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1-[5-(4-Methoxyphenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazol-1-yl]ethanone

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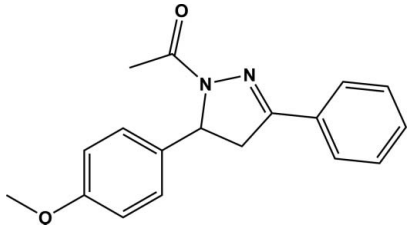
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.164; data-to-parameter ratio = 17.2.

The title molecule, $C_{18}H_{18}N_2O_2$, is V-shaped with the pyrazoline moiety being inclined to the adjacent phenyl ring by an angle of 6.49 (9)°, while the 4-methoxy-substituted ring is inclined to the pyrazoline ring by 82.99 (9)°. In the crystal, adjacent molecules are linked by C—H···O interactions, forming chains propagating in [100]. There are also C—H···π interactions involving adjacent molecules and those related by an inversion center.

Related literature

For the biological and pharmacological activity of 2-pyrazoline derivatives, see: Hatheway *et al.* (1978); Lombardino & Ottemes (1981); Parmar *et al.* (1974); Rathish *et al.* (2009); Subbaramaiah *et al.* (2002). For the synthesis and crystal structure of alkoxy group-bearing 2-pyrazoline derivatives, see: Abbas *et al.* (2010); Bai *et al.* (2009); Lu *et al.* (2008); Fahrni *et al.* (2003); Jian *et al.* (2008).



Experimental

Crystal data

$C_{18}H_{18}N_2O_2$
M_r = 294.34
Triclinic, $P\overline{1}$
a = 6.2762 (9) Å
b = 7.2081 (9) Å
c = 18.570 (2) Å
α = 85.939 (9)°
β = 85.384 (9)°
γ = 64.709 (8)°
V = 756.51 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.983
7199 measured reflections
3448 independent reflections
2584 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.164
S = 1.08
3448 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

Cg1 and *Cg3* are the centroids of the N1,N2,C8–C10 and C11–C16 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2^{i}	0.93	2.47	3.331 (2)	154
C1—H1*C*···*Cg*1^{ii}	0.96	2.96	3.755 (2)	141
C12—H12···*Cg*1^{iii}	0.93	2.96	3.7783 (18)	148
C18—H18*A*···*Cg*3^{iv}	0.96	2.63	3.544 (2)	159

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

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: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); 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: SU2223).

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supplementary materials

Acta Cryst. (2010). E**66**, o3174 [**doi:10.1107/S1600536810045861**]

1-[5-(4-Methoxyphenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazol-1-yl]ethanone

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Comment

Pyrazoline systems are well known nitrogen-containing heterocyclic compounds which possess a wide range of biological and pharmacological activities such as antitumor (Hatheway *et al.*, 1978), immunosuppressive (Lombardino *et al.*,1981), psychoanaleptic (Parmar *et al.*, 1974), anti-inflammation (Rathish *et al.*, 2009), and anticancer (Subbaramaiah *et al.*, 2002). In continuation of previous structural studies of alkoxy group bearing pyrazoline derivatives (Abbas *et al.*, 2010), the title compound was synthesized and its crystal structure is reported on herein.

The molecular structure of the title compound is shown in Fig. 1. All the bond lengths and bond angles are similar to those observed in similar structures (Fahrni *et al.*, 2003; Bai *et al.*, 2009; Lu *et al.*, 2008). In the pyrazolinyl ring, the C8—N2 and C10=N1 bond lengths, 1.483 (2) and 1.2860 (18) Å, respectively, are comparable with those in similar structures [C—N 1.482 (2)–1.515 (9) A°, C=N 1.291 (2)–1.300 (10) A°]. The N1—N2 bond length of 1.3867 (16) Å is slightly longer than that found in a similar structure [N–N 1.373 (2)–1.380 (8) A°] (Jian *et al.*, 2008). The plane containing the pyrazoline moiety is inclined to the adjacent phenyl ring (C16-C21) by 6.49 (9)\%, while the 4-methoxy substituted phenyl ring (C2-C7) is inclined to the pyrazoline moiety by 82.99 (9) °.

In the crystal adjacent molecules are linked by a C-H···O interaction forming chains propagating in [100]. There are also C-H···π interactions involving adjacent molecules and those related by an inversion center; see Table 1 for details.

Experimental

To a mixture of *(E)*-3-(4-(methoxy)phenyl)-1-phenylprop-2-en-1-one (2.94 g, 10 mmol) and hydrazine hydrate (1.0 g, 20 mmol) in acetic acid (25 ml), were added two drops of concentrated hydrochloric acid. The mixture was refluxed for 5 h. The precipitated solids were filtered, dried and recrystallized from ethanol. The crystals, suitable for X-ray diffraction analysis, were obtained from a mixture of ethyl acetate and dichloromethane (v:v / 1:1) by slow evaporation.

Refinement

The H-atoms were placed at calculated positions and were treated as riding: C-H = 0.93, 0.96, 0.97 and 0.98 Å for CH(aromatic), methylene, methyl and methine H-atoms, respectively, with $U_{iso}(H) = k \times U_{eq}(C)$, where k = 1.5 for methyl H-atoms and 1.2 for all other H-atoms.

Figures

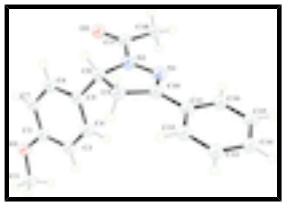


Fig. 1. A view of the molecular structure of the title molecule, showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

1-[5-(4-Methoxyphenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazol-1-yl]ethanone

Crystal data

$C_{18}H_{18}N_2O_2$	$Z = 2$
$M_r = 294.34$	$F(000) = 312$
Triclinic, $P\overline{1}$	$D_x = 1.292$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.2762$ (9) Å	Cell parameters from 2249 reflections
$b = 7.2081$ (9) Å	$\theta = 3.1$–$26.2°$
$c = 18.570$ (2) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 85.939$ (9)°	$T = 296$ K
$\beta = 85.384$ (9)°	Block, white
$\gamma = 64.709$ (8)°	0.30 × 0.30 × 0.20 mm
$V = 756.51$ (17) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	3448 independent reflections
Radiation source: fine-focus sealed tube	2584 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.026$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 1.1°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -8 \rightarrow 7$
$T_{min} = 0.975$, $T_{max} = 0.983$	$k = -9 \rightarrow 9$
7199 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.050$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.164$	H-atom parameters constrained
$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.0912P)^2 + 0.0545P]$ where $P = (F_o^2 + 2F_c^2)/3$

3448 reflections	$(\Delta/\sigma)_{max} < 0.001$
201 parameters	$\Delta\rho_{max} = 0.18$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.26$ 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	0.4631 (3)	−0.2736 (2)	0.45861 (9)	0.0843 (5)
C3	0.4986 (3)	−0.0139 (3)	0.37307 (9)	0.0537 (4)
H3	0.6618	−0.0701	0.3751	0.064*
C4	0.3831 (3)	0.1595 (3)	0.32925 (9)	0.0500 (4)
H4	0.4709	0.2180	0.3018	0.060*
O2	−0.1965 (2)	0.2057 (2)	0.21830 (7)	0.0643 (4)
C16	0.4222 (3)	0.6534 (2)	0.08234 (9)	0.0494 (4)
H16	0.3703	0.5800	0.0546	0.059*
N2	0.0349 (2)	0.3699 (2)	0.20010 (7)	0.0452 (3)
N1	0.1673 (2)	0.44578 (18)	0.15426 (7)	0.0401 (3)
C1	0.7049 (4)	−0.3530 (3)	0.47300 (13)	0.0760 (6)
H1A	0.7996	−0.3994	0.4291	0.114*
H1B	0.7424	−0.4661	0.5077	0.114*
H1C	0.7366	−0.2475	0.4920	0.114*
C2	0.3689 (3)	−0.1025 (3)	0.41372 (9)	0.0564 (4)
C5	0.1405 (3)	0.2471 (2)	0.32553 (8)	0.0456 (4)
C8	0.0129 (3)	0.4317 (2)	0.27581 (8)	0.0472 (4)
H8	−0.1543	0.4988	0.2920	0.057*
C9	0.1164 (3)	0.5910 (3)	0.26675 (9)	0.0511 (4)
H9A	−0.0054	0.7288	0.2738	0.061*
H9B	0.2381	0.5615	0.3005	0.061*
C10	0.2176 (2)	0.5667 (2)	0.19012 (8)	0.0388 (3)
C11	0.3582 (3)	0.6705 (2)	0.15576 (8)	0.0399 (3)
C15	0.5613 (3)	0.7436 (3)	0.05020 (10)	0.0601 (5)
H15	0.6047	0.7297	0.0011	0.072*
C14	0.6364 (3)	0.8549 (3)	0.09092 (11)	0.0597 (5)
H14	0.7331	0.9138	0.0694	0.072*
C13	0.5693 (3)	0.8791 (3)	0.16288 (10)	0.0558 (4)
H13	0.6178	0.9566	0.1899	0.067*

C12	0.4290 (3)	0.7881 (2)	0.19563 (9)	0.0481 (4)
H12	0.3823	0.8059	0.2444	0.058*
C17	−0.0737 (3)	0.2610 (2)	0.17608 (9)	0.0460 (4)
C18	−0.0336 (3)	0.2129 (3)	0.09780 (10)	0.0546 (4)
H18A	0.1118	0.0928	0.0906	0.082*
H18B	−0.0251	0.3269	0.0697	0.082*
H18C	−0.1617	0.1882	0.0828	0.082*
C6	0.0143 (3)	0.1551 (3)	0.36706 (9)	0.0538 (4)
H6	−0.1492	0.2116	0.3657	0.065*
C7	0.1271 (3)	−0.0172 (3)	0.40986 (10)	0.0599 (5)
H7	0.0396	−0.0774	0.4366	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0905 (11)	0.0808 (10)	0.0967 (11)	−0.0527 (9)	−0.0259 (9)	0.0337 (8)
C3	0.0521 (9)	0.0614 (10)	0.0550 (10)	−0.0316 (8)	0.0020 (7)	−0.0057 (8)
C4	0.0551 (9)	0.0630 (10)	0.0458 (8)	−0.0396 (8)	0.0082 (7)	−0.0047 (7)
O2	0.0651 (8)	0.0827 (9)	0.0682 (8)	−0.0548 (7)	0.0016 (6)	0.0011 (7)
C16	0.0627 (10)	0.0455 (8)	0.0521 (9)	−0.0349 (8)	0.0060 (7)	−0.0092 (7)
N2	0.0524 (8)	0.0529 (7)	0.0433 (7)	−0.0356 (6)	0.0019 (6)	−0.0019 (6)
N1	0.0424 (6)	0.0418 (6)	0.0435 (7)	−0.0257 (5)	−0.0004 (5)	0.0006 (5)
C1	0.0838 (15)	0.0640 (12)	0.0780 (14)	−0.0283 (11)	−0.0145 (11)	0.0035 (10)
C2	0.0732 (12)	0.0592 (10)	0.0508 (9)	−0.0416 (9)	−0.0063 (8)	0.0018 (8)
C5	0.0541 (9)	0.0554 (9)	0.0390 (7)	−0.0353 (8)	0.0072 (6)	−0.0070 (6)
C8	0.0514 (9)	0.0537 (9)	0.0443 (8)	−0.0307 (7)	0.0068 (7)	−0.0067 (7)
C9	0.0660 (10)	0.0497 (9)	0.0473 (9)	−0.0343 (8)	0.0059 (7)	−0.0084 (7)
C10	0.0407 (7)	0.0358 (7)	0.0438 (8)	−0.0201 (6)	−0.0016 (6)	−0.0021 (6)
C11	0.0418 (7)	0.0324 (7)	0.0492 (8)	−0.0194 (6)	−0.0034 (6)	0.0003 (6)
C15	0.0774 (12)	0.0567 (10)	0.0590 (10)	−0.0433 (9)	0.0167 (9)	−0.0087 (8)
C14	0.0634 (11)	0.0516 (10)	0.0783 (13)	−0.0400 (9)	0.0057 (9)	−0.0007 (9)
C13	0.0650 (11)	0.0491 (9)	0.0698 (11)	−0.0387 (8)	−0.0122 (9)	−0.0011 (8)
C12	0.0571 (9)	0.0458 (8)	0.0504 (9)	−0.0297 (7)	−0.0062 (7)	−0.0014 (7)
C17	0.0424 (8)	0.0482 (8)	0.0566 (9)	−0.0282 (7)	−0.0051 (7)	0.0034 (7)
C18	0.0631 (10)	0.0573 (10)	0.0587 (10)	−0.0387 (9)	−0.0103 (8)	−0.0033 (8)
C6	0.0554 (10)	0.0712 (11)	0.0497 (9)	−0.0426 (9)	0.0052 (7)	−0.0016 (8)
C7	0.0717 (12)	0.0772 (12)	0.0520 (9)	−0.0541 (10)	0.0013 (8)	0.0071 (8)

Geometric parameters (Å, °)

O1—C2	1.370 (2)	C8—C9	1.537 (2)
O1—C1	1.415 (2)	C8—H8	0.9800
C3—C2	1.384 (2)	C9—C10	1.501 (2)
C3—C4	1.388 (2)	C9—H9A	0.9700
C3—H3	0.9300	C9—H9B	0.9700
C4—C5	1.382 (2)	C10—C11	1.467 (2)
C4—H4	0.9300	C11—C12	1.389 (2)
O2—C17	1.2202 (19)	C15—C14	1.380 (3)
C16—C15	1.374 (2)	C15—H15	0.9300

C16—C11	1.389 (2)	C14—C13	1.369 (3)
C16—H16	0.9300	C14—H14	0.9300
N2—C17	1.3544 (19)	C13—C12	1.388 (2)
N2—N1	1.3867 (16)	C13—H13	0.9300
N2—C8	1.483 (2)	C12—H12	0.9300
N1—C10	1.2860 (18)	C17—C18	1.495 (2)
C1—H1A	0.9600	C18—H18A	0.9600
C1—H1B	0.9600	C18—H18B	0.9600
C1—H1C	0.9600	C18—H18C	0.9600
C2—C7	1.379 (3)	C6—C7	1.370 (3)
C5—C6	1.393 (2)	C6—H6	0.9300
C5—C8	1.516 (2)	C7—H7	0.9300
C2—O1—C1	118.98 (16)	C8—C9—H9B	111.2
C2—C3—C4	119.52 (16)	H9A—C9—H9B	109.1
C2—C3—H3	120.2	N1—C10—C11	120.66 (14)
C4—C3—H3	120.2	N1—C10—C9	113.99 (13)
C5—C4—C3	121.48 (15)	C11—C10—C9	125.34 (13)
C5—C4—H4	119.3	C16—C11—C12	118.70 (14)
C3—C4—H4	119.3	C16—C11—C10	120.40 (13)
C15—C16—C11	120.83 (15)	C12—C11—C10	120.90 (14)
C15—C16—H16	119.6	C16—C15—C14	119.84 (17)
C11—C16—H16	119.6	C16—C15—H15	120.1
C17—N2—N1	122.42 (13)	C14—C15—H15	120.1
C17—N2—C8	124.22 (13)	C13—C14—C15	120.30 (15)
N1—N2—C8	113.24 (11)	C13—C14—H14	119.8
C10—N1—N2	108.02 (12)	C15—C14—H14	119.8
O1—C1—H1A	109.5	C14—C13—C12	120.07 (15)
O1—C1—H1B	109.5	C14—C13—H13	120.0
H1A—C1—H1B	109.5	C12—C13—H13	120.0
O1—C1—H1C	109.5	C13—C12—C11	120.19 (16)
H1A—C1—H1C	109.5	C13—C12—H12	119.9
H1B—C1—H1C	109.5	C11—C12—H12	119.9
O1—C2—C7	115.83 (16)	O2—C17—N2	119.62 (16)
O1—C2—C3	124.75 (17)	O2—C17—C18	123.10 (14)
C7—C2—C3	119.42 (16)	N2—C17—C18	117.28 (13)
C4—C5—C6	117.83 (15)	C17—C18—H18A	109.5
C4—C5—C8	122.07 (14)	C17—C18—H18B	109.5
C6—C5—C8	120.04 (15)	H18A—C18—H18B	109.5
N2—C8—C5	110.93 (13)	C17—C18—H18C	109.5
N2—C8—C9	100.75 (12)	H18A—C18—H18C	109.5
C5—C8—C9	115.68 (13)	H18B—C18—H18C	109.5
N2—C8—H8	109.7	C7—C6—C5	121.05 (16)
C5—C8—H8	109.7	C7—C6—H6	119.5
C9—C8—H8	109.7	C5—C6—H6	119.5
C10—C9—C8	102.96 (12)	C6—C7—C2	120.69 (16)
C10—C9—H9A	111.2	C6—C7—H7	119.7
C8—C9—H9A	111.2	C2—C7—H7	119.7
C10—C9—H9B	111.2		

C2—C3—C4—C5	0.4 (3)	C8—C9—C10—C11	−173.86 (14)
C17—N2—N1—C10	170.50 (14)	C15—C16—C11—C12	2.7 (2)
C8—N2—N1—C10	−5.73 (17)	C15—C16—C11—C10	−177.55 (15)
C1—O1—C2—C7	−171.49 (18)	N1—C10—C11—C16	5.5 (2)
C1—O1—C2—C3	8.9 (3)	C9—C10—C11—C16	−173.24 (14)
C4—C3—C2—O1	179.81 (17)	N1—C10—C11—C12	−174.79 (13)
C4—C3—C2—C7	0.2 (3)	C9—C10—C11—C12	6.5 (2)
C3—C4—C5—C6	−0.3 (2)	C11—C16—C15—C14	−0.8 (3)
C3—C4—C5—C8	−177.65 (15)	C16—C15—C14—C13	−1.2 (3)
C17—N2—C8—C5	70.55 (18)	C15—C14—C13—C12	1.3 (3)
N1—N2—C8—C5	−113.30 (14)	C14—C13—C12—C11	0.7 (3)
C17—N2—C8—C9	−166.43 (15)	C16—C11—C12—C13	−2.7 (2)
N1—N2—C8—C9	9.72 (16)	C10—C11—C12—C13	177.64 (14)
C4—C5—C8—N2	77.68 (18)	N1—N2—C17—O2	−176.77 (14)
C6—C5—C8—N2	−99.57 (17)	C8—N2—C17—O2	−1.0 (2)
C4—C5—C8—C9	−36.3 (2)	N1—N2—C17—C18	3.8 (2)
C6—C5—C8—C9	146.50 (15)	C8—N2—C17—C18	179.57 (14)
N2—C8—C9—C10	−9.34 (15)	C4—C5—C6—C7	−0.3 (3)
C5—C8—C9—C10	110.31 (14)	C8—C5—C6—C7	177.01 (16)
N2—N1—C10—C11	179.75 (12)	C5—C6—C7—C2	1.0 (3)
N2—N1—C10—C9	−1.36 (17)	O1—C2—C7—C6	179.48 (17)
C8—C9—C10—N1	7.31 (17)	C3—C2—C7—C6	−0.8 (3)

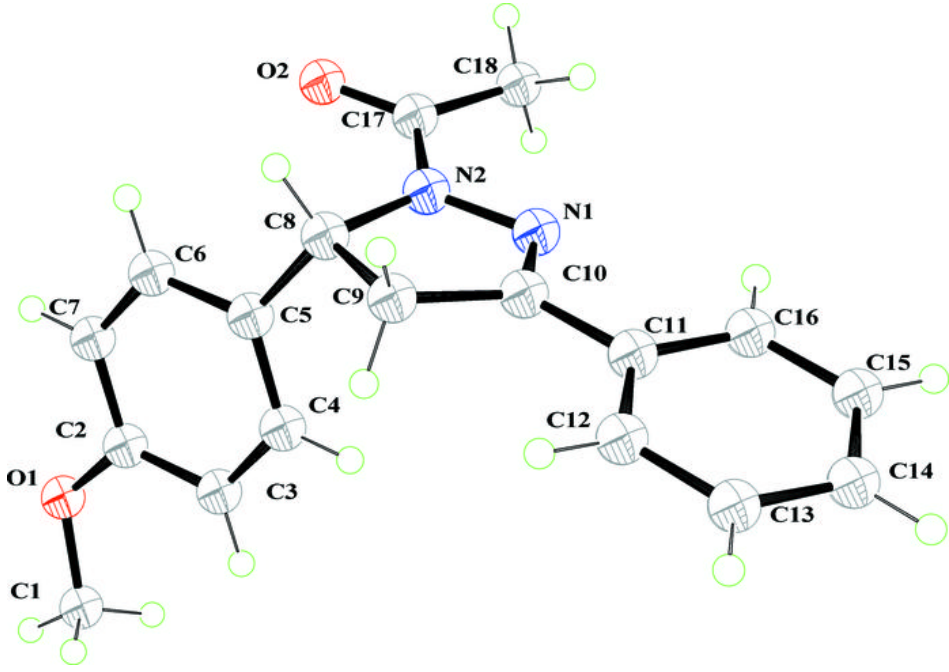
Hydrogen-bond geometry (Å, °)

Cg1 and *Cg3* are the centroids of the N1,N2,C8–C10 and C11–C16 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.93	2.47	3.331 (2)	154
C1—H1C···Cg1^{ii}	0.96	2.96	3.755 (2)	141
C12—H12···Cg1^{iii}	0.93	2.96	3.7783 (18)	148
C18—H18A···Cg3^{iv}	0.96	2.63	3.544 (2)	159

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

Fig. 1


O2
C18
C17
N2
N1
C8
C6
C10
C7
C5
C9
C11
C16
C15
C4
C12
C2
C14
O1
C3
C13
C1