Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 1-{5-Methyl-1-[8-(trifluoromethyl)-quinolin-4-yl]-1*H*-1,2,3-triazol-4-yl}-ethanone

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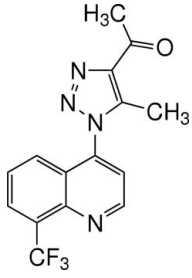
Received 3 November 2007; accepted 14 November 2007

Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.043; $wR$ factor = 0.126; data-to-parameter ratio = 22.0.

In the title molecule, $C_{15}H_{11}F_3N_4O$, the quinoline unit is nearly planar. The dihedral angle between the pyridine ring and the fused benzene ring is 2.45 (6)°. The triazole ring makes dihedral angles of 63.7 (1) and 64.7 (1)° with the pyridine and benzene rings, respectively. The ethanone group is coplanar with the attached triazole ring, except for the methyl H atoms. C—H···O, C—H···N and C—H···F hydrogen bonds are found in the crystal structure.

## Related literature

For the uses of 1,2,3-triazoles and their benzo derivatives, see Banu *et al.* (1999); Biagi *et al.* (2004); Chen *et al.* (2000); Jilino & Stevens (1998); Kreutzberger & Stratmann (1980); Manfredini *et al.* (2000); Melo *et al.* (2003); Passannanti *et al.* (1988); Peter & Roger (2004); Safonova *et al.* (2003); Sanghvi *et al.* (1990); Sherement *et al.* (2004).




## Experimental

### Crystal data

$C_{15}H_{11}F_3N_4O$
$M_r$ = 320.28
Monoclinic, $P2_1/n$
$a$ = 11.7974 (4) Å
$b$ = 8.2946 (2) Å
$c$ = 14.6706 (4) Å
$\beta$ = 106.273 (3)°
$V$ = 1378.07 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 200 (2) K
0.44 × 0.37 × 0.22 mm

### Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.962, $T_{max}$ = 1.000 (expected range = 0.935–0.972)
13863 measured reflections
4615 independent reflections
2511 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.126
$S$ = 0.96
4615 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C12—H12···N3$^{i}$ | 0.95 | 2.61 | 3.559 (2) | 173 |
| C15—H15···N2 | 0.95 | 2.55 | 3.101 (2) | 117 |
| C17—H17···F1 | 0.95 | 2.31 | 2.668 (2) | 102 |
| C17—H17···O41$^{ii}$ | 0.95 | 2.43 | 3.196 (2) | 138 |
| C42—H42$A$···F1$^{iii}$ | 0.98 | 2.52 | 3.373 (2) | 146 |
| C42—H42$B$···F3$^{iv}$ | 0.98 | 2.48 | 3.434 (2) | 165 |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer. AT thanks the UGC, India, for the award of a Minor Research Project [File No. MRP-2355/06(UGC-SERO), Link No. 2355, 10/01/2007].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2045).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4813-o4814 [ **doi:10.1107/S1600536807059193** ]

# 1-{5-Methyl-1-[8-(trifluoromethyl)quinolin-4-yl]-1*H*-1,2,3-triazol-4-yl}ethanone

**A. Thiruvalluvar, M. Subramanyam, R. J. Butcher and M. Mahalinga**

## Comment

1,2,3-Triazoles and their benzoderivatives have attracted considerable attention because of their theoretical interest and synthetic value. They also find numerous applications in industry and agriculture due to their extensive biological activities and successful application as fluorescent whiteners, light stabilizers and optical brightening agents (Sanghvi, *et al.*, 1990). Many 1,2,3-triazoles are found to be potent antimicrobial (Chen, *et al.*, 2000; Sherement, *et al.*, 2004), analgesic (Kreutzberger & Stratmann, 1980), anti- inflammatory, local anesthetic (Banu, *et al.*, 1999), anticonvulsant (Peter & Roger, 2004), antineoplastic (Passannanti, *et al.*, 1998), antimalarial (Jilino & Stevens, 1998) and antiviral agents (Safonova, *et al.*, 2003). Some of them also exhibited antiproliferative (Manfredini, *et al.*, 2000) and anticancer activity (Melo, *et al.*, 2003). A good number of derivatives of 1,2,3-triazoles are used as DNA cleaving agents and potassium channel activators (Biagi, *et al.*, 2004).

In the title molecule, $C_{15}H_{11}F_3N_4O$, Fig.1., the quinoline unit is nearly planar. The dihedral angle between the pyridine ring and the fused benzene ring is 2.45 (6)°. The triazole ring makes a dihedral angle of 63.7 (1)° and 64.7 (1)°, with that of pyridine and benzene rings respectively. The ethanone group is coplanar with the attached triazole ring, except the methyl H atoms. C—H···O, C—H···N and C—H···F hydrogen bonds are found in the crystal structure; see Fig.2 and hydrogen bond table. Furthermore, there is a short intermolecular C12···C12 contact which is caused by an intermolecular hydrogen bond H12 is involved in as well as by π-stacking effects.

## Experimental

4-Azido-8-trifluoromethyl quinoline (15 g, 0.06 mol) was treated with acetylacetone (6.4 g, 0.06 mol) in methanol (75 ml) and the mixture was cooled to 273 K. Sodium methoxide (3.5 g, 0.06 mol) was added under nitrogen atmosphere to the above mixture and then stirred at ambient temperature for 6–8 h. Progress of the reaction was monitored by TLC (ethylacetate:n-hexane: 2:3, *v*/*v*). The reaction mass was poured into ice cold water, precipitated solid was filtered and washed with water. The crude product was recrystallized from methanol. Yield 13.5 g (65%).

## Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95–0.98Å and $U_{iso}$=1.2–1.5 times $U_{eq}$(C).

## Figures

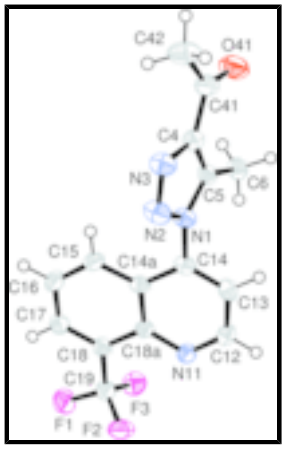


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

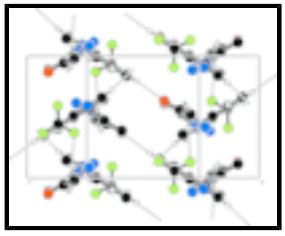

Fig. 2. The packing of the title compound, viewed down the *c* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

### 1-{5-Methyl-1-[8-(trifluoromethyl)quinolin-4-yl]-1*H*-1,2,3-triazol- 4-yl}ethanone

*Crystal data*

| | |
|---|---|
| $C_{15}H_{11}F_3N_4O$ | $F_{000}$ = 656 |
| $M_r$ = 320.28 | $D_x$ = 1.544 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Melting point: 459(1) K |
| Hall symbol: -P 2yn | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| *a* = 11.7974 (4) Å | Cell parameters from 5005 reflections |
| *b* = 8.2946 (2) Å | θ = 4.6–32.5º |
| *c* = 14.6706 (4) Å | μ = 0.13 mm$^{-1}$ |
| β = 106.273 (3)º | *T* = 200 (2) K |
| *V* = 1378.07 (7) Å$^3$ | Plate, colourless |
| *Z* = 4 | 0.44 × 0.37 × 0.22 mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini diffractometer | 4615 independent reflections |
| Radiation source: fine-focus sealed tube | 2511 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.027 |
| *T* = 200(2) K | $\theta_{max}$ = 32.6º |
| φ and ω scans | $\theta_{min}$ = 4.6º |
| Absorption correction: multi-scan | *h* = −17→17 |

(CrysAlis RED; Oxford Diffraction, 2007)

$T_{min}$ = 0.962, $T_{max}$ = 1.000

13863 measured reflections

$k$ = −12→11

$l$ = −22→20

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.043

$wR(F^2)$ = 0.126

$S$ = 0.96

4615 reflections

210 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = <0.001

$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$

$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

Extinction correction: none

*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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.65453 (7) | 0.13558 (11) | 0.67581 (5) | 0.0531 (3) |
| F2 | 0.73949 (7) | −0.09155 (11) | 0.67264 (5) | 0.0470 (3) |
| F3 | 0.83628 (7) | 0.12893 (9) | 0.67695 (5) | 0.0445 (3) |
| O41 | 0.87328 (10) | 0.13080 (14) | −0.00685 (7) | 0.0567 (4) |
| N1 | 0.77553 (9) | −0.04634 (13) | 0.22873 (7) | 0.0309 (3) |
| N2 | 0.67283 (10) | −0.11480 (14) | 0.17371 (7) | 0.0410 (4) |
| N3 | 0.66767 (9) | −0.08334 (14) | 0.08593 (7) | 0.0380 (3) |
| N11 | 0.86194 (9) | −0.09327 (13) | 0.52759 (7) | 0.0303 (3) |
| C4 | 0.76499 (10) | 0.00397 (14) | 0.08307 (8) | 0.0296 (3) |
| C5 | 0.83557 (10) | 0.02833 (14) | 0.17441 (8) | 0.0281 (3) |
| C6 | 0.95054 (10) | 0.11275 (16) | 0.21160 (9) | 0.0343 (4) |
| C12 | 0.92664 (11) | −0.15856 (14) | 0.47733 (8) | 0.0308 (3) |
| C13 | 0.90248 (10) | −0.14431 (15) | 0.37815 (8) | 0.0317 (4) |
| C14 | 0.80417 (10) | −0.06296 (15) | 0.32991 (8) | 0.0279 (3) |
| C14A | 0.72793 (10) | 0.00695 (14) | 0.37893 (8) | 0.0268 (3) |
| C15 | 0.62311 (11) | 0.09220 (15) | 0.33425 (9) | 0.0321 (4) |

| | | | | |
|---|---|---|---|---|
| C16 | 0.55839 (11) | 0.16221 (16) | 0.38699 (9) | 0.0359 (4) |
| C17 | 0.59412 (11) | 0.15093 (15) | 0.48661 (9) | 0.0342 (4) |
| C18 | 0.69379 (10) | 0.06727 (15) | 0.53191 (8) | 0.0289 (4) |
| C18A | 0.76407 (10) | −0.00955 (14) | 0.47940 (8) | 0.0267 (3) |
| C19 | 0.73096 (11) | 0.05847 (17) | 0.63863 (9) | 0.0350 (4) |
| C41 | 0.78389 (12) | 0.05745 (16) | −0.00728 (9) | 0.0370 (4) |
| C42 | 0.69031 (14) | 0.0203 (2) | −0.09740 (9) | 0.0514 (5) |
| H6A | 0.97595 | 0.10527 | 0.28105 | 0.0515* |
| H6B | 1.00988 | 0.06222 | 0.18563 | 0.0515* |
| H6C | 0.94153 | 0.22637 | 0.19263 | 0.0515* |
| H12 | 0.99402 | −0.21921 | 0.51019 | 0.0370* |
| H13 | 0.95383 | −0.19059 | 0.34570 | 0.0380* |
| H15 | 0.59782 | 0.10056 | 0.26699 | 0.0385* |
| H16 | 0.48832 | 0.21932 | 0.35621 | 0.0431* |
| H17 | 0.54873 | 0.20176 | 0.52263 | 0.0410* |
| H42A | 0.69885 | 0.09280 | −0.14779 | 0.0771* |
| H42B | 0.69863 | −0.09168 | −0.11590 | 0.0771* |
| H42C | 0.61224 | 0.03535 | −0.08746 | 0.0771* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0538 (5) | 0.0722 (7) | 0.0382 (4) | 0.0185 (4) | 0.0211 (4) | −0.0015 (4) |
| F2 | 0.0608 (5) | 0.0461 (5) | 0.0365 (4) | 0.0014 (4) | 0.0178 (4) | 0.0109 (3) |
| F3 | 0.0427 (4) | 0.0504 (5) | 0.0361 (4) | −0.0019 (4) | 0.0042 (3) | −0.0039 (3) |
| O41 | 0.0561 (7) | 0.0696 (8) | 0.0486 (6) | −0.0104 (6) | 0.0216 (5) | 0.0131 (5) |
| N1 | 0.0315 (5) | 0.0346 (6) | 0.0267 (5) | −0.0062 (4) | 0.0083 (4) | −0.0024 (4) |
| N2 | 0.0389 (6) | 0.0516 (8) | 0.0316 (6) | −0.0177 (5) | 0.0082 (5) | −0.0046 (5) |
| N3 | 0.0402 (6) | 0.0415 (7) | 0.0313 (5) | −0.0097 (5) | 0.0084 (5) | −0.0037 (5) |
| N11 | 0.0289 (5) | 0.0302 (6) | 0.0310 (5) | 0.0015 (4) | 0.0072 (4) | 0.0024 (4) |
| C4 | 0.0316 (6) | 0.0274 (6) | 0.0294 (6) | −0.0006 (5) | 0.0079 (5) | −0.0011 (5) |
| C5 | 0.0300 (6) | 0.0243 (6) | 0.0326 (6) | 0.0015 (5) | 0.0130 (5) | 0.0004 (5) |
| C6 | 0.0290 (6) | 0.0344 (7) | 0.0406 (7) | −0.0041 (5) | 0.0115 (5) | −0.0005 (5) |
| C12 | 0.0267 (6) | 0.0285 (6) | 0.0343 (6) | 0.0011 (5) | 0.0037 (5) | 0.0000 (5) |
| C13 | 0.0292 (6) | 0.0337 (7) | 0.0333 (6) | −0.0029 (5) | 0.0107 (5) | −0.0065 (5) |
| C14 | 0.0296 (6) | 0.0290 (7) | 0.0249 (5) | −0.0078 (5) | 0.0071 (5) | −0.0020 (5) |
| C14A | 0.0282 (6) | 0.0259 (6) | 0.0258 (6) | −0.0053 (5) | 0.0066 (5) | 0.0014 (5) |
| C15 | 0.0310 (6) | 0.0334 (7) | 0.0287 (6) | −0.0007 (5) | 0.0033 (5) | 0.0072 (5) |
| C16 | 0.0288 (6) | 0.0369 (7) | 0.0393 (7) | 0.0044 (5) | 0.0051 (5) | 0.0088 (6) |
| C17 | 0.0309 (6) | 0.0344 (7) | 0.0389 (7) | 0.0014 (5) | 0.0126 (5) | 0.0020 (5) |
| C18 | 0.0286 (6) | 0.0299 (7) | 0.0288 (6) | −0.0023 (5) | 0.0091 (5) | 0.0014 (5) |
| C18A | 0.0261 (6) | 0.0244 (6) | 0.0293 (6) | −0.0019 (5) | 0.0072 (5) | 0.0032 (5) |
| C19 | 0.0351 (7) | 0.0401 (8) | 0.0314 (6) | 0.0052 (6) | 0.0119 (5) | 0.0020 (6) |
| C41 | 0.0464 (8) | 0.0334 (7) | 0.0332 (7) | 0.0026 (6) | 0.0145 (6) | 0.0018 (6) |
| C42 | 0.0752 (11) | 0.0481 (9) | 0.0289 (7) | −0.0060 (8) | 0.0115 (7) | −0.0021 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| F1—C19 | 1.3399 (16) | C14A—C18A | 1.4216 (16) |

| | | | |
|---|---|---|---|
| F2—C19 | 1.3339 (17) | C15—C16 | 1.3601 (19) |
| F3—C19 | 1.3454 (16) | C16—C17 | 1.4061 (18) |
| O41—C41 | 1.2160 (19) | C17—C18 | 1.3667 (18) |
| N1—N2 | 1.3762 (16) | C18—C18A | 1.4300 (17) |
| N1—C5 | 1.3553 (16) | C18—C19 | 1.5047 (17) |
| N1—C14 | 1.4337 (15) | C41—C42 | 1.4979 (19) |
| N2—N3 | 1.2986 (14) | C6—H6A | 0.9800 |
| N3—C4 | 1.3680 (16) | C6—H6B | 0.9800 |
| N11—C12 | 1.3172 (16) | C6—H6C | 0.9800 |
| N11—C18A | 1.3630 (16) | C12—H12 | 0.9500 |
| C4—C5 | 1.3800 (16) | C13—H13 | 0.9500 |
| C4—C41 | 1.4728 (17) | C15—H15 | 0.9500 |
| C5—C6 | 1.4876 (17) | C16—H16 | 0.9500 |
| C12—C13 | 1.4071 (16) | C17—H17 | 0.9500 |
| C13—C14 | 1.3570 (17) | C42—H42A | 0.9800 |
| C14—C14A | 1.4230 (17) | C42—H42B | 0.9800 |
| C14A—C15 | 1.4158 (18) | C42—H42C | 0.9800 |
| F1···C6$^{i}$ | 3.3366 (15) | C12···C13$^{ii}$ | 3.5320 (17) |
| F2···N11 | 2.8876 (13) | C13···N11$^{ii}$ | 3.3713 (16) |
| F3···N11 | 2.9431 (13) | C13···C6 | 3.4080 (18) |
| F3···C6$^{ii}$ | 3.2730 (15) | C13···C12$^{ii}$ | 3.5320 (17) |
| F1···H42A$^{iii}$ | 2.5200 | C15···N2$^{vi}$ | 3.4457 (18) |
| F1···H6C$^{i}$ | 2.8300 | C15···N1$^{vi}$ | 3.4485 (17) |
| F1···H17 | 2.3100 | C15···N2 | 3.1005 (17) |
| F2···H42A$^{iv}$ | 2.7700 | C16···C4$^{vi}$ | 3.4724 (18) |
| F2···H16$^{v}$ | 2.8100 | C16···C5$^{vi}$ | 3.4972 (18) |
| F3···H42B$^{vi}$ | 2.4800 | C17···O41$^{i}$ | 3.1961 (18) |
| F3···H6B$^{ii}$ | 2.8000 | C17···C17$^{v}$ | 3.4415 (18) |
| F3···H13$^{ii}$ | 2.6400 | C41···N11$^{vi}$ | 3.3399 (17) |
| O41···C6 | 3.0801 (16) | C41···C12$^{vi}$ | 3.5387 (19) |
| O41···C17$^{vii}$ | 3.1961 (18) | C5···H13 | 3.1000 |
| O41···H6B | 2.8900 | C13···H15$^{iv}$ | 3.0000 |
| O41···H6C | 2.9200 | C13···H6A | 2.7900 |
| O41···H17$^{vii}$ | 2.4300 | C14···H6A | 2.7200 |
| N1···C15$^{iv}$ | 3.4485 (17) | C14A···H6C$^{iv}$ | 3.0600 |
| N2···C15 | 3.1005 (17) | C19···H42B$^{vi}$ | 3.0600 |
| N2···C6$^{iv}$ | 3.3807 (17) | H6A···C13 | 2.7900 |
| N2···C15$^{iv}$ | 3.4457 (18) | H6A···C14 | 2.7200 |
| N11···C41$^{iv}$ | 3.3399 (17) | H6A···N11$^{ii}$ | 2.9200 |
| N11···F3 | 2.9431 (13) | H6B···O41 | 2.8900 |
| N11···C13$^{ii}$ | 3.3713 (16) | H6B···F3$^{ii}$ | 2.8000 |
| N11···F2 | 2.8876 (13) | H6C···O41 | 2.9200 |
| N11···C12$^{ii}$ | 3.2696 (17) | H6C···C14A$^{vi}$ | 3.0600 |
| N1···H15 | 2.6200 | H6C···F1$^{vii}$ | 2.8300 |

| | | | |
|---|---|---|---|
| N2···H15 | 2.5500 | H12···N3$^{ix}$ | 2.6100 |
| N3···H12$^{viii}$ | 2.6100 | H13···C5 | 3.1000 |
| N3···H42C | 2.6300 | H13···H15$^{iv}$ | 2.3500 |
| N11···H6A$^{ii}$ | 2.9200 | H13···F3$^{ii}$ | 2.6400 |
| C4···C12$^{vi}$ | 3.5509 (17) | H15···N1 | 2.6200 |
| C4···C16$^{iv}$ | 3.4724 (18) | H15···N2 | 2.5500 |
| C5···C16$^{iv}$ | 3.4972 (18) | H15···C13$^{vi}$ | 3.0000 |
| C6···C13 | 3.4080 (18) | H15···H13$^{vi}$ | 2.3500 |
| C6···O41 | 3.0801 (16) | H16···F2$^{v}$ | 2.8100 |
| C6···F1$^{vii}$ | 3.3366 (15) | H17···F1 | 2.3100 |
| C6···N2$^{vi}$ | 3.3807 (17) | H17···O41$^{i}$ | 2.4300 |
| C6···F3$^{ii}$ | 3.2730 (15) | H42A···F1$^{x}$ | 2.5200 |
| C12···C4$^{iv}$ | 3.5509 (17) | H42A···F2$^{vi}$ | 2.7700 |
| C12···C12$^{ii}$ | 3.1164 (17) | H42B···F3$^{iv}$ | 2.4800 |
| C12···C41$^{iv}$ | 3.5387 (19) | H42B···C19$^{iv}$ | 3.0600 |
| C12···N11$^{ii}$ | 3.2696 (17) | H42C···N3 | 2.6300 |
| N2—N1—C5 | 111.28 (9) | F1—C19—F3 | 105.70 (10) |
| N2—N1—C14 | 118.75 (10) | F1—C19—C18 | 111.55 (11) |
| C5—N1—C14 | 129.97 (11) | F2—C19—F3 | 106.55 (10) |
| N1—N2—N3 | 106.72 (10) | F2—C19—C18 | 113.82 (11) |
| N2—N3—C4 | 109.29 (10) | F3—C19—C18 | 112.30 (11) |
| C12—N11—C18A | 117.30 (10) | O41—C41—C4 | 119.73 (12) |
| N3—C4—C5 | 109.33 (10) | O41—C41—C42 | 122.08 (12) |
| N3—C4—C41 | 121.81 (11) | C4—C41—C42 | 118.19 (12) |
| C5—C4—C41 | 128.87 (11) | C5—C6—H6A | 109.00 |
| N1—C5—C4 | 103.39 (10) | C5—C6—H6B | 109.00 |
| N1—C5—C6 | 124.93 (10) | C5—C6—H6C | 109.00 |
| C4—C5—C6 | 131.69 (11) | H6A—C6—H6B | 109.00 |
| N11—C12—C13 | 124.27 (11) | H6A—C6—H6C | 109.00 |
| C12—C13—C14 | 118.49 (11) | H6B—C6—H6C | 109.00 |
| N1—C14—C13 | 120.45 (11) | N11—C12—H12 | 118.00 |
| N1—C14—C14A | 119.02 (10) | C13—C12—H12 | 118.00 |
| C13—C14—C14A | 120.53 (11) | C12—C13—H13 | 121.00 |
| C14—C14A—C15 | 124.28 (11) | C14—C13—H13 | 121.00 |
| C14—C14A—C18A | 115.87 (11) | C14A—C15—H15 | 120.00 |
| C15—C14A—C18A | 119.83 (11) | C16—C15—H15 | 120.00 |
| C14A—C15—C16 | 120.44 (12) | C15—C16—H16 | 120.00 |
| C15—C16—C17 | 120.68 (12) | C17—C16—H16 | 120.00 |
| C16—C17—C18 | 120.38 (12) | C16—C17—H17 | 120.00 |
| C17—C18—C18A | 120.93 (11) | C18—C17—H17 | 120.00 |
| C17—C18—C19 | 119.39 (11) | C41—C42—H42A | 109.00 |
| C18A—C18—C19 | 119.67 (11) | C41—C42—H42B | 109.00 |
| N11—C18A—C14A | 123.45 (11) | C41—C42—H42C | 109.00 |
| N11—C18A—C18 | 118.84 (10) | H42A—C42—H42B | 109.00 |
| C14A—C18A—C18 | 117.71 (11) | H42A—C42—H42C | 109.00 |

| | | | |
|---|---|---|---|
| F1—C19—F2 | 106.37 (10) | H42B—C42—H42C | 109.00 |
| C5—N1—N2—N3 | −0.27 (14) | C12—C13—C14—C14A | 0.38 (18) |
| C14—N1—N2—N3 | −179.85 (11) | N1—C14—C14A—C15 | 0.63 (18) |
| N2—N1—C5—C4 | 0.37 (13) | N1—C14—C14A—C18A | −177.90 (11) |
| N2—N1—C5—C6 | −179.34 (11) | C13—C14—C14A—C15 | −179.30 (12) |
| C14—N1—C5—C4 | 179.89 (12) | C13—C14—C14A—C18A | 2.17 (17) |
| C14—N1—C5—C6 | 0.2 (2) | C14—C14A—C15—C16 | −176.69 (12) |
| N2—N1—C14—C13 | 116.76 (13) | C18A—C14A—C15—C16 | 1.79 (19) |
| N2—N1—C14—C14A | −63.17 (15) | C14—C14A—C18A—N11 | −3.21 (17) |
| C5—N1—C14—C13 | −62.72 (18) | C14—C14A—C18A—C18 | 176.32 (11) |
| C5—N1—C14—C14A | 117.34 (14) | C15—C14A—C18A—N11 | 178.19 (11) |
| N1—N2—N3—C4 | 0.04 (13) | C15—C14A—C18A—C18 | −2.28 (17) |
| N2—N3—C4—C5 | 0.19 (14) | C14A—C15—C16—C17 | −0.2 (2) |
| N2—N3—C4—C41 | 179.89 (12) | C15—C16—C17—C18 | −0.9 (2) |
| C18A—N11—C12—C13 | 1.42 (18) | C16—C17—C18—C18A | 0.36 (19) |
| C12—N11—C18A—C14A | 1.48 (18) | C16—C17—C18—C19 | 179.32 (12) |
| C12—N11—C18A—C18 | −178.05 (11) | C17—C18—C18A—N11 | −179.22 (12) |
| N3—C4—C5—N1 | −0.34 (13) | C17—C18—C18A—C14A | 1.23 (18) |
| N3—C4—C5—C6 | 179.35 (12) | C19—C18—C18A—N11 | 1.82 (17) |
| C41—C4—C5—N1 | 179.97 (12) | C19—C18—C18A—C14A | −177.73 (11) |
| C41—C4—C5—C6 | −0.3 (2) | C17—C18—C19—F1 | 1.58 (17) |
| N3—C4—C41—O41 | −177.86 (13) | C17—C18—C19—F2 | 121.95 (13) |
| N3—C4—C41—C42 | 2.76 (19) | C17—C18—C19—F3 | −116.87 (13) |
| C5—C4—C41—O41 | 1.8 (2) | C18A—C18—C19—F1 | −179.45 (11) |
| C5—C4—C41—C42 | −177.60 (13) | C18A—C18—C19—F2 | −59.08 (16) |
| N11—C12—C13—C14 | −2.36 (19) | C18A—C18—C19—F3 | 62.10 (16) |
| C12—C13—C14—N1 | −179.56 (11) | | |

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+2, −*y*, −*z*+1; (iii) *x*, *y*, *z*+1; (iv) −*x*+3/2, *y*−1/2, −*z*+1/2; (v) −*x*+1, −*y*, −*z*+1; (vi) −*x*+3/2, *y*+1/2, −*z*+1/2; (vii) *x*+1/2, −*y*+1/2, *z*−1/2; (viii) *x*−1/2, −*y*−1/2, *z*−1/2; (ix) *x*+1/2, −*y*−1/2, *z*+1/2; (x) *x*, *y*, *z*−1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···N3$^{ix}$ | 0.95 | 2.61 | 3.559 (2) | 173.00 |
| C15—H15···N2 | 0.95 | 2.55 | 3.101 (2) | 117.00 |
| C17—H17···F1 | 0.95 | 2.31 | 2.668 (2) | 102.00 |
| C17—H17···O41$^{i}$ | 0.95 | 2.43 | 3.196 (2) | 138.00 |
| C42—H42A···F1$^{x}$ | 0.98 | 2.52 | 3.373 (2) | 146.00 |
| C42—H42B···F3$^{iv}$ | 0.98 | 2.48 | 3.434 (2) | 165.00 |

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

**Fig. 1**

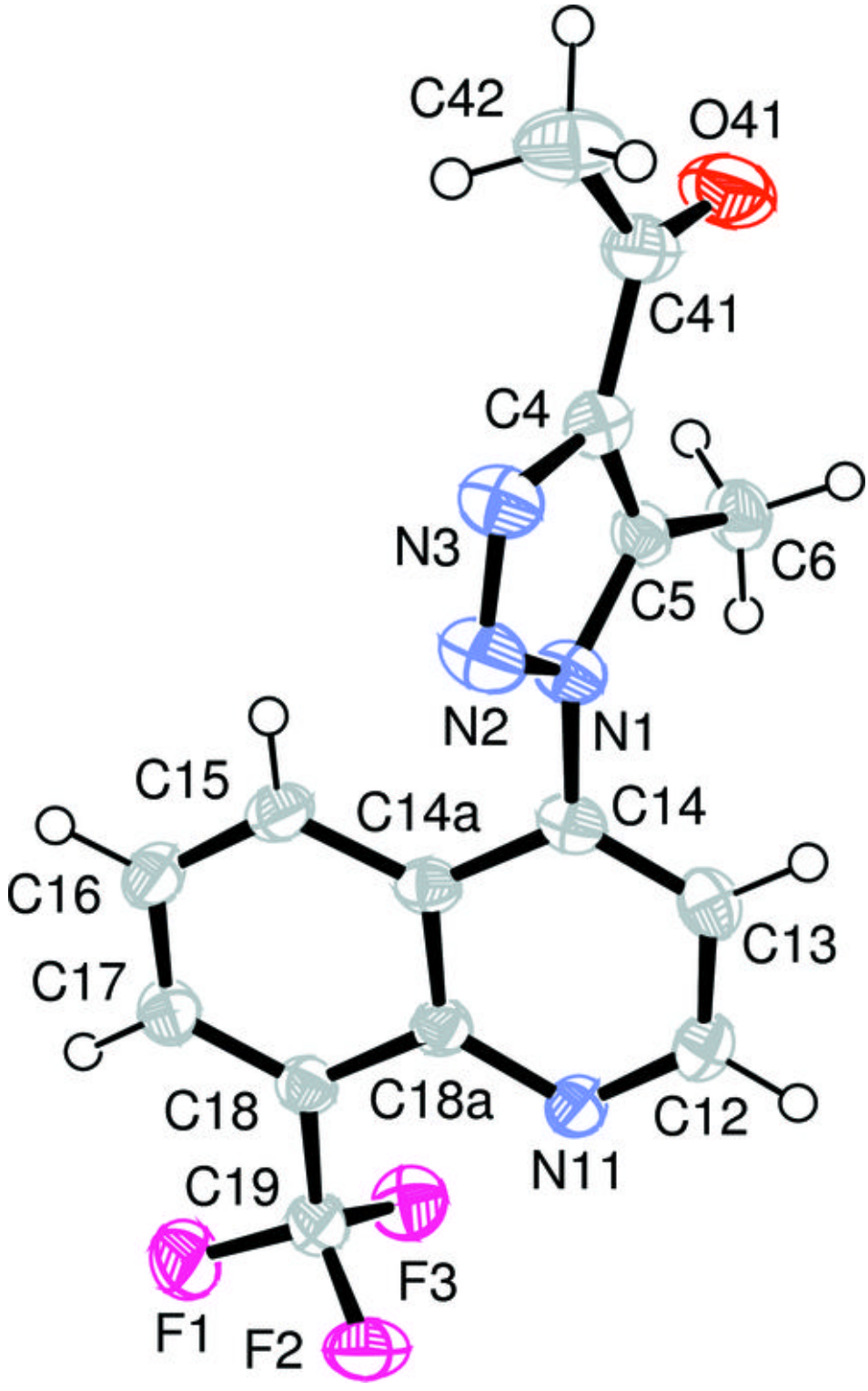
C42
O41
C41
C4
N3
C5
C6
N2
N1
C15
C14a
C14
C16
C13
C17
C18
C18a
C12
N11
C19
F3
F1
F2

**Fig. 2**