

4,4'-Di-*tert*-butyl-2,2'-bipyridine–hexafluorobenzene (1/1)Andrei S. Batsanov,\*  
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## Key indicators

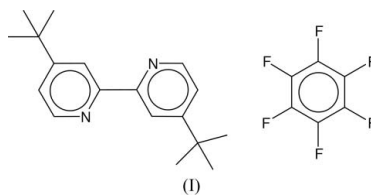
Single-crystal X-ray study  
 $T = 120$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.045  
 $wR$  factor = 0.138  
Data-to-parameter ratio = 13.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title structure,  $\text{C}_{18}\text{H}_{24}\text{N}_2 \cdot \text{C}_6\text{F}_6$ , comprises mixed stacks of alternating 4,4'-di-*tert*-butyl-2,2'-bipyridine and hexafluorobenzene molecules, both lying on crystallographic mirror planes. There are weak  $\text{C}-\text{H} \cdots \text{N}$  (2.46–2.51 Å) and  $\text{C}-\text{H} \cdots \text{F}$  (2.52–2.74 Å) hydrogen bonds lying on the mirror planes, as well as  $\pi$ - $\pi$  interactions between stacked aromatic molecules (as indicated by interplanar distances of 3.35 Å).

Received 3 December 2006  
Accepted 27 January 2007Arene–perfluoroarene inter-  
actions in crystal engineering.  
Part XVI. For Part XV, see  
Batsanov *et al.* (2006).

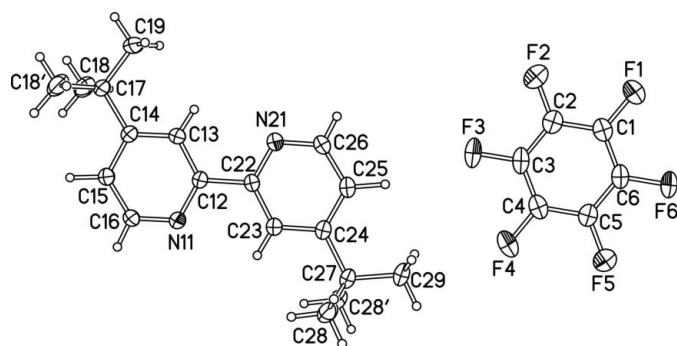
## Comment

Numerous arenes and perfluoroarenes readily co-crystallize in a 1:1 stoichiometry with a mixed-stack packing motif (Patrick & Prosser, 1960; Dahl, 1988; Collings *et al.*, 2002). However, only three complexes of pyridine derivatives with perfluoroarenes have been reported to date. In 1:1 complexes of hexafluorobenzene (HFB) with 6-phenyl- or 6,6'-diphenyl derivatives of 4,4'-di-*tert*-butyl-2,2'-bipyridine, DTBPy (Mkhaliid *et al.*, 2006), the HFB molecule is stacked with the phenyl substituent rather than with the bipyridine core of the DTBPy. In  $Q \cdot 2.5\text{C}_6\text{F}_6$ , where  $Q = 5,10,15$ -{(1,3,5-triamido-mesitylene)-tris(*o*-phenylene)}-2-(2-pivaloylaminophenyl)porphyrin,  $\text{C}_{61}\text{H}_{46}\text{N}_8\text{O}_4$  (Sleboznick *et al.*, 1996), an HFB molecule is in face-to-face contact with the porphyrin, at a distance of 3.21 Å, implying  $\pi$ - $\pi$  interactions (Hunter & Sanders, 1990; Bacchi *et al.*, 2006), but no continuous stacks exist. Here, we report the title DTBPy·HFB complex, (I), which has infinite heteroarene/HFB mixed stacks.

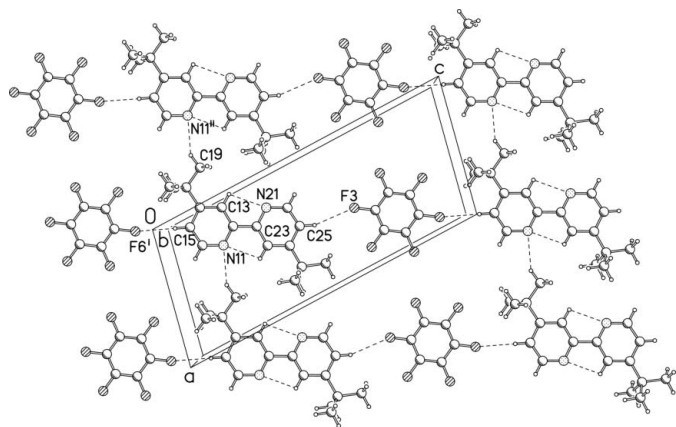


The entire HFB molecule of (I) (Fig. 1) lies on a crystallographic mirror plane (Wyckoff position e), as does the DTBPy molecule, except for the methyl groups  $\text{C}18\text{H}_3$  and  $\text{C}28\text{H}_3$  and their symmetry equivalents ( $\text{C}18'\text{H}_3$  and  $\text{C}28'\text{H}_3$  in Fig. 1), as well as two symmetry-related pairs of H atoms on atoms C19 and C29. The DTBPy molecule adopts a *trans* conformation around the central  $\text{C}12$ – $\text{C}22$  bond, as in 6-phenyl-DTBPy·HFB, which shows the same motif of alternating molecules lying on mirror planes, whereas in 6,6'-diphenyl-DTBPy·HFB, this unit is twisted by 19° from a perfect *trans* conformation (Mkhaliid *et al.*, 2006).

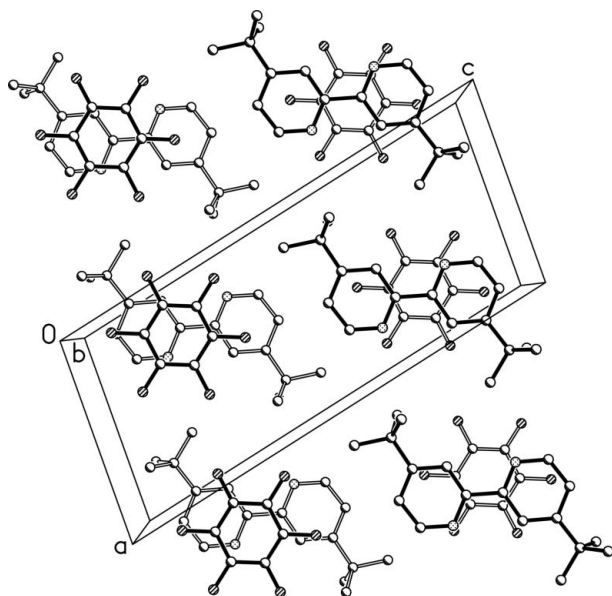
Table 1 lists the shortest intra- (lines 1 and 2) and intermolecular contacts (all located in the mirror plane; Fig. 2),

**Figure 1**

The molecular structure of HFB and DTBPy in (I), viewed down the *b* axis. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are related to unprimed atoms by  $(x, \frac{3}{2} - y, z)$ .

**Figure 2**

The molecular packing of (I) in the  $(x, \frac{3}{4}, z)$  plane. [Symmetry codes: (i)  $x - 1, y, z - 1$ ; (ii)  $x - 1, y, z$ .]

**Figure 3**

The overlap between molecules of two adjacent layers. H atoms have been omitted for clarity.

which satisfy the definition of ‘weak hydrogen bonds’ as proposed by Taylor & Kennard (1982), Jeffrey (1997) or Desiraju & Steiner (1999). The low dissociation energy of the

shortest C15—H15...F6<sup>i</sup> interaction in (I) can be estimated by analogy with the C—H...F—C interactions in the gaseous CH<sub>3</sub>·CH<sub>3</sub>F complex (Caminati *et al.*, 2005), with similar H...F distances of 2.43 (1) Å. The dissociation energy in the latter compound is only 1.8 kJ mol<sup>-1</sup> per H...F link.

The overlap between adjacent layers in (I) is shown in Fig. 3, whereas in the perpendicular direction, [010], runs an infinite columnar (rather than slanted) stack of alternating rigorously parallel HFB and DTBPy molecules with a uniform interplanar separation of 3.35 Å (or *b*/2), which indicates π–π electron interaction between the aromatic rings (see above).

The structure of (I) shows pseudo-symmetry of space group *I2/m* (in the same setting), disturbed by the orientation of the *tert*-butyl groups in DTBPy and by small shifts of the molecular centroids (for HFB,  $x = 0.7287$  and  $z = 0.7694$ ; for DTBPy,  $x = 0.2751$  and  $z = 0.2658$ ) from the pseudo-2/*m* special positions ( $x = z = \frac{3}{4}$  and  $x = z = \frac{1}{4}$ , respectively).

## Experimental

Compound (I) was obtained by hydrolysis of the B—C bond during an attempt to recrystallize the borylation product 4,4′-di-*tert*-butyl-6-Bpin-2,2′-bipyridine (Bpin = BOCMe<sub>2</sub>CMe<sub>2</sub>O) from HFB solution, which was permitted to evaporate slowly at room temperature. Crystals of (I) were obtained as blocks of irregular shape (with rounded edges) of 0.1 to 0.3 mm in size.

### Crystal data

C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> ·C <sub>6</sub> F <sub>6</sub>	<i>Z</i> = 2
<i>M<sub>r</sub></i> = 454.45	<i>D<sub>x</sub></i> = 1.408 Mg m <sup>-3</sup>
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>m</i>	Mo <i>K</i> α radiation
<i>a</i> = 8.5150 (7) Å	$\mu$ = 0.12 mm <sup>-1</sup>
<i>b</i> = 6.6964 (5) Å	<i>T</i> = 120 (2) K
<i>c</i> = 19.2756 (18) Å	Block, colourless
$\beta$ = 102.73 (1)°	0.32 × 0.25 × 0.21 mm
<i>V</i> = 1072.08 (16) Å <sup>3</sup>	

### Data collection

Bruker SMART 6K CCD area-detector diffractometer	2669 independent reflections
$\omega$ scans	1962 reflections with $I > 2\sigma(I)$
Absorption correction: none	<i>R</i> <sub>int</sub> = 0.047
12337 measured reflections	$\theta_{\max}$ = 27.5°

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 0.0675P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.138$	$(\Delta/\sigma)_{\max} < 0.001$
<i>S</i> = 1.06	$\Delta\rho_{\max} = 0.35 \text{ e \AA}^{-3}$
2669 reflections	$\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$
193 parameters	
H-atom parameters constrained	

**Table 1**

Geometry of C—H...N and C—H...F interactions (Å, °).

<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>
C13—H13...N21	0.95	2.50	2.819 (2)	100
C23—H23...N11	0.95	2.46	2.793 (2)	100
C15—H15...F6 <sup>i</sup>	0.95	2.52	3.472 (2)	180
C25—H25...F3	0.95	2.74	3.649 (2)	160
C19—H19...N11 <sup>ii</sup>	0.98	2.51	3.388 (2)	149

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

All H atoms were observed in a difference Fourier map but were treated as riding in idealized positions, with bond lengths C–H = 0.95 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aryl H atoms and C–H = 0.98 Å for methyl groups, of which C18H<sub>3</sub> and C28H<sub>3</sub> were permitted to rotate around the C–C bonds and C19H<sub>3</sub> and C29H<sub>3</sub> had fixed orientations due to mirror symmetry. The H atoms of each methyl group were assigned the same  $U_{\text{iso}}(\text{H})$  value, which was refined.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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## supporting information

*Acta Cryst.* (2007). E63, o1196–o1198 [https://doi.org/10.1107/S160053680700445X]

4,4'-Di-*tert*-butyl-2,2'-bipyridine–hexafluorobenzene (1/1)

Andrei S. Batsanov, Ibraheem A. I. Mkhaliid and Todd B. Marder

4,4'-Di-*tert*-butyl-2,2'-bipyridine–hexafluorobenzene (1/1)*Crystal data*

$C_{18}H_{24}N_2 \cdot C_6F_6$

$M_r = 454.45$

Monoclinic,  $P2_1/m$

Hall symbol:  $-P\ 2yb$

$a = 8.5150$  (7) Å

$b = 6.6964$  (5) Å

$c = 19.2756$  (18) Å

$\beta = 102.73$  (1)°

$V = 1072.08$  (16) Å<sup>3</sup>

$Z = 2$

$F(000) = 472$

$D_x = 1.408$  Mg m<sup>-3</sup>

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

Cell parameters from 4097 reflections

$\theta = 2.5$ – $27.5$ °

$\mu = 0.12$  mm<sup>-1</sup>

$T = 120$  K

Block, colourless

$0.32 \times 0.25 \times 0.21$  mm

*Data collection*

Bruker SMART 6K CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 5.6 pixels mm<sup>-1</sup>

$\omega$  scans

12337 measured reflections

2669 independent reflections

1962 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.047$

$\theta_{max} = 27.5$ °,  $\theta_{min} = 2.2$ °

$h = -11 \rightarrow 11$

$k = -8 \rightarrow 8$

$l = -25 \rightarrow 25$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.138$

$S = 1.06$

2669 reflections

193 parameters

0 restraints

50 constraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 0.0675P]$

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

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

$\Delta\rho_{max} = 0.35$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.20$  e Å<sup>-3</sup>

*Special details*

**Experimental.** The data collection nominally covered full sphere of reciprocal space, by a combination of 3 runs of narrow-frame  $\omega$ -scans (scan width  $0.3^\circ \omega$ , 5 s exposure), every run at a different  $\varphi$  angle. Crystal to detector distance 4.84 cm.

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6571 (2)	0.7500	0.82701 (10)	0.0336 (4)
C2	0.5633 (2)	0.7500	0.75872 (11)	0.0339 (4)
C3	0.6353 (3)	0.7500	0.70135 (10)	0.0336 (4)
C4	0.7999 (3)	0.7500	0.71175 (10)	0.0341 (4)
C5	0.8943 (2)	0.7500	0.77986 (10)	0.0335 (4)
C6	0.8220 (2)	0.7500	0.83733 (10)	0.0331 (4)
F1	0.58793 (15)	0.7500	0.88277 (6)	0.0465 (3)
F2	0.40304 (15)	0.7500	0.74889 (7)	0.0482 (3)
F3	0.54412 (16)	0.7500	0.63522 (6)	0.0459 (3)
F4	0.86995 (17)	0.7500	0.65629 (6)	0.0468 (3)
F5	1.05383 (15)	0.7500	0.78996 (7)	0.0475 (3)
F6	0.91353 (15)	0.7500	0.90366 (6)	0.0446 (3)
N11	0.32420 (17)	0.7500	0.17729 (8)	0.0274 (3)
C12	0.2315 (2)	0.7500	0.22505 (9)	0.0231 (4)
C13	0.0633 (2)	0.7500	0.20553 (9)	0.0250 (4)
H13	0.0020	0.7500	0.2412	0.030*
C14	-0.0145 (2)	0.7500	0.13405 (9)	0.0268 (4)
C15	0.0835 (2)	0.7500	0.08478 (9)	0.0302 (4)
H15	0.0368	0.7500	0.0352	0.036*
C16	0.2491 (2)	0.7500	0.10847 (9)	0.0303 (4)
H16	0.3133	0.7500	0.0739	0.036*
C17	-0.1979 (2)	0.7500	0.10838 (9)	0.0326 (4)
C19	-0.2816 (2)	0.7500	0.17042 (11)	0.0534 (7)
H191	-0.3986	0.7500	0.1524	0.054 (4)*
H192	-0.2500	0.8687	0.2000	0.054 (4)*
N21	0.22538 (18)	0.7500	0.34977 (8)	0.0270 (3)
C22	0.3176 (2)	0.7500	0.30150 (8)	0.0223 (4)
C23	0.4850 (2)	0.7500	0.32017 (9)	0.0238 (4)
H23	0.5451	0.7500	0.2841	0.029*
C24	0.5657 (2)	0.7500	0.39175 (9)	0.0246 (4)
C25	0.4695 (2)	0.7500	0.44138 (9)	0.0298 (4)
H25	0.5171	0.7500	0.4908	0.036*
C26	0.3029 (2)	0.7500	0.41801 (9)	0.0307 (4)
H26	0.2398	0.7500	0.4530	0.037*
C27	0.7500 (2)	0.7500	0.41172 (9)	0.0276 (4)
C29	0.8142 (2)	0.7500	0.49233 (10)	0.0369 (5)
H291	0.9322	0.7500	0.5034	0.048 (4)*
H292	0.7745	0.6315	0.5129	0.048 (4)*
C18	-0.24974 (16)	0.9365 (2)	0.06286 (8)	0.0419 (4)
H181	-0.3670	0.9364	0.0459	0.054 (3)*
H182	-0.1984	0.9360	0.0221	0.054 (3)*

H183	-0.2168	1.0564	0.0916	0.054 (3)*
C28	0.81300 (15)	0.5629 (2)	0.38063 (7)	0.0354 (3)
H281	0.9310	0.5641	0.3921	0.043 (2)*
H282	0.7737	0.5617	0.3289	0.043 (2)*
H283	0.7744	0.4433	0.4011	0.043 (2)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0425 (11)	0.0295 (9)	0.0289 (9)	0.000	0.0079 (8)	0.000
C2	0.0372 (11)	0.0271 (9)	0.0347 (10)	0.000	0.0022 (8)	0.000
C3	0.0485 (12)	0.0238 (9)	0.0233 (9)	0.000	-0.0033 (8)	0.000
C4	0.0492 (12)	0.0266 (9)	0.0269 (9)	0.000	0.0094 (9)	0.000
C5	0.0347 (10)	0.0322 (10)	0.0313 (10)	0.000	0.0024 (8)	0.000
C6	0.0419 (11)	0.0309 (10)	0.0236 (9)	0.000	0.0010 (8)	0.000
F1	0.0513 (8)	0.0575 (8)	0.0336 (6)	0.000	0.0157 (6)	0.000
F2	0.0358 (7)	0.0531 (8)	0.0517 (8)	0.000	0.0012 (6)	0.000
F3	0.0584 (8)	0.0437 (7)	0.0268 (6)	0.000	-0.0094 (5)	0.000
F4	0.0651 (9)	0.0485 (7)	0.0298 (6)	0.000	0.0172 (6)	0.000
F5	0.0367 (7)	0.0596 (8)	0.0449 (7)	0.000	0.0063 (5)	0.000
F6	0.0465 (7)	0.0580 (8)	0.0237 (6)	0.000	-0.0043 (5)	0.000
N11	0.0224 (7)	0.0365 (8)	0.0228 (7)	0.000	0.0040 (6)	0.000
C12	0.0217 (8)	0.0259 (8)	0.0208 (8)	0.000	0.0028 (6)	0.000
C13	0.0216 (8)	0.0312 (9)	0.0229 (8)	0.000	0.0066 (6)	0.000
C14	0.0210 (8)	0.0342 (9)	0.0244 (8)	0.000	0.0035 (7)	0.000
C15	0.0246 (9)	0.0452 (11)	0.0204 (8)	0.000	0.0038 (7)	0.000
C16	0.0250 (9)	0.0458 (11)	0.0212 (8)	0.000	0.0073 (7)	0.000
C17	0.0192 (8)	0.0545 (12)	0.0230 (8)	0.000	0.0022 (7)	0.000
C19	0.0201 (9)	0.109 (2)	0.0310 (11)	0.000	0.0054 (8)	0.000
N21	0.0264 (8)	0.0322 (8)	0.0222 (7)	0.000	0.0052 (6)	0.000
C22	0.0251 (8)	0.0219 (8)	0.0195 (8)	0.000	0.0042 (6)	0.000
C23	0.0243 (9)	0.0250 (8)	0.0216 (8)	0.000	0.0042 (6)	0.000
C24	0.0260 (9)	0.0231 (8)	0.0225 (8)	0.000	0.0007 (7)	0.000
C25	0.0333 (10)	0.0346 (10)	0.0197 (8)	0.000	0.0019 (7)	0.000
C26	0.0312 (10)	0.0403 (10)	0.0214 (8)	0.000	0.0079 (7)	0.000
C27	0.0249 (9)	0.0311 (9)	0.0237 (8)	0.000	-0.0017 (7)	0.000
C29	0.0326 (10)	0.0460 (12)	0.0264 (9)	0.000	-0.0055 (8)	0.000
C18	0.0265 (7)	0.0523 (9)	0.0424 (8)	0.0064 (6)	-0.0021 (6)	0.0006 (7)
C28	0.0270 (7)	0.0376 (7)	0.0376 (7)	0.0047 (5)	-0.0017 (5)	-0.0029 (6)

*Geometric parameters (Å, °)*

C1—F1	1.334 (2)	C17—C18	1.5343 (18)
C1—C6	1.374 (3)	C19—H191	0.9800
C1—C2	1.381 (3)	C19—H192	0.9800
C2—F2	1.336 (2)	N21—C26	1.335 (2)
C2—C3	1.377 (3)	N21—C22	1.343 (2)
C3—F3	1.338 (2)	C22—C23	1.391 (2)

C3—C4	1.371 (3)	C23—C24	1.399 (2)
C4—F4	1.334 (2)	C23—H23	0.9500
C4—C5	1.380 (3)	C24—C25	1.390 (2)
C5—F5	1.329 (2)	C24—C27	1.531 (2)
C5—C6	1.381 (3)	C25—C26	1.390 (3)
C6—F6	1.343 (2)	C25—H25	0.9500
N11—C12	1.338 (2)	C26—H26	0.9500
N11—C16	1.340 (2)	C27—C29	1.529 (2)
C12—C13	1.399 (2)	C27—C28	1.5359 (17)
C12—C22	1.494 (2)	C27—C28 <sup>i</sup>	1.5360 (17)
C13—C14	1.391 (2)	C29—H291	0.9800
C13—H13	0.9500	C29—H292	0.9800
C14—C15	1.396 (2)	C18—H181	0.9800
C14—C17	1.531 (2)	C18—H182	0.9800
C15—C16	1.382 (3)	C18—H183	0.9800
C15—H15	0.9500	C28—H281	0.9800
C16—H16	0.9500	C28—H282	0.9800
C17—C19	1.521 (3)	C28—H283	0.9800
C17—C18 <sup>i</sup>	1.5343 (18)		
F1—C1—C6	120.10 (17)	C17—C19—H191	109.7
F1—C1—C2	120.18 (19)	C17—C19—H192	109.9
C6—C1—C2	119.72 (19)	H191—C19—H192	109.5
F2—C2—C3	120.51 (17)	C26—N21—C22	116.41 (15)
F2—C2—C1	119.55 (18)	N21—C22—C23	122.88 (15)
C3—C2—C1	119.94 (19)	N21—C22—C12	116.63 (14)
F3—C3—C4	119.93 (18)	C23—C22—C12	120.48 (15)
F3—C3—C2	119.82 (19)	C22—C23—C24	120.48 (15)
C4—C3—C2	120.25 (17)	C22—C23—H23	119.8
F4—C4—C3	120.39 (17)	C24—C23—H23	119.8
F4—C4—C5	119.50 (19)	C25—C24—C23	116.31 (15)
C3—C4—C5	120.11 (19)	C25—C24—C27	123.63 (15)
F5—C5—C4	120.11 (19)	C23—C24—C27	120.06 (15)
F5—C5—C6	120.30 (17)	C24—C25—C26	119.40 (16)
C4—C5—C6	119.59 (19)	C24—C25—H25	120.3
F6—C6—C1	119.87 (17)	C26—C25—H25	120.3
F6—C6—C5	119.73 (18)	N21—C26—C25	124.52 (16)
C1—C6—C5	120.39 (17)	N21—C26—H26	117.7
C12—N11—C16	117.11 (14)	C25—C26—H26	117.8
N11—C12—C13	122.64 (15)	C29—C27—C24	111.87 (15)
N11—C12—C22	116.28 (14)	C29—C27—C28	108.61 (10)
C13—C12—C22	121.08 (15)	C24—C27—C28	109.18 (9)
C14—C13—C12	120.17 (16)	C29—C27—C28 <sup>i</sup>	108.61 (10)
C14—C13—H13	119.9	C24—C27—C28 <sup>i</sup>	109.18 (9)
C12—C13—H13	119.9	C28—C27—C28 <sup>i</sup>	109.35 (16)
C13—C14—C15	116.62 (16)	C27—C29—H291	110.0
C13—C14—C17	123.34 (15)	C27—C29—H292	109.5
C15—C14—C17	120.05 (15)	H291—C29—H292	109.9

C16—C15—C14	119.63 (16)	C17—C18—H181	109.5
C16—C15—H15	120.2	C17—C18—H182	109.4
C14—C15—H15	120.2	H181—C18—H182	109.5
N11—C16—C15	123.83 (16)	C17—C18—H183	109.5
N11—C16—H16	118.1	H181—C18—H183	109.5
C15—C16—H16	118.1	H182—C18—H183	109.5
C19—C17—C14	111.54 (15)	C27—C28—H281	109.5
C19—C17—C18 <sup>i</sup>	108.91 (11)	C27—C28—H282	109.5
C14—C17—C18 <sup>i</sup>	109.22 (10)	H281—C28—H282	109.5
C19—C17—C18	108.91 (11)	C27—C28—H283	109.4
C14—C17—C18	109.22 (10)	H281—C28—H283	109.5
C18 <sup>i</sup> —C17—C18	109.00 (16)	H282—C28—H283	109.5

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

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C13—H13 $\cdots$ N21	0.95	2.50	2.819 (2)	100
C23—H23 $\cdots$ N11	0.95	2.46	2.793 (2)	100
C15—H15 $\cdots$ F6 <sup>ii</sup>	0.95	2.52	3.472 (2)	180
C25—H25 $\cdots$ F3	0.95	2.74	3.649 (2)	160
C19—H191 $\cdots$ N11 <sup>iii</sup>	0.98	2.51	3.388 (2)	149

Symmetry codes: (ii)  $x-1, y, z-1$ ; (iii)  $x-1, y, z$ .