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

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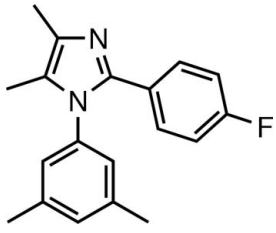
Key indicators: single-crystal X-ray study; $T$ = 170 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.052; $wR$ factor = 0.159; data-to-parameter ratio = 15.0.

In the title compound, $C_{19}H_{19}FN_2$, the imidazole ring is essentially planar [maximum deviation of 0.0015 (9) Å] and makes dihedral angles of 77.61 (9) and 26.93 (10)° with the benzene rings attached to nitrogen and carbon, respectively. The dihedral angle between the two benzene rings is 78.84 (8)°. A C—H$\cdots\pi$ interaction is found in the crystal structure.

## Related literature

For related structures and applications of imidazole derivatives, see: Gayathri *et al.* (2010); Rosepriya *et al.* (2011).




## Experimental

### Crystal data

$C_{19}H_{19}FN_2$
$M_r$ = 294.36
Triclinic, $P\overline{1}$
$a$ = 8.4226 (10) Å
$b$ = 9.5572 (10) Å
$c$ = 11.0351 (11) Å
$\alpha$ = 105.423 (9)°
$\beta$ = 105.677 (9)°
$\gamma$ = 95.781 (9)°
$V$ = 810.07 (17) Å$^3$
$Z$ = 2
Cu $K\alpha$ radiation
$\mu$ = 0.63 mm$^{-1}$
$T$ = 170 K
0.25 × 0.20 × 0.15 mm

### Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
$T_{min}$ = 0.858, $T_{max}$ = 0.911
5121 measured reflections
3054 independent reflections
2771 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.011

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.159
$S$ = 1.07
3054 reflections
203 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

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

*Cg*3 is the centroid of the C21–C26 ring.

| $D$—H$\cdots$$A$ | $D$—H | H$\cdots$$A$ | $D\cdots A$ | $D$—H$\cdots$$A$ |
|---|---|---|---|---|
| C12—H12$\cdots$*Cg*3$^{i}$ | 0.95 | 2.86 | 3.7969 (19) | 169 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5018).

## References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gayathri, P., Thiruvalluvar, A., Srinivasan, N., Jayabharathi, J. & Butcher, R. J. (2010). *Acta Cryst.* E**66**, o2776.
Oxford Diffraction (2010). *CrysAlis PRO* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
Rosepriya, S., Thiruvalluvar, A., Jayabharathi, J., Venkatesh Perumal, M., Butcher, R. J., Jasinski, J. P. & Golen, J. A. (2011). *Acta Cryst.* E**67**, o989.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supplementary materials

*Acta Cryst.* (2011). E**67**, o1065 [ **doi:10.1107/S1600536811012098** ]

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

**S. Rosepriya, A. Thiruvalluvar, J. Jayabharathi, N. Srinivasan, R. J. Butcher, J. P. Jasinski and J. A. Golen**

## Comment

Rosepriya *et al.* (2011) have reported the crystal structure of 1,2-Diphenyl-1*H*-imidazo[4,5-*f*][1,10]phenanthroline. As part of our research (Gayathri *et al.*, (2010)), we have synthesized the title compound (I) and report its crystal structure here. Since our group doing the research in organic light emitting devices, we are interested to use the title compound as ligand for synthesizing Ir(III) complexes.

In the title compound (Fig. 1), $C_{19}H_{19}FN_2$, the imidazole ring is essentially planar [maximum deviation of 0.0015 (9) Å for C4]. The imidazole ring makes dihedral angles of 77.61 (9) and 26.93 (10)° with the benzene rings attached to N1 and C2, respectively. The dihedral angle between the two benzene rings is 78.84 (8)°. A C12—H12···π interaction involving (C21—C26) ring is found in the crystal structure (Table 1).

## Experimental

To pure butane-2,3-dione (1.48 g, 15 mmol) in ethanol (10 ml), 3,5-xylidine (1.8 g, 15 mmol), ammonium acetate (1.15 g, 15 mmol) and 4-fluorobenzaldehyde (1.7 g, 15 mmol) was added about 1 h by maintaining the temperature 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: 2.1 g (48%). Crystals suitable for X-ray diffraction studies were grown by slow solvent evaporation of a solution of the compound in dichloromethane.

## Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 - 0.98 Å; $U_{iso}$(H) = k$U_{eq}$(C), where k = 1.5 for methyl and 1.2 for all other H atoms.

## Figures

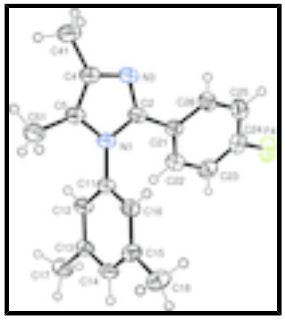


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius.

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

*Crystal data*

| | |
|---|---|
| $C_{19}H_{19}FN_2$ | $Z = 2$ |
| $M_r = 294.36$ | $F(000) = 312$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.207$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 377 K |
| $a = 8.4226$ (10) Å | Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å |
| $b = 9.5572$ (10) Å | Cell parameters from 3721 reflections |
| $c = 11.0351$ (11) Å | $\theta = 5.6$–$71.2°$ |
| $\alpha = 105.423$ (9)° | $\mu = 0.63$ mm$^{-1}$ |
| $\beta = 105.677$ (9)° | $T = 170$ K |
| $\gamma = 95.781$ (9)° | Block, colourless |
| $V = 810.07$ (17) Å$^3$ | 0.25 × 0.20 × 0.15 mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Eos Gemini diffractometer | 3054 independent reflections |
| Radiation source: Enhance (Cu) X-ray Source | 2771 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.011$ |
| Detector resolution: 16.1500 pixels mm$^{-1}$ | $\theta_{max} = 71.3°$, $\theta_{min} = 5.6°$ |
| ω scans | $h = -9 \rightarrow 10$ |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010) | $k = -11 \rightarrow 11$ |
| $T_{min} = 0.858$, $T_{max} = 0.911$ | $l = -13 \rightarrow 10$ |
| 5121 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 |
| $R[F^2 > 2\sigma(F^2)] = 0.052$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.159$ | H-atom parameters constrained |
| $S = 1.07$ | $w = 1/[\sigma^2(F_o^2) + (0.0944P)^2 + 0.144P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3054 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 203 parameters | $\Delta\rho_{max} = 0.31$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.23$ 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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F4 | 0.29950 (19) | 0.53513 (14) | 0.86850 (14) | 0.0964 (5) |
| N1 | 0.19985 (15) | −0.06005 (14) | 0.37504 (12) | 0.0449 (4) |
| N3 | 0.32289 (16) | −0.11576 (15) | 0.55605 (13) | 0.0520 (4) |
| C2 | 0.27033 (18) | −0.00885 (17) | 0.50979 (14) | 0.0453 (4) |
| C4 | 0.2859 (2) | −0.23874 (19) | 0.44868 (16) | 0.0532 (5) |
| C5 | 0.20944 (19) | −0.20827 (17) | 0.33550 (15) | 0.0488 (5) |
| C11 | 0.14226 (18) | 0.02522 (16) | 0.28741 (14) | 0.0435 (4) |
| C12 | −0.02859 (18) | 0.01651 (18) | 0.23336 (15) | 0.0480 (5) |
| C13 | −0.08585 (19) | 0.10368 (18) | 0.15377 (15) | 0.0494 (5) |
| C14 | 0.0323 (2) | 0.19566 (17) | 0.12941 (14) | 0.0515 (5) |
| C15 | 0.2035 (2) | 0.20141 (16) | 0.17950 (15) | 0.0487 (5) |
| C16 | 0.25852 (18) | 0.11506 (16) | 0.26059 (14) | 0.0464 (4) |
| C17 | −0.2713 (2) | 0.0990 (2) | 0.0987 (2) | 0.0692 (7) |
| C18 | 0.3276 (3) | 0.2979 (2) | 0.1464 (2) | 0.0698 (7) |
| C21 | 0.28022 (18) | 0.14031 (17) | 0.59540 (15) | 0.0472 (5) |
| C22 | 0.1660 (2) | 0.2313 (2) | 0.56533 (17) | 0.0566 (5) |
| C23 | 0.1740 (3) | 0.3655 (2) | 0.6562 (2) | 0.0654 (6) |
| C24 | 0.2952 (3) | 0.4060 (2) | 0.77740 (19) | 0.0660 (6) |
| C25 | 0.4109 (2) | 0.3201 (2) | 0.81121 (19) | 0.0655 (6) |
| C26 | 0.4030 (2) | 0.1881 (2) | 0.71957 (16) | 0.0558 (5) |
| C41 | 0.3314 (3) | −0.3824 (2) | 0.4636 (2) | 0.0787 (8) |
| C51 | 0.1442 (2) | −0.3012 (2) | 0.19482 (17) | 0.0623 (6) |
| H12 | −0.10645 | −0.04873 | 0.25055 | 0.0575* |
| H14 | −0.00553 | 0.25686 | 0.07653 | 0.0618* |
| H16 | 0.37514 | 0.11800 | 0.29712 | 0.0556* |
| H17A | −0.29302 | 0.13147 | 0.01961 | 0.1037* |
| H17B | −0.30948 | 0.16460 | 0.16526 | 0.1037* |
| H17C | −0.33197 | −0.00229 | 0.07526 | 0.1037* |
| H18A | 0.34608 | 0.24283 | 0.06431 | 0.1046* |
| H18B | 0.43413 | 0.32742 | 0.21839 | 0.1046* |
| H18C | 0.28339 | 0.38610 | 0.13490 | 0.1046* |
| H22 | 0.08176 | 0.20091 | 0.48163 | 0.0679* |
| H23 | 0.09729 | 0.42825 | 0.63510 | 0.0784* |
| H25 | 0.49398 | 0.35114 | 0.89552 | 0.0785* |

| | | | | |
|---|---|---|---|---|
| H26 | 0.48261 | 0.12777 | 0.74092 | 0.0670* |
| H41A | 0.45009 | −0.38100 | 0.47068 | 0.1181* |
| H41B | 0.26202 | −0.46386 | 0.38633 | 0.1181* |
| H41C | 0.31177 | −0.39629 | 0.54360 | 0.1181* |
| H51A | 0.14887 | −0.40467 | 0.18925 | 0.0934* |
| H51B | 0.21302 | −0.26845 | 0.14515 | 0.0934* |
| H51C | 0.02775 | −0.29169 | 0.15728 | 0.0934* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F4 | 0.1034 (10) | 0.0696 (8) | 0.0947 (9) | 0.0084 (7) | 0.0297 (8) | −0.0060 (7) |
| N1 | 0.0417 (6) | 0.0541 (7) | 0.0451 (7) | 0.0131 (5) | 0.0125 (5) | 0.0248 (5) |
| N3 | 0.0508 (7) | 0.0622 (8) | 0.0497 (7) | 0.0169 (6) | 0.0121 (6) | 0.0291 (6) |
| C2 | 0.0399 (7) | 0.0568 (9) | 0.0451 (7) | 0.0108 (6) | 0.0128 (6) | 0.0250 (6) |
| C4 | 0.0533 (9) | 0.0573 (9) | 0.0561 (9) | 0.0180 (7) | 0.0150 (7) | 0.0279 (7) |
| C5 | 0.0466 (8) | 0.0547 (9) | 0.0516 (8) | 0.0152 (6) | 0.0156 (6) | 0.0243 (7) |
| C11 | 0.0430 (7) | 0.0527 (8) | 0.0410 (7) | 0.0148 (6) | 0.0131 (6) | 0.0222 (6) |
| C12 | 0.0418 (8) | 0.0586 (9) | 0.0494 (8) | 0.0121 (6) | 0.0143 (6) | 0.0250 (7) |
| C13 | 0.0469 (8) | 0.0581 (9) | 0.0445 (8) | 0.0182 (7) | 0.0102 (6) | 0.0187 (7) |
| C14 | 0.0634 (10) | 0.0533 (9) | 0.0448 (8) | 0.0218 (7) | 0.0150 (7) | 0.0243 (7) |
| C15 | 0.0567 (9) | 0.0479 (8) | 0.0496 (8) | 0.0139 (6) | 0.0223 (7) | 0.0206 (6) |
| C16 | 0.0418 (7) | 0.0533 (8) | 0.0490 (8) | 0.0134 (6) | 0.0155 (6) | 0.0207 (6) |
| C17 | 0.0519 (10) | 0.0793 (12) | 0.0756 (12) | 0.0238 (9) | 0.0056 (8) | 0.0327 (10) |
| C18 | 0.0764 (12) | 0.0665 (11) | 0.0864 (13) | 0.0152 (9) | 0.0385 (11) | 0.0419 (10) |
| C21 | 0.0437 (7) | 0.0569 (9) | 0.0481 (8) | 0.0075 (6) | 0.0178 (6) | 0.0248 (7) |
| C22 | 0.0565 (9) | 0.0630 (10) | 0.0535 (9) | 0.0151 (7) | 0.0163 (7) | 0.0224 (8) |
| C23 | 0.0670 (11) | 0.0609 (10) | 0.0762 (12) | 0.0192 (8) | 0.0287 (9) | 0.0248 (9) |
| C24 | 0.0680 (11) | 0.0561 (10) | 0.0684 (11) | −0.0007 (8) | 0.0275 (9) | 0.0082 (8) |
| C25 | 0.0548 (10) | 0.0716 (11) | 0.0589 (10) | −0.0022 (8) | 0.0124 (8) | 0.0123 (8) |
| C26 | 0.0460 (8) | 0.0654 (10) | 0.0559 (9) | 0.0054 (7) | 0.0132 (7) | 0.0227 (8) |
| C41 | 0.1018 (16) | 0.0660 (12) | 0.0736 (12) | 0.0332 (11) | 0.0157 (11) | 0.0351 (10) |
| C51 | 0.0685 (11) | 0.0640 (10) | 0.0532 (9) | 0.0186 (8) | 0.0135 (8) | 0.0192 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| F4—C24 | 1.359 (2) | C24—C25 | 1.375 (3) |
| N1—C2 | 1.3713 (19) | C25—C26 | 1.374 (3) |
| N1—C5 | 1.385 (2) | C12—H12 | 0.9500 |
| N1—C11 | 1.442 (2) | C14—H14 | 0.9500 |
| N3—C2 | 1.322 (2) | C16—H16 | 0.9500 |
| N3—C4 | 1.367 (2) | C17—H17A | 0.9800 |
| C2—C21 | 1.466 (2) | C17—H17B | 0.9800 |
| C4—C5 | 1.362 (2) | C17—H17C | 0.9800 |
| C4—C41 | 1.500 (3) | C18—H18A | 0.9800 |
| C5—C51 | 1.486 (2) | C18—H18B | 0.9800 |
| C11—C12 | 1.385 (2) | C18—H18C | 0.9800 |
| C11—C16 | 1.381 (2) | C22—H22 | 0.9500 |
| C12—C13 | 1.393 (2) | C23—H23 | 0.9500 |

| | | | |
|---|---|---|---|
| C13—C14 | 1.389 (2) | C25—H25 | 0.9500 |
| C13—C17 | 1.507 (2) | C26—H26 | 0.9500 |
| C14—C15 | 1.387 (2) | C41—H41A | 0.9800 |
| C15—C16 | 1.394 (2) | C41—H41B | 0.9800 |
| C15—C18 | 1.506 (3) | C41—H41C | 0.9800 |
| C21—C22 | 1.393 (2) | C51—H51A | 0.9800 |
| C21—C26 | 1.401 (2) | C51—H51B | 0.9800 |
| C22—C23 | 1.385 (3) | C51—H51C | 0.9800 |
| C23—C24 | 1.374 (3) | | |
| C2—N1—C5 | 107.12 (13) | C13—C14—H14 | 119.00 |
| C2—N1—C11 | 127.30 (14) | C15—C14—H14 | 119.00 |
| C5—N1—C11 | 125.28 (12) | C11—C16—H16 | 120.00 |
| C2—N3—C4 | 106.09 (13) | C15—C16—H16 | 120.00 |
| N1—C2—N3 | 110.65 (14) | C13—C17—H17A | 109.00 |
| N1—C2—C21 | 126.33 (14) | C13—C17—H17B | 109.00 |
| N3—C2—C21 | 122.95 (13) | C13—C17—H17C | 109.00 |
| N3—C4—C5 | 110.80 (16) | H17A—C17—H17B | 110.00 |
| N3—C4—C41 | 121.02 (15) | H17A—C17—H17C | 109.00 |
| C5—C4—C41 | 128.18 (16) | H17B—C17—H17C | 110.00 |
| N1—C5—C4 | 105.35 (14) | C15—C18—H18A | 109.00 |
| N1—C5—C51 | 122.36 (14) | C15—C18—H18B | 109.00 |
| C4—C5—C51 | 132.29 (16) | C15—C18—H18C | 109.00 |
| N1—C11—C12 | 119.20 (14) | H18A—C18—H18B | 109.00 |
| N1—C11—C16 | 119.31 (14) | H18A—C18—H18C | 109.00 |
| C12—C11—C16 | 121.49 (15) | H18B—C18—H18C | 110.00 |
| C11—C12—C13 | 119.80 (15) | C21—C22—H22 | 120.00 |
| C12—C13—C14 | 118.19 (15) | C23—C22—H22 | 120.00 |
| C12—C13—C17 | 120.13 (16) | C22—C23—H23 | 121.00 |
| C14—C13—C17 | 121.67 (16) | C24—C23—H23 | 121.00 |
| C13—C14—C15 | 122.39 (15) | C24—C25—H25 | 121.00 |
| C14—C15—C16 | 118.59 (15) | C26—C25—H25 | 121.00 |
| C14—C15—C18 | 120.88 (16) | C21—C26—H26 | 119.00 |
| C16—C15—C18 | 120.54 (16) | C25—C26—H26 | 119.00 |
| C11—C16—C15 | 119.50 (15) | C4—C41—H41A | 109.00 |
| C2—C21—C22 | 123.84 (14) | C4—C41—H41B | 109.00 |
| C2—C21—C26 | 117.57 (15) | C4—C41—H41C | 109.00 |
| C22—C21—C26 | 118.34 (16) | H41A—C41—H41B | 109.00 |
| C21—C22—C23 | 120.67 (17) | H41A—C41—H41C | 109.00 |
| C22—C23—C24 | 118.6 (2) | H41B—C41—H41C | 109.00 |
| F4—C24—C23 | 118.8 (2) | C5—C51—H51A | 109.00 |
| F4—C24—C25 | 118.53 (18) | C5—C51—H51B | 109.00 |
| C23—C24—C25 | 122.71 (19) | C5—C51—H51C | 109.00 |
| C24—C25—C26 | 118.09 (17) | H51A—C51—H51B | 109.00 |
| C21—C26—C25 | 121.54 (17) | H51A—C51—H51C | 109.00 |
| C11—C12—H12 | 120.00 | H51B—C51—H51C | 109.00 |
| C13—C12—H12 | 120.00 | | |
| C5—N1—C2—N3 | 0.02 (19) | C41—C4—C5—C51 | 1.4 (3) |
| C5—N1—C2—C21 | −176.74 (15) | N1—C11—C12—C13 | 176.87 (14) |

| | | | |
|---|---|---|---|
| C11—N1—C2—N3 | −173.88 (14) | C16—C11—C12—C13 | −2.3 (2) |
| C11—N1—C2—C21 | 9.4 (3) | N1—C11—C16—C15 | −177.86 (14) |
| C2—N1—C5—C4 | −0.20 (18) | C12—C11—C16—C15 | 1.3 (2) |
| C2—N1—C5—C51 | 179.77 (15) | C11—C12—C13—C14 | 1.1 (2) |
| C11—N1—C5—C4 | 173.87 (15) | C11—C12—C13—C17 | −177.75 (15) |
| C11—N1—C5—C51 | −6.2 (2) | C12—C13—C14—C15 | 1.1 (2) |
| C2—N1—C11—C12 | −105.84 (19) | C17—C13—C14—C15 | 179.93 (15) |
| C2—N1—C11—C16 | 73.4 (2) | C13—C14—C15—C16 | −2.1 (2) |
| C5—N1—C11—C12 | 81.3 (2) | C13—C14—C15—C18 | 177.47 (16) |
| C5—N1—C11—C16 | −99.51 (18) | C14—C15—C16—C11 | 0.9 (2) |
| C4—N3—C2—N1 | 0.16 (18) | C18—C15—C16—C11 | −178.71 (15) |
| C4—N3—C2—C21 | 177.05 (15) | C2—C21—C22—C23 | 174.03 (18) |
| C2—N3—C4—C5 | −0.3 (2) | C26—C21—C22—C23 | 0.0 (3) |
| C2—N3—C4—C41 | 178.74 (17) | C2—C21—C26—C25 | −173.55 (16) |
| N1—C2—C21—C22 | 27.5 (3) | C22—C21—C26—C25 | 0.9 (3) |
| N1—C2—C21—C26 | −158.45 (16) | C21—C22—C23—C24 | −1.0 (3) |
| N3—C2—C21—C22 | −148.95 (17) | C22—C23—C24—F4 | −177.64 (19) |
| N3—C2—C21—C26 | 25.2 (2) | C22—C23—C24—C25 | 1.3 (3) |
| N3—C4—C5—N1 | 0.30 (19) | F4—C24—C25—C26 | 178.47 (18) |
| N3—C4—C5—C51 | −179.66 (17) | C23—C24—C25—C26 | −0.5 (3) |
| C41—C4—C5—N1 | −178.63 (19) | C24—C25—C26—C21 | −0.7 (3) |

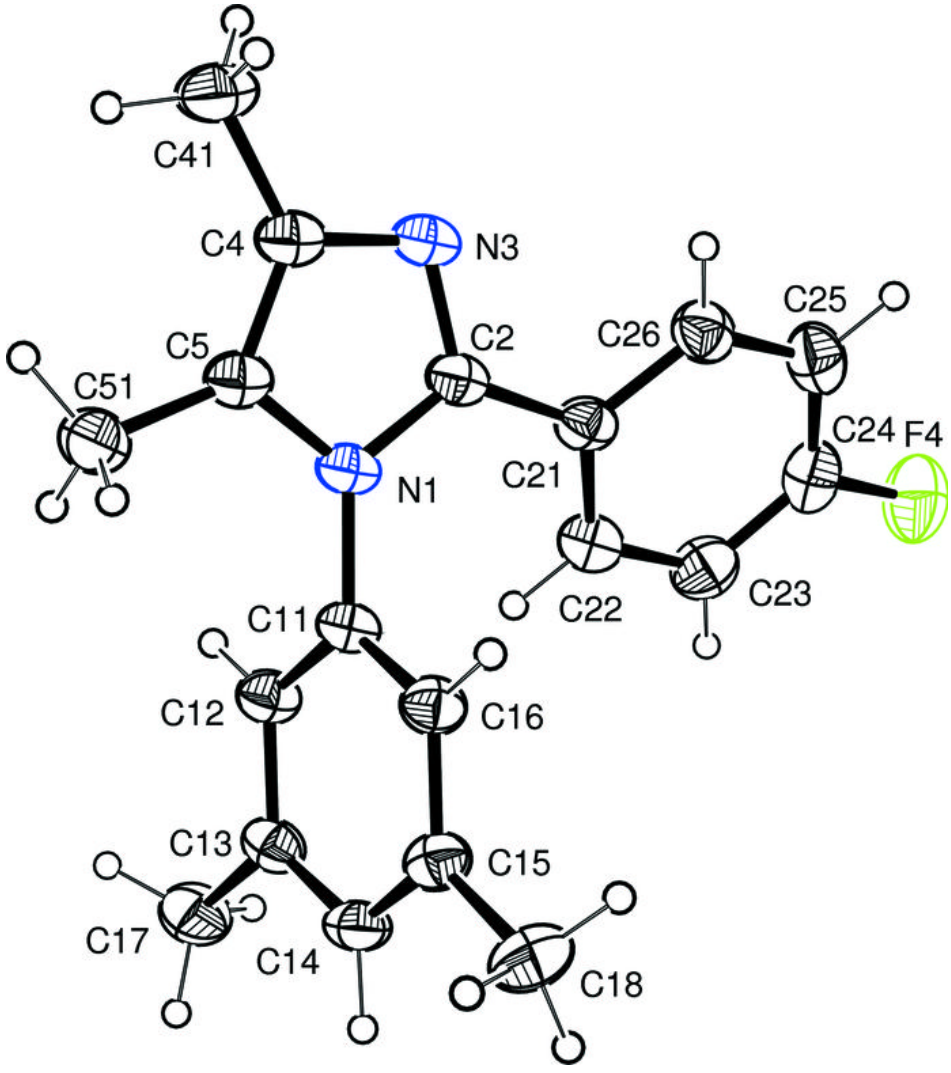
*Hydrogen-bond geometry (Å, °)*

Cg3 is the centroid of the C21–C26 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···Cg3$^{i}$ | 0.95 | 2.86 | 3.7969 (19) | 169 |

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

**Fig. 1**


C41
C4
N3
C5
C2
C26
C25
C51
C24
F4
N1
C21
C22
C23
C11
C12
C16
C13
C15
C17
C14
C18