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# *N*-[4-Cyano-3-(trifluoromethyl)phenyl]-2-ethoxybenzamide

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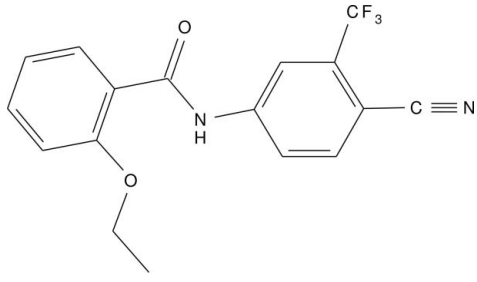
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.049; $wR$ factor = 0.176; data-to-parameter ratio = 12.5.

In the title compound, $C_{17}H_{13}F_3N_2O_2$, the two aromatic rings are essentially coplanar, forming a dihedral angle of 2.78 (12)°. The non-H atoms of the ethoxy group are coplanar with the attached ring [maximum deviation = 0.271 (3) Å]. An intramolecular N—H···O hydrogen bond occurs. In the crystal structure, molecules are linked by intermolecular C—H···N and C—H···F hydrogen bonds.

## Related literature

For background to the biological activity of ethoxybenzamides, see: Mantelingu *et al.* (2007). For related structures, see: Ma *et al.* (2009); Saeed *et al.* (2010).




## Experimental

### Crystal data

$C_{17}H_{13}F_3N_2O_2$
$M_r$ = 334.29
Monoclinic, $P2_1/n$
$a$ = 10.5010 (13) Å
$b$ = 12.8830 (16) Å
$c$ = 11.6130 (14) Å
$\beta$ = 101.653 (6)°
$V$ = 1538.7 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 293 K
0.32 × 0.30 × 0.27 mm

### Data collection

MacScience DIPLabo 32001 diffractometer
5043 measured reflections
2704 independent reflections
1896 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.176
$S$ = 1.02
2704 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N7—H1···O15 | 0.96 | 1.82 | 2.661 (2) | 145 |
| C1—H16···N19$^{i}$ | 0.96 | 2.47 | 3.377 (3) | 157 |
| C13—H18···F23$^{ii}$ | 0.96 | 2.50 | 3.365 (3) | 150 |

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

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2389).

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# supporting information

*Acta Cryst.* (2010). E**66**, o1533 [doi:10.1107/S1600536810019811]

## *N*-[4-Cyano-3-(trifluoromethyl)phenyl]-2-ethoxybenzamide

**S. Naveen, Basappa, H. R. Manjunath, M. A. Sridhar, J. Shashidhara Prasad and K. S. Rangappa**

### S1. Comment

Histone acetyl transfereses (HAT) are enzymes that acetylate conserved lysine amino acids on histone proteins by transferring the acetyl group from acetyl CoA to form *ε*-*N*-acetyl lysine. HAT functions to promote transcriptional activation and has significant histone acetyl transferase activity with core histones (H3 and H4), and also with nucleosome core particles. In addition, HAT inhibits cell-cycle progression and counteracts the mitogenic activity of the adenoviral oncoprotein E1A. A literature survey revealed that the small molecule KCN weakly activated the p300 histone acetyl transferase (Mantelingu *et al.* 2007). With this background, the title compound was synthesized and we report its crystal structure here.

A perspective view of the title compound is shown in Fig. 1. The bond lengths and bond angles are normal and are comparable with values reported earlier for *N*-(3,4-diethoxyphenyl)acetamide (Ma *et al.* 2009). The dihedral angle between the two aromatic rings is 2.78 (12)°, indicating that the two aromatic rings are essentially coplanar. This value differs from the value of 55.69 (3)° reported earlier (Saeed *et al.* 2010). The carbamide group connecting the two rings is -*anti*-*periplanar*, as indicated by the torsion angle value of -177.2 (2)° for C5—N7—C8—C9. The non-H atoms of the ethoxy group lie within the plane of the aromatic ring, as confirmed by the torsion angle value of 174.3 (2)° for C14—O15—C16—C17. In the crystal structure, the molecules exhibit both intramolecular N—H···O and intermolecular hydrogen bonds of the type C—H···N and C—H···F. The molecules exhibit layered stacking when viewed down the *b* axis, as shown in Fig. 2.

### S2. Experimental

*N*-(4-Cyano-3-(trifluoromethyl)phenyl)-2-ethoxybenzamide was synthesized according to the procedure reported earlier (Mantelingu *et al.* 2007). The final product was obtained by crystallization using methanol as solvent. Slow evaporation of the solvent yielded colorless crystals after three days.

### S3. Refinement

H atoms were placed at idealized positions and allowed to ride on their parent atoms with C—H and N—H distances set equal to 0.96 Å; $U_{iso}$(H) = 1.2$U_{eq}$(carrier atom) for all H atoms.

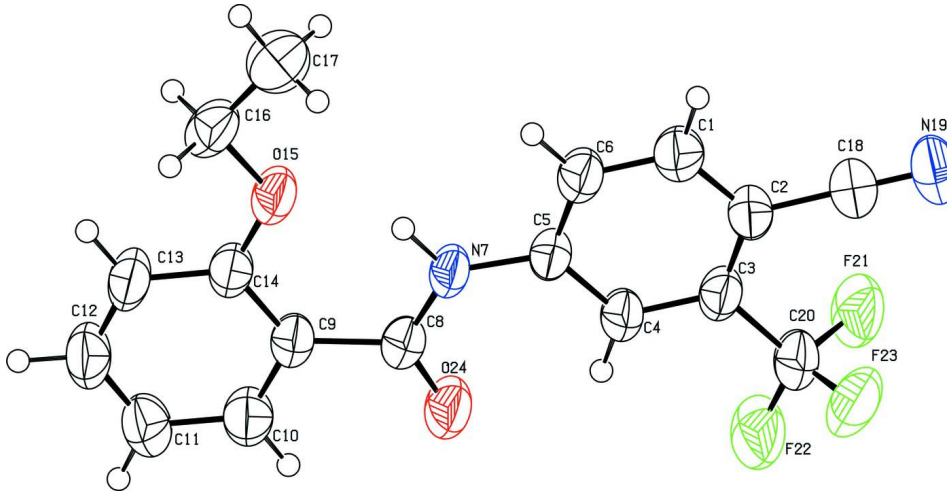


**Figure 1**

A view of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen atoms are shown as spheres of arbitrary radius.

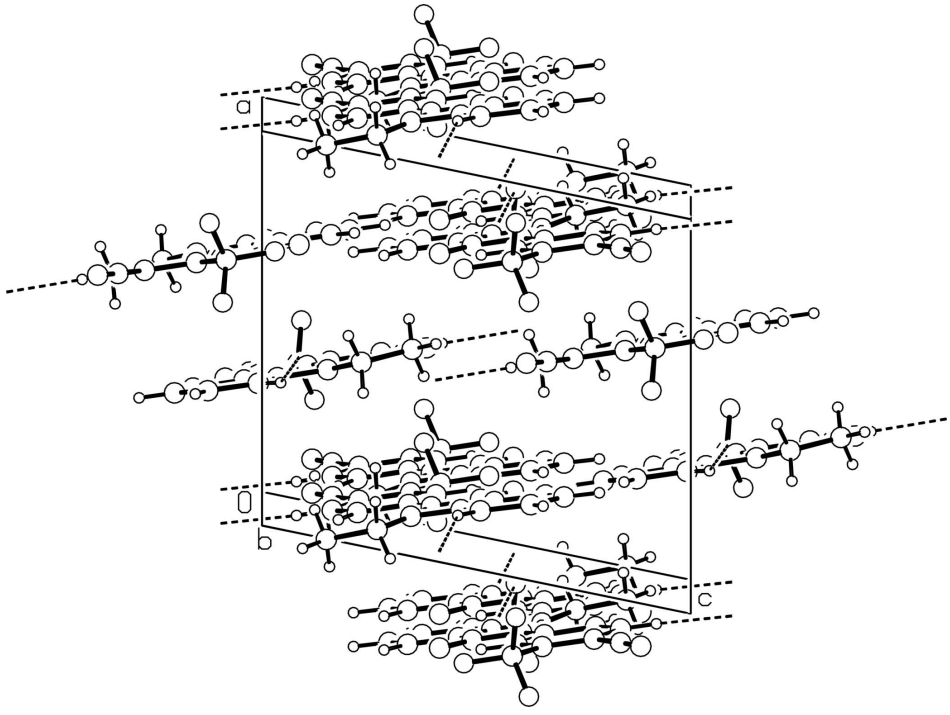


**Figure 2**

Packing diagram of the molecules, viewed down the *b* axis. The dashed lines represent hydrogen bonds. H atoms not involved in the hydrogen bond interactions have been omitted for clarity.

### *N*-(4-cyano-3-(trifluromethyl)phenyl)-2-ethoxybenzamide

*Crystal data*

$C_{17}H_{13}F_3N_2O_2$
$M_r$ = 334.29

Monoclinic, $P2_1/n$
Hall symbol: -P 2yn

$a$ = 10.5010 (13) Å
$b$ = 12.8830 (16) Å
$c$ = 11.6130 (14) Å
$\beta$ = 101.653 (6)°
$V$ = 1538.7 (3) Å$^3$
$Z$ = 4
$F$(000) = 688

$D_x$ = 1.443 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
$\mu$ = 0.12 mm$^{-1}$
$T$ = 293 K
Block, colorless
0.32 × 0.30 × 0.27 mm

*Data collection*

MacScience DIPLabo 32001 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\omega$ scan
5043 measured reflections

2704 independent reflections
1896 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.4°
$h$ = −12→12
$k$ = −15→15
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.176
$S$ = 1.02
2704 reflections
217 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
$w = 1/[\sigma^2(F_o^2) + (0.1179P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N7 | 0.87506 (17) | 0.12966 (13) | 0.60529 (15) | 0.0493 (5) |
| H1 | 0.8991 | 0.0685 | 0.6519 | 0.059* |
| O24 | 0.7968 (2) | 0.17185 (12) | 0.41408 (15) | 0.0740 (6) |
| O15 | 0.89269 (17) | −0.07252 (11) | 0.65288 (15) | 0.0610 (5) |
| F21 | 0.75451 (17) | 0.57018 (11) | 0.62234 (16) | 0.0844 (5) |
| F22 | 0.79874 (19) | 0.49654 (12) | 0.47046 (14) | 0.0996 (7) |
| C6 | 0.9373 (2) | 0.23273 (17) | 0.7779 (2) | 0.0566 (6) |
| H6 | 0.9602 | 0.1701 | 0.8220 | 0.068* |
| C14 | 0.8480 (2) | −0.09241 (16) | 0.5358 (2) | 0.0513 (6) |
| C5 | 0.8896 (2) | 0.22760 (15) | 0.6581 (2) | 0.0474 (5) |
| C9 | 0.8176 (2) | −0.00775 (16) | 0.45831 (19) | 0.0489 (5) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.9212 (2) | 0.41873 (16) | 0.7744 (2) | 0.0537 (6) |
| C8 | 0.8285 (2) | 0.10574 (17) | 0.4903 (2) | 0.0501 (6) |
| F23 | 0.94844 (17) | 0.57372 (11) | 0.59172 (17) | 0.0881 (6) |
| C10 | 0.7724 (2) | −0.0286 (2) | 0.3392 (2) | 0.0608 (6) |
| H13 | 0.7506 | 0.0277 | 0.2847 | 0.073* |
| C4 | 0.8589 (2) | 0.31994 (16) | 0.5946 (2) | 0.0516 (6) |
| H14 | 0.8274 | 0.3167 | 0.5111 | 0.062* |
| C18 | 0.9345 (2) | 0.51680 (19) | 0.8361 (2) | 0.0638 (6) |
| C1 | 0.9528 (2) | 0.32671 (18) | 0.8361 (2) | 0.0602 (6) |
| H16 | 0.9846 | 0.3279 | 0.9196 | 0.072* |
| C3 | 0.8748 (2) | 0.41397 (16) | 0.6531 (2) | 0.0519 (6) |
| C13 | 0.8323 (3) | −0.19283 (18) | 0.4910 (2) | 0.0645 (7) |
| H18 | 0.8507 | −0.2510 | 0.5433 | 0.077* |
| N19 | 0.9424 (3) | 0.59476 (17) | 0.8833 (2) | 0.0817 (7) |
| C20 | 0.8439 (3) | 0.51243 (18) | 0.5837 (2) | 0.0641 (7) |
| C16 | 0.9363 (3) | −0.15806 (18) | 0.7317 (2) | 0.0650 (7) |
| H21A | 0.8635 | −0.2019 | 0.7358 | 0.078* |
| H21B | 1.0002 | −0.1970 | 0.7014 | 0.078* |
| C11 | 0.7590 (3) | −0.1291 (2) | 0.2959 (2) | 0.0684 (7) |
| H22 | 0.7290 | −0.1410 | 0.2133 | 0.082* |
| C12 | 0.7889 (3) | −0.2104 (2) | 0.3733 (3) | 0.0699 (7) |
| H23 | 0.7802 | −0.2804 | 0.3444 | 0.084* |
| C17 | 0.9919 (3) | −0.1132 (2) | 0.8500 (2) | 0.0771 (8) |
| H24A | 1.0226 | −0.1674 | 0.9054 | 0.092* |
| H24B | 0.9264 | −0.0736 | 0.8771 | 0.092* |
| H24C | 1.0631 | −0.0686 | 0.8426 | 0.092* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N7 | 0.0650 (11) | 0.0285 (9) | 0.0529 (11) | 0.0026 (8) | 0.0082 (8) | 0.0020 (7) |
| O24 | 0.1173 (15) | 0.0391 (9) | 0.0591 (11) | 0.0047 (9) | 0.0021 (10) | 0.0044 (8) |
| O15 | 0.0839 (11) | 0.0346 (8) | 0.0620 (11) | 0.0028 (8) | 0.0085 (8) | 0.0058 (7) |
| F21 | 0.0949 (11) | 0.0477 (9) | 0.1143 (14) | 0.0226 (8) | 0.0300 (10) | 0.0033 (8) |
| F22 | 0.1628 (18) | 0.0520 (9) | 0.0731 (11) | 0.0248 (10) | −0.0023 (10) | 0.0071 (8) |
| C6 | 0.0748 (15) | 0.0384 (12) | 0.0545 (14) | 0.0010 (11) | 0.0080 (11) | 0.0026 (10) |
| C14 | 0.0574 (13) | 0.0365 (11) | 0.0605 (14) | −0.0025 (9) | 0.0134 (10) | −0.0019 (9) |
| C5 | 0.0554 (12) | 0.0329 (10) | 0.0547 (13) | −0.0006 (9) | 0.0129 (9) | −0.0007 (9) |
| C9 | 0.0533 (12) | 0.0353 (11) | 0.0585 (14) | 0.0004 (9) | 0.0118 (10) | −0.0014 (10) |
| C2 | 0.0624 (13) | 0.0408 (12) | 0.0594 (15) | −0.0033 (10) | 0.0159 (11) | −0.0071 (10) |
| C8 | 0.0585 (13) | 0.0361 (11) | 0.0557 (14) | 0.0011 (9) | 0.0117 (10) | 0.0022 (10) |
| F23 | 0.1009 (12) | 0.0474 (8) | 0.1229 (15) | −0.0056 (8) | 0.0386 (10) | 0.0167 (8) |
| C10 | 0.0701 (15) | 0.0484 (13) | 0.0618 (15) | −0.0015 (11) | 0.0080 (11) | −0.0035 (11) |
| C4 | 0.0682 (14) | 0.0342 (11) | 0.0521 (13) | 0.0048 (10) | 0.0116 (10) | −0.0004 (9) |
| C18 | 0.0779 (16) | 0.0476 (14) | 0.0669 (15) | −0.0019 (12) | 0.0174 (12) | −0.0099 (12) |
| C1 | 0.0761 (16) | 0.0492 (13) | 0.0534 (13) | −0.0027 (11) | 0.0084 (11) | −0.0021 (11) |
| C3 | 0.0587 (13) | 0.0338 (11) | 0.0657 (15) | 0.0021 (9) | 0.0187 (11) | 0.0008 (10) |
| C13 | 0.0798 (16) | 0.0325 (11) | 0.0818 (18) | −0.0040 (11) | 0.0178 (13) | −0.0010 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N19 | 0.110 (2) | 0.0529 (13) | 0.0824 (17) | −0.0022 (12) | 0.0193 (14) | −0.0211 (12) |
| C20 | 0.0848 (17) | 0.0377 (12) | 0.0706 (17) | 0.0092 (12) | 0.0173 (13) | −0.0013 (11) |
| C16 | 0.0742 (15) | 0.0465 (13) | 0.0750 (17) | 0.0069 (12) | 0.0167 (13) | 0.0178 (12) |
| C11 | 0.0798 (17) | 0.0554 (15) | 0.0681 (16) | −0.0080 (13) | 0.0105 (13) | −0.0169 (13) |
| C12 | 0.0812 (17) | 0.0438 (13) | 0.086 (2) | −0.0117 (12) | 0.0192 (14) | −0.0166 (13) |
| C17 | 0.0840 (18) | 0.0718 (18) | 0.0721 (18) | 0.0127 (15) | 0.0080 (14) | 0.0129 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N7—C8 | 1.362 (3) | F23—C20 | 1.340 (3) |
| N7—C5 | 1.398 (3) | C10—C11 | 1.386 (3) |
| N7—H1 | 0.9600 | C10—H13 | 0.9600 |
| O24—C8 | 1.225 (3) | C4—C3 | 1.382 (3) |
| O15—C14 | 1.370 (3) | C4—H14 | 0.9598 |
| O15—C16 | 1.447 (3) | C18—N19 | 1.139 (3) |
| F21—C20 | 1.344 (3) | C1—H16 | 0.9599 |
| F22—C20 | 1.321 (3) | C3—C20 | 1.503 (3) |
| C6—C1 | 1.380 (3) | C13—C12 | 1.370 (4) |
| C6—C5 | 1.381 (3) | C13—H18 | 0.9600 |
| C6—H6 | 0.9600 | C16—C17 | 1.496 (4) |
| C14—C13 | 1.392 (3) | C16—H21A | 0.9600 |
| C14—C9 | 1.409 (3) | C16—H21B | 0.9599 |
| C5—C4 | 1.403 (3) | C11—C12 | 1.374 (4) |
| C9—C10 | 1.395 (3) | C11—H22 | 0.9600 |
| C9—C8 | 1.507 (3) | C12—H23 | 0.9601 |
| C2—C1 | 1.390 (3) | C17—H24A | 0.9600 |
| C2—C3 | 1.395 (3) | C17—H24B | 0.9600 |
| C2—C18 | 1.445 (3) | C17—H24C | 0.9600 |
| | | | |
| C8—N7—C5 | 128.36 (18) | C2—C1—H16 | 120.3 |
| C8—N7—H1 | 111.7 | C4—C3—C2 | 121.2 (2) |
| C5—N7—H1 | 120.0 | C4—C3—C20 | 119.0 (2) |
| C14—O15—C16 | 119.14 (18) | C2—C3—C20 | 119.9 (2) |
| C1—C6—C5 | 121.2 (2) | C12—C13—C14 | 121.1 (2) |
| C1—C6—H6 | 118.9 | C12—C13—H18 | 119.2 |
| C5—C6—H6 | 119.9 | C14—C13—H18 | 119.7 |
| O15—C14—C13 | 122.4 (2) | F22—C20—F23 | 106.6 (2) |
| O15—C14—C9 | 118.49 (19) | F22—C20—F21 | 106.5 (2) |
| C13—C14—C9 | 119.1 (2) | F23—C20—F21 | 105.6 (2) |
| C6—C5—N7 | 118.07 (19) | F22—C20—C3 | 113.5 (2) |
| C6—C5—C4 | 119.1 (2) | F23—C20—C3 | 112.1 (2) |
| N7—C5—C4 | 122.8 (2) | F21—C20—C3 | 112.2 (2) |
| C10—C9—C14 | 118.1 (2) | O15—C16—C17 | 107.6 (2) |
| C10—C9—C8 | 115.14 (19) | O15—C16—H21A | 109.1 |
| C14—C9—C8 | 126.7 (2) | C17—C16—H21A | 110.4 |
| C1—C2—C3 | 118.8 (2) | O15—C16—H21B | 108.7 |
| C1—C2—C18 | 120.0 (2) | C17—C16—H21B | 111.5 |
| C3—C2—C18 | 121.2 (2) | H21A—C16—H21B | 109.5 |

| | | | |
|---|---|---|---|
| O24—C8—N7 | 122.9 (2) | C12—C11—C10 | 118.8 (2) |
| O24—C8—C9 | 120.1 (2) | C12—C11—H22 | 121.2 |
| N7—C8—C9 | 117.08 (18) | C10—C11—H22 | 120.1 |
| C11—C10—C9 | 122.0 (2) | C13—C12—C11 | 120.9 (2) |
| C11—C10—H13 | 118.2 | C13—C12—H23 | 119.5 |
| C9—C10—H13 | 119.8 | C11—C12—H23 | 119.7 |
| C3—C4—C5 | 119.5 (2) | C16—C17—H24A | 110.5 |
| C3—C4—H14 | 121.1 | C16—C17—H24B | 109.5 |
| C5—C4—H14 | 119.4 | H24A—C17—H24B | 109.5 |
| N19—C18—C2 | 178.5 (3) | C16—C17—H24C | 108.4 |
| C6—C1—C2 | 120.2 (2) | H24A—C17—H24C | 109.5 |
| C6—C1—H16 | 119.4 | H24B—C17—H24C | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N7—H1···O15 | 0.96 | 1.82 | 2.661 (2) | 145 |
| C1—H16···N19$^{i}$ | 0.96 | 2.47 | 3.377 (3) | 157 |
| C13—H18···F23$^{ii}$ | 0.96 | 2.50 | 3.365 (3) | 150 |

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