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2-(4-Methoxyphenyl)-4-oxo-4-phenylbutanenitrile

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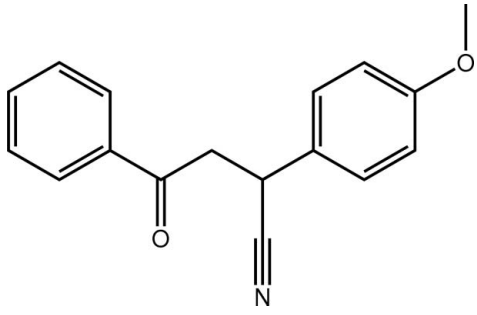
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 15.3.

The title molecule, $C_{17}H_{15}NO_2$, is twisted, the dihedral angle between the terminal benzene rings being 63.30 (6)°. In the crystal, C—H···O and C—H···N interactions lead to supramolecular layers in the *ab* plane. These are connected along the *c* axis *via* C—H···π interactions.

Related literature

For background to the synthetic applications of 2,4-diaryl-4-oxo-butanenitriles, see: Coudert *et al.* (1990), 1988); Iida *et al.* (2007). For the preparation of the title compound, see: Coudert *et al.* (1990). For the structure of the unsubstituted parent compound, see: Abdel-Aziz *et al.* (2012).



Experimental

Crystal data

$C_{17}H_{15}NO_2$
M_r = 265.30
Orthorhombic, *Pbca*
a = 9.5730 (2) Å
b = 8.7748 (2) Å
c = 32.0620 (7) Å
V = 2693.25 (10) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 100 K
0.30 × 0.30 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.651, T_{max} = 1.000
6569 measured reflections
2764 independent reflections
2410 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.02
2764 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

Cg is the centroid of the C11–C16 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8b···O1^{i}	0.99	2.44	3.3102 (16)	147
C15—H15···N1^{ii}	0.95	2.62	3.4250 (17)	143
C4—H4···*Cg*^{iii}	0.95	2.82	3.5787 (14)	138
C17—H17c···*Cg*^{iv}	0.98	2.89	3.6754 (15)	138

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5470).

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supplementary materials

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2-(4-Methoxyphenyl)-4-oxo-4-phenylbutanenitrile

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Comment

An important class of difunctional intermediates for both the synthesis of biologically active heterocycles, such as pyridazine derivatives, and as a source ketone (Coudert *et al.*, 1990; Coudert *et al.*, 1988; Iida *et al.*, 2007) are the 2,4-diaryl-4-oxo-butanenitriles. Herein, the crystal structure of a 2,4-diaryl-4-oxo-butanenitrile derivative, 4-(4-methoxyphenyl)-4-oxo-2-phenylbutanenitrile (I), is described. The structure of the parent compound is known (Abdel-Aziz *et al.*, 2012).

In (I), Fig. 1, the terminal benzene rings form a dihedral angle of 63.30 (6)° indicating a considerable twist in the molecule. The benzyl group is twisted out of the plane of the benzene ring to which it is connected [the C2—C1—C7—C8 torsion angle is -8.58 (17)°] and in addition there is a twist around the C8—C9 bond [the C7—C8—C9—C11 torsion angle is 173.19 (10)°]. The methoxy group is co-planar with the benzene ring to which it is connected [the C17—O2—C14—C13 torsion angle is 3.03 (17)°].

In the crystal packing, molecules are linked by C—H···O and C—H···N interactions into supramolecular layers in the *ab* plane, Fig. 2 and Table 1. Layers are connected along the *c* axis *via* C—H···π interactions involving the (C11–C16) ring, Fig. 3 and Table 1.

Experimental

Acetone cyanohydrin (0.045 mol) and 10% aqueous sodium carbonate (0.0015 mol and 1.5 ml water) were added to solution of 3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (0.015 mol) in ethanol (50 ml). The mixture was heated at reflux temperature for 4 h. After cooling, the product which separated out was filtered off and recrystallized from methanol solution.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 1.00 Å, U_{iso}(H) = 1.2–1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

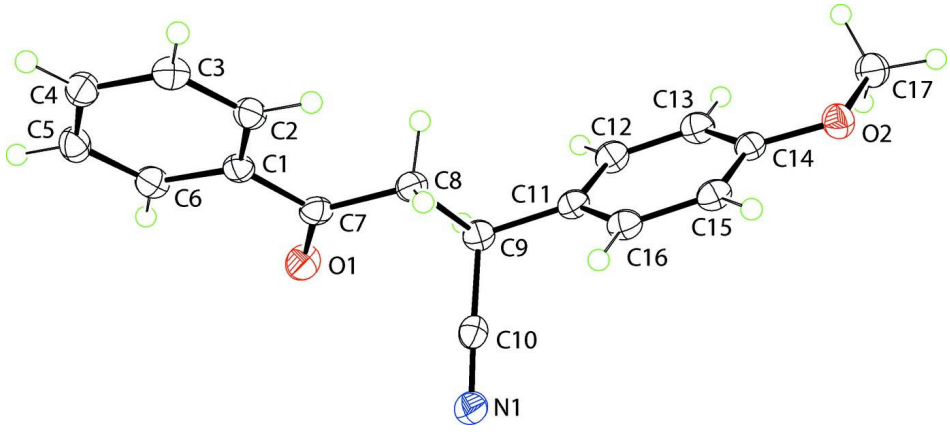

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

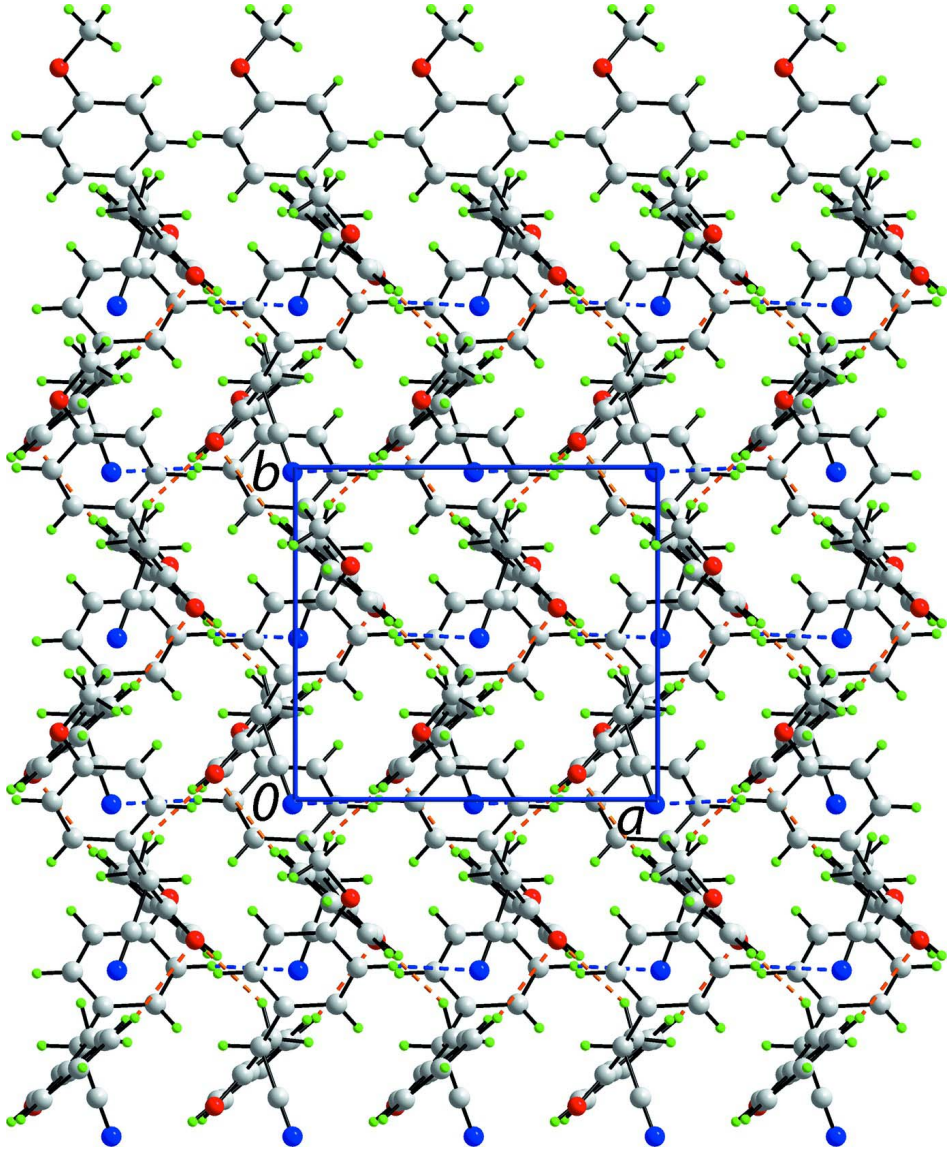

Figure 2

A view of the supramolecular array in the *ab* plane in (I). The C—H···O and C—H···N interactions are shown as orange and blue dashed lines, respectively.

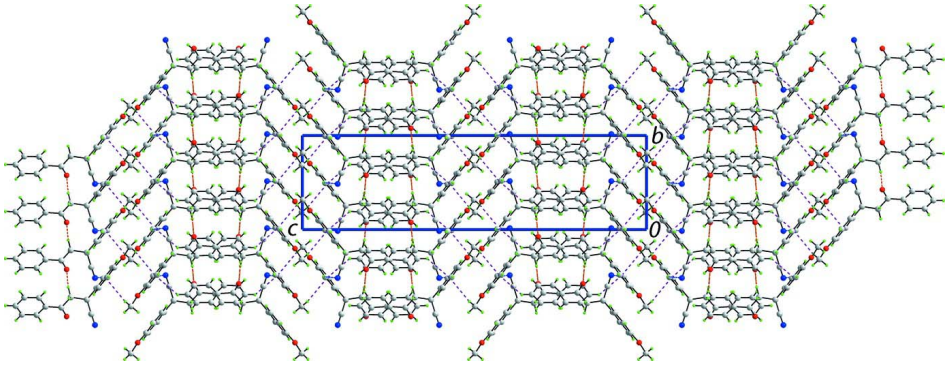

Figure 3

A view in projection down the *a* axis of the unit-cell contents for (I). The C—H···O, C—H···N and C—H···π interactions are shown as orange, blue and purple dashed lines, respectively.

2-(4-Methoxyphenyl)-4-oxo-4-phenylbutanenitrile

Crystal data

$C_{17}H_{15}NO_2$
$M_r = 265.30$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 9.5730\ (2)$ Å
$b = 8.7748\ (2)$ Å
$c = 32.0620\ (7)$ Å
$V = 2693.25\ (10)$ Å^3
$Z = 8$
$F(000) = 1120$
$D_x = 1.309$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 2587 reflections
$\theta = 2.8$–$76.0°$
$\mu = 0.69$ mm^{-1}
$T = 100$ K
Prism, colourless
0.30 × 0.30 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.651$, $T_{max} = 1.000$
6569 measured reflections
2764 independent reflections
2410 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 76.2°$, $\theta_{min} = 2.8°$
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 10$
$l = -33 \rightarrow 39$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.101$
$S = 1.02$
2764 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.8432P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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	0.27711 (10)	0.07603 (11)	0.68494 (3)	0.0294 (2)
O2	0.65190 (10)	0.70231 (10)	0.52150 (3)	0.0267 (2)
N1	0.49228 (12)	−0.01483 (13)	0.60258 (3)	0.0282 (3)
C1	0.37272 (13)	0.18133 (13)	0.74651 (4)	0.0214 (3)
C2	0.47344 (13)	0.27465 (14)	0.76484 (4)	0.0235 (3)
H2	0.5322	0.3358	0.7478	0.028*
C3	0.48802 (14)	0.27836 (15)	0.80803 (4)	0.0261 (3)
H3	0.5570	0.3418	0.8204	0.031*
C4	0.40215 (14)	0.18967 (15)	0.83309 (4)	0.0262 (3)
H4	0.4124	0.1922	0.8625	0.031*
C5	0.30090 (14)	0.09693 (15)	0.81498 (4)	0.0268 (3)
H5	0.2420	0.0364	0.8321	0.032*
C6	0.28593 (13)	0.09281 (15)	0.77198 (4)	0.0244 (3)
H6	0.2165	0.0297	0.7598	0.029*
C7	0.35473 (13)	0.17095 (14)	0.70034 (4)	0.0225 (3)
C8	0.43447 (13)	0.28103 (14)	0.67269 (4)	0.0231 (3)
H8A	0.5359	0.2687	0.6777	0.028*
H8B	0.4086	0.3868	0.6802	0.028*
C9	0.40397 (13)	0.25499 (14)	0.62604 (4)	0.0228 (3)
H9	0.3005	0.2589	0.6220	0.027*
C10	0.45287 (13)	0.10206 (15)	0.61327 (4)	0.0230 (3)
C11	0.46935 (13)	0.37597 (14)	0.59828 (4)	0.0222 (3)
C12	0.38502 (13)	0.48068 (15)	0.57791 (4)	0.0251 (3)
H12	0.2867	0.4759	0.5816	0.030*
C13	0.44116 (14)	0.59264 (15)	0.55215 (4)	0.0252 (3)
H13	0.3818	0.6640	0.5386	0.030*
C14	0.58517 (14)	0.59909 (14)	0.54638 (4)	0.0219 (3)
C15	0.67095 (13)	0.49409 (14)	0.56660 (4)	0.0230 (3)
H15	0.7693	0.4985	0.5628	0.028*
C16	0.61369 (13)	0.38362 (14)	0.59212 (4)	0.0233 (3)
H16	0.6730	0.3122	0.6056	0.028*
C17	0.56675 (16)	0.81515 (16)	0.50178 (4)	0.0293 (3)
H17A	0.6249	0.8788	0.4836	0.044*
H17B	0.5226	0.8790	0.5231	0.044*
H17C	0.4944	0.7650	0.4851	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0261 (5)	0.0329 (5)	0.0292 (5)	−0.0061 (4)	0.0019 (4)	−0.0041 (4)
O2	0.0286 (5)	0.0262 (5)	0.0254 (4)	0.0001 (4)	0.0000 (4)	0.0033 (4)
N1	0.0313 (6)	0.0268 (6)	0.0264 (5)	−0.0021 (5)	0.0035 (5)	−0.0028 (4)
C1	0.0201 (6)	0.0188 (6)	0.0252 (6)	0.0040 (5)	0.0029 (5)	0.0002 (4)
C2	0.0228 (6)	0.0201 (6)	0.0276 (6)	0.0005 (5)	0.0042 (5)	0.0007 (5)
C3	0.0250 (6)	0.0240 (6)	0.0294 (6)	0.0010 (5)	−0.0003 (5)	−0.0027 (5)
C4	0.0283 (6)	0.0264 (7)	0.0239 (6)	0.0055 (5)	0.0015 (5)	0.0021 (5)
C5	0.0247 (6)	0.0264 (6)	0.0294 (6)	0.0027 (5)	0.0066 (5)	0.0053 (5)
C6	0.0203 (6)	0.0220 (6)	0.0309 (6)	0.0003 (5)	0.0023 (5)	0.0004 (5)
C7	0.0188 (5)	0.0213 (6)	0.0274 (6)	0.0032 (5)	0.0024 (5)	−0.0028 (5)
C8	0.0235 (6)	0.0227 (6)	0.0232 (6)	0.0008 (5)	0.0013 (5)	−0.0022 (5)
C9	0.0204 (6)	0.0239 (6)	0.0241 (6)	0.0012 (5)	−0.0005 (5)	−0.0009 (5)
C10	0.0227 (6)	0.0268 (7)	0.0197 (5)	−0.0034 (5)	0.0005 (5)	−0.0003 (5)
C11	0.0234 (6)	0.0236 (6)	0.0197 (5)	0.0014 (5)	−0.0005 (5)	−0.0029 (5)
C12	0.0202 (6)	0.0281 (7)	0.0269 (6)	0.0029 (5)	−0.0003 (5)	−0.0013 (5)
C13	0.0255 (6)	0.0255 (6)	0.0246 (6)	0.0048 (5)	−0.0035 (5)	0.0000 (5)
C14	0.0263 (6)	0.0208 (6)	0.0186 (5)	−0.0005 (5)	−0.0001 (5)	−0.0028 (4)
C15	0.0193 (6)	0.0260 (6)	0.0237 (6)	0.0015 (5)	−0.0010 (5)	−0.0041 (5)
C16	0.0235 (6)	0.0238 (6)	0.0225 (6)	0.0043 (5)	−0.0032 (5)	−0.0023 (5)
C17	0.0375 (7)	0.0271 (7)	0.0233 (6)	0.0032 (6)	−0.0012 (5)	0.0035 (5)

Geometric parameters (Å, º)

O1—C7	1.2205 (15)	C8—H8A	0.9900
O2—C14	1.3656 (15)	C8—H8B	0.9900
O2—C17	1.4299 (15)	C9—C10	1.4791 (17)
N1—C10	1.1454 (17)	C9—C11	1.5201 (17)
C1—C2	1.3949 (17)	C9—H9	1.0000
C1—C6	1.4002 (17)	C11—C12	1.3865 (17)
C1—C7	1.4931 (17)	C11—C16	1.3975 (18)
C2—C3	1.3921 (18)	C12—C13	1.3915 (18)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.3881 (18)	C13—C14	1.3920 (18)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.3924 (19)	C14—C15	1.3941 (17)
C4—H4	0.9500	C15—C16	1.3818 (18)
C5—C6	1.3865 (18)	C15—H15	0.9500
C5—H5	0.9500	C16—H16	0.9500
C6—H6	0.9500	C17—H17A	0.9800
C7—C8	1.5172 (17)	C17—H17B	0.9800
C8—C9	1.5409 (16)	C17—H17C	0.9800
C14—O2—C17	116.80 (10)	C11—C9—C8	112.75 (10)
C2—C1—C6	119.34 (11)	C10—C9—H9	108.0
C2—C1—C7	122.23 (11)	C11—C9—H9	108.0
C6—C1—C7	118.43 (11)	C8—C9—H9	108.0
C3—C2—C1	120.14 (12)	N1—C10—C9	178.38 (13)

C3—C2—H2	119.9	C12—C11—C16	118.50 (12)
C1—C2—H2	119.9	C12—C11—C9	119.93 (11)
C4—C3—C2	120.21 (12)	C16—C11—C9	121.57 (11)
C4—C3—H3	119.9	C11—C12—C13	121.51 (12)
C2—C3—H3	119.9	C11—C12—H12	119.2
C3—C4—C5	119.91 (12)	C13—C12—H12	119.2
C3—C4—H4	120.0	C14—C13—C12	119.34 (12)
C5—C4—H4	120.0	C14—C13—H13	120.3
C6—C5—C4	120.12 (12)	C12—C13—H13	120.3
C6—C5—H5	119.9	O2—C14—C13	124.60 (11)
C4—C5—H5	119.9	O2—C14—C15	115.75 (11)
C5—C6—C1	120.28 (12)	C13—C14—C15	119.65 (12)
C5—C6—H6	119.9	C16—C15—C14	120.35 (12)
C1—C6—H6	119.9	C16—C15—H15	119.8
O1—C7—C1	120.86 (11)	C14—C15—H15	119.8
O1—C7—C8	120.30 (11)	C15—C16—C11	120.64 (12)
C1—C7—C8	118.85 (11)	C15—C16—H16	119.7
C7—C8—C9	112.17 (10)	C11—C16—H16	119.7
C7—C8—H8A	109.2	O2—C17—H17A	109.5
C9—C8—H8A	109.2	O2—C17—H17B	109.5
C7—C8—H8B	109.2	H17A—C17—H17B	109.5
C9—C8—H8B	109.2	O2—C17—H17C	109.5
H8A—C8—H8B	107.9	H17A—C17—H17C	109.5
C10—C9—C11	109.95 (10)	H17B—C17—H17C	109.5
C10—C9—C8	110.08 (10)		

C6—C1—C2—C3	0.58 (18)	C10—C9—C11—C12	126.52 (12)
C7—C1—C2—C3	−178.79 (11)	C8—C9—C11—C12	−110.23 (13)
C1—C2—C3—C4	−0.23 (19)	C10—C9—C11—C16	−52.54 (15)
C2—C3—C4—C5	−0.13 (19)	C8—C9—C11—C16	70.70 (15)
C3—C4—C5—C6	0.13 (19)	C16—C11—C12—C13	−0.69 (18)
C4—C5—C6—C1	0.23 (19)	C9—C11—C12—C13	−179.78 (11)
C2—C1—C6—C5	−0.58 (18)	C11—C12—C13—C14	0.55 (19)
C7—C1—C6—C5	178.81 (11)	C17—O2—C14—C13	3.03 (17)
C2—C1—C7—O1	171.59 (11)	C17—O2—C14—C15	−177.49 (10)
C6—C1—C7—O1	−7.78 (17)	C12—C13—C14—O2	179.13 (11)
C2—C1—C7—C8	−8.58 (17)	C12—C13—C14—C15	−0.33 (18)
C6—C1—C7—C8	172.05 (11)	O2—C14—C15—C16	−179.24 (10)
O1—C7—C8—C9	−0.11 (16)	C13—C14—C15—C16	0.27 (18)
C1—C7—C8—C9	−179.94 (10)	C14—C15—C16—C11	−0.42 (18)
C7—C8—C9—C10	−63.64 (13)	C12—C11—C16—C15	0.62 (18)
C7—C8—C9—C11	173.19 (10)	C9—C11—C16—C15	179.70 (11)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8b···O1^{i}	0.99	2.44	3.3102 (16)	147
C15—H15···N1^{ii}	0.95	2.62	3.4250 (17)	143

C4—H4···Cg^{iii}	0.95	2.82	3.5787 (14)	138
C17—H17c···Cg^{iv}	0.98	2.89	3.6754 (15)	138

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