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1-Acetyl-5-(4-fluorophenyl)-3-(4-nitrophenyl)-2-pyrazoline

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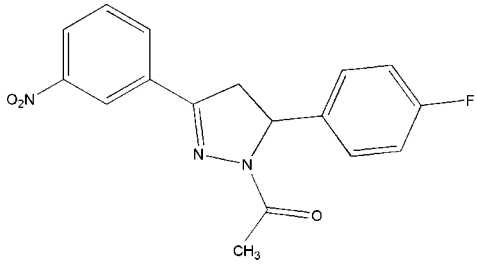
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.109; data-to-parameter ratio = 13.0.

The title compound, $C_{17}H_{14}FN_3O_3$, was prepared by the reaction of hydrazine and 1-(4-nitrophenyl)-3-(4-fluorophenyl)-2-propenyl-1-ketone. The dihedral angle between the benzene ring bearing the nitro substituent and the pyrazoline ring is 3.82 (8)° and the dihedral angle between the two benzene rings is 70.27 (8)°. Weak intermolecular C—H···O hydrogen bonds are present in the crystal structure.

Related literature

The medicinal and biological properties of pyrazoline derivatives has been reported previously (Rawal *et al.*, 1963; Dhal *et al.*, 1975; Lombardino & Ottemes, 1981; Manna *et al.*, 2002). The bond lengths and angles of the title compound are similar to those in related structures (Fahrni *et al.*, 2003; Kimura *et al.*, 1977; Guo *et al.*, 2007).



Experimental

Crystal data

$C_{17}H_{14}FN_3O_3$
M_r = 327.31
Monoclinic, $P2_1/c$
a = 5.7992 (11) Å
b = 16.661 (3) Å
c = 16.056 (3) Å
β = 99.387 (2)°
V = 1530.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.50 × 0.25 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
7736 measured reflections
2826 independent reflections
2326 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.109
S = 1.05
2826 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O2^{i}	0.97	2.53	3.271 (2)	133
C12—H12···O1^{ii}	0.93	2.41	3.150 (2)	136

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2419).

References

Bruker (1997). *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Versions 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Dhal, P. N., Acharya, T. E. & Nayak, A. (1975). *J. Indian Chem. Soc.* **52**, 1196–1200.
Fahrni, C. J., Yang, L. C. & VanDerveer, D. G. (2003). *J. Am. Chem. Soc.* **125**, 3799–3812.
Guo, H.-M., Jian, F.-F., Zhao, P.-S., Sun, X.-Z. & Lin, C.-H. (2007). *Acta Cryst.* E**63**, o2618–o2619.
Kimura, T., Kai, Y., Yasuoka, N. & Kasai, N. (1977). *Acta Cryst.* B**33**, 1786–1792.
Lombardino, G. & Ottemes, I. G. (1981). *J. Med. Chem.* **24**, 830–834.
Manna, F., Chimenti, F., Bolasco, A., Secci, D., Bizzarri, B., Befani, O., Turini, P., Mondovi, B., Alcaro, S. & Tafi, A. (2002). *Bioorg. Med. Chem. Lett.* **12**, 3629–3635.
Rawal, A. A., Thakor, V. M. & Shah, N. M. (1963). *J. Indian Chem. Soc.* **40**, 323–326.
Sheldrick, G. M. (1990). *SHELXTL/PC*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

Acta Cryst. (2007). E**63**, o3179 [**doi:10.1107/S1600536807027833**]

1-Acetyl-5-(4-fluorophenyl)-3-(4-nitrophenyl)-2-pyrazoline

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Comment

Pyrazoline and its derivatives are useful compounds found to possess antiviral (Rawal *et al.*, 1963), antifungal (Dhal *et al.*, 1975), and immunosuppressive (Lombardino & Ottemes, 1981) activities. 1-Acetyl-3,5-diaryl-2-pyrazoline has been found to inhibit the monoamine oxidases (Manna *et al.*, 2002). As part of our ongoing investgation of pyrazolines and their metal complexes, we report here the crystal strucutre of the title compound.

In the molecule (Fig. 1), all of the bond lengthes and bond angles fall in the normal ranges (Fahrni *et al.*, 2003; Kimura *et al.*, 1977; Guo *et al.*, 2007). The dihedral angles formed by pyrazolinyl ring with phenyl groups at positions 3 and 5 of the pyrazoline are 3.82 (8) and 66.57 (8)°, respectively. Intermolecular C—H···O hydrogen bonds help stabilize the crystal structure of.

Experimental

1-(*p*-Nitrophenyl)-3-(*p*-fluorophenyl)-2-propenyl-1-ketone (0.02 mol)and hydrazine (0.02 mol)were mixed in 99.5% acetic acid (40 ml) and stirred in refluxing for 6 h, then the mixture was poured into ice-water to afford a colourless solid. This solid was filtered and washed with water until the pH of the solution was *ca* 7.0. Finally, the solid was dry at room temperature. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from EtOH at room temperature.

Refinement

H atoms were fixed geometrically and allowed to ride on their parent atoms, C—H distances 0.93–0.96 Å,respectively, and with U_{iso} = 1.2–1.5U_{eq} of the parent atoms.

Figures

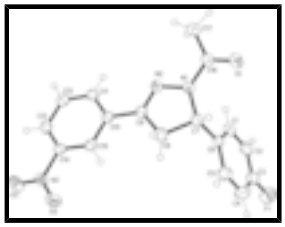


Fig. 1. The molecular structure and atom-labeling scheme with displacement ellipsoids drawn at the 30% probability level.

1-Acetyl-5-(4-fluorophenyl)-3-(4-nitrophenyl)-2-pyrazoline

Crystal data

$C_{17}H_{14}FN_3O_3$	F_{000} = 680
M_r = 327.31	D_x = 1.420 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3251 reflections
a = 5.7992 (11) Å	θ = 2.5–26.6º
b = 16.661 (3) Å	μ = 0.11 mm^{-1}
c = 16.056 (3) Å	T = 298 (2) K
β = 99.387 (2)º	Bar, colourless
V = 1530.5 (5) Å^3	0.50 × 0.25 × 0.21 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2326 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.023
Monochromator: graphite	θ_{max} = 25.5º
T = 298(2) K	θ_{min} = 1.8º
φ and ω scans	h = −6→7
Absorption correction: none	k = −17→20
7736 measured reflections	l = −19→17
2826 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.109	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.2585P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
2826 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
218 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.1716 (3)	0.28095 (9)	0.31214 (10)	0.0497 (4)
H1	0.0514	0.2449	0.2940	0.060*
C2	0.1713 (3)	0.32338 (10)	0.38636 (10)	0.0576 (4)
H2	0.0515	0.3163	0.4178	0.069*
C3	0.3486 (3)	0.37541 (10)	0.41247 (10)	0.0591 (4)
C4	0.5251 (4)	0.38828 (12)	0.36756 (12)	0.0691 (5)
H4	0.6436	0.4248	0.3862	0.083*
C5	0.5239 (3)	0.34580 (11)	0.29357 (11)	0.0584 (4)
H5	0.6436	0.3538	0.2623	0.070*
C6	0.3472 (2)	0.29139 (8)	0.26500 (9)	0.0422 (3)
C7	0.3543 (3)	0.24768 (9)	0.18283 (9)	0.0459 (4)
H7	0.4945	0.2140	0.1882	0.055*
C8	0.3488 (3)	0.30551 (11)	0.10788 (9)	0.0525 (4)
H8A	0.3740	0.3606	0.1269	0.063*
H8B	0.4653	0.2911	0.0735	0.063*
C9	0.1069 (3)	0.29371 (9)	0.06089 (8)	0.0419 (3)
C10	−0.0012 (3)	0.34281 (8)	−0.01095 (8)	0.0392 (3)
C11	−0.2240 (3)	0.32545 (9)	−0.05429 (9)	0.0447 (4)
H11	−0.3050	0.2816	−0.0378	0.054*
C12	−0.3259 (3)	0.37190 (10)	−0.12099 (9)	0.0486 (4)
H12	−0.4751	0.3595	−0.1489	0.058*
C13	−0.2074 (3)	0.43700 (9)	−0.14678 (9)	0.0465 (4)
H13	−0.2756	0.4693	−0.1913	0.056*
C14	0.0134 (3)	0.45268 (8)	−0.10489 (8)	0.0401 (3)
C15	0.1209 (3)	0.40736 (8)	−0.03730 (8)	0.0398 (3)
H15	0.2709	0.4197	−0.0102	0.048*
C16	0.1205 (3)	0.12039 (10)	0.17533 (10)	0.0548 (4)
C17	−0.0864 (4)	0.07640 (11)	0.13026 (12)	0.0713 (6)
H17A	−0.0725	0.0708	0.0718	0.107*
H17B	−0.2260	0.1058	0.1350	0.107*
H17C	−0.0942	0.0242	0.1550	0.107*
F1	0.3487 (2)	0.41655 (7)	0.48573 (7)	0.0914 (4)
N1	0.1449 (2)	0.19873 (8)	0.15372 (7)	0.0490 (3)
N2	−0.0014 (2)	0.23332 (7)	0.08576 (7)	0.0466 (3)
N3	0.1435 (2)	0.52153 (7)	−0.13096 (8)	0.0483 (3)
O1	0.2651 (3)	0.09008 (7)	0.22967 (8)	0.0733 (4)
O2	0.3452 (2)	0.53098 (7)	−0.09699 (8)	0.0662 (4)
O3	0.0411 (2)	0.56620 (7)	−0.18506 (8)	0.0696 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0534 (10)	0.0437 (8)	0.0520 (9)	−0.0073 (7)	0.0088 (7)	0.0059 (7)
C2	0.0713 (12)	0.0525 (10)	0.0529 (9)	0.0023 (8)	0.0215 (8)	0.0073 (7)
C3	0.0758 (12)	0.0501 (10)	0.0496 (9)	0.0042 (9)	0.0046 (8)	−0.0025 (7)
C4	0.0653 (12)	0.0657 (12)	0.0723 (12)	−0.0146 (9)	−0.0012 (10)	−0.0138 (9)
C5	0.0499 (10)	0.0642 (11)	0.0617 (10)	−0.0105 (8)	0.0105 (8)	−0.0009 (8)
C6	0.0426 (8)	0.0395 (8)	0.0431 (8)	0.0004 (6)	0.0028 (6)	0.0096 (6)
C7	0.0446 (8)	0.0470 (8)	0.0459 (8)	−0.0014 (7)	0.0065 (7)	0.0067 (7)
C8	0.0512 (10)	0.0637 (10)	0.0430 (8)	−0.0079 (8)	0.0093 (7)	0.0111 (7)
C9	0.0494 (9)	0.0407 (8)	0.0371 (7)	−0.0017 (6)	0.0118 (6)	−0.0015 (6)
C10	0.0463 (8)	0.0379 (7)	0.0352 (7)	0.0011 (6)	0.0120 (6)	−0.0032 (6)
C11	0.0482 (9)	0.0427 (8)	0.0451 (8)	−0.0039 (6)	0.0129 (6)	−0.0024 (6)
C12	0.0442 (9)	0.0531 (9)	0.0474 (8)	−0.0013 (7)	0.0039 (7)	−0.0049 (7)
C13	0.0532 (9)	0.0457 (8)	0.0405 (8)	0.0081 (7)	0.0067 (7)	0.0014 (6)
C14	0.0500 (9)	0.0334 (7)	0.0387 (7)	0.0018 (6)	0.0126 (6)	−0.0026 (6)
C15	0.0436 (8)	0.0389 (7)	0.0376 (7)	−0.0006 (6)	0.0084 (6)	−0.0038 (6)
C16	0.0752 (12)	0.0448 (9)	0.0433 (8)	−0.0074 (8)	0.0062 (8)	0.0038 (7)
C17	0.0936 (15)	0.0519 (10)	0.0634 (11)	−0.0215 (10)	−0.0018 (10)	0.0059 (8)
F1	0.1220 (11)	0.0845 (8)	0.0669 (7)	0.0009 (7)	0.0134 (7)	−0.0266 (6)
N1	0.0603 (8)	0.0426 (7)	0.0417 (6)	−0.0075 (6)	0.0011 (6)	0.0059 (5)
N2	0.0562 (8)	0.0426 (7)	0.0399 (6)	−0.0049 (6)	0.0045 (6)	0.0026 (5)
N3	0.0611 (9)	0.0362 (7)	0.0501 (7)	0.0019 (6)	0.0164 (6)	0.0012 (6)
O1	0.0935 (10)	0.0537 (7)	0.0648 (8)	−0.0072 (6)	−0.0107 (7)	0.0180 (6)
O2	0.0631 (8)	0.0568 (7)	0.0771 (8)	−0.0177 (6)	0.0060 (7)	0.0093 (6)
O3	0.0817 (9)	0.0512 (7)	0.0761 (8)	0.0083 (6)	0.0138 (7)	0.0260 (6)

Geometric parameters (Å, °)

C1—C6	1.375 (2)	C10—C15	1.391 (2)
C1—C2	1.386 (2)	C10—C11	1.394 (2)
C1—H1	0.9300	C11—C12	1.374 (2)
C2—C3	1.358 (3)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.383 (2)
C3—F1	1.3613 (19)	C12—H12	0.9300
C3—C4	1.362 (3)	C13—C14	1.371 (2)
C4—C5	1.382 (2)	C13—H13	0.9300
C4—H4	0.9300	C14—C15	1.3842 (19)
C5—C6	1.389 (2)	C14—N3	1.4709 (19)
C5—H5	0.9300	C15—H15	0.9300
C6—C7	1.513 (2)	C16—O1	1.217 (2)
C7—N1	1.4745 (19)	C16—N1	1.364 (2)
C7—C8	1.538 (2)	C16—C17	1.489 (2)
C7—H7	0.9800	C17—H17A	0.9600
C8—C9	1.494 (2)	C17—H17B	0.9600
C8—H8A	0.9700	C17—H17C	0.9600
C8—H8B	0.9700	N1—N2	1.3930 (17)

C9—N2	1.2841 (18)	N3—O2	1.2176 (17)
C9—C10	1.4686 (19)	N3—O3	1.2219 (17)
C6—C1—C2	120.90 (15)	C15—C10—C9	119.73 (13)
C6—C1—H1	119.5	C11—C10—C9	121.26 (13)
C2—C1—H1	119.5	C12—C11—C10	121.21 (14)
C3—C2—C1	118.94 (16)	C12—C11—H11	119.4
C3—C2—H2	120.5	C10—C11—H11	119.4
C1—C2—H2	120.5	C11—C12—C13	120.20 (14)
C2—C3—F1	118.79 (17)	C11—C12—H12	119.9
C2—C3—C4	122.27 (16)	C13—C12—H12	119.9
F1—C3—C4	118.94 (17)	C14—C13—C12	118.20 (14)
C3—C4—C5	118.41 (17)	C14—C13—H13	120.9
C3—C4—H4	120.8	C12—C13—H13	120.9
C5—C4—H4	120.8	C13—C14—C15	123.10 (14)
C4—C5—C6	121.22 (16)	C13—C14—N3	119.37 (13)
C4—C5—H5	119.4	C15—C14—N3	117.51 (13)
C6—C5—H5	119.4	C14—C15—C10	118.25 (14)
C1—C6—C5	118.26 (14)	C14—C15—H15	120.9
C1—C6—C7	123.15 (14)	C10—C15—H15	120.9
C5—C6—C7	118.58 (13)	O1—C16—N1	119.46 (15)
N1—C7—C6	113.84 (12)	O1—C16—C17	123.41 (15)
N1—C7—C8	100.81 (11)	N1—C16—C17	117.13 (15)
C6—C7—C8	112.37 (13)	C16—C17—H17A	109.5
N1—C7—H7	109.8	C16—C17—H17B	109.5
C6—C7—H7	109.8	H17A—C17—H17B	109.5
C8—C7—H7	109.8	C16—C17—H17C	109.5
C9—C8—C7	102.17 (12)	H17A—C17—H17C	109.5
C9—C8—H8A	111.3	H17B—C17—H17C	109.5
C7—C8—H8A	111.3	C16—N1—N2	121.34 (13)
C9—C8—H8B	111.3	C16—N1—C7	124.25 (13)
C7—C8—H8B	111.3	N2—N1—C7	112.62 (11)
H8A—C8—H8B	109.2	C9—N2—N1	107.54 (12)
N2—C9—C10	120.84 (13)	O2—N3—O3	124.03 (14)
N2—C9—C8	114.40 (13)	O2—N3—C14	118.26 (13)
C10—C9—C8	124.69 (13)	O3—N3—C14	117.70 (14)
C15—C10—C11	119.01 (13)		
C6—C1—C2—C3	−0.4 (2)	C10—C11—C12—C13	0.4 (2)
C1—C2—C3—F1	−179.51 (14)	C11—C12—C13—C14	0.9 (2)
C1—C2—C3—C4	1.0 (3)	C12—C13—C14—C15	−1.2 (2)
C2—C3—C4—C5	−0.9 (3)	C12—C13—C14—N3	180.00 (12)
F1—C3—C4—C5	179.60 (16)	C13—C14—C15—C10	0.1 (2)
C3—C4—C5—C6	0.3 (3)	N3—C14—C15—C10	178.97 (12)
C2—C1—C6—C5	−0.2 (2)	C11—C10—C15—C14	1.16 (19)
C2—C1—C6—C7	−179.00 (14)	C9—C10—C15—C14	−179.63 (12)
C4—C5—C6—C1	0.3 (2)	O1—C16—N1—N2	172.89 (15)
C4—C5—C6—C7	179.14 (16)	C17—C16—N1—N2	−7.4 (2)
C1—C6—C7—N1	5.5 (2)	O1—C16—N1—C7	9.3 (2)
C5—C6—C7—N1	−173.28 (14)	C17—C16—N1—C7	−170.99 (15)

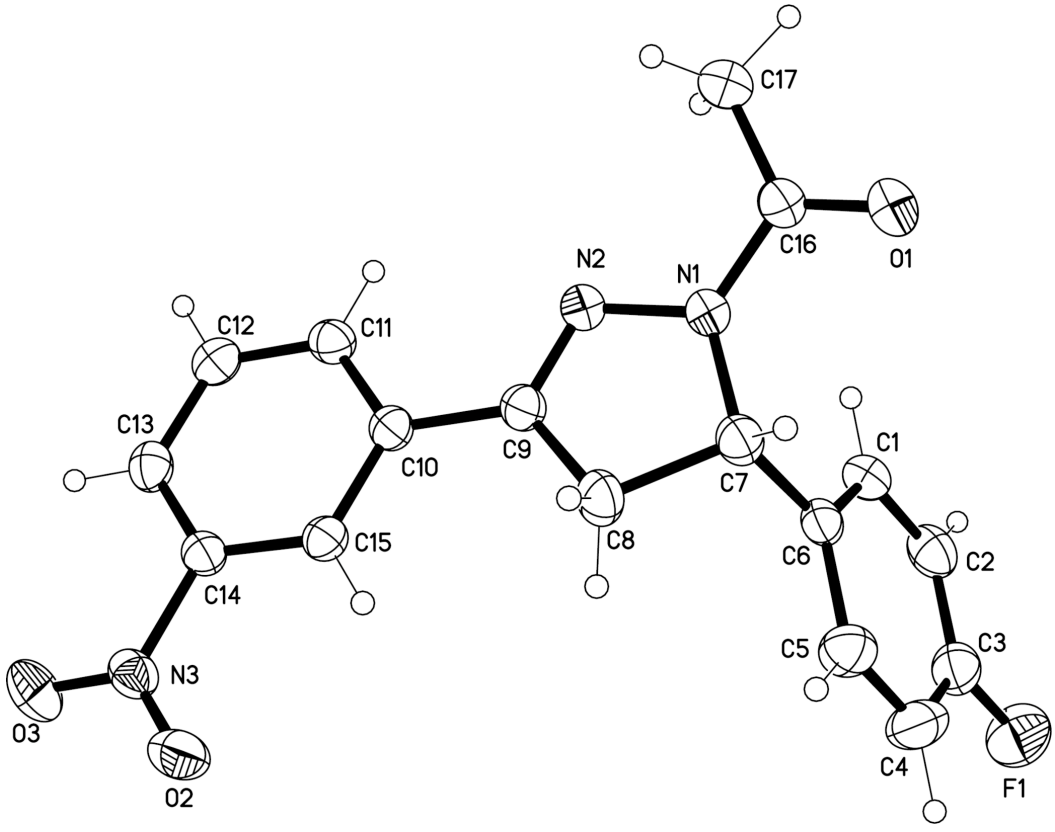
C1—C6—C7—C8	119.32 (15)	C6—C7—N1—C16	−89.44 (18)
C5—C6—C7—C8	−59.47 (18)	C8—C7—N1—C16	150.03 (15)
N1—C7—C8—C9	14.43 (15)	C6—C7—N1—N2	105.70 (14)
C6—C7—C8—C9	−107.14 (14)	C8—C7—N1—N2	−14.83 (16)
C7—C8—C9—N2	−11.41 (17)	C10—C9—N2—N1	179.48 (12)
C7—C8—C9—C10	171.64 (13)	C8—C9—N2—N1	2.40 (17)
N2—C9—C10—C15	−179.24 (13)	C16—N1—N2—C9	−156.81 (14)
C8—C9—C10—C15	−2.5 (2)	C7—N1—N2—C9	8.55 (17)
N2—C9—C10—C11	−0.1 (2)	C13—C14—N3—O2	−174.83 (13)
C8—C9—C10—C11	176.70 (14)	C15—C14—N3—O2	6.29 (19)
C15—C10—C11—C12	−1.4 (2)	C13—C14—N3—O3	5.8 (2)
C9—C10—C11—C12	179.36 (12)	C15—C14—N3—O3	−173.06 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8A···O2^{i}	0.97	2.53	3.271 (2)	133
C12—H12···O1^{ii}	0.93	2.41	3.150 (2)	136

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

Fig. 1


C17
C16
O1
N2
N1
C12
C11
C13
C10
C9
C7
C1
C8
C6
C2
C15
C14
C5
C3
N3
O3
O2
C4
F1