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N,*N*-Bis(2,6-difluorobenzyl)-1,3,4-thiadiazol-2-amine

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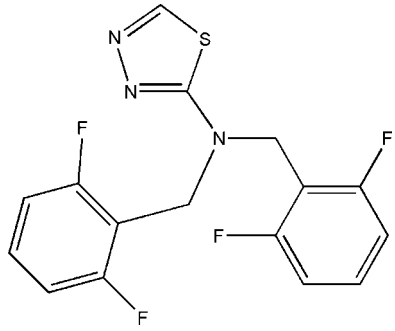
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.076; data-to-parameter ratio = 22.0.

In the title compound, $C_{16}H_{11}F_4N_3S$, the dihedral angles between the thiadiazole ring and the difluorobenzyl rings are 81.95 (7) and 81.96 (7)°, whereas the dihedral angle between the difluorobenzyl rings is 11.41 (7)°. In the crystal structure, C—H···N and C—H···F interactions link the molecules into two-dimensional arrays parallel to the *bc* plane.

Related literature

For the synthesis of pharmaceutically condensed heterocyclic thiadiazole derivatives as antimicrobials, see: Swamy *et al.* (2006). For the synthesis and anti-inflammatory, analgesic, ulcerogenic and lipid peroxidation activity of some new acetic acid derivatives, see: Amir & Shikha (2004). For new bis-aminomercaptotriazoles and bis-triazolothiadiazoles as possible anticancer agents, see: Holla *et al.* (2002). For the synthesis and biological evaluation of thiadiazole derivatives as a novel class of potential anti-tumor agents, see: Ibrahim (2009). For related structures, see: Wang *et al.* (2009*a*,*b*); Yin *et al.* (2008). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{16}H_{11}F_4N_3S$
M_r = 353.34
Orthorhombic, $Pca2_1$
a = 32.6678 (6) Å
b = 5.8515 (1) Å
c = 7.8140 (2) Å
V = 1493.69 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 100 K
0.46 × 0.33 × 0.14 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.887, T_{max} = 0.965
17980 measured reflections
4796 independent reflections
4299 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.076
S = 1.02
4796 reflections
218 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 1935 Friedel pairs
Flack parameter: 0.20 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···N1^{i}	0.93	2.58	3.392 (2)	146
C3—H3B···F3^{ii}	0.97	2.47	3.0226 (16)	116
C8—H8A···F4^{iii}	0.93	2.54	3.144 (2)	123
C10—H10B···N2^{iv}	0.97	2.56	3.4191 (17)	148

Symmetry codes: (i) $-x+\frac{3}{2}, y, z-\frac{1}{2}$; (ii) $x, y+1, z$; (iii) $x, y-1, z+1$; (iv) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2527).

‡ Thomson Reuters ResearcherID: A-3561-2009.

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Acta Cryst. (2009). E**65**, o2166–o2167 [doi:10.1107/S1600536809031675]

N,*N*-Bis(2,6-difluorobenzyl)-1,3,4-thiadiazol-2-amine

Hoong-Kun Fun, Wei-Ching Liew, B. Chandrakantha and Arun M. Isloor

S1. Comment

Heterocycles bearing 1,3,4-thiadiazole moieties represent an interesting class of compounds possessing a wide spectrum of biological activity (Swamy *et al.*, 2006) such as anti-inflammatory, anti-viral and anti-microbial properties (Amir & Shikha, 2004). Recently, 1,3,4-thiadiazoles have attracted particular attention due to their analgesic, ulcerogenic and lipidperoxidation activities (Holla *et al.*, 2002). In particular, the derivatives of variously substituted 1,3,4-thiadiazoles are also known to exhibit anti-depressant and anxiolitic agents (Ibrahim, 2009). Herein, the crystal structure of the title compound (I) is reported.

In (I), Fig. 1, the bond lengths and angles are comparable to related structures (Wang *et al.*, 2009*a* & *b*; Yin *et al.*, 2008). The dihedral angles between the thiadiazole ring (C1—C2/S1/N1—N2) and the difluorobenzyl rings [(C4—C9) and (C11—C16)] are 81.95 (7)° and 81.86 (7)°, respectively whereas the dihedral angle between the difluorobenzyl rings is 11.41 (7)°. These data indicate that all the three rings are twisted from each other.

The crystal packing (Fig. 2) is consolidated by C—H···N and C—H···F interactions (Table 1) that link molecules into two-dimensional arrays parallel to the *bc* plane.

S2. Experimental

Anhydrous potassium carbonate (5.4 g, 0.0395 mol) was added to a solution of 1,3,4-thiadiazole-2-amine (2 g, 0.0197 mol) in dry acetonitrile (25 ml). The reaction mixture was stirred for 15 min. 2,6-Difluorobenzyl bromide (8.18 g, 0.0395 mol) was added drop-wise to the mixture. After addition, the reaction mixture was stirred at room temperature for 18 h, filtered, and the filtrate was concentrated. The crude product was purified by column chromatography using 60–120 silica gel. The fraction eluted with 10% ethyl acetate in hexane was concentrated to produce (I) as a pale-yellow crystalline solid. Yield 5.0 g, 71.63%. *m.p.* 421–423 K.

S3. Refinement

C-bound H atoms were positioned geometrically [C—H = 0.93 and 0.97 Å] and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C).

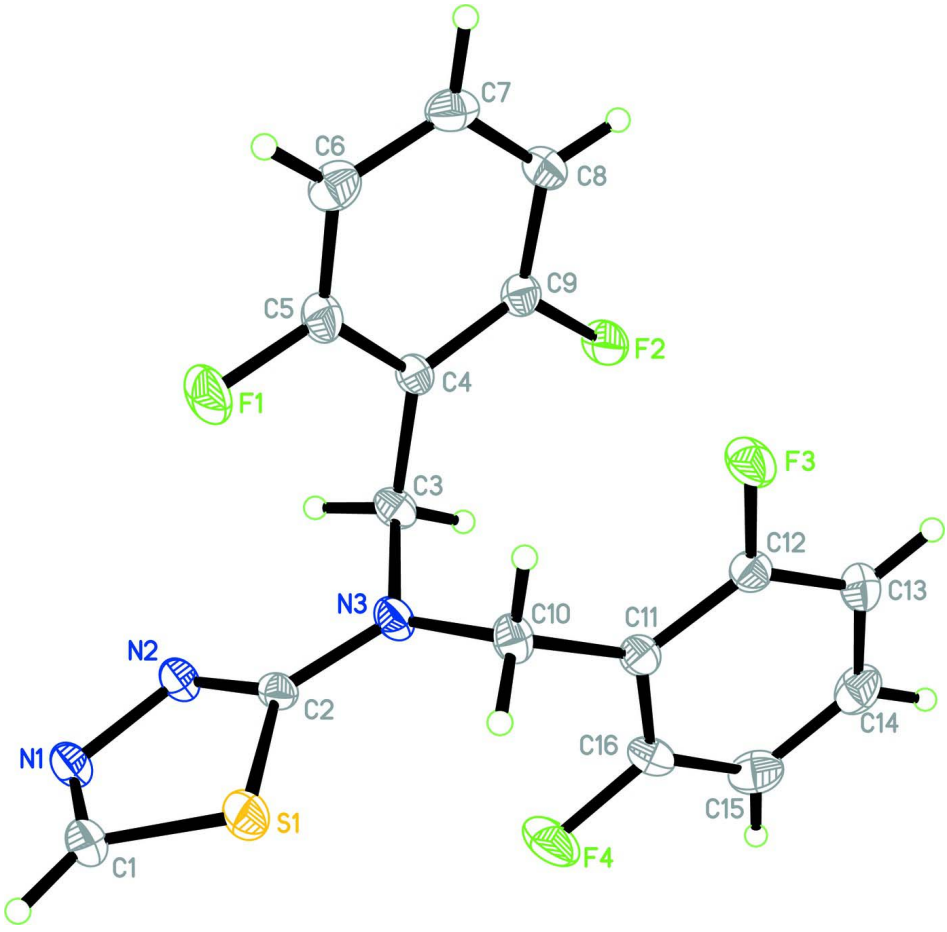

Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom numbering scheme.

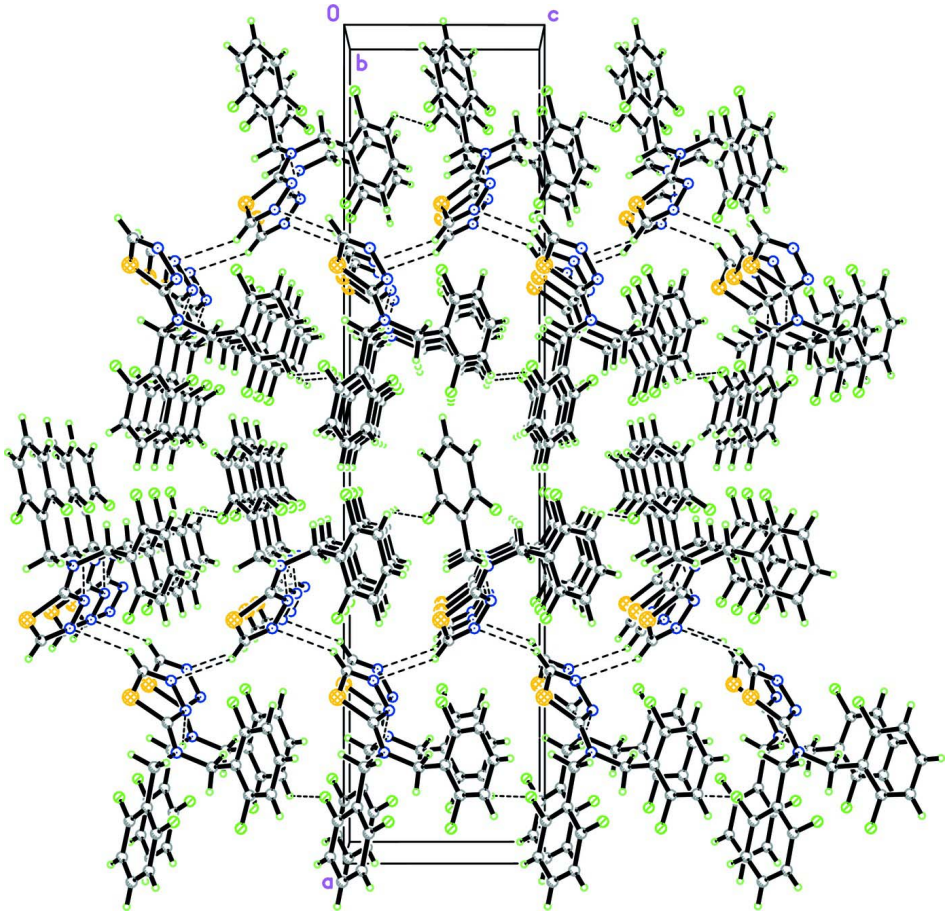

Figure 2

Crystal packing viewed along the *b*-axis. C-H···N and C-H···F interactions are shown as dashed lines.

N,*N*-Bis(2,6-difluorobenzyl)-1,3,4-thiadiazol-2-amine

Crystal data

$C_{16}H_{11}F_4N_3S$
$M_r = 353.34$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 32.6678$ (6) Å
$b = 5.8515$ (1) Å
$c = 7.8140$ (2) Å
$V = 1493.69$ (5) Å^3
$Z = 4$

$F(000) = 720$
$D_x = 1.571$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9387 reflections
$\theta = 2.9$–$33.7°$
$\mu = 0.26$ mm^{-1}
$T = 100$ K
Block, pale-yellow
0.46 × 0.33 × 0.14 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.887$, $T_{max} = 0.965$

17980 measured reflections
4796 independent reflections
4299 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 32.5°$, $\theta_{min} = 2.5°$
$h = -48 \rightarrow 46$
$k = -8 \rightarrow 8$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.076$
$S = 1.02$
4796 reflections
218 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.2893P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Absolute structure: Flack (1983), 1935 Friedel pairs
Absolute structure parameter: 0.20 (5)

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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}
S1	0.794704 (10)	0.52906 (6)	−0.01577 (5)	0.02346 (8)
F1	0.79830 (2)	0.37874 (17)	0.48808 (16)	0.0338 (2)
F2	0.94005 (2)	0.27091 (16)	0.53340 (11)	0.0261 (2)
F3	0.92412 (3)	−0.07230 (15)	0.24104 (14)	0.0264 (2)
F4	0.91204 (3)	0.60294 (17)	−0.07755 (14)	0.0338 (2)
N1	0.78098 (4)	0.8994 (2)	0.14916 (18)	0.0236 (3)
N2	0.81456 (4)	0.8012 (2)	0.22916 (17)	0.0209 (2)
N3	0.85771 (4)	0.4805 (2)	0.21110 (16)	0.0190 (2)
C1	0.76794 (4)	0.7789 (3)	0.0214 (2)	0.0249 (3)
H1A	0.7458	0.8235	−0.0455	0.030*
C2	0.82545 (4)	0.6085 (2)	0.15657 (18)	0.0160 (2)
C3	0.87577 (4)	0.5273 (2)	0.3784 (2)	0.0187 (3)
H3A	0.8637	0.6655	0.4249	0.022*
H3B	0.9049	0.5537	0.3647	0.022*
C4	0.86929 (4)	0.3330 (2)	0.50333 (18)	0.0162 (2)
C5	0.83046 (4)	0.2629 (3)	0.5541 (2)	0.0213 (3)
C6	0.82293 (5)	0.0864 (3)	0.6657 (2)	0.0242 (3)
H6A	0.7963	0.0468	0.6955	0.029*
C7	0.85629 (5)	−0.0312 (3)	0.7328 (2)	0.0238 (3)
H7A	0.8520	−0.1523	0.8078	0.029*
C8	0.89596 (5)	0.0308 (3)	0.68863 (19)	0.0220 (3)

H8A	0.9184	−0.0466	0.7334	0.026*
C9	0.90109 (4)	0.2105 (2)	0.57631 (19)	0.0181 (3)
C10	0.87024 (4)	0.2743 (2)	0.1207 (2)	0.0194 (3)
H10A	0.8557	0.2656	0.0126	0.023*
H10B	0.8627	0.1417	0.1882	0.023*
C11	0.91598 (4)	0.2685 (2)	0.08670 (19)	0.0175 (3)
C12	0.94120 (4)	0.0961 (2)	0.14585 (18)	0.0184 (3)
C13	0.98273 (5)	0.0831 (3)	0.1130 (2)	0.0234 (3)
H13A	0.9984	−0.0374	0.1548	0.028*
C14	1.00032 (4)	0.2553 (3)	0.0158 (2)	0.0260 (3)
H14A	1.0282	0.2512	−0.0072	0.031*
C15	0.97688 (5)	0.4331 (3)	−0.0475 (2)	0.0272 (3)
H15A	0.9886	0.5489	−0.1125	0.033*
C16	0.93555 (4)	0.4336 (2)	−0.0113 (2)	0.0218 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01673 (15)	0.03179 (18)	0.02187 (15)	0.00300 (13)	−0.00547 (14)	−0.00224 (18)
F1	0.0139 (4)	0.0423 (5)	0.0451 (5)	0.0051 (4)	−0.0022 (4)	0.0137 (6)
F2	0.0124 (4)	0.0360 (5)	0.0298 (5)	0.0007 (3)	−0.0012 (3)	0.0101 (4)
F3	0.0237 (4)	0.0208 (4)	0.0345 (5)	0.0013 (3)	0.0037 (4)	0.0108 (4)
F4	0.0341 (5)	0.0282 (5)	0.0390 (5)	0.0040 (4)	−0.0034 (4)	0.0175 (4)
N1	0.0206 (6)	0.0248 (6)	0.0253 (6)	0.0062 (5)	−0.0010 (5)	0.0065 (5)
N2	0.0187 (6)	0.0213 (6)	0.0226 (6)	0.0044 (4)	−0.0020 (5)	0.0032 (5)
N3	0.0181 (5)	0.0192 (5)	0.0196 (5)	0.0039 (4)	−0.0049 (4)	−0.0013 (5)
C1	0.0165 (6)	0.0339 (8)	0.0243 (7)	0.0059 (6)	−0.0018 (5)	0.0044 (6)
C2	0.0127 (6)	0.0192 (6)	0.0161 (5)	−0.0015 (5)	−0.0012 (4)	0.0041 (5)
C3	0.0192 (6)	0.0172 (6)	0.0198 (6)	−0.0007 (5)	−0.0054 (5)	0.0006 (5)
C4	0.0132 (5)	0.0177 (6)	0.0177 (6)	0.0003 (4)	−0.0022 (5)	0.0000 (5)
C5	0.0150 (6)	0.0230 (7)	0.0258 (7)	0.0015 (5)	−0.0015 (5)	0.0003 (6)
C6	0.0199 (7)	0.0277 (8)	0.0250 (7)	−0.0054 (6)	0.0019 (5)	0.0003 (6)
C7	0.0296 (8)	0.0218 (7)	0.0200 (7)	−0.0022 (6)	0.0024 (6)	0.0032 (6)
C8	0.0220 (7)	0.0233 (7)	0.0206 (7)	0.0039 (6)	−0.0031 (5)	0.0030 (6)
C9	0.0141 (6)	0.0208 (6)	0.0193 (6)	−0.0005 (5)	−0.0004 (5)	0.0001 (5)
C10	0.0167 (6)	0.0180 (6)	0.0235 (7)	0.0011 (5)	−0.0027 (5)	−0.0023 (6)
C11	0.0167 (6)	0.0176 (6)	0.0181 (6)	0.0001 (5)	−0.0012 (5)	0.0001 (5)
C12	0.0203 (6)	0.0164 (6)	0.0185 (6)	−0.0009 (5)	0.0014 (5)	0.0005 (5)
C13	0.0201 (7)	0.0243 (7)	0.0259 (7)	0.0049 (5)	0.0009 (5)	−0.0005 (6)
C14	0.0184 (6)	0.0345 (8)	0.0252 (8)	−0.0026 (6)	0.0044 (5)	−0.0024 (7)
C15	0.0278 (8)	0.0299 (8)	0.0238 (8)	−0.0075 (6)	0.0042 (6)	0.0053 (6)
C16	0.0252 (7)	0.0191 (6)	0.0211 (6)	0.0009 (5)	−0.0027 (6)	0.0058 (7)

Geometric parameters (Å, º)

S1—C1	1.7278 (16)	C6—C7	1.392 (2)
S1—C2	1.7431 (14)	C6—H6A	0.9300
F1—C5	1.3527 (16)	C7—C8	1.389 (2)

F2—C9	1.3630 (15)	C7—H7A	0.9300
F3—C12	1.3548 (17)	C8—C9	1.380 (2)
F4—C16	1.3566 (16)	C8—H8A	0.9300
N1—C1	1.295 (2)	C10—C11	1.5179 (19)
N1—N2	1.3872 (16)	C10—H10A	0.9700
N2—C2	1.3114 (19)	C10—H10B	0.9700
N3—C2	1.3613 (17)	C11—C12	1.3824 (19)
N3—C10	1.4570 (18)	C11—C16	1.388 (2)
N3—C3	1.4598 (19)	C12—C13	1.383 (2)
C1—H1A	0.9300	C13—C14	1.387 (2)
C3—C4	1.514 (2)	C13—H13A	0.9300
C3—H3A	0.9700	C14—C15	1.383 (2)
C3—H3B	0.9700	C14—H14A	0.9300
C4—C9	1.3848 (18)	C15—C16	1.380 (2)
C4—C5	1.3906 (19)	C15—H15A	0.9300
C5—C6	1.374 (2)		

C1—S1—C2	86.35 (7)	C9—C8—C7	118.05 (14)
C1—N1—N2	112.47 (13)	C9—C8—H8A	121.0
C2—N2—N1	112.07 (13)	C7—C8—H8A	121.0
C2—N3—C10	121.42 (12)	F2—C9—C8	117.87 (12)
C2—N3—C3	119.33 (12)	F2—C9—C4	117.72 (12)
C10—N3—C3	118.42 (11)	C8—C9—C4	124.41 (13)
N1—C1—S1	115.07 (11)	N3—C10—C11	112.32 (11)
N1—C1—H1A	122.5	N3—C10—H10A	109.1
S1—C1—H1A	122.5	C11—C10—H10A	109.1
N2—C2—N3	123.20 (13)	N3—C10—H10B	109.1
N2—C2—S1	114.03 (10)	C11—C10—H10B	109.1
N3—C2—S1	122.77 (11)	H10A—C10—H10B	107.9
N3—C3—C4	112.33 (11)	C12—C11—C16	114.68 (12)
N3—C3—H3A	109.1	C12—C11—C10	122.98 (12)
C4—C3—H3A	109.1	C16—C11—C10	122.31 (13)
N3—C3—H3B	109.1	F3—C12—C11	117.97 (12)
C4—C3—H3B	109.1	F3—C12—C13	117.77 (13)
H3A—C3—H3B	107.9	C11—C12—C13	124.25 (13)
C9—C4—C5	114.46 (13)	C12—C13—C14	117.94 (14)
C9—C4—C3	123.33 (11)	C12—C13—H13A	121.0
C5—C4—C3	122.21 (12)	C14—C13—H13A	121.0
F1—C5—C6	118.65 (13)	C15—C14—C13	120.85 (14)
F1—C5—C4	116.87 (13)	C15—C14—H14A	119.6
C6—C5—C4	124.48 (14)	C13—C14—H14A	119.6
C5—C6—C7	118.08 (14)	C16—C15—C14	118.03 (14)
C5—C6—H6A	121.0	C16—C15—H15A	121.0
C7—C6—H6A	121.0	C14—C15—H15A	121.0
C8—C7—C6	120.51 (14)	F4—C16—C15	118.49 (13)
C8—C7—H7A	119.7	F4—C16—C11	117.26 (12)
C6—C7—H7A	119.7	C15—C16—C11	124.24 (13)

C1—N1—N2—C2	0.11 (18)	C7—C8—C9—C4	−0.5 (2)
N2—N1—C1—S1	0.64 (17)	C5—C4—C9—F2	−179.53 (12)
C2—S1—C1—N1	−0.89 (12)	C3—C4—C9—F2	0.5 (2)
N1—N2—C2—N3	179.58 (13)	C5—C4—C9—C8	0.9 (2)
N1—N2—C2—S1	−0.80 (15)	C3—C4—C9—C8	−179.07 (14)
C10—N3—C2—N2	−176.38 (13)	C2—N3—C10—C11	131.34 (14)
C3—N3—C2—N2	14.2 (2)	C3—N3—C10—C11	−59.13 (17)
C10—N3—C2—S1	4.04 (19)	N3—C10—C11—C12	121.31 (15)
C3—N3—C2—S1	−165.40 (10)	N3—C10—C11—C16	−60.72 (19)
C1—S1—C2—N2	0.94 (11)	C16—C11—C12—F3	−179.37 (13)
C1—S1—C2—N3	−179.44 (13)	C10—C11—C12—F3	−1.3 (2)
C2—N3—C3—C4	113.44 (14)	C16—C11—C12—C13	0.1 (2)
C10—N3—C3—C4	−56.32 (16)	C10—C11—C12—C13	178.17 (14)
N3—C3—C4—C9	118.26 (15)	F3—C12—C13—C14	−179.93 (14)
N3—C3—C4—C5	−61.69 (18)	C11—C12—C13—C14	0.6 (2)
C9—C4—C5—F1	179.22 (13)	C12—C13—C14—C15	−0.6 (2)
C3—C4—C5—F1	−0.8 (2)	C13—C14—C15—C16	−0.1 (2)
C9—C4—C5—C6	−0.6 (2)	C14—C15—C16—F4	−177.79 (14)
C3—C4—C5—C6	179.38 (14)	C14—C15—C16—C11	0.9 (2)
F1—C5—C6—C7	−179.92 (14)	C12—C11—C16—F4	177.85 (13)
C4—C5—C6—C7	−0.1 (2)	C10—C11—C16—F4	−0.3 (2)
C5—C6—C7—C8	0.6 (2)	C12—C11—C16—C15	−0.9 (2)
C6—C7—C8—C9	−0.3 (2)	C10—C11—C16—C15	−178.99 (15)
C7—C8—C9—F2	179.95 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···N1^{i}	0.93	2.58	3.392 (2)	146
C3—H3*A*···N2	0.97	2.36	2.8155 (18)	108
C3—H3*B*···F2	0.97	2.41	2.8508 (15)	107
C3—H3*B*···F3^{ii}	0.97	2.47	3.0226 (16)	116
C8—H8*A*···F4^{iii}	0.93	2.54	3.144 (2)	123
C10—H10*A*···S1	0.97	2.53	3.0738 (14)	115
C10—H10*B*···F3	0.97	2.40	2.8453 (16)	107
C10—H10*B*···N2^{iv}	0.97	2.56	3.4191 (17)	148

Symmetry codes: (i) −*x*+3/2, *y*, *z*−1/2; (ii) *x*, *y*+1, *z*; (iii) *x*, *y*−1, *z*+1; (iv) *x*, *y*−1, *z*.