) | 0.50575 (9) | 0.0497 (3) |
| H8A | 0.2364 | −0.0137 | 0.5148 | 0.060* |
| C9 | 0.37566 (19) | −0.21468 (15) | 0.57977 (9) | 0.0460 (3) |
| H9A | 0.4334 | −0.3300 | 0.5689 | 0.055* |
| C10 | 0.38354 (17) | −0.14415 (15) | 0.67833 (8) | 0.0419 (3) |
| C11 | 0.33505 (18) | 0.03198 (16) | 0.69527 (9) | 0.0455 (3) |
| H11A | 0.2967 | 0.1094 | 0.6436 | 0.055* |
| C12 | 0.34453 (19) | 0.09026 (18) | 0.78952 (10) | 0.0522 (3) |
| C13 | 0.3995 (2) | −0.0188 (2) | 0.86864 (11) | 0.0644 (4) |
| H13A | 0.4044 | 0.0240 | 0.9316 | 0.077* |
| C14 | 0.4467 (2) | −0.1924 (2) | 0.85189 (11) | 0.0685 (4) |
| H14A | 0.4839 | −0.2685 | 0.9044 | 0.082* |
| C15 | 0.4399 (2) | −0.25623 (18) | 0.75773 (10) | 0.0542 (3) |
| H15A | 0.4732 | −0.3743 | 0.7476 | 0.065* |
| C16 | 0.0965 (3) | 0.34867 (17) | 0.39303 (15) | 0.0703 (5) |
| H16A | 0.1164 | 0.3956 | 0.4541 | 0.105* |
| H16B | −0.0333 | 0.3808 | 0.3876 | 0.105* |
| H16C | 0.1665 | 0.3928 | 0.3344 | 0.105* |
| C17 | 0.1863 (3) | −0.3918 (2) | 0.07001 (13) | 0.0749 (5) |
| H17A | 0.1741 | −0.4357 | 0.0063 | 0.112* |
| H17B | 0.1195 | −0.4461 | 0.1256 | 0.112* |
| H17C | 0.3152 | −0.4158 | 0.0772 | 0.112* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0856 (7) | 0.0345 (4) | 0.0589 (6) | −0.0060 (4) | −0.0224 (5) | −0.0149 (4) |
| O2 | 0.0998 (9) | 0.0582 (6) | 0.0452 (5) | −0.0064 (5) | −0.0298 (5) | −0.0119 (4) |
| O3 | 0.1363 (12) | 0.0367 (5) | 0.0692 (7) | 0.0086 (6) | −0.0573 (7) | −0.0125 (4) |
| O4 | 0.1368 (14) | 0.0526 (7) | 0.1063 (11) | −0.0103 (8) | −0.0283 (10) | −0.0141 (7) |
| O5 | 0.1285 (13) | 0.1081 (11) | 0.1059 (11) | −0.0205 (10) | −0.0210 (10) | −0.0706 (9) |
| N1 | 0.0739 (9) | 0.0682 (8) | 0.0789 (9) | −0.0184 (7) | −0.0019 (7) | −0.0394 (7) |
| C1 | 0.0446 (6) | 0.0331 (5) | 0.0452 (6) | −0.0076 (4) | −0.0069 (4) | −0.0070 (4) |
| C2 | 0.0549 (7) | 0.0347 (5) | 0.0548 (7) | −0.0055 (5) | −0.0117 (5) | 0.0014 (5) |
| C3 | 0.0566 (7) | 0.0475 (6) | 0.0456 (6) | −0.0065 (5) | −0.0153 (5) | 0.0041 (5) |
| C4 | 0.0543 (7) | 0.0467 (6) | 0.0374 (5) | −0.0092 (5) | −0.0113 (5) | −0.0068 (4) |
| C5 | 0.0517 (7) | 0.0342 (5) | 0.0396 (5) | −0.0050 (4) | −0.0113 (5) | −0.0071 (4) |
| C6 | 0.0440 (6) | 0.0332 (5) | 0.0374 (5) | −0.0066 (4) | −0.0085 (4) | −0.0057 (4) |
| C7 | 0.0595 (7) | 0.0365 (5) | 0.0418 (6) | −0.0074 (5) | −0.0172 (5) | −0.0058 (4) |
| C8 | 0.0688 (8) | 0.0402 (6) | 0.0402 (6) | −0.0060 (5) | −0.0158 (5) | −0.0082 (4) |
| C9 | 0.0570 (7) | 0.0386 (5) | 0.0439 (6) | −0.0076 (5) | −0.0149 (5) | −0.0072 (4) |
| C10 | 0.0441 (6) | 0.0451 (6) | 0.0376 (5) | −0.0091 (5) | −0.0100 (4) | −0.0048 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0509 (7) | 0.0473 (6) | 0.0404 (6) | −0.0124 (5) | −0.0090 (5) | −0.0070 (4) |
| C12 | 0.0499 (7) | 0.0577 (7) | 0.0500 (7) | −0.0112 (6) | −0.0058 (5) | −0.0204 (6) |
| C13 | 0.0604 (9) | 0.0892 (11) | 0.0426 (7) | −0.0066 (8) | −0.0139 (6) | −0.0193 (7) |
| C14 | 0.0716 (10) | 0.0849 (11) | 0.0427 (7) | 0.0005 (8) | −0.0199 (6) | 0.0043 (7) |
| C15 | 0.0583 (8) | 0.0526 (7) | 0.0484 (7) | −0.0022 (6) | −0.0151 (6) | 0.0014 (5) |
| C16 | 0.0901 (12) | 0.0352 (6) | 0.0849 (11) | −0.0072 (7) | −0.0160 (9) | −0.0185 (7) |
| C17 | 0.1071 (14) | 0.0604 (9) | 0.0567 (8) | −0.0066 (9) | −0.0215 (8) | −0.0245 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.3585 (13) | C8—H8A | 0.9300 |
| O1—C16 | 1.4140 (15) | C9—C10 | 1.4689 (15) |
| O2—C4 | 1.3725 (13) | C9—H9A | 0.9300 |
| O2—C17 | 1.4114 (18) | C10—C11 | 1.3911 (16) |
| O3—C7 | 1.2186 (14) | C10—C15 | 1.3941 (16) |
| O4—N1 | 1.214 (2) | C11—C12 | 1.3775 (16) |
| O5—N1 | 1.2241 (18) | C11—H11A | 0.9300 |
| N1—C12 | 1.477 (2) | C12—C13 | 1.375 (2) |
| C1—C2 | 1.4006 (17) | C13—C14 | 1.372 (2) |
| C1—C6 | 1.4007 (14) | C13—H13A | 0.9300 |
| C2—C3 | 1.3736 (18) | C14—C15 | 1.3894 (19) |
| C2—H2A | 0.9300 | C14—H14A | 0.9300 |
| C3—C4 | 1.3876 (17) | C15—H15A | 0.9300 |
| C3—H3A | 0.9300 | C16—H16A | 0.9600 |
| C4—C5 | 1.3781 (16) | C16—H16B | 0.9600 |
| C5—C6 | 1.4035 (14) | C16—H16C | 0.9600 |
| C5—H5A | 0.9300 | C17—H17A | 0.9600 |
| C6—C7 | 1.4986 (15) | C17—H17B | 0.9600 |
| C7—C8 | 1.4754 (15) | C17—H17C | 0.9600 |
| C8—C9 | 1.3121 (17) | | |
| | | | |
| C1—O1—C16 | 119.72 (11) | C10—C9—H9A | 117.1 |
| C4—O2—C17 | 117.66 (10) | C11—C10—C15 | 118.74 (11) |
| O4—N1—O5 | 124.18 (17) | C11—C10—C9 | 121.88 (10) |
| O4—N1—C12 | 118.90 (13) | C15—C10—C9 | 119.38 (11) |
| O5—N1—C12 | 116.90 (18) | C12—C11—C10 | 119.18 (12) |
| O1—C1—C2 | 122.18 (10) | C12—C11—H11A | 120.4 |
| O1—C1—C6 | 118.48 (10) | C10—C11—H11A | 120.4 |
| C2—C1—C6 | 119.33 (10) | C13—C12—C11 | 122.74 (13) |
| C3—C2—C1 | 121.03 (11) | C13—C12—N1 | 119.30 (13) |
| C3—C2—H2A | 119.5 | C11—C12—N1 | 117.96 (13) |
| C1—C2—H2A | 119.5 | C14—C13—C12 | 118.00 (12) |
| C2—C3—C4 | 120.09 (11) | C14—C13—H13A | 121.0 |
| C2—C3—H3A | 120.0 | C12—C13—H13A | 121.0 |
| C4—C3—H3A | 120.0 | C13—C14—C15 | 121.00 (13) |
| O2—C4—C5 | 124.45 (11) | C13—C14—H14A | 119.5 |
| O2—C4—C3 | 115.96 (10) | C15—C14—H14A | 119.5 |
| C5—C4—C3 | 119.58 (10) | C14—C15—C10 | 120.34 (13) |

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| C4—C5—C6 | 121.45 (10) | C14—C15—H15A | 119.8 |
| C4—C5—H5A | 119.3 | C10—C15—H15A | 119.8 |
| C6—C5—H5A | 119.3 | O1—C16—H16A | 109.5 |
| C1—C6—C5 | 118.51 (10) | O1—C16—H16B | 109.5 |
| C1—C6—C7 | 126.70 (9) | H16A—C16—H16B | 109.5 |
| C5—C6—C7 | 114.78 (9) | O1—C16—H16C | 109.5 |
| O3—C7—C8 | 119.73 (10) | H16A—C16—H16C | 109.5 |
| O3—C7—C6 | 118.73 (10) | H16B—C16—H16C | 109.5 |
| C8—C7—C6 | 121.54 (10) | O2—C17—H17A | 109.5 |
| C9—C8—C7 | 122.75 (11) | O2—C17—H17B | 109.5 |
| C9—C8—H8A | 118.6 | H17A—C17—H17B | 109.5 |
| C7—C8—H8A | 118.6 | O2—C17—H17C | 109.5 |
| C8—C9—C10 | 125.75 (11) | H17A—C17—H17C | 109.5 |
| C8—C9—H9A | 117.1 | H17B—C17—H17C | 109.5 |

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| C16—O1—C1—C2 | −1.1 (2) | C5—C6—C7—C8 | −173.92 (12) |
| C16—O1—C1—C6 | 178.45 (13) | O3—C7—C8—C9 | 4.2 (2) |
| O1—C1—C2—C3 | 178.92 (12) | C6—C7—C8—C9 | −175.88 (13) |
| C6—C1—C2—C3 | −0.6 (2) | C7—C8—C9—C10 | −179.56 (12) |
| C1—C2—C3—C4 | 1.0 (2) | C8—C9—C10—C11 | −12.8 (2) |
| C17—O2—C4—C5 | −6.0 (2) | C8—C9—C10—C15 | 166.73 (14) |
| C17—O2—C4—C3 | 175.36 (15) | C15—C10—C11—C12 | 0.15 (19) |
| C2—C3—C4—O2 | 178.06 (13) | C9—C10—C11—C12 | 179.72 (12) |
| C2—C3—C4—C5 | −0.6 (2) | C10—C11—C12—C13 | −0.3 (2) |
| O2—C4—C5—C6 | −178.65 (12) | C10—C11—C12—N1 | 179.37 (12) |
| C3—C4—C5—C6 | −0.1 (2) | O4—N1—C12—C13 | −168.10 (17) |
| O1—C1—C6—C5 | −179.64 (11) | O5—N1—C12—C13 | 10.5 (2) |
| C2—C1—C6—C5 | −0.08 (18) | O4—N1—C12—C11 | 12.2 (2) |
| O1—C1—C6—C7 | −0.96 (19) | O5—N1—C12—C11 | −169.16 (15) |
| C2—C1—C6—C7 | 178.60 (12) | C11—C12—C13—C14 | 0.1 (2) |
| C4—C5—C6—C1 | 0.41 (19) | N1—C12—C13—C14 | −179.54 (15) |
| C4—C5—C6—C7 | −178.42 (12) | C12—C13—C14—C15 | 0.2 (3) |
| C1—C6—C7—O3 | −172.69 (14) | C13—C14—C15—C10 | −0.4 (2) |
| C5—C6—C7—O3 | 6.03 (19) | C11—C10—C15—C14 | 0.2 (2) |
| C1—C6—C7—C8 | 7.4 (2) | C9—C10—C15—C14 | −179.40 (13) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3*A*···O2$^{i}$ | 0.93 | 2.55 | 3.4773 (18) | 172 |
| C8—H8*A*···O1 | 0.93 | 2.12 | 2.7727 (16) | 126 |
| C17—H17*A*···O5$^{ii}$ | 0.96 | 2.50 | 3.309 (2) | 142 |

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