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# (*E*)-3-(4-Methoxyphenyl)-1-[4-(piperidin-1-yl)phenyl]prop-2-en-1-one

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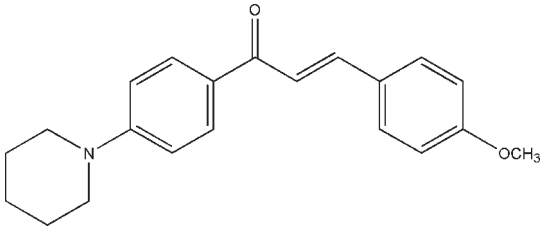
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.052; $wR$ factor = 0.151; data-to-parameter ratio = 22.3.

The piperidine ring in the title compound, $C_{21}H_{23}NO_2$, is in a slightly distorted chair conformation. The dihedral angle between the two benzene rings is 5.6 (4)°. The dihedral angles between the propenone unit and the benzene and methoxy-substituted benzene rings are 5.6 (7) and 10.7 (8)°, respectively. Weak intermolecular C—H···O hydrogen bonds and weak C—H···$\pi$ interactions contribute to the stability of the crystal structure.

## Related literature

For the synthesis and biological evaluation of simple methoxylated chalcones as anticancer, anti-inflammatory and antioxidant agents, see: Bandgar *et al.* (2010). For anti-inflammatory chalcones, see: Nowakowska (2007). For related structures, see: Ahmad *et al.*(2010); Arai *et al.*(1994); Jasinski *et al.* (2010); Li *et al.* (1992); Patil *et al.* (2007); Shettigar *et al.* (2006). For standard bond lengths, see; Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{21}H_{23}NO_2$
$M_r$ = 321.40
Triclinic, $P\overline{1}$
$a$ = 6.0963 (11) Å
$b$ = 10.985 (2) Å
$c$ = 13.133 (3) Å
$\alpha$ = 74.188 (3)°
$\beta$ = 88.674 (3)°
$\gamma$ = 77.393 (3)°
$V$ = 825.2 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 100 K
0.47 × 0.36 × 0.21 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.962, $T_{max}$ = 0.983
10674 measured reflections
4861 independent reflections
3562 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.151
$S$ = 1.05
4861 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

*Cg*2 and *Cg*3 are the centroids of the C1–C6 and C15–C20 rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C20—H20···O2$^{i}$ | 0.93 | 2.47 | 3.2105 (16) | 137 |
| C8—H8$A$···$Cg3^{ii}$ | 0.97 | 2.66 | 3.623 (2) | 171 |
| C21—H21$A$···$Cg2^{iii}$ | 0.96 | 2.90 | 3.823 (2) | 162 |

Symmetry codes: (i) $-x+2, -y+2, -z$; (ii) $x, y, z+1$; (iii) $-x+1, -y+2, -z$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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).

BN thanks the UGC (New Delhi) for the SAP chemical grant. HSY thanks UOM for sabbatical leave. JPJ thanks Dr Matthias Zeller and the YSU Department of Chemistry for their assistance with the data collection. The diffractometer was funded by NSF grant 0087210, by the Ohio Board of Regents grant CAP-491, and by YSU.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5070).

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# supporting information

*Acta Cryst.* (2010). E**66**, o1996 [https://doi.org/10.1107/S1600536810026218]

## (*E*)-3-(4-Methoxyphenyl)-1-[4-(piperidin-1-yl)phenyl]prop-2-en-1-one

**Jerry P. Jasinski, Curtis J. Guild, B. Narayana, Prakash S. Nayak and H. S. Yathirajan**

### S1. Comment

The chalcone skeleton (1,3-diphenyl-2-propen-1-one) is a unique template that is associated with various biological activities. A review of anti- infective and anti-inflammatory chalcones is published (Nowakowska, 2007). The synthesis and biological evaluation of simple methoxylated chalcones as anticancer, anti-inflammatory and antioxidant agents is recently reported (Bandgar *et al.*, 2010). The crystal structures of some related chalcones containing methoxy substituents, *viz*., 4-bromo-4′-methoxy-chalcone (Li *et al.*, 1992), 4-bromo-4′-methoxychalcone (Arai *et al.*, 1994), 1-(4-bromophenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Shettigar *et al.*, 2006) and 1-(4-bromophenyl)-3-(3-methoxy-phenyl) prop-2-en-1-one (Patil *et al.*, 2007), a monoclinic polymorph of 1-(4-chlorophenyl)-3- (4-methoxyphenyl)prop-2-en-1-one (Jasinski *et al.*, 2010) and (*E*)-3-(3-chlorophenyl)-1-(4-methoxyphenyl) prop-2-en-1-one (Ahmad *et al.*, 2010) have been reported. Hence in continuation with the synthesis and crystal structure of chalcones and their derivatives, this new chalcone containing the piperidine moiety was synthesized and its crystal structure is reported herein.

The title compound contains phenyl-4-methoxy and phenyl-4-piperidine groups on opposite sides of a 2-propen-1-one moiety (Fig. 1). Bond distances (Allen *et al.*, 1987) and angles are in normal ranges. The piperidine ring is in a slightly distorted chair conformation. The dihedral angles between the two benzene rings is 5.6 (4)°. The dihedral angles between the propenone moiety and the benzene and methoxy-benzene rings are 5.6 (7)° and 10.7 (8)°. A weak intermolecular hydrogen bond and weak intermolecular C—H···$\pi$-ring interactions contribute to the stability of crystal packing (Fig. 2).

### S2. Experimental

A 30% KOH solution was added to a mixture of 1-[4-(piperidin-1-yl)phenyl] ethanone (0.01 mol, 2.03 g) and 4-methoxy benzaldehyde (0.01 mol, 1.36 g) in 50 ml of ethanol (Fig. 3). The mixture was stirred for an hour at room temperature and the precipitate was collected by filtration and purified by recrystallization from ethanol. The single-crystal was grown from 1:1 mixture of acetone and toluene by slow evaporation method and yield of the compound was 68% (m.p.391–394 K). Analytical data: Found (Calculated): C %: 78.41 (78.47); H%: 7.18 (7.21); N%: 4.33 (4.36).

### S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.93–0.97 Å, and with $U_{iso}$(H) = 1.17–1.51$U_{eq}$(C).

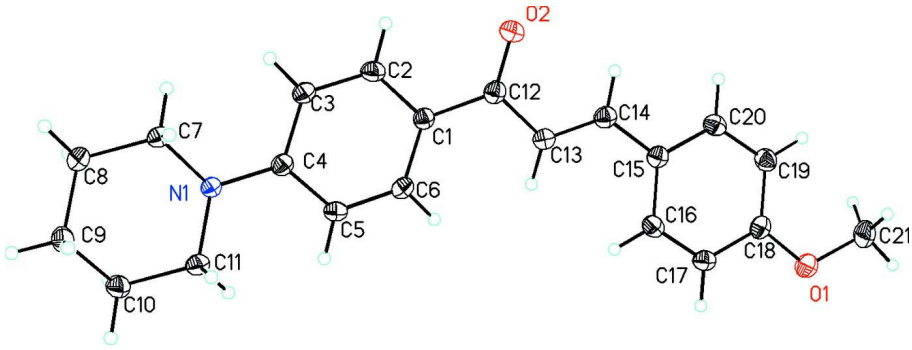


**Figure 1**

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

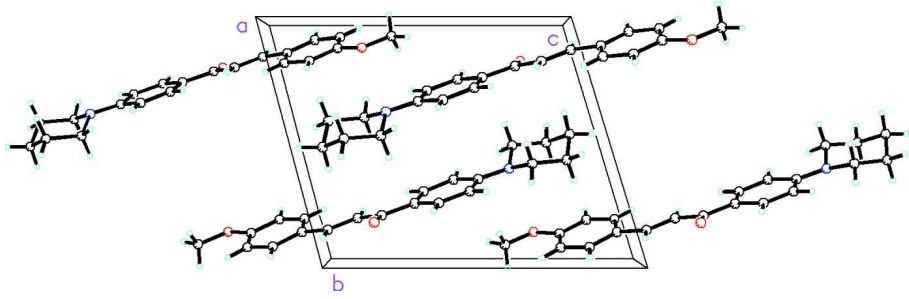


**Figure 2**

Packing of the title compound viewed along the *a* axis.

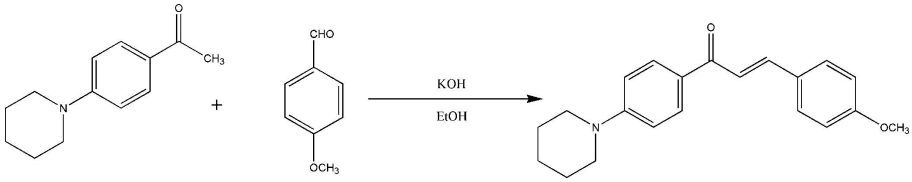


**Figure 3**

Reaction Scheme of $C_{21}H_{23}N_1O_2$,.

**(*E*)-3-(4-Methoxyphenyl)-1-[4-(piperidin-1-yl)phenyl]prop-2-en-1-one**

*Crystal data*

$C_{21}H_{23}NO_2$
$M_r = 321.40$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.0963$ (11) Å
$b = 10.985$ (2) Å
$c = 13.133$ (3) Å
$\alpha = 74.188$ (3)°
$\beta = 88.674$ (3)°
$\gamma = 77.393$ (3)°
$V = 825.2$ (3) Å$^3$
$Z = 2$
$F(000) = 344$
$D_x = 1.294$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1958 reflections
$\theta = 2.2$–30.9°
$\mu = 0.08$ mm$^{-1}$
$T = 100$ K
Block, red
0.47 × 0.36 × 0.21 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*APEX2*; Bruker, 2008)
$T_{min}$ = 0.962, $T_{max}$ = 0.983
10674 measured reflections
4861 independent reflections
3562 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 31.3°, $\theta_{min}$ = 1.6°
$h$ = −8→8
$k$ = −15→15
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.151
$S$ = 1.05
4861 reflections
218 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
$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.1716P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.23178 (16) | 0.88147 (10) | −0.30730 (7) | 0.0256 (2) |
| O2 | 1.10171 (16) | 0.82032 (10) | 0.20063 (7) | 0.0233 (2) |
| N1 | 0.76112 (17) | 0.61303 (11) | 0.66686 (8) | 0.0172 (2) |
| C1 | 0.8660 (2) | 0.75063 (12) | 0.33849 (9) | 0.0166 (2) |
| C2 | 1.0241 (2) | 0.74601 (13) | 0.41547 (10) | 0.0197 (3) |
| H2 | 1.1548 | 0.7748 | 0.3940 | 0.024* |
| C3 | 0.9928 (2) | 0.70016 (13) | 0.52239 (10) | 0.0201 (3) |
| H3 | 1.1021 | 0.6994 | 0.5710 | 0.024* |
| C4 | 0.7989 (2) | 0.65444 (12) | 0.55956 (9) | 0.0168 (2) |
| C5 | 0.6400 (2) | 0.65849 (13) | 0.48138 (10) | 0.0208 (3) |
| H5 | 0.5103 | 0.6282 | 0.5022 | 0.025* |
| C6 | 0.6729 (2) | 0.70647 (13) | 0.37468 (10) | 0.0199 (3) |
| H6 | 0.5630 | 0.7094 | 0.3256 | 0.024* |
| C7 | 0.9508 (2) | 0.59163 (14) | 0.74157 (10) | 0.0202 (3) |
| H7A | 1.0243 | 0.6641 | 0.7201 | 0.024* |
| H7B | 1.0594 | 0.5139 | 0.7385 | 0.024* |

| | | | | |
|---|---|---|---|---|
| C8 | 0.8785 (2) | 0.57739 (14) | 0.85498 (10) | 0.0210 (3) |
| H8A | 0.7896 | 0.6599 | 0.8606 | 0.025* |
| H8B | 1.0111 | 0.5548 | 0.9015 | 0.025* |
| C9 | 0.7413 (2) | 0.47408 (13) | 0.89082 (10) | 0.0204 (3) |
| H9A | 0.8332 | 0.3896 | 0.8921 | 0.025* |
| H9B | 0.6895 | 0.4714 | 0.9616 | 0.025* |
| C10 | 0.5413 (2) | 0.50756 (13) | 0.81348 (9) | 0.0194 (3) |
| H10A | 0.4555 | 0.4405 | 0.8336 | 0.023* |
| H10B | 0.4440 | 0.5888 | 0.8171 | 0.023* |
| C11 | 0.6156 (2) | 0.51976 (13) | 0.70057 (10) | 0.0187 (3) |
| H11B | 0.6961 | 0.4354 | 0.6951 | 0.022* |
| H11A | 0.4836 | 0.5471 | 0.6532 | 0.022* |
| C12 | 0.9153 (2) | 0.79733 (12) | 0.22544 (9) | 0.0174 (2) |
| C13 | 0.7416 (2) | 0.81181 (12) | 0.14373 (10) | 0.0182 (3) |
| H13 | 0.6061 | 0.7885 | 0.1641 | 0.022* |
| C14 | 0.7769 (2) | 0.85811 (12) | 0.04061 (10) | 0.0179 (3) |
| H14 | 0.9108 | 0.8853 | 0.0243 | 0.021* |
| C15 | 0.6283 (2) | 0.87041 (12) | −0.04869 (9) | 0.0174 (2) |
| C16 | 0.4309 (2) | 0.82206 (13) | −0.03711 (10) | 0.0195 (3) |
| H16 | 0.3856 | 0.7857 | 0.0304 | 0.023* |
| C17 | 0.3037 (2) | 0.82786 (13) | −0.12444 (10) | 0.0202 (3) |
| H17 | 0.1744 | 0.7948 | −0.1154 | 0.024* |
| C18 | 0.3679 (2) | 0.88308 (13) | −0.22624 (10) | 0.0198 (3) |
| C19 | 0.5590 (2) | 0.93488 (13) | −0.23992 (10) | 0.0210 (3) |
| H19 | 0.6008 | 0.9739 | −0.3074 | 0.025* |
| C20 | 0.6865 (2) | 0.92747 (12) | −0.15117 (10) | 0.0190 (3) |
| H20 | 0.8146 | 0.9616 | −0.1604 | 0.023* |
| C21 | 0.3004 (3) | 0.93119 (15) | −0.41233 (10) | 0.0265 (3) |
| H21A | 0.3054 | 1.0207 | −0.4238 | 0.040* |
| H21B | 0.1949 | 0.9240 | −0.4624 | 0.040* |
| H21C | 0.4470 | 0.8823 | −0.4214 | 0.040* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0261 (5) | 0.0332 (6) | 0.0188 (5) | −0.0104 (4) | −0.0024 (4) | −0.0061 (4) |
| O2 | 0.0210 (5) | 0.0296 (5) | 0.0216 (5) | −0.0118 (4) | 0.0029 (4) | −0.0060 (4) |
| N1 | 0.0154 (5) | 0.0228 (6) | 0.0143 (5) | −0.0079 (4) | −0.0008 (4) | −0.0038 (4) |
| C1 | 0.0178 (6) | 0.0159 (6) | 0.0169 (6) | −0.0039 (4) | 0.0006 (4) | −0.0054 (4) |
| C2 | 0.0153 (6) | 0.0257 (7) | 0.0190 (6) | −0.0080 (5) | 0.0009 (4) | −0.0047 (5) |
| C3 | 0.0164 (6) | 0.0268 (7) | 0.0173 (6) | −0.0080 (5) | −0.0019 (5) | −0.0036 (5) |
| C4 | 0.0157 (6) | 0.0182 (6) | 0.0166 (6) | −0.0035 (4) | −0.0005 (4) | −0.0050 (5) |
| C5 | 0.0161 (6) | 0.0295 (7) | 0.0192 (6) | −0.0103 (5) | 0.0014 (5) | −0.0065 (5) |
| C6 | 0.0186 (6) | 0.0262 (7) | 0.0168 (6) | −0.0085 (5) | −0.0009 (5) | −0.0064 (5) |
| C7 | 0.0172 (6) | 0.0281 (7) | 0.0171 (6) | −0.0097 (5) | −0.0012 (4) | −0.0054 (5) |
| C8 | 0.0211 (6) | 0.0274 (7) | 0.0167 (6) | −0.0094 (5) | −0.0003 (5) | −0.0066 (5) |
| C9 | 0.0206 (6) | 0.0244 (7) | 0.0154 (6) | −0.0059 (5) | 0.0011 (5) | −0.0032 (5) |
| C10 | 0.0167 (6) | 0.0240 (6) | 0.0174 (6) | −0.0068 (5) | 0.0010 (4) | −0.0034 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0166 (6) | 0.0222 (6) | 0.0183 (6) | −0.0072 (5) | −0.0004 (5) | −0.0048 (5) |
| C12 | 0.0201 (6) | 0.0161 (6) | 0.0163 (6) | −0.0044 (5) | 0.0000 (5) | −0.0047 (5) |
| C13 | 0.0180 (6) | 0.0190 (6) | 0.0183 (6) | −0.0054 (5) | 0.0003 (5) | −0.0052 (5) |
| C14 | 0.0177 (6) | 0.0179 (6) | 0.0185 (6) | −0.0039 (5) | 0.0002 (5) | −0.0057 (5) |
| C15 | 0.0187 (6) | 0.0154 (6) | 0.0182 (6) | −0.0036 (4) | 0.0007 (4) | −0.0048 (5) |
| C16 | 0.0201 (6) | 0.0204 (6) | 0.0177 (6) | −0.0057 (5) | 0.0031 (5) | −0.0039 (5) |
| C17 | 0.0175 (6) | 0.0213 (6) | 0.0224 (6) | −0.0058 (5) | 0.0015 (5) | −0.0057 (5) |
| C18 | 0.0201 (6) | 0.0210 (6) | 0.0182 (6) | −0.0031 (5) | −0.0016 (5) | −0.0062 (5) |
| C19 | 0.0226 (6) | 0.0219 (6) | 0.0177 (6) | −0.0064 (5) | 0.0012 (5) | −0.0029 (5) |
| C20 | 0.0188 (6) | 0.0181 (6) | 0.0197 (6) | −0.0052 (5) | 0.0020 (5) | −0.0038 (5) |
| C21 | 0.0305 (8) | 0.0312 (8) | 0.0177 (6) | −0.0068 (6) | −0.0013 (5) | −0.0063 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C18 | 1.3711 (15) | C9—H9B | 0.9700 |
| O1—C21 | 1.4277 (16) | C10—C11 | 1.5194 (17) |
| O2—C12 | 1.2346 (15) | C10—H10A | 0.9700 |
| N1—C4 | 1.3882 (16) | C10—H10B | 0.9700 |
| N1—C7 | 1.4706 (15) | C11—H11B | 0.9700 |
| N1—C11 | 1.4713 (16) | C11—H11A | 0.9700 |
| C1—C6 | 1.3942 (17) | C12—C13 | 1.4779 (17) |
| C1—C2 | 1.3963 (16) | C13—C14 | 1.3408 (17) |
| C1—C12 | 1.4797 (17) | C13—H13 | 0.9300 |
| C2—C3 | 1.3806 (17) | C14—C15 | 1.4575 (17) |
| C2—H2 | 0.9300 | C14—H14 | 0.9300 |
| C3—C4 | 1.4097 (17) | C15—C20 | 1.3948 (17) |
| C3—H3 | 0.9300 | C15—C16 | 1.4071 (17) |
| C4—C5 | 1.4130 (16) | C16—C17 | 1.3785 (17) |
| C5—C6 | 1.3830 (17) | C16—H16 | 0.9300 |
| C5—H5 | 0.9300 | C17—C18 | 1.3949 (18) |
| C6—H6 | 0.9300 | C17—H17 | 0.9300 |
| C7—C8 | 1.5197 (17) | C18—C19 | 1.3920 (18) |
| C7—H7A | 0.9700 | C19—C20 | 1.3897 (17) |
| C7—H7B | 0.9700 | C19—H19 | 0.9300 |
| C8—C9 | 1.5212 (18) | C20—H20 | 0.9300 |
| C8—H8A | 0.9700 | C21—H21A | 0.9600 |
| C8—H8B | 0.9700 | C21—H21B | 0.9600 |
| C9—C10 | 1.5207 (17) | C21—H21C | 0.9600 |
| C9—H9A | 0.9700 | | |

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| C18—O1—C21 | 116.56 (10) | C11—C10—H10B | 109.3 |
| C4—N1—C7 | 117.45 (10) | C9—C10—H10B | 109.3 |
| C4—N1—C11 | 117.85 (10) | H10A—C10—H10B | 108.0 |
| C7—N1—C11 | 113.84 (10) | N1—C11—C10 | 112.56 (10) |
| C6—C1—C2 | 116.73 (11) | N1—C11—H11B | 109.1 |
| C6—C1—C12 | 124.41 (11) | C10—C11—H11B | 109.1 |
| C2—C1—C12 | 118.84 (11) | N1—C11—H11A | 109.1 |
| C3—C2—C1 | 122.16 (11) | C10—C11—H11A | 109.1 |

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| C3—C2—H2 | 118.9 | H11B—C11—H11A | 107.8 |
| C1—C2—H2 | 118.9 | O2—C12—C13 | 121.02 (11) |
| C2—C3—C4 | 121.43 (11) | O2—C12—C1 | 119.88 (11) |
| C2—C3—H3 | 119.3 | C13—C12—C1 | 119.07 (11) |
| C4—C3—H3 | 119.3 | C14—C13—C12 | 120.87 (12) |
| N1—C4—C3 | 121.98 (11) | C14—C13—H13 | 119.6 |
| N1—C4—C5 | 121.74 (11) | C12—C13—H13 | 119.6 |
| C3—C4—C5 | 116.22 (11) | C13—C14—C15 | 127.06 (12) |
| C6—C5—C4 | 121.47 (12) | C13—C14—H14 | 116.5 |
| C6—C5—H5 | 119.3 | C15—C14—H14 | 116.5 |
| C4—C5—H5 | 119.3 | C20—C15—C16 | 117.66 (11) |
| C5—C6—C1 | 121.97 (11) | C20—C15—C14 | 119.35 (11) |
| C5—C6—H6 | 119.0 | C16—C15—C14 | 122.93 (11) |
| C1—C6—H6 | 119.0 | C17—C16—C15 | 120.88 (12) |
| N1—C7—C8 | 112.76 (10) | C17—C16—H16 | 119.6 |
| N1—C7—H7A | 109.0 | C15—C16—H16 | 119.6 |
| C8—C7—H7A | 109.0 | C16—C17—C18 | 120.37 (12) |
| N1—C7—H7B | 109.0 | C16—C17—H17 | 119.8 |
| C8—C7—H7B | 109.0 | C18—C17—H17 | 119.8 |
| H7A—C7—H7B | 107.8 | O1—C18—C19 | 124.56 (12) |
| C7—C8—C9 | 112.12 (10) | O1—C18—C17 | 115.48 (11) |
| C7—C8—H8A | 109.2 | C19—C18—C17 | 119.96 (11) |
| C9—C8—H8A | 109.2 | C20—C19—C18 | 119.01 (12) |
| C7—C8—H8B | 109.2 | C20—C19—H19 | 120.5 |
| C9—C8—H8B | 109.2 | C18—C19—H19 | 120.5 |
| H8A—C8—H8B | 107.9 | C19—C20—C15 | 122.08 (12) |
| C10—C9—C8 | 108.32 (10) | C19—C20—H20 | 119.0 |
| C10—C9—H9A | 110.0 | C15—C20—H20 | 119.0 |
| C8—C9—H9A | 110.0 | O1—C21—H21A | 109.5 |
| C10—C9—H9B | 110.0 | O1—C21—H21B | 109.5 |
| C8—C9—H9B | 110.0 | H21A—C21—H21B | 109.5 |
| H9A—C9—H9B | 108.4 | O1—C21—H21C | 109.5 |
| C11—C10—C9 | 111.56 (10) | H21A—C21—H21C | 109.5 |
| C11—C10—H10A | 109.3 | H21B—C21—H21C | 109.5 |
| C9—C10—H10A | 109.3 | | |

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| C6—C1—C2—C3 | 0.01 (19) | C6—C1—C12—O2 | −171.55 (13) |
| C12—C1—C2—C3 | −178.13 (12) | C2—C1—C12—O2 | 6.44 (18) |
| C1—C2—C3—C4 | 0.5 (2) | C6—C1—C12—C13 | 6.57 (19) |
| C7—N1—C4—C3 | −12.83 (18) | C2—C1—C12—C13 | −175.44 (11) |
| C11—N1—C4—C3 | −154.97 (12) | O2—C12—C13—C14 | −4.24 (19) |
| C7—N1—C4—C5 | 170.04 (11) | C1—C12—C13—C14 | 177.66 (11) |
| C11—N1—C4—C5 | 27.90 (18) | C12—C13—C14—C15 | 176.00 (11) |
| C2—C3—C4—N1 | −177.33 (12) | C13—C14—C15—C20 | 176.56 (12) |
| C2—C3—C4—C5 | −0.05 (19) | C13—C14—C15—C16 | −6.3 (2) |
| N1—C4—C5—C6 | 176.42 (12) | C20—C15—C16—C17 | 1.80 (19) |
| C3—C4—C5—C6 | −0.9 (2) | C14—C15—C16—C17 | −175.43 (12) |
| C4—C5—C6—C1 | 1.4 (2) | C15—C16—C17—C18 | −0.6 (2) |

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| C2—C1—C6—C5 | −0.95 (19) | C21—O1—C18—C19 | 3.18 (19) |
| C12—C1—C6—C5 | 177.09 (12) | C21—O1—C18—C17 | −176.80 (11) |
| C4—N1—C7—C8 | 166.66 (11) | C16—C17—C18—O1 | 178.77 (11) |
| C11—N1—C7—C8 | −49.73 (15) | C16—C17—C18—C19 | −1.2 (2) |
| N1—C7—C8—C9 | 53.10 (15) | O1—C18—C19—C20 | −178.31 (12) |
| C7—C8—C9—C10 | −55.90 (15) | C17—C18—C19—C20 | 1.7 (2) |
| C8—C9—C10—C11 | 56.61 (14) | C18—C19—C20—C15 | −0.4 (2) |
| C4—N1—C11—C10 | −165.90 (11) | C16—C15—C20—C19 | −1.33 (19) |
| C7—N1—C11—C10 | 50.64 (15) | C14—C15—C20—C19 | 176.00 (12) |
| C9—C10—C11—N1 | −54.75 (15) | | |

*Hydrogen-bond geometry (Å, º)*

Cg2 and Cg3 are the centroids of the C1–C6 and C15–C20 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C20—H20···O2$^{i}$ | 0.93 | 2.47 | 3.2105 (16) | 137 |
| C8—H8*A*···*Cg*3$^{ii}$ | 0.97 | 2.66 | 3.623 (2) | 171 |
| C21—H21*A*···*Cg*2$^{iii}$ | 0.96 | 2.90 | 3.823 (2) | 162 |

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