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# 1-Methyl-4-phenyl-3-[4-(trifluoromethyl)phenyl]-1*H*-pyrazolo[3,4-*d*]pyrimidine

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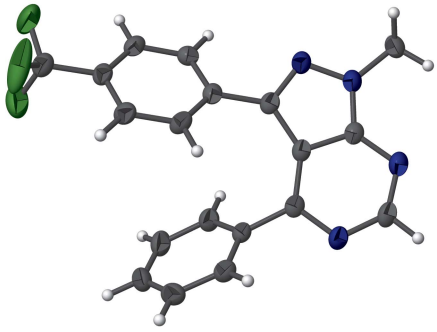
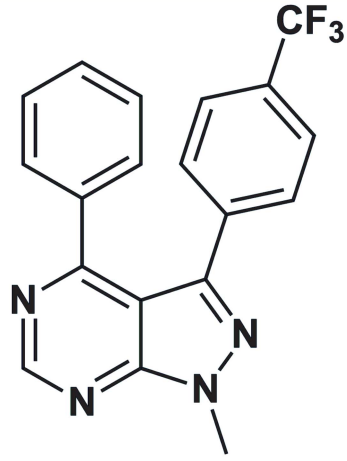
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{19}H_{13}F_3N_4$, the pyrazolopyrimidine unit is slightly non-planar [dihedral angle between the five- and six-membered rings = 3.03 (15)°]. In the crystal, offset head-to-tail $\pi$-stacking interactions between pyrazolopyrimidine units [centroid–centroid separation = 3.665 (2) Å] together with weak C—H···N hydrogen bonds form stepped chains propagating along the *c*-axis direction. The structure was refined as a two-component twin.

3D view



Chemical scheme




## Structure description

Pyrazolo [3,4-*d*] pyrimidine derivatives display a broad spectrum of biological properties, such as antiviral (Bektemirov *et al.*, 1981), antibacterial (Rostamizadeh *et al.*, 2013) and antitumor (Tintori *et al.*, 2015). The present work is a continuation of our studies of pyrazolo[3,4-*d*]pyrimidine derivatives (El Hafi *et al.*, 2017).

In the title molecule (Fig. 1), the pyrazolopyrimidine unit is slightly non-planar as indicated by the dihedral angle of 3.03 (15)° between the mean planes of the five- and six-membered rings. The plane of the C7–C12 benzene ring bearing the $CF_3$ substituent is inclined to the pyrazole moiety by 31.98 (16)° while the plane of the C14–C19 benzene ring is inclined by 50.69 (14)° to that of the pyrimidine ring.

In the crystal, offset, head-to-tail $\pi$-stacking interactions between adjacent pyrazolopyrimidine units reinforced by weak, complementary C6—H6*B*···N1 hydrogen bonds form centrosymmetric dimers, which are connected into stepped chains along the *c* axis direction by weak, complementary C4—H4···N2 hydrogen bonds (Table 1 and Figs. 2 and 3). The centroid–centroid distance for the $\pi$-stacking interaction is 3.665 (2) Å.

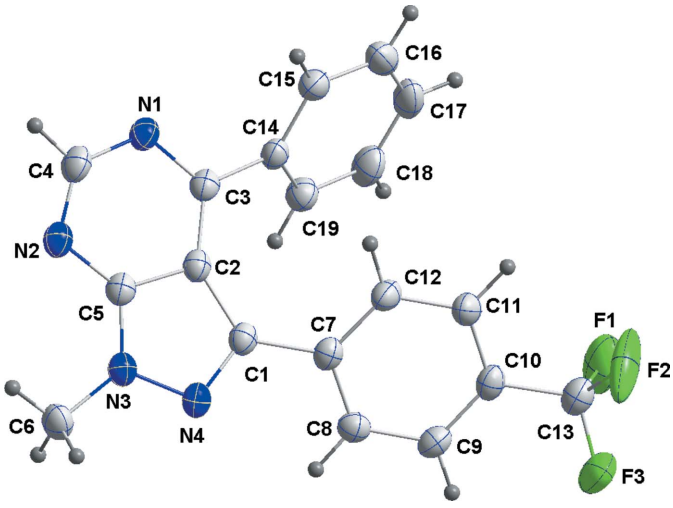



**Figure 1**
The title molecule with 50% probability ellipsoids.

## Synthesis and crystallization

A mixture 1-methyl-4-phenyl-1*H*-pyrazolo [3,4-*d*] pyrimidine (0.1 g, 0.47 mmol), 4-iodobenzotrifluoride (0.26 g, 0.95 mmol), $Cs_2CO_3$ (0.46 g, 1.42 mmol), $K_3PO_4$ (0.25 g, 1.18 mmol), 1,10-phenanthroline (0.034 g, 0.19 mmol), and $Pd(OAc)_2$ (0.021 g, 0.094 mmol) was dissolved/suspended in DMA (3 ml). The resulting mixture was flushed with argon and heated to 165°C for 48 h. After completion of the reaction, the mixture was cooled to room temperature, and the solvent was removed under reduced pressure. Water (15 ml) was added, and the resulting aqueous phase was extracted with $CH_2Cl_2$ (3 × 15 ml). The combined organic layers were dried with $MgSO_4$ and concentrated under vacuum. The residue was purified by column chromatography on silica gel (mixed solvents of EtOAc/ petroleum ether). The title compound was recrystallized from ethanol solution at room temperature in the form of colourless plates (yield: 65%; m.p. 418–420 K).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as a two-component twin.

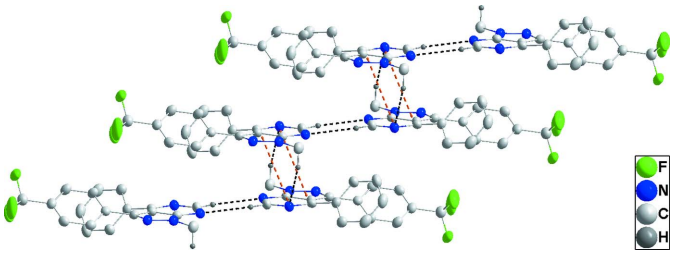



**Figure 2**
Detail of the stepped chain formed by C—H···N hydrogen bonds (black dashed lines) and offset $\pi$-stacking interactions (orange dashed lines).

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4···N2$^{i}$ | 0.96 (3) | 2.66 (3) | 3.588 (4) | 162 (2) |
| C6—H6$B$···N1$^{ii}$ | 1.01 (4) | 2.64 (3) | 3.346 (4) | 127 (2) |

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y+1, -z+1$.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{19}H_{13}F_3N_4$ |
| $M_r$ | 354.33 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 150 |
| $a, b, c$ (Å) | 15.0553 (10), 15.7338 (12), 6.9701 (5) |
| $\beta$ (°) | 99.540 (4) |
| $V$ (Å$^3$) | 1628.2 (2) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.96 |
| Crystal size (mm) | 0.19 × 0.12 × 0.02 |
| Data collection | |
| Diffractometer | Bruker D8 VENTURE PHOTON 100 CMOS |
| Absorption correction | Multi-scan (*TWINABS*; Sheldrick, 2009) |
| $T_{min}$, $T_{max}$ | 0.84, 0.98 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 17099, 16740, 12748 |
| $R_{int}$ | 0.046 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.618 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.060, 0.147, 1.03 |
| No. of reflections | 16740 |
| No. of parameters | 288 |
| H-atom treatment | All H-atom parameters refined |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.45, −0.44 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012), *SHELXTL* (Sheldrick, 2008*a*) and *CELL_NOW* (Sheldrick, 2008*b*).

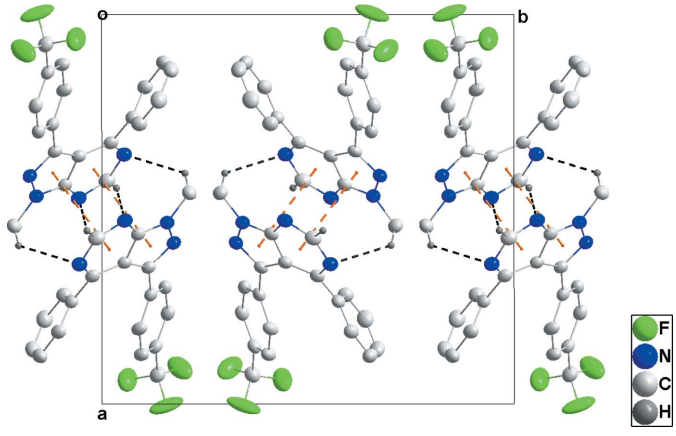



**Figure 3**
Packing projected along the *c*-axis direction giving end views of three adjacent chains. Intermolecular interactions are depicted as in Fig. 2.

## Funding information

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# full crystallographic data

*IUCrData* (2018). **3**, x180875 [https://doi.org/10.1107/S2414314618008751]

## 1-Methyl-4-phenyl-3-[4-(trifluoromethyl)phenyl]-1*H*-pyrazolo[3,4-*d*]pyrimidine

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### 1-Methyl-4-phenyl-3-[4-(trifluoromethyl)phenyl]-1*H*-pyrazolo[3,4-*d*]pyrimidine

*Crystal data*

$C_{19}H_{13}F_3N_4$
$M_r$ = 354.33
Monoclinic, $P2_1/c$
$a$ = 15.0553 (10) Å
$b$ = 15.7338 (12) Å
$c$ = 6.9701 (5) Å
$\beta$ = 99.540 (4)°
$V$ = 1628.2 (2) Å$^3$
$Z$ = 4
$F(000)$ = 728
$D_x$ = 1.445 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 9981 reflections
$\theta$ = 3.0–72.5°
$\mu$ = 0.96 mm$^{-1}$
$T$ = 150 K
Plate, colourless
0.19 × 0.12 × 0.02 mm

*Data collection*

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC I$\mu$S micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
$T_{min}$ = 0.84, $T_{max}$ = 0.98
17099 measured reflections
16740 independent reflections
12748 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046
$\theta_{max}$ = 72.5°, $\theta_{min}$ = 3.0°
$h$ = −18→18
$k$ = −18→18
$l$ = −8→8

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.147
$S$ = 1.02
16740 reflections
288 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.8087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.44 e Å$^{-3}$

*Special details*

**Experimental**. Analysis of 1332 reflections having I/$\sigma$(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008b) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about the *a* axis. The raw data were processed using the multi-component version of*SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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. Refined as a 2-component twin.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.93746 (17) | 0.43794 (15) | −0.1891 (4) | 0.0744 (8) |
| F2 | 1.00377 (15) | 0.3438 (2) | −0.0044 (4) | 0.0895 (10) |
| F3 | 0.90729 (18) | 0.31053 (18) | −0.2496 (4) | 0.0824 (9) |
| N1 | 0.64088 (16) | 0.55427 (16) | 0.7611 (4) | 0.0311 (6) |
| N2 | 0.52893 (16) | 0.44411 (16) | 0.7545 (4) | 0.0315 (6) |
| N3 | 0.53400 (15) | 0.34150 (15) | 0.4998 (4) | 0.0300 (6) |
| N4 | 0.58613 (15) | 0.32541 (15) | 0.3609 (4) | 0.0305 (6) |
| C1 | 0.64887 (18) | 0.38622 (18) | 0.3746 (4) | 0.0277 (6) |
| C2 | 0.63661 (18) | 0.44456 (18) | 0.5265 (4) | 0.0266 (6) |
| C3 | 0.67118 (18) | 0.52239 (18) | 0.6055 (4) | 0.0274 (6) |
| C4 | 0.5736 (2) | 0.5126 (2) | 0.8265 (5) | 0.0337 (7) |
| H4 | 0.5549 (19) | 0.5358 (19) | 0.941 (5) | 0.031 (8)* |
| C5 | 0.56320 (18) | 0.41149 (18) | 0.6036 (4) | 0.0274 (6) |
| C6 | 0.4576 (2) | 0.2875 (2) | 0.5169 (6) | 0.0353 (7) |
| H6A | 0.477 (2) | 0.228 (2) | 0.522 (6) | 0.048 (10)* |
| H6B | 0.407 (2) | 0.298 (2) | 0.405 (6) | 0.036 (9)* |
| H6C | 0.435 (2) | 0.305 (2) | 0.635 (7) | 0.053 (11)* |
| C7 | 0.71865 (19) | 0.38123 (18) | 0.2509 (4) | 0.0272 (6) |
| C8 | 0.6999 (2) | 0.34624 (19) | 0.0652 (5) | 0.0294 (7) |
| H8 | 0.641 (2) | 0.3240 (17) | 0.017 (5) | 0.023 (7)* |
| C9 | 0.7662 (2) | 0.33996 (19) | −0.0502 (5) | 0.0311 (7) |
| H9 | 0.753 (2) | 0.315 (2) | −0.175 (6) | 0.048 (10)* |
| C10 | 0.8521 (2) | 0.36943 (18) | 0.0192 (5) | 0.0306 (7) |
| C11 | 0.8724 (2) | 0.4041 (2) | 0.2034 (5) | 0.0338 (7) |
| H11 | 0.935 (2) | 0.425 (2) | 0.253 (6) | 0.045 (10)* |
| C12 | 0.8064 (2) | 0.4091 (2) | 0.3195 (5) | 0.0322 (7) |
| H12 | 0.821 (2) | 0.434 (2) | 0.447 (5) | 0.036 (9)* |
| C13 | 0.9243 (2) | 0.3649 (2) | −0.1037 (5) | 0.0370 (8) |
| C14 | 0.73663 (19) | 0.57372 (18) | 0.5194 (5) | 0.0282 (7) |
| C15 | 0.8139 (2) | 0.6051 (2) | 0.6335 (5) | 0.0333 (7) |
| H15 | 0.828 (2) | 0.592 (2) | 0.772 (6) | 0.042 (10)* |
| C16 | 0.8760 (2) | 0.6503 (2) | 0.5480 (6) | 0.0405 (8) |
| H16 | 0.931 (2) | 0.668 (2) | 0.627 (6) | 0.044 (10)* |
| C17 | 0.8595 (2) | 0.6674 (2) | 0.3512 (6) | 0.0427 (9) |
| H17 | 0.903 (3) | 0.698 (2) | 0.296 (6) | 0.053 (11)* |
| C18 | 0.7813 (2) | 0.6387 (2) | 0.2375 (6) | 0.0418 (8) |

| | | | | |
|---|---|---|---|---|
| H18 | 0.768 (2) | 0.652 (2) | 0.110 (6) | 0.052 (11)* |
| C19 | 0.7201 (2) | 0.5910 (2) | 0.3209 (5) | 0.0341 (7) |
| H19 | 0.668 (2) | 0.570 (2) | 0.245 (6) | 0.040 (9)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0874 (17) | 0.0592 (15) | 0.092 (2) | 0.0045 (12) | 0.0588 (16) | 0.0163 (13) |
| F2 | 0.0474 (13) | 0.177 (3) | 0.0493 (14) | 0.0533 (16) | 0.0231 (12) | 0.0258 (17) |
| F3 | 0.0830 (17) | 0.0977 (19) | 0.0802 (19) | −0.0278 (14) | 0.0537 (15) | −0.0485 (16) |
| N1 | 0.0312 (13) | 0.0380 (14) | 0.0253 (13) | 0.0007 (10) | 0.0077 (11) | −0.0008 (11) |
| N2 | 0.0297 (13) | 0.0390 (15) | 0.0268 (14) | 0.0030 (10) | 0.0075 (11) | 0.0033 (11) |
| N3 | 0.0280 (12) | 0.0331 (14) | 0.0300 (14) | 0.0000 (10) | 0.0082 (11) | 0.0020 (11) |
| N4 | 0.0287 (12) | 0.0319 (14) | 0.0322 (14) | 0.0037 (10) | 0.0092 (12) | 0.0026 (11) |
| C1 | 0.0245 (14) | 0.0318 (16) | 0.0268 (15) | 0.0046 (11) | 0.0039 (12) | 0.0009 (13) |
| C2 | 0.0235 (13) | 0.0323 (16) | 0.0239 (15) | 0.0031 (11) | 0.0039 (12) | 0.0022 (12) |
| C3 | 0.0256 (14) | 0.0339 (16) | 0.0222 (15) | 0.0036 (11) | 0.0024 (12) | 0.0016 (12) |
| C4 | 0.0343 (16) | 0.0433 (19) | 0.0252 (16) | 0.0038 (13) | 0.0100 (13) | 0.0014 (13) |
| C5 | 0.0263 (14) | 0.0322 (16) | 0.0233 (15) | 0.0041 (11) | 0.0033 (12) | 0.0033 (12) |
| C6 | 0.0327 (16) | 0.0340 (18) | 0.041 (2) | −0.0034 (13) | 0.0116 (16) | 0.0027 (14) |
| C7 | 0.0288 (14) | 0.0261 (15) | 0.0274 (16) | 0.0045 (11) | 0.0065 (13) | 0.0034 (12) |
| C8 | 0.0300 (15) | 0.0268 (15) | 0.0308 (17) | 0.0003 (12) | 0.0030 (13) | 0.0002 (13) |
| C9 | 0.0369 (16) | 0.0306 (16) | 0.0259 (16) | 0.0040 (12) | 0.0059 (14) | −0.0024 (13) |
| C10 | 0.0314 (15) | 0.0287 (15) | 0.0336 (17) | 0.0063 (12) | 0.0108 (13) | 0.0017 (13) |
| C11 | 0.0268 (15) | 0.0361 (17) | 0.0388 (18) | 0.0023 (12) | 0.0063 (14) | −0.0069 (14) |
| C12 | 0.0279 (15) | 0.0385 (18) | 0.0297 (18) | 0.0054 (12) | 0.0034 (13) | −0.0074 (13) |
| C13 | 0.0396 (17) | 0.0376 (18) | 0.0360 (19) | 0.0053 (13) | 0.0125 (15) | −0.0004 (14) |
| C14 | 0.0272 (14) | 0.0285 (16) | 0.0303 (17) | 0.0028 (11) | 0.0089 (13) | −0.0023 (13) |
| C15 | 0.0316 (16) | 0.0360 (17) | 0.0324 (18) | 0.0016 (12) | 0.0060 (14) | −0.0053 (14) |
| C16 | 0.0328 (17) | 0.0355 (18) | 0.054 (2) | −0.0033 (13) | 0.0105 (17) | −0.0080 (17) |
| C17 | 0.0418 (19) | 0.0365 (19) | 0.055 (2) | −0.0040 (15) | 0.0250 (18) | −0.0006 (17) |
| C18 | 0.049 (2) | 0.043 (2) | 0.038 (2) | 0.0016 (15) | 0.0202 (17) | 0.0044 (15) |
| C19 | 0.0342 (17) | 0.0399 (18) | 0.0287 (18) | −0.0001 (14) | 0.0070 (14) | 0.0000 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C13 | 1.324 (4) | C7—C12 | 1.399 (4) |
| F2—C13 | 1.321 (4) | C8—C9 | 1.385 (4) |
| F3—C13 | 1.321 (4) | C8—H8 | 0.96 (3) |
| N1—C3 | 1.342 (4) | C9—C10 | 1.383 (4) |
| N1—C4 | 1.348 (4) | C9—H9 | 0.95 (4) |
| N2—C4 | 1.324 (4) | C10—C11 | 1.382 (5) |
| N2—C5 | 1.347 (4) | C10—C13 | 1.493 (4) |
| N3—C5 | 1.350 (4) | C11—C12 | 1.384 (4) |
| N3—N4 | 1.367 (3) | C11—H11 | 1.00 (4) |
| N3—C6 | 1.451 (4) | C12—H12 | 0.97 (4) |
| N4—C1 | 1.337 (4) | C14—C15 | 1.387 (4) |
| C1—C2 | 1.436 (4) | C14—C19 | 1.392 (5) |

| | | | |
|---|---|---|---|
| C1—C7 | 1.468 (4) | C15—C16 | 1.386 (5) |
| C2—C3 | 1.406 (4) | C15—H15 | 0.98 (4) |
| C2—C5 | 1.406 (4) | C16—C17 | 1.379 (6) |
| C3—C14 | 1.476 (4) | C16—H16 | 0.96 (4) |
| C4—H4 | 0.96 (3) | C17—C18 | 1.382 (5) |
| C6—H6A | 0.99 (4) | C17—H17 | 0.94 (4) |
| C6—H6B | 1.01 (4) | C18—C19 | 1.387 (5) |
| C6—H6C | 0.98 (5) | C18—H18 | 0.90 (4) |
| C7—C8 | 1.392 (4) | C19—H19 | 0.94 (4) |

| | | | |
|---|---|---|---|
| C3—N1—C4 | 117.8 (3) | C8—C9—H9 | 121 (2) |
| C4—N2—C5 | 111.7 (3) | C11—C10—C9 | 120.5 (3) |
| C5—N3—N4 | 110.9 (2) | C11—C10—C13 | 118.8 (3) |
| C5—N3—C6 | 128.7 (3) | C9—C10—C13 | 120.7 (3) |
| N4—N3—C6 | 120.4 (3) | C10—C11—C12 | 119.7 (3) |
| C1—N4—N3 | 107.4 (2) | C10—C11—H11 | 120 (2) |
| N4—C1—C2 | 109.6 (2) | C12—C11—H11 | 120 (2) |
| N4—C1—C7 | 119.1 (3) | C11—C12—C7 | 120.8 (3) |
| C2—C1—C7 | 131.3 (3) | C11—C12—H12 | 119.0 (19) |
| C3—C2—C5 | 115.8 (3) | C7—C12—H12 | 120.2 (19) |
| C3—C2—C1 | 139.5 (3) | F3—C13—F2 | 106.5 (3) |
| C5—C2—C1 | 104.5 (2) | F3—C13—F1 | 103.9 (3) |
| N1—C3—C2 | 119.2 (3) | F2—C13—F1 | 105.3 (3) |
| N1—C3—C14 | 117.6 (3) | F3—C13—C10 | 114.0 (3) |
| C2—C3—C14 | 123.1 (3) | F2—C13—C10 | 113.2 (3) |
| N2—C4—N1 | 129.1 (3) | F1—C13—C10 | 113.2 (3) |
| N2—C4—H4 | 115.1 (18) | C15—C14—C19 | 119.7 (3) |
| N1—C4—H4 | 115.8 (19) | C15—C14—C3 | 121.0 (3) |
| N2—C5—N3 | 126.6 (3) | C19—C14—C3 | 119.3 (3) |
| N2—C5—C2 | 125.7 (3) | C16—C15—C14 | 119.9 (3) |
| N3—C5—C2 | 107.7 (2) | C16—C15—H15 | 119 (2) |
| N3—C6—H6A | 109 (2) | C14—C15—H15 | 121 (2) |
| N3—C6—H6B | 110.0 (19) | C17—C16—C15 | 120.3 (3) |
| H6A—C6—H6B | 112 (3) | C17—C16—H16 | 121 (2) |
| N3—C6—H6C | 108 (2) | C15—C16—H16 | 119 (2) |
| H6A—C6—H6C | 112 (3) | C16—C17—C18 | 120.2 (3) |
| H6B—C6—H6C | 106 (3) | C16—C17—H17 | 119 (2) |
| C8—C7—C12 | 118.4 (3) | C18—C17—H17 | 121 (2) |
| C8—C7—C1 | 120.9 (3) | C17—C18—C19 | 119.9 (3) |
| C12—C7—C1 | 120.7 (3) | C17—C18—H18 | 121 (2) |
| C9—C8—C7 | 120.9 (3) | C19—C18—H18 | 119 (3) |
| C9—C8—H8 | 118.9 (19) | C18—C19—C14 | 120.1 (3) |
| C7—C8—H8 | 120.1 (19) | C18—C19—H19 | 121 (2) |
| C10—C9—C8 | 119.6 (3) | C14—C19—H19 | 119 (2) |
| C10—C9—H9 | 120 (2) | | |

| | | | |
|---|---|---|---|
| C5—N3—N4—C1 | −0.6 (3) | C2—C1—C7—C12 | 30.2 (5) |
| C6—N3—N4—C1 | 177.9 (3) | C12—C7—C8—C9 | −0.7 (4) |

| | | | |
|---|---|---|---|
| N3—N4—C1—C2 | −0.6 (3) | C1—C7—C8—C9 | −178.7 (3) |
| N3—N4—C1—C7 | 175.7 (2) | C7—C8—C9—C10 | −0.5 (4) |
| N4—C1—C2—C3 | −173.5 (3) | C8—C9—C10—C11 | 0.8 (5) |
| C7—C1—C2—C3 | 10.8 (6) | C8—C9—C10—C13 | −178.9 (3) |
| N4—C1—C2—C5 | 1.6 (3) | C9—C10—C11—C12 | 0.2 (5) |
| C7—C1—C2—C5 | −174.1 (3) | C13—C10—C11—C12 | 179.8 (3) |
| C4—N1—C3—C2 | −4.5 (4) | C10—C11—C12—C7 | −1.5 (5) |
| C4—N1—C3—C14 | 172.5 (3) | C8—C7—C12—C11 | 1.7 (4) |
| C5—C2—C3—N1 | 8.1 (4) | C1—C7—C12—C11 | 179.7 (3) |
| C1—C2—C3—N1 | −177.2 (3) | C11—C10—C13—F3 | 161.7 (3) |
| C5—C2—C3—C14 | −168.7 (3) | C9—C10—C13—F3 | −18.7 (4) |
| C1—C2—C3—C14 | 5.9 (6) | C11—C10—C13—F2 | 39.8 (4) |
| C5—N2—C4—N1 | 5.2 (5) | C9—C10—C13—F2 | −140.6 (3) |
| C3—N1—C4—N2 | −2.7 (5) | C11—C10—C13—F1 | −79.9 (4) |
| C4—N2—C5—N3 | 179.1 (3) | C9—C10—C13—F1 | 99.7 (4) |
| C4—N2—C5—C2 | −0.6 (4) | N1—C3—C14—C15 | 51.8 (4) |
| N4—N3—C5—N2 | −178.2 (3) | C2—C3—C14—C15 | −131.3 (3) |
| C6—N3—C5—N2 | 3.4 (5) | N1—C3—C14—C19 | −128.0 (3) |
| N4—N3—C5—C2 | 1.6 (3) | C2—C3—C14—C19 | 48.9 (4) |
| C6—N3—C5—C2 | −176.8 (3) | C19—C14—C15—C16 | −2.7 (5) |
| C3—C2—C5—N2 | −5.7 (4) | C3—C14—C15—C16 | 177.5 (3) |
| C1—C2—C5—N2 | 177.9 (3) | C14—C15—C16—C17 | 2.7 (5) |
| C3—C2—C5—N3 | 174.6 (2) | C15—C16—C17—C18 | −0.7 (5) |
| C1—C2—C5—N3 | −1.9 (3) | C16—C17—C18—C19 | −1.3 (5) |
| N4—C1—C7—C8 | 32.8 (4) | C17—C18—C19—C14 | 1.3 (5) |
| C2—C1—C7—C8 | −151.9 (3) | C15—C14—C19—C18 | 0.7 (5) |
| N4—C1—C7—C12 | −145.2 (3) | C3—C14—C19—C18 | −179.5 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4···N2$^{i}$ | 0.96 (3) | 2.66 (3) | 3.588 (4) | 162 (2) |
| C6—H6*B*···N1$^{ii}$ | 1.01 (4) | 2.64 (3) | 3.346 (4) | 127 (2) |

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