



## Crystal structure of (4*E*)-4-(8-methoxy-2*H*-chromen-2-ylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

Muhammad Salim,<sup>a</sup> Munawar Ali Munawar,<sup>a</sup>  
Muhammad Nawaz Tahir,<sup>b\*</sup> Muhammad Shahid<sup>a</sup> and  
Khizar Iqbal Malik<sup>a</sup>

<sup>a</sup>Department of Chemistry, University of the Punjab, Lahore, Punjab, Pakistan, and

<sup>b</sup>Department of Physics, University of Sargodha, Sargodha, Punjab, Pakistan.

\*Correspondence e-mail: dmntahir\_uos@yahoo.com

Received 6 May 2015; accepted 18 May 2015

Edited by W. Imhof, University Koblenz-Landau, Germany

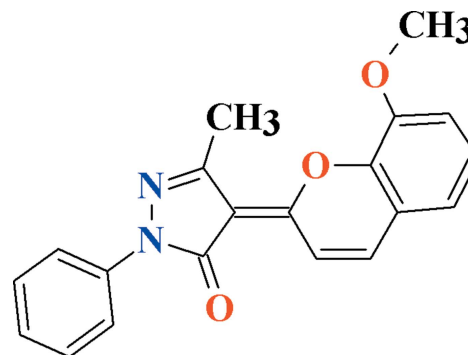
In the title compound, C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>, the phenyl substituent attached to the pyrazole ring makes a dihedral angle of 4.87 (7)° with the rest of the molecule. In the crystal, molecules are connected into inversion dimers of the R<sub>2</sub><sup>2</sup>(14) type by pairs of C—H···O interactions. π–π interactions exist between the benzene and pyrazole rings at a distance of 3.701 (1) Å. Similarly, π–π interactions are present at a centroid–centroid distance of 3.601 (1) Å between the oxygen-containing heterocyclic ring and methoxy substituted aromatic ring of a neighbouring molecule. Additional C—H···π and C=O···π interactions are also observed.

**Keywords:** crystal structure; pyrazolone; π–π interactions.

**CCDC reference:** 1401584

### 1. Related literature

For related structures, see: Chaudhry *et al.* (2012); Holzer *et al.* (1999); Malik *et al.* (2009).



### 2. Experimental

#### 2.1. Crystal data

C <sub>20</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	<i>V</i> = 3157.7 (10) Å <sup>3</sup>
<i>M<sub>r</sub></i> = 332.35	<i>Z</i> = 8
Monoclinic, <i>C</i> 2/ <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 28.179 (5) Å	<i>μ</i> = 0.10 mm <sup>-1</sup>
<i>b</i> = 4.7108 (8) Å	<i>T</i> = 296 K
<i>c</i> = 23.819 (5) Å	0.40 × 0.22 × 0.18 mm
<i>β</i> = 92.957 (7)°	

#### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer	13056 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	3419 independent reflections
<i>T</i> <sub>min</sub> = 0.961, <i>T</i> <sub>max</sub> = 0.985	2389 reflections with <i>I</i> > 2σ( <i>I</i> )
	<i>R</i> <sub>int</sub> = 0.033

#### 2.3. Refinement

<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.042	229 parameters
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.127	H-atom parameters constrained
<i>S</i> = 1.06	Δ <i>ρ</i> <sub>max</sub> = 0.22 e Å <sup>-3</sup>
3419 reflections	Δ <i>ρ</i> <sub>min</sub> = -0.16 e Å <sup>-3</sup>

**Table 1**

Hydrogen-bond geometry and C—H···π and C=O···π interactions (Å, °).

Cg1 and Cg2 are the centroids of the N1/N2/C7–C9 and C11–C14/C19/O2 rings, respectively.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C6—H6···O1	0.93	2.28	2.911 (2)	124
C12—H12···O1	0.93	2.38	3.004 (2)	124
C13—H13···O1 <sup>i</sup>	0.93	2.53	3.2577 (19)	136
C10—H10A···Cg1 <sup>ii</sup>	0.96	2.79	3.6812 (17)	155
C7—O1···Cg2 <sup>iii</sup>	1.23 (1)	3.65 (1)	3.9797 (18)	96 (1)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

### Acknowledgements

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: IM2465).

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## supporting information

*Acta Cryst.* (2015). E71, o414–o415 [doi:10.1107/S2056989015009445]

## Crystal structure of (4E)-4-(8-methoxy-2H-chromen-2-ylidene)-3-methyl-1-phenyl-1H-pyrazol-5(4H)-one

Muhammad Salim, Munawar Ali Munawar, Muhammad Nawaz Tahir, Muhammad Shahid and Khizar Iqbal Malik

### S1. Comment

The crystal structures of 5-methyl-2-phenyl-4-((E)-3-phenyl-2-hydroxy-prop-2-enylidene)-1,2-dihydro-3H-pyrazol-3-one (Holzer *et al.*, 1999), (4Z)-4-((2E)-1-hydroxy-3-(4-methoxyphenyl)prop-2-en-1-ylidene)-3-methyl-1-phenyl-1H-pyrazol-5(4H)-one (Malik *et al.*, 2009) and (4Z)-4-((2E)-1-hydroxy-3-(3-nitrophenyl)prop-2-en-1-ylidene)-3-methyl-1-(4-methylphenyl)-1H-pyrazol-5(4H)-one (Chaudhry, *et al.*, 2012) have been published which are related to the title compound (I, Fig. 1). No crystal structure has been found containing a 8-methoxy-2H-chromene subunit. (I) is synthesized for the biological studies *etc.*

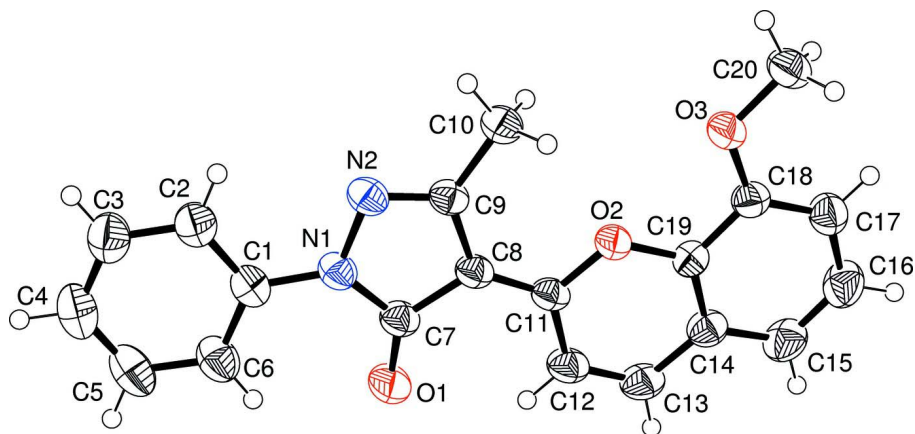
In (I), the benzene ring A (C1–C6) and the (4E)-4-(8-methoxy-2H-chromen-2-ylidene)-5-methyl-2,4-dihydro-3H-pyrazol-3-one (C7–C20/N1/N2/O1/O2/O3) part of the molecule are planar with r. m. s. deviations of 0.0053 and 0.0108 Å, respectively. The dihedral angle between A/B is 4.87 (7)°. The molecules are dimerized due to C—H···O interactions completing  $R_2^2$  (14) Motifs. Molecules are connected to inversion dimers dimerized of the  $R_2^2$  (14) type by C—H···O interactions. There exist  $\pi$ – $\pi$  interactions at a distance of 3.7011 (12) Å between the centeroids of Cg1—Cg3<sup>i</sup> and Cg3—Cg1<sup>ii</sup> [*i* = *x*, -1 + *y*, *z* and *ii* = *x*, 1 + *y*, *z*], where Cg1 and Cg3 are the centeroids of heterocyclic ring C (N1/N2/C7/C8/C9) and benzene ring A, respectively. Similarly, there exist  $\pi$ – $\pi$  interaction at a distance of 3.6012 (11) Å between the centeroids of Cg2—Cg4<sup>ii</sup> and Cg4—Cg2<sup>i</sup> [*i* = *x*, -1 + *y*, *z* and *ii* = *x*, 1 + *y*, *z*], where Cg2 and Cg4 are the centeroids of heterocyclic ring D (C11—C14/C19/O2) and methoxy containing benzene ring E (C14—C19), respectively. There exist C—H··· $\pi$  and C=O··· $\pi$  interactions (Table 1).

### S2. Experimental

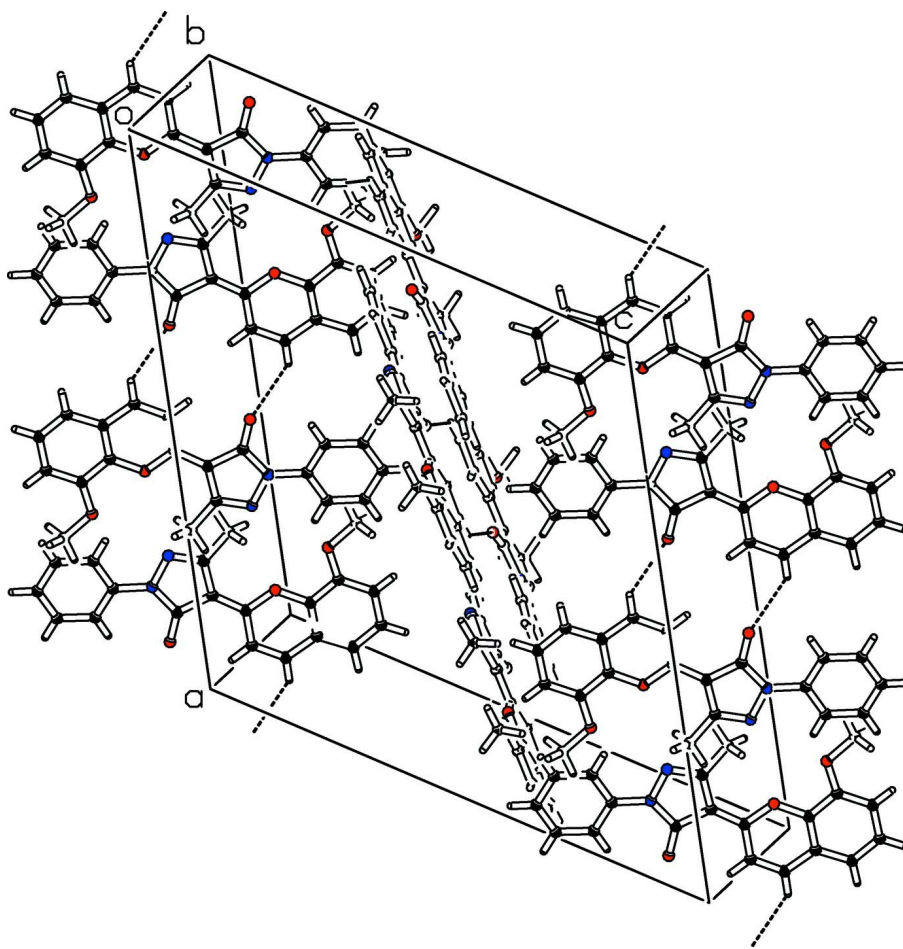
For the preparation of title compound (I), a mixture of 4-acetyl-3-methyl-1-phenyl-5-hydroxy pyrazole (0.218 g, 1 mmol), 2-methoxybenzaldehyde (0.205 g, 1.5 mmol) was refluxed for 8 h in glacial acetic acid (15 ml) and concentrated sulfuric acid (0.2 ml). The reaction mixture was diluted with distilled water (60 ml). The precipitate was filtered, washed with methanol and dried. The crude product was purified by column chromatography using n-hexane and ethyl acetate mixtures as eluents. The product was recrystallized using n-hexane to afford red needles (yield = 63%, m.p. 503 K)

### S3. Refinement

H-atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with  $U_{iso}(H) = xU_{eq}(C, O)$ , where *x* = 1.5 for methyl and *x* = 1.2 for aromatic H-atoms.

**Figure 1**

View of the title compound with the atom numbering scheme. Thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii.

**Figure 2**

Partial packing (*PLATON*; Spek, 2009) which shows that molecules are dimerized due to C—H...O bondings.

**(4E)-4-(8-Methoxy-2H-chromen-2-ylidene)-3-methyl-1-phenyl-1H-pyrazol-5(4H)-one***Crystal data*C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub> $M_r = 332.35$ Monoclinic, *C2/c* $a = 28.179$  (5) Å $b = 4.7108$  (8) Å $c = 23.819$  (5) Å $\beta = 92.957$  (7)° $V = 3157.7$  (10) Å<sup>3</sup> $Z = 8$  $F(000) = 1392$  $D_x = 1.398$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2389 reflections

 $\theta = 2.9$ – $27.0$ ° $\mu = 0.10$  mm<sup>-1</sup> $T = 296$  K

Needle, red

 $0.40 \times 0.22 \times 0.18$  mm*Data collection*Bruker Kappa APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 7.70 pixels mm<sup>-1</sup> $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2005)

 $T_{\min} = 0.961$ ,  $T_{\max} = 0.985$ 

13056 measured reflections

3419 independent reflections

2389 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.033$  $\theta_{\max} = 27.0$ °,  $\theta_{\min} = 2.9$ ° $h = -35 \rightarrow 35$  $k = -6 \rightarrow 5$  $l = -24 \rightarrow 30$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.042$  $wR(F^2) = 0.127$  $S = 1.06$ 

3419 reflections

229 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.6123P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.22$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.16$  e Å<sup>-3</sup>Extinction correction: *SHELXL2014* (Sheldrick,  
2015),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ 

Extinction coefficient: 0.0021 (4)

*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<sup>2</sup>)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.06562 (4)	1.0410 (2)	0.06364 (5)	0.0601 (4)
O2	0.11680 (3)	0.3975 (2)	-0.05229 (4)	0.0405 (3)
O3	0.16619 (4)	0.0352 (2)	-0.10799 (5)	0.0504 (3)

N1	0.14466 (4)	0.9876 (2)	0.09568 (5)	0.0407 (3)
N2	0.18451 (4)	0.8288 (2)	0.08158 (6)	0.0417 (3)
C1	0.14967 (6)	1.1800 (3)	0.14142 (6)	0.0410 (4)
C2	0.19424 (6)	1.2193 (3)	0.16813 (7)	0.0501 (4)
H2	0.2202	1.1180	0.1563	0.060*
C3	0.19992 (7)	1.4086 (4)	0.21225 (8)	0.0575 (5)
H3	0.2298	1.4329	0.2301	0.069*
C4	0.16197 (8)	1.5617 (4)	0.23019 (8)	0.0593 (5)
H4	0.1661	1.6913	0.2595	0.071*
C5	0.11808 (7)	1.5206 (4)	0.20427 (8)	0.0619 (5)
H5	0.0923	1.6222	0.2164	0.074*
C6	0.11134 (7)	1.3295 (3)	0.16006 (7)	0.0541 (5)
H6	0.0812	1.3025	0.1431	0.065*
C7	0.10494 (5)	0.9304 (3)	0.06052 (7)	0.0410 (4)
C8	0.12183 (5)	0.7169 (3)	0.02175 (6)	0.0372 (4)
C9	0.17098 (5)	0.6713 (3)	0.03861 (7)	0.0370 (4)
C10	0.20563 (5)	0.4738 (3)	0.01377 (7)	0.0451 (4)
H10A	0.1932	0.2840	0.0139	0.068*
H10B	0.2352	0.4800	0.0356	0.068*
H10C	0.2108	0.5304	-0.0242	0.068*
C11	0.09468 (5)	0.5939 (3)	-0.02107 (6)	0.0368 (4)
C12	0.04599 (5)	0.6554 (3)	-0.03528 (7)	0.0455 (4)
H12	0.0304	0.7917	-0.0149	0.055*
C13	0.02230 (6)	0.5199 (3)	-0.07759 (7)	0.0492 (4)
H13	-0.0096	0.5601	-0.0856	0.059*
C14	0.04580 (5)	0.3138 (3)	-0.11063 (7)	0.0435 (4)
C15	0.02414 (6)	0.1660 (4)	-0.15629 (8)	0.0562 (5)
H15	-0.0078	0.1959	-0.1664	0.067*
C16	0.05019 (7)	-0.0228 (4)	-0.18596 (8)	0.0583 (5)
H16	0.0357	-0.1184	-0.2164	0.070*
C17	0.09766 (6)	-0.0735 (3)	-0.17137 (7)	0.0490 (4)
H17	0.1146	-0.2024	-0.1921	0.059*
C18	0.12003 (5)	0.0664 (3)	-0.12619 (7)	0.0404 (4)
C19	0.09317 (5)	0.2600 (3)	-0.09639 (6)	0.0373 (4)
C20	0.19362 (6)	-0.1685 (4)	-0.13639 (8)	0.0533 (5)
H20A	0.1797	-0.3531	-0.1328	0.080*
H20B	0.2255	-0.1704	-0.1201	0.080*
H20C	0.1942	-0.1191	-0.1754	0.080*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0403 (7)	0.0647 (7)	0.0753 (9)	0.0165 (6)	0.0028 (6)	-0.0223 (7)
O2	0.0332 (6)	0.0421 (5)	0.0463 (7)	0.0051 (4)	0.0011 (5)	-0.0075 (5)
O3	0.0370 (6)	0.0583 (7)	0.0556 (7)	0.0076 (5)	0.0004 (5)	-0.0180 (6)
N1	0.0402 (7)	0.0393 (6)	0.0429 (8)	0.0073 (5)	0.0044 (6)	-0.0023 (6)
N2	0.0404 (8)	0.0400 (6)	0.0450 (8)	0.0098 (5)	0.0040 (6)	0.0006 (6)
C1	0.0522 (10)	0.0341 (7)	0.0372 (9)	0.0036 (6)	0.0069 (7)	0.0040 (7)

C2	0.0550 (11)	0.0476 (9)	0.0477 (10)	-0.0008 (7)	0.0044 (8)	-0.0021 (8)
C3	0.0697 (13)	0.0533 (10)	0.0496 (11)	-0.0105 (9)	0.0030 (9)	-0.0022 (9)
C4	0.0898 (16)	0.0451 (9)	0.0432 (11)	-0.0025 (9)	0.0052 (10)	-0.0037 (8)
C5	0.0816 (15)	0.0547 (10)	0.0501 (11)	0.0199 (9)	0.0104 (10)	-0.0039 (9)
C6	0.0592 (11)	0.0539 (9)	0.0491 (11)	0.0147 (8)	0.0022 (9)	-0.0044 (9)
C7	0.0380 (9)	0.0383 (7)	0.0472 (10)	0.0053 (6)	0.0059 (7)	0.0001 (7)
C8	0.0347 (8)	0.0346 (7)	0.0427 (9)	0.0040 (6)	0.0070 (7)	0.0010 (7)
C9	0.0369 (8)	0.0331 (7)	0.0413 (9)	0.0045 (6)	0.0063 (7)	0.0037 (7)
C10	0.0390 (9)	0.0433 (8)	0.0531 (10)	0.0080 (6)	0.0040 (7)	-0.0034 (7)
C11	0.0342 (8)	0.0340 (7)	0.0430 (9)	0.0046 (6)	0.0084 (7)	0.0028 (7)
C12	0.0368 (9)	0.0446 (8)	0.0554 (11)	0.0090 (7)	0.0066 (8)	0.0007 (8)
C13	0.0324 (9)	0.0537 (9)	0.0609 (11)	0.0080 (7)	-0.0020 (8)	0.0042 (8)
C14	0.0364 (9)	0.0443 (8)	0.0493 (10)	0.0028 (6)	-0.0020 (7)	0.0039 (7)
C15	0.0417 (10)	0.0619 (10)	0.0634 (12)	0.0029 (8)	-0.0131 (9)	0.0000 (9)
C16	0.0561 (11)	0.0632 (11)	0.0541 (12)	-0.0012 (9)	-0.0139 (9)	-0.0080 (9)
C17	0.0504 (10)	0.0507 (9)	0.0457 (10)	0.0016 (7)	0.0004 (8)	-0.0065 (8)
C18	0.0358 (9)	0.0419 (8)	0.0434 (9)	0.0002 (6)	0.0017 (7)	0.0006 (7)
C19	0.0366 (8)	0.0362 (7)	0.0388 (9)	-0.0014 (6)	0.0000 (7)	0.0013 (7)
C20	0.0453 (10)	0.0585 (10)	0.0565 (11)	0.0111 (8)	0.0060 (8)	-0.0096 (9)

*Geometric parameters (Å, °)*

O1—C7	1.2299 (17)	C8—C9	1.438 (2)
O2—C11	1.3584 (17)	C9—C10	1.4931 (19)
O2—C19	1.3766 (17)	C10—H10A	0.9600
O3—C18	1.3578 (18)	C10—H10B	0.9600
O3—C20	1.4244 (18)	C10—H10C	0.9600
N1—C7	1.389 (2)	C11—C12	1.426 (2)
N1—N2	1.4046 (16)	C12—C13	1.341 (2)
N1—C1	1.419 (2)	C12—H12	0.9300
N2—C9	1.3048 (19)	C13—C14	1.433 (2)
C1—C6	1.382 (2)	C13—H13	0.9300
C1—C2	1.390 (2)	C14—C19	1.384 (2)
C2—C3	1.381 (2)	C14—C15	1.404 (2)
C2—H2	0.9300	C15—C16	1.372 (2)
C3—C4	1.376 (3)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.385 (2)
C4—C5	1.367 (3)	C16—H16	0.9300
C4—H4	0.9300	C17—C18	1.385 (2)
C5—C6	1.391 (2)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.401 (2)
C6—H6	0.9300	C20—H20A	0.9600
C7—C8	1.462 (2)	C20—H20B	0.9600
C8—C11	1.371 (2)	C20—H20C	0.9600
C11—O2—C19	121.38 (11)	C9—C10—H10C	109.5
C18—O3—C20	117.11 (12)	H10A—C10—H10C	109.5
C7—N1—N2	112.43 (12)	H10B—C10—H10C	109.5

C7—N1—C1	129.21 (13)	O2—C11—C8	116.14 (13)
N2—N1—C1	118.35 (12)	O2—C11—C12	118.14 (14)
C9—N2—N1	106.59 (12)	C8—C11—C12	125.72 (14)
C6—C1—C2	119.19 (15)	C13—C12—C11	121.15 (15)
C6—C1—N1	121.59 (15)	C13—C12—H12	119.4
C2—C1—N1	119.22 (14)	C11—C12—H12	119.4
C3—C2—C1	120.04 (16)	C12—C13—C14	120.59 (14)
C3—C2—H2	120.0	C12—C13—H13	119.7
C1—C2—H2	120.0	C14—C13—H13	119.7
C4—C3—C2	120.87 (18)	C19—C14—C15	118.31 (15)
C4—C3—H3	119.6	C19—C14—C13	117.17 (14)
C2—C3—H3	119.6	C15—C14—C13	124.52 (15)
C5—C4—C3	118.99 (17)	C16—C15—C14	119.84 (16)
C5—C4—H4	120.5	C16—C15—H15	120.1
C3—C4—H4	120.5	C14—C15—H15	120.1
C4—C5—C6	121.25 (18)	C15—C16—C17	121.19 (16)
C4—C5—H5	119.4	C15—C16—H16	119.4
C6—C5—H5	119.4	C17—C16—H16	119.4
C1—C6—C5	119.64 (18)	C16—C17—C18	120.50 (16)
C1—C6—H6	120.2	C16—C17—H17	119.7
C5—C6—H6	120.2	C18—C17—H17	119.7
O1—C7—N1	125.57 (15)	O3—C18—C17	125.90 (14)
O1—C7—C8	130.78 (15)	O3—C18—C19	116.25 (13)
N1—C7—C8	103.65 (12)	C17—C18—C19	117.84 (14)
C11—C8—C9	129.57 (13)	O2—C19—C14	121.56 (13)
C11—C8—C7	124.98 (13)	O2—C19—C18	116.12 (13)
C9—C8—C7	105.45 (13)	C14—C19—C18	122.31 (14)
N2—C9—C8	111.87 (13)	O3—C20—H20A	109.5
N2—C9—C10	119.63 (13)	O3—C20—H20B	109.5
C8—C9—C10	128.50 (14)	H20A—C20—H20B	109.5
C9—C10—H10A	109.5	O3—C20—H20C	109.5
C9—C10—H10B	109.5	H20A—C20—H20C	109.5
H10A—C10—H10B	109.5	H20B—C20—H20C	109.5
C7—N1—N2—C9	-0.36 (16)	C19—O2—C11—C12	-0.2 (2)
C1—N1—N2—C9	-179.67 (12)	C9—C8—C11—O2	0.7 (2)
C7—N1—C1—C6	5.1 (2)	C7—C8—C11—O2	-179.45 (13)
N2—N1—C1—C6	-175.68 (14)	C9—C8—C11—C12	-179.11 (15)
C7—N1—C1—C2	-174.84 (15)	C7—C8—C11—C12	0.8 (2)
N2—N1—C1—C2	4.3 (2)	O2—C11—C12—C13	1.2 (2)
C6—C1—C2—C3	-0.8 (2)	C8—C11—C12—C13	-179.03 (15)
N1—C1—C2—C3	179.12 (14)	C11—C12—C13—C14	-1.5 (2)
C1—C2—C3—C4	-0.4 (3)	C12—C13—C14—C19	0.8 (2)
C2—C3—C4—C5	1.1 (3)	C12—C13—C14—C15	-178.71 (16)
C3—C4—C5—C6	-0.6 (3)	C19—C14—C15—C16	-1.0 (3)
C2—C1—C6—C5	1.4 (2)	C13—C14—C15—C16	178.53 (16)
N1—C1—C6—C5	-178.61 (14)	C14—C15—C16—C17	0.7 (3)
C4—C5—C6—C1	-0.7 (3)	C15—C16—C17—C18	0.0 (3)



N2—N1—C7—O1	-179.78 (15)	C20—O3—C18—C17	-2.8 (2)
C1—N1—C7—O1	-0.6 (3)	C20—O3—C18—C19	177.68 (14)
N2—N1—C7—C8	0.35 (16)	C16—C17—C18—O3	-179.84 (15)
C1—N1—C7—C8	179.58 (13)	C16—C17—C18—C19	-0.3 (2)
O1—C7—C8—C11	0.0 (3)	C11—O2—C19—C14	-0.5 (2)
N1—C7—C8—C11	179.86 (14)	C11—O2—C19—C18	178.69 (12)
O1—C7—C8—C9	179.92 (17)	C15—C14—C19—O2	179.76 (14)
N1—C7—C8—C9	-0.22 (15)	C13—C14—C19—O2	0.2 (2)
N1—N2—C9—C8	0.20 (16)	C15—C14—C19—C18	0.6 (2)
N1—N2—C9—C10	-179.44 (12)	C13—C14—C19—C18	-178.94 (14)
C11—C8—C9—N2	179.93 (14)	O3—C18—C19—O2	0.4 (2)
C7—C8—C9—N2	0.02 (17)	C17—C18—C19—O2	-179.14 (13)
C11—C8—C9—C10	-0.5 (3)	O3—C18—C19—C14	179.59 (14)
C7—C8—C9—C10	179.61 (14)	C17—C18—C19—C14	0.0 (2)
C19—O2—C11—C8	-179.97 (12)		

*Hydrogen-bond geometry (Å, °)*

Cg1 and Cg2 are the centroids of the N1/N2/C7—C9 and C11—C14/C19/O2 rings, respectively.

<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>
C6—H6 $\cdots$ O1	0.93	2.28	2.911 (2)	124
C12—H12 $\cdots$ O1	0.93	2.38	3.004 (2)	124
C13—H13 $\cdots$ O1 <sup>i</sup>	0.93	2.53	3.2577 (19)	136
C10—H10 <i>A</i> $\cdots$ Cg1 <sup>ii</sup>	0.96	2.79	3.6812 (17)	155
C7—O1 $\cdots$ Cg2 <sup>iii</sup>	1.23 (1)	3.65 (1)	3.9797 (18)	96 (1)

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