Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 5-methoxy-2-trifluoromethyl-1*H*-indole-3-carboxylate

Aurelien Crochet,[a]* Isak Alimi,[b] Christian G. Bochet[b] and Katharina M. Fromm[b]

[a]Fribourg Center for Nanomaterials, FriMat, University of Fribourg, Chemin du Musee 3, CH-1700 Fribourg, Switzerland, and [b]Chemistry Department, University of Fribourg, Chemin du Musee 9, CH-1700 Fribourg, Switzerland
Correspondence e-mail: aurelien.crochet@unifr.ch

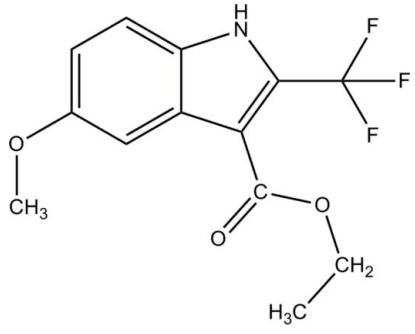
Received 16 January 2013; accepted 25 January 2013

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 11.5.

The title compound, $C_{13}H_{12}F_3NO_3$, is almost planar if one excludes the F atoms of the –CF_3 group [maximum deviation for the other hetero atoms = 0.069 (1) Å], and the dihedral angle between the pyrrole and benzene ring of the indole system is 2.54 (8)°. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming chains propagating along the *a*-axis direction. These chains are linked *via* C—H···O and C—H···F hydrogen bonds, forming a three-dimensional network.

Related literature

For indoles, see: Kochanowska-Karamyan & Hamann (2010); Debieux & Bochet (2009); Helgen & Bochet (2003); Oppolzer *et al.* (1994), and for their synthesis, see: Chen *et al.* (2008); Barton *et al.* (1977). For photochemical methods for the synthesis of substituted indoles, see: Bochet & Blanc (2010); Bochet & Mercier (2009); Debieux & Bochet (2012); Streit & Bochet (2011); Alimi & Bochet (2013).



Experimental

Crystal data

$C_{13}H_{12}F_3NO_3$
M_r = 287.24
Orthorhombic, *Pbca*
a = 13.9211 (8) Å
b = 8.6383 (4) Å
c = 21.5316 (7) Å
V = 2589.3 (2) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 200 K
0.74 × 0.39 × 0.14 mm

Data collection

Stoe IPDS 2T diffractometer
Absorption correction: integration (*X-SHAPE*; Stoe & Cie, 2001)
T_{min} = 0.610, T_{max} = 0.850
15525 measured reflections
2130 independent reflections
1894 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.09
2130 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.835 (19)	2.109 (19)	2.8623 (16)	149.8 (16)
C6—H6···O3^{ii}	0.95	2.53	3.460 (2)	168
C11—H11*B*···F2^{iii}	0.99	2.50	3.336 (2)	142

Symmetry codes: (i) $x+\frac{1}{2}, y, -z+\frac{1}{2}$; (ii) $-x+2, -y+2, -z+1$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors thank the Swiss National Science Foundation and the Fribourg Center for Nanomaterials (FriMat) for generous support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2553).

References

Alimi, I. & Bochet, C. G. (2013). Unpublished data.
Barton, D. H. R., Hesse, R. H., Jackman, G. P. & Pechet, M. M. (1977). *J. Chem. Soc. Perkin Trans. 1*, pp. 2604–2608.
Bochet, C. G. & Blanc, A. (2010). In *Handbook of Synthetic Photochemistry*, edited by A. Albini & M. Fagnoni, pp. 417–447. Weinheim: Wiley-VCH.
Bochet, C. G. & Mercier, S. (2009). In *Linker Strategies in Solid-Phase Organic Synthesis*, edited by P. Scott, pp. 151–193. New York: John Wiley.
Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Chen, Y., Wang, Y., Sun, Z. & Ma, D. (2008). *Org. Lett.* **4**, 625-628.
Debieux, J.-L. & Bochet, C. G. (2009). *J. Org. Chem.***74**, 4519–4524.
Debieux, J.-L. & Bochet, C. G. (2012). *Chem. Sci.* **3**, 405–406.
Helgen, C. & Bochet, C. G. (2003). *J. Org. Chem.* **68**, 2483–2486.
Kochanowska-Karamyan, A. J. & Hamann, M. T. (2010). *Chem. Rev.* **110**, 4489–4497.
Oppolzer, W., Spivey, A. C. & Bochet, C. G. (1994). *J. Am. Chem. Soc.* **116**, 3139–3140.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2001). *X-AREA*, *X-RED32* and *X-SHAPE*. Stoe & Cie GmbH, Darmstadt, Germany.
Streit, U. & Bochet, C. G. (2011). *Beilstein J. Org. Chem.* **7**, 525–542.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2013). E**69**, o339 [doi:10.1107/S1600536813002614]

Ethyl 5-methoxy-2-trifluoromethyl-1*H*-indole-3-carboxylate

Aurelien Crochet, Isak Alimi, Christian G. Bochet and Katharina M. Fromm

Comment

Indoles exhibit a plethora of biological applications (Kochanowska-Karamyan & Hamann, 2010), and a wide range of synthetic methods have been developed to synthesize them (Chen *et al.*, 2008; Barton *et al.*, 1977). Recently an efficient photochemical method for the synthesis of substituted indoles, based on a [3 + 2] cycloaddition of azide and alcynes, has been developed (Alimi & Bochet, 2013). During this work the title compound was synthesized and we report herein on its crystal structure.

The molecular structure of the title molecule is illustrated in Fig. 1. The molecule is almost planar [mean deviation for atoms (O1-O3,N1,C1-C8,C10-C13) is 0.069 (1) Å] with small deviations for the C9, CF_3 group. The dihedral angle between the pyrrole (N1/C1-C3/C8) and the benzene (C3-C8) ring is only 2.54 (8)°.

In the crystal, N-H···O hydrogen bonds link the molecules to form chains propagating along the a axis direction (Table 1 and Fig. 2). These chains are linked via C-H···O and C-H···F hydrogen bonds forming a three-dimensional network (Table 1 and Fig. 3).

Experimental

Ethyl 1-(4-methoxyphenyl)-5-(trifluoromethyl)-1*H*-1,2,3-triazole-4-carboxylate (101.7 g, 323 mmol) was dissolved in MeCN (15 ml) and irradiated during 10 h at 254 nm. The solution was concentrated *in vacuo* and purified with flash chromatography (Pentane: EtOAc, 4:1) to afford the title compound as a white solid [60.5 g, 211 mmol, 65.3% yield; M.p. 416 - 419 K; HRMS 310.0662 ($C_{13}H_{12}F_3NO_3 + Na^+$; calcd. 310.0661]. The compound was recrystallized from chloroform to afford colourless block-like crystals suitable for X-ray analysis. Spectroscopic and other analytical data for the title compound are available in the archived CIF.

Refinement

The NH H-atom was located in a difference Fourier map and refined with $U_{iso}(H) = 1.2U_{eq}(N)$. The C-bound H-atoms were included in calculated positions and treated as riding atoms: C-H = 0.93, 0.97 and 0.96 Å for CH, CH_2 and CH_3 H-atoms, respectively, with $U_{iso}(H) = k \times U_{eq}$(parent C-atom), where k = 1.5 for CH_3 H-atoms and = 1.2 for other H-atoms.

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA* (Stoe & Cie, 2001); data reduction: *X-RED32* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

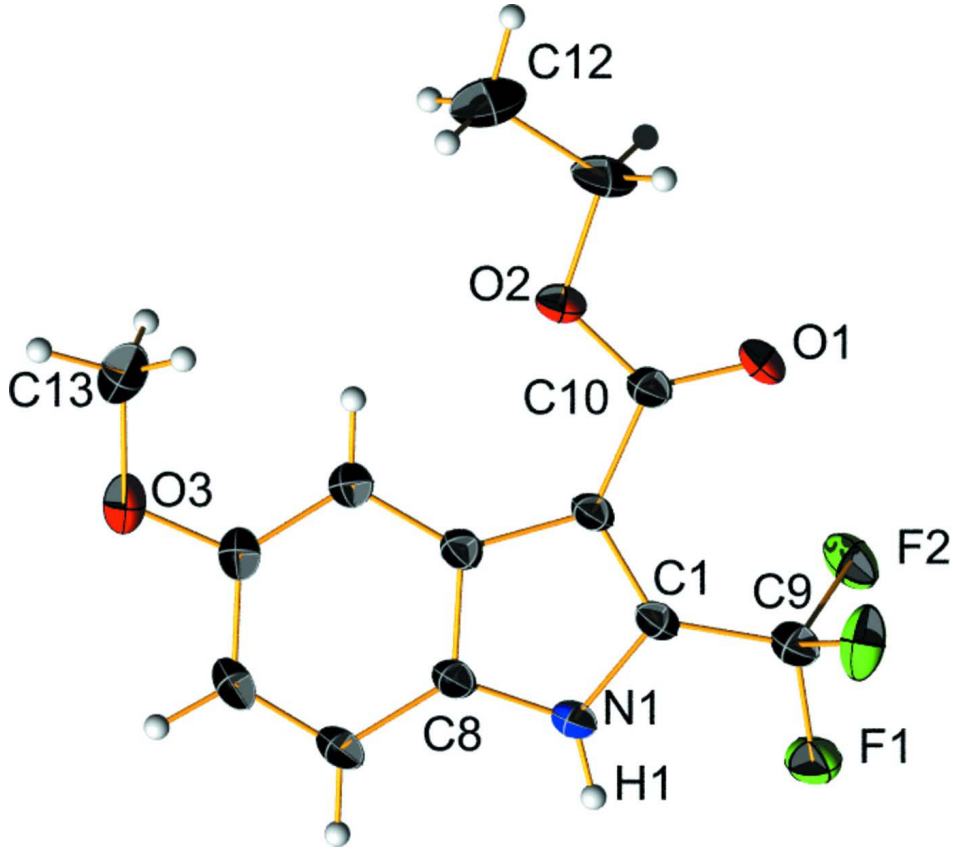


Figure 1

A view of the molecular structure of the title molecule, with atom labelling. The displacement ellipsoids are drawn at the 50% probability level.

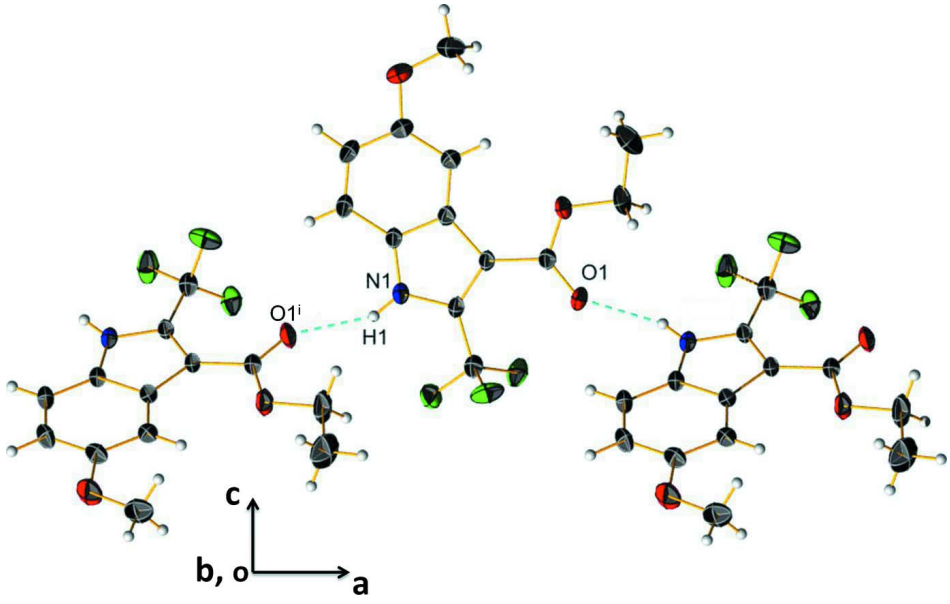


Figure 2

A view normal to the ac plane showing the N-H···O hydrogen bonded (dashed lines) chains propagating along the a axis direction in the crystal structure of the title compound [symmetry code: (i) x+1/2, y, -z+1/2; see Table 1 for details].

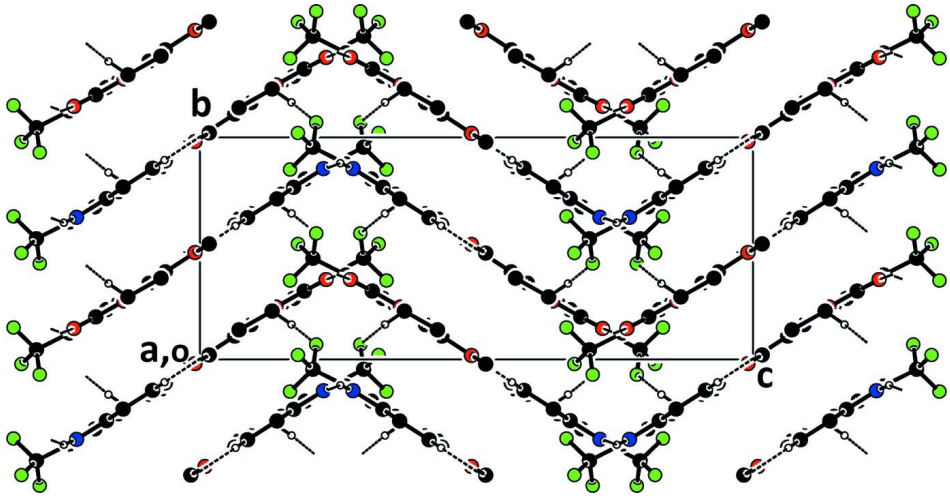


Figure 3

A view along the a axis of the crystal packing of the title compound. H atoms not involved in the C-H···O and C-H···F hydrogen bonds (dashed lines; see Table 1 for details) have been omitted for clarity.

Ethyl 5-methoxy-2-trifluoromethyl-1*H*-indole-3-carboxylate

Crystal data

$C_{13}H_{12}F_3NO_3$
M_r = 287.24
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 13.9211 (8) Å
b = 8.6383 (4) Å
c = 21.5316 (7) Å
V = 2589.3 (2) Å^3
Z = 8
F(000) = 1184
D_x = 1.474 Mg m^{-3}
Melting point: 416 K
Cu *Kα* radiation, *λ* = 1.54186 Å
Cell parameters from 35241 reflections

θ = 3.2–67.3°
μ = 1.16 mm^{-1}
T = 200 K

Block, colourless
0.74 × 0.39 × 0.14 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-SHAPE*; Stoe & Cie, 2001)
T_{min} = 0.610, T_{max} = 0.850

15525 measured reflections
2130 independent reflections
1894 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 65.0°, θ_{min} = 6.4°
h = −16→16
k = −9→9
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.09
2130 reflections
186 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
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 1.0298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Experimental. Spectroscopic data for the title compound: ^{1}H NMR (360 MHz, $CDCl_3$) δ p.p.m. 8.88 (br. s., 1 H) 7.74 (s, 1 H) 7.36 (d, J = 8.63 Hz, 1 H) 7.05 (d, J = 9.08 Hz, 1 H) 4.44 (q, J = 6.96 Hz, 2 H) 3.90 (s, 3 H) 1.44 (t, J = 7.04 Hz, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$) d p.p.m. 163.48, 156.43, 129.48, 128.97, 128.84, 128.45, 127.94, 127.62, 125.75, 122.17, 118.60, 116.85, 115.03, 112.92, 107.77 (d, J=2.20 Hz, 1 C) 102.90, 60.57, 55.58, 14.05. IR (neat, cm^{-1}) 3280, 2995, 2833, 1681, 1550, 1467, 1439, 1309, 1209, 1166, 1154, 1112, 1032, 845, 824, 713, 637. Rf 0.42 (Pentane: EtOAc 4:1).

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2$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}
F1	0.83489 (7)	0.47973 (13)	0.17707 (5)	0.0429 (3)
F2	0.69256 (7)	0.43215 (11)	0.21010 (5)	0.0352 (3)
F3	0.72136 (8)	0.64436 (11)	0.16278 (4)	0.0399 (3)
O1	0.57084 (7)	0.64000 (15)	0.27202 (5)	0.0348 (4)
O2	0.59337 (7)	0.76352 (14)	0.36252 (5)	0.0342 (4)
O3	0.86605 (9)	0.98158 (18)	0.49087 (5)	0.0471 (5)
N1	0.87955 (9)	0.64042 (15)	0.27672 (6)	0.0241 (4)
C1	0.78495 (10)	0.61930 (17)	0.26378 (7)	0.0209 (4)
C2	0.72915 (10)	0.68707 (17)	0.30968 (6)	0.0210 (4)

C3	0.79547 (10)	0.75592 (18)	0.35320 (6)	0.0223 (4)
C4	0.78425 (11)	0.8434 (2)	0.40791 (7)	0.0281 (5)
C5	0.86630 (12)	0.8946 (2)	0.43723 (7)	0.0327 (5)
C6	0.95870 (12)	0.8613 (2)	0.41420 (8)	0.0377 (6)
C7	0.97083 (11)	0.7768 (2)	0.36098 (7)	0.0329 (5)
C8	0.88812 (10)	0.72466 (18)	0.33081 (7)	0.0240 (4)
C9	0.75746 (11)	0.54400 (17)	0.20418 (7)	0.0249 (4)
C10	0.62433 (10)	0.69181 (18)	0.31147 (7)	0.0243 (4)
C11	0.49061 (12)	0.7820 (3)	0.36956 (9)	0.0467 (7)
C12	0.47534 (15)	0.8662 (3)	0.42942 (11)	0.0636 (9)
C13	0.77531 (14)	1.0206 (3)	0.51655 (8)	0.0439 (6)
H1	0.9254 (14)	0.616 (2)	0.2537 (8)	0.0290*
H4	0.72230	0.86620	0.42400	0.0340*
H6	1.01350	0.89810	0.43590	0.0450*
H7	1.03300	0.75450	0.34520	0.0390*
H11A	0.45860	0.67970	0.37070	0.0560*
H11B	0.46390	0.84220	0.33450	0.0560*
H12A	0.50170	0.80480	0.46370	0.0950*
H12B	0.40640	0.88220	0.43600	0.0950*
H12C	0.50790	0.96660	0.42770	0.0950*
H13A	0.73750	1.07770	0.48570	0.0660*
H13B	0.78460	1.08520	0.55350	0.0660*
H13C	0.74110	0.92570	0.52820	0.0660*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0257 (5)	0.0536 (7)	0.0493 (6)	0.0019 (5)	0.0055 (4)	−0.0246 (5)
F2	0.0295 (5)	0.0287 (5)	0.0473 (6)	−0.0098 (4)	−0.0046 (4)	−0.0037 (4)
F3	0.0607 (7)	0.0331 (6)	0.0260 (5)	0.0016 (5)	−0.0127 (4)	0.0004 (4)
O1	0.0156 (5)	0.0566 (8)	0.0322 (6)	0.0001 (5)	−0.0052 (4)	−0.0080 (5)
O2	0.0154 (6)	0.0534 (7)	0.0339 (6)	0.0031 (5)	0.0021 (4)	−0.0119 (5)
O3	0.0381 (7)	0.0734 (10)	0.0299 (6)	−0.0043 (7)	−0.0059 (5)	−0.0191 (6)
N1	0.0140 (6)	0.0334 (7)	0.0249 (6)	0.0002 (5)	0.0015 (5)	−0.0004 (5)
C1	0.0145 (7)	0.0239 (8)	0.0242 (7)	−0.0004 (5)	−0.0021 (5)	0.0027 (6)
C2	0.0136 (7)	0.0270 (8)	0.0225 (7)	−0.0008 (6)	−0.0015 (5)	0.0030 (6)
C3	0.0176 (7)	0.0288 (8)	0.0204 (7)	−0.0012 (6)	−0.0018 (5)	0.0039 (6)
C4	0.0224 (8)	0.0403 (9)	0.0217 (7)	−0.0007 (7)	−0.0007 (6)	0.0009 (7)
C5	0.0294 (9)	0.0460 (10)	0.0227 (8)	−0.0045 (7)	−0.0047 (6)	−0.0033 (7)
C6	0.0233 (8)	0.0581 (12)	0.0318 (9)	−0.0098 (8)	−0.0086 (7)	−0.0034 (8)
C7	0.0167 (8)	0.0507 (11)	0.0313 (8)	−0.0062 (7)	−0.0029 (6)	0.0010 (7)
C8	0.0152 (7)	0.0338 (9)	0.0230 (7)	−0.0020 (6)	−0.0007 (6)	0.0025 (6)
C9	0.0197 (7)	0.0239 (8)	0.0310 (8)	0.0006 (6)	−0.0004 (6)	−0.0006 (6)
C10	0.0165 (7)	0.0326 (9)	0.0237 (7)	0.0008 (6)	−0.0002 (6)	0.0016 (6)
C11	0.0165 (8)	0.0685 (14)	0.0552 (12)	0.0071 (8)	0.0061 (7)	−0.0133 (10)
C12	0.0418 (12)	0.0882 (18)	0.0607 (14)	0.0105 (11)	0.0208 (10)	−0.0212 (12)
C13	0.0476 (11)	0.0566 (12)	0.0274 (9)	0.0025 (9)	0.0004 (7)	−0.0096 (8)

Geometric parameters (Å, º)

F1—C9	1.3457 (18)	C4—C5	1.378 (2)
F2—C9	1.3289 (18)	C5—C6	1.408 (2)
F3—C9	1.3412 (18)	C6—C7	1.369 (2)
O1—C10	1.2150 (18)	C7—C8	1.397 (2)
O2—C10	1.3333 (19)	C11—C12	1.495 (3)
O2—C11	1.447 (2)	C4—H4	0.9500
O3—C5	1.378 (2)	C6—H6	0.9500
O3—C13	1.420 (2)	C7—H7	0.9500
N1—C1	1.3584 (19)	C11—H11A	0.9900
N1—C8	1.379 (2)	C11—H11B	0.9900
N1—H1	0.835 (19)	C12—H12A	0.9800
C1—C2	1.387 (2)	C12—H12B	0.9800
C1—C9	1.489 (2)	C12—H12C	0.9800
C2—C3	1.4437 (19)	C13—H13A	0.9800
C2—C10	1.460 (2)	C13—H13B	0.9800
C3—C8	1.403 (2)	C13—H13C	0.9800
C3—C4	1.408 (2)		
C10—O2—C11	117.20 (13)	F2—C9—C1	114.19 (13)
C5—O3—C13	117.27 (14)	O1—C10—O2	123.32 (13)
C1—N1—C8	109.15 (12)	O1—C10—C2	125.71 (14)
C8—N1—H1	124.7 (13)	O2—C10—C2	110.97 (12)
C1—N1—H1	125.8 (13)	O2—C11—C12	106.53 (15)
N1—C1—C9	118.99 (13)	C3—C4—H4	121.00
C2—C1—C9	130.91 (13)	C5—C4—H4	121.00
N1—C1—C2	109.89 (13)	C5—C6—H6	119.00
C3—C2—C10	127.62 (13)	C7—C6—H6	119.00
C1—C2—C3	106.16 (12)	C6—C7—H7	121.00
C1—C2—C10	126.19 (13)	C8—C7—H7	121.00
C4—C3—C8	119.51 (13)	O2—C11—H11A	110.00
C2—C3—C4	133.88 (13)	O2—C11—H11B	110.00
C2—C3—C8	106.59 (12)	C12—C11—H11A	110.00
C3—C4—C5	117.62 (14)	C12—C11—H11B	110.00
C4—C5—C6	122.02 (15)	H11A—C11—H11B	109.00
O3—C5—C4	123.85 (15)	C11—C12—H12A	109.00
O3—C5—C6	114.13 (14)	C11—C12—H12B	109.00
C5—C6—C7	121.08 (15)	C11—C12—H12C	109.00
C6—C7—C8	117.36 (14)	H12A—C12—H12B	110.00
N1—C8—C7	129.39 (13)	H12A—C12—H12C	110.00
C3—C8—C7	122.41 (14)	H12B—C12—H12C	110.00
N1—C8—C3	108.20 (12)	O3—C13—H13A	109.00
F1—C9—C1	110.38 (12)	O3—C13—H13B	110.00
F1—C9—F2	106.63 (12)	O3—C13—H13C	109.00
F1—C9—F3	106.17 (12)	H13A—C13—H13B	110.00
F3—C9—C1	112.76 (12)	H13A—C13—H13C	109.00
F2—C9—F3	106.20 (12)	H13B—C13—H13C	109.00
C11—O2—C10—O1	−1.4 (2)	C1—C2—C3—C8	−0.23 (16)

C11—O2—C10—C2	177.83 (15)	C10—C2—C3—C4	0.3 (3)
C10—O2—C11—C12	−179.41 (16)	C10—C2—C3—C8	−178.02 (14)
C13—O3—C5—C4	−0.5 (3)	C1—C2—C10—O1	−1.9 (3)
C13—O3—C5—C6	179.56 (16)	C1—C2—C10—O2	178.96 (14)
C8—N1—C1—C2	−0.98 (17)	C3—C2—C10—O1	175.48 (15)
C8—N1—C1—C9	174.28 (13)	C3—C2—C10—O2	−3.7 (2)
C1—N1—C8—C3	0.82 (17)	C2—C3—C4—C5	−178.23 (16)
C1—N1—C8—C7	−178.31 (16)	C8—C3—C4—C5	−0.1 (2)
N1—C1—C2—C3	0.74 (17)	C2—C3—C8—N1	−0.35 (17)
N1—C1—C2—C10	178.57 (14)	C2—C3—C8—C7	178.85 (14)
C9—C1—C2—C3	−173.78 (15)	C4—C3—C8—N1	−178.96 (14)
C9—C1—C2—C10	4.1 (3)	C4—C3—C8—C7	0.2 (2)
N1—C1—C9—F1	12.34 (19)	C3—C4—C5—O3	179.75 (15)
N1—C1—C9—F2	132.45 (14)	C3—C4—C5—C6	−0.3 (2)
N1—C1—C9—F3	−106.22 (16)	O3—C5—C6—C7	−179.55 (16)
C2—C1—C9—F1	−173.56 (15)	C4—C5—C6—C7	0.5 (3)
C2—C1—C9—F2	−53.5 (2)	C5—C6—C7—C8	−0.3 (2)
C2—C1—C9—F3	67.9 (2)	C6—C7—C8—N1	178.97 (16)
C1—C2—C3—C4	178.10 (17)	C6—C7—C8—C3	−0.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.835 (19)	2.109 (19)	2.8623 (16)	149.8 (16)
C6—H6···O3^{ii}	0.95	2.53	3.460 (2)	168
C11—H11*B*···F2^{iii}	0.99	2.50	3.336 (2)	142

Symmetry codes: (i) *x*+1/2, *y*, −*z*+1/2; (ii) −*x*+2, −*y*+2, −*z*+1; (iii) −*x*+1, *y*+1/2, −*z*+1/2.