The structures of 1,4-diaryl-5-trifluoromethyl-1*H*-1,2,3-triazoles related to J147, a drug for treating Alzheimer's disease

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J147 [*N*-(2,4-dimethylphenyl)-2,2,2-trifluoro-*N'*-(3-methoxybenzylidene)acetohydrazide] has recently been reported as a promising new drug for the treatment of Alzheimer's disease. The X-ray structures of seven new 1,4-diaryl-5-trifluoromethyl-1*H*-1,2,3-triazoles, namely 1-(3,4-dimethylphenyl)-4-phenyl-5-trifluoromethyl-1*H*-1,2,3-triazole (C₁₇H₁₄F₃N₃, **1**), 1-(3,4-dimethylphenyl)-4-(3-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (C₁₈H₁₆F₃N₃O, **2**), 1-(3,4-dimethylphenyl)-4-(4-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (C₁₈H₁₆F₃N₃O, **3**), 1-(2,4-dimethylphenyl)-4-(4-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (C₁₈H₁₆F₃N₃O, **4**), 1-[2,4-bis(trifluoromethyl)phenyl]-4-(3-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (C₁₈H₁₀F₉N₃O, **5**), 1-(3,4-dimethoxyphenyl)-4-(3,4-dimethoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (C₁₉H₁₈F₃N₃O₄, **6**) and 3-[4-(3,4-dimethoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazol-1-yl]phenol (C₁₇H₁₄F₃N₃O₃, **7**), have been determined and compared to that of **J147**. B3LYP/6-311++G(d,p) calculations have been performed to determine the potential surface and molecular electrostatic potential (MEP) of **J147**, and to examine the correlation between hydrazone **J147** and the 1,2,3-triazoles, both bearing a CF₃ substituent. Using MEPs, it was found that the minimum-energy conformation of **4**, which is nearly identical to its X-ray structure, is closely related to one of the **J147** seven minima.

1. Introduction

In the past few years, we have been interested in preparing compounds that could be used to treat Alzheimer's disease (Martínez, 2010) and other neurodegenerative pathologies (Nieto *et al.*, 2015; Martí-Centelles *et al.*, 2016). Recently, two compounds, namely **J147** (Chen *et al.*, 2011; Prior *et al.*, 2014; Daugherty *et al.*, 2017) and **CAD-31** [*N*-(2,4-dimethylphenyl)-2,2,2-trifluoro-*N'*-[3-(trifluoromethoxy)benzylidene]acetohydrazide; Prior *et al.*, 2016; Daugherty *et al.*, 2017], have shown in

Figure 1 J147 CAD-31
Relationship between **J147**, **CAD-31** and 1,4-diaryl-5-trifluoromethyl-1*H*-1,2,3-triazoles.

mice models a substantial improvement in cognitive deficits even when administered at the late stages of the disease. Structural variations starting from these compounds led us to a series of heterocyclic compounds, amongst them the 1,4-diaryl-5-trifluoromethyl-1*H*-1,2,3-triazoles (Fig. 1).

Schubert's compounds, **J147** and **CAD-31**, are not the only representatives of active pharmaceutical ingredients (APIs) bearing CF₃ substituents (Betageri *et al.*, 2005; Nenajdenko, 2014); consider, for instance, fluoxetine [*N*-methyl-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propan-1-amine], used for the treatment of depression, celecoxib [4-[5-(4-methylphenyl)-3-(trifluoromethyl)-1*H*-pyrazol-1-yl]benzenesulfonamide], used for the treatment of pain or inflammation, or riluzole (6-trifluoromethoxy-1,3-benzothiazol-2-amine), used for the treatment of amyotrophic lateral sclerosis.

However, examples in the literature of 4(5)-CF₃-substituted 1*H*-1,2,3-triazoles are scarce (Kobayashi *et al.*, 1984; Meazza & Zanardi, 1991), being prepared by 1,3-dipolar cycloaddition between different aryltrifluoromethylacetylenes and aryl azides. One drawback of this method is the lack of regioselectivity, giving two regioisomers, the 1,4-diaryl-substituted 1,2,3-triazole being the major one. This lack of regioselectivity could be circumvented using click chemistry (Huisgen, 1984; Padwa, 1991; Fan & Katritzky, 1996). Nowadays, metal-free 1,3-dipolar cycloadditions have proven to be an alternative method for obtaining 1,2,3-triazoles (Lima *et al.*, 2015), although the synthesis of substituted phenyltrifluoromethylacetylenes is still challenging and requires expensive catalysts.

When preparing these compounds for pharmacological evaluation (Scheme 1), we decided to determine their X-ray crystal structures to see if they would shed any light on the interactions and properties of the CF₃ group. This has been a topic of great interest related to F...F interactions; it should be noted that some authors doubted their existence, as we discussed in an earlier paper, where we reported one of the

Figure 2
The X-ray molecular structure of **J147** [adapted and coloured from Chen *et al.* (2011)].

shortest F...F distances determined by X-ray crystallography (Pérez-Torrallba *et al.*, 2014). Very recently, two papers appeared where these interactions were ascertained using an inelastic tunnelling probe (itProbe) on a metal surface (Han *et al.*, 2017; Neaton, 2017).

Concerning those involving a CF₃ group, the answer is more nuanced. The volumes of the CH₃ (54 Å³) and CF₃ (94 Å³) groups and their relative solubilities, as well as the intramolecular O—H...F hydrogen bonds involving CF₃, have been discussed in a collective book (Ojima, 2009) and in a review on intramolecular hydrogen bonding involving organic fluorine, where examples of N—H...F—C hydrogen bonds in CF₃-substituted benzanilides and related compounds based on NMR and DFT (density functional theory) calculations have been reported (Mishra & Suryaprakash, 2017).

Attention should be paid to the fact that until now the X-ray crystal structures of **J147** and **CAD-31** have not yet been deposited in the Cambridge Structural Database (CSD, Version 5.37; Groom *et al.*, 2016); only a poor-quality picture of the **J147** structure (Fig. 2) has been published (Chen *et al.*, 2011).

2. Experimental

2.1. Synthesis and crystallization

Compounds **1–6** have been synthesized using **method A** and compound **7** has been synthesized using **method B**, as depicted in Fig. 3. Melting points were measured in a ThermoGalen 10 Hot Stage Microscope.

The 1,1,1-trifluoro-3-(*X*-methoxyphenyl)propan-2-ones (**K1–K4**) were prepared from the corresponding phenylacetic acid, trifluoroacetate and lithium diisopropylamide (LDA) at low temperature (Reeves *et al.*, 2008). Azides **A1–A4** (Barral *et al.*, 2007) and azide **A5** (Budruv *et al.*, 2016) were obtained according to literature procedures.

Method A: in a round-bottomed flask, 1 equivalent of 1,1,1-trifluoro-3-(*X*-methoxyphenyl)propan-2-one was dissolved in 3 equivalents of triethylamine and, after a few minutes, 1 equivalent of aryl azide was added to the reaction mixture,

Figure 3

Compounds **1–6** were synthesized using **method A** and compound **7** was synthesized using **method B**.

which was warmed to 348 K and heated overnight. After that, the reaction mixture was dissolved in a few millilitres of dichloromethane and brought to dryness at reduced pressure. The residue was purified by column chromatography (silica gel) using as eluent a hexane–ethyl acetate mixture (0–40% gradient). Triazoles **1–6** were obtained in good to moderate yields.

Method B: 1.5 equivalents of aryl azide **A5** was dissolved in dimethyl sulfoxide (DMSO, 0.5 ml) and 1 equivalent of 3-(3,4-dimethoxyphenyl)-1,1,1-trifluoropropan-2-one (**K4**) in the presence of 10 mol% of Et₃N or DBU (1,8-diazabicyclo[5.4.0]undec-7-ene) was added. The reaction was allowed to stir for 5–6 h at room temperature. After the reaction was complete, a saturated solution of ammonium chloride (5 ml) was added and the reaction mixture was extracted with chloroform (3 × 10 ml). The chloroform extracts were combined, the solvent evaporated at reduced pressure and the residue purified by column chromatography using 2% methanol in dichloromethane as eluent.

2.2. Analytical data

Analytical data for **1**: 30% yield, m.p. 374–375 K (hexane). Analysis calculated for C₁₇H₁₄F₃N₃ (%): C 64.35, H 4.45, N 13.24; found: C 63.95, H 4.45, N 13.02. ¹H NMR (400.13 MHz, CDCl₃): δ 7.71 (*m*, 2H, H6'', H2''), 7.53–7.44 (*m*, 3H, H3'', H4'', H5''), 7.35–7.25 (*m*, 3H, H5', H6', H2'), 2.36 and 2.37 (*s*, 6H, CH₃, CH₃). ¹³C NMR (100.61 MHz, CDCl₃): δ 148.16, 139.66, 138.16, 133.74, 130.32, 129.41 (2C), 129.06 (2C), 128.86, 128.51, 126.46, 124.02 (*q*, ²J_{CF} = 40 Hz, C5), 122.76, 120.08 (*q*, ¹J_{CF} = 270 Hz, CF₃), 19.80 (CH₃), 19.67 (CH₃). ¹⁹F NMR (379.5 MHz, CDCl₃): δ –55.40 (5-CF₃).

Analytical data for **2**: 40% yield, m.p. 338–339 K (hexane). Analysis calculated for C₁₈H₁₆F₃N₃O (%): C 62.24, H 4.64, N 12.10; found: C 62.02, H 4.49, N 11.89. ¹H NMR (400.13 MHz,

CDCl₃): δ 7.40 (*t*, ³J = 8.1 Hz, 1H, H5''), 7.32 (*s*, 1H, H6'), 7.31–7.24 (*m*, 4H, H2', H5', H2'', H6''), 7.02 (*ddd*, ³J = 8.2, ⁴J = 2.4, ⁴J = 1.0 Hz, 1H, H4''), 3.87 (*s*, 3H, OCH₃), 2.37 (*s*, 3H, CH₃), 2.36 (*s*, 3H, CH₃). ¹³C NMR (100.61 MHz, CDCl₃): δ 159.59, 148.02, 139.65, 138.13, 133.77, 130.31, 130.08, 129.54, 126.48, 122.77, 121.52, 124.09 (*q*, ²J_{CF} = 40 Hz, C5), 120.08 (*q*, ¹J_{CF} = 270 Hz, CF₃), 115.48, 114.29, 55.32 (OCH₃), 19.74 (CH₃), 19.61 (CH₃). ¹⁹F NMR (379.5 MHz, CDCl₃): δ –55.33 (5-CF₃).

Analytical data for **3**: 50% yield, m.p. 424–426 K (hexane). Analysis calculated for C₁₈H₁₆F₃N₃O (%): C 62.24, H 4.64, N 12.10; found: C 62.19, H 4.51, N 12.05. ¹H NMR (400.13 MHz, CDCl₃): δ 7.65 (*dd*, ³J = 8.7, ⁴J = 3.3 Hz, 2H, H2'', H6''), 7.34–7.28 (*m*, 2H, H5', H6'), 7.27–7.23 (*m*, 1H, H2'), 7.02 (*m*, 2H, H3'', H5''), 3.88 (*s*, 3H, OCH₃), 2.37 (*s*, 3H, CH₃), 2.36 (*s*, 3H, CH₃). ¹³C NMR (100.61 MHz, CDCl₃): δ 160.55, 148.03, 139.54, 138.11, 133.89, 130.39 (2C), 130.29, 126.49, 123.45 (*q*, ²J_{CF} = 40 Hz, C5), 122.77, 121.29, 120.24 (*q*, ¹J_{CF} = 270 Hz, CF₃), 114.02 (2C), 55.33 (OCH₃), 19.78 (CH₃), 19.64 (CH₃). ¹⁹F NMR (379.5 MHz, CDCl₃): δ –55.34 (5-CF₃).

Analytical data for **4**: 60% yield; m.p. 372–373 K (hexane). Analysis calculated for C₁₈H₁₆F₃N₃O (%): C 62.24, H 4.64, N 12.10; found: C 61.89, H 4.49, N 12.06. ¹H NMR (400.13 MHz, CDCl₃): δ 7.68 (*d*, ³J = 8.6 Hz, 2H, H2'', H6''), 7.30–7.13 (*m*, 3H, H3', H5', H6'), 7.02 (*m*, 2H, H3'', H5''), 3.88 (*s*, 3H, OCH₃), 2.43 (*s*, 3H, CH₃), 2.08 (*s*, 3H, CH₃). ¹³C NMR (100.61 MHz, CDCl₃): δ 160.56, 147.46, 141.25, 135.21, 132.70, 131.76, 130.38 (2C), 127.28, 126.94, 124.10 (*q*, ²J_{CF} = 40 Hz, C5), 121.22, 120.17 (*q*, ¹J_{CF} = 270 Hz, CF₃), 114.04 (2C), 55.34 (OCH₃), 21.27 (CH₃), 16.94 (CH₃). ¹⁹F NMR (379.5 MHz, CDCl₃): δ –56.60 (5-CF₃).

Analytical data for **5**: 66% yield; m.p. 381–382 K (hexane). Analysis calculated for C₁₈H₁₀F₉N₃O (%): C 47.49, H 2.21, N 9.23; found: C 47.43, H 2.18, N 9.18. ¹H NMR (400.13 MHz, CDCl₃): δ 8.19 (*m*, 1H, H3'), 8.08 (*dd*, *J* = 8.2, 1.9 Hz, 1H, H5'), 7.71 (*d*, ³J = 8.2 Hz, 1H, H6'), 7.43 (*dd*, ³J = ³J = 8.2 Hz, 1H,

H5''), 7.37–7.30 (*m*, 2H, H2'', H6''), 7.05 (*ddd*, $^3J = 8.2$, $^4J = 2.6$, $^4J = 0.9$ Hz, 1H, H4''), 3.89 (*s*, 3H, OCH₃). ¹³C NMR (100.61 MHz, CDCl₃): δ 159.78, 148.01, 136.12, 134.15 (*q*, $^2J_{CF} = 34$ Hz), 130.44, 129.88 (*q*, $^3J_{CF} = 4$ Hz), 129.10 (*q*, $^2J_{CF} = 34$ Hz), 129.82, 128.99, 125.24 (*qq*, $^3J_{CF} = ^3J_{CF} = 4$ Hz), 123.77 (*q*, $^2J_{CF} = 40$ Hz, C5), 122.50 (*q*, $^1J_{CF} = 270$ Hz, CF₃), 121.63 (*q*, $^1J_{CF} = 270$ Hz, CF₃), 121.23, 119.76 (*q*, $^1J_{CF} = 270$ Hz, CF₃), 116.01, 114.07, 55.39 (OCH₃). ¹⁹F NMR (379.5 MHz, CDCl₃): δ –55.6 (5-CF₃), –60.8 (*o*-CF₃), –63.7 (*p*-CF₃).

Analytical data for **6**: 50% yield; m.p. 438–441 K (hexane). Analysis calculated for C₁₉H₁₈F₃N₃O₄ (%): C 55.75, H 4.43, N 10.26; found: C 55.34, H 4.32, N 9.97. ¹H NMR (400.13 MHz, CDCl₃): δ 7.30–7.24 (*m*, 2H, H2', H6'), 7.12 (*dd*, $^3J = 8.5$, $^4J = 2.4$ Hz, 1H, H6''), 7.05 (*d*, $^4J = 2.4$ Hz, 1H, H2''), 6.99 (*d*, $J = 8.5$ Hz, 1H, H5''), 6.98 (*d*, $^3J = 8.5$ Hz, 1H, H5'), 3.98 (*s*, 3H, OCH₃), 3.95 (*s*, 3H, OCH₃), 3.95 (*s*, 3H, OCH₃), 3.93 (*s*, 3H, OCH₃). ¹³C NMR (100.61 MHz, CDCl₃): δ 150.80, 150.18, 149.37, 148.97, 148.12, 128.94, 121.93, 121.73 (*q*, $^2J_{CF} = 40$ Hz, C5), 121.31, 120.20 (*q*, $^1J_{CF} = 270$ Hz, CF₃), 118.13, 112.15, 111.05, 110.83, 109.17, 56.18 (OCH₃, OCH₃), 55.96 (OCH₃), 55.94 (OCH₃). ¹⁹F NMR (379.5 MHz, CDCl₃): δ –55.50 (5-CF₃).

Analytical data for **7**: 20% yield; m.p. 480–482 K (methanol). Analysis calculated for C₁₇H₁₄F₃N₃O₃ (%): C 55.89, H 3.86, N 11.50; found: C 55.85, H 3.75, N 11.40. ¹H NMR (400.13 MHz, acetone-*d*₆): δ 9.12 (*s*, 1H, OH), 7.49 (*dd*, $^3J = ^3J = 8.5$ Hz, 1H, H5'), 7.30 (*d*, $^4J = 2.0$ Hz, 1H, H2''), 7.27–7.22 (*m*, 1H, H6''), 7.18–7.08 (*m*, 4H, H2', H4', H6', H5''), 3.90 (*s*, 6H, OCH₃, OCH₃). ¹³C NMR (100.61 MHz, CDCl₃): δ 159.25, 151.70, 150.51, 149.41, 138.27, 131.06, 122.77, 122.43, 121.48 (*q*, $^1J_{CF} = 270$ Hz, CF₃), 118.76, 117.73, 113.94, 113.58, 112.66, 56.33 (OCH₃), 56.25 (OCH₃) (C5 was not detected). ¹⁹F NMR (379.5 MHz, CDCl₃): δ –55.53 (5-CF₃).

2.3. NMR experiments

NMR spectra were recorded on a Bruker DRX 400 (9.4 Tesla, 400.13 MHz for ¹H, 100.61 MHz for ¹³C and 40.54 MHz for ¹⁵N), using a 5 mm inverse-detection H-X probe equipped with a z-gradient coil, at 300 K. Chemical shifts (δ in ppm) are given from internal solvent; CDCl₃ 7.26 and 77.0 and acetone-*d*₆ 2.05 and 29.92 for ¹H and ¹³C were used as external references. Signals were characterized as *s* (singlet), *d* (doublet), *t* (triplet), *q* (quartet) and *m* (multiplet), and *J* couplings are given in Hz.

Typical parameters for ¹H NMR spectra were a spectral width of 4800 Hz and a pulse width of 9.5 μ s at an attenuation level of 0 dB. Typical parameters for ¹³C NMR spectra were a spectral width of 21 kHz, a pulse width of 12.5 μ s at an attenuation level of –6 dB and a relaxation delay of 2 s. WALTZ-16 was used for broadband proton decoupling; the FIDS were multiplied by an exponential weighting (lb = 1 Hz) before Fourier transformation.

Inverse proton-detected heteronuclear shift correlation spectra, (¹H–¹³C) gs-HMQC and (¹H–¹³C) gs-HMBC, were acquired and processed using standard Bruker NMR software and in nonphase-sensitive mode. Gradient selection was

achieved through a 5% sine truncated shaped pulse gradient of 1 ms.

Selected parameters for (¹H–¹³C) gs-HMQC and (¹H–¹³C) gs-HMBC spectra were a spectral width of 4800 Hz for ¹H and 20.5 kHz for ¹³C, 1024 $\times$ 256 data set, number of scans 2 (gs-HMQC) or 4 (gs-HMBC) and a relaxation delay of 1 s. The FIDs were processed using zero filling in the *F*₁ domain and a sine-bell window function in both dimensions was applied prior to Fourier transformation. In the gs-HMQC experiments, GARP modulation of ¹³C was used for decoupling.

¹⁹F NMR spectra were recorded on the same spectrometer (376.50 for ¹⁹F), using a 5 mm QNP direct-detection probe head equipped with a z-gradient coil, at 300 K. Chemical shifts (δ in ppm) are given from CFCl₃ as external reference [one drop of CFCl₃ in CDCl₃ (0.00)]. Typical parameters for ¹⁹F NMR spectra were a spectral width of 55 kHz, a pulse width of 13.75 μ s at an attenuation level of –6 dB and a relaxation delay of 1 s. WALTZ-16 was used for broadband proton decoupling ¹⁹F{¹H} and the FIDS were multiplied by an exponential weighting (lb = 1 Hz) before Fourier transformation.

2.4. X-ray data collection and structure refinement

Crystals of good quality for X-ray diffraction analyses were obtained for compounds **1–5** from hexane and compounds **6** and **7** from methanol. Data collection was carried out at room temperature on a Bruker SMART CCD diffractometer for compounds **2–7** and on an Xcalibur Atlas CCD diffractometer for **1**. They were operating at 50 kV and 25 mA for **2**, and at 35 mA for the remainder of the compounds using, in all cases, exposure times of 20 s and graphite-monochromated Mo *K* α radiation ($\lambda = 0.71073$ Å). Crystal data, data collection and structure refinement details are summarized in Table 1.

All H atoms were included in their calculated positions and refined as riding on the respective bonded atoms. In compound **7**, atom H3 linked to atom O3 was located in a difference Fourier map and refined as riding on the O atom.

Concerning the positional disorder of the trifluoromethyl groups, compound **1** crystallizes with two molecules; one of them presents CF₃ disorder that was modelled and refined with displacement parameters restrained and occupancies in a 65:35 ratio. All the remaining compounds, except for **2** and **7**, also present positional disorder for their F atoms, which were modelled similarly in two different positions for the sake of simplicity and clarity, and were refined with occupancies around 50% for **3** and **4**, ratios of 62:38 (for C6-F₃ and C19-F₃) and 73:27 (for C20-F₃) for **5**, and a ratio of 70:30 for **6**.

Compound **6** shows a different kind of positional disorder that affects atoms N1 and C4 on the triazole ring. This disorder was modelled and refined with occupancies of 45% N and 55% C for the first position and a ratio of 55:45 for the second position.

2.5. Computational details

B3LYP/6-311++G(d,p) calculations (Ditchfield *et al.*, 1971; Frisch *et al.*, 1984) were carried out using the GAUSSIAN16

Table 1
Experimental details.

	1	2	3	4
Crystal data				
Chemical formula	C ₁₇ H ₁₄ F ₃ N ₃	C ₁₈ H ₁₆ F ₃ N ₃ O	C ₁₈ H ₁₆ F ₃ N ₃ O	C ₁₈ H ₁₆ F ₃ N ₃ O
<i>M_r</i>	317.31	347.34	347.34	347.34
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>n</i>	Orthorhombic, <i>Pbca</i>	Monoclinic, <i>P</i> ₂ ₁ / <i>n</i>	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	296	296	296	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.001 (8), 20.82 (2), 15.124 (7)	9.5097 (13), 17.921 (2), 20.011 (3)	15.1368 (16), 7.7224 (9), 15.4446 (18)	8.829 (2), 9.513 (2), 11.598 (3)
α , β , γ (°)	90, 96.12 (5), 90	90, 90, 90	90, 112.454 (2), 90	106.105 (4), 95.554 (4), 110.049 (4)
<i>V</i> (Å ³)	3131 (5)	3410.3 (8)	1668.5 (3)	859.1 (4)
<i>Z</i>	8	8	4	2
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.11	0.11	0.11	0.11
Crystal size (mm)	0.46 × 0.12 × 0.07	0.78 × 0.37 × 0.32	0.36 × 0.23 × 0.2	0.72 × 0.23 × 0.13
Data collection				
Diffractometer	Agilent Xcalibur Atlas CCD	Bruker SMART CCD area detector	Bruker SMART CCD area detector	Bruker SMART CCD area detector
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2013)	—	—	—
<i>T</i> _{min} , <i>T</i> _{max}	0.859, 1.000	—	—	—
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	14744, 5504, 2879	24398, 3001, 1986	12266, 2930, 1644	6496, 3096, 1709
<i>R</i> _{int}	0.045	0.070	0.045	0.092
(sin θ / λ) _{max} (Å ⁻¹)	0.594	0.595	0.595	0.606
Refinement				
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.053, 0.125, 1.01	0.037, 0.114, 1.02	0.038, 0.114, 1.01	0.053, 0.153, 0.98
No. of reflections	5504	3001	2930	3096
No. of parameters	447	226	254	254
No. of restraints	36	0	0	292
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.15, -0.22	0.13, -0.17	0.15, -0.13	0.23, -0.14
	5	6	7	
Crystal data				
Chemical formula	C ₁₈ H ₁₀ F ₉ N ₃ O	C ₁₉ H ₁₈ F ₃ N ₃ O ₄	C ₁₇ H ₁₄ F ₃ N ₃ O ₃	
<i>M_r</i>	455.29	409.36	365.31	
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>n</i>	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>	
Temperature (K)	296	293	293	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.9633 (8), 7.8453 (5), 20.0446 (14)	30.656 (2), 8.3363 (6), 7.6723 (6)	12.267 (2), 8.4334 (14), 15.686 (3)	
α , β , γ (°)	90, 95.191 (1), 90	90, 94.627 (1), 90	90, 93.904 (3), 90	
<i>V</i> (Å ³)	1873.6 (2)	1954.3 (3)	1619.0 (5)	
<i>Z</i>	4	4	4	
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α	
μ (mm ⁻¹)	0.16	0.12	0.13	
Crystal size (mm)	0.52 × 0.20 × 0.13	0.41 × 0.29 × 0.09	0.59 × 0.11 × 0.07	
Data collection				
Diffractometer	Bruker SMART CCD area detector	Bruker SMART CCD area detector	Bruker SMART CCD area detector	
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	16580, 3688, 2142	16559, 3634, 1881	14139, 3188, 1336	
<i>R</i> _{int}	0.040	0.049	0.146	
(sin θ / λ) _{max} (Å ⁻¹)	0.617	0.606	0.617	
Refinement				
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.037, 0.107, 1.01	0.042, 0.133, 1.04	0.057, 0.189, 0.97	
No. of reflections	3688	3634	3188	
No. of parameters	365	289	235	
No. of restraints	484	36	0	
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.13, -0.17	0.14, -0.14	0.26, -0.26	

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SAINT* (Bruker, 2002), *SMART* (Bruker, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

facilities (Frisch *et al.*, 2016). Frequency calculations show that all the reported structures are minima (number of imaginary frequencies = 0). Maps of electrostatic potential were calculated with the *GAUSSIAN16* program and represented with the *Jmol* viewer (*Jmol*, 2018).

3. Results and discussion

In this article, we will discuss the crystal and molecular structures of seven 1,2,3-triazoles (denoted **1–7**). Scheme 1 shows the compounds under study and the numbering systems

Figure 4

The molecular structures of **1–7** (with displacement ellipsoids at the 20 and 30% probability levels), showing the labelling of the asymmetric units from the crystal structure analyses.

used for their NMR characterization (see Figs. S1–S21 in the supporting information).

Triazoles **1–6** were synthesized using a metal-free domino reaction from aryl trifluoromethyl ketones and aryl azides in the presence of a base (DBU or triethylamine) in a 1:1:3 ratio (Sosnovskikh & Usachev, 2002; Usachev *et al.*, 2011, 2014). Triazole **7**, which contains a hydroxy group, was prepared at room temperature using a catalytic amount of base DBU or trimethylamine from enolizable aryl trifluoromethyl ketones and aryl azides (Shashank *et al.*, 2014) (Fig. 3).

3.1. Crystal structures

The compounds under study crystallize in triclinic, monoclinic and orthorhombic systems, in the space groups $P\bar{1}$ (for **4**), $P2_1/n$ (for **1**, **3** and **5**), $P2_1/c$ (for **6** and **7**) and $Pbca$ (for **2**). Fig. 4 displays the molecular structures of the different derivatives with the labelling schemes of their corresponding asymmetric units. All of them have one molecule per asymmetric unit, with the exception of **1**, which shows two crystallographically independent molecules.

Compound **1** crystallizes with two types of molecules showing positional disorder for the F atoms of the CF₃ group in one of them, which was refined with occupancies of a 65:35 ratio. The remainder of the compounds, excluding **2** and **7**, also show positional disorder for the F atoms, being modelled in two different positions with occupancies of about 50% for **3** and **4**, and nearly a 70:30 ratio for **5** and **6**. Additionally, compound **6** showed positional disorder for atoms N1 and C4 on the triazole ring. This disorder was modelled and refined with occupancies of 45% N and 55% C for the first position and a 55:45 ratio for the second position.

Compound **1** has both molecules in an eclipsed orientation of its triazole rings. As expected, they are not planar because of the twisting of the aromatic rings on the triazole unit in order to minimize the steric hindrance of their substituents. Thus, the dihedral angle between the planes of the triazole ring and the *N*-3,4-dimethylphenyl group is about 35° for both

Table 2

Rotational disorder of the trifluoromethyl groups in compounds **1–7**.

N1–C5–C–F torsion angle (°) defined selecting the F atom of the CF₃ group closer to 0, 90 or 180°.

Compound	Comments		Experimental	Close conformation
1	Molecule A	Disorder	–94.2	90
			176.7	180
2	Molecule B	No disorder	89.9	90
		No disorder	–92.7	90
3	–	Disorder	–177.4	180
			–163.6	180
4	–	Disorder	–169.0	180
			101.9	90
5	–	Disorder	–75.0	90
			7.0	0
6	Disorder C/N	Disorder	–103.8	90
			168.1	180
7	–	No disorder	94.8	90

molecules, while that with the *C*-phenyl ring is higher, with values of 63.3 (3) and 85.4 (3)° for molecules **1** and **2**, respectively. The distinct values of the latter angle for the different types of molecules could be related to the positional disorder of the CF₃ group in the type 2 molecules that introduces more steric hindrance in that part of the molecule and, consequently, a larger twist.

The remainder of the derivatives show a similar behaviour. Thus, the dihedral angles in compounds **2–5** vary between 36.7 (2) and 42.5 (2)° for the methoxyphenyl ring, and between 71.4 (2) and 86.2 (3)° for the disubstituted ring, the differences in these values being attributed to the diverse positions of the substituents. The highest value for this angle (seen in **5**) is related to the presence of the larger CF₃ group compared to the CH₃ groups.

In contrast, compound **6**, with symmetrical methoxy substituents of larger size, shows similar intermediate values for both dihedral angles, *i.e.* 55.1 (2) and 56.0 (2)°. This symmetry is associated with a positional disorder in the first and fourth positions on the triazole moiety. Consequently, atoms N1A and C4B occupy the first position in a 45:55 ratio, while atoms N1B and C4A occupy the fourth position in a 55:45 ratio. This fact seems to affect slightly the distribution of the electronic delocalization on the triazole ring.

Finally, these angles are significantly smaller, *i.e.* 49.1 (4) and 30.1 (4)°, in **7**. This fact is related to the existence of intermolecular hydrogen bonds between the triazole N3 atom and the hydroxy group of neighbouring molecules.

The nonplanarity of these molecules along with their bond lengths and angles indicate that the electronic delocalization

Figure 5
View of the crystal packing of **7** along the *a* axis, showing the interactions (hydrogen bonds are red and π – π interactions are blue) between the chains.

Figure 6

Definition of the rotation angles studied in the theoretical calculations; for the *syn/anti* isomerism, note that $\phi_3 = 0^\circ$ corresponds to the *Z* configuration and $\phi_3 = 180^\circ$ to the *E* configuration.

on the triazole ring is not extended to its substituents and it is mainly focused on the shortest N2—N3 bond with a length of about 1.31 Å.

Also remarkable is the positional disorder of the CF₃ groups displayed by most of derivatives that possibly contributes to the twisting of the molecules, preventing any interactions with their neighbours.

In that context, the crystal packing for these compounds is similar and consists of crystallographically isolated molecules with no significant interactions between them. This fact is probably due to the steric hindrance introduced by the substituents and the nonplanarity of the molecules. However, the crystal packing for **7** consists of a supramolecular bidimensional network formed by intermolecular hydrogen bonds, as mentioned, between atom N3 and the H3—O3 hydroxy groups of adjacent molecules [$\text{O3}-\text{H3} \cdots \text{N3}(-x+1, y+\frac{1}{2}, -z-\frac{1}{2}) = 2.02 \text{ Å}$ and 163°] (see Fig. S22 of the supporting information). This interaction extends along the *b* axis, resulting in zigzag chains that interpenetrate each other. The chains are interconnected along the *c* axis owed to a partial overlapping of the benzene rings of centrosymmetric molecules of different chains (shortest C···C distance $\sim 3.3 \text{ Å}$), leading to the supramolecular network, as shown in Fig. 5.

In summary, from the results discussed above, the following observations can be made:

(a) *Generalities.* Concerning the 5-CF₃ rotational disorder, Table 2 summarizes the findings. There are seven conformations of the 90° type (*syn*- or *anticlinal*), five of the 180° type and one of the 0° type (in the last six, either *syn*- or *anti*-periplanar types are present).

As was already mentioned, the torsions involving both aryl groups are due to the steric effect of the CF₃ group. For instance, for compound **1** (two independent molecules), the torsion angles N2—N1—C1'—C2' and N3—C4—C1''—C2'' (see chemical numbering in Scheme 1) are about 35° (3,4-dimethylphenyl) and about 63 and 85° (*C*-phenyl). For a similar compound, in terms of the absence of *ortho* substituents, with *N*-4-methoxyphenyl and *C*-phenyl (CSD refcode SOVWIL; Adluri *et al.*, 2014), these angles are approximately 50 and 9° . One increases by 15° , but the other decreases by between 54 and 76° , confirming that CF₃ is larger than CH₃, but also that torsions in the solid state are not simply due to steric effects.

Why are there no C_{ar}—H···F—C intramolecular contacts? That is because the geometry is unfavourable due to torsion of the two aryl groups. If the aryl groups were coplanar with the triazole ring, the C—F and the C—H atoms would be too close. Thus, the steric effect is more efficient than the weak hydrogen bond.

(b) *Singularities.* The only compound which clearly shows a hydrogen bond (O—H···N) is compound **7**. The hydrogen bond is established with atom N3 and not with N2; this is due to the fact that N3 is more basic, as well as being a better hydrogen-bond acceptor, than N2 (Abboud *et al.*, 2001; McDonald *et al.*, 2010). The role of a more favourable geometry cannot be excluded.

The shortest F···F intermolecular contact between the F atoms of the CF₃ substituents is seen for compound **5**, *i.e.* $2.875/2.826 \text{ Å}$, which are longer than the $2.5\text{--}2.7 \text{ Å}$ limit for F···F contacts (the shortest distance we found in other structures was 2.596 Å ; Pérez-Torralba *et al.*, 2014). Note that other authors extend the C—F···F—C histograms to 3.0 (Reichenbacher *et al.*, 2005) and 3.4 Å (Karnoukhova *et al.*, 2016).

Figure 7

Reported and calculated structures of **J147**.

Table 3

Angles φ_1 , φ_2 and φ_3 ($^\circ$).

Relative energies (kJ mol^{-1}) of the seven minima (types 1–7) for **J147**. The bold entries relate to the *E/Z* isomerism about the C=N bond (*Z*: $\varphi_3 = 0^\circ$; *E*: $\varphi_3 = 180^\circ$).

Geometry/Energy	Types 1–7 minima	
Optimized geom ($^\circ$)	Type 1: $-11.5/63.9/\mathbf{4.8}$	Type 2: $-3.4/5.6/\mathbf{180.0}$
Relative energy (E_{rel})	Type 1: 49.5	Type 2: 20.7
Optimized geom ($^\circ$)	Type 3: $-15.0/94.6/-\mathbf{0.4}$	Type 4: $0.9/177.5/-\mathbf{179.9}$
Relative energy (E_{rel})	Type 3: 53.2	Type 4: 17.2
Optimized geom ($^\circ$)	Type 5: $165.9/93.6/\mathbf{178.9}$	Type 6: $-168.0/-169.7/\mathbf{5.7}$
Relative energy (E_{rel})	Type 5: 32.9	Type 6: 49.0
Optimized geom ($^\circ$)	Type 7: $178.1/-178.6/\mathbf{179.8}$	X-ray: $178.5/-178.7/\mathbf{179.9}$
Relative energy (E_{rel})	Type 7: 0.0	X-ray: 0.2

The N1/C4 positional disorder of compound **6** is related to the general topic of positional solid-solution, *i.e.* a homogeneous nonstoichiometric crystalline phase in which some of the molecules are substituted by identical molecules ordered differently, so the lattice dimensions are changed only slightly (Kitaigorodsky, 1984; Jacques *et al.*, 1994; Oliveira *et al.*, 2008; Santa María *et al.*, 2009).

3.2. Theoretical calculations

We started exploring the conformational/configurational space of **J147**, limiting ourselves to the angles φ_1 , φ_2 and φ_3 defined in Fig. 6; φ_1 and φ_2 correspond to rotations about single bonds, while φ_3 corresponds to the *E/Z* isomerism of the C=N bond. The rotations about the N-aryl, C-aryl and C-OCH₃ single bonds were not explored.

We have found seven minima that are reported in Table 3 and the two most significant are depicted in Figs. 7 and 8; the geometries of the remaining ones are given in the supporting information.

The minimum is close to an all-*trans* geometry (angles close to $|180^\circ|$, *E* isomer). The positions of the *ortho*-methyl group (position 2'-Me) and that of the methyl group of the methoxy substituent (position 3''-OMe) are different from the positions they occupy in the crystal (Chen *et al.*, 2011). Therefore, we optimized an all-*trans* geometry similar to that obtained by crystallography, obtaining another minimum 0.2 kJ mol^{-1} higher in energy than the absolute minimum but with very similar φ_1 , φ_2 and φ_3 angles (Fig. 7).

Note from Table 3 that the *E/Z* isomerism (φ_3) always shows small deformations between 0.1 and 5.7° from 0 and 180° . The single bond corresponding to the φ_1 angle is not far (maximum value 19.2°) from being 0 or 180° . By contrast, the central φ_2 angle has in some isomers angles close to 90° (63.9 , 93.6 , 94.6 and 118.6°) due to the steric hindrance that results from angles close to 0 or to 180° .

Clearly the minimum of **J147** Type 7 ($178.1/-178.6/179.8^\circ$) of Table 3 (very similar to the X-ray structure) is very different from **4** (Fig. 8). But, on the other hand, the **J147** Type 1 ($-11.5/63.9/4.8^\circ$) of Table 3, which lies 49.5 kJ mol^{-1} higher in energy, is close to that found in the X-ray structure for compound **4**. Would such a difference in energy be too high for both structures to fit the same receptor? There has been much

interest in comparing the structures of the ligands inside a receptor/protein with those of the free molecules, both determined by X-ray crystallography. While the X-ray geometry usually, as in the present case, matches the minimum-energy geometry calculated theoretically (both after optimization which relaxes the geometry), the geometry of the small molecule within the receptor only coincides in some cases; in others it differs by as much as 40 kJ mol^{-1} (Boström *et al.*, 1998; Perola & Charifson, 2004; Fu *et al.*, 2011; Sitzmann *et al.*, 2012; Krall *et al.*, 2017; Hawkins, 2017). Therefore, it is reasonable to assume that they act on the same receptor.

4. Conclusions

A series of closely related 1,4-diaryl-5-trifluoromethyl-1*H*-1,2,3-triazoles have been prepared and their X-ray structures were determined. Some generalities (CF₃ disorder and conformation; C—F...F—C contacts) and some peculiarities of these structures have been discussed. Amongst the latter, of note are an O—H...N hydrogen bond with the most basic N atom of 1,2,3-triazole (N3), a short F...F contact and an N1/C4 positional disorder related to solid solutions. Theoretical calculations found seven minima in the **J147** potential surface, with the absolute minimum coinciding with the X-ray structure (estimated), and the structure that most resembles compound **4** (as a model of the seven triazoles) lies nearly 50 kJ mol^{-1} above the minimum. Although this is a high gap, it is still possible that both types of compounds share the same receptor.

Figure 8
X-ray geometries and MEPs of the minima of compounds **4** and **J147**.

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supporting information

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The structures of 1,4-diaryl-5-trifluoromethyl-1*H*-1,2,3-triazoles related to J147, a drug for treating Alzheimer's disease

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2013) for 1_triazol34; *SAINT* (Bruker, 2002) for 2_C18H16F3N3O_3OMe34, 3_C18H16F3N3O_4OMe34, 5_C18H10F9N3O_abc13, 6_C19H18F3N3O4_ABC23, 7_C17H14F3N3O3; *SMART* (Bruker, 2002) for 4_4OMe24Me. Cell refinement: *CrysAlis PRO* (Agilent, 2013) for 1_triazol34; *SMART* (Bruker, 2002) for 2_C18H16F3N3O_3OMe34, 3_C18H16F3N3O_4OMe34, 4_4OMe24Me, 5_C18H10F9N3O_abc13, 6_C19H18F3N3O4_ABC23, 7_C17H14F3N3O3. Data reduction: *CrysAlis PRO* (Agilent, 2013) for 1_triazol34; *SAINT* (Bruker, 2002) for 2_C18H16F3N3O_3OMe34, 3_C18H16F3N3O_4OMe34, 4_4OMe24Me, 5_C18H10F9N3O_abc13, 6_C19H18F3N3O4_ABC23, 7_C17H14F3N3O3. Program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) for 1_triazol34, 2_C18H16F3N3O_3OMe34, 4_4OMe24Me, 5_C18H10F9N3O_abc13, 7_C17H14F3N3O3. For all structures, program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

1-(3,4-Dimethylphenyl)-4-phenyl-5-trifluoromethyl-1*H*-1,2,3-triazole (1_triazol34)

Crystal data

$C_{17}H_{14}F_3N_3$	$F(000) = 1312$
$M_r = 317.31$	$D_x = 1.346 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 10.001 (8) \text{ \AA}$	Cell parameters from 2404 reflections
$b = 20.82 (2) \text{ \AA}$	$\theta = 2.7\text{--}21.1^\circ$
$c = 15.124 (7) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$\beta = 96.12 (5)^\circ$	$T = 296 \text{ K}$
$V = 3131 (5) \text{ \AA}^3$	Needle, colourless
$Z = 8$	$0.46 \times 0.12 \times 0.07 \text{ mm}$

Data collection

Agilent Xcalibur Atlas CCD diffractometer	5504 independent reflections
ω scans	2879 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2013)	$R_{\text{int}} = 0.045$
$T_{\text{min}} = 0.859$, $T_{\text{max}} = 1.000$	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.3^\circ$
14744 measured reflections	$h = -11 \rightarrow 11$
	$k = -24 \rightarrow 15$
	$l = -17 \rightarrow 17$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.053$ $wR(F^2) = 0.125$ $S = 1.01$

5504 reflections

447 parameters

36 restraints

Primary atom site location: structure-invariant
direct methodsHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.037P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$ *Special details*

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
F11	0.42912 (15)	0.08479 (9)	0.68419 (10)	0.0856 (6)	
F21	0.45733 (15)	0.06191 (9)	0.82172 (9)	0.0839 (6)	
F31	0.58601 (17)	0.02044 (9)	0.73286 (11)	0.0852 (5)	
N11	0.6481 (2)	0.17013 (11)	0.70246 (12)	0.0528 (6)	
N21	0.7302 (2)	0.21710 (12)	0.73692 (13)	0.0688 (7)	
N31	0.7509 (2)	0.20703 (12)	0.82346 (13)	0.0650 (7)	
C41	0.6827 (2)	0.15327 (13)	0.84497 (14)	0.0474 (6)	
C51	0.6154 (2)	0.12982 (13)	0.76785 (14)	0.0453 (6)	
C61	0.5227 (3)	0.07490 (16)	0.75157 (16)	0.0578 (8)	
C71	0.6910 (2)	0.13053 (14)	0.93810 (14)	0.0474 (7)	
C81	0.7027 (2)	0.17509 (14)	1.00691 (14)	0.0578 (7)	
H81	0.7046	0.2188	0.9943	0.069*	
C91	0.7117 (3)	0.15420 (16)	1.09445 (16)	0.0696 (9)	
H91	0.7201	0.1841	1.1404	0.084*	
C101	0.7084 (3)	0.08990 (17)	1.11375 (17)	0.0720 (9)	
H101	0.7129	0.0763	1.1726	0.086*	
C111	0.6985 (3)	0.04554 (15)	1.04609 (17)	0.0732 (9)	
H111	0.6969	0.0019	1.0591	0.088*	
C121	0.6909 (3)	0.06582 (15)	0.95877 (16)	0.0605 (8)	
H121	0.6857	0.0356	0.9133	0.073*	
C131	0.6151 (2)	0.16775 (14)	0.60726 (14)	0.0506 (7)	
C141	0.6584 (3)	0.11626 (14)	0.56026 (15)	0.0594 (7)	
H141	0.7049	0.0829	0.5907	0.071*	
C151	0.6335 (3)	0.11360 (15)	0.46829 (16)	0.0606 (8)	
C161	0.5621 (3)	0.16355 (16)	0.42371 (15)	0.0597 (8)	
C171	0.5198 (3)	0.21443 (16)	0.47268 (16)	0.0681 (9)	
H171	0.4729	0.2480	0.4429	0.082*	
C181	0.5450 (3)	0.21710 (15)	0.56441 (16)	0.0646 (8)	
H181	0.5150	0.2516	0.5961	0.078*	

C191	0.6868 (4)	0.05717 (17)	0.41909 (18)	0.1046 (12)	
H19D	0.7449	0.0726	0.3772	0.157*	
H19E	0.6129	0.0342	0.3881	0.157*	
H19F	0.7363	0.0290	0.4609	0.157*	
C201	0.5346 (3)	0.16413 (17)	0.32280 (15)	0.0869 (11)	
H20D	0.4949	0.1240	0.3028	0.130*	
H20E	0.6176	0.1702	0.2972	0.130*	
H20F	0.4741	0.1986	0.3047	0.130*	
N12	1.1457 (2)	0.16125 (11)	0.69086 (12)	0.0547 (6)	
N22	1.2317 (2)	0.20708 (12)	0.72382 (14)	0.0744 (7)	
N32	1.2519 (2)	0.19872 (12)	0.81027 (13)	0.0710 (7)	
C42	1.1791 (2)	0.14733 (13)	0.83428 (15)	0.0502 (7)	
C52	1.1122 (2)	0.12240 (13)	0.75798 (15)	0.0481 (7)	
C62	1.0304 (3)	0.06363 (16)	0.74120 (18)	0.0575 (8)	
C72	1.1848 (3)	0.12982 (13)	0.92950 (15)	0.0502 (7)	
C82	1.3046 (3)	0.13797 (14)	0.98363 (15)	0.0624 (8)	
H82	1.3806	0.1529	0.9596	0.075*	
C92	1.3110 (3)	0.12394 (16)	1.07320 (17)	0.0809 (10)	
H92	1.3912	0.1298	1.1094	0.097*	
C102	1.1990 (4)	0.10122 (18)	1.10928 (19)	0.0901 (11)	
H102	1.2041	0.0913	1.1695	0.108*	
C112	1.0816 (3)	0.09340 (18)	1.0568 (2)	0.0875 (11)	
H112	1.0061	0.0784	1.0813	0.105*	
C122	1.0731 (3)	0.10753 (15)	0.96716 (17)	0.0698 (9)	
H122	0.9919	0.1021	0.9318	0.084*	
C132	1.0998 (3)	0.16084 (13)	0.59666 (15)	0.0512 (7)	
C142	1.1766 (3)	0.13100 (14)	0.53780 (15)	0.0591 (8)	
H142	1.2562	0.1106	0.5594	0.071*	
C152	1.1370 (3)	0.13094 (14)	0.44753 (15)	0.0573 (7)	
C162	1.0183 (3)	0.16287 (14)	0.41608 (15)	0.0556 (7)	
C172	0.9446 (3)	0.19259 (15)	0.47672 (17)	0.0641 (8)	
H172	0.8658	0.2138	0.4557	0.077*	
C182	0.9832 (3)	0.19211 (14)	0.56720 (16)	0.0592 (8)	
H182	0.9316	0.2123	0.6067	0.071*	
C192	1.2217 (3)	0.09732 (18)	0.38449 (16)	0.0876 (11)	
H19A	1.3009	0.0800	0.4174	0.131*	
H19B	1.2473	0.1275	0.3414	0.131*	
H19C	1.1706	0.0631	0.3547	0.131*	
C202	0.9720 (3)	0.16489 (16)	0.31767 (15)	0.0827 (10)	
H20A	0.8882	0.1876	0.3081	0.124*	
H20B	0.9601	0.1219	0.2954	0.124*	
H20C	1.0383	0.1865	0.2870	0.124*	
F12A	1.0336 (15)	0.0375 (4)	0.6609 (5)	0.103 (3)	0.66 (3)
F22A	0.8992 (10)	0.0729 (7)	0.7457 (10)	0.107 (3)	0.66 (3)
F32A	1.0656 (14)	0.0176 (6)	0.7983 (10)	0.100 (3)	0.66 (3)
F12B	0.914 (2)	0.0751 (12)	0.708 (2)	0.114 (7)	0.34 (3)
F22B	1.016 (4)	0.0322 (16)	0.813 (2)	0.120 (8)	0.34 (3)
F32B	1.091 (3)	0.0270 (9)	0.690 (2)	0.127 (7)	0.34 (3)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F11	0.0735 (10)	0.1017 (16)	0.0738 (10)	−0.0230 (10)	−0.0278 (8)	0.0097 (10)
F21	0.0792 (11)	0.1035 (17)	0.0699 (10)	−0.0329 (10)	0.0121 (9)	0.0038 (9)
F31	0.0955 (13)	0.0521 (13)	0.1063 (13)	−0.0073 (10)	0.0024 (10)	−0.0199 (10)
N11	0.0615 (14)	0.0521 (17)	0.0430 (12)	−0.0079 (12)	−0.0023 (10)	−0.0035 (11)
N21	0.0935 (18)	0.0613 (19)	0.0499 (13)	−0.0245 (15)	−0.0006 (12)	−0.0035 (12)
N31	0.0840 (17)	0.0622 (19)	0.0470 (13)	−0.0191 (14)	−0.0012 (11)	−0.0075 (12)
C41	0.0502 (15)	0.0459 (19)	0.0451 (14)	−0.0015 (14)	0.0012 (12)	−0.0024 (13)
C51	0.0468 (14)	0.0469 (18)	0.0412 (13)	0.0000 (13)	0.0002 (12)	−0.0034 (13)
C61	0.0589 (18)	0.063 (2)	0.0500 (15)	−0.0063 (17)	−0.0041 (14)	−0.0021 (15)
C71	0.0491 (15)	0.049 (2)	0.0426 (14)	0.0034 (14)	−0.0003 (11)	−0.0037 (13)
C81	0.0705 (18)	0.054 (2)	0.0482 (15)	0.0064 (15)	0.0015 (13)	−0.0065 (14)
C91	0.096 (2)	0.069 (3)	0.0423 (15)	0.0120 (19)	0.0024 (14)	−0.0113 (15)
C101	0.097 (2)	0.071 (3)	0.0471 (16)	0.013 (2)	0.0053 (15)	0.0061 (17)
C111	0.101 (2)	0.055 (2)	0.0612 (18)	0.0097 (18)	0.0002 (16)	0.0068 (17)
C121	0.0771 (19)	0.052 (2)	0.0496 (15)	0.0101 (16)	−0.0040 (13)	−0.0075 (14)
C131	0.0584 (17)	0.054 (2)	0.0386 (13)	−0.0041 (15)	−0.0009 (12)	−0.0012 (14)
C141	0.0719 (18)	0.052 (2)	0.0516 (15)	0.0029 (15)	−0.0055 (13)	−0.0007 (14)
C151	0.0677 (18)	0.063 (2)	0.0506 (16)	−0.0058 (16)	0.0025 (14)	−0.0086 (15)
C161	0.0612 (18)	0.073 (2)	0.0445 (14)	−0.0115 (17)	0.0023 (13)	0.0003 (16)
C171	0.081 (2)	0.068 (2)	0.0537 (17)	0.0094 (18)	−0.0030 (15)	0.0118 (16)
C181	0.083 (2)	0.060 (2)	0.0499 (16)	0.0093 (17)	0.0013 (14)	0.0008 (15)
C191	0.147 (3)	0.093 (3)	0.073 (2)	0.016 (3)	0.005 (2)	−0.032 (2)
C201	0.094 (2)	0.121 (3)	0.0449 (15)	−0.019 (2)	0.0031 (15)	0.0051 (17)
N12	0.0667 (14)	0.0497 (17)	0.0461 (12)	−0.0061 (12)	−0.0017 (11)	0.0068 (11)
N22	0.1057 (19)	0.0608 (19)	0.0535 (14)	−0.0314 (16)	−0.0068 (13)	0.0044 (13)
N32	0.1008 (19)	0.0614 (19)	0.0485 (13)	−0.0240 (15)	−0.0032 (12)	0.0044 (12)
C42	0.0542 (16)	0.0463 (19)	0.0497 (15)	−0.0010 (14)	0.0035 (12)	0.0043 (13)
C52	0.0503 (15)	0.0439 (18)	0.0489 (14)	−0.0021 (14)	0.0000 (12)	0.0065 (14)
C62	0.063 (2)	0.057 (2)	0.0503 (18)	−0.0059 (18)	−0.0008 (17)	0.0072 (17)
C72	0.0587 (17)	0.0447 (19)	0.0474 (14)	0.0058 (14)	0.0071 (13)	0.0005 (13)
C82	0.0664 (19)	0.068 (2)	0.0526 (16)	−0.0019 (16)	0.0046 (14)	−0.0053 (14)
C92	0.097 (2)	0.092 (3)	0.0508 (17)	0.007 (2)	−0.0055 (16)	−0.0061 (17)
C102	0.129 (3)	0.095 (3)	0.0486 (18)	0.022 (3)	0.019 (2)	0.0097 (18)
C112	0.094 (3)	0.103 (3)	0.071 (2)	0.011 (2)	0.0340 (19)	0.019 (2)
C122	0.0626 (19)	0.081 (3)	0.0661 (18)	0.0058 (17)	0.0096 (15)	0.0101 (16)
C132	0.0591 (17)	0.0470 (19)	0.0459 (14)	−0.0036 (15)	−0.0021 (13)	0.0076 (13)
C142	0.0598 (17)	0.063 (2)	0.0517 (16)	0.0102 (15)	−0.0068 (13)	0.0039 (14)
C152	0.0571 (17)	0.062 (2)	0.0520 (15)	0.0008 (15)	−0.0001 (13)	0.0013 (14)
C162	0.0619 (17)	0.055 (2)	0.0474 (14)	−0.0058 (15)	−0.0055 (13)	0.0053 (14)
C172	0.0580 (17)	0.065 (2)	0.0655 (17)	0.0067 (16)	−0.0091 (14)	0.0071 (16)
C182	0.0600 (17)	0.060 (2)	0.0577 (16)	0.0037 (16)	0.0050 (14)	0.0015 (15)
C192	0.079 (2)	0.120 (3)	0.0635 (17)	0.012 (2)	0.0055 (15)	−0.0206 (19)
C202	0.090 (2)	0.095 (3)	0.0578 (17)	0.002 (2)	−0.0149 (15)	0.0055 (17)
F12A	0.149 (7)	0.094 (4)	0.068 (3)	−0.063 (4)	0.028 (3)	−0.021 (3)
F22A	0.058 (3)	0.101 (6)	0.166 (8)	−0.015 (3)	0.023 (5)	−0.014 (6)

F32A	0.120 (6)	0.055 (4)	0.113 (8)	−0.020 (3)	−0.042 (5)	0.033 (4)
F12B	0.049 (8)	0.115 (10)	0.166 (15)	−0.031 (8)	−0.041 (9)	0.046 (12)
F22B	0.17 (2)	0.092 (15)	0.084 (6)	−0.065 (12)	−0.020 (13)	0.040 (10)
F32B	0.127 (12)	0.073 (7)	0.189 (16)	−0.027 (7)	0.050 (11)	−0.082 (9)

Geometric parameters (Å, °)

F11—C61	1.324 (3)	N12—C132	1.449 (3)
F21—C61	1.332 (3)	N22—N32	1.313 (3)
F31—C61	1.343 (3)	N32—C42	1.365 (3)
N11—N21	1.345 (3)	C42—C52	1.373 (3)
N11—C51	1.363 (3)	C42—C72	1.481 (3)
N11—C131	1.443 (3)	C52—C62	1.479 (4)
N21—N31	1.320 (3)	C62—F12A	1.334 (7)
N31—C41	1.368 (3)	C62—F22A	1.335 (10)
C41—C51	1.373 (3)	C62—F32A	1.313 (14)
C41—C71	1.480 (3)	C62—F12B	1.236 (18)
C51—C61	1.476 (4)	C62—F22B	1.29 (3)
C71—C81	1.390 (3)	C62—F32B	1.280 (14)
C71—C121	1.383 (4)	C72—C82	1.388 (3)
C81—H81	0.9300	C72—C122	1.387 (3)
C81—C91	1.387 (3)	C82—H82	0.9300
C91—H91	0.9300	C82—C92	1.381 (3)
C91—C101	1.371 (4)	C92—H92	0.9300
C101—H101	0.9300	C92—C102	1.381 (4)
C101—C111	1.374 (4)	C102—H102	0.9300
C111—H111	0.9300	C102—C112	1.355 (4)
C111—C121	1.381 (3)	C112—H112	0.9300
C121—H121	0.9300	C112—C122	1.381 (3)
C131—C141	1.381 (4)	C122—H122	0.9300
C131—C181	1.367 (4)	C132—C142	1.383 (3)
C141—H141	0.9300	C132—C182	1.369 (3)
C141—C151	1.388 (3)	C142—H142	0.9300
C151—C161	1.394 (4)	C142—C152	1.380 (3)
C151—C191	1.517 (4)	C152—C162	1.399 (4)
C161—C171	1.384 (4)	C152—C192	1.513 (3)
C161—C201	1.522 (3)	C162—C172	1.382 (3)
C171—H171	0.9300	C162—C202	1.511 (3)
C171—C181	1.384 (3)	C172—H172	0.9300
C181—H181	0.9300	C172—C182	1.382 (3)
C191—H19D	0.9600	C182—H182	0.9300
C191—H19E	0.9600	C192—H19A	0.9600
C191—H19F	0.9600	C192—H19B	0.9600
C201—H20D	0.9600	C192—H19C	0.9600
C201—H20E	0.9600	C202—H20A	0.9600
C201—H20F	0.9600	C202—H20B	0.9600
N12—N22	1.344 (3)	C202—H20C	0.9600
N12—C52	1.367 (3)		

N21—N11—C51	110.48 (19)	N32—N22—N12	107.5 (2)
N21—N11—C131	118.5 (2)	N22—N32—C42	109.8 (2)
C51—N11—C131	131.0 (2)	N32—C42—C52	107.4 (2)
N31—N21—N11	107.1 (2)	N32—C42—C72	119.0 (2)
N21—N31—C41	109.6 (2)	C52—C42—C72	133.6 (3)
N31—C41—C51	107.5 (2)	N12—C52—C42	105.3 (2)
N31—C41—C71	120.6 (2)	N12—C52—C62	122.5 (2)
C51—C41—C71	131.9 (3)	C42—C52—C62	131.9 (2)
N11—C51—C41	105.3 (2)	F12A—C62—C52	115.3 (4)
N11—C51—C61	123.4 (2)	F12A—C62—F22A	102.9 (6)
C41—C51—C61	131.2 (2)	F22A—C62—C52	113.6 (6)
F11—C61—F21	106.1 (2)	F32A—C62—C52	112.8 (7)
F11—C61—F31	106.2 (2)	F32A—C62—F12A	105.7 (7)
F11—C61—C51	112.8 (3)	F32A—C62—F22A	105.5 (7)
F21—C61—F31	106.2 (3)	F12B—C62—C52	112.8 (11)
F21—C61—C51	112.2 (2)	F12B—C62—F22B	104.6 (13)
F31—C61—C51	112.8 (2)	F12B—C62—F32B	110.7 (12)
C81—C71—C41	119.4 (3)	F22B—C62—C52	112.7 (13)
C121—C71—C41	121.7 (2)	F32B—C62—C52	108.0 (8)
C121—C71—C81	118.9 (2)	F32B—C62—F22B	108.0 (12)
C71—C81—H81	120.1	C82—C72—C42	119.0 (2)
C91—C81—C71	119.8 (3)	C122—C72—C42	122.1 (2)
C91—C81—H81	120.1	C122—C72—C82	118.8 (2)
C81—C91—H91	119.7	C72—C82—H82	120.0
C101—C91—C81	120.6 (3)	C92—C82—C72	120.0 (3)
C101—C91—H91	119.7	C92—C82—H82	120.0
C91—C101—H101	120.0	C82—C92—H92	119.8
C91—C101—C111	119.9 (3)	C82—C92—C102	120.4 (3)
C111—C101—H101	120.0	C102—C92—H92	119.8
C101—C111—H111	120.0	C92—C102—H102	120.1
C101—C111—C121	119.9 (3)	C112—C102—C92	119.9 (3)
C121—C111—H111	120.0	C112—C102—H102	120.1
C71—C121—H121	119.6	C102—C112—H112	119.7
C111—C121—C71	120.8 (3)	C102—C112—C122	120.6 (3)
C111—C121—H121	119.6	C122—C112—H112	119.7
C141—C131—N11	119.3 (2)	C72—C122—H122	119.8
C181—C131—N11	119.9 (2)	C112—C122—C72	120.4 (3)
C181—C131—C141	120.8 (2)	C112—C122—H122	119.8
C131—C141—H141	119.5	C142—C132—N12	119.7 (2)
C131—C141—C151	120.9 (3)	C182—C132—N12	119.1 (2)
C151—C141—H141	119.5	C182—C132—C142	121.1 (2)
C141—C151—C161	118.9 (3)	C132—C142—H142	119.5
C141—C151—C191	119.2 (3)	C152—C142—C132	121.1 (2)
C161—C151—C191	121.9 (2)	C152—C142—H142	119.5
C151—C161—C201	121.3 (3)	C142—C152—C162	118.7 (2)
C171—C161—C151	118.8 (2)	C142—C152—C192	120.2 (2)
C171—C161—C201	119.9 (3)	C162—C152—C192	121.2 (2)

C161—C171—H171	118.9	C152—C162—C202	120.5 (2)
C181—C171—C161	122.2 (3)	C172—C162—C152	118.7 (2)
C181—C171—H171	118.9	C172—C162—C202	120.8 (2)
C131—C181—C171	118.3 (3)	C162—C172—H172	118.6
C131—C181—H181	120.9	C182—C172—C162	122.8 (3)
C171—C181—H181	120.9	C182—C172—H172	118.6
C151—C191—H19D	109.5	C132—C182—C172	117.7 (2)
C151—C191—H19E	109.5	C132—C182—H182	121.2
C151—C191—H19F	109.5	C172—C182—H182	121.2
H19D—C191—H19E	109.5	C152—C192—H19A	109.5
H19D—C191—H19F	109.5	C152—C192—H19B	109.5
H19E—C191—H19F	109.5	C152—C192—H19C	109.5
C161—C201—H20D	109.5	H19A—C192—H19B	109.5
C161—C201—H20E	109.5	H19A—C192—H19C	109.5
C161—C201—H20F	109.5	H19B—C192—H19C	109.5
H20D—C201—H20E	109.5	C162—C202—H20A	109.5
H20D—C201—H20F	109.5	C162—C202—H20B	109.5
H20E—C201—H20F	109.5	C162—C202—H20C	109.5
N22—N12—C52	110.0 (2)	H20A—C202—H20B	109.5
N22—N12—C132	119.5 (2)	H20A—C202—H20C	109.5
C52—N12—C132	130.5 (2)	H20B—C202—H20C	109.5

1-(3,4-Dimethylphenyl)-4-(3-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (2_C18H16F3N3O_3OMe34)

Crystal data

C₁₈H₁₆F₃N₃O*M_r* = 347.34Orthorhombic, *Pbca**a* = 9.5097 (13) Å*b* = 17.921 (2) Å*c* = 20.011 (3) Å*V* = 3410.3 (8) Å³*Z* = 8*F*(000) = 1440*D_x* = 1.353 Mg m⁻³Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 6163 reflections

θ = 2.5–23.0°

μ = 0.11 mm⁻¹*T* = 296 K

Prism, colourless

0.78 × 0.37 × 0.32 mm

Data collection

Bruker SMART CCD area detector
diffractometer

phi and ω scans

24398 measured reflections

3001 independent reflections

1986 reflections with *I* > 2σ(*I*)*R*_{int} = 0.070θ_{max} = 25.0°, θ_{min} = 2.0°*h* = -11→11*k* = -21→18*l* = -23→22

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.037*wR*(*F*²) = 0.114*S* = 1.02

3001 reflections

226 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0523*P*)² + 0.6011*P*]where *P* = (*F_o*² + 2*F_c*²)/3(Δ/σ)_{max} < 0.001

$$\Delta\rho_{\max} = 0.13 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$$

Special details

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C4	0.45657 (19)	0.13444 (10)	0.53652 (8)	0.0517 (5)
C5	0.51589 (19)	0.11231 (10)	0.47700 (8)	0.0513 (5)
C6	0.4518 (2)	0.08305 (12)	0.41461 (10)	0.0624 (5)
C7	0.30890 (18)	0.14475 (10)	0.55692 (9)	0.0515 (5)
C8	0.27036 (18)	0.12856 (10)	0.62260 (9)	0.0539 (5)
H8	0.336611	0.109980	0.652467	0.065*
C9	0.1333 (2)	0.14023 (11)	0.64313 (10)	0.0616 (5)
C10	0.0346 (2)	0.16762 (11)	0.59890 (12)	0.0689 (6)
H10	−0.057596	0.175192	0.612864	0.083*
C11	0.0726 (2)	0.18369 (12)	0.53428 (12)	0.0681 (6)
H11	0.005582	0.202003	0.504652	0.082*
C12	0.2090 (2)	0.17299 (11)	0.51278 (10)	0.0623 (5)
H12	0.234105	0.184570	0.469075	0.075*
C13	0.77078 (19)	0.10712 (11)	0.43884 (9)	0.0547 (5)
C14	0.7871 (2)	0.15926 (11)	0.38891 (9)	0.0594 (5)
H14	0.725376	0.199398	0.386202	0.071*
C15	0.8952 (2)	0.15240 (12)	0.34245 (9)	0.0627 (5)
C16	0.9859 (2)	0.09124 (13)	0.34746 (10)	0.0636 (5)
C17	0.9668 (2)	0.04048 (12)	0.39842 (11)	0.0694 (6)
H17	1.028383	0.000337	0.401877	0.083*
C18	0.8598 (2)	0.04716 (11)	0.44441 (11)	0.0646 (5)
H18	0.848183	0.012082	0.478216	0.078*
C19	0.9127 (3)	0.21093 (14)	0.28922 (11)	0.0925 (8)
H19A	0.829265	0.240984	0.286963	0.139*
H19B	0.928131	0.187197	0.246845	0.139*
H19C	0.991846	0.241980	0.299887	0.139*
C20	1.1031 (2)	0.07970 (17)	0.29777 (13)	0.0988 (8)
H20A	1.160591	0.038568	0.311813	0.148*
H20B	1.159390	0.124064	0.295249	0.148*
H20C	1.063802	0.069116	0.254602	0.148*
C21	0.1781 (3)	0.09107 (18)	0.75216 (12)	0.1067 (9)
H21A	0.205598	0.043296	0.734837	0.160*
H21B	0.131728	0.084499	0.794364	0.160*
H21C	0.260040	0.121655	0.758145	0.160*
F1	0.33196 (13)	0.04803 (7)	0.42676 (6)	0.0849 (4)
F2	0.42400 (15)	0.13635 (8)	0.37093 (6)	0.0985 (5)
F3	0.53445 (14)	0.03468 (8)	0.38283 (6)	0.0935 (4)
N1	0.65692 (16)	0.11688 (9)	0.48613 (7)	0.0562 (4)

N2	0.68475 (17)	0.13996 (10)	0.54906 (8)	0.0681 (5)
N3	0.56389 (16)	0.14978 (10)	0.57937 (8)	0.0642 (5)
O1	0.08504 (15)	0.12619 (10)	0.70658 (8)	0.0888 (5)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C4	0.0570 (10)	0.0560 (12)	0.0421 (10)	−0.0035 (8)	−0.0041 (9)	0.0061 (8)
C5	0.0544 (11)	0.0558 (11)	0.0436 (10)	−0.0080 (8)	−0.0023 (8)	0.0065 (8)
C6	0.0669 (13)	0.0722 (14)	0.0480 (11)	−0.0098 (11)	0.0004 (10)	0.0004 (10)
C7	0.0547 (10)	0.0512 (11)	0.0487 (10)	−0.0029 (9)	−0.0038 (8)	−0.0003 (8)
C8	0.0525 (11)	0.0588 (12)	0.0504 (11)	0.0035 (9)	−0.0018 (8)	0.0020 (9)
C9	0.0608 (12)	0.0607 (13)	0.0633 (12)	0.0039 (10)	0.0056 (10)	−0.0009 (10)
C10	0.0523 (11)	0.0661 (14)	0.0885 (16)	0.0042 (10)	−0.0008 (11)	−0.0039 (12)
C11	0.0631 (13)	0.0621 (13)	0.0792 (16)	0.0038 (10)	−0.0217 (11)	−0.0005 (11)
C12	0.0708 (13)	0.0622 (13)	0.0539 (11)	−0.0003 (10)	−0.0116 (10)	0.0025 (10)
C13	0.0544 (11)	0.0603 (12)	0.0495 (11)	−0.0084 (9)	0.0020 (8)	−0.0011 (9)
C14	0.0705 (12)	0.0559 (12)	0.0519 (11)	0.0019 (9)	0.0072 (9)	−0.0029 (9)
C15	0.0761 (13)	0.0641 (13)	0.0479 (11)	−0.0129 (11)	0.0075 (10)	−0.0089 (10)
C16	0.0538 (11)	0.0788 (15)	0.0580 (12)	−0.0047 (11)	0.0017 (9)	−0.0170 (11)
C17	0.0598 (12)	0.0726 (14)	0.0758 (14)	0.0081 (10)	−0.0046 (11)	−0.0095 (12)
C18	0.0648 (12)	0.0610 (13)	0.0680 (13)	−0.0042 (10)	−0.0021 (10)	0.0060 (10)
C19	0.130 (2)	0.0872 (17)	0.0604 (14)	−0.0072 (15)	0.0313 (14)	0.0029 (13)
C20	0.0790 (15)	0.143 (2)	0.0744 (16)	0.0114 (16)	0.0131 (13)	−0.0189 (16)
C21	0.0996 (19)	0.154 (3)	0.0662 (15)	0.0239 (18)	0.0215 (14)	0.0312 (17)
F1	0.0766 (8)	0.1095 (10)	0.0685 (8)	−0.0362 (7)	−0.0014 (6)	−0.0132 (7)
F2	0.1292 (12)	0.1098 (11)	0.0566 (7)	−0.0205 (9)	−0.0288 (7)	0.0222 (7)
F3	0.0889 (9)	0.1118 (11)	0.0798 (9)	−0.0044 (8)	0.0009 (7)	−0.0407 (8)
N1	0.0566 (9)	0.0673 (11)	0.0447 (9)	−0.0071 (7)	0.0004 (7)	0.0026 (7)
N2	0.0585 (10)	0.0978 (14)	0.0480 (9)	−0.0076 (9)	−0.0043 (8)	−0.0046 (9)
N3	0.0567 (10)	0.0892 (13)	0.0467 (9)	−0.0045 (8)	−0.0032 (8)	−0.0030 (8)
O1	0.0748 (10)	0.1169 (13)	0.0747 (10)	0.0205 (9)	0.0239 (8)	0.0132 (10)

Geometric parameters ($\text{\AA}$, $^\circ$)

C4—C5	1.376 (2)	C11—C12	1.381 (3)
C4—C7	1.474 (2)	C13—C14	1.377 (3)
C4—N3	1.361 (2)	C13—C18	1.373 (3)
C5—C6	1.485 (3)	C13—N1	1.449 (2)
C5—N1	1.356 (2)	C14—C15	1.392 (3)
C6—F1	1.324 (2)	C15—C16	1.398 (3)
C6—F2	1.321 (2)	C15—C19	1.504 (3)
C6—F3	1.332 (2)	C16—C17	1.378 (3)
C7—C8	1.395 (2)	C16—C20	1.507 (3)
C7—C12	1.392 (2)	C17—C18	1.377 (3)
C8—C9	1.383 (3)	C21—O1	1.418 (3)
C9—C10	1.380 (3)	N1—N2	1.352 (2)
C9—O1	1.373 (2)	N2—N3	1.311 (2)

C10—C11	1.373 (3)		
C5—C4—C7	131.78 (16)	C10—C11—C12	120.76 (19)
N3—C4—C5	107.22 (15)	C11—C12—C7	119.61 (19)
N3—C4—C7	120.98 (16)	C14—C13—N1	118.45 (17)
C4—C5—C6	131.40 (17)	C18—C13—C14	121.38 (18)
N1—C5—C4	105.74 (15)	C18—C13—N1	120.17 (17)
N1—C5—C6	122.71 (16)	C13—C14—C15	120.54 (19)
F1—C6—C5	111.49 (16)	C14—C15—C16	118.50 (18)
F1—C6—F3	106.69 (17)	C14—C15—C19	119.5 (2)
F2—C6—C5	112.53 (18)	C16—C15—C19	121.96 (19)
F2—C6—F1	106.95 (17)	C15—C16—C20	121.1 (2)
F2—C6—F3	105.84 (16)	C17—C16—C15	119.28 (18)
F3—C6—C5	112.92 (17)	C17—C16—C20	119.7 (2)
C8—C7—C4	119.02 (16)	C18—C17—C16	122.3 (2)
C12—C7—C4	121.32 (17)	C13—C18—C17	118.00 (19)
C12—C7—C8	119.61 (17)	C5—N1—C13	130.09 (15)
C9—C8—C7	119.75 (17)	N2—N1—C5	109.74 (15)
C10—C9—C8	120.29 (19)	N2—N1—C13	119.94 (14)
O1—C9—C8	124.19 (18)	N3—N2—N1	107.47 (14)
O1—C9—C10	115.53 (18)	N2—N3—C4	109.81 (15)
C11—C10—C9	119.98 (19)	C9—O1—C21	117.87 (16)
C4—C5—C6—F1	−27.8 (3)	C13—C14—C15—C19	−178.75 (19)
C4—C5—C6—F2	92.4 (2)	C13—N1—N2—N3	175.11 (16)
C4—C5—C6—F3	−147.9 (2)	C14—C13—C18—C17	0.1 (3)
C4—C5—N1—C13	−173.58 (18)	C14—C13—N1—C5	68.0 (3)
C4—C5—N1—N2	0.8 (2)	C14—C13—N1—N2	−105.9 (2)
C4—C7—C8—C9	177.89 (17)	C14—C15—C16—C17	−0.9 (3)
C4—C7—C12—C11	−178.29 (18)	C14—C15—C16—C20	178.61 (19)
C5—C4—C7—C8	145.9 (2)	C15—C16—C17—C18	1.0 (3)
C5—C4—C7—C12	−36.7 (3)	C16—C17—C18—C13	−0.6 (3)
C5—C4—N3—N2	1.4 (2)	C18—C13—C14—C15	0.0 (3)
C5—N1—N2—N3	0.1 (2)	C18—C13—N1—C5	−112.2 (2)
C6—C5—N1—C13	10.4 (3)	C18—C13—N1—N2	73.9 (2)
C6—C5—N1—N2	−175.27 (17)	C19—C15—C16—C17	178.3 (2)
C7—C4—C5—C6	−7.7 (4)	C19—C15—C16—C20	−2.3 (3)
C7—C4—C5—N1	176.71 (18)	C20—C16—C17—C18	−178.5 (2)
C7—C4—N3—N2	−176.86 (16)	N1—C5—C6—F1	147.14 (18)
C7—C8—C9—C10	0.2 (3)	N1—C5—C6—F2	−92.7 (2)
C7—C8—C9—O1	−179.90 (19)	N1—C5—C6—F3	27.0 (3)
C8—C7—C12—C11	−0.9 (3)	N1—C13—C14—C15	179.78 (16)
C8—C9—C10—C11	−0.3 (3)	N1—C13—C18—C17	−179.72 (17)
C8—C9—O1—C21	−6.1 (3)	N1—N2—N3—C4	−0.9 (2)
C9—C10—C11—C12	−0.2 (3)	N3—C4—C5—C6	174.3 (2)
C10—C9—O1—C21	173.8 (2)	N3—C4—C5—N1	−1.3 (2)
C10—C11—C12—C7	0.8 (3)	N3—C4—C7—C8	−36.3 (3)
C12—C7—C8—C9	0.4 (3)	N3—C4—C7—C12	141.13 (19)

C13—C14—C15—C16 0.4 (3) O1—C9—C10—C11 179.77 (19)

1-(3,4-Dimethylphenyl)-4-(4-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (3_C18H16F3N3O_4OMe34)

Crystal data

C₁₈H₁₆F₃N₃O

M_r = 347.34

Monoclinic, *P*2₁/*n*

a = 15.1368 (16) Å

b = 7.7224 (9) Å

c = 15.4446 (18) Å

β = 112.454 (2)°

V = 1668.5 (3) Å³

Z = 4

F(000) = 720

D_x = 1.383 Mg m^{−3}

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 2495 reflections

θ = 2.4–22.3°

μ = 0.11 mm^{−1}

T = 296 K

Prism, colourless

0.36 × 0.23 × 0.2 mm

Data collection

Bruker SMART CCD area detector
diffractometer

Graphite monochromator

phi and ω scans

12266 measured reflections

2930 independent reflections

1644 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.045

θ_{max} = 25.0°, θ_{min} = 1.6°

h = −13→18

k = −6→9

l = −18→18

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.038

wR (*F*²) = 0.114

S = 1.00

2930 reflections

254 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.053*P*)² + 0.0053*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.15 e Å^{−3}

Δρ_{min} = −0.13 e Å^{−3}

Special details

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}	Occ. (<1)
C4	0.93725 (15)	0.4081 (3)	0.12782 (13)	0.0499 (5)	
C5	0.86075 (15)	0.2987 (3)	0.09070 (13)	0.0508 (5)	
N1	0.78596 (12)	0.3801 (2)	0.10140 (11)	0.0547 (5)	
C7	1.03822 (14)	0.3954 (2)	0.14026 (13)	0.0494 (5)	
C12	1.06877 (16)	0.3365 (3)	0.07057 (13)	0.0568 (6)	
H12	1.023688	0.300023	0.013383	0.068*	
C11	1.16373 (16)	0.3317 (3)	0.08504 (14)	0.0602 (6)	
H11	1.182349	0.291691	0.037771	0.072*	
C10	1.23252 (16)	0.3859 (3)	0.16955 (14)	0.0561 (6)	
C9	1.20406 (16)	0.4474 (3)	0.23901 (14)	0.0597 (6)	

H9	1.249274	0.485992	0.295640	0.072*	
C8	1.10823 (16)	0.4510 (3)	0.22363 (13)	0.0577 (6)	
H8	1.089851	0.492092	0.270839	0.069*	
C13	0.68774 (15)	0.3272 (3)	0.07683 (15)	0.0543 (5)	
C14	0.62510 (15)	0.3317 (2)	−0.01507 (14)	0.0560 (6)	
H14	0.646474	0.367211	−0.061250	0.067*	
C15	0.52962 (16)	0.2833 (2)	−0.03990 (14)	0.0547 (6)	
C16	0.49917 (16)	0.2331 (3)	0.03122 (16)	0.0575 (6)	
C17	0.56329 (18)	0.2312 (3)	0.12258 (16)	0.0694 (7)	
H17	0.542310	0.198475	0.169471	0.083*	
C18	0.65795 (18)	0.2765 (3)	0.14683 (15)	0.0656 (6)	
H18	0.700601	0.272849	0.208944	0.079*	
C21	1.39830 (16)	0.4186 (3)	0.26503 (18)	0.0847 (8)	
H21A	1.390735	0.537335	0.279363	0.127*	
H21B	1.459662	0.403551	0.261226	0.127*	
H21C	1.393847	0.345369	0.313420	0.127*	
C19	0.46274 (16)	0.2853 (3)	−0.14122 (15)	0.0798 (7)	
H19A	0.496027	0.327359	−0.178884	0.120*	
H19B	0.409508	0.359779	−0.148830	0.120*	
H19C	0.440024	0.170028	−0.160587	0.120*	
C20	0.39630 (16)	0.1806 (3)	0.00797 (18)	0.0801 (7)	
H20A	0.386211	0.161333	0.064915	0.120*	
H20B	0.382839	0.076031	−0.028404	0.120*	
H20C	0.354595	0.271102	−0.027359	0.120*	
C6	0.8518 (2)	0.1193 (4)	0.0541 (2)	0.0735 (8)	
N2	0.81480 (14)	0.5342 (2)	0.14348 (12)	0.0667 (5)	
N3	0.90597 (14)	0.5511 (2)	0.15941 (12)	0.0632 (5)	
O1	1.32510 (11)	0.3737 (2)	0.17768 (11)	0.0741 (5)	
F1	0.9321 (10)	0.0565 (19)	0.0516 (13)	0.091 (3)	0.52 (2)
F2	0.7859 (4)	0.0920 (10)	−0.0236 (6)	0.084 (3)	0.52 (2)
F3	0.8295 (8)	0.0123 (10)	0.1138 (6)	0.107 (3)	0.52 (2)
F1'	0.9333 (11)	0.051 (2)	0.0709 (16)	0.108 (5)	0.48 (2)
F2'	0.8105 (15)	0.136 (2)	−0.0456 (10)	0.186 (6)	0.48 (2)
F3'	0.8016 (14)	0.0178 (14)	0.076 (2)	0.180 (6)	0.48 (2)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C4	0.0551 (14)	0.0482 (13)	0.0428 (11)	0.0035 (11)	0.0147 (10)	−0.0022 (9)
C5	0.0499 (14)	0.0481 (13)	0.0497 (12)	0.0044 (11)	0.0138 (10)	−0.0031 (9)
N1	0.0529 (12)	0.0529 (11)	0.0537 (10)	0.0015 (9)	0.0152 (8)	−0.0078 (8)
C7	0.0580 (14)	0.0417 (12)	0.0459 (11)	0.0012 (10)	0.0171 (10)	0.0003 (9)
C12	0.0656 (16)	0.0557 (14)	0.0441 (11)	0.0009 (11)	0.0154 (11)	−0.0050 (10)
C11	0.0717 (17)	0.0607 (15)	0.0517 (13)	0.0023 (12)	0.0274 (12)	−0.0029 (10)
C10	0.0582 (15)	0.0506 (14)	0.0611 (14)	−0.0001 (11)	0.0247 (12)	0.0006 (10)
C9	0.0577 (16)	0.0634 (15)	0.0523 (13)	−0.0043 (11)	0.0146 (11)	−0.0097 (10)
C8	0.0623 (16)	0.0615 (15)	0.0493 (12)	−0.0013 (11)	0.0213 (11)	−0.0115 (10)
C13	0.0528 (15)	0.0491 (13)	0.0589 (13)	0.0075 (10)	0.0190 (11)	−0.0002 (10)

C14	0.0632 (16)	0.0515 (13)	0.0548 (13)	0.0040 (11)	0.0241 (11)	0.0014 (10)
C15	0.0546 (15)	0.0443 (12)	0.0620 (13)	0.0071 (10)	0.0188 (11)	0.0009 (10)
C16	0.0595 (16)	0.0456 (13)	0.0743 (16)	0.0093 (11)	0.0333 (13)	0.0010 (11)
C17	0.0794 (19)	0.0693 (16)	0.0721 (16)	0.0071 (13)	0.0430 (15)	0.0075 (12)
C18	0.0694 (17)	0.0720 (16)	0.0562 (13)	0.0084 (13)	0.0248 (12)	0.0050 (11)
C21	0.0561 (16)	0.092 (2)	0.100 (2)	−0.0124 (13)	0.0228 (14)	−0.0208 (15)
C19	0.0715 (17)	0.0875 (19)	0.0698 (16)	0.0022 (13)	0.0151 (13)	0.0000 (13)
C20	0.0707 (18)	0.0686 (17)	0.113 (2)	0.0049 (13)	0.0481 (15)	0.0022 (14)
C6	0.0541 (19)	0.0656 (19)	0.090 (2)	0.0054 (16)	0.0160 (19)	−0.0199 (16)
N2	0.0631 (14)	0.0611 (13)	0.0744 (13)	0.0006 (10)	0.0244 (10)	−0.0171 (10)
N3	0.0620 (14)	0.0568 (12)	0.0696 (12)	−0.0001 (10)	0.0238 (10)	−0.0150 (9)
O1	0.0613 (11)	0.0850 (12)	0.0791 (11)	−0.0036 (9)	0.0302 (9)	−0.0090 (9)
F1	0.065 (6)	0.070 (6)	0.147 (7)	−0.012 (5)	0.051 (5)	−0.053 (5)
F2	0.070 (5)	0.077 (4)	0.077 (4)	0.012 (2)	−0.006 (3)	−0.038 (3)
F3	0.157 (7)	0.047 (3)	0.129 (5)	−0.019 (3)	0.070 (4)	0.011 (3)
F1'	0.079 (7)	0.061 (5)	0.157 (9)	0.022 (5)	0.014 (5)	−0.013 (5)
F2'	0.263 (10)	0.160 (8)	0.087 (5)	0.036 (7)	0.014 (6)	−0.063 (5)
F3'	0.123 (8)	0.088 (6)	0.377 (19)	−0.045 (5)	0.149 (12)	−0.090 (9)

Geometric parameters (Å, °)

C4—C5	1.369 (3)	C13—C18	1.378 (3)
C4—C7	1.469 (3)	C14—C15	1.397 (3)
C4—N3	1.363 (2)	C15—C16	1.399 (3)
C5—N1	1.359 (2)	C15—C19	1.505 (3)
C5—C6	1.483 (3)	C16—C17	1.374 (3)
N1—C13	1.446 (2)	C16—C20	1.514 (3)
N1—N2	1.346 (2)	C17—C18	1.381 (3)
C7—C12	1.400 (3)	C21—O1	1.424 (2)
C7—C8	1.387 (3)	C6—F1	1.323 (14)
C12—C11	1.368 (3)	C6—F2	1.250 (7)
C11—C10	1.387 (3)	C6—F3	1.373 (8)
C10—C9	1.384 (3)	C6—F1'	1.274 (15)
C10—O1	1.362 (2)	C6—F2'	1.429 (14)
C9—C8	1.378 (3)	C6—F3'	1.224 (12)
C13—C14	1.374 (3)	N2—N3	1.313 (2)
C5—C4—C7	133.23 (19)	C14—C15—C16	118.38 (19)
N3—C4—C5	107.20 (19)	C14—C15—C19	119.8 (2)
N3—C4—C7	119.55 (18)	C16—C15—C19	121.8 (2)
C4—C5—C6	132.5 (2)	C15—C16—C20	120.4 (2)
N1—C5—C4	105.93 (18)	C17—C16—C15	119.6 (2)
N1—C5—C6	121.3 (2)	C17—C16—C20	120.0 (2)
C5—N1—C13	131.18 (17)	C16—C17—C18	121.9 (2)
N2—N1—C5	109.63 (17)	C13—C18—C17	118.4 (2)
N2—N1—C13	119.19 (17)	F1—C6—C5	113.7 (6)
C12—C7—C4	123.63 (18)	F1—C6—F3	105.3 (9)
C8—C7—C4	119.27 (18)	F2—C6—C5	116.5 (4)

C8—C7—C12	117.0 (2)	F2—C6—F1	108.3 (8)
C11—C12—C7	121.22 (19)	F2—C6—F3	103.5 (6)
C12—C11—C10	120.6 (2)	F3—C6—C5	108.4 (5)
C9—C10—C11	119.3 (2)	F1'—C6—C5	111.5 (8)
O1—C10—C11	116.22 (19)	F1'—C6—F2'	104.3 (10)
O1—C10—C9	124.50 (19)	F2'—C6—C5	105.5 (7)
C8—C9—C10	119.48 (19)	F3'—C6—C5	118.0 (7)
C9—C8—C7	122.34 (19)	F3'—C6—F1'	109.6 (11)
C14—C13—N1	119.93 (19)	F3'—C6—F2'	106.8 (8)
C14—C13—C18	121.0 (2)	N3—N2—N1	107.59 (16)
C18—C13—N1	119.10 (19)	N2—N3—C4	109.66 (17)
C13—C14—C15	120.7 (2)	C10—O1—C21	118.13 (17)
C4—C5—N1—C13	−179.11 (19)	C12—C7—C8—C9	−0.8 (3)
C4—C5—N1—N2	0.1 (2)	C12—C11—C10—C9	−0.9 (3)
C4—C5—C6—F1	−4.8 (10)	C12—C11—C10—O1	179.03 (17)
C4—C5—C6—F2	−131.9 (6)	C11—C10—C9—C8	1.1 (3)
C4—C5—C6—F3	111.9 (6)	C11—C10—O1—C21	−176.53 (19)
C4—C5—C6—F1'	9.0 (12)	C10—C9—C8—C7	−0.3 (3)
C4—C5—C6—F2'	−103.7 (12)	C9—C10—O1—C21	3.3 (3)
C4—C5—C6—F3'	137.1 (15)	C8—C7—C12—C11	1.0 (3)
C4—C7—C12—C11	178.24 (18)	C13—N1—N2—N3	179.25 (16)
C4—C7—C8—C9	−178.14 (18)	C13—C14—C15—C16	1.0 (3)
C5—C4—C7—C12	45.3 (3)	C13—C14—C15—C19	−178.63 (19)
C5—C4—C7—C8	−137.5 (2)	C14—C13—C18—C17	−0.4 (3)
C5—C4—N3—N2	0.0 (2)	C14—C15—C16—C17	−0.5 (3)
C5—N1—C13—C14	−75.4 (3)	C14—C15—C16—C20	179.64 (18)
C5—N1—C13—C18	106.0 (2)	C15—C16—C17—C18	−0.5 (3)
C5—N1—N2—N3	0.0 (2)	C16—C17—C18—C13	1.0 (3)
N1—C5—C6—F1	−177.4 (9)	C18—C13—C14—C15	−0.5 (3)
N1—C5—C6—F2	55.5 (7)	C19—C15—C16—C17	179.12 (19)
N1—C5—C6—F3	−60.7 (6)	C19—C15—C16—C20	−0.7 (3)
N1—C5—C6—F1'	−163.6 (11)	C20—C16—C17—C18	179.37 (19)
N1—C5—C6—F2'	83.7 (12)	C6—C5—N1—C13	−4.8 (3)
N1—C5—C6—F3'	−35.5 (16)	C6—C5—N1—N2	174.4 (2)
N1—C13—C14—C15	−179.10 (17)	N2—N1—C13—C14	105.5 (2)
N1—C13—C18—C17	178.13 (18)	N2—N1—C13—C18	−73.1 (2)
N1—N2—N3—C4	0.0 (2)	N3—C4—C5—N1	−0.1 (2)
C7—C4—C5—N1	178.12 (19)	N3—C4—C5—C6	−173.5 (2)
C7—C4—C5—C6	4.7 (4)	N3—C4—C7—C12	−136.7 (2)
C7—C4—N3—N2	−178.43 (16)	N3—C4—C7—C8	40.5 (3)
C7—C12—C11—C10	−0.2 (3)	O1—C10—C9—C8	−178.80 (18)

1-(2,4-Dimethylphenyl)-4-(4-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole (4_4OMe24Me)*Crystal data*C₁₈H₁₆F₃N₃O $M_r = 347.34$ Triclinic, $P\bar{1}$ $a = 8.829$ (2) Å $b = 9.513$ (2) Å $c = 11.598$ (3) Å $\alpha = 106.105$ (4)° $\beta = 95.554$ (4)° $\gamma = 110.049$ (4)° $V = 859.1$ (4) Å³ $Z = 2$ $F(000) = 360$ $D_x = 1.343$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1698 reflections

 $\theta = 2.4\text{--}23.5^\circ$ $\mu = 0.11$ mm⁻¹ $T = 293$ K

Prismatic, colorless

 $0.72 \times 0.23 \times 0.13$ mm*Data collection*Bruker SMART CCD area detector
diffractometerphi and ω scans

6496 measured reflections

3096 independent reflections

1709 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.092$ $\theta_{\text{max}} = 25.5^\circ$, $\theta_{\text{min}} = 1.9^\circ$ $h = -10 \rightarrow 10$ $k = -11 \rightarrow 11$ $l = -14 \rightarrow 11$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.053$ $wR(F^2) = 0.153$ $S = 0.98$

3096 reflections

254 parameters

292 restraints

Primary atom site location: structure-invariant
direct methodsHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0648P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.14$ e Å⁻³*Special details*

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C21	−0.2723 (3)	0.4401 (5)	0.1277 (3)	0.1030 (12)	
H21A	−0.349309	0.396692	0.050371	0.155*	
H21B	−0.308799	0.373940	0.176948	0.155*	
H21C	−0.265738	0.545027	0.169772	0.155*	
F1A	0.5992 (16)	0.863 (2)	0.3572 (15)	0.121 (5)	0.48 (3)
F2A	0.8012 (19)	0.816 (2)	0.416 (2)	0.110 (4)	0.48 (3)
F3A	0.772 (2)	1.0149 (11)	0.5188 (11)	0.127 (4)	0.48 (3)
C4	0.4271 (3)	0.6786 (3)	0.5017 (2)	0.0469 (6)	
N1	0.6568 (2)	0.7876 (2)	0.63995 (18)	0.0516 (5)	
N2	0.5401 (3)	0.7010 (3)	0.6858 (2)	0.0646 (6)	

C8	0.1354 (3)	0.6176 (3)	0.4205 (2)	0.0523 (6)	
H8	0.125932	0.655038	0.501384	0.063*	
O1	−0.1156 (2)	0.4471 (3)	0.10743 (17)	0.0830 (6)	
C5	0.5900 (3)	0.7766 (3)	0.5244 (2)	0.0464 (6)	
N3	0.4021 (3)	0.6347 (3)	0.6036 (2)	0.0641 (6)	
C7	0.2876 (3)	0.6213 (3)	0.3969 (2)	0.0476 (6)	
C18	0.9423 (3)	0.8184 (3)	0.6932 (2)	0.0592 (7)	
H18	0.918317	0.722985	0.630980	0.071*	
C12	0.2975 (3)	0.5641 (3)	0.2750 (2)	0.0583 (7)	
H12	0.397518	0.563510	0.256550	0.070*	
C10	0.0121 (3)	0.5060 (3)	0.2072 (2)	0.0585 (7)	
C9	−0.0025 (3)	0.5598 (3)	0.3273 (2)	0.0563 (7)	
H9	−0.103664	0.557199	0.345213	0.068*	
C11	0.1630 (3)	0.5088 (3)	0.1820 (2)	0.0647 (7)	
H11	0.172788	0.472726	0.101015	0.078*	
C13	0.8214 (3)	0.8776 (3)	0.7137 (2)	0.0488 (6)	
C14	0.8521 (3)	1.0193 (3)	0.8045 (3)	0.0637 (7)	
C17	1.0983 (3)	0.9015 (4)	0.7652 (3)	0.0695 (8)	
H17	1.179193	0.860479	0.752133	0.083*	
C15	1.0117 (4)	1.0987 (4)	0.8744 (3)	0.0792 (9)	
H15	1.035990	1.193929	0.936856	0.095*	
C6	0.6859 (3)	0.8668 (3)	0.4524 (3)	0.0599 (7)	
F2B	0.8099 (12)	0.9917 (15)	0.5138 (9)	0.108 (3)	0.52 (3)
F3B	0.5899 (16)	0.9137 (18)	0.3889 (16)	0.106 (4)	0.52 (3)
F1B	0.734 (3)	0.7772 (16)	0.3677 (14)	0.120 (4)	0.52 (3)
C16	1.1371 (3)	1.0440 (4)	0.8563 (3)	0.0728 (8)	
C20	1.3089 (4)	1.1376 (5)	0.9345 (4)	0.1147 (13)	
H20A	1.311734	1.233108	0.992634	0.172*	
H20B	1.338856	1.075074	0.977604	0.172*	
H20C	1.385341	1.164288	0.883001	0.172*	
C19	0.7210 (4)	1.0866 (4)	0.8254 (4)	0.1035 (12)	
H19A	0.766548	1.185267	0.892332	0.155*	
H19B	0.682842	1.104232	0.752394	0.155*	
H19C	0.630178	1.012962	0.844895	0.155*	

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C21	0.0532 (18)	0.166 (4)	0.066 (2)	0.015 (2)	0.0017 (16)	0.042 (2)
F1A	0.065 (5)	0.179 (11)	0.098 (6)	−0.017 (5)	−0.007 (4)	0.104 (7)
F2A	0.109 (7)	0.132 (9)	0.147 (11)	0.067 (7)	0.089 (6)	0.086 (7)
F3A	0.191 (11)	0.042 (4)	0.118 (6)	0.006 (4)	0.046 (6)	0.027 (3)
C4	0.0461 (14)	0.0468 (14)	0.0522 (14)	0.0160 (11)	0.0166 (12)	0.0235 (12)
N1	0.0462 (12)	0.0570 (13)	0.0559 (13)	0.0158 (10)	0.0119 (10)	0.0304 (11)
N2	0.0498 (13)	0.0872 (16)	0.0631 (14)	0.0154 (12)	0.0138 (12)	0.0474 (13)
C8	0.0529 (14)	0.0575 (15)	0.0430 (14)	0.0188 (12)	0.0110 (12)	0.0145 (12)
O1	0.0617 (12)	0.1139 (16)	0.0495 (11)	0.0094 (11)	0.0024 (10)	0.0253 (11)
C5	0.0492 (14)	0.0481 (14)	0.0468 (14)	0.0183 (12)	0.0134 (11)	0.0226 (11)

N3	0.0473 (12)	0.0807 (15)	0.0659 (15)	0.0134 (11)	0.0115 (11)	0.0414 (13)
C7	0.0464 (14)	0.0444 (13)	0.0518 (15)	0.0128 (11)	0.0122 (12)	0.0208 (11)
C18	0.0531 (15)	0.0571 (16)	0.0694 (18)	0.0211 (13)	0.0179 (14)	0.0227 (14)
C12	0.0529 (15)	0.0635 (16)	0.0584 (16)	0.0182 (13)	0.0214 (13)	0.0222 (14)
C10	0.0542 (15)	0.0608 (16)	0.0463 (15)	0.0075 (12)	0.0039 (13)	0.0175 (13)
C9	0.0478 (14)	0.0652 (17)	0.0544 (16)	0.0189 (13)	0.0126 (13)	0.0206 (13)
C11	0.0647 (17)	0.0735 (18)	0.0448 (15)	0.0138 (14)	0.0185 (14)	0.0169 (14)
C13	0.0442 (13)	0.0483 (14)	0.0550 (15)	0.0124 (11)	0.0090 (12)	0.0262 (13)
C14	0.0636 (17)	0.0575 (16)	0.0682 (18)	0.0238 (14)	0.0103 (14)	0.0188 (14)
C17	0.0517 (16)	0.082 (2)	0.083 (2)	0.0263 (15)	0.0159 (15)	0.0386 (17)
C15	0.080 (2)	0.0717 (19)	0.0649 (19)	0.0157 (16)	0.0099 (16)	0.0102 (16)
C6	0.0527 (17)	0.0632 (19)	0.0606 (18)	0.0119 (15)	0.0118 (15)	0.0290 (15)
F2B	0.071 (4)	0.123 (7)	0.079 (5)	−0.041 (4)	−0.016 (3)	0.066 (4)
F3B	0.090 (4)	0.136 (6)	0.144 (9)	0.050 (5)	0.031 (4)	0.115 (6)
F1B	0.155 (11)	0.116 (5)	0.120 (8)	0.060 (7)	0.098 (7)	0.055 (5)
C16	0.0588 (17)	0.092 (2)	0.0617 (18)	0.0173 (16)	0.0045 (15)	0.0339 (17)
C20	0.068 (2)	0.141 (3)	0.098 (3)	0.009 (2)	−0.012 (2)	0.034 (2)
C19	0.100 (2)	0.085 (2)	0.124 (3)	0.053 (2)	0.023 (2)	0.012 (2)

Geometric parameters (Å, °)

C21—O1	1.409 (3)	C7—C12	1.390 (3)
F1A—C6	1.266 (13)	C18—C13	1.378 (3)
F2A—C6	1.323 (13)	C18—C17	1.373 (3)
F3A—C6	1.306 (9)	C12—C11	1.363 (3)
C4—C5	1.371 (3)	C10—C9	1.380 (4)
C4—N3	1.371 (3)	C10—C11	1.384 (3)
C4—C7	1.474 (3)	C13—C14	1.380 (3)
N1—N2	1.338 (3)	C14—C15	1.387 (4)
N1—C5	1.372 (3)	C14—C19	1.512 (4)
N1—C13	1.442 (3)	C17—C16	1.374 (4)
N2—N3	1.306 (3)	C15—C16	1.385 (4)
C8—C7	1.387 (3)	C6—F2B	1.267 (9)
C8—C9	1.382 (3)	C6—F3B	1.335 (11)
O1—C10	1.370 (3)	C6—F1B	1.318 (12)
C5—C6	1.478 (4)	C16—C20	1.508 (4)
C5—C4—N3	107.1 (2)	C18—C13—N1	119.1 (2)
C5—C4—C7	133.2 (2)	C18—C13—C14	122.1 (2)
N3—C4—C7	119.7 (2)	C14—C13—N1	118.8 (2)
N2—N1—C5	109.65 (19)	C13—C14—C15	116.1 (2)
N2—N1—C13	119.69 (19)	C13—C14—C19	122.3 (2)
C5—N1—C13	130.6 (2)	C15—C14—C19	121.6 (3)
N3—N2—N1	108.13 (19)	C18—C17—C16	121.3 (3)
C9—C8—C7	122.0 (2)	C16—C15—C14	123.7 (3)
C10—O1—C21	118.5 (2)	F1A—C6—F2A	106.8 (9)
C4—C5—N1	105.5 (2)	F1A—C6—F3A	108.6 (9)
C4—C5—C6	131.9 (2)	F1A—C6—C5	114.0 (7)

N1—C5—C6	122.5 (2)	F2A—C6—C5	112.4 (7)
N2—N3—C4	109.6 (2)	F3A—C6—F2A	102.4 (8)
C8—C7—C4	118.6 (2)	F3A—C6—C5	111.8 (6)
C8—C7—C12	117.6 (2)	F2B—C6—C5	116.0 (5)
C12—C7—C4	123.7 (2)	F2B—C6—F3B	105.5 (7)
C17—C18—C13	119.5 (2)	F2B—C6—F1B	108.6 (8)
C11—C12—C7	121.1 (2)	F3B—C6—C5	109.9 (7)
O1—C10—C9	124.1 (2)	F1B—C6—C5	111.7 (7)
O1—C10—C11	116.1 (2)	F1B—C6—F3B	104.2 (9)
C9—C10—C11	119.8 (2)	C17—C16—C15	117.4 (3)
C10—C9—C8	119.0 (2)	C17—C16—C20	121.7 (3)
C12—C11—C10	120.6 (2)	C15—C16—C20	120.9 (3)
C21—O1—C10—C9	−0.1 (4)	C5—N1—C13—C18	−81.6 (3)
C21—O1—C10—C11	179.5 (3)	C5—N1—C13—C14	99.6 (3)
C4—C5—C6—F1A	6.5 (13)	N3—C4—C5—N1	0.0 (2)
C4—C5—C6—F2A	−115.3 (11)	N3—C4—C5—C6	−176.1 (2)
C4—C5—C6—F3A	130.2 (9)	N3—C4—C7—C8	41.1 (3)
C4—C5—C6—F2B	152.2 (9)	N3—C4—C7—C12	−136.1 (3)
C4—C5—C6—F3B	32.6 (9)	C7—C4—C5—N1	178.6 (2)
C4—C5—C6—F1B	−82.6 (11)	C7—C4—C5—C6	2.5 (4)
C4—C7—C12—C11	178.3 (2)	C7—C4—N3—N2	−178.6 (2)
N1—N2—N3—C4	−0.4 (3)	C7—C8—C9—C10	−0.8 (4)
N1—C5—C6—F1A	−169.0 (13)	C7—C12—C11—C10	−1.1 (4)
N1—C5—C6—F2A	69.2 (11)	C18—C13—C14—C15	−0.3 (4)
N1—C5—C6—F3A	−45.3 (9)	C18—C13—C14—C19	178.5 (3)
N1—C5—C6—F2B	−23.3 (9)	C18—C17—C16—C15	1.4 (5)
N1—C5—C6—F3B	−142.9 (8)	C18—C17—C16—C20	−178.9 (3)
N1—C5—C6—F1B	101.9 (11)	C9—C8—C7—C4	−177.5 (2)
N1—C13—C14—C15	178.5 (2)	C9—C8—C7—C12	−0.1 (4)
N1—C13—C14—C19	−2.7 (4)	C9—C10—C11—C12	0.1 (4)
N2—N1—C5—C4	−0.2 (2)	C11—C10—C9—C8	0.8 (4)
N2—N1—C5—C6	176.3 (2)	C13—N1—N2—N3	178.3 (2)
N2—N1—C13—C18	100.9 (3)	C13—N1—C5—C4	−177.9 (2)
N2—N1—C13—C14	−77.9 (3)	C13—N1—C5—C6	−1.3 (4)
C8—C7—C12—C11	1.1 (4)	C13—C18—C17—C16	−1.1 (4)
O1—C10—C9—C8	−179.7 (2)	C13—C14—C15—C16	0.7 (5)
O1—C10—C11—C12	−179.5 (2)	C14—C15—C16—C17	−1.3 (5)
C5—C4—N3—N2	0.3 (3)	C14—C15—C16—C20	179.0 (3)
C5—C4—C7—C8	−137.4 (3)	C17—C18—C13—N1	−178.3 (2)
C5—C4—C7—C12	45.4 (4)	C17—C18—C13—C14	0.5 (4)
C5—N1—N2—N3	0.4 (3)	C19—C14—C15—C16	−178.1 (3)

1-[2,4-Bis(trifluoromethyl)phenyl]-4-(3-methoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole
(5_C18H10F9N3O_abc13)

Crystal data

C₁₈H₁₀F₉N₃O

$M_r = 455.29$

Monoclinic, $P2_1/n$

$a = 11.9633$ (8) Å

$b = 7.8453$ (5) Å

$c = 20.0446$ (14) Å

$\beta = 95.191$ (1)°

$V = 1873.6$ (2) Å³

$Z = 4$

$F(000) = 912$

$D_x = 1.614$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4121 reflections

$\theta = 3.1\text{--}22.9^\circ$

$\mu = 0.16$ mm⁻¹

$T = 296$ K

Prism, colourless

$0.52 \times 0.20 \times 0.13$ mm

Data collection

Bruker SMART CCD area detector
diffractometer

Graphite monochromator

phi and ω scans

16580 measured reflections

3688 independent reflections

2142 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.9^\circ$

$h = -14 \rightarrow 14$

$k = -9 \rightarrow 9$

$l = -24 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.107$

$S = 1.01$

3688 reflections

365 parameters

484 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.098P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\text{max}} = 0.13$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Special details

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
F1A	0.3825 (6)	0.3118 (13)	−0.0220 (5)	0.095 (2)	0.626 (15)
F2A	0.2105 (5)	0.3767 (8)	−0.0419 (4)	0.1102 (17)	0.626 (15)
F3A	0.3308 (10)	0.4986 (6)	−0.09522 (19)	0.113 (3)	0.626 (15)
F7B	0.3743 (5)	1.0807 (6)	−0.28047 (18)	0.136 (2)	0.734 (8)
F8B	0.2181 (2)	1.1783 (5)	−0.26167 (19)	0.1004 (15)	0.734 (8)
F9B	0.3667 (4)	1.3003 (5)	−0.21996 (18)	0.1081 (17)	0.734 (8)
F4A	0.0987 (6)	0.6882 (8)	−0.0612 (6)	0.134 (2)	0.620 (16)
F6B	0.0334 (6)	0.9334 (10)	−0.0899 (4)	0.111 (2)	0.620 (16)
F5A	0.1185 (5)	0.8984 (18)	0.0042 (2)	0.136 (3)	0.620 (16)

O1	0.46377 (12)	0.29856 (19)	0.29415 (7)	0.0758 (4)	
N1	0.33818 (12)	0.74393 (19)	0.00276 (7)	0.0501 (4)	
N2	0.35630 (14)	0.8316 (2)	0.06057 (8)	0.0621 (4)	
N3	0.35712 (14)	0.7222 (2)	0.10989 (7)	0.0610 (4)	
C4	0.33866 (14)	0.5615 (2)	0.08472 (9)	0.0489 (4)	
C5	0.32760 (14)	0.5742 (2)	0.01598 (9)	0.0487 (4)	
C6	0.3174 (2)	0.4433 (3)	−0.03777 (11)	0.0657 (6)	
C7	0.33157 (15)	0.4170 (2)	0.13091 (9)	0.0501 (4)	
C8	0.40093 (15)	0.4144 (2)	0.19032 (9)	0.0513 (5)	
H8	0.454350	0.499710	0.198705	0.062*	
C9	0.39184 (15)	0.2869 (2)	0.23727 (9)	0.0534 (5)	
C10	0.31385 (18)	0.1596 (3)	0.22494 (11)	0.0677 (6)	
H10	0.307093	0.073612	0.256262	0.081*	
C11	0.2457 (2)	0.1606 (3)	0.16566 (12)	0.0827 (7)	
H11	0.193608	0.073546	0.157030	0.099*	
C12	0.25323 (18)	0.2876 (3)	0.11909 (11)	0.0717 (6)	
H12	0.205832	0.286856	0.079671	0.086*	
C13	0.33133 (15)	0.8405 (2)	−0.05893 (8)	0.0485 (4)	
C14	0.22819 (15)	0.9007 (2)	−0.08746 (9)	0.0514 (5)	
C15	0.22641 (16)	1.0011 (2)	−0.14440 (9)	0.0553 (5)	
H15	0.158391	1.041789	−0.164324	0.066*	
C16	0.32444 (17)	1.0409 (2)	−0.17166 (9)	0.0535 (5)	
C17	0.42625 (17)	0.9818 (3)	−0.14259 (10)	0.0597 (5)	
H17	0.492424	1.009808	−0.161049	0.072*	
C18	0.42920 (16)	0.8810 (3)	−0.08594 (9)	0.0580 (5)	
H18	0.497443	0.840753	−0.066171	0.070*	
C19	0.4509 (2)	0.1815 (3)	0.34683 (11)	0.0865 (7)	
H19A	0.461358	0.067508	0.331159	0.130*	
H19B	0.376924	0.192423	0.361352	0.130*	
H19C	0.505663	0.205420	0.383647	0.130*	
C20	0.3220 (2)	1.1516 (3)	−0.23262 (12)	0.0724 (6)	
C21	0.1204 (2)	0.8655 (4)	−0.05801 (13)	0.0787 (7)	
F1B	0.3421 (19)	0.295 (2)	−0.0180 (8)	0.126 (5)	0.374 (15)
F2B	0.2263 (7)	0.430 (2)	−0.0729 (7)	0.111 (4)	0.374 (15)
F3B	0.3927 (11)	0.4804 (17)	−0.0852 (7)	0.129 (4)	0.374 (15)
F9A	0.2730 (18)	1.2947 (14)	−0.2183 (5)	0.175 (8)	0.266 (8)
F8A	0.2848 (15)	1.0999 (14)	−0.2817 (4)	0.130 (6)	0.266 (8)
F7A	0.4276 (10)	1.1975 (19)	−0.2463 (5)	0.146 (5)	0.266 (8)
F5B	0.1142 (11)	1.002 (2)	−0.0109 (9)	0.156 (5)	0.380 (16)
F6A	0.0349 (9)	0.886 (3)	−0.0992 (7)	0.146 (5)	0.380 (16)
F4B	0.1114 (8)	0.743 (2)	−0.0248 (8)	0.117 (4)	0.380 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1A	0.121 (3)	0.075 (4)	0.083 (3)	0.050 (3)	−0.019 (2)	−0.022 (2)
F2A	0.119 (3)	0.112 (3)	0.093 (4)	−0.027 (2)	−0.027 (2)	−0.038 (3)
F3A	0.231 (7)	0.070 (2)	0.0372 (17)	0.012 (4)	0.008 (3)	−0.0027 (13)

F7B	0.201 (5)	0.149 (3)	0.066 (2)	0.067 (3)	0.059 (3)	0.0319 (19)
F8B	0.0919 (18)	0.116 (3)	0.089 (3)	0.0009 (14)	−0.0169 (14)	0.051 (2)
F9B	0.154 (3)	0.075 (2)	0.090 (2)	−0.049 (2)	−0.018 (2)	0.0219 (16)
F4A	0.090 (2)	0.107 (3)	0.212 (7)	−0.012 (2)	0.052 (4)	0.018 (4)
F6B	0.063 (3)	0.152 (4)	0.120 (4)	0.054 (3)	0.019 (3)	0.055 (3)
F5A	0.092 (3)	0.258 (9)	0.061 (2)	0.029 (5)	0.0281 (17)	0.005 (4)
O1	0.0770 (10)	0.0879 (11)	0.0597 (9)	−0.0165 (8)	−0.0098 (7)	0.0242 (8)
N1	0.0573 (9)	0.0505 (9)	0.0413 (8)	0.0033 (7)	−0.0026 (7)	−0.0011 (7)
N2	0.0835 (12)	0.0543 (10)	0.0473 (9)	−0.0026 (8)	−0.0007 (8)	−0.0043 (9)
N3	0.0828 (12)	0.0541 (10)	0.0449 (9)	−0.0029 (8)	0.0002 (8)	−0.0006 (8)
C4	0.0497 (10)	0.0519 (11)	0.0443 (10)	0.0009 (8)	−0.0007 (8)	−0.0011 (9)
C5	0.0530 (10)	0.0460 (11)	0.0458 (10)	0.0032 (8)	−0.0033 (8)	−0.0010 (9)
C6	0.0861 (17)	0.0556 (14)	0.0523 (14)	0.0058 (12)	−0.0110 (12)	−0.0035 (11)
C7	0.0514 (10)	0.0514 (11)	0.0472 (10)	−0.0014 (9)	0.0027 (8)	−0.0001 (9)
C8	0.0522 (10)	0.0517 (11)	0.0499 (10)	−0.0047 (9)	0.0032 (8)	0.0006 (9)
C9	0.0514 (11)	0.0592 (12)	0.0496 (11)	−0.0009 (9)	0.0047 (9)	0.0051 (10)
C10	0.0733 (14)	0.0628 (13)	0.0668 (14)	−0.0126 (11)	0.0058 (11)	0.0134 (11)
C11	0.0913 (17)	0.0748 (16)	0.0792 (16)	−0.0364 (13)	−0.0076 (13)	0.0092 (13)
C12	0.0747 (14)	0.0743 (15)	0.0630 (13)	−0.0171 (12)	−0.0113 (11)	0.0042 (12)
C13	0.0571 (11)	0.0463 (10)	0.0415 (10)	0.0034 (8)	0.0013 (8)	0.0006 (8)
C14	0.0544 (11)	0.0547 (11)	0.0448 (10)	0.0106 (9)	0.0030 (8)	−0.0008 (9)
C15	0.0627 (12)	0.0542 (12)	0.0478 (11)	0.0139 (9)	−0.0018 (9)	−0.0031 (9)
C16	0.0728 (13)	0.0434 (11)	0.0437 (10)	0.0020 (9)	0.0017 (9)	−0.0037 (9)
C17	0.0627 (12)	0.0616 (13)	0.0553 (12)	−0.0064 (10)	0.0079 (9)	−0.0001 (10)
C18	0.0530 (12)	0.0638 (13)	0.0563 (12)	0.0044 (9)	0.0000 (9)	0.0024 (10)
C19	0.0921 (17)	0.0991 (19)	0.0667 (14)	−0.0047 (14)	−0.0013 (12)	0.0309 (14)
C20	0.1018 (19)	0.0600 (15)	0.0547 (14)	−0.0037 (14)	0.0041 (13)	0.0019 (12)
C21	0.0638 (15)	0.106 (2)	0.0676 (16)	0.0233 (14)	0.0104 (12)	0.0208 (16)
F1B	0.252 (15)	0.049 (3)	0.069 (4)	0.024 (8)	−0.029 (8)	−0.008 (3)
F2B	0.078 (4)	0.164 (8)	0.083 (6)	0.026 (4)	−0.030 (4)	−0.058 (5)
F3B	0.145 (7)	0.133 (6)	0.123 (7)	−0.034 (5)	0.086 (5)	−0.057 (5)
F9A	0.360 (19)	0.076 (7)	0.093 (7)	0.084 (11)	0.049 (11)	0.031 (6)
F8A	0.214 (14)	0.117 (9)	0.051 (5)	−0.064 (10)	−0.027 (8)	0.002 (5)
F7A	0.170 (7)	0.169 (12)	0.097 (7)	−0.086 (7)	0.008 (5)	0.042 (7)
F5B	0.124 (6)	0.168 (9)	0.192 (9)	−0.023 (6)	0.102 (6)	−0.075 (7)
F6A	0.049 (5)	0.272 (13)	0.111 (6)	−0.041 (6)	−0.021 (4)	0.054 (7)
F4B	0.068 (4)	0.129 (8)	0.160 (10)	0.025 (5)	0.045 (6)	0.078 (7)

Geometric parameters (Å, °)

F1A—C6	1.315 (8)	C6—F3B	1.398 (8)
F2A—C6	1.376 (6)	C7—C8	1.389 (2)
F3A—C6	1.254 (5)	C7—C12	1.387 (3)
F7B—C20	1.315 (4)	C8—C9	1.384 (2)
F8B—C20	1.341 (4)	C9—C10	1.374 (3)
F9B—C20	1.299 (4)	C10—C11	1.379 (3)
F4A—C21	1.415 (7)	C11—C12	1.374 (3)
F6B—C21	1.286 (6)	C13—C14	1.395 (2)

F5A—C21	1.275 (6)	C13—C18	1.371 (3)
O1—C9	1.368 (2)	C14—C15	1.385 (2)
O1—C19	1.418 (2)	C14—C21	1.492 (3)
N1—N2	1.3481 (19)	C15—C16	1.374 (3)
N1—C5	1.366 (2)	C16—C17	1.382 (3)
N1—C13	1.446 (2)	C16—C20	1.497 (3)
N2—N3	1.308 (2)	C17—C18	1.381 (3)
N3—C4	1.369 (2)	C20—F9A	1.311 (9)
C4—C5	1.376 (2)	C20—F8A	1.118 (7)
C4—C7	1.471 (2)	C20—F7A	1.365 (10)
C5—C6	1.485 (3)	C21—F5B	1.436 (9)
C6—F1B	1.253 (14)	C21—F6A	1.264 (10)
C6—F2B	1.247 (7)	C21—F4B	1.181 (9)
C9—O1—C19	118.36 (17)	C18—C13—N1	118.35 (15)
N2—N1—C5	109.94 (14)	C18—C13—C14	120.98 (17)
N2—N1—C13	117.40 (15)	C13—C14—C21	122.64 (18)
C5—N1—C13	132.64 (15)	C15—C14—C13	118.53 (17)
N3—N2—N1	107.74 (14)	C15—C14—C21	118.81 (18)
N2—N3—C4	109.61 (14)	C16—C15—C14	120.45 (17)
N3—C4—C5	107.47 (16)	C15—C16—C17	120.52 (17)
N3—C4—C7	119.64 (15)	C15—C16—C20	120.14 (19)
C5—C4—C7	132.87 (17)	C17—C16—C20	119.3 (2)
N1—C5—C4	105.23 (15)	C18—C17—C16	119.64 (18)
N1—C5—C6	122.43 (17)	C13—C18—C17	119.88 (18)
C4—C5—C6	132.11 (18)	F7B—C20—F8B	103.5 (3)
F1A—C6—F2A	104.1 (5)	F7B—C20—C16	112.0 (2)
F1A—C6—C5	111.1 (5)	F8B—C20—C16	113.2 (2)
F2A—C6—C5	108.8 (3)	F9B—C20—F7B	107.9 (3)
F3A—C6—F1A	111.8 (6)	F9B—C20—F8B	107.1 (3)
F3A—C6—F2A	105.7 (3)	F9B—C20—C16	112.6 (2)
F3A—C6—C5	114.7 (3)	F9A—C20—C16	107.1 (4)
F1B—C6—C5	114.2 (8)	F9A—C20—F7A	105.0 (9)
F1B—C6—F3B	105.0 (9)	F8A—C20—C16	119.0 (5)
F2B—C6—C5	118.4 (4)	F8A—C20—F9A	110.7 (9)
F2B—C6—F1B	105.8 (9)	F8A—C20—F7A	102.8 (7)
F2B—C6—F3B	102.6 (5)	F7A—C20—C16	111.5 (4)
F3B—C6—C5	109.5 (5)	F4A—C21—C14	109.0 (4)
C8—C7—C4	119.15 (17)	F6B—C21—F4A	104.4 (5)
C12—C7—C4	122.20 (17)	F6B—C21—C14	114.6 (4)
C12—C7—C8	118.54 (17)	F5A—C21—F4A	102.9 (5)
C9—C8—C7	121.06 (17)	F5A—C21—F6B	108.5 (5)
O1—C9—C8	115.87 (17)	F5A—C21—C14	116.2 (4)
O1—C9—C10	124.34 (18)	F5B—C21—C14	102.7 (5)
C10—C9—C8	119.79 (18)	F6A—C21—C14	113.3 (7)
C9—C10—C11	119.3 (2)	F6A—C21—F5B	104.5 (8)
C12—C11—C10	121.3 (2)	F4B—C21—C14	120.0 (4)
C11—C12—C7	119.97 (19)	F4B—C21—F5B	103.0 (6)

C14—C13—N1

120.52 (16)

F4B—C21—F6A

111.1 (9)

1-(3,4-Dimethoxyphenyl)-4-(3,4-dimethoxyphenyl)-5-trifluoromethyl-1*H*-1,2,3-triazole
(6_C19H18F3N3O4_ABC23)

*Crystal data*C₁₉H₁₈F₃N₃O₄ $M_r = 409.36$ Monoclinic, $P2_1/c$ $a = 30.656$ (2) Å $b = 8.3363$ (6) Å $c = 7.6723$ (6) Å $\beta = 94.627$ (1)° $V = 1954.3$ (3) Å³ $Z = 4$ $F(000) = 848$ $D_x = 1.391$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3310 reflections

 $\theta = 2.5$ – 22.8° $\mu = 0.12$ mm⁻¹ $T = 293$ K

Prismatic, colorless

 $0.41 \times 0.29 \times 0.09$ mm*Data collection*Bruker SMART CCD area detector
diffractometerphi and ω scans

16559 measured reflections

3634 independent reflections

1881 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.049$ $\theta_{\text{max}} = 25.5^\circ$, $\theta_{\text{min}} = 1.3^\circ$ $h = -37 \rightarrow 37$ $k = -10 \rightarrow 10$ $l = -9 \rightarrow 9$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.042$ $wR(F^2) = 0.133$ $S = 1.04$

3634 reflections

289 parameters

36 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.1371P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.13$ e Å⁻³*Special details*

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
F2A	0.2870 (3)	0.3129 (14)	0.2864 (16)	0.134 (4)	0.7
F3A	0.22126 (15)	0.2948 (10)	0.3284 (11)	0.111 (3)	0.7
F1A	0.2596 (2)	0.4880 (9)	0.4359 (8)	0.158 (3)	0.7
F2B	0.2885 (6)	0.357 (3)	0.338 (3)	0.106 (8)	0.3
F3B	0.2256 (6)	0.260 (3)	0.272 (3)	0.135 (8)	0.3
F1B	0.2339 (3)	0.4560 (17)	0.4402 (16)	0.089 (4)	0.3
C21	0.00296 (8)	0.2878 (4)	0.1042 (4)	0.0729 (8)	
H21A	−0.024987	0.277532	0.151248	0.109*	
H21B	−0.000800	0.336655	−0.009313	0.109*	

H21C	0.015824	0.183513	0.094428	0.109*	
C22	0.10824 (10)	0.6225 (4)	0.5701 (4)	0.0926 (11)	
H22A	0.091879	0.644599	0.668942	0.139*	
H22B	0.133474	0.559165	0.606916	0.139*	
H22C	0.117444	0.721630	0.521047	0.139*	
C19	0.38750 (10)	0.3769 (5)	−0.3573 (4)	0.1066 (12)	
H19A	0.408395	0.342779	−0.436377	0.160*	
H19B	0.371110	0.285849	−0.322403	0.160*	
H19C	0.367917	0.453771	−0.414532	0.160*	
C20	0.47877 (9)	0.6290 (5)	0.2087 (5)	0.1183 (14)	
H20A	0.509219	0.620553	0.189121	0.177*	
H20B	0.471363	0.739649	0.224605	0.177*	
H20C	0.473104	0.569331	0.311511	0.177*	
O1	0.08186 (5)	0.5380 (2)	0.4439 (2)	0.0581 (5)	
O2	0.03110 (4)	0.3858 (2)	0.2180 (2)	0.0555 (5)	
C8	0.14225 (7)	0.5312 (3)	0.2570 (3)	0.0482 (6)	
H8	0.160656	0.587718	0.337495	0.058*	
C9	0.09994 (7)	0.4962 (3)	0.2936 (3)	0.0427 (6)	
N1A	0.27051 (7)	0.5588 (3)	0.0331 (3)	0.0521 (6)	0.45
C4A	0.20101 (6)	0.5240 (3)	0.0568 (3)	0.0512 (6)	0.45
C4B	0.27051 (7)	0.5588 (3)	0.0331 (3)	0.0521 (6)	0.55
N1B	0.20101 (6)	0.5240 (3)	0.0568 (3)	0.0512 (6)	0.55
O3	0.40974 (5)	0.4479 (2)	−0.2079 (3)	0.0781 (6)	
C13	0.31806 (7)	0.5609 (3)	0.0491 (3)	0.0527 (7)	
C10	0.07240 (7)	0.4131 (3)	0.1707 (3)	0.0448 (6)	
O4	0.45308 (5)	0.5661 (3)	0.0623 (3)	0.0861 (7)	
N2	0.24820 (7)	0.6257 (3)	−0.1071 (3)	0.0694 (7)	
C12	0.13043 (8)	0.3983 (3)	−0.0189 (3)	0.0576 (7)	
H12	0.140840	0.364073	−0.123250	0.069*	
C11	0.08784 (7)	0.3650 (3)	0.0163 (3)	0.0559 (7)	
H11	0.069537	0.309429	−0.065309	0.067*	
C7	0.15721 (7)	0.4819 (3)	0.1001 (3)	0.0473 (6)	
C5	0.24118 (7)	0.4937 (3)	0.1386 (3)	0.0488 (6)	
N3	0.20629 (7)	0.6058 (3)	−0.0935 (3)	0.0688 (7)	
C14	0.34016 (7)	0.5020 (3)	−0.0884 (3)	0.0525 (6)	
H14	0.324414	0.460671	−0.187031	0.063*	
C16	0.40865 (8)	0.5681 (3)	0.0668 (4)	0.0594 (7)	
C15	0.38522 (8)	0.5041 (3)	−0.0799 (3)	0.0552 (7)	
C18	0.34132 (8)	0.6228 (3)	0.1930 (4)	0.0689 (8)	
H18	0.326684	0.662158	0.285641	0.083*	
C6	0.25045 (10)	0.3951 (4)	0.2961 (5)	0.0694 (8)	
C17	0.38671 (8)	0.6273 (4)	0.2017 (4)	0.0730 (9)	
H17	0.402323	0.670610	0.299480	0.088*	

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F2A	0.079 (5)	0.120 (5)	0.206 (10)	0.054 (4)	0.042 (4)	0.096 (6)

F3A	0.053 (2)	0.131 (6)	0.149 (7)	−0.006 (3)	0.008 (2)	0.095 (6)
F1A	0.248 (8)	0.137 (4)	0.083 (3)	−0.007 (6)	−0.026 (5)	0.022 (3)
F2B	0.038 (7)	0.152 (18)	0.122 (10)	−0.007 (9)	−0.032 (7)	0.067 (10)
F3B	0.198 (15)	0.086 (7)	0.121 (10)	−0.049 (8)	0.011 (8)	0.025 (6)
F1B	0.085 (6)	0.125 (10)	0.060 (5)	0.034 (6)	0.019 (5)	0.019 (5)
C21	0.0466 (15)	0.090 (2)	0.081 (2)	−0.0172 (14)	−0.0018 (14)	−0.0081 (17)
C22	0.090 (2)	0.126 (3)	0.062 (2)	−0.034 (2)	0.0058 (17)	−0.031 (2)
C19	0.085 (2)	0.159 (4)	0.078 (2)	−0.015 (2)	0.0207 (19)	−0.049 (2)
C20	0.0512 (18)	0.173 (4)	0.129 (3)	−0.014 (2)	−0.0041 (19)	−0.059 (3)
O1	0.0516 (10)	0.0647 (12)	0.0585 (11)	−0.0025 (8)	0.0067 (9)	−0.0146 (9)
O2	0.0363 (9)	0.0678 (12)	0.0624 (11)	−0.0073 (8)	0.0036 (8)	−0.0056 (9)
C8	0.0409 (13)	0.0427 (15)	0.0596 (17)	−0.0009 (10)	−0.0040 (12)	−0.0011 (12)
C9	0.0396 (13)	0.0387 (14)	0.0498 (15)	0.0066 (10)	0.0031 (11)	−0.0003 (11)
N1A	0.0416 (13)	0.0476 (14)	0.0682 (17)	−0.0001 (10)	0.0113 (12)	0.0052 (12)
C4A	0.0418 (13)	0.0480 (14)	0.0650 (16)	0.0016 (10)	0.0107 (11)	0.0107 (12)
C4B	0.0416 (13)	0.0476 (14)	0.0682 (17)	−0.0001 (10)	0.0113 (12)	0.0052 (12)
N1B	0.0418 (13)	0.0480 (14)	0.0650 (16)	0.0016 (10)	0.0107 (11)	0.0107 (12)
O3	0.0547 (11)	0.1072 (16)	0.0747 (14)	−0.0044 (10)	0.0205 (10)	−0.0245 (12)
C13	0.0430 (14)	0.0465 (16)	0.0698 (19)	−0.0043 (11)	0.0112 (13)	−0.0003 (13)
C10	0.0341 (13)	0.0451 (15)	0.0550 (16)	0.0004 (10)	0.0028 (11)	0.0014 (12)
O4	0.0410 (10)	0.1157 (18)	0.1023 (16)	−0.0095 (10)	0.0108 (10)	−0.0308 (13)
N2	0.0481 (13)	0.0769 (17)	0.0845 (18)	0.0015 (12)	0.0134 (12)	0.0215 (14)
C12	0.0500 (15)	0.0644 (18)	0.0597 (17)	−0.0005 (13)	0.0127 (13)	−0.0089 (14)
C11	0.0495 (15)	0.0591 (17)	0.0589 (17)	−0.0077 (12)	0.0036 (13)	−0.0127 (13)
C7	0.0364 (13)	0.0448 (15)	0.0609 (17)	0.0052 (11)	0.0050 (12)	0.0027 (13)
C5	0.0426 (14)	0.0415 (14)	0.0631 (17)	0.0017 (11)	0.0083 (12)	0.0058 (13)
N3	0.0489 (14)	0.0799 (17)	0.0783 (17)	0.0028 (11)	0.0104 (11)	0.0222 (14)
C14	0.0475 (15)	0.0496 (16)	0.0613 (17)	−0.0040 (11)	0.0085 (12)	0.0004 (13)
C16	0.0401 (14)	0.0642 (18)	0.0746 (19)	−0.0068 (12)	0.0094 (13)	−0.0107 (15)
C15	0.0460 (15)	0.0571 (17)	0.0649 (18)	−0.0032 (12)	0.0183 (13)	−0.0062 (14)
C18	0.0550 (17)	0.075 (2)	0.080 (2)	−0.0080 (14)	0.0225 (15)	−0.0204 (16)
C6	0.055 (2)	0.065 (2)	0.088 (3)	0.0046 (17)	0.0057 (19)	0.017 (2)
C17	0.0534 (17)	0.088 (2)	0.079 (2)	−0.0133 (15)	0.0124 (15)	−0.0280 (17)

Geometric parameters (Å, °)

F2A—C6	1.320 (11)	C4A—N3	1.360 (3)
F3A—C6	1.264 (7)	C4B—C13	1.453 (3)
F1A—C6	1.334 (7)	C4B—N2	1.348 (3)
F2B—C6	1.227 (17)	C4B—C5	1.369 (3)
F3B—C6	1.36 (2)	N1B—C7	1.452 (3)
F1B—C6	1.351 (13)	N1B—C5	1.360 (3)
C21—O2	1.433 (3)	N1B—N3	1.360 (3)
C22—O1	1.400 (3)	O3—C15	1.366 (3)
C19—O3	1.416 (3)	C13—C14	1.389 (3)
C20—O4	1.420 (3)	C13—C18	1.367 (3)
O1—C9	1.365 (3)	C10—C11	1.371 (3)
O2—C10	1.364 (2)	O4—C16	1.365 (3)

C8—C9	1.380 (3)	N2—N3	1.308 (2)
C8—C7	1.385 (3)	C12—C11	1.383 (3)
C9—C10	1.398 (3)	C12—C7	1.368 (3)
N1A—C13	1.453 (3)	C5—C6	1.470 (4)
N1A—N2	1.348 (3)	C14—C15	1.378 (3)
N1A—C5	1.369 (3)	C16—C15	1.392 (3)
C4A—C7	1.452 (3)	C16—C17	1.371 (3)
C4A—C5	1.360 (3)	C18—C17	1.388 (3)
C9—O1—C22	117.50 (19)	C8—C7—N1B	120.3 (2)
C10—O2—C21	117.31 (18)	C12—C7—C8	120.6 (2)
C9—C8—C7	119.7 (2)	C12—C7—C4A	119.1 (2)
O1—C9—C8	124.8 (2)	C12—C7—N1B	119.1 (2)
O1—C9—C10	115.61 (19)	N1A—C5—C6	127.9 (2)
C8—C9—C10	119.6 (2)	C4A—C5—N1A	105.5 (2)
N2—N1A—C13	120.2 (2)	C4A—C5—C6	126.2 (2)
N2—N1A—C5	108.70 (19)	C4B—C5—C6	127.9 (2)
C5—N1A—C13	131.1 (2)	N1B—C5—C4B	105.5 (2)
C5—C4A—C7	132.0 (2)	N1B—C5—C6	126.2 (2)
N3—C4A—C7	119.4 (2)	N2—N3—C4A	108.44 (19)
N3—C4A—C5	108.61 (19)	N2—N3—N1B	108.44 (19)
N2—C4B—C13	120.2 (2)	C15—C14—C13	120.5 (2)
N2—C4B—C5	108.70 (19)	O4—C16—C15	115.2 (2)
C5—C4B—C13	131.1 (2)	O4—C16—C17	125.1 (2)
C5—N1B—C7	132.0 (2)	C17—C16—C15	119.7 (2)
N3—N1B—C7	119.4 (2)	O3—C15—C14	124.7 (2)
N3—N1B—C5	108.61 (19)	O3—C15—C16	115.7 (2)
C15—O3—C19	117.9 (2)	C14—C15—C16	119.6 (2)
C14—C13—N1A	118.6 (2)	C13—C18—C17	120.3 (2)
C14—C13—C4B	118.6 (2)	F2A—C6—F1A	102.9 (6)
C18—C13—N1A	121.8 (2)	F2A—C6—C5	110.6 (6)
C18—C13—C4B	121.8 (2)	F3A—C6—F2A	106.5 (6)
C18—C13—C14	119.5 (2)	F3A—C6—F1A	109.4 (6)
O2—C10—C9	115.2 (2)	F3A—C6—C5	116.0 (4)
O2—C10—C11	125.0 (2)	F1A—C6—C5	110.5 (4)
C11—C10—C9	119.7 (2)	F2B—C6—F3B	109.2 (15)
C16—O4—C20	117.8 (2)	F2B—C6—F1B	107.0 (13)
N3—N2—N1A	108.77 (19)	F2B—C6—C5	118.7 (13)
N3—N2—C4B	108.77 (19)	F3B—C6—C5	106.4 (9)
C7—C12—C11	119.8 (2)	F1B—C6—F3B	100.2 (10)
C10—C11—C12	120.5 (2)	F1B—C6—C5	113.7 (6)
C8—C7—C4A	120.3 (2)	C16—C17—C18	120.4 (3)
C21—O2—C10—C9	−174.1 (2)	N2—C4B—C13—C18	125.0 (3)
C21—O2—C10—C11	5.6 (3)	N2—C4B—C5—N1B	0.0 (3)
C22—O1—C9—C8	0.0 (3)	N2—C4B—C5—C6	173.5 (3)
C22—O1—C9—C10	−179.6 (2)	C11—C12—C7—C8	1.0 (4)
C19—O3—C15—C14	−2.5 (4)	C11—C12—C7—C4A	−176.5 (2)

C19—O3—C15—C16	178.0 (3)	C11—C12—C7—N1B	−176.5 (2)
C20—O4—C16—C15	−179.6 (3)	C7—C8—C9—O1	179.6 (2)
C20—O4—C16—C17	0.5 (4)	C7—C8—C9—C10	−0.8 (3)
O1—C9—C10—O2	0.3 (3)	C7—C4A—C5—N1A	178.0 (2)
O1—C9—C10—C11	−179.4 (2)	C7—C4A—C5—C6	4.4 (4)
O2—C10—C11—C12	−179.8 (2)	C7—C4A—N3—N2	−178.1 (2)
C8—C9—C10—O2	−179.30 (19)	C7—N1B—C5—C4B	178.0 (2)
C8—C9—C10—C11	1.0 (3)	C7—N1B—C5—C6	4.4 (4)
C9—C8—C7—C4A	177.3 (2)	C7—N1B—N3—N2	−178.1 (2)
C9—C8—C7—N1B	177.3 (2)	C7—C12—C11—C10	−0.9 (4)
C9—C8—C7—C12	−0.2 (3)	C5—N1A—C13—C14	124.8 (3)
C9—C10—C11—C12	−0.1 (4)	C5—N1A—C13—C18	−56.9 (4)
N1A—C13—C14—C15	179.0 (2)	C5—N1A—N2—N3	0.2 (3)
N1A—C13—C18—C17	−178.1 (2)	C5—C4A—C7—C8	58.8 (4)
N1A—N2—N3—C4A	−0.4 (3)	C5—C4A—C7—C12	−123.7 (3)
C4B—C13—C14—C15	179.0 (2)	C5—C4A—N3—N2	0.4 (3)
C4B—C13—C18—C17	−178.1 (2)	C5—C4B—C13—C14	124.8 (3)
C4B—N2—N3—N1B	−0.4 (3)	C5—C4B—C13—C18	−56.9 (4)
C13—N1A—N2—N3	178.7 (2)	C5—C4B—N2—N3	0.2 (3)
C13—N1A—C5—C4A	−178.2 (2)	C5—N1B—C7—C8	58.8 (4)
C13—N1A—C5—C6	−4.8 (5)	C5—N1B—C7—C12	−123.7 (3)
C13—C4B—N2—N3	178.7 (2)	C5—N1B—N3—N2	0.4 (3)
C13—C4B—C5—N1B	−178.2 (2)	N3—C4A—C7—C8	−123.1 (3)
C13—C4B—C5—C6	−4.8 (5)	N3—C4A—C7—C12	54.4 (3)
C13—C14—C15—O3	179.6 (2)	N3—C4A—C5—N1A	−0.2 (3)
C13—C14—C15—C16	−0.9 (4)	N3—C4A—C5—C6	−173.8 (3)
C13—C18—C17—C16	−0.7 (4)	N3—N1B—C7—C8	−123.1 (3)
O4—C16—C15—O3	0.1 (3)	N3—N1B—C7—C12	54.4 (3)
O4—C16—C15—C14	−179.4 (2)	N3—N1B—C5—C4B	−0.2 (3)
O4—C16—C17—C18	−179.8 (3)	N3—N1B—C5—C6	−173.8 (3)
N2—N1A—C13—C14	−53.3 (3)	C14—C13—C18—C17	0.2 (4)
N2—N1A—C13—C18	125.0 (3)	C15—C16—C17—C18	0.3 (4)
N2—N1A—C5—C4A	0.0 (3)	C18—C13—C14—C15	0.6 (4)
N2—N1A—C5—C6	173.5 (3)	C17—C16—C15—O3	−180.0 (2)
N2—C4B—C13—C14	−53.3 (3)	C17—C16—C15—C14	0.5 (4)

3-[4-(3,4-Dimethoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazol-1-yl]phenol (7_C17H14F3N3O3)

Crystal data

C₁₇H₁₄F₃N₃O₃*M_r* = 365.31Monoclinic, *P*2₁/*c**a* = 12.267 (2) Å*b* = 8.4334 (14) Å*c* = 15.686 (3) Å*β* = 93.904 (3)°*V* = 1619.0 (5) Å³*Z* = 4*F*(000) = 752*D_x* = 1.499 Mg m^{−3}Mo *Kα* radiation, *λ* = 0.71073 Å

Cell parameters from 1754 reflections

θ = 2.6–20.7°*μ* = 0.13 mm^{−1}*T* = 293 K

Prismatic, colorless

0.59 × 0.11 × 0.07 mm

Data collection

Bruker SMART CCD area detector
diffractometer
phi and ω scans
14139 measured reflections
3188 independent reflections
1336 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.146$
 $\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.7^\circ$
 $h = -15 \rightarrow 15$
 $k = -10 \rightarrow 10$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.189$
 $S = 0.97$
3188 reflections
235 parameters
0 restraints

Primary atom site location: structure-invariant
direct methods
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0845P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.26 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.26 \text{ e } \text{\AA}^{-3}$

Special details

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C20	0.8329 (3)	−0.0079 (7)	0.3176 (3)	0.0541 (14)
H20A	0.8974	−0.0300	0.3536	0.081*
H20B	0.7871	0.0645	0.3461	0.081*
H20C	0.7937	−0.1047	0.3054	0.081*
C19	0.9660 (4)	0.2263 (7)	0.0204 (3)	0.0740 (19)
H19A	1.0445	0.2267	0.0249	0.111*
H19B	0.9404	0.1596	−0.0264	0.111*
H19C	0.9397	0.3323	0.0105	0.111*
F1	0.3156 (2)	0.2140 (3)	0.06978 (18)	0.0623 (9)
F3	0.30635 (19)	0.4482 (3)	0.01740 (16)	0.0558 (8)
F2	0.43554 (19)	0.3871 (3)	0.10946 (16)	0.0560 (8)
N1	0.4142 (2)	0.2988 (4)	−0.1121 (2)	0.0298 (9)
N3	0.5783 (2)	0.2093 (4)	−0.1062 (2)	0.0343 (9)
O3	0.2226 (2)	0.6087 (4)	−0.3331 (2)	0.0562 (10)
H3	0.2850	0.6383	−0.3401	0.067*
O2	0.8630 (2)	0.0614 (4)	0.23952 (17)	0.0465 (9)
N2	0.4966 (2)	0.2538 (4)	−0.1594 (2)	0.0355 (9)
O1	0.9269 (2)	0.1674 (4)	0.09764 (19)	0.0560 (10)
C9	0.8163 (3)	0.1585 (5)	0.1025 (3)	0.0348 (11)
C5	0.4442 (3)	0.2821 (5)	−0.0270 (3)	0.0283 (10)
C11	0.6711 (3)	0.0847 (5)	0.1904 (3)	0.0376 (11)
H11	0.6476	0.0467	0.2417	0.045*

C15	0.2243 (3)	0.5046 (5)	−0.2670 (3)	0.0352 (11)
C10	0.7820 (3)	0.1010 (5)	0.1802 (3)	0.0347 (11)
C7	0.6277 (3)	0.1829 (5)	0.0482 (3)	0.0304 (10)
C14	0.3199 (3)	0.4599 (5)	−0.2209 (3)	0.0324 (11)
H14	0.3868	0.5033	−0.2332	0.039*
C12	0.5949 (3)	0.1252 (5)	0.1242 (3)	0.0354 (11)
H12	0.5208	0.1129	0.1315	0.042*
C8	0.7407 (3)	0.1984 (5)	0.0379 (3)	0.0337 (11)
H8	0.7640	0.2362	−0.0135	0.040*
C18	0.2155 (3)	0.2837 (5)	−0.1356 (3)	0.0394 (12)
H18	0.2129	0.2092	−0.0921	0.047*
C16	0.1246 (3)	0.4426 (6)	−0.2464 (3)	0.0432 (12)
H16	0.0603	0.4751	−0.2761	0.052*
C4	0.5508 (3)	0.2235 (5)	−0.0238 (3)	0.0293 (10)
C6	0.3750 (3)	0.3312 (6)	0.0421 (3)	0.0372 (11)
C13	0.3138 (3)	0.3506 (5)	−0.1571 (2)	0.0283 (10)
C17	0.1217 (3)	0.3337 (6)	−0.1824 (3)	0.0447 (13)
H17	0.0547	0.2915	−0.1697	0.054*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C20	0.044 (3)	0.084 (4)	0.033 (3)	0.006 (3)	−0.004 (2)	0.022 (3)
C19	0.028 (3)	0.143 (6)	0.053 (4)	−0.012 (3)	0.011 (2)	0.027 (4)
F1	0.0571 (17)	0.071 (2)	0.063 (2)	−0.0048 (15)	0.0358 (15)	0.0066 (17)
F3	0.0469 (16)	0.070 (2)	0.0505 (17)	0.0315 (14)	0.0032 (13)	−0.0029 (15)
F2	0.0472 (16)	0.081 (2)	0.0382 (16)	0.0115 (14)	−0.0073 (12)	−0.0202 (15)
N1	0.0139 (16)	0.048 (2)	0.027 (2)	0.0033 (15)	0.0009 (14)	0.0024 (18)
N3	0.0168 (17)	0.057 (3)	0.029 (2)	0.0028 (16)	−0.0017 (15)	0.0025 (19)
O3	0.0237 (16)	0.088 (3)	0.056 (2)	−0.0011 (16)	−0.0024 (14)	0.029 (2)
O2	0.0275 (16)	0.080 (3)	0.0314 (17)	0.0019 (15)	−0.0021 (13)	0.0190 (17)
N2	0.0194 (17)	0.057 (3)	0.030 (2)	0.0038 (16)	0.0027 (16)	−0.0012 (18)
O1	0.0181 (16)	0.104 (3)	0.046 (2)	−0.0025 (16)	0.0031 (14)	0.0230 (19)
C9	0.020 (2)	0.054 (3)	0.031 (2)	0.0016 (19)	0.0020 (18)	0.004 (2)
C5	0.0159 (19)	0.039 (3)	0.030 (2)	0.0034 (18)	0.0021 (17)	−0.001 (2)
C11	0.027 (2)	0.059 (3)	0.027 (2)	0.004 (2)	0.0041 (18)	0.012 (2)
C15	0.025 (2)	0.050 (3)	0.030 (2)	0.003 (2)	−0.0001 (18)	0.007 (2)
C10	0.023 (2)	0.048 (3)	0.032 (2)	0.002 (2)	−0.0029 (18)	0.005 (2)
C7	0.021 (2)	0.039 (3)	0.031 (2)	0.0039 (18)	−0.0027 (18)	0.001 (2)
C14	0.016 (2)	0.050 (3)	0.031 (2)	−0.0018 (18)	−0.0024 (17)	0.005 (2)
C12	0.018 (2)	0.051 (3)	0.037 (3)	0.0003 (19)	0.0023 (18)	0.007 (2)
C8	0.019 (2)	0.054 (3)	0.028 (2)	−0.0006 (19)	0.0043 (17)	0.007 (2)
C18	0.025 (2)	0.053 (3)	0.041 (3)	−0.001 (2)	0.0003 (19)	0.010 (2)
C16	0.018 (2)	0.065 (4)	0.046 (3)	−0.002 (2)	−0.0045 (19)	0.004 (3)
C4	0.023 (2)	0.036 (3)	0.029 (2)	−0.0018 (18)	−0.0005 (18)	−0.003 (2)
C6	0.033 (2)	0.046 (3)	0.033 (3)	0.006 (2)	0.007 (2)	0.001 (2)
C13	0.015 (2)	0.045 (3)	0.025 (2)	0.0034 (18)	−0.0009 (16)	0.001 (2)
C17	0.017 (2)	0.062 (4)	0.055 (3)	−0.001 (2)	0.004 (2)	0.006 (3)

Geometric parameters (Å, °)

C20—H20A	0.9600	C9—C8	1.369 (5)
C20—H20B	0.9600	C5—C4	1.396 (5)
C20—H20C	0.9600	C5—C6	1.480 (5)
C20—O2	1.428 (5)	C11—H11	0.9300
C19—H19A	0.9600	C11—C10	1.388 (5)
C19—H19B	0.9600	C11—C12	1.392 (5)
C19—H19C	0.9600	C15—C14	1.388 (5)
C19—O1	1.423 (5)	C15—C16	1.388 (5)
F1—C6	1.319 (5)	C7—C12	1.373 (5)
F3—C6	1.337 (5)	C7—C8	1.413 (5)
F2—C6	1.336 (5)	C7—C4	1.461 (5)
N1—N2	1.349 (4)	C14—H14	0.9300
N1—C5	1.368 (5)	C14—C13	1.366 (5)
N1—C13	1.446 (5)	C12—H12	0.9300
N3—N2	1.315 (4)	C8—H8	0.9300
N3—C4	1.363 (5)	C18—H18	0.9300
O3—H3	0.8200	C18—C13	1.393 (5)
O3—C15	1.357 (5)	C18—C17	1.388 (6)
O2—C10	1.356 (4)	C16—H16	0.9300
O1—C9	1.366 (4)	C16—C17	1.362 (6)
C9—C10	1.402 (6)	C17—H17	0.9300
H20A—C20—H20B	109.5	C11—C10—C9	119.3 (4)
H20A—C20—H20C	109.5	C12—C7—C8	118.6 (4)
H20B—C20—H20C	109.5	C12—C7—C4	122.8 (3)
O2—C20—H20A	109.5	C8—C7—C4	118.5 (4)
O2—C20—H20B	109.5	C15—C14—H14	120.7
O2—C20—H20C	109.5	C13—C14—C15	118.6 (4)
H19A—C19—H19B	109.5	C13—C14—H14	120.7
H19A—C19—H19C	109.5	C11—C12—H12	119.5
H19B—C19—H19C	109.5	C7—C12—C11	120.9 (4)
O1—C19—H19A	109.5	C7—C12—H12	119.5
O1—C19—H19B	109.5	C9—C8—C7	120.9 (4)
O1—C19—H19C	109.5	C9—C8—H8	119.5
N2—N1—C5	110.3 (3)	C7—C8—H8	119.5
N2—N1—C13	117.5 (3)	C13—C18—H18	121.7
C5—N1—C13	132.2 (3)	C17—C18—H18	121.7
N2—N3—C4	110.5 (3)	C17—C18—C13	116.7 (4)
C15—O3—H3	109.5	C15—C16—H16	120.2
C10—O2—C20	117.9 (3)	C17—C16—C15	119.6 (4)
N3—N2—N1	107.3 (3)	C17—C16—H16	120.2
C9—O1—C19	117.4 (3)	N3—C4—C5	106.8 (3)
O1—C9—C10	115.2 (3)	N3—C4—C7	121.6 (3)
O1—C9—C8	124.8 (4)	C5—C4—C7	131.6 (4)
C8—C9—C10	120.0 (4)	F1—C6—F3	107.3 (3)
N1—C5—C4	105.1 (3)	F1—C6—F2	107.1 (4)

N1—C5—C6	123.7 (3)	F1—C6—C5	112.8 (4)
C4—C5—C6	131.0 (4)	F3—C6—C5	112.1 (3)
C10—C11—H11	119.9	F2—C6—F3	105.9 (4)
C10—C11—C12	120.2 (4)	F2—C6—C5	111.2 (3)
C12—C11—H11	119.9	C14—C13—N1	118.3 (3)
O3—C15—C14	122.8 (4)	C14—C13—C18	122.9 (4)
O3—C15—C16	117.0 (4)	C18—C13—N1	118.8 (4)
C16—C15—C14	120.2 (4)	C18—C17—H17	118.9
O2—C10—C9	115.6 (3)	C16—C17—C18	122.1 (4)
O2—C10—C11	125.1 (4)	C16—C17—H17	118.9
C20—O2—C10—C9	−175.8 (4)	C10—C11—C12—C7	−0.6 (7)
C20—O2—C10—C11	2.5 (7)	C14—C15—C16—C17	−2.1 (7)
C19—O1—C9—C10	−179.5 (4)	C12—C11—C10—O2	−178.2 (4)
C19—O1—C9—C8	1.7 (7)	C12—C11—C10—C9	0.0 (7)
N1—C5—C4—N3	0.2 (4)	C12—C7—C8—C9	−0.8 (6)
N1—C5—C4—C7	179.2 (4)	C12—C7—C4—N3	−149.1 (4)
N1—C5—C6—F1	94.9 (5)	C12—C7—C4—C5	32.0 (7)
N1—C5—C6—F3	−26.4 (6)	C8—C9—C10—O2	178.6 (4)
N1—C5—C6—F2	−144.8 (4)	C8—C9—C10—C11	0.2 (7)
O3—C15—C14—C13	−178.0 (4)	C8—C7—C12—C11	1.0 (6)
O3—C15—C16—C17	177.9 (4)	C8—C7—C4—N3	28.5 (6)
N2—N1—C5—C4	−0.1 (4)	C8—C7—C4—C5	−150.4 (5)
N2—N1—C5—C6	175.8 (4)	C16—C15—C14—C13	2.0 (6)
N2—N1—C13—C14	−48.9 (5)	C4—N3—N2—N1	0.3 (5)
N2—N1—C13—C18	129.1 (4)	C4—C5—C6—F1	−90.4 (5)
N2—N3—C4—C5	−0.3 (5)	C4—C5—C6—F3	148.3 (4)
N2—N3—C4—C7	−179.5 (4)	C4—C5—C6—F2	29.9 (7)
O1—C9—C10—O2	−0.3 (6)	C4—C7—C12—C11	178.6 (4)
O1—C9—C10—C11	−178.7 (4)	C4—C7—C8—C9	−178.5 (4)
O1—C9—C8—C7	179.0 (4)	C6—C5—C4—N3	−175.2 (4)
C5—N1—N2—N3	−0.1 (4)	C6—C5—C4—C7	3.8 (8)
C5—N1—C13—C14	132.6 (5)	C13—N1—N2—N3	−179.0 (3)
C5—N1—C13—C18	−49.4 (6)	C13—N1—C5—C4	178.5 (4)
C15—C14—C13—N1	177.1 (4)	C13—N1—C5—C6	−5.6 (7)
C15—C14—C13—C18	−0.9 (7)	C13—C18—C17—C16	0.1 (7)
C15—C16—C17—C18	1.0 (7)	C17—C18—C13—N1	−178.1 (4)
C10—C9—C8—C7	0.2 (7)	C17—C18—C13—C14	−0.2 (7)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H3 $\cdots$ N3 ⁱ	0.82	2.02	2.813 (4)	163

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