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2-[(*E*)-(Naphthalen-2-ylimino)methyl]-4-(trifluoromethoxy)phenol

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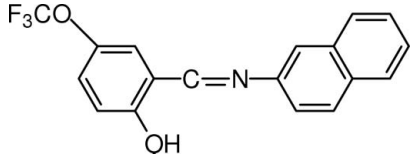
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.130; data-to-parameter ratio = 13.1.

In the title compound, $C_{18}H_{12}F_3NO_2$, the planes of the benzene ring and the naphthalene system form a dihedral angle of 47.21 (3)°. The hydroxy group is involved in an intramolecular O—H···N hydrogen bond. In the crystal, weak C—H···O and C—H···F interactions link the molecules related by translations along the c and a axes, respectively, into sheets.

Related literature

For background to photochromic and thermochromic characteristics and tautomerism of Schiff bases, see: Cohen *et al.* (1964); Hadjoudis *et al.* (1987). For related structures, see: Gül *et al.* (2007); Yüce *et al.* (2004). For classification of hydrogen-bonding patterns, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{18}H_{12}F_3NO_2$
M_r = 331.29
Monoclinic, $P2_1/c$
a = 17.0813 (10) Å
b = 14.1248 (8) Å
c = 6.1900 (5) Å
β = 99.669 (6)°
V = 1472.25 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 123 K
0.50 × 0.40 × 0.18 mm

Data collection

Oxford Diffraction Gemini-R diffractometer
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2007) based on Clark & Reid (1995)
T_{min} = 0.941, T_{max} = 0.978
15270 measured reflections
2892 independent reflections
2497 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.130
S = 1.09
2892 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.90 (3)	1.77 (3)	2.5904 (18)	150 (2)
C10—H10···O1^{i}	0.93	2.57	3.473 (2)	165
C5—H5···F2^{ii}	0.93	2.57	3.487 (2)	170

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2007); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5250).

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supplementary materials

Acta Cryst. (2012). E**68**, o1024 [doi:10.1107/S1600536812009361]

2-[(*E*)-(Naphthalen-2-ylimino)methyl]-4-(trifluoromethoxy)phenol

Merve Pekdemir, Zarife Sibel Şahin, Şamil Işık, Ayşen Alaman Ağar, Sema Öztürk Yıldırım and Ray J. Butcher

Comment

There are two characteristic properties of Schiff bases, *viz*. photochromism and thermochromism (Cohen *et al.*, 1964). These properties result from proton transfer from the hydroxyl O atom to the imine N atom (Hadjoudis *et al.*, 1987). There are two types of intramolecular hydrogen bonds in Schiff bases, which may be stabilized in keto-amine (N—H···O hydrogen bond) or phenol-imine (N···H—O hydrogen bond) tautomeric forms (Hadjoudis *et al.*, 1987). Herewith we present the title compound (I), which exhibits the phenol-imine tautomeric form (Fig. 1).

In (I), the C1—N1 bond length of 1.417 (2) Å agrees with the matching distance in 1-{4-[2-hydroxy-benzyl-idene)amino]phenyl}ethanone [1.4138 (17) Å; Yüce *et al.*, 2004]. The N1═C11 bond length of 1.284 (2) Å is typical of a double bond, like to the matching bond length in (*E*)-2-[(3-trifluoromenthylphenylimino)methyl]-4-methylphenol [1.280 (2) Å; Gül *et al.*, 2007]. The O1—C17 distance of 1.349 (2) Å is similar to the worth of 1.352 (3) Å in (*E*)-2-[(3-trifluoromenthylphenylimino)methyl]-4-methylphenol (Gül *et al.*, 2007). Fig.1 additionally shows a strong intramolecular hyrogen bond (O1—H1···N1) can be defined as an S(6) motif (Bernstein *et al.*, 1995). The O1—N1 distance of 2.590 (2) Å is comparable to those observed for same hydrogen bonds in 1-{4-[(2-hydroxy-benzylidene)amino]phenyl}ethanone [2.594 (2) Å; Yüce *et al.*, 2004].

The molecules are linked into sheets by a combination of C—H···O and C—H···F interactions (Table 1). The atom C10 in the reference molecule at (*x*, *y*, *z*) acts as a hydrogen-bond donor, *via* H10, to atom O1 in the molecule at (*x*, *y*, *z* + 1), so forming a C(8) chain running parallel to the [001] direction. Similarly, atom C5 in the molecule at (*x*, *y*, *z*) acts as a hydrogen-bond donor, *via* H5, to atom F2 in the molecule at (*x* + 1, *y*, *z*), so forming a C(14) chain running parallel to the [100] direction. The combination of the C(8) and C(14) chains generates a chain edge-fused $R_5^5(36)$ rings running parallel to the *ac* plane (Fig.2)

Experimental

The title compound, (I), was prepared by reflux a mixture of a solution containing 2-hydroxy-5-(trifluoromethoxy)-benzaldehyde (0.045 g 0.23 mmol) in 20 ml e thanol and a solution containing 2-Naphthyamine (0.033 g 0.23 mmol) in 20 ml e thanol. The reaction mixture was stirred for 1 hunder reflux. The crystals of (I) suitable for X-ray analysis were obtained from ethylalcohol by slow evaporation (yield % 68; m.p.369–371 K).

Refinement

The H1 atom was located in a difference map, and isotropically refined with restraint of O—H=0.82 (2) Å. All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H=0.93 Å and U_{iso}(H)=1.2U_{eq}(C).

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2007); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

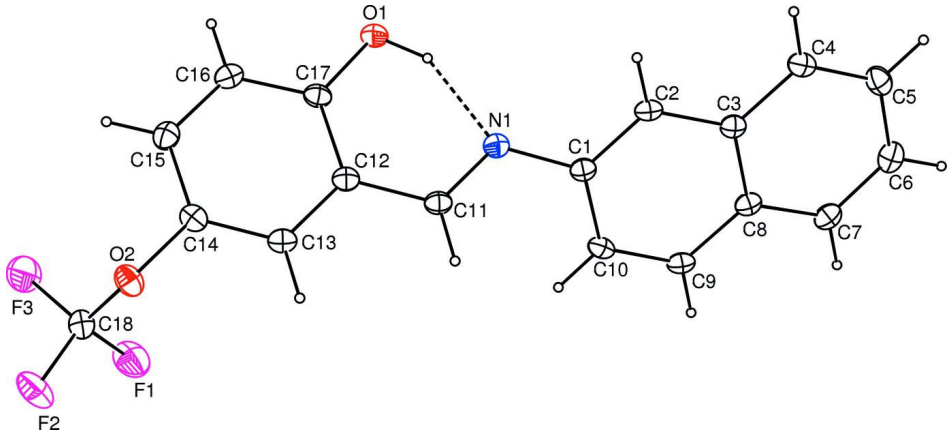

Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability. Dashed line denotes hydrogen bond.

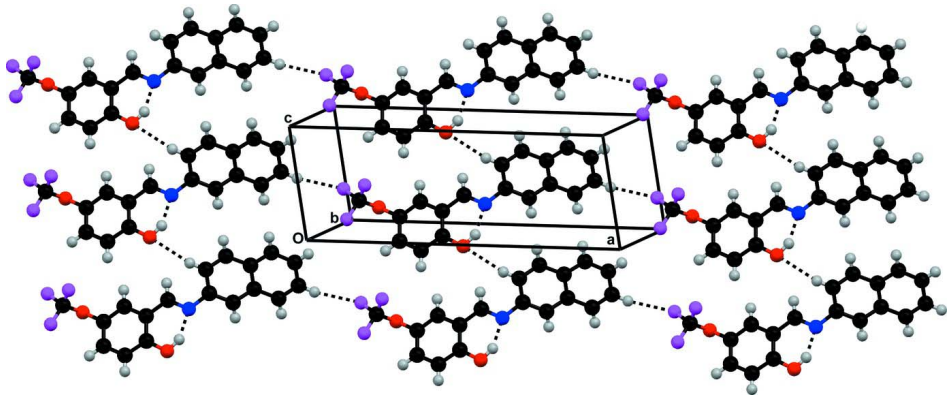

Figure 2

A portion of the crystal packing showing hydrogen bonds as dashed lines.

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Crystal data

$C_{18}H_{12}F_3NO_2$
$M_r = 331.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.0813\ (10)$ Å
$b = 14.1248\ (8)$ Å
$c = 6.1900\ (5)$ Å
$\beta = 99.669\ (6)°$
$V = 1472.25\ (17)$ Å^3
$Z = 4$

$F(000) = 680$
$D_x = 1.495$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5076 reflections
$\theta = 3.1–34.9°$
$\mu = 0.12$ mm^{-1}
$T = 123$ K
Plate, yellow
0.50 × 0.40 × 0.18 mm

Data collection

Oxford Diffraction Gemini-R diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2007) based on Clark & Reid (1995)

T_{min} = 0.941, T_{max} = 0.978
15270 measured reflections
2892 independent reflections
2497 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.0°, θ_{min} = 3.1°
h = −20→21
k = −17→17
l = −7→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.130
S = 1.09
2892 reflections
221 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.5277P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
C1	0.52707 (9)	0.88417 (11)	0.3403 (3)	0.0225 (4)
C2	0.59465 (10)	0.90836 (11)	0.2604 (3)	0.0225 (3)
H2	0.5903	0.9338	0.1203	0.027*
C3	0.67071 (9)	0.89512 (10)	0.3876 (3)	0.0222 (3)
C4	0.74184 (10)	0.91509 (11)	0.3061 (3)	0.0268 (4)
H4	0.7390	0.9413	0.1672	0.032*
C5	0.81420 (10)	0.89635 (12)	0.4287 (3)	0.0313 (4)
H5	0.8601	0.9103	0.3729	0.038*
C6	0.82014 (11)	0.85608 (12)	0.6391 (3)	0.0320 (4)
H6	0.8698	0.8424	0.7201	0.038*
C7	0.75296 (10)	0.83705 (11)	0.7244 (3)	0.0275 (4)
H7	0.7573	0.8114	0.8642	0.033*
C8	0.67680 (10)	0.85604 (11)	0.6021 (3)	0.0232 (4)
C9	0.60574 (10)	0.83457 (11)	0.6822 (3)	0.0246 (4)
H9	0.6089	0.8110	0.8237	0.029*
C10	0.53290 (10)	0.84767 (11)	0.5564 (3)	0.0244 (4)

H10	0.4871	0.8327	0.6121	0.029*
C11	0.38798 (10)	0.90319 (11)	0.2662 (3)	0.0241 (4)
H11	0.3894	0.9215	0.4112	0.029*
C12	0.31186 (10)	0.89349 (11)	0.1221 (3)	0.0236 (4)
C13	0.24206 (10)	0.92206 (11)	0.1940 (3)	0.0246 (4)
H13	0.2443	0.9475	0.3334	0.030*
C14	0.17025 (10)	0.91238 (11)	0.0580 (3)	0.0265 (4)
C15	0.16428 (10)	0.87238 (12)	−0.1487 (3)	0.0285 (4)
H15	0.1150	0.8661	−0.2381	0.034*
C16	0.23260 (10)	0.84183 (12)	−0.2206 (3)	0.0279 (4)
H16	0.2290	0.8130	−0.3570	0.034*
C17	0.30663 (10)	0.85398 (11)	−0.0901 (3)	0.0248 (4)
C18	0.05121 (10)	0.89134 (14)	0.1960 (3)	0.0335 (4)
F1	0.08590 (7)	0.83013 (9)	0.3436 (2)	0.0551 (4)
F2	−0.00045 (7)	0.94076 (10)	0.2849 (2)	0.0537 (4)
F3	0.01029 (7)	0.84060 (11)	0.0357 (2)	0.0614 (4)
N1	0.45326 (8)	0.88684 (9)	0.1961 (2)	0.0241 (3)
O1	0.37203 (7)	0.82747 (9)	−0.1701 (2)	0.0301 (3)
O2	0.10202 (7)	0.95092 (8)	0.1277 (2)	0.0328 (3)
H1	0.4140 (16)	0.8422 (18)	−0.067 (5)	0.066 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0276 (8)	0.0185 (8)	0.0218 (8)	0.0017 (6)	0.0051 (7)	−0.0016 (6)
C2	0.0325 (9)	0.0176 (7)	0.0184 (8)	0.0003 (6)	0.0072 (7)	0.0002 (6)
C3	0.0282 (8)	0.0162 (7)	0.0228 (8)	0.0003 (6)	0.0060 (7)	−0.0030 (6)
C4	0.0327 (9)	0.0225 (8)	0.0268 (9)	−0.0017 (7)	0.0095 (7)	−0.0011 (7)
C5	0.0279 (9)	0.0273 (9)	0.0402 (10)	−0.0031 (7)	0.0102 (8)	−0.0038 (8)
C6	0.0299 (9)	0.0266 (9)	0.0370 (10)	0.0026 (7)	−0.0018 (8)	−0.0041 (8)
C7	0.0349 (9)	0.0205 (8)	0.0256 (9)	0.0014 (6)	0.0013 (7)	−0.0025 (6)
C8	0.0317 (9)	0.0158 (7)	0.0220 (8)	0.0005 (6)	0.0043 (7)	−0.0026 (6)
C9	0.0345 (9)	0.0215 (8)	0.0185 (8)	0.0009 (6)	0.0070 (7)	0.0011 (6)
C10	0.0282 (8)	0.0223 (8)	0.0253 (9)	−0.0004 (6)	0.0118 (7)	−0.0016 (6)
C11	0.0304 (9)	0.0207 (8)	0.0222 (8)	0.0005 (6)	0.0069 (7)	−0.0012 (6)
C12	0.0292 (8)	0.0191 (8)	0.0231 (8)	−0.0001 (6)	0.0063 (7)	0.0026 (6)
C13	0.0323 (9)	0.0191 (8)	0.0235 (8)	0.0006 (6)	0.0076 (7)	−0.0003 (6)
C14	0.0277 (8)	0.0224 (8)	0.0303 (9)	0.0020 (6)	0.0080 (7)	0.0031 (7)
C15	0.0291 (9)	0.0270 (8)	0.0282 (9)	−0.0026 (7)	0.0014 (7)	0.0036 (7)
C16	0.0350 (9)	0.0264 (8)	0.0221 (8)	−0.0016 (7)	0.0041 (7)	0.0003 (7)
C17	0.0303 (9)	0.0213 (8)	0.0245 (9)	−0.0010 (6)	0.0092 (7)	0.0010 (6)
C18	0.0257 (9)	0.0413 (11)	0.0330 (10)	0.0012 (7)	0.0035 (8)	−0.0022 (8)
F1	0.0503 (7)	0.0630 (8)	0.0554 (8)	0.0110 (6)	0.0188 (6)	0.0264 (6)
F2	0.0386 (7)	0.0587 (8)	0.0701 (9)	0.0065 (5)	0.0274 (6)	−0.0067 (6)
F3	0.0440 (7)	0.0829 (10)	0.0581 (8)	−0.0267 (7)	0.0108 (6)	−0.0259 (7)
N1	0.0275 (7)	0.0215 (7)	0.0236 (7)	−0.0009 (5)	0.0052 (6)	0.0006 (5)
O1	0.0299 (7)	0.0375 (7)	0.0244 (6)	0.0001 (5)	0.0085 (5)	−0.0058 (5)
O2	0.0283 (6)	0.0289 (7)	0.0428 (8)	0.0036 (5)	0.0103 (5)	−0.0008 (5)

Geometric parameters (Å, º)

C1—C2	1.373 (2)	C11—N1	1.284 (2)
C1—N1	1.417 (2)	C11—C12	1.454 (2)
C1—C10	1.421 (2)	C11—H11	0.9300
C2—C3	1.414 (2)	C12—C13	1.400 (2)
C2—H2	0.9300	C12—C17	1.416 (2)
C3—C4	1.420 (2)	C13—C14	1.373 (2)
C3—C8	1.425 (2)	C13—H13	0.9300
C4—C5	1.363 (2)	C14—C15	1.387 (2)
C4—H4	0.9300	C14—O2	1.4176 (19)
C5—C6	1.409 (3)	C15—C16	1.386 (2)
C5—H5	0.9300	C15—H15	0.9300
C6—C7	1.368 (3)	C16—C17	1.392 (2)
C6—H6	0.9300	C16—H16	0.9300
C7—C8	1.416 (2)	C17—O1	1.349 (2)
C7—H7	0.9300	C18—F2	1.316 (2)
C8—C9	1.419 (2)	C18—F1	1.324 (2)
C9—C10	1.365 (2)	C18—F3	1.324 (2)
C9—H9	0.9300	C18—O2	1.328 (2)
C10—H10	0.9300	O1—H1	0.90 (3)
C2—C1—N1	118.63 (14)	N1—C11—C12	120.90 (15)
C2—C1—C10	119.94 (15)	N1—C11—H11	119.5
N1—C1—C10	121.10 (14)	C12—C11—H11	119.5
C1—C2—C3	121.05 (15)	C13—C12—C17	118.92 (15)
C1—C2—H2	119.5	C13—C12—C11	119.96 (15)
C3—C2—H2	119.5	C17—C12—C11	121.11 (15)
C2—C3—C4	122.47 (15)	C14—C13—C12	119.83 (15)
C2—C3—C8	119.10 (14)	C14—C13—H13	120.1
C4—C3—C8	118.35 (15)	C12—C13—H13	120.1
C5—C4—C3	120.90 (16)	C13—C14—C15	121.73 (15)
C5—C4—H4	119.6	C13—C14—O2	118.08 (15)
C3—C4—H4	119.6	C15—C14—O2	120.04 (15)
C4—C5—C6	120.71 (16)	C16—C15—C14	119.18 (16)
C4—C5—H5	119.6	C16—C15—H15	120.4
C6—C5—H5	119.6	C14—C15—H15	120.4
C7—C6—C5	120.07 (16)	C15—C16—C17	120.49 (16)
C7—C6—H6	120.0	C15—C16—H16	119.8
C5—C6—H6	120.0	C17—C16—H16	119.8
C6—C7—C8	120.76 (16)	O1—C17—C16	118.72 (15)
C6—C7—H7	119.6	O1—C17—C12	121.51 (15)
C8—C7—H7	119.6	C16—C17—C12	119.77 (15)
C7—C8—C9	122.39 (15)	F2—C18—F1	108.15 (15)
C7—C8—C3	119.20 (15)	F2—C18—F3	107.09 (14)
C9—C8—C3	118.38 (15)	F1—C18—F3	106.41 (17)
C10—C9—C8	121.55 (15)	F2—C18—O2	108.49 (16)
C10—C9—H9	119.2	F1—C18—O2	113.14 (14)
C8—C9—H9	119.2	F3—C18—O2	113.28 (15)
C9—C10—C1	119.93 (15)	C11—N1—C1	121.55 (14)

C9—C10—H10	120.0	C17—O1—H1	106.7 (17)
C1—C10—H10	120.0	C18—O2—C14	117.93 (13)
N1—C1—C2—C3	−171.57 (13)	C17—C12—C13—C14	−0.7 (2)
C10—C1—C2—C3	1.8 (2)	C11—C12—C13—C14	−179.68 (14)
C1—C2—C3—C4	176.90 (14)	C12—C13—C14—C15	1.8 (2)
C1—C2—C3—C8	0.0 (2)	C12—C13—C14—O2	−173.65 (14)
C2—C3—C4—C5	−176.17 (15)	C13—C14—C15—C16	−0.4 (2)
C8—C3—C4—C5	0.8 (2)	O2—C14—C15—C16	174.97 (14)
C3—C4—C5—C6	0.4 (3)	C14—C15—C16—C17	−2.1 (2)
C4—C5—C6—C7	−1.3 (3)	C15—C16—C17—O1	−176.85 (14)
C5—C6—C7—C8	1.0 (3)	C15—C16—C17—C12	3.2 (2)
C6—C7—C8—C9	178.00 (15)	C13—C12—C17—O1	178.27 (14)
C6—C7—C8—C3	0.2 (2)	C11—C12—C17—O1	−2.7 (2)
C2—C3—C8—C7	175.98 (14)	C13—C12—C17—C16	−1.8 (2)
C4—C3—C8—C7	−1.1 (2)	C11—C12—C17—C16	177.22 (14)
C2—C3—C8—C9	−1.9 (2)	C12—C11—N1—C1	−171.85 (13)
C4—C3—C8—C9	−178.95 (14)	C2—C1—N1—C11	−151.42 (15)
C7—C8—C9—C10	−175.68 (15)	C10—C1—N1—C11	35.3 (2)
C3—C8—C9—C10	2.1 (2)	F2—C18—O2—C14	170.19 (14)
C8—C9—C10—C1	−0.4 (2)	F1—C18—O2—C14	50.2 (2)
C2—C1—C10—C9	−1.6 (2)	F3—C18—O2—C14	−71.0 (2)
N1—C1—C10—C9	171.60 (14)	C13—C14—O2—C18	−105.77 (18)
N1—C11—C12—C13	−172.63 (14)	C15—C14—O2—C18	78.7 (2)
N1—C11—C12—C17	8.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.90 (3)	1.77 (3)	2.5904 (18)	150 (2)
C10—H10···O1^{i}	0.93	2.57	3.473 (2)	165
C5—H5···F2^{ii}	0.93	2.57	3.487 (2)	170

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) *x*+1, *y*, *z*.