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2-Fluoro-*N*-[(*E*)-1-(6-methoxy-2-naphthyl)methylidene]-5-(trifluoromethyl)aniline

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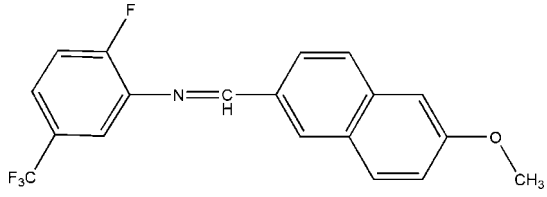
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.096; wR factor = 0.206; data-to-parameter ratio = 11.8.

In the title Schiff base, $C_{19}H_{13}F_4NO$, there is intramolecular C—H···F hydrogen bonding. A C—H···π interaction of 3.97 (6) Å forms an infinite tape parallel to the c axis. The trifluoromethyl group is disordered over two positions, with site occupancy factors of approximately 0.6:0.4.

Related literature

For related literature, see: Alemi & Shaabani (2000); Alizadeh *et al.* (1999); Kim & Shin (1999); Johnson *et al.* (1996); Wang & Zheng (2007).



Experimental

Crystal data

$C_{19}H_{13}F_4NO$
M_r = 347.30
Monoclinic, $P2_1/c$
a = 14.815 (9) Å
b = 6.192 (4) Å
c = 17.989 (11) Å
β = 106.127 (11)°
V = 1585.3 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 (2) K
0.38 × 0.31 × 0.19 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.955, T_{max} = 0.977
7985 measured reflections
2841 independent reflections
2522 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.096
$wR(F^2)$ = 0.206
S = 1.15
2841 reflections
240 parameters
138 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···F3	0.93	2.45	2.737 (14)	98
C8—H8···F4	0.93	2.46	2.835 (4)	104

Data collection: *SMART* (Bruker,1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2054).

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supplementary materials

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2-Fluoro-*N*-[(*E*)-1-(6-methoxy-2-naphthyl)methylidene]-5-(trifluoromethyl)aniline

G.-B. Yan, L.-G. Wang and C.-N. Zhang

Comment

Schiff base ligands have significant importance in chemistry, especially in the development of Schiff base complexes, (Johnson *et al.*, 1996; Alizadeh *et al.*, 1999; Wang & Zheng, 2007). Schiff bases that have solvent-dependent UV/vis spectra (solvatochromicity) can be suitable NLO (nonlinear optically active) materials (Alemi & Shaabani, 2000). They are also useful in the asymmetric oxidation of methyl phenyl sulfide and can be enantioselective (Kim & Shim, 1999). In this paper, we report the synthesis and crystal structure of the title compound, (I).

The molecular structure of the title compound (Fig. 1) contains one intermolecular hydrogen bonds (C3—H3···F3; C8—H8···F4) (Table 1). The C8—N1 bond length is 1.262 (4) Å, indicative of a C═N double bond. The C—F, C—O and C—C distances are unremarkable (Table.1).

Intramolecular C—H···F hydrogen bonding and C—H···/p interaction form an infinite tape parallel to the *c* axis.

Experimental

Under nitrogen, a mixture of 6-methoxy-1-naphthaldehyde (1.87 g,10 mmol), Na_2SO_4 (3.0 g) and 5-fluoro-2-trifluoromethylaniline (1.58 g, 10 mmol) in absolute ethanol (20 ml) was refluxed for about 12 h to yield a yellow precipitate. The product was collected by vacuum filtration and washed with ethanol. The crude solid was redissolved in CH_2Cl_2 (100 ml) and washed with water (2 *x* 15 ml) and brine (8 ml). After drying over Na_2SO_4, the solvent was removed under vacuum, and a yellow solid was isolated in 92% yield (3.1 g). Colourless single crystals of the Schiff base, (I), suitable for X-ray analysis were grown from CH_2Cl_2 and absolute ethanol (4:1) by slow evaporation of the solvents at room temperature over a period of about one week.

Refinement

All H atoms were placed in calculated positions [Csp^2—H = 0.93 Å] and refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C). The trifluoromethyl group was found to be disordered, the two components being rotated by about 60°. Atoms C1, F1, F2 and F3 were refined over two positions [occupancies 0.609 (4) for the primed and 0.391 (4) for the unprimed atoms] and the C—F distances restrained.

Figures

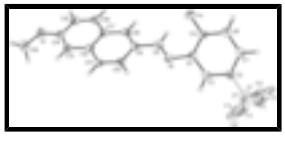


Fig. 1. The molecular structure of (I), showing the atomic numbering scheme (CF_3 component is disordered). Probability displacement ellipsoids are drawn at the 30% level.

2-Fluoro-*N*-[(*E*)-1-(6-methoxy-2-naphthyl)methylidene]-5-(trifluoromethyl)aniline

Crystal data

$C_{19}H_{13}F_4NO$	F_{000} = 712
M_r = 347.30	D_x = 1.455 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2493 reflections
a = 14.815 (9) Å	θ = 2.4–24.5º
b = 6.192 (4) Å	μ = 0.12 mm^{-1}
c = 17.989 (11) Å	T = 298 (2) K
β = 106.127 (11)º	Block, colourless
V = 1585.3 (17) Å^3	0.38 × 0.31 × 0.19 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	2841 independent reflections
Radiation source: fine-focus sealed tube	2522 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 298(2) K	θ_{max} = 25.2º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −17→16
T_{min} = 0.955, T_{max} = 0.977	k = −7→6
7985 measured reflections	l = −19→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.096	H-atom parameters constrained
$wR(F^2)$ = 0.206	$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 2.7345P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.15	$(\Delta/\sigma)_{max}$ = 0.001
2841 reflections	$\Delta\rho_{max}$ = 0.64 e Å^{-3}
240 parameters	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
138 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.9123 (9)	0.7965 (18)	0.0535 (5)	0.0750 (14)	0.391 (4)
F1	0.9885 (6)	0.6777 (17)	0.0554 (7)	0.117 (2)	0.391 (4)
F2	0.9043 (6)	0.9304 (19)	−0.0065 (5)	0.1122 (19)	0.391 (4)
F3	0.9411 (9)	0.9277 (17)	0.1148 (6)	0.119 (2)	0.391 (4)
C1'	0.9213 (6)	0.7832 (10)	0.0569 (3)	0.0750 (14)	0.609 (4)
F1'	0.9923 (4)	0.7061 (11)	0.1142 (4)	0.117 (2)	0.609 (4)
F2'	0.9500 (4)	0.7608 (12)	−0.0071 (3)	0.1122 (19)	0.609 (4)
F3'	0.9197 (6)	0.9953 (10)	0.0713 (5)	0.119 (2)	0.609 (4)
F4	0.58472 (16)	0.3569 (4)	0.03359 (14)	0.0622 (7)	
O1	0.1144 (2)	1.0983 (5)	0.24659 (18)	0.0684 (9)	
N1	0.6066 (2)	0.7862 (5)	0.09222 (17)	0.0468 (8)	
C2	0.8304 (3)	0.6720 (6)	0.0503 (2)	0.0505 (10)	
C3	0.7613 (3)	0.7712 (6)	0.0756 (2)	0.0489 (9)	
H3	0.7713	0.9101	0.0959	0.059*	
C4	0.6768 (2)	0.6681 (6)	0.07158 (19)	0.0414 (8)	
C5	0.6658 (3)	0.4624 (6)	0.0399 (2)	0.0448 (9)	
C6	0.7326 (3)	0.3628 (6)	0.0121 (2)	0.0530 (10)	
H6	0.7217	0.2265	−0.0103	0.064*	
C7	0.8160 (3)	0.4681 (7)	0.0181 (2)	0.0563 (11)	
H7	0.8625	0.4022	0.0004	0.068*	
C8	0.5562 (3)	0.6978 (6)	0.1298 (2)	0.0457 (9)	
H8	0.5699	0.5575	0.1478	0.055*	
C9	0.4770 (2)	0.8105 (6)	0.14573 (19)	0.0426 (8)	
C10	0.4475 (3)	1.0150 (6)	0.1130 (2)	0.0451 (9)	
H10	0.4803	1.0817	0.0821	0.054*	
C11	0.3723 (3)	1.1148 (6)	0.1261 (2)	0.0462 (9)	
H11	0.3541	1.2493	0.1041	0.055*	
C12	0.3205 (2)	1.0184 (6)	0.17287 (19)	0.0434 (9)	
C13	0.2404 (3)	1.1187 (7)	0.1858 (2)	0.0499 (9)	
H13	0.2203	1.2517	0.1632	0.060*	
C14	0.1926 (3)	1.0203 (7)	0.2314 (2)	0.0532 (10)	
C15	0.2244 (3)	0.8213 (7)	0.2667 (2)	0.0573 (11)	
H15	0.1922	0.7574	0.2987	0.069*	

C16	0.3005 (3)	0.7208 (7)	0.2554 (2)	0.0536 (10)
H16	0.3199	0.5892	0.2794	0.064*
C17	0.3506 (3)	0.8145 (6)	0.20723 (19)	0.0429 (8)
C18	0.4291 (3)	0.7146 (6)	0.1921 (2)	0.0454 (9)
H18	0.4488	0.5806	0.2140	0.054*
C19	0.0753 (3)	1.2934 (8)	0.2097 (3)	0.0781 (14)
H19A	0.1204	1.4078	0.2250	0.117*
H19B	0.0198	1.3289	0.2247	0.117*
H19C	0.0594	1.2752	0.1546	0.117*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.053 (3)	0.064 (3)	0.120 (4)	−0.009 (2)	0.045 (3)	−0.005 (3)
F1	0.050 (2)	0.147 (4)	0.142 (5)	−0.017 (2)	0.006 (4)	0.030 (5)
F2	0.085 (4)	0.158 (5)	0.111 (3)	−0.054 (3)	0.055 (3)	−0.012 (4)
F3	0.084 (4)	0.074 (4)	0.208 (8)	−0.032 (3)	0.057 (5)	−0.009 (4)
C1'	0.053 (3)	0.064 (3)	0.120 (4)	−0.009 (2)	0.045 (3)	−0.005 (3)
F1'	0.050 (2)	0.147 (4)	0.142 (5)	−0.017 (2)	0.006 (4)	0.030 (5)
F2'	0.085 (4)	0.158 (5)	0.111 (3)	−0.054 (3)	0.055 (3)	−0.012 (4)
F3'	0.084 (4)	0.074 (4)	0.208 (8)	−0.032 (3)	0.057 (5)	−0.009 (4)
F4	0.0546 (14)	0.0554 (14)	0.0793 (16)	−0.0163 (11)	0.0231 (12)	−0.0134 (12)
O1	0.0547 (18)	0.081 (2)	0.076 (2)	0.0017 (16)	0.0305 (15)	−0.0072 (17)
N1	0.0472 (18)	0.0431 (17)	0.0500 (18)	−0.0024 (15)	0.0132 (14)	−0.0003 (14)
C2	0.046 (2)	0.049 (2)	0.057 (2)	0.0012 (18)	0.0135 (18)	0.0055 (19)
C3	0.056 (2)	0.040 (2)	0.049 (2)	−0.0023 (18)	0.0116 (18)	−0.0020 (17)
C4	0.0406 (19)	0.043 (2)	0.0407 (19)	0.0007 (16)	0.0109 (15)	0.0040 (16)
C5	0.046 (2)	0.042 (2)	0.045 (2)	−0.0059 (17)	0.0112 (16)	0.0042 (16)
C6	0.061 (2)	0.041 (2)	0.057 (2)	0.0018 (19)	0.0175 (19)	−0.0049 (18)
C7	0.048 (2)	0.054 (2)	0.071 (3)	0.0071 (19)	0.025 (2)	0.000 (2)
C8	0.050 (2)	0.040 (2)	0.045 (2)	0.0002 (17)	0.0091 (17)	−0.0006 (16)
C9	0.047 (2)	0.043 (2)	0.0376 (18)	−0.0030 (17)	0.0097 (15)	−0.0026 (16)
C10	0.050 (2)	0.043 (2)	0.046 (2)	−0.0048 (17)	0.0186 (17)	0.0044 (16)
C11	0.055 (2)	0.0365 (19)	0.047 (2)	−0.0023 (17)	0.0147 (17)	0.0056 (16)
C12	0.047 (2)	0.044 (2)	0.0373 (18)	−0.0037 (17)	0.0086 (15)	−0.0049 (16)
C13	0.051 (2)	0.048 (2)	0.050 (2)	0.0021 (18)	0.0120 (18)	−0.0052 (18)
C14	0.047 (2)	0.063 (3)	0.051 (2)	−0.008 (2)	0.0166 (18)	−0.011 (2)
C15	0.062 (3)	0.061 (3)	0.055 (2)	−0.013 (2)	0.028 (2)	0.001 (2)
C16	0.064 (3)	0.048 (2)	0.052 (2)	−0.006 (2)	0.0215 (19)	0.0047 (18)
C17	0.048 (2)	0.041 (2)	0.0399 (18)	−0.0042 (17)	0.0130 (16)	−0.0023 (16)
C18	0.055 (2)	0.0383 (19)	0.0400 (19)	0.0001 (17)	0.0091 (16)	0.0024 (16)
C19	0.061 (3)	0.077 (3)	0.103 (4)	0.007 (3)	0.033 (3)	−0.017 (3)

Geometric parameters (Å, °)

C1—F1	1.3396 (12)	C8—C9	1.460 (5)
C1—F2	1.3399 (12)	C8—H8	0.9300
C1—F3	1.3400 (12)	C9—C18	1.371 (5)
C1—C2	1.425 (15)	C9—C10	1.414 (5)

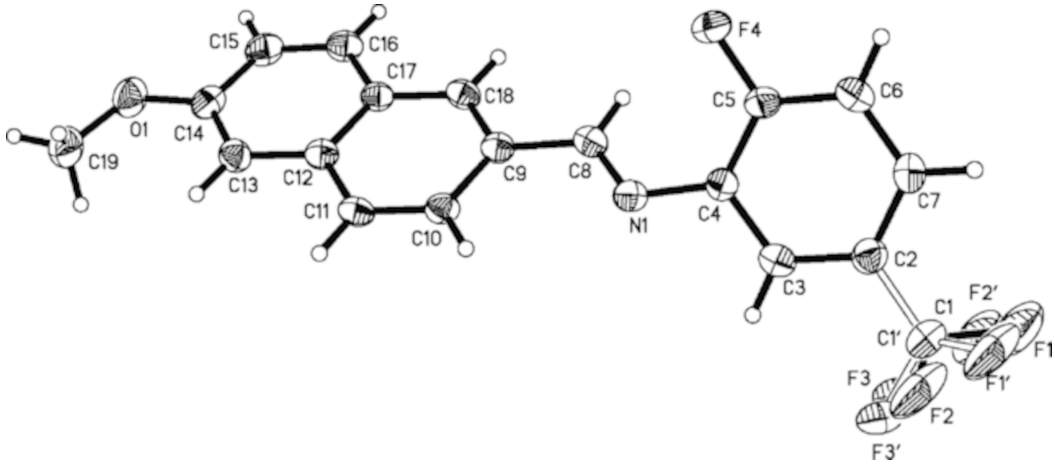
C1'—F2'	1.3395 (13)	C10—C11	1.352 (5)
C1'—F1'	1.3396 (12)	C10—H10	0.9300
C1'—F3'	1.3399 (13)	C11—C12	1.417 (5)
C1'—C2	1.486 (10)	C11—H11	0.9300
F4—C5	1.344 (4)	C12—C13	1.414 (5)
O1—C14	1.352 (5)	C12—C17	1.422 (5)
O1—C19	1.421 (6)	C13—C14	1.368 (5)
N1—C8	1.263 (5)	C13—H13	0.9300
N1—C4	1.404 (5)	C14—C15	1.406 (6)
C2—C3	1.376 (5)	C15—C16	1.352 (6)
C2—C7	1.381 (6)	C15—H15	0.9300
C3—C4	1.388 (5)	C16—C17	1.413 (5)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.386 (5)	C17—C18	1.409 (5)
C5—C6	1.373 (5)	C18—H18	0.9300
C6—C7	1.374 (6)	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—H7	0.9300	C19—H19C	0.9600
F1—C1—F2	104.3 (9)	C9—C8—H8	119.2
F1—C1—F3	103.8 (9)	C18—C9—C10	119.3 (3)
F2—C1—F3	103.0 (9)	C18—C9—C8	119.5 (3)
F1—C1—C2	113.9 (9)	C10—C9—C8	121.2 (3)
F2—C1—C2	114.7 (9)	C11—C10—C9	120.7 (3)
F3—C1—C2	115.7 (10)	C11—C10—H10	119.6
F2'—C1'—F1'	104.8 (5)	C9—C10—H10	119.6
F2'—C1'—F3'	107.1 (6)	C10—C11—C12	121.3 (3)
F1'—C1'—F3'	104.6 (6)	C10—C11—H11	119.3
F2'—C1'—C2	112.3 (5)	C12—C11—H11	119.3
F1'—C1'—C2	113.3 (6)	C13—C12—C11	122.0 (4)
F3'—C1'—C2	113.9 (6)	C13—C12—C17	119.7 (3)
C14—O1—C19	118.0 (4)	C11—C12—C17	118.4 (3)
C8—N1—C4	120.5 (3)	C14—C13—C12	120.0 (4)
C3—C2—C7	120.3 (4)	C14—C13—H13	120.0
C3—C2—C1	116.7 (5)	C12—C13—H13	120.0
C7—C2—C1	122.9 (5)	O1—C14—C13	125.3 (4)
C3—C2—C1'	120.5 (4)	O1—C14—C15	114.8 (4)
C7—C2—C1'	119.3 (4)	C13—C14—C15	119.9 (4)
C1—C2—C1'	5.5 (4)	C16—C15—C14	121.5 (4)
C2—C3—C4	121.4 (4)	C16—C15—H15	119.2
C2—C3—H3	119.3	C14—C15—H15	119.2
C4—C3—H3	119.3	C15—C16—C17	120.4 (4)
C5—C4—C3	116.4 (3)	C15—C16—H16	119.8
C5—C4—N1	125.2 (3)	C17—C16—H16	119.8
C3—C4—N1	118.1 (3)	C18—C17—C16	122.8 (4)
F4—C5—C6	117.9 (3)	C18—C17—C12	118.8 (3)
F4—C5—C4	118.8 (3)	C16—C17—C12	118.4 (3)
C6—C5—C4	123.2 (3)	C9—C18—C17	121.5 (3)
C5—C6—C7	118.8 (4)	C9—C18—H18	119.3
C5—C6—H6	120.6	C17—C18—H18	119.3

C7—C6—H6	120.6	O1—C19—H19A	109.5
C6—C7—C2	119.9 (4)	O1—C19—H19B	109.5
C6—C7—H7	120.1	H19A—C19—H19B	109.5
C2—C7—H7	120.1	O1—C19—H19C	109.5
N1—C8—C9	121.7 (3)	H19A—C19—H19C	109.5
N1—C8—H8	119.2	H19B—C19—H19C	109.5
F1—C1—C2—C3	157.3 (6)	C5—C6—C7—C2	−1.2 (6)
F2—C1—C2—C3	−82.6 (8)	C3—C2—C7—C6	−0.7 (6)
F3—C1—C2—C3	37.1 (8)	C1—C2—C7—C6	−175.6 (5)
F1—C1—C2—C7	−27.6 (8)	C1'—C2—C7—C6	179.5 (4)
F2—C1—C2—C7	92.4 (7)	C4—N1—C8—C9	−174.1 (3)
F3—C1—C2—C7	−147.8 (6)	N1—C8—C9—C18	−174.7 (3)
F1—C1—C2—C1'	23 (4)	N1—C8—C9—C10	6.5 (5)
F2—C1—C2—C1'	143 (5)	C18—C9—C10—C11	−0.9 (5)
F3—C1—C2—C1'	−98 (4)	C8—C9—C10—C11	177.9 (3)
F2'—C1'—C2—C3	−136.8 (5)	C9—C10—C11—C12	0.0 (5)
F1'—C1'—C2—C3	104.7 (5)	C10—C11—C12—C13	−178.6 (3)
F3'—C1'—C2—C3	−14.8 (6)	C10—C11—C12—C17	1.2 (5)
F2'—C1'—C2—C7	42.9 (6)	C11—C12—C13—C14	−179.9 (3)
F1'—C1'—C2—C7	−75.6 (6)	C17—C12—C13—C14	0.3 (5)
F3'—C1'—C2—C7	164.9 (5)	C19—O1—C14—C13	3.1 (6)
F2'—C1'—C2—C1	−89 (4)	C19—O1—C14—C15	−176.9 (4)
F1'—C1'—C2—C1	152 (5)	C12—C13—C14—O1	−178.6 (3)
F3'—C1'—C2—C1	33 (4)	C12—C13—C14—C15	1.3 (6)
C7—C2—C3—C4	1.8 (6)	O1—C14—C15—C16	178.4 (4)
C1—C2—C3—C4	177.0 (5)	C13—C14—C15—C16	−1.6 (6)
C1'—C2—C3—C4	−178.5 (4)	C14—C15—C16—C17	0.1 (6)
C2—C3—C4—C5	−0.8 (5)	C15—C16—C17—C18	−178.6 (4)
C2—C3—C4—N1	−174.5 (3)	C15—C16—C17—C12	1.5 (6)
C8—N1—C4—C5	45.9 (5)	C13—C12—C17—C18	178.4 (3)
C8—N1—C4—C3	−141.0 (4)	C11—C12—C17—C18	−1.4 (5)
C3—C4—C5—F4	−179.0 (3)	C13—C12—C17—C16	−1.8 (5)
N1—C4—C5—F4	−5.8 (5)	C11—C12—C17—C16	178.4 (3)
C3—C4—C5—C6	−1.2 (5)	C10—C9—C18—C17	0.6 (5)
N1—C4—C5—C6	172.1 (4)	C8—C9—C18—C17	−178.2 (3)
F4—C5—C6—C7	−180.0 (3)	C16—C17—C18—C9	−179.3 (3)
C4—C5—C6—C7	2.2 (6)	C12—C17—C18—C9	0.5 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···F3	0.93	2.45	2.737 (14)	98
C8—H8···F4	0.93	2.46	2.835 (4)	104

Fig. 1


C15
C16
C17
C18
F4
C5
C6
O1
C14
C19
C13
C12
C9
C8
C7
C11
N1
C4
C10
C2
C3
C1
F2'
C1'
F1
F3
F1'
F2
F3'