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2-(1*H*-Imidazol-1-yl)-4-[3-(trifluoromethyl)phenyl]-1,3-thiazole

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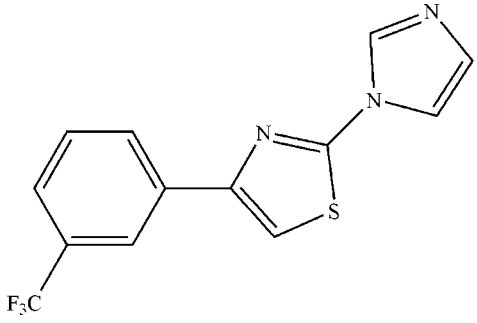
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.103; data-to-parameter ratio = 12.8.

The title compound, $C_{13}H_8F_3N_3S$, consists of three linked aromatic rings. The whole molecule (except for the three F atoms) is planar to within 0.225 (2) Å. In the crystal, adjacent molecules are linked into chains along the *ac* diagonal by weak C—H···N interactions.

Related literature

For general background to the synthesis of imidazolothiazoles by copper-catalysed coupling, see: Zhu *et al.* (2007).



Experimental

Crystal data

$C_{13}H_8F_3N_3S$
M_r = 295.28
Monoclinic, $P2_1/c$
a = 8.4152 (7) Å
b = 19.2403 (15) Å
c = 8.4105 (7) Å
β = 114.210 (1)°
V = 1241.98 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 150 K
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.893, T_{max} = 0.972
9797 measured reflections
2716 independent reflections
2164 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 1.07
2716 reflections
213 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···N3^{i}	0.95 (2)	2.34 (2)	3.278 (2)	169.4 (18)

Symmetry code: (i) $x+1, y, z+1$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: FF2095).

References

Bruker (2008). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhu, L., Guo, P., Li, G., Lan, J., Xie, R. & You, J. (2007). *J. Org. Chem.* **72**, 8535–8538.

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2-(1*H*-Imidazol-1-yl)-4-[3-(trifluoromethyl)phenyl]-1,3-thiazole

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S1. Comment

The title compound, $C_{13}H_8F_3N_3S$, which is a potential anticancer agent, consists of the three linked aromatic and heteroaromatic cycles, which were condensed by copper-catalyzed method (Fig. 1). The whole molecule (except three fluorine atoms) is planar within 0.225 (2) Å (Fig. 2).

In the crystal, the adjacent molecules are combined in chains along *ac*-diagonal by weak C—H···N interactions (Fig. 3). The C···N separation is equal to 3.278 (2) Å and C—H···N angle is close to linear (169 (2) °).

S2. Experimental

2-Bromo-4-(3-(trifluoromethyl)phenyl)thiazole (0.800 g, 2.60 mmol) was added to a stirred suspension of imidazole (0.345 g, 5.07 mmol), CuI (0.209 g, 1.10 mmol) and Cs_2CO_3 (1.830 g, 5.62 mmol) in 30 ml of DMF under argon atmosphere. The reaction mixture was stirred for 8 h at rt and then for 7 h at 115 °C. After cooling to the ambient temperature the reaction mixture was filtered and precipitate was washed with 30 ml of DMF. The solution was concentrated under vacuum and residue was diluted with 80 ml of ethyl acetate. Organic phase was washed with water (2 *x* 10 ml) and saturated solution of NH_4Cl (1 *x* 10 ml), dried over Na_2SO_4, concentrated and purified by column chromatography on silica gel 60 (particle size 0.040–0.063 mm) using $CHCl_3$—MeOH (gradient from 1:0 to 50:1) as eluent. 2-(1*H*-Imidazol-1-yl)-4-(3-(trifluoromethyl)phenyl)thiazole, yield 368 mg (48%), yellowish crystals, mp 99–100°C. ^{1}H NMR (400 MHz, $CDCl_3$/DMSO-d_6 5:1): δ 7.16 (s, 1H), 7.52–7.56 (m, 2H), 7.67 (s, 1H), 7.75 (s, 1H), 8.09–8.11 (m, 1H), 8.15 (s, 1H), 8.40 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$/DMSO-d_6 5:1): δ 111.88, 118.24, 122.95, 122.98, 125.00, 125.03, 129.59, 129.66, 130.17, 130.62, 134.35, 135.63, 150.89, 157.05. Found, %: C, 52.95; H, 2.69; N, 14.20. $C_{13}H_8F_3N_3S$. Calculated, %: C, 52.88; H, 2.73; N, 14.23. The crystals were obtained by slow evaporation of the $CDCl_3$/DMSO-d_6 (5:1) solution.

S3. Refinement

All hydrogen atoms were located in a difference Fourier map and refined with isotropic thermal parameters.

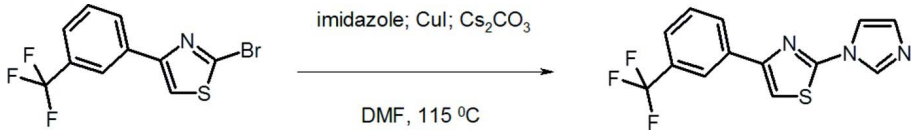

Figure 1

Reaction scheme.

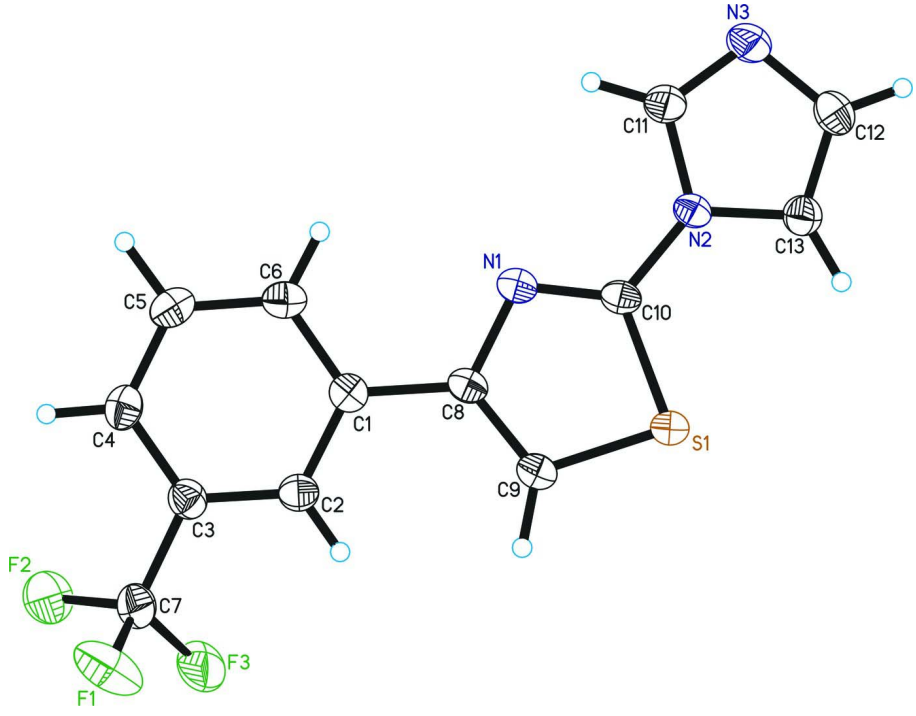

Figure 2

The molecular structure of the title compound, showing the numbering scheme adopted. Displacement ellipsoids are shown at the 50% probability level.

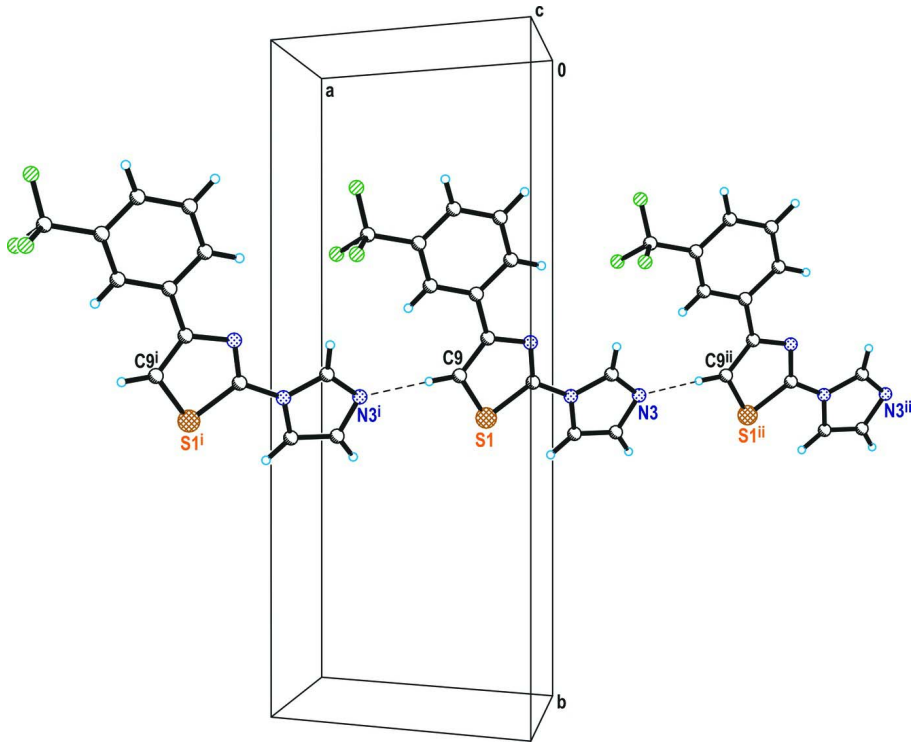

Figure 3

Chains along *ac*-diagonal in the structure of the title compound. C—H···N interactions are shown as dashed lines. [Symmetry codes: (i) 1 + *x*, *y*, 1 + *z*; (ii) -1 + *x*, *y*, -1 + *z*.]

2-(1*H*-Imidazol-1-yl)-4-[3-(trifluoromethyl)phenyl]-1,3-thiazole

Crystal data

$C_{13}H_8F_3N_3S$
$M_r = 295.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.4152\ (7)$ Å
$b = 19.2403\ (15)$ Å
$c = 8.4105\ (7)$ Å
$\beta = 114.210\ (1)°$
$V = 1241.98\ (18)$ Å^3
$Z = 4$
$F(000) = 600$
$D_x = 1.579$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1717 reflections
$\theta = 3.1–24.5°$
$\mu = 0.29$ mm^{-1}
$T = 150$ K
Block, colourless
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.893$, $T_{max} = 0.972$
9797 measured reflections
2716 independent reflections
2164 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.1°$
$h = -10\rightarrow9$
$k = -24\rightarrow24$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.103$
$S = 1.07$
2716 reflections
213 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.2754P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.22949 (6)	0.55985 (2)	0.40649 (6)	0.02492 (15)
N1	0.0577 (2)	0.44567 (7)	0.36963 (19)	0.0214 (3)
N2	−0.0844 (2)	0.52744 (7)	0.14612 (18)	0.0207 (3)
N3	−0.3431 (2)	0.52646 (9)	−0.0761 (2)	0.0306 (4)
F1	0.62622 (19)	0.32402 (8)	1.15343 (17)	0.0571 (4)
F2	0.64762 (19)	0.22590 (6)	1.0452 (2)	0.0571 (4)
F3	0.74065 (16)	0.31841 (7)	0.97113 (19)	0.0530 (4)
C1	0.2432 (2)	0.37530 (9)	0.6250 (2)	0.0215 (4)
C2	0.4056 (3)	0.36375 (10)	0.7611 (2)	0.0234 (4)
C3	0.4358 (3)	0.30371 (9)	0.8600 (2)	0.0250 (4)
C4	0.3055 (3)	0.25486 (10)	0.8277 (3)	0.0277 (4)
C5	0.1440 (3)	0.26582 (10)	0.6924 (3)	0.0288 (5)
C6	0.1129 (3)	0.32528 (10)	0.5908 (3)	0.0256 (4)
C7	0.6105 (3)	0.29265 (10)	1.0058 (3)	0.0331 (5)
C8	0.2102 (2)	0.43953 (9)	0.5201 (2)	0.0204 (4)
C9	0.3176 (3)	0.49573 (9)	0.5588 (2)	0.0240 (4)
C10	0.0540 (2)	0.50577 (9)	0.2999 (2)	0.0205 (4)
C11	−0.2399 (3)	0.49374 (10)	0.0647 (2)	0.0285 (5)
C12	−0.2503 (3)	0.58436 (11)	−0.0854 (3)	0.0286 (4)
C13	−0.0922 (3)	0.58620 (10)	0.0485 (2)	0.0266 (4)
H9	0.425 (3)	0.5042 (10)	0.656 (3)	0.028 (5)*
H6	0.004 (3)	0.3331 (10)	0.496 (3)	0.028 (5)*
H2	0.489 (3)	0.3964 (11)	0.783 (3)	0.031 (6)*
H11	−0.263 (3)	0.4517 (11)	0.113 (3)	0.035 (6)*
H5	0.053 (3)	0.2292 (11)	0.670 (3)	0.040 (6)*

H4	0.328 (3)	0.2144 (11)	0.900 (3)	0.037 (6)*
H12	−0.298 (3)	0.6159 (12)	−0.176 (3)	0.043 (7)*
H13	0.002 (3)	0.6192 (12)	0.080 (3)	0.044 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0198 (3)	0.0248 (2)	0.0255 (3)	−0.00220 (19)	0.00454 (19)	0.00161 (18)
N1	0.0189 (8)	0.0255 (8)	0.0196 (8)	0.0012 (6)	0.0077 (6)	−0.0024 (6)
N2	0.0192 (8)	0.0238 (7)	0.0172 (7)	0.0011 (6)	0.0055 (6)	−0.0012 (6)
N3	0.0268 (9)	0.0364 (9)	0.0214 (8)	−0.0014 (7)	0.0028 (7)	0.0014 (7)
F1	0.0494 (9)	0.0731 (10)	0.0318 (7)	0.0124 (8)	−0.0007 (6)	−0.0037 (7)
F2	0.0446 (9)	0.0321 (7)	0.0713 (10)	0.0094 (6)	0.0003 (7)	0.0201 (6)
F3	0.0223 (7)	0.0689 (10)	0.0589 (9)	0.0053 (6)	0.0076 (6)	0.0279 (7)
C1	0.0230 (10)	0.0223 (9)	0.0209 (9)	0.0020 (7)	0.0107 (8)	−0.0022 (7)
C2	0.0210 (10)	0.0251 (9)	0.0244 (10)	0.0001 (8)	0.0096 (8)	−0.0013 (7)
C3	0.0256 (11)	0.0233 (9)	0.0250 (10)	0.0028 (8)	0.0094 (8)	0.0007 (7)
C4	0.0315 (11)	0.0222 (9)	0.0319 (11)	0.0007 (8)	0.0155 (9)	0.0025 (8)
C5	0.0257 (11)	0.0260 (10)	0.0361 (11)	−0.0043 (8)	0.0142 (9)	−0.0040 (8)
C6	0.0214 (10)	0.0273 (10)	0.0270 (10)	−0.0003 (8)	0.0088 (8)	−0.0046 (8)
C7	0.0315 (12)	0.0276 (10)	0.0357 (12)	0.0029 (9)	0.0092 (9)	0.0084 (8)
C8	0.0176 (9)	0.0250 (9)	0.0186 (9)	0.0028 (7)	0.0074 (7)	−0.0018 (7)
C9	0.0198 (10)	0.0267 (10)	0.0229 (9)	0.0014 (8)	0.0059 (8)	0.0008 (7)
C10	0.0179 (9)	0.0257 (9)	0.0176 (9)	0.0005 (7)	0.0068 (7)	−0.0029 (7)
C11	0.0274 (11)	0.0297 (10)	0.0220 (10)	−0.0044 (8)	0.0037 (8)	−0.0012 (8)
C12	0.0307 (11)	0.0316 (10)	0.0224 (10)	0.0043 (9)	0.0099 (8)	0.0034 (8)
C13	0.0259 (11)	0.0282 (10)	0.0255 (10)	−0.0005 (8)	0.0104 (8)	0.0036 (8)

Geometric parameters (Å, º)

S1—C9	1.7128 (19)	C2—C3	1.385 (3)
S1—C10	1.7266 (18)	C2—H2	0.90 (2)
N1—C10	1.291 (2)	C3—C4	1.384 (3)
N1—C8	1.390 (2)	C3—C7	1.494 (3)
N2—C11	1.367 (2)	C4—C5	1.385 (3)
N2—C13	1.383 (2)	C4—H4	0.96 (2)
N2—C10	1.403 (2)	C5—C6	1.387 (3)
N3—C11	1.307 (2)	C5—H5	1.00 (2)
N3—C12	1.381 (3)	C6—H6	0.95 (2)
F1—C7	1.337 (3)	C8—C9	1.360 (3)
F2—C7	1.331 (2)	C9—H9	0.95 (2)
F3—C7	1.339 (3)	C11—H11	0.96 (2)
C1—C2	1.394 (3)	C12—C13	1.346 (3)
C1—C6	1.397 (3)	C12—H12	0.93 (2)
C1—C8	1.477 (2)	C13—H13	0.96 (2)
C9—S1—C10	88.27 (9)	F2—C7—F1	106.30 (17)
C10—N1—C8	109.34 (15)	F2—C7—F3	106.36 (18)

C11—N2—C13	106.72 (15)	F1—C7—F3	104.87 (18)
C11—N2—C10	125.71 (16)	F2—C7—C3	113.16 (17)
C13—N2—C10	127.57 (16)	F1—C7—C3	112.79 (18)
C11—N3—C12	105.01 (17)	F3—C7—C3	112.71 (17)
C2—C1—C6	118.77 (17)	C9—C8—N1	115.14 (16)
C2—C1—C8	120.30 (17)	C9—C8—C1	125.36 (16)
C6—C1—C8	120.93 (17)	N1—C8—C1	119.50 (16)
C3—C2—C1	120.20 (18)	C8—C9—S1	110.65 (14)
C3—C2—H2	121.4 (13)	C8—C9—H9	130.2 (12)
C1—C2—H2	118.4 (13)	S1—C9—H9	119.0 (12)
C4—C3—C2	120.85 (18)	N1—C10—N2	122.77 (16)
C4—C3—C7	119.88 (17)	N1—C10—S1	116.59 (13)
C2—C3—C7	119.25 (17)	N2—C10—S1	120.64 (13)
C3—C4—C5	119.30 (18)	N3—C11—N2	111.68 (18)
C3—C4—H4	119.6 (14)	N3—C11—H11	128.1 (13)
C5—C4—H4	121.1 (14)	N2—C11—H11	120.2 (13)
C4—C5—C6	120.36 (19)	C13—C12—N3	111.19 (17)
C4—C5—H5	117.8 (13)	C13—C12—H12	128.0 (14)
C6—C5—H5	121.8 (13)	N3—C12—H12	120.8 (14)
C5—C6—C1	120.50 (18)	C12—C13—N2	105.38 (17)
C5—C6—H6	121.5 (12)	C12—C13—H13	131.8 (14)
C1—C6—H6	118.0 (12)	N2—C13—H13	122.8 (14)

C6—C1—C2—C3	−0.1 (3)	C2—C1—C8—N1	170.46 (17)
C8—C1—C2—C3	179.52 (17)	C6—C1—C8—N1	−9.9 (3)
C1—C2—C3—C4	−1.0 (3)	N1—C8—C9—S1	0.5 (2)
C1—C2—C3—C7	−179.66 (18)	C1—C8—C9—S1	−178.79 (15)
C2—C3—C4—C5	1.2 (3)	C10—S1—C9—C8	−0.46 (15)
C7—C3—C4—C5	179.87 (19)	C8—N1—C10—N2	−179.81 (16)
C3—C4—C5—C6	−0.3 (3)	C8—N1—C10—S1	−0.2 (2)
C4—C5—C6—C1	−0.8 (3)	C11—N2—C10—N1	9.5 (3)
C2—C1—C6—C5	1.0 (3)	C13—N2—C10—N1	−171.01 (18)
C8—C1—C6—C5	−178.61 (18)	C11—N2—C10—S1	−170.05 (15)
C4—C3—C7—F2	26.1 (3)	C13—N2—C10—S1	9.4 (3)
C2—C3—C7—F2	−155.26 (19)	C9—S1—C10—N1	0.41 (16)
C4—C3—C7—F1	−94.6 (2)	C9—S1—C10—N2	180.00 (16)
C2—C3—C7—F1	84.0 (2)	C12—N3—C11—N2	−0.4 (2)
C4—C3—C7—F3	146.84 (19)	C13—N2—C11—N3	0.4 (2)
C2—C3—C7—F3	−34.5 (3)	C10—N2—C11—N3	180.00 (17)
C10—N1—C8—C9	−0.2 (2)	C11—N3—C12—C13	0.2 (2)
C10—N1—C8—C1	179.13 (16)	N3—C12—C13—N2	0.0 (2)
C2—C1—C8—C9	−10.3 (3)	C11—N2—C13—C12	−0.3 (2)
C6—C1—C8—C9	169.30 (18)	C10—N2—C13—C12	−179.81 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C9—H9···N3^{i}	0.95 (2)	2.34 (2)	3.278 (2)	169.4 (18)

Symmetry code: (i) $x+1, y, z+1$.