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## 2-(3-Methoxyphenoxy)pyrimidine

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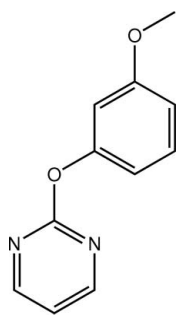
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  
 $R$  factor = 0.032;  $wR$  factor = 0.086; data-to-parameter ratio = 8.4.

In the title compound,  $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2$ , the benzene ring faces towards one of the pyrimidine N atoms, and is almost orthogonal to the plane through the pyrimidine ring [dihedral angle =  $84.40(14)^\circ$ ]. In the crystal, the presence of  $\text{C}-\text{H}\cdots\pi$  and  $\pi-\pi$  [centroid-centroid separation =  $3.7658(18)$  Å] interactions leads to a supramolecular array in the  $ac$  plane. The layers thus formed interdigitate along the  $b$  axis.

## Related literature

For background to the fluorescence properties of compounds related to the title compound, see: Kawai *et al.* (2001); Abdullah (2005).



## Experimental

## Crystal data

 $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2$   
 $M_r = 202.21$   
 Monoclinic,  $Cc$ 
 $a = 8.8120(16)$  Å  
 $b = 18.215(3)$  Å  
 $c = 7.2094(10)$  Å

 $\beta = 119.380(2)^\circ$   
 $V = 1008.4(3)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation

 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.40 \times 0.30 \times 0.08$  mm

## Data collection

 Bruker SMART APEX CCD  
 diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.889$ ,  $T_{\max} = 1.000$ 

 4725 measured reflections  
 1165 independent reflections  
 897 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.033$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.086$   
 $S = 1.02$   
 1165 reflections  
 138 parameters

 2 restraints  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.10$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.10$  e Å<sup>-3</sup>  
 Absolute structure: nd

Table 1

Hydrogen-bond geometry (Å, °).

 $Cg_2$  is the centroid of the C5–C10 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C4-H4\cdots Cg_2^i$	0.93	2.89	3.710 (4)	148

 Symmetry code: (i)  $x - 1, -y, z - \frac{1}{2}$ .

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; 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: HB5584).

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## supporting information

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## 2-(3-Methoxyphenoxy)pyrimidine

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### S1. Comment

Interest in the title compound stems from interesting fluorescence properties of related compounds (Kawai *et al.* 2001; Abdullah, 2005). In (I), the least-squares plane through the pyrimidine ring bisects the plane through the benzene ring with the C5 and C8 atoms of the latter lying in the plane; the dihedral angle between the planes is 84.40 (14) °. The benzene ring lies to one side of the pyrimidine ring, being proximate to the N1 atom. The methoxy group is almost coplanar with the benzene ring to which is bonded as seen in the value of the C11–O2–C7–C6 torsion angle of 171.7 (2) °.

In the crystal, the presence of C–H··· $\pi$  interactions, formed between pyrimidine-H atoms and benzene rings, and  $\pi$ – $\pi$  interactions [centroid-centroid separation = 3.7658 (18) Å], formed between pyrimidine rings, leads to the formation of layers in the *ac* plane, Fig. 2 and Table 1. Layers comprise alternating rows of pyrimidine and benzene molecules, and interdigitate along the *b* axis as shown in Fig. 3.

### S2. Experimental

3-Methoxyphenol (2.2 ml, 20 mmol) was mixed with sodium hydroxide (0.8 g, 20 mmol) in several drops of water. The water was then evaporated. The paste was heated with 2-chloropyrimidine (2.3 g, 20 mmol) at 423–433 K for 5 h. The product was dissolved in water and the solution extracted with chloroform. The chloroform phase was dried over sodium sulfate; the evaporation of the solvent gave well shaped colourless prisms of (I).

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 to 0.96 Å) and were included in the refinement in the riding model approximation, with  $U_{\text{iso}}(\text{H})$  set to 1.2 to 1.5 $U_{\text{equiv}}(\text{C})$ . In the absence of significant anomalous scattering effects, 985 Friedel pairs were averaged in the final refinement.

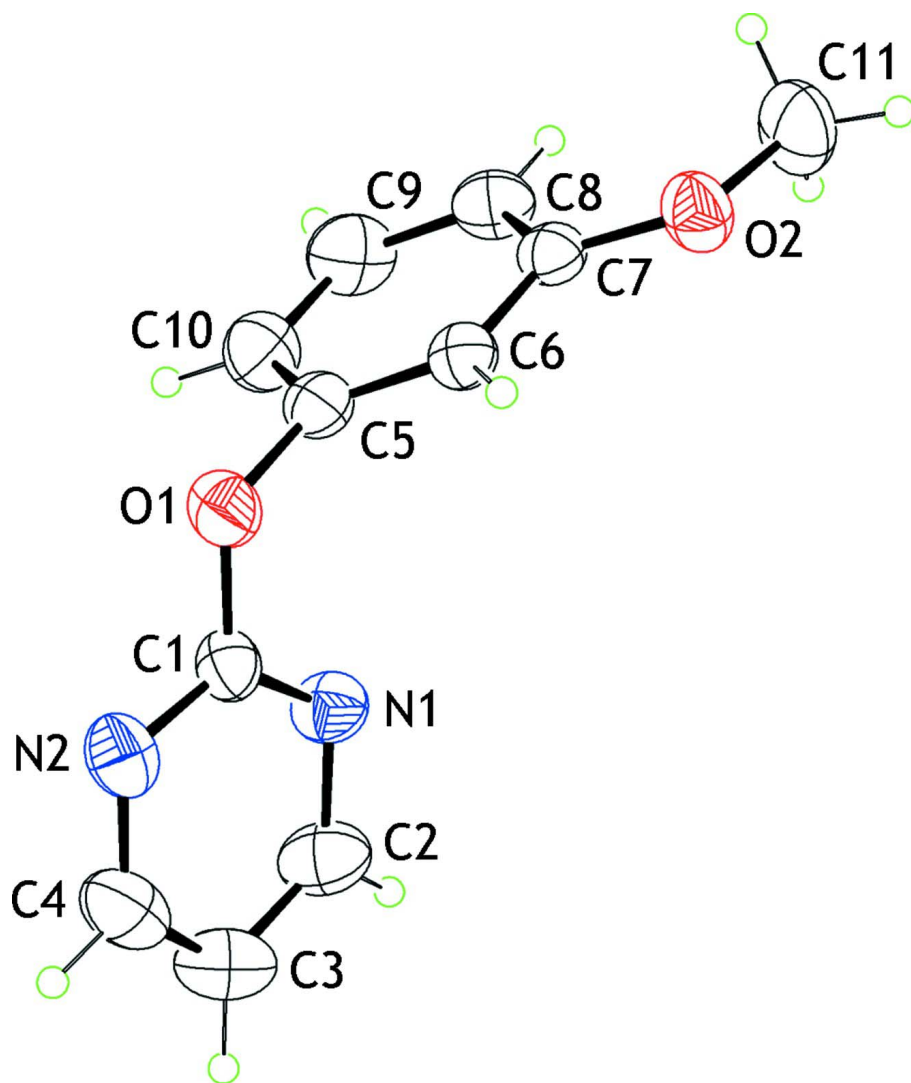
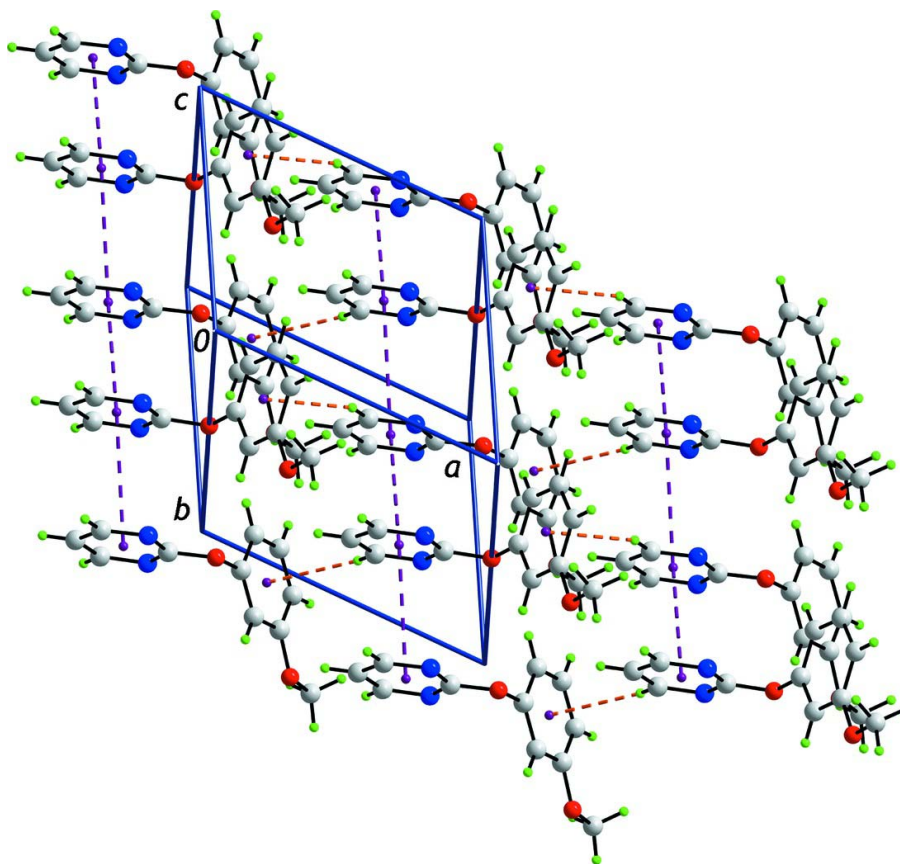


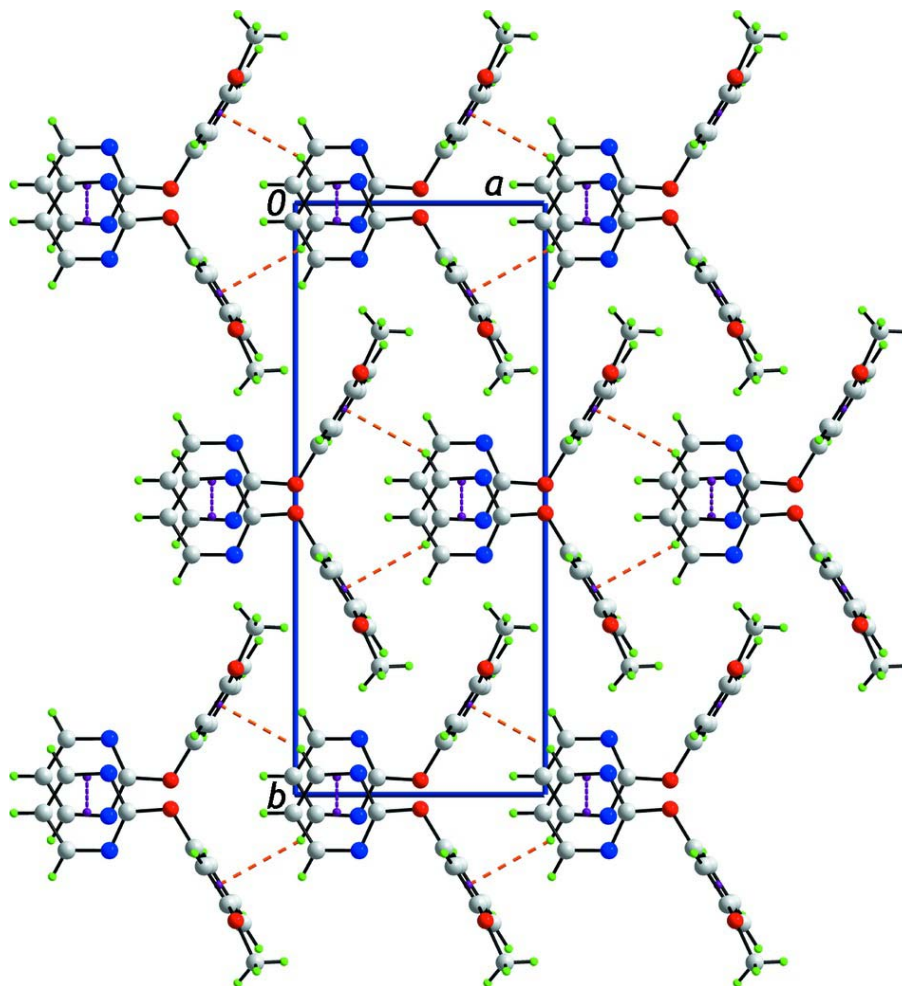
Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 35% probability level.



**Figure 2**

Supramolecular layer in (I) mediated by C-H... $\pi$  and  $\pi$ - $\pi$  interactions, shown as orange and purple dashed lines, respectively.



**Figure 3**

Unit-cell contents shown in projection down the  $c$  axis in (I), highlighting the stacking of layers. The C–H $\cdots$  $\pi$  and  $\pi$ – $\pi$  interactions are shown as orange and purple dashed lines, respectively.

### 2-(3-Methoxyphenoxy)pyrimidine

#### Crystal data

$C_{11}H_{10}N_2O_2$

$M_r = 202.21$

Monoclinic,  $Cc$

Hall symbol:  $C -2yc$

$a = 8.8120$  (16) Å

$b = 18.215$  (3) Å

$c = 7.2094$  (10) Å

$\beta = 119.380$  (2)°

$V = 1008.4$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 424$

$D_x = 1.332$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1361 reflections

$\theta = 2.2$ – $21.9$ °

$\mu = 0.09$  mm<sup>-1</sup>

$T = 293$  K

Prism, colourless

$0.40 \times 0.30 \times 0.08$  mm

*Data collection*

Bruker SMART APEX CCD diffractometer	4725 measured reflections
Radiation source: fine-focus sealed tube	1165 independent reflections
Graphite monochromator	897 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.033$
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	$\theta_{\text{max}} = 27.5^\circ$ , $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.889$ , $T_{\text{max}} = 1.000$	$h = -11 \rightarrow 11$
	$k = -23 \rightarrow 23$
	$l = -9 \rightarrow 9$

*Refinement*

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.0614P]$
$wR(F^2) = 0.086$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1165 reflections	$\Delta\rho_{\text{max}} = 0.10 \text{ e } \text{\AA}^{-3}$
138 parameters	$\Delta\rho_{\text{min}} = -0.10 \text{ e } \text{\AA}^{-3}$
2 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.016 (3)
Secondary atom site location: difference Fourier map	Absolute structure: nd

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.5000 (2)	0.02433 (8)	0.5000 (3)	0.0629 (5)
O2	0.7604 (2)	0.21319 (8)	0.3071 (3)	0.0628 (5)
N1	0.2553 (3)	0.09456 (10)	0.4018 (3)	0.0595 (5)
N2	0.2520 (3)	-0.03621 (10)	0.4056 (4)	0.0655 (6)
C1	0.3265 (3)	0.02912 (11)	0.4325 (4)	0.0510 (5)
C2	0.0840 (4)	0.09409 (16)	0.3359 (5)	0.0756 (8)
H2	0.0262	0.1387	0.3129	0.091*
C3	-0.0084 (4)	0.03096 (19)	0.3015 (5)	0.0828 (9)
H3	-0.1272	0.0314	0.2555	0.099*
C4	0.0819 (4)	-0.03306 (17)	0.3379 (5)	0.0789 (8)
H4	0.0213	-0.0770	0.3141	0.095*
C5	0.5948 (3)	0.09030 (11)	0.5548 (4)	0.0531 (6)
C6	0.6335 (3)	0.12134 (10)	0.4098 (4)	0.0484 (5)
H6	0.5954	0.0995	0.2776	0.058*
C7	0.7304 (3)	0.18570 (11)	0.4623 (3)	0.0488 (5)

C8	0.7882 (3)	0.21731 (13)	0.6603 (4)	0.0624 (6)
H8	0.8527	0.2605	0.6970	0.075*
C9	0.7481 (4)	0.18335 (17)	0.8027 (4)	0.0771 (8)
H9	0.7870	0.2045	0.9359	0.093*
C10	0.6533 (3)	0.11978 (16)	0.7543 (4)	0.0697 (7)
H10	0.6292	0.0973	0.8529	0.084*
C11	0.8382 (4)	0.28395 (15)	0.3411 (5)	0.0868 (9)
H11A	0.8443	0.2986	0.2169	0.130*
H11B	0.9535	0.2823	0.4615	0.130*
H11C	0.7692	0.3187	0.3676	0.130*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0614 (11)	0.0435 (8)	0.0919 (13)	0.0088 (7)	0.0438 (11)	0.0096 (8)
O2	0.0722 (11)	0.0520 (9)	0.0643 (10)	-0.0123 (8)	0.0335 (8)	-0.0019 (8)
N1	0.0551 (11)	0.0530 (11)	0.0691 (12)	0.0075 (9)	0.0294 (10)	-0.0016 (10)
N2	0.0773 (15)	0.0501 (12)	0.0735 (14)	-0.0070 (10)	0.0403 (12)	-0.0005 (10)
C1	0.0553 (14)	0.0481 (12)	0.0565 (14)	0.0034 (10)	0.0329 (12)	0.0045 (10)
C2	0.0570 (16)	0.0763 (17)	0.087 (2)	0.0111 (14)	0.0299 (15)	-0.0078 (15)
C3	0.0562 (17)	0.101 (2)	0.087 (2)	-0.0074 (16)	0.0322 (15)	-0.0199 (17)
C4	0.076 (2)	0.0799 (19)	0.084 (2)	-0.0262 (17)	0.0412 (16)	-0.0136 (15)
C5	0.0468 (12)	0.0451 (12)	0.0666 (14)	0.0094 (9)	0.0273 (11)	0.0057 (10)
C6	0.0480 (12)	0.0415 (10)	0.0535 (12)	0.0036 (9)	0.0231 (10)	-0.0013 (9)
C7	0.0427 (11)	0.0464 (10)	0.0546 (13)	0.0040 (9)	0.0219 (10)	0.0008 (10)
C8	0.0555 (13)	0.0619 (13)	0.0614 (15)	-0.0069 (11)	0.0223 (12)	-0.0156 (12)
C9	0.0779 (19)	0.097 (2)	0.0549 (15)	-0.0069 (16)	0.0315 (14)	-0.0186 (15)
C10	0.0733 (17)	0.0811 (18)	0.0651 (17)	0.0059 (14)	0.0419 (14)	0.0032 (14)
C11	0.103 (2)	0.0589 (16)	0.088 (2)	-0.0223 (14)	0.0389 (19)	0.0037 (14)

*Geometric parameters (Å, °)*

O1—C1	1.361 (3)	C5—C6	1.372 (3)
O1—C5	1.405 (3)	C5—C10	1.377 (3)
O2—C7	1.365 (3)	C6—C7	1.389 (3)
O2—C11	1.424 (3)	C6—H6	0.9300
N1—C1	1.314 (3)	C7—C8	1.384 (3)
N1—C2	1.342 (3)	C8—C9	1.384 (4)
N2—C1	1.327 (3)	C8—H8	0.9300
N2—C4	1.330 (4)	C9—C10	1.369 (4)
C2—C3	1.360 (4)	C9—H9	0.9300
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.363 (4)	C11—H11A	0.9600
C3—H3	0.9300	C11—H11B	0.9600
C4—H4	0.9300	C11—H11C	0.9600
C1—O1—C5	117.01 (16)	C5—C6—H6	120.3
C7—O2—C11	117.50 (19)	C7—C6—H6	120.3

C1—N1—C2	114.5 (2)	O2—C7—C8	124.9 (2)
C1—N2—C4	113.7 (2)	O2—C7—C6	115.23 (18)
N1—C1—N2	128.9 (2)	C8—C7—C6	119.9 (2)
N1—C1—O1	118.57 (19)	C7—C8—C9	118.7 (2)
N2—C1—O1	112.54 (19)	C7—C8—H8	120.7
N1—C2—C3	122.6 (3)	C9—C8—H8	120.7
N1—C2—H2	118.7	C10—C9—C8	122.4 (3)
C3—C2—H2	118.7	C10—C9—H9	118.8
C2—C3—C4	116.6 (3)	C8—C9—H9	118.8
C2—C3—H3	121.7	C9—C10—C5	117.7 (2)
C4—C3—H3	121.7	C9—C10—H10	121.2
N2—C4—C3	123.6 (3)	C5—C10—H10	121.2
N2—C4—H4	118.2	O2—C11—H11A	109.5
C3—C4—H4	118.2	O2—C11—H11B	109.5
C6—C5—C10	122.0 (2)	H11A—C11—H11B	109.5
C6—C5—O1	118.3 (2)	O2—C11—H11C	109.5
C10—C5—O1	119.6 (2)	H11A—C11—H11C	109.5
C5—C6—C7	119.3 (2)	H11B—C11—H11C	109.5
C2—N1—C1—N2	0.6 (4)	C10—C5—C6—C7	-2.0 (3)
C2—N1—C1—O1	-179.8 (2)	O1—C5—C6—C7	-178.59 (19)
C4—N2—C1—N1	0.1 (4)	C11—O2—C7—C8	-8.0 (3)
C4—N2—C1—O1	-179.5 (2)	C11—O2—C7—C6	171.7 (2)
C5—O1—C1—N1	6.9 (3)	C5—C6—C7—O2	-179.02 (19)
C5—O1—C1—N2	-173.5 (2)	C5—C6—C7—C8	0.7 (3)
C1—N1—C2—C3	-0.7 (4)	O2—C7—C8—C9	180.0 (2)
N1—C2—C3—C4	0.2 (5)	C6—C7—C8—C9	0.3 (3)
C1—N2—C4—C3	-0.8 (4)	C7—C8—C9—C10	-0.1 (4)
C2—C3—C4—N2	0.6 (5)	C8—C9—C10—C5	-1.1 (4)
C1—O1—C5—C6	-100.4 (2)	C6—C5—C10—C9	2.1 (4)
C1—O1—C5—C10	82.8 (3)	O1—C5—C10—C9	178.7 (2)

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

Cg2 is the centroid of the C5—C10 ring.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C4—H4 $\cdots$ Cg2 <sup>i</sup>	0.93	2.89	3.710 (4)	148

Symmetry code: (i)  $x-1, -y, z-1/2$ .