

1,3,4-Triphenyl-7-trifluoromethyl-1H-pyrazolo[3,4-*b*]quinoline at 293 and 100 K

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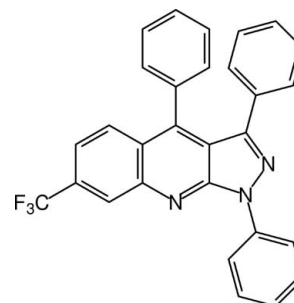
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In the structure of the title compound, C₂₉H₁₈F₃N₃, belonging to the space group *P*6₅ (or *P*6₁), three symmetry-independent molecules are arranged in two chains, with two molecules alternating along the 3₂ axes, whereas the remaining molecule forms a chain along [0001] due to the 6₅ screw axis. The conformation of each of the molecules is stabilized by an intramolecular C—H···N hydrogen bond, with C···N distances in the range 2.964 (6)–3.069 (5) Å at room temperature (293 K) and 2.943 (4)–3.084 (4) Å at low temperature (100 K). One molecule has its –CF₃ group ordered even at 293 K, which can be explained only by considering its involvement in two weak intermolecular C—H···F interactions, with C···F distances in the range 3.084 (6)–3.302 (5) Å at 293 K and 3.070 (3)–3.196 (3) Å at 100 K, and also a C—F···N interaction, with a C···N distance of 3.823 (5) Å at 293 K and 3.722 (4) Å at 100 K. The trifluoromethyl groups in the two remaining molecules are disordered at 293 K, whereas at 100 K the continuous (dynamic) positional disorder of one of the –CF₃ groups (of the molecule forming the chain along [0001]) is totally eliminated while the –CF₃ group disorder remains for the third molecule.

Comment

As part of a continuing study of organic materials for electroluminescence and OLED (organic light-emitting diode) preparation, new 1*H*-pyrazolo[3,4-*b*]quinoline derivatives containing trifluoromethyl substituents were obtained. Among them the title compound, 1,3,4-triphenyl-7-trifluoromethyl-1*H*-pyrazolo[3,4-*b*]quinoline, (I), has a very interesting crystal structure, belonging to the chiral space group *P*6₅ (or *P*6₁), rarely observed for achiral planar organic molecules. In the Cambridge Structural Database (CSD, Version of 2009; Allen, 2002), only three structures could be considered for comparison, *viz.* CIHMAI (1,3-diisopropylperimidinium chloride, space group *P*6₅; Bazinet *et al.*, 2007), ROLHAB

(phenanthro[5,6-*d*][1,2,3]trithiole, *P*6₁; Ogawa *et al.*, 1996) and SUHVUM (3-methylcarboxy-1*H*-indazole, *P*6₁ or *P*6₅; Glaser *et al.*, 1993).



(I)

Compound (I) shows fluorescence both in solution and in the solid state, which suggests that electroluminescence should also be observed for this material (Thomas *et al.*, 2004; Yeh *et al.*, 2004; Garbuzow *et al.*, 1996). A trifluoromethyl group at C7 is expected to have a significant influence on the absorption and emission properties of the molecule, causing bathochromic shifts of emission bands (Koścień *et al.*, 2009*a,b*) compared with 1*H*-pyrazolo[3,4-*b*]quinoline derivatives without trifluoromethyl substituents (Gondek *et al.*, 2006).

The crystal structure of (I) was determined at both room temperature (293 K) and low temperature (100 K). It consists of three symmetry-independent molecules, denoted (Ia), (Ib) and (Ic), and shown in Fig. 1 according to the data at 100 K. The molecular core of 1*H*-pyrazolo[3,4-*b*]quinoline is almost planar and aromatic [r.m.s. deviations of 0.0301, 0.0211 and 0.0229 Å for molecules (Ia), (Ib) and (Ic), respectively, at 293 K, and 0.0367, 0.0209 and 0.0244 Å, respectively, at 100 K].

The conformations of the molecules are defined in terms of just three dihedral angles (Table 1). Among the three phenyl substituents, only that at N1 could be approximately coplanar with the core moiety according to the conjugation effect. From Table 1, the expected coplanarity of the phenyl substituent (C11–C16) at N1 with the core moiety is observed only in the case of molecule (Ib). The two remaining phenyl substituents at C3 (C31–C36) and C4 (C41–C46) adopt synclinal (+*sc* or –*sc*) conformations due to steric hindrance. The distances between the centres of gravity of the rings are in the range 4.179 (6)–4.349 (7) Å at 293 K and 4.220 (4)–4.376 (4) Å at 100 K. The appropriate angles between the best planes of the rings are in the range 36.1 (2)–39.2 (2)° at 293 K and 36.9 (1)–39.2 (1)° at 100 K. The behaviour of the phenyl substituents is similar for all symmetry-independent molecules and is comparable with that of 6-fluoro-1,3,4-triphenyl-1*H*-pyrazolo[3,4-*b*]quinoline (PQ6F; Szlachcic & Stadnicka, 2010).

In all three symmetry-independent molecules of (I), a significant shortening of the N2–C3 and N9–C9a bond lengths is observed, with average values of 1.310 (5) and 1.321 (5) Å, respectively, at 293 K, and 1.316 (3) and 1.318 (4) Å, respectively, at 100 K. The endocyclic angles at N1 and N2 follow the geometry of a five-membered aromatic ring, whereas the endocyclic angle at N9 is smaller than those observed for unsubstituted pyridine in certain solvates (Morris

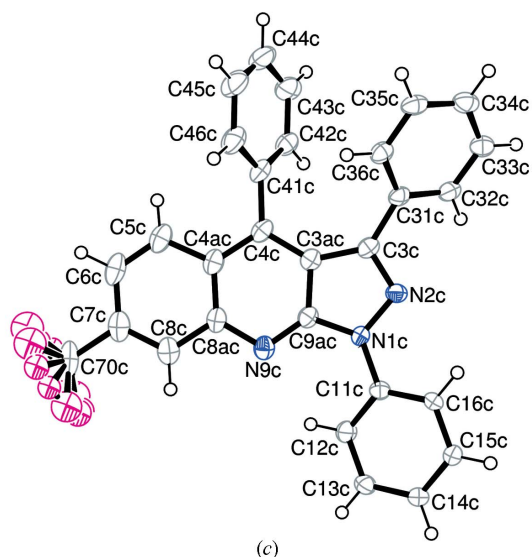
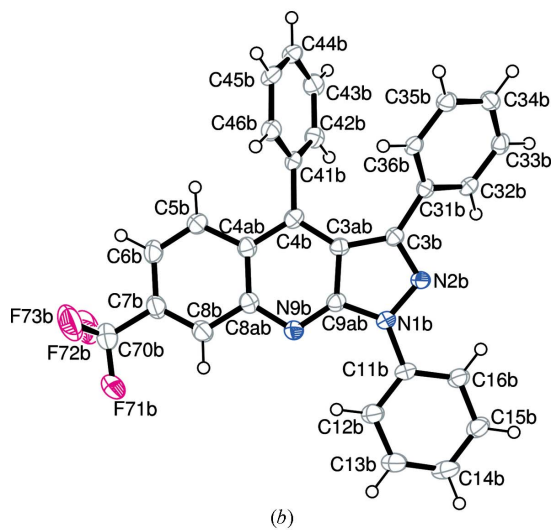
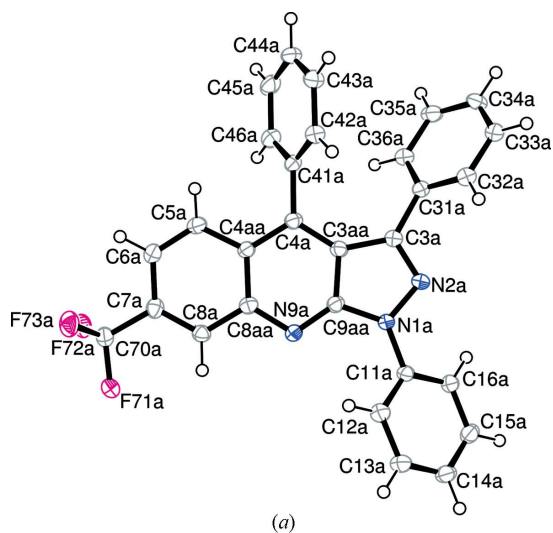


Figure 1
The three independent molecules of (I) at 100 K, showing (a) molecule (Ia), (b) molecule (Ib) and (c) molecule (Ic), together with the atom-labelling schemes. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

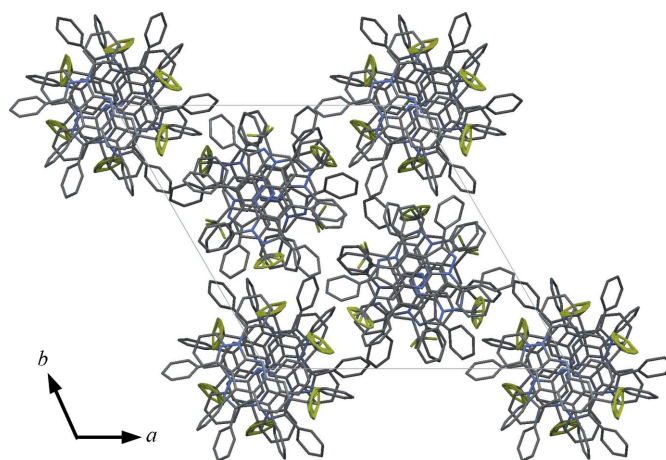


Figure 2
A projection of the unit-cell contents of (I) at 293 K along [001]. The disordered $-\text{CF}_3$ groups of molecules (Ib) and (Ic) can be seen. H atoms have been omitted for clarity.

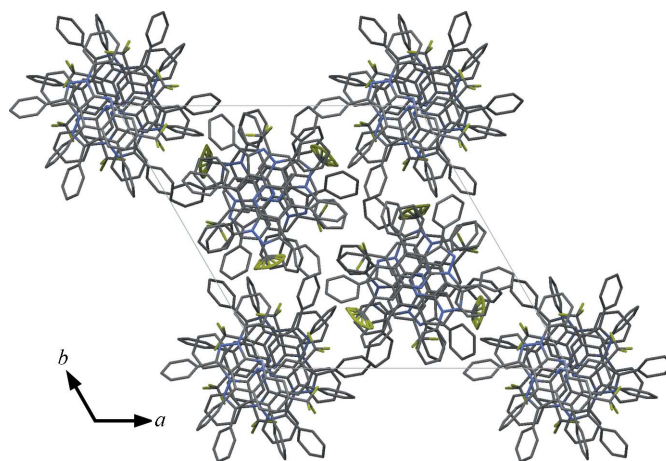


Figure 3
A projection of the unit-cell contents of (I) at 100 K along [001]. The disordered $-\text{CF}_3$ groups are observed only for the molecule (Ic). H atoms have been omitted for clarity.

et al., 2006; Chantrapromma *et al.*, 2001) but in good agreement with the values found for pyrazolo[3,4-*b*]pyridines (Portilla *et al.*, 2007; Low *et al.*, 2002, 2007). Among the torsion angles, the most important showing conformational variation between the molecules are those defining the orientation of the phenyl substituents with respect to the core moiety, namely N2–N1–C11–C16, N2–C3–C31–C32 and C3a–C4–C41–C42 (see Tables 2 and 4 for the 293 and 100 K data, respectively).

For all three symmetry-independent molecules, weak intramolecular C–H...N interactions are observed (C12–H12...N9), the geometry of which is given in Tables 3 and 5 for the 293 and 100 K data, respectively.

Despite the different torsion angles, the three molecules also exhibit different behaviour of the trifluoromethyl substituents: at 293 K, the $-\text{CF}_3$ group of (Ia) is ordered, and those of (Ib) and (Ic) are disordered, whereas at 100 K, the $-\text{CF}_3$ groups of (Ia) and (Ib) are ordered and only that of (Ic) still shows the continuous (static or dynamic) positional

disorder (compare Figs. 2 and 3). It is worth noting that the same behaviour of the $-\text{CF}_3$ groups was observed for several investigated crystals, which means that the phenomenon is a specific quality for the crystal structure and not for a particular crystal. The only explanation for the ordered trifluoromethyl group of (*Ia*) is its involvement in very weak intermolecular interactions: two of $\text{C}-\text{H}\cdots\text{F}$ type [despite relatively long $\text{C}\cdots\text{F}$ distances of 3.084 (6)–3.302 (5) Å at 293 K and 3.070 (3)–3.196 (3) Å at 100 K] and one of $\text{C}-\text{F}\cdots\text{N}$ type [$\text{C}\cdots\text{N}$ distance of 3.823 (5) Å at 293 K and 3.722 (4) Å at 100 K]. The trifluoromethyl groups of molecules (*Ib*) and (*Ic*) face each other, with the shortest intermolecular $\text{F}\cdots\text{F}$ distance being 3.573 (19) Å at 293 K and 3.460 (6) Å at 100 K, much longer than the sum of the van der Waals radii for F atoms ($r = 1.47$ Å for F; Bondi, 1964). This type of dynamic disorder of trifluoromethyl groups is often observed, *e.g.* in ethyl 4-[2-nitro-4-(trifluoromethyl)phenyl]piperazine-1-carboxylate (Lynch & McClenaghan, 2004) or {2-[3,5-bis(trifluoromethyl)-1*H*-pyrazol-1-ylmethyl]-6-(3,5-dimethyl-1*H*-pyrazol-1-ylmethyl)pyridine}methylpalladium(II) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate at 100 K (Guzei *et al.*, 2008).

In the crystal structure of (*I*), molecules (*Ib*) form a helix of symmetry 6_5 (Fig. 4), with a distance between the planar cores of adjacent molecules of 3.687 (3) Å at 293 K and 3.619 (3) Å at 100 K, but the molecules are not exactly parallel, with the angles between their best planes being 17.25 (8) and 17.90 (5)° at 293 K and 100 K, respectively. The shortest distances

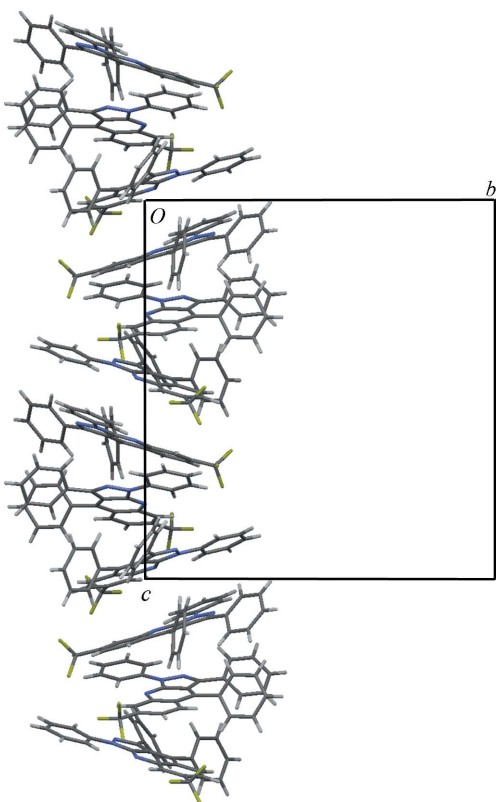


Figure 4
Part of the crystal structure of compound (*I*) at 100 K, showing the helix built of (*Ib*) molecules related by the 6_5 screw axis. The view is along [100].

between the centres of gravity of the rings were found for the pyridine rings, *viz.* 3.937 (8) Å at 293 K and 3.888 (4) Å at 100 K.

Molecules (*Ia*) and (*Ic*) alternate along the 3_2 axes (Fig. 5), forming pairs through π - π interactions between the following rings of the molecular core (distances are given at 293 and 100 K, respectively): the pyrazole ring of (*Ia*) and the benzene ring of (*Ic*), with centroid-centroid ($\text{Cg}\cdots\text{Cg}$) distances of 3.729 (7) and 3.671 (5) Å; the pyridine ring of (*Ia*) and the pyridine ring of (*Ic*), with $\text{Cg}\cdots\text{Cg}$ distances of 3.801 (7) and 3.746 (5) Å; and the benzene ring of (*Ia*) and the pyrazole ring of (*Ic*), with $\text{Cg}\cdots\text{Cg}$ distances of 3.747 (7) and 3.677 (5) Å. The molecules in the pair are almost parallel to each other, with angles between their best planes of 4.86 (7)° at 293 K and 5.09 (4)° at 100 K. This pair of molecules interacts with the next closest one, rotated by 120° about the 3_2 axis, due to π - π interactions between the benzene ring of (*Ia*) and the pyridine ring of (*Ic*) at symmetry position $(-x + y, -x + 1, z + \frac{1}{3})$, and also between the pyridine ring of (*Ic*) and the benzene ring of (*Ia*) at symmetry position $(-y + 1, x - y + 1, z - \frac{1}{3})$, with a $\text{Cg}\cdots\text{Cg}$ distance of 3.889 (8) Å at 293 K and 3.793 (5) Å at 100 K.

The geometry of the other weak interactions, mainly those of the $\text{C}-\text{H}\cdots\pi$ type, is characterized in Tables 3 and 5 for the 293 and 100 K data, respectively.

It is worth noting that, in the three structures obtained from the CSD and listed above, containing condensed aromatic ring systems (CSD refcodes CIHMAI, ROLHAB and SUHVUM),

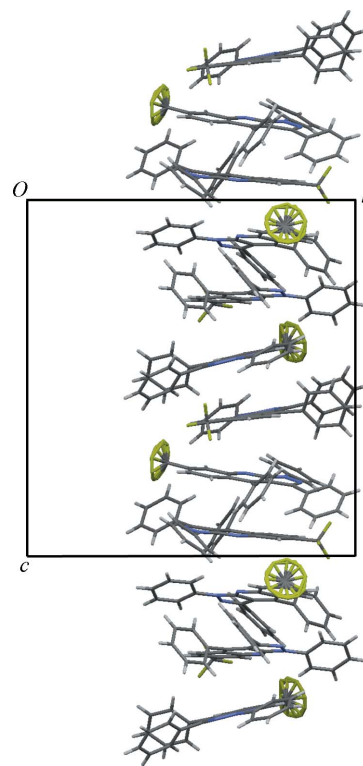


Figure 5
Part of the crystal structure of compound (*I*) at 100 K, showing molecules (*Ia*) and (*Ic*) alternating along the 3_2 screw axis. The $-\text{CF}_3$ group of the (*Ic*) molecule is disordered. The view is along [100].

π - π interactions between the molecules were also observed. The resulting distances between the best planes of the molecules along the sixfold screw axis were 3.411, 3.277 and 3.367 Å, respectively. In the case of SUHVUM, the arrangement of the three independent molecules of 3-methylcarboxy-1*H*-indazole is similar to the structure of (I): one of the molecules is related by the 6_1 (6_5) screw axis, with benzene ring $Cg \cdots Cg$ distances of 3.929 Å, while the two remaining molecules alternate along 3_1 (3_2) and form dimers due to π - π interactions, with benzene ring $Cg \cdots Cg$ distances of 4.002 Å.

Experimental

The title compound was synthesized, using a procedure already described in the literature (Chaczatrian *et al.*, 2003, 2007), from 3-trifluoromethylaniline, benzaldehyde and 2,5-diphenyl-2,4-dihydropyrazol-3-one (50 mmol of each substrate, ethylene glycol as solvent). The product was purified by column chromatography on SilicaGel 60 with toluene as eluent (repeated twice) to give 1.86 g of (I) (8% yield) as a yellow crystalline solid (m.p. 449–450.5 K). ^1H NMR (CDCl_3 , 300 MHz): δ 7.04–7.10 (*m*, 2H), 7.12–7.15 (*m*, 2H), 7.17–7.29 (*m*, 5H), 7.32–7.39 (*m*, 2H), 7.54 (*ddd*, $J = 9.0, 1.9$ and 0.4 Hz, 1H), 7.57–7.63 (*m*, 2H), 8.04 (*dt*, $J = 9.0$ and 0.8 Hz, 1H), 8.57–8.60 (*m*, 3H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 116.0, 119.4 (*q*, $J_{\text{C-F}} = 3.1$ Hz), 121.0, 124.6, 125.8, 127.1 (*q*, $J_{\text{C-F}} = 4.6$ Hz), 127.6, 127.8, 128.1, 128.6, 128.8, 129.0, 129.1, 130.3, 131.7, 132.2, 133.8, 139.6, 144.9, 146.9, 147.3, 150.6. Single crystals of (I) suitable for X-ray diffraction were grown by slow evaporation of a solution in toluene. The experimental data at 293 and 100 K were obtained from two different crystals.

Compound (I) at 293 K

Crystal data

$\text{C}_{29}\text{H}_{18}\text{F}_3\text{N}_3$	$Z = 18$
$M_r = 465.46$	Mo $K\alpha$ radiation
Hexagonal, $P6_5$	$\mu = 0.10 \text{ mm}^{-1}$
$a = 23.2368$ (3) Å	$T = 293 \text{ K}$
$c = 22.1155$ (3) Å	$0.50 \times 0.27 \times 0.25 \text{ mm}$
$V = 10341.4$ (2) Å ³	

Data collection

Nonius KappaCCD diffractometer	70213 measured reflections
Absorption correction: multi-scan (<i>DENZO</i> and <i>SCALEPACK</i> ; Otwinowski & Minor, 1997)	8110 independent reflections
	4772 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.080$
$T_{\text{min}} = 0.953, T_{\text{max}} = 0.976$	

Table 1

Comparison of the dihedral angles ($^\circ$) between the best planes of the phenyl substituents and the core of the molecule (the 1*H*-pyrazolo[3,4-*b*]quinoline moiety) for (I) and 6-fluoro-1,3,4-triphenyl-1*H*-pyrazolo[3,4-*b*]quinoline (PQ6F).

<i>T</i> (K)	Molecule	C11–C16 ring	C31–C36 ring	C41–C46 ring
293	(Ia)	32.75 (15)	50.35 (14)	64.58 (13)
293	(Ib)	5.3 (2)	43.37 (15)	63.65 (16)
293	(Ic)	18.24 (17)	40.42 (14)	61.25 (17)
100	(Ia)	34.02 (9)	49.91 (7)	62.79 (7)
100	(Ib)	4.69 (11)	42.25 (9)	63.33 (9)
100	(Ic)	19.24 (9)	37.74 (8)	58.17 (8)
293	PQ6F†	29.66 (7)	44.59 (7)	67.94 (6)

† Szlachcic & Stadnicka (2010).

Table 2

Selected torsion angles ($^\circ$) for (I) at 293 K.

N2A–N1A–C11A–C16A	–31.4 (6)	$\text{C3aB–C4B–C41B–C42B}$	63.2 (6)
N2A–C3A–C31A–C32A	–48.3 (6)	N2C–N1C–C11C–C16C	14.8 (6)
$\text{C3aA–C4A–C41A–C42A}$	–65.3 (6)	N2C–C3C–C31C–C32C	36.6 (6)
N2B–N1B–C11B–C16B	–3.0 (7)	$\text{C3aC–C4C–C41C–C42C}$	59.7 (7)
N2B–C3B–C31B–C32B	39.0 (6)		

Table 3

Hydrogen-bond geometry (Å, $^\circ$) for (I) at 293 K.

$Cg1$ is the centroid of the phenyl substituent at C1 of molecule (Ib), $Cg2$ that of the pyrazole ring of (Ib) and $Cg4$ that of the phenyl substituent at C4 of (Ia).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
$\text{C12A–H12A}\cdots\text{N9A}$	0.93	2.57	3.069 (5)	114
$\text{C12B–H12B}\cdots\text{N9B}$	0.93	2.32	2.972 (6)	127
$\text{C12C–H12C}\cdots\text{N9C}$	0.93	2.37	2.964 (6)	121
$\text{C32B–H32B}\cdots\text{Cg1}^1$	0.93	2.77	3.61	151
$\text{C42B–H42B}\cdots\text{Cg2}^1$	0.93	2.95	3.90	163
$\text{C44B–H44B}\cdots\text{Cg4}$	0.93	3.18	3.99	148

Symmetry code: (i) $x - y + 1, x + 1, z - \frac{1}{6}$.

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$	45 restraints
$wR(F^2) = 0.162$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$
8110 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$
971 parameters	

Compound (I) at 100 K

Crystal data

$\text{C}_{29}\text{H}_{18}\text{F}_3\text{N}_3$	$Z = 18$
$M_r = 465.46$	Mo $K\alpha$ radiation
Hexagonal, $P6_5$	$\mu = 0.10 \text{ mm}^{-1}$
$a = 23.0675$ (3) Å	$T = 100 \text{ K}$
$c = 21.7160$ (4) Å	$0.32 \times 0.30 \times 0.25 \text{ mm}$
$V = 10007.2$ (3) Å ³	

Data collection

Nonius KappaCCD diffractometer	25552 measured reflections
Absorption correction: multi-scan (<i>DENZO</i> and <i>SCALEPACK</i> ; Otwinowski & Minor, 1997)	7805 independent reflections
	6555 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.045$
$T_{\text{min}} = 0.969, T_{\text{max}} = 0.975$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	26 restraints
$wR(F^2) = 0.105$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$
7805 reflections	$\Delta\rho_{\text{min}} = -0.47 \text{ e \AA}^{-3}$
976 parameters	

Table 4

Selected torsion angles ($^\circ$) for (I) at 100 K.

N2A–N1A–C11A–C16A	–31.1 (4)	$\text{C3aB–C4B–C41B–C42B}$	62.3 (4)
N2A–C3A–C31A–C32A	–47.9 (4)	N2C–N1C–C11C–C16C	16.5 (4)
$\text{C3aA–C4A–C41A–C42A}$	–62.7 (4)	N2C–C3C–C31C–C32C	34.0 (4)
N2B–N1B–C11B–C16B	–2.8 (4)	$\text{C3aC–C4C–C41C–C42C}$	56.6 (4)
N2B–C3B–C31B–C32B	39.3 (4)		

Table 5

Hydrogen-bond geometry (Å, °) for (I) at 100 K.

Cg1 is the centroid of the phenyl substituent at C1 of molecule (Ib), Cg2 that of the pyrazole ring of (Ib), Cg3 that of the phenyl substituent at C3 of (Ic), Cg4 that of the phenyl substituent at C4 of (Ia) and Cg5 that of the phenyl substituent at C1 of (Ia).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C12A—H12A...N9A	0.95	2.59	3.084 (4)	113
C12B—H12B...N9B	0.95	2.33	2.983 (4)	125
C12C—H12C...N9C	0.95	2.34	2.943 (4)	121
C32B—H32B...Cg1 ⁱ	0.95	2.65	3.49	149
C42B—H42B...Cg2 ⁱ	0.95	2.92	3.83	161
C45B—H45B...Cg3 ⁱⁱ	0.95	2.96	3.90	176
C44B—H44B...Cg4	0.95	3.04	3.87	147
C46C—H46C...Cg5	0.95	3.08	3.90	145

Symmetry codes: (i) $x - y + 1, x + 1, z - \frac{1}{6}$; (ii) $-x + y, -x + 1, z + \frac{1}{3}$.

H atoms were found in difference Fourier maps and included in geometrically calculated positions, with C—H = 0.93 (293 K) or 0.95 Å (100 K), and constrained as part of a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ for the aromatic CH groups. At 293 K, two of the three —CF₃ groups are disordered. Three orientations were defined for the —CF₃ groups at C70B and C70C. At 100 K, only the —CF₃ at C70C is disordered, with four orientations of the group being defined. In each case the sum of the site-occupation factors of the F atoms within a disordered group was restrained to 1.0000 (1). Furthermore, bond length and angle restraints (DFIX and DANG in *SHELXL97*; Sheldrick, 2008) were applied as follows: C—F = 1.336 (2) Å and F...F = 2.125 (10) Å for the 293 K data, and C—F = 1.341 (2) Å and F...F = 2.150 (10) Å for the 100 K data. The F atoms of the disordered —CF₃ groups were also refined with isotropic displacement parameters.

For both determinations, data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GG3239). Services for accessing these data are described at the back of the journal.

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