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# 2-[4-(Trifluoromethoxy)phenyl]-1*H*-benzimidazole

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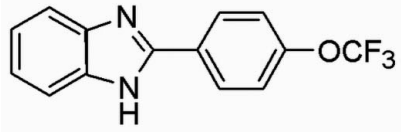
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.064; $wR$ factor = 0.157; data-to-parameter ratio = 10.5.

In the title compound, $C_{14}H_9F_3N_2O$, the best planes of the benzimidazole group and benzene ring form a dihedral angle of 26.68 (3)°. In the crystal, N—H···N hydrogen bonds link the molecules into infinite chains parallel to the $c$ axis. Stacking interactions between the benzimidazole groups [centroid–centroid distance = 3.594 (5) Å] assemble the molecules into layers parallel to (100). The trifluoromethyl group is disordered over three sets of sites with site-occupancy factors of 0.787 (4), 0.107 (7) and 0.106 (7).

## Related literature

For therapeutic and medicinal properties of benzimidazole derivatives, see: Chimirri *et al.* (1991); Benavides *et al.* (1995); Ishihara *et al.* (1994); Kubo *et al.* (1993). For related structures, see: Jian *et al.* (2006); Rashid, Tahir, Yusof *et al.* (2007); Rashid, Tahir, Kanwal *et al.* (2007).




## Experimental

### Crystal data

$C_{14}H_9F_3N_2O$
$M_r$ = 278.23
Monoclinic, $P2_1/c$
$a$ = 14.476 (6) Å
$b$ = 9.312 (4) Å
$c$ = 9.835 (4) Å
$\beta$ = 108.192 (8)°
$V$ = 1259.5 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 296 K
0.18 × 0.16 × 0.16 mm

### Data collection

Bruker SMART APEX CCD detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.978, $T_{max}$ = 0.980
6284 measured reflections
2209 independent reflections
1333 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.077

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.157
$S$ = 1.00
2209 reflections
210 parameters
21 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H21···N1$^{i}$ | 0.86 | 2.07 | 2.864 (4) | 154 |

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2550).

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# supporting information

*Acta Cryst.* (2013). E**69**, o264 [doi:10.1107/S1600536813001220]

## 2-[4-(Trifluoromethoxy)phenyl]-1*H*-benzimidazole

**Nikhath Fathima, M. S. Krishnamurthy and Noor Shahina Begum**

### S1. Comment

Benzimidazole and its derivatives are known to exhibit a wide variety of pharmacological activities such as anti-HIV (Chimirri *et al.*, 1991), antihistaminic (Benavides *et al.*, 1995), antiulcer (Ishihara *et al.*, 1994), antihypertensive (Kubo *et al.*, 1993). The benzimidazole and phenyl groups form a dihedral angle of 26.68 (3)°. The bond lengths and angles of the benzimidazole moiety in the title compound are in good agreement with those observed in other benzimidazole derivatives (Jian *et al.*, 2006; Rashid, Tahir, Yusof *et al.*, 2007; Rashid, Tahir, Kanwal *et al.*, 2007). The N1—C8 and N2—C8 distances were found to be 1.338 (5) Å and 1.356 (5) Å, respectively. The trifluoromethyl group is disordered over three sites with occupancy factors 0.787 (4), 0.107 (7) and 0.106 (7). The molecules are linked by intermolecular N—H···N hydrogen bonds to form infinite chains parallel to the *c* axis. Additionally, the crystal packing is further stabilized by $\pi$ -$\pi$ stacking interactions between the benzimidazole groups [interplanar distance 3.594 (5) Å].

### S2. Experimental

A mixture of 4-(trifluoromethoxy)benzaldehyde (10 mmol, 0.19 g) and *o*-phenyldiamine (10 mmol, 0.19 g) in benzene (2 ml) was refluxed for 6 h on a water bath. The reaction mixture was cooled. The solid separated, was filtered and dried (yield: 0.26 g, 75% and m.p. 503–508 K). Pale yellow crystals of the title compound were obtained by slow evaporation from a solution in ethyl acetate.

### S3. Refinement

All H atoms were included in calculated positions, with C—H bond distances of 0.93 Å and N—H = 0.86 Å and refined in a riding model approximation with $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*). The trifluoromethyl group is disordered over three sites with the occupancy factors 0.787 (4), 0.107 (7) and 0.106 (7). The atoms of the minor components were refined isotropically with a common displacement parameter for each group. The geometry of the minor components was restrained to that of the major component with the SAME instruction of *SHELXL97* (Sheldrick, 2008).

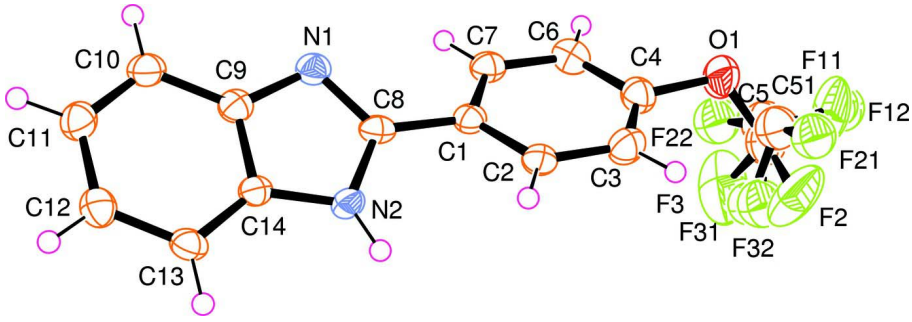


**Figure 1**

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.The trifluoromethyl group is disordered over three sites.

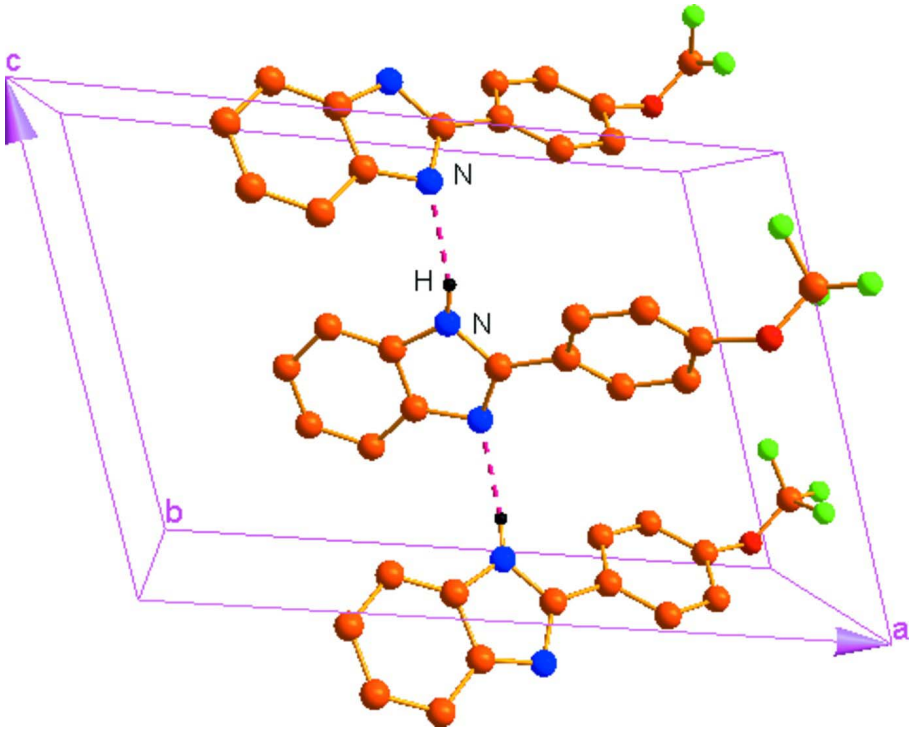


**Figure 2**

A view of the intermolecular hydrogen bonds(dotted lines) in the crystal structure of the title compound. H atoms non participating in H-bonding and minor components of the disordered $CF_3$ group were omitted for clarity.

### 2-[4-(Trifluoromethoxy)phenyl]-1*H*-benzimidazole

*Crystal data*

$C_{14}H_9F_3N_2O$
$M_r = 278.23$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.476$ (6) Å
$b = 9.312$ (4) Å
$c = 9.835$ (4) Å
$\beta = 108.192$ (8)°
$V = 1259.5$ (9) Å$^3$
$Z = 4$
$F(000) = 568$
$D_x = 1.467$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2209 reflections

$\theta$ = 2.6–25.0°
$\mu$ = 0.13 mm$^{-1}$
$T$ = 296 K

Block, yellow
0.18 × 0.16 × 0.16 mm

*Data collection*

Bruker SMART APEX CCD detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.978, $T_{max}$ = 0.980

6284 measured reflections
2209 independent reflections
1333 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.077
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.6°
$h$ = −17→15
$k$ = −8→11
$l$ = −11→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.157
$S$ = 1.00
2209 reflections
210 parameters
21 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
$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.3459 (2) | 0.8348 (3) | 0.4611 (3) | 0.0246 (8) | |
| C2 | 0.3309 (2) | 0.9562 (3) | 0.3748 (3) | 0.0297 (8) | |
| H2 | 0.3786 | 0.9857 | 0.3359 | 0.036* | |
| C3 | 0.2445 (2) | 1.0344 (4) | 0.3460 (4) | 0.0361 (9) | |
| H3 | 0.2352 | 1.1177 | 0.2912 | 0.043* | |
| C4 | 0.1735 (2) | 0.9856 (4) | 0.4004 (4) | 0.0333 (9) | |
| C6 | 0.1860 (2) | 0.8644 (3) | 0.4854 (3) | 0.0321 (9) | |
| H6 | 0.1368 | 0.8332 | 0.5206 | 0.039* | |
| C7 | 0.2734 (2) | 0.7900 (3) | 0.5172 (3) | 0.0284 (8) | |
| H7 | 0.2836 | 0.7097 | 0.5763 | 0.034* | |
| C8 | 0.4390 (2) | 0.7578 (3) | 0.4969 (3) | 0.0245 (8) | |
| C9 | 0.5675 (2) | 0.6361 (3) | 0.6072 (3) | 0.0260 (8) | |
| C10 | 0.6411 (2) | 0.5565 (3) | 0.7050 (3) | 0.0316 (9) | |

| | | | | | |
|---|---|---|---|---|---|
| H10 | 0.6339 | 0.5228 | 0.7901 | 0.038* | |
| C11 | 0.7245 (2) | 0.5305 (3) | 0.6695 (4) | 0.0327 (9) | |
| H11 | 0.7743 | 0.4778 | 0.7323 | 0.039* | |
| C12 | 0.7367 (2) | 0.5806 (3) | 0.5422 (3) | 0.0311 (8) | |
| H12 | 0.7946 | 0.5624 | 0.5233 | 0.037* | |
| C13 | 0.6639 (2) | 0.6567 (3) | 0.4443 (3) | 0.0277 (8) | |
| H13 | 0.6709 | 0.6883 | 0.3583 | 0.033* | |
| C14 | 0.5804 (2) | 0.6840 (3) | 0.4794 (3) | 0.0233 (8) | |
| O1 | 0.08661 (17) | 1.0648 (3) | 0.3804 (3) | 0.0460 (7) | |
| N1 | 0.47847 (18) | 0.6843 (3) | 0.6176 (3) | 0.0272 (7) | |
| N2 | 0.49671 (18) | 0.7606 (3) | 0.4113 (3) | 0.0260 (7) | |
| H21 | 0.4836 | 0.8024 | 0.3295 | 0.031* | |
| C5 | 0.0271 (4) | 1.0787 (7) | 0.2470 (6) | 0.0534 (16) | 0.787 (4) |
| F1 | −0.0537 (4) | 1.1368 (8) | 0.2540 (9) | 0.0740 (15) | 0.787 (4) |
| F2 | 0.0616 (3) | 1.1639 (8) | 0.1658 (6) | 0.0954 (17) | 0.787 (4) |
| F3 | 0.0071 (4) | 0.9548 (6) | 0.1788 (7) | 0.110 (2) | 0.787 (4) |
| C51 | 0.0312 (14) | 1.109 (2) | 0.268 (3) | 0.047 (6)* | 0.107 (7) |
| F11 | −0.0580 (16) | 1.145 (3) | 0.259 (7) | 0.047 (6)* | 0.107 (7) |
| F21 | 0.0781 (14) | 1.2304 (19) | 0.261 (3) | 0.047 (6)* | 0.107 (7) |
| F31 | 0.030 (3) | 1.033 (3) | 0.154 (4) | 0.047 (6)* | 0.107 (7) |
| C52 | 0.010 (2) | 1.062 (3) | 0.270 (3) | 0.056 (7)* | 0.106 (7) |
| F12 | −0.066 (4) | 1.144 (3) | 0.251 (8) | 0.056 (7)* | 0.106 (7) |
| F22 | −0.0187 (16) | 0.928 (2) | 0.282 (3) | 0.056 (7)* | 0.106 (7) |
| F32 | 0.037 (4) | 1.064 (4) | 0.154 (4) | 0.056 (7)* | 0.106 (7) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0277 (18) | 0.0240 (18) | 0.0207 (17) | −0.0013 (14) | 0.0055 (14) | −0.0033 (14) |
| C2 | 0.031 (2) | 0.037 (2) | 0.0256 (18) | 0.0045 (15) | 0.0146 (15) | 0.0039 (16) |
| C3 | 0.040 (2) | 0.038 (2) | 0.033 (2) | 0.0027 (17) | 0.0134 (17) | 0.0087 (17) |
| C4 | 0.030 (2) | 0.035 (2) | 0.032 (2) | 0.0030 (16) | 0.0069 (16) | −0.0047 (17) |
| C6 | 0.030 (2) | 0.033 (2) | 0.035 (2) | −0.0056 (15) | 0.0115 (16) | −0.0059 (17) |
| C7 | 0.033 (2) | 0.0275 (19) | 0.0244 (18) | −0.0029 (15) | 0.0087 (15) | −0.0031 (15) |
| C8 | 0.0320 (19) | 0.0228 (18) | 0.0204 (17) | −0.0048 (14) | 0.0105 (15) | −0.0034 (14) |
| C9 | 0.0305 (19) | 0.0217 (18) | 0.0248 (18) | −0.0018 (14) | 0.0069 (14) | −0.0029 (14) |
| C10 | 0.043 (2) | 0.028 (2) | 0.0243 (19) | 0.0028 (16) | 0.0104 (16) | −0.0006 (15) |
| C11 | 0.038 (2) | 0.0272 (19) | 0.030 (2) | 0.0044 (16) | 0.0060 (16) | −0.0005 (16) |
| C12 | 0.032 (2) | 0.0268 (19) | 0.034 (2) | 0.0023 (15) | 0.0106 (16) | −0.0014 (16) |
| C13 | 0.036 (2) | 0.0242 (18) | 0.0250 (18) | 0.0006 (15) | 0.0132 (15) | −0.0037 (15) |
| C14 | 0.0318 (19) | 0.0179 (17) | 0.0206 (17) | −0.0004 (14) | 0.0087 (14) | −0.0005 (14) |
| O1 | 0.0353 (15) | 0.0582 (18) | 0.0454 (16) | 0.0162 (12) | 0.0137 (13) | 0.0099 (13) |
| N1 | 0.0327 (16) | 0.0248 (15) | 0.0238 (15) | −0.0002 (12) | 0.0085 (12) | −0.0020 (12) |
| N2 | 0.0335 (16) | 0.0241 (15) | 0.0207 (14) | 0.0028 (12) | 0.0089 (12) | 0.0042 (12) |
| C5 | 0.038 (3) | 0.065 (5) | 0.054 (4) | 0.012 (3) | 0.010 (3) | 0.003 (4) |
| F1 | 0.026 (2) | 0.084 (3) | 0.111 (3) | 0.0205 (17) | 0.021 (2) | 0.043 (2) |
| F2 | 0.056 (2) | 0.154 (5) | 0.086 (3) | 0.030 (3) | 0.034 (2) | 0.078 (3) |
| F3 | 0.076 (3) | 0.085 (3) | 0.116 (4) | 0.016 (3) | −0.045 (3) | −0.042 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.390 (4) | C11—C12 | 1.397 (5) |
| C1—C7 | 1.393 (4) | C11—H11 | 0.9300 |
| C1—C8 | 1.469 (4) | C12—C13 | 1.380 (4) |
| C2—C3 | 1.397 (4) | C12—H12 | 0.9300 |
| C2—H2 | 0.9300 | C13—C14 | 1.380 (4) |
| C3—C4 | 1.376 (5) | C13—H13 | 0.9300 |
| C3—H3 | 0.9300 | C14—N2 | 1.385 (4) |
| C4—C6 | 1.382 (4) | O1—C5 | 1.332 (6) |
| C4—O1 | 1.417 (4) | N2—H21 | 0.8600 |
| C6—C7 | 1.391 (4) | C5—F1 | 1.309 (5) |
| C6—H6 | 0.9300 | C5—F3 | 1.321 (7) |
| C7—H7 | 0.9300 | C5—F2 | 1.329 (8) |
| C8—N1 | 1.334 (4) | C51—F11 | 1.309 (5) |
| C8—N2 | 1.358 (4) | C51—F31 | 1.321 (7) |
| C9—N1 | 1.399 (4) | C51—F21 | 1.329 (8) |
| C9—C14 | 1.400 (4) | C52—F12 | 1.309 (5) |
| C9—C10 | 1.403 (4) | C52—F32 | 1.321 (7) |
| C10—C11 | 1.379 (5) | C52—F22 | 1.329 (8) |
| C10—H10 | 0.9300 | | |
| | | | |
| C2—C1—C7 | 119.5 (3) | C10—C11—H11 | 118.9 |
| C2—C1—C8 | 120.0 (3) | C12—C11—H11 | 118.9 |
| C7—C1—C8 | 120.4 (3) | C13—C12—C11 | 121.0 (3) |
| C1—C2—C3 | 120.5 (3) | C13—C12—H12 | 119.5 |
| C1—C2—H2 | 119.8 | C11—C12—H12 | 119.5 |
| C3—C2—H2 | 119.8 | C14—C13—C12 | 117.2 (3) |
| C4—C3—C2 | 118.6 (3) | C14—C13—H13 | 121.4 |
| C4—C3—H3 | 120.7 | C12—C13—H13 | 121.4 |
| C2—C3—H3 | 120.7 | C13—C14—N2 | 132.6 (3) |
| C3—C4—C6 | 122.1 (3) | C13—C14—C9 | 122.6 (3) |
| C3—C4—O1 | 120.8 (3) | N2—C14—C9 | 104.8 (3) |
| C6—C4—O1 | 116.9 (3) | C5—O1—C4 | 117.5 (3) |
| C4—C6—C7 | 118.7 (3) | C8—N1—C9 | 104.3 (3) |
| C4—C6—H6 | 120.6 | C8—N2—C14 | 107.8 (3) |
| C7—C6—H6 | 120.6 | C8—N2—H21 | 126.1 |
| C6—C7—C1 | 120.4 (3) | C14—N2—H21 | 126.1 |
| C6—C7—H7 | 119.8 | F1—C5—F3 | 109.3 (5) |
| C1—C7—H7 | 119.8 | F1—C5—F2 | 107.1 (5) |
| N1—C8—N2 | 112.7 (3) | F3—C5—F2 | 106.3 (6) |
| N1—C8—C1 | 124.7 (3) | F1—C5—O1 | 107.6 (5) |
| N2—C8—C1 | 122.5 (3) | F3—C5—O1 | 112.8 (5) |
| N1—C9—C14 | 110.4 (3) | F2—C5—O1 | 113.6 (5) |
| N1—C9—C10 | 129.7 (3) | F11—C51—F31 | 109.3 (5) |
| C14—C9—C10 | 119.9 (3) | F11—C51—F21 | 107.1 (5) |
| C11—C10—C9 | 117.1 (3) | F31—C51—F21 | 106.3 (6) |
| C11—C10—H10 | 121.4 | F12—C52—F32 | 109.3 (5) |

| | | | |
|---|---|---|---|
| C9—C10—H10 | 121.4 | F12—C52—F22 | 107.1 (5) |
| C10—C11—C12 | 122.2 (3) | F32—C52—F22 | 106.3 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H21···N1$^{i}$ | 0.86 | 2.07 | 2.864 (4) | 154 |

Symmetry code: (i) $x$, $-y+3/2$, $z-1/2$.