Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(3,5-Dimethoxyphenyl)-2-(4-fluorophenyl)-4,5-dimethyl-1*H*-imidazole

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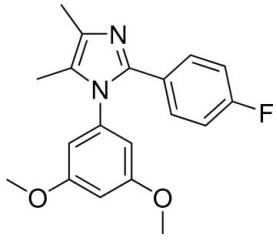
Received 20 December 2011; accepted 21 December 2011

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.046; wR factor = 0.138; data-to-parameter ratio = 14.7.

In the title compound, $C_{19}H_{19}FN_2O_2$, the imidazole ring is essentially planar [maximum deviation = 0.0030 (8) Å] and makes dihedral angles of 66.45 (7) and 29.98 (7)° with the benzene rings attached to the ring N and C atoms, respectively. The dihedral angle between the two benzene rings is 64.79 (7)°. A C—H$\cdots\pi$ interaction is found in the crystal structure. The two methoxy groups were found to be disordered over two sets of sites with occupancy factors of 0.803 (4) and 0.197 (4). The F atom is disordered over two sites with occupancy factors of 0.929 (4) and 0.071 (4).

Related literature

For general background to the use of imidazole derivatives as drugs, see: Dooley *et al.* (1992); Jackson *et al.* (2000); Banfi *et al.* (2006). For a related structure and applications of imidazole derivatives, see: Rosepriya *et al.* (2011).



Experimental

Crystal data

$C_{19}H_{19}FN_2O_2$
M_r = 326.36
Monoclinic, $P2_1/n$
a = 6.9654 (1) Å
b = 17.8520 (3) Å
c = 13.7121 (3) Å
β = 97.833 (2)°
V = 1689.14 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 295 K
0.47 × 0.38 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan *CrysAlis PRO* (Oxford Diffraction, 2010)
T_{min} = 0.558, T_{max} = 1.000
7744 measured reflections
3533 independent reflections
2723 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.138
S = 1.06
3533 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1 is the centroid of the N1/C2/N3/C4/C5 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C23—H23$\cdots Cg1^{i}$	0.93	2.99	3.8714 (16)	159

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); 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); software used to prepare material for publication: *PLATON* (Spek, 2009).

JJ is thankful to the Department of Science and Technology [No. SR/S1/IC-07/2007] and the University Grants Commission [F. No. 36–21/2008 (SR)] for providing funding for this research work. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5156).

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supplementary materials

Acta Cryst. (2012). E**68**, o256 [**doi:10.1107/S1600536811055012**]

1-(3,5-Dimethoxyphenyl)-2-(4-fluorophenyl)-4,5-dimethyl-1*H*-imidazole

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Comment

For multidrug-resistant Tuberculosis (Dooley *et al.*,(1992)), antifungal and antimycobacterial activity (Banfi *et al.* 2006), and bactericidal effects (Jackson *et al.* 2000), the use of imidazole based compounds were reported. Rosepriya *et al.* 2011 have reported the crystal structure of 1-(3,5-Dimethylphenyl)-2-(4-fluorophenyl)-4,5-dimethyl-1*H*-imidazole. As part of our research (Rosepriya *et al.* 2011), we have synthesized the title compound (I) and report its crystal structure here.

In the title compound, Fig. 1, $C_{19}H_{19}FN_2O_2$, the imidazole ring is essentially planar [maximum deviation of 0.0030 (8) Å for C4]. The imidazole ring makes dihedral angles of 66.45 (7) and 29.98 (7)° with the benzene rings attached to nitrogen and carbon, respectively. The dihedral angle between the two benzene rings is 64.79 (7)°. A C23—H23···π interaction involving the imidazole (N1,C2,N3,C4,C5) ring is found in the crystal structure (Table 1). The two methoxy groups at C13 and C15 were found to be disordered over two positions with occupancy factors of 0.803 (4) and 0.197 (4). The F atom at C24 is disordered over two positions with occupancy factors of 0.929 (4) and 0.071 (4).

Experimental

To pure butane-2,3-dione (1.48 g, 15 mmol) in ethanol (10 ml), 3,5-dimethoxyaniline (2.29 g, 15 mmol), ammonium acetate (1.15 g, 15 mmol) and 4-fluorobenzaldehyde (1.8 g, 15 mmol) was added over 1 hr with the temperature maintained at 333 K. The reaction mixture was refluxed for 7 days and extracted with dichloromethane. The solid separated was purified by column chromatography using Hexane: Ethyl acetate as the eluent. Yield: 2.20 g (45%). Crystals suitable for X-ray diffraction studies were grown by slow solvent evaporation of a solution of the compound in dichloromethane.

Refinement

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 - 0.96 Å; U_{iso}(H) = kU_{eq}(C), where k = 1.5 for methyl and 1.2 for all other H atoms. The two methoxy groups were found to be disordered over two positions with occupancy factors of 0.803 (4) and 0.197 (4). The F atom is disordered over two positions with occupancy factors of 0.929 (4) and 0.071 (4).

Figures

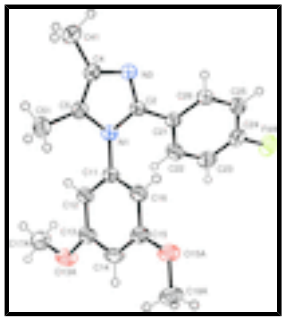


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius. The minor component of methoxy and F atoms are omitted for clarity.

1-(3,5-Dimethoxyphenyl)-2-(4-fluorophenyl)-4,5-dimethyl-1*H*-imidazole

Crystal data

$C_{19}H_{19}FN_2O_2$	$F(000) = 688$
$M_r = 326.36$	$D_x = 1.283$ Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 420 K
Hall symbol: -P 2yn	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
$a = 6.9654$ (1) Å	Cell parameters from 3957 reflections
$b = 17.8520$ (3) Å	$\theta = 5.0$–$77.4°$
$c = 13.7121$ (3) Å	$\mu = 0.75$ mm^{-1}
$\beta = 97.833$ (2)°	$T = 295$ K
$V = 1689.14$ (5) Å^3	Plate, colourless
$Z = 4$	0.47 × 0.38 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer	3533 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2723 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.024$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{max} = 77.6°$, $\theta_{min} = 5.0°$
ω scans	$h = -4 \rightarrow 8$
Absorption correction: multi-scan *CrysAlis PRO* (Oxford Diffraction, 2010)	$k = -22 \rightarrow 21$
$T_{min} = 0.558$, $T_{max} = 1.000$	$l = -17 \rightarrow 17$
7744 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.138$	H-atom parameters constrained

S = 1.06	$w = 1/[\sigma^2(F_o^2) + (0.0917P)^2 + 0.0185P]$ where $P = (F_o^2 + 2F_c^2)/3$
3533 reflections	$(\Delta/\sigma)_{max} = 0.001$
240 parameters	$\Delta\rho_{max} = 0.21$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\sigma(F^2)$ 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.

A damping factor (DAMP 200 15 in the final refinement cycles) was applied to avoid large displacements of the less occupied methoxy and fluorine atoms with EADP F4A F4B, EADP O13A O13B, EADP O15A O15B, EADP C17A C17B, EADP C18A C18B.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
F4A	−0.29421 (17)	0.18280 (10)	0.14002 (10)	0.0827 (4)	0.929 (4)
O13A	0.7091 (3)	0.45839 (10)	0.22912 (15)	0.0748 (6)	0.803 (4)
O15A	0.2065 (3)	0.45966 (11)	0.43181 (19)	0.0728 (6)	0.803 (4)
N1	0.55071 (14)	0.23172 (5)	0.40039 (8)	0.0452 (3)	
N3	0.48548 (15)	0.11225 (6)	0.42587 (9)	0.0513 (3)	
C2	0.42077 (16)	0.17418 (6)	0.38065 (9)	0.0446 (3)	
C4	0.66338 (17)	0.12988 (7)	0.47766 (10)	0.0513 (3)	
C5	0.70736 (16)	0.20299 (7)	0.46281 (10)	0.0493 (3)	
C11	0.52171 (16)	0.30968 (6)	0.37642 (9)	0.0459 (3)	
C12	0.64059 (19)	0.34342 (7)	0.31551 (11)	0.0533 (4)	
C13	0.6101 (2)	0.41860 (8)	0.29299 (12)	0.0600 (4)	
C14	0.4653 (2)	0.45903 (7)	0.33020 (13)	0.0643 (5)	
C15	0.3491 (2)	0.42387 (7)	0.38983 (11)	0.0564 (4)	
C16	0.37798 (17)	0.34825 (7)	0.41430 (10)	0.0502 (4)	
C17A	0.8558 (4)	0.4227 (2)	0.1871 (3)	0.0874 (9)	0.803 (4)
C18A	0.1764 (5)	0.53712 (15)	0.4144 (3)	0.0865 (12)	0.803 (4)
C21	0.23453 (16)	0.17930 (6)	0.31576 (9)	0.0446 (3)	
C22	0.2032 (2)	0.22706 (8)	0.23517 (10)	0.0562 (4)	
C23	0.0262 (2)	0.22827 (9)	0.17545 (11)	0.0642 (4)	
C24	−0.11786 (19)	0.18160 (8)	0.19783 (11)	0.0571 (4)	
C25	−0.09381 (19)	0.13336 (7)	0.27609 (11)	0.0551 (4)	
C26	0.08443 (18)	0.13216 (7)	0.33465 (10)	0.0500 (3)	
C41	0.7816 (2)	0.07173 (10)	0.53699 (14)	0.0737 (5)	
C51	0.8802 (2)	0.24892 (9)	0.50026 (13)	0.0651 (5)	
C17B	0.898 (2)	0.4240 (10)	0.2150 (14)	0.0874 (9)	0.197 (4)

C18B	0.135 (2)	0.5285 (8)	0.3807 (13)	0.0865 (12)	0.197 (4)
O13B	0.7483 (14)	0.4621 (5)	0.2658 (7)	0.0748 (6)	0.197 (4)
O15B	0.1779 (16)	0.4481 (5)	0.4134 (10)	0.0728 (6)	0.197 (4)
F4B	−0.253 (3)	0.2120 (13)	0.1380 (16)	0.0827 (4)	0.071 (4)
H16	0.30133	0.32452	0.45545	0.0602*	
H17A	0.94989	0.40279	0.23819	0.1309*	0.803 (4)
H12	0.73740	0.31646	0.29069	0.0639*	
H14	0.44718	0.50951	0.31489	0.0771*	
H22	0.30229	0.25856	0.22119	0.0675*	
H23	0.00548	0.26006	0.12131	0.0770*	
H25	−0.19419	0.10232	0.28952	0.0662*	
H26	0.10444	0.09926	0.38765	0.0600*	
H41A	0.86731	0.04817	0.49709	0.1106*	
H41B	0.69719	0.03475	0.55904	0.1106*	
H41C	0.85625	0.09493	0.59293	0.1106*	
H51A	0.96450	0.22046	0.54767	0.0976*	
H51B	0.83938	0.29349	0.53081	0.0976*	
H51C	0.94812	0.26244	0.44646	0.0976*	
H17B	0.91718	0.45800	0.14857	0.1309*	0.803 (4)
H17C	0.80126	0.38258	0.14554	0.1309*	0.803 (4)
H18A	0.29026	0.56430	0.44132	0.1298*	0.803 (4)
H18B	0.06803	0.55363	0.44518	0.1298*	0.803 (4)
H18C	0.15032	0.54600	0.34477	0.1298*	0.803 (4)
H17D	0.99679	0.40337	0.26325	0.1309*	0.197 (4)
H17E	0.95528	0.45968	0.17517	0.1309*	0.197 (4)
H17F	0.83856	0.38452	0.17401	0.1309*	0.197 (4)
H18D	0.25069	0.55810	0.39539	0.1298*	0.197 (4)
H18E	0.03553	0.54860	0.41504	0.1298*	0.197 (4)
H18F	0.09270	0.52961	0.31114	0.1298*	0.197 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F4A	0.0562 (6)	0.1013 (10)	0.0835 (6)	0.0048 (5)	−0.0161 (5)	−0.0034 (7)
O13A	0.0855 (9)	0.0547 (6)	0.0943 (13)	0.0053 (6)	0.0491 (9)	0.0201 (8)
O15A	0.0821 (9)	0.0435 (8)	0.1025 (12)	0.0134 (6)	0.0473 (8)	0.0021 (7)
N1	0.0446 (4)	0.0365 (4)	0.0546 (5)	−0.0007 (3)	0.0076 (4)	−0.0003 (4)
N3	0.0490 (5)	0.0410 (5)	0.0638 (6)	0.0016 (4)	0.0079 (4)	0.0075 (4)
C2	0.0466 (5)	0.0357 (5)	0.0523 (6)	−0.0006 (4)	0.0092 (4)	0.0016 (4)
C4	0.0472 (5)	0.0477 (6)	0.0594 (7)	0.0056 (5)	0.0090 (5)	0.0059 (5)
C5	0.0443 (5)	0.0474 (6)	0.0564 (6)	0.0030 (4)	0.0075 (4)	−0.0035 (5)
C11	0.0481 (5)	0.0349 (5)	0.0552 (6)	−0.0017 (4)	0.0086 (4)	−0.0018 (4)
C12	0.0532 (6)	0.0419 (6)	0.0685 (8)	0.0010 (5)	0.0218 (5)	−0.0016 (5)
C13	0.0636 (7)	0.0450 (6)	0.0767 (9)	−0.0020 (5)	0.0287 (6)	0.0070 (6)
C14	0.0749 (8)	0.0362 (6)	0.0872 (10)	0.0049 (5)	0.0309 (7)	0.0091 (6)
C15	0.0604 (7)	0.0421 (6)	0.0707 (8)	0.0061 (5)	0.0237 (6)	−0.0004 (5)
C16	0.0528 (6)	0.0414 (6)	0.0589 (7)	−0.0013 (5)	0.0168 (5)	0.0020 (5)
C17A	0.0810 (14)	0.0824 (12)	0.110 (2)	0.0107 (12)	0.0532 (13)	0.0286 (14)

C18A	0.0976 (16)	0.0484 (10)	0.123 (3)	0.0222 (10)	0.0493 (15)	0.0015 (12)
C21	0.0472 (5)	0.0360 (5)	0.0510 (6)	0.0010 (4)	0.0080 (4)	−0.0026 (4)
C22	0.0589 (7)	0.0536 (7)	0.0559 (7)	−0.0060 (5)	0.0070 (5)	0.0071 (6)
C23	0.0724 (8)	0.0631 (8)	0.0545 (7)	0.0051 (6)	−0.0003 (6)	0.0091 (6)
C24	0.0488 (6)	0.0609 (8)	0.0592 (7)	0.0081 (5)	−0.0011 (5)	−0.0104 (6)
C25	0.0484 (6)	0.0497 (6)	0.0677 (8)	−0.0033 (5)	0.0094 (5)	−0.0097 (6)
C26	0.0531 (6)	0.0394 (5)	0.0575 (7)	−0.0017 (5)	0.0077 (5)	0.0014 (5)
C41	0.0584 (7)	0.0687 (9)	0.0917 (11)	0.0116 (7)	0.0019 (7)	0.0249 (8)
C51	0.0499 (6)	0.0632 (8)	0.0799 (10)	−0.0034 (6)	0.0008 (6)	−0.0123 (7)
C17B	0.0810 (14)	0.0824 (12)	0.110 (2)	0.0107 (12)	0.0532 (13)	0.0286 (14)
C18B	0.0976 (16)	0.0484 (10)	0.123 (3)	0.0222 (10)	0.0493 (15)	0.0015 (12)
O13B	0.0855 (9)	0.0547 (6)	0.0943 (13)	0.0053 (6)	0.0491 (9)	0.0201 (8)
O15B	0.0821 (9)	0.0435 (8)	0.1025 (12)	0.0134 (6)	0.0473 (8)	0.0021 (7)
F4B	0.0562 (6)	0.1013 (10)	0.0835 (6)	0.0048 (5)	−0.0161 (5)	−0.0034 (7)

Geometric parameters (Å, °)

F4A—C24	1.3683 (19)	C23—C24	1.371 (2)
F4B—C24	1.28 (2)	C24—C25	1.368 (2)
O13A—C17A	1.394 (4)	C25—C26	1.3838 (19)
O13A—C13	1.383 (3)	C12—H12	0.9300
O13B—C17B	1.494 (19)	C14—H14	0.9300
O13B—C13	1.329 (10)	C16—H16	0.9300
O15A—C15	1.372 (3)	C17A—H17A	0.9600
O15A—C18A	1.414 (3)	C17A—H17B	0.9600
O15B—C15	1.349 (11)	C17A—H17C	0.9600
O15B—C18B	1.521 (17)	C17B—H17F	0.9600
N1—C2	1.3714 (14)	C17B—H17E	0.9600
N1—C5	1.3898 (16)	C17B—H17D	0.9600
N1—C11	1.4379 (14)	C18A—H18C	0.9600
N3—C4	1.3780 (17)	C18A—H18B	0.9600
N3—C2	1.3167 (16)	C18A—H18A	0.9600
C2—C21	1.4725 (16)	C18B—H18F	0.9600
C4—C5	1.3623 (18)	C18B—H18E	0.9600
C4—C41	1.495 (2)	C18B—H18D	0.9600
C5—C51	1.4889 (19)	C22—H22	0.9300
C11—C16	1.3740 (17)	C23—H23	0.9300
C11—C12	1.3909 (18)	C25—H25	0.9300
C12—C13	1.3870 (19)	C26—H26	0.9300
C13—C14	1.392 (2)	C41—H41B	0.9600
C14—C15	1.378 (2)	C41—H41A	0.9600
C15—C16	1.3990 (18)	C41—H41C	0.9600
C21—C22	1.3892 (18)	C51—H51C	0.9600
C21—C26	1.3936 (17)	C51—H51A	0.9600
C22—C23	1.384 (2)	C51—H51B	0.9600
C13—O13A—C17A	119.0 (2)	C15—C14—H14	120.00
C13—O13B—C17B	116.3 (9)	C11—C16—H16	121.00
C15—O15A—C18A	118.9 (2)	C15—C16—H16	121.00
C15—O15B—C18B	112.1 (9)	O13A—C17A—H17A	109.00

C5—N1—C11	124.89 (10)	O13A—C17A—H17B	110.00
C2—N1—C5	106.66 (9)	O13A—C17A—H17C	109.00
C2—N1—C11	127.70 (10)	H17A—C17A—H17B	110.00
C2—N3—C4	106.08 (10)	H17A—C17A—H17C	109.00
N1—C2—C21	125.18 (10)	H17B—C17A—H17C	109.00
N3—C2—C21	123.61 (10)	H17E—C17B—H17F	109.00
N1—C2—N3	111.20 (10)	H17D—C17B—H17F	109.00
C5—C4—C41	128.92 (12)	O13B—C17B—H17E	109.00
N3—C4—C5	110.28 (11)	O13B—C17B—H17F	110.00
N3—C4—C41	120.78 (12)	O13B—C17B—H17D	109.00
C4—C5—C51	131.59 (12)	H17D—C17B—H17E	109.00
N1—C5—C51	122.63 (11)	O15A—C18A—H18C	109.00
N1—C5—C4	105.78 (10)	H18A—C18A—H18B	109.00
N1—C11—C16	119.05 (10)	O15A—C18A—H18B	109.00
C12—C11—C16	122.28 (11)	O15A—C18A—H18A	109.00
N1—C11—C12	118.67 (10)	H18A—C18A—H18C	109.00
C11—C12—C13	117.85 (12)	H18B—C18A—H18C	109.00
O13A—C13—C14	114.49 (14)	O15B—C18B—H18D	109.00
O13A—C13—C12	124.31 (14)	H18E—C18B—H18F	110.00
O13B—C13—C14	112.9 (4)	H18D—C18B—H18F	109.00
C12—C13—C14	121.10 (13)	O15B—C18B—H18E	110.00
O13B—C13—C12	122.2 (4)	O15B—C18B—H18F	110.00
C13—C14—C15	119.66 (12)	H18D—C18B—H18E	109.00
C14—C15—C16	120.34 (12)	C21—C22—H22	120.00
O15A—C15—C14	123.67 (14)	C23—C22—H22	120.00
O15A—C15—C16	115.94 (14)	C24—C23—H23	121.00
O15B—C15—C16	110.8 (4)	C22—C23—H23	121.00
O15B—C15—C14	127.3 (5)	C24—C25—H25	121.00
C11—C16—C15	118.77 (12)	C26—C25—H25	121.00
C2—C21—C26	118.14 (11)	C21—C26—H26	119.00
C2—C21—C22	123.28 (11)	C25—C26—H26	119.00
C22—C21—C26	118.55 (11)	C4—C41—H41B	109.00
C21—C22—C23	120.72 (13)	C4—C41—H41C	109.00
C22—C23—C24	118.57 (14)	H41A—C41—H41B	109.00
C23—C24—C25	122.89 (13)	C4—C41—H41A	109.00
F4B—C24—C23	95.5 (10)	H41A—C41—H41C	109.00
F4B—C24—C25	140.3 (10)	H41B—C41—H41C	109.00
F4A—C24—C25	117.94 (13)	H51B—C51—H51C	109.00
F4A—C24—C23	119.18 (14)	H51A—C51—H51B	109.00
C24—C25—C26	117.98 (12)	H51A—C51—H51C	109.00
C21—C26—C25	121.28 (12)	C5—C51—H51A	109.00
C11—C12—H12	121.00	C5—C51—H51B	109.00
C13—C12—H12	121.00	C5—C51—H51C	109.00
C13—C14—H14	120.00		
C17A—O13A—C13—C14	−179.4 (2)	C41—C4—C5—N1	178.65 (14)
C17A—O13A—C13—C12	−3.0 (3)	N3—C4—C5—C51	−179.23 (14)
C18A—O15A—C15—C14	−0.6 (3)	C41—C4—C5—C51	−1.1 (3)
C18A—O15A—C15—C16	176.7 (2)	C16—C11—C12—C13	−0.2 (2)
C2—N1—C5—C4	−0.21 (14)	N1—C11—C16—C15	−179.31 (12)

C11—N1—C2—N3	−170.50 (11)	C12—C11—C16—C15	0.7 (2)
C11—N1—C2—C21	10.84 (19)	N1—C11—C12—C13	179.83 (12)
C11—N1—C5—C51	−9.77 (19)	C11—C12—C13—C14	0.1 (2)
C5—N1—C2—C21	−178.82 (11)	C11—C12—C13—O13A	−176.12 (16)
C2—N1—C11—C16	60.35 (17)	O13A—C13—C14—C15	176.05 (16)
C5—N1—C11—C12	71.66 (16)	C12—C13—C14—C15	−0.5 (2)
C5—N1—C11—C16	−108.35 (14)	C13—C14—C15—C16	1.0 (2)
C2—N1—C11—C12	−119.64 (14)	C13—C14—C15—O15A	178.23 (18)
C5—N1—C2—N3	−0.15 (14)	O15A—C15—C16—C11	−178.53 (15)
C2—N1—C5—C51	179.54 (12)	C14—C15—C16—C11	−1.1 (2)
C11—N1—C5—C4	170.48 (11)	C2—C21—C22—C23	178.55 (12)
C4—N3—C2—N1	0.45 (14)	C26—C21—C22—C23	0.6 (2)
C2—N3—C4—C41	−178.92 (13)	C2—C21—C26—C25	−179.31 (12)
C2—N3—C4—C5	−0.59 (15)	C22—C21—C26—C25	−1.22 (19)
C4—N3—C2—C21	179.14 (11)	C21—C22—C23—C24	0.3 (2)
N1—C2—C21—C26	−151.86 (12)	C22—C23—C24—F4A	179.31 (14)
N3—C2—C21—C22	−148.36 (13)	C22—C23—C24—C25	−0.6 (2)
N3—C2—C21—C26	29.64 (18)	F4A—C24—C25—C26	−179.94 (14)
N1—C2—C21—C22	30.15 (19)	C23—C24—C25—C26	0.0 (2)
N3—C4—C5—N1	0.50 (15)	C24—C25—C26—C21	0.9 (2)

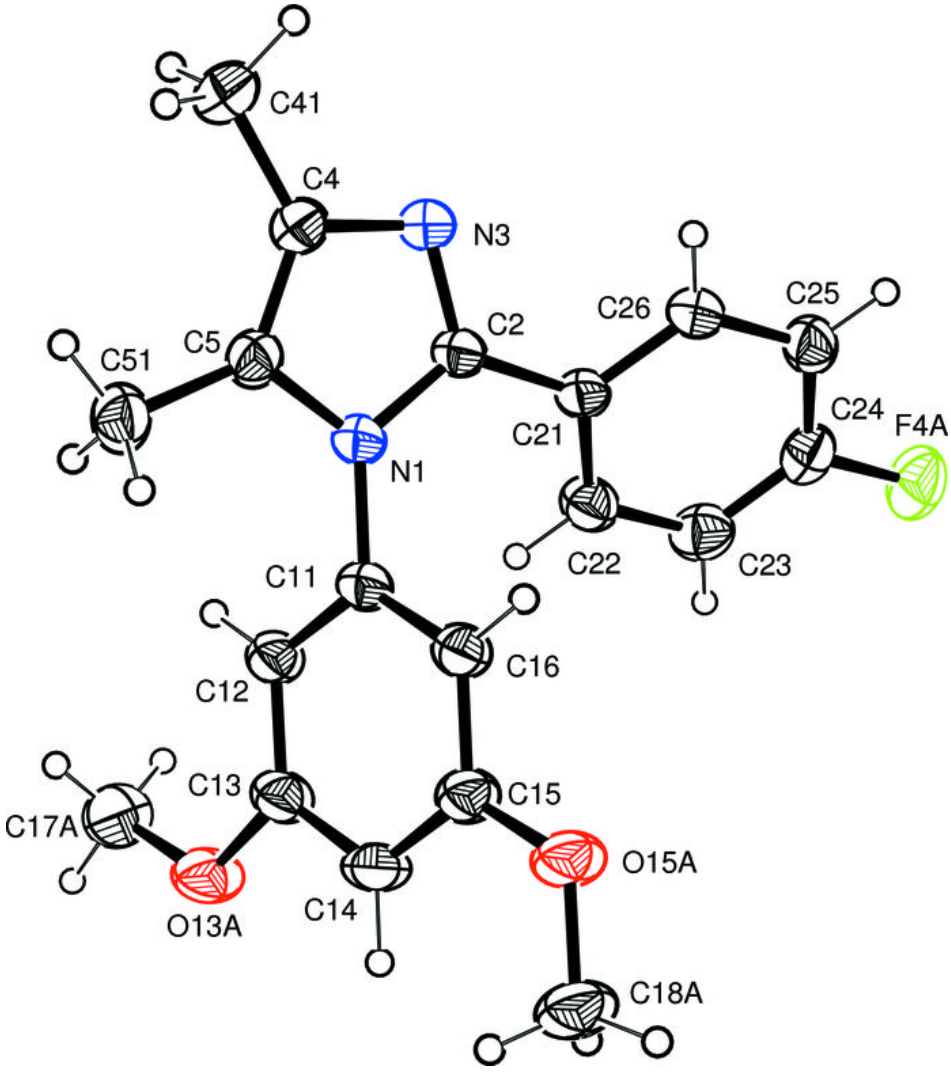
Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the N1/C2/N3/C4/C5 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23···Cg1^{i}	0.93	2.99	3.8714 (16)	159

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

Fig. 1


C41
C4
N3
C26
C25
C2
C5
C51
C21
C24
F4A
N1
C22
C23
C11
C16
C12
C13
C15
C17A
O15A
O13A
C14
C18A