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

# 4-[2-(4-Fluorophenyl)-1*H*-pyrrol-3-yl]-pyridine

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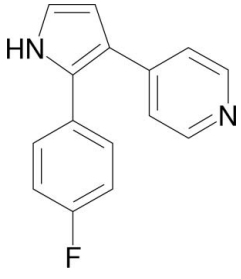
Received 23 January 2009; accepted 29 January 2009

Key indicators: single-crystal X-ray study; $T$ = 193 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.042; $wR$ factor = 0.120; data-to-parameter ratio = 13.3.

In the crystal structure of the title compound, $C_{15}H_{11}FN_2$, the pyrrole ring makes dihedral angles of 33.19 (9) and 36.33 (10)° with the pyridine and 4-fluorophenyl rings, respectively. The pyridine ring makes a dihedral angle of 46.59 (9)° with the 4-fluorophenyl ring. In the crystal structure, an N—H···N hydrogen bond joins the molecules into chains.

## Related literature

Many 1-(4-fluorophenyl)-2-(pyridin-4-yl)pyrrol derivatives have been prepared and their biological activities studied; see: de Laszlo *et al.* (1998); Revesz *et al.* (2000, 2002); Qian *et al.* (2006). For the synthesis of the title compound, see: Qian *et al.* (2006).




## Experimental

### Crystal data

$C_{15}H_{11}FN_2$
$M_r$ = 238.26
Orthorhombic, *Pbca*
$a$ = 9.2966 (7) Å
$b$ = 8.1966 (5) Å
$c$ = 30.5738 (19) Å
$V$ = 2329.7 (3) Å$^3$
$Z$ = 8
Cu $K\alpha$ radiation
$\mu$ = 0.76 mm$^{-1}$
$T$ = 193 (2) K
0.25 × 0.20 × 0.18 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2175 measured reflections
2175 independent reflections
1744 reflections with $I > 2\sigma(I)$
3 standard reflections
frequency: 60 min
intensity decay: 2%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
$S$ = 1.03
2175 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N16$^{i}$ | 0.93 | 1.97 | 2.8696 (19) | 161 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CORINC* (Dräger & Gattow, 1971); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors thank the Alexander von Humbolt Foundation (AvH) for funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2858).

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# supporting information

*Acta Cryst.* (2009). E**65**, o457 [doi:10.1107/S160053680900364X]

## 4-[2-(4-Fluorophenyl)-1*H*-pyrrol-3-yl]pyridine

**Bassam Abu Thaher, Pierre Koch, Dieter Schollmeyer and Stefan Laufer**

### S1. Comment

Functionalized 1-(4-fluorophenyl)-2-(pyridin-4-yl)pyrrols can be used as anticoccidial agents (Qian *et al.* 2006) or as p38 MAP kinase inhibitors (de Laszlo *et al.* 1998; Revesz *et al.* 2000, 2002).

The analysis of the crystal structure of the title compound is shown in Fig. 1. The pyrrole ring makes dihedral angles of 33.19 (9)° and 36.33 (10)° to the pyridine ring and the 4-fluorophenyl ring, respectively. The pyridine ring makes a dihedral angle of 46.59 (9)° to the 4-fluorophenyl ring.

The crystal packing (Fig. 2) shows that N1—H1 of the pyrrole ring forms an intermolecular N—H···N hydrogen bond to the pyridine ring (N16) resulting in a chain parallel to the *a* axis.

### S2. Experimental

Ammonium acetate (2.20 g, 34.9 mmol) was added to a solution of 4-(4-fluorophenyl)-4-oxo-3-(pyridin-4-yl)butanal (0.50 g) in glacial acetic acid (10 ml). The resulting mixture was heated to 388–393 K for 2 h. The solvent was removed under reduced pressure and the residue was diluted with ethyl acetate and aq. $NaHCO_3$ solution. Solid $Na_2CO_3$ was added until effervescence ceased. The organic phase was washed with aq. $NaHCO_3$ solution and brine, dried over $Na_2SO_4$ and the solvent was evaporated under reduced pressure to give crude **I**. The residue was dissolved in ethyl acetate (7 ml) and filtered, then purified by flash chromatography ($SiO_2$, petroleum ether/ethyl acetate 1:1 to 1:4). Yield 135 mg. For X-ray suitable crystals of compound **I** were obtained by slow evaporation at 298 K of a solution of n-hexane–ethyl acetate.

### S3. Refinement

All atoms were located in a differerence Fourier map. Nevertheless, they were placed at calculated positions with C—H = 0.95 Å or N—H = 0.94 Å and they were refined in the riding-model approximation with isotropic displacement parameters set to 1.2 times of the $U_{eq}$ of the parent atom.

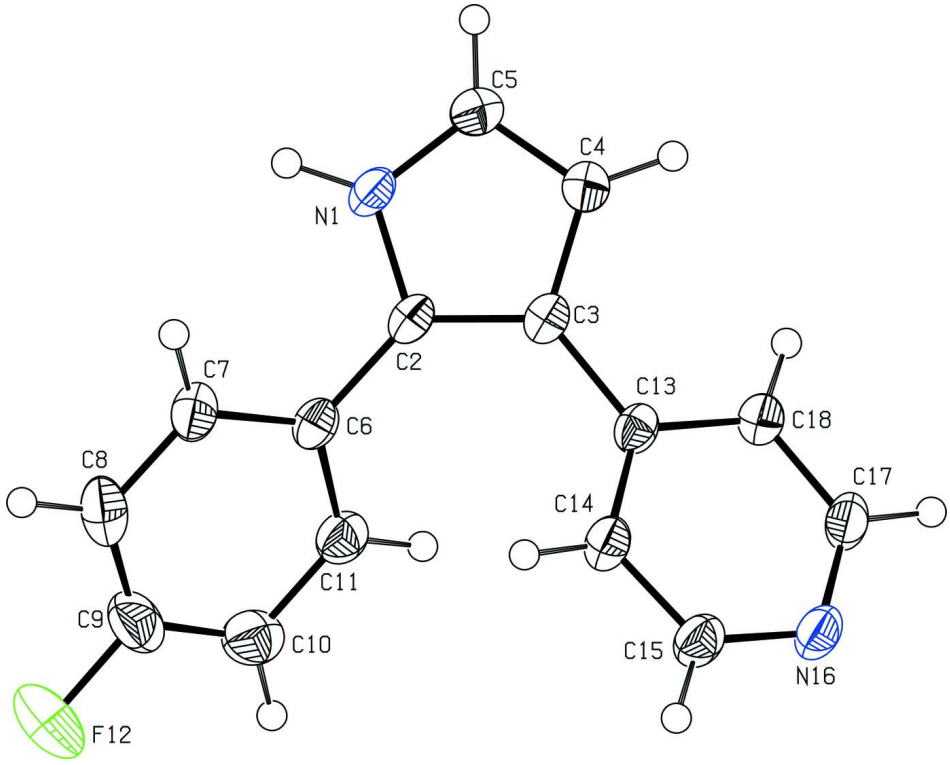


**Figure 1**

View of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are depicted as circles of arbitrary size.

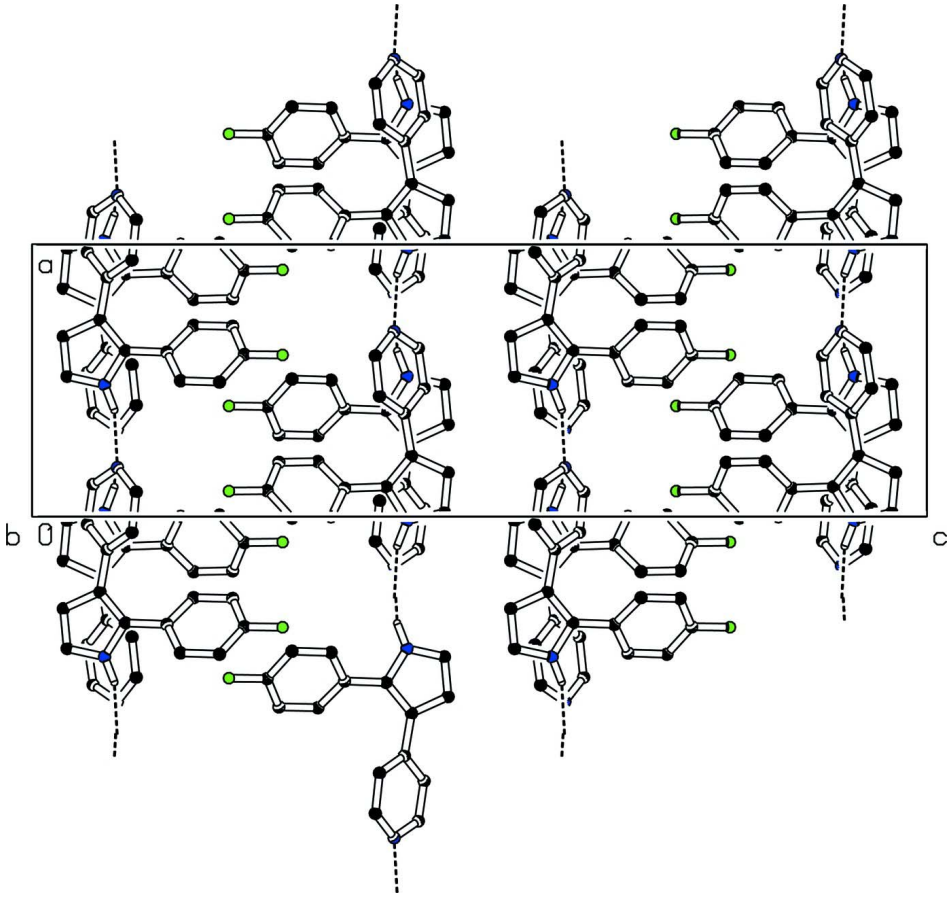


**Figure 2**

Crystal packing of the title compound. The hydrogen bond is shown with dashed lines. View along the *b* axis.

### 4-[2-(4-Fluorophenyl)-1*H*-pyrrol-3-yl]pyridine

*Crystal data*

$C_{15}H_{11}FN_2$
$M_r = 238.26$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 9.2966\ (7)$ Å
$b = 8.1966\ (5)$ Å
$c = 30.5738\ (19)$ Å
$V = 2329.7\ (3)$ Å$^3$
$Z = 8$
$F(000) = 992$
$D_x = 1.359$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 30–51.7°$
$\mu = 0.76$ mm$^{-1}$
$T = 193$ K
Plate, light brown
0.25 × 0.20 × 0.18 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: rotating anode
Graphite monochromator
$\omega/2\theta$ scans
2175 measured reflections
2175 independent reflections
1744 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 69.5°$, $\theta_{min} = 2.9°$
$h = 0\rightarrow11$
$k = -9\rightarrow0$
$l = -36\rightarrow0$
3 standard reflections every 60 min
intensity decay: 2%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.120$
$S = 1.03$
2175 reflections
164 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.5148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00086 (16)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.51524 (14) | 0.21406 (17) | 0.41905 (5) | 0.0278 (3) |
| H1 | 0.6083 | 0.2266 | 0.4081 | 0.033* |
| C2 | 0.39066 (16) | 0.2347 (2) | 0.39570 (6) | 0.0249 (4) |
| C3 | 0.27690 (16) | 0.2008 (2) | 0.42407 (5) | 0.0255 (4) |
| C4 | 0.33869 (18) | 0.1586 (2) | 0.46491 (6) | 0.0311 (4) |
| H4 | 0.2876 | 0.1288 | 0.4906 | 0.037* |
| C5 | 0.48474 (18) | 0.1684 (2) | 0.46075 (6) | 0.0317 (4) |
| H5 | 0.5531 | 0.1470 | 0.4831 | 0.038* |
| C6 | 0.39610 (16) | 0.2800 (2) | 0.34938 (5) | 0.0264 (4) |
| C7 | 0.50091 (18) | 0.3890 (2) | 0.33407 (6) | 0.0331 (4) |
| H7 | 0.5698 | 0.4322 | 0.3539 | 0.040* |
| C8 | 0.5055 (2) | 0.4345 (3) | 0.29053 (6) | 0.0421 (5) |
| H8 | 0.5773 | 0.5075 | 0.2802 | 0.051* |
| C9 | 0.4047 (2) | 0.3721 (3) | 0.26266 (6) | 0.0429 (5) |
| C10 | 0.3009 (2) | 0.2630 (3) | 0.27593 (6) | 0.0395 (5) |
| H10 | 0.2329 | 0.2207 | 0.2557 | 0.047* |
| C11 | 0.29785 (18) | 0.2163 (2) | 0.31936 (6) | 0.0311 (4) |
| H11 | 0.2279 | 0.1397 | 0.3289 | 0.037* |
| F12 | 0.40632 (16) | 0.4201 (2) | 0.22006 (4) | 0.0706 (5) |
| C13 | 0.12145 (16) | 0.20955 (19) | 0.41599 (5) | 0.0244 (4) |
| C14 | 0.05747 (18) | 0.3235 (2) | 0.38834 (6) | 0.0292 (4) |
| H14 | 0.1155 | 0.3991 | 0.3727 | 0.035* |
| C15 | −0.09026 (18) | 0.3267 (2) | 0.38362 (6) | 0.0318 (4) |

| | | | | |
|---|---|---|---|---|
| H15 | −0.1307 | 0.4053 | 0.3644 | 0.038* |
| N16 | −0.17994 (14) | 0.2253 (2) | 0.40458 (5) | 0.0329 (4) |
| C17 | −0.11823 (18) | 0.1169 (2) | 0.43157 (6) | 0.0320 (4) |
| H17 | −0.1791 | 0.0442 | 0.4472 | 0.038* |
| C18 | 0.02834 (17) | 0.1046 (2) | 0.43807 (5) | 0.0286 (4) |
| H18 | 0.0657 | 0.0248 | 0.4575 | 0.034* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0166 (6) | 0.0319 (8) | 0.0348 (8) | −0.0002 (6) | −0.0004 (5) | 0.0008 (6) |
| C2 | 0.0176 (7) | 0.0249 (8) | 0.0322 (9) | 0.0008 (6) | 0.0008 (6) | −0.0021 (6) |
| C3 | 0.0207 (8) | 0.0253 (8) | 0.0304 (8) | −0.0006 (6) | 0.0015 (6) | −0.0009 (7) |
| C4 | 0.0258 (8) | 0.0379 (10) | 0.0297 (9) | 0.0005 (7) | 0.0018 (7) | 0.0050 (7) |
| C5 | 0.0266 (8) | 0.0359 (10) | 0.0327 (9) | 0.0011 (7) | −0.0036 (7) | 0.0037 (7) |
| C6 | 0.0199 (7) | 0.0276 (8) | 0.0316 (9) | 0.0044 (6) | 0.0034 (6) | −0.0020 (6) |
| C7 | 0.0267 (8) | 0.0374 (10) | 0.0353 (9) | −0.0029 (7) | 0.0064 (7) | −0.0013 (7) |
| C8 | 0.0413 (10) | 0.0452 (11) | 0.0399 (10) | −0.0017 (9) | 0.0160 (9) | 0.0048 (8) |
| C9 | 0.0483 (11) | 0.0538 (12) | 0.0266 (9) | 0.0098 (10) | 0.0091 (8) | 0.0025 (8) |
| C10 | 0.0377 (10) | 0.0475 (11) | 0.0332 (10) | 0.0072 (9) | −0.0022 (8) | −0.0071 (8) |
| C11 | 0.0253 (8) | 0.0342 (9) | 0.0339 (9) | 0.0030 (7) | 0.0007 (7) | −0.0027 (7) |
| F12 | 0.0869 (11) | 0.0956 (11) | 0.0292 (6) | −0.0015 (9) | 0.0080 (6) | 0.0113 (7) |
| C13 | 0.0204 (8) | 0.0262 (8) | 0.0264 (8) | −0.0003 (6) | 0.0028 (6) | −0.0052 (6) |
| C14 | 0.0226 (8) | 0.0289 (9) | 0.0361 (9) | 0.0001 (7) | 0.0041 (7) | 0.0013 (7) |
| C15 | 0.0232 (8) | 0.0343 (9) | 0.0380 (10) | 0.0042 (7) | 0.0013 (7) | 0.0012 (8) |
| N16 | 0.0197 (7) | 0.0426 (9) | 0.0362 (8) | 0.0000 (6) | 0.0031 (6) | −0.0027 (7) |
| C17 | 0.0237 (8) | 0.0384 (10) | 0.0339 (9) | −0.0049 (7) | 0.0065 (7) | 0.0000 (7) |
| C18 | 0.0244 (8) | 0.0326 (9) | 0.0286 (8) | −0.0009 (7) | 0.0025 (6) | 0.0005 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C5 | 1.358 (2) | C9—F12 | 1.360 (2) |
| N1—C2 | 1.371 (2) | C9—C10 | 1.377 (3) |
| N1—H1 | 0.9339 | C10—C11 | 1.382 (3) |
| C2—C3 | 1.396 (2) | C10—H10 | 0.9500 |
| C2—C6 | 1.465 (2) | C11—H11 | 0.9500 |
| C3—C4 | 1.417 (2) | C13—C14 | 1.393 (2) |
| C3—C13 | 1.468 (2) | C13—C18 | 1.395 (2) |
| C4—C5 | 1.366 (2) | C14—C15 | 1.381 (2) |
| C4—H4 | 0.9500 | C14—H14 | 0.9500 |
| C5—H5 | 0.9500 | C15—N16 | 1.340 (2) |
| C6—C11 | 1.396 (2) | C15—H15 | 0.9500 |
| C6—C7 | 1.402 (2) | N16—C17 | 1.341 (2) |
| C7—C8 | 1.383 (3) | C17—C18 | 1.381 (2) |
| C7—H7 | 0.9500 | C17—H17 | 0.9500 |
| C8—C9 | 1.366 (3) | C18—H18 | 0.9500 |
| C8—H8 | 0.9500 | | |

| | | | |
|---|---|---|---|
| C5—N1—C2 | 110.27 (14) | F12—C9—C10 | 118.54 (19) |
| C5—N1—H1 | 124.1 | C8—C9—C10 | 122.70 (18) |
| C2—N1—H1 | 125.6 | C9—C10—C11 | 118.50 (18) |
| N1—C2—C3 | 106.96 (15) | C9—C10—H10 | 120.8 |
| N1—C2—C6 | 120.37 (14) | C11—C10—H10 | 120.8 |
| C3—C2—C6 | 132.65 (15) | C10—C11—C6 | 120.97 (17) |
| C2—C3—C4 | 106.80 (14) | C10—C11—H11 | 119.5 |
| C2—C3—C13 | 129.17 (15) | C6—C11—H11 | 119.5 |
| C4—C3—C13 | 124.00 (15) | C14—C13—C18 | 116.25 (15) |
| C5—C4—C3 | 107.84 (15) | C14—C13—C3 | 123.73 (15) |
| C5—C4—H4 | 126.1 | C18—C13—C3 | 119.96 (15) |
| C3—C4—H4 | 126.1 | C15—C14—C13 | 120.04 (16) |
| N1—C5—C4 | 108.13 (15) | C15—C14—H14 | 120.0 |
| N1—C5—H5 | 125.9 | C13—C14—H14 | 120.0 |
| C4—C5—H5 | 125.9 | N16—C15—C14 | 123.85 (17) |
| C11—C6—C7 | 118.26 (16) | N16—C15—H15 | 118.1 |
| C11—C6—C2 | 121.19 (15) | C14—C15—H15 | 118.1 |
| C7—C6—C2 | 120.55 (15) | C15—N16—C17 | 116.02 (14) |
| C8—C7—C6 | 120.96 (18) | N16—C17—C18 | 123.98 (16) |
| C8—C7—H7 | 119.5 | N16—C17—H17 | 118.0 |
| C6—C7—H7 | 119.5 | C18—C17—H17 | 118.0 |
| C9—C8—C7 | 118.57 (18) | C17—C18—C13 | 119.86 (16) |
| C9—C8—H8 | 120.7 | C17—C18—H18 | 120.1 |
| C7—C8—H8 | 120.7 | C13—C18—H18 | 120.1 |
| F12—C9—C8 | 118.76 (19) | | |

| | | | |
|---|---|---|---|
| C5—N1—C2—C3 | 0.13 (19) | C7—C8—C9—C10 | −1.6 (3) |
| C5—N1—C2—C6 | −178.44 (15) | F12—C9—C10—C11 | −178.99 (17) |
| N1—C2—C3—C4 | −0.29 (18) | C8—C9—C10—C11 | 0.8 (3) |
| C6—C2—C3—C4 | 178.03 (17) | C9—C10—C11—C6 | 1.0 (3) |
| N1—C2—C3—C13 | 177.86 (16) | C7—C6—C11—C10 | −1.9 (2) |
| C6—C2—C3—C13 | −3.8 (3) | C2—C6—C11—C10 | 178.16 (16) |
| C2—C3—C4—C5 | 0.4 (2) | C2—C3—C13—C14 | −33.5 (3) |
| C13—C3—C4—C5 | −177.92 (16) | C4—C3—C13—C14 | 144.40 (18) |
| C2—N1—C5—C4 | 0.1 (2) | C2—C3—C13—C18 | 149.46 (17) |
| C3—C4—C5—N1 | −0.3 (2) | C4—C3—C13—C18 | −32.7 (2) |
| N1—C2—C6—C11 | 142.67 (16) | C18—C13—C14—C15 | −0.8 (2) |
| C3—C2—C6—C11 | −35.5 (3) | C3—C13—C14—C15 | −177.95 (16) |
| N1—C2—C6—C7 | −37.2 (2) | C13—C14—C15—N16 | 0.4 (3) |
| C3—C2—C6—C7 | 144.63 (19) | C14—C15—N16—C17 | 0.3 (3) |
| C11—C6—C7—C8 | 1.1 (3) | C15—N16—C17—C18 | −0.7 (3) |
| C2—C6—C7—C8 | −178.99 (17) | N16—C17—C18—C13 | 0.3 (3) |
| C6—C7—C8—C9 | 0.6 (3) | C14—C13—C18—C17 | 0.4 (2) |
| C7—C8—C9—F12 | 178.17 (18) | C3—C13—C18—C17 | 177.73 (16) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···N16$^{i}$ | 0.93 | 1.97 | 2.8696 (19) | 161 |

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