

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(2,3-Difluorophenyl)(4-tosylpiperazin-1-yl)methanone

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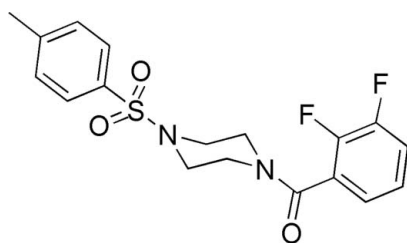
Received 19 December 2012; accepted 22 December 2012

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.033; wR factor = 0.092; data-to-parameter ratio = 10.0.

In the title compound, $C_{18}H_{18}F_2N_2O_3S$, the piperazine ring adopts a chair conformation. The dihedral angle between the sulfonyl-bound benzene ring and the best fit plane through the six non-H atoms of the piperazine ring is $69.4(2)^\circ$, while those between the fluorobenzene and sulfonyl rings and the fluorobenzene and piperazine rings are $30.97(2)$ and $75.98(2)^\circ$, respectively. In the crystal, molecules are connected to form a tetrameric unit through $C-H \cdots O$ hydrogen bonds. The structure is further stabilized by weak intermolecular $C-H \cdots F$ interactions, generating $C(8)$ and $C(7)$ chains running along $[100]$.

Related literature

For the synthesis, characterization and biological activity of piperazine and its derivatives, see: Gan *et al.* (2009*a,b*). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $C_{18}H_{18}F_2N_2O_3S$
 $M_r = 380.40$

Monoclinic, $P2_1/c$
 $a = 17.0456(4)$ Å
 $b = 7.6026(1)$ Å
 $c = 15.5113(3)$ Å
 $\beta = 113.513(1)^\circ$
 $V = 1843.22(6)$ Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.22$ mm⁻¹
 $T = 298$ K
 $0.28 \times 0.26 \times 0.20$ mm

Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)
 $T_{min} = 0.942$, $T_{max} = 0.958$

11988 measured reflections
2359 independent reflections
1930 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.023$
 $\theta_{max} = 22.4^\circ$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.092$
 $S = 1.06$
2359 reflections

236 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 0.15$ e Å⁻³
 $\Delta\rho_{min} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C4-H4 \cdots O3^i$	0.93	2.58	3.495 (3)	169
$C8-H8A \cdots O3^{ii}$	0.97	2.34	3.255 (3)	157
$C10-H10B \cdots O1^{iii}$	0.97	2.48	3.402 (3)	159
$C8-H8B \cdots F1^{iv}$	0.97	2.57	3.518 (3)	165
$C11-H11A \cdots F2^{iv}$	0.97	2.56	3.296 (3)	133

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

The authors thank Dr S. C. Sharma, Vice Chancellor, Tumkur University, for his constant encouragement. JT also thanks the DST, New Delhi, for the SCXRD facility under the PURSE Grant (SR/S9/Z-23/2008/11, 2009) at USIC, Karnatak University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5290).

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supporting information

Acta Cryst. (2013). E69, o185 [doi:10.1107/S1600536812051690]

(2,3-Difluorophenyl)(4-tosylpiperazin-1-yl)methanone

S. Sreenivasa, K. E. ManojKumar, P. A. Suchetan, J. Tonannavar, Yashshwita Chavan and B. S. Palakshamurthy

S1. Comment

Numerous piperazine derivatives such as aryl amides, sulphonamides, Mannich bases, Schiff's bases, thiazolidinones, azetidinones, imidazolinones have shown a wide spectrum of biological activities *viz.* anti-inflammatory, antibacterial, antimalarial, anticonvulsant, antipyretic, antitumor, anthelmintics, analgesic, antidepressant, antifungal, antitubercular, anticancer, antidiabetic effects (Gan *et al.*, 2009a, 2009b). Keeping this in mind, we synthesized the title compound to study its crystal structure.

The compound crystallizes in monoclinic crystal system and the space group $P2_1/c$. In the crystal structure, the piperazine ring adopts chair conformation. The dihedral angle between the sulfonyl bound benzene ring and the best fit plane through all six atoms of the piperazine ring is $69.4(2)^\circ$, while those between the fluorobenzene and the sulfonyl rings and the fluorobenzene and the piperazine rings are $30.97(2)^\circ$ and $75.98(2)^\circ$ respectively. In the crystal structure molecules form a tetrameric unit generating alternate $R_2^2(22)$, (C8—H8A \cdots O3, C10—H10B \cdots O1) and inversion related C4—H4 \cdots O3 $R_2^2(10)$ rings (Bernstein *et al.* 1995). The structure is further stabilized by weak intermolecular C11—H11A \cdots F2 and C8—H8B \cdots F1 interactions.

S2. Experimental

1-Tosylpiperazine (0.01 mmol) and triethylamine (0.02 mmol) were dissolved in 10 ml of dichloromethane (CH_2Cl_2). The mixture was cooled to 0°C and 1-propanephosphonic acid anhydride (0.02 mmol) and 2,4-difluorobenzoic acid (0.01 mmol) added. The reaction mixture was stirred at 80°C for 14 h. The reaction was monitored by TLC and the solvent removed yielding the crude product. The crude mass was purified by chromatography on 230–400 silica gel with petroleum ether and ethyl acetate as eluents. Single crystals of the title compound were obtained from slow evaporation of a solution of the compound in petroleum ether and ethyl acetate (1:4).

S3. Refinement

H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 - 0.97 Å. The isotropic displacement parameters for all H atoms were set to 1.2 times U_{eq} of the parent atom or 1.5 times that of the parent atom for CH_3 .

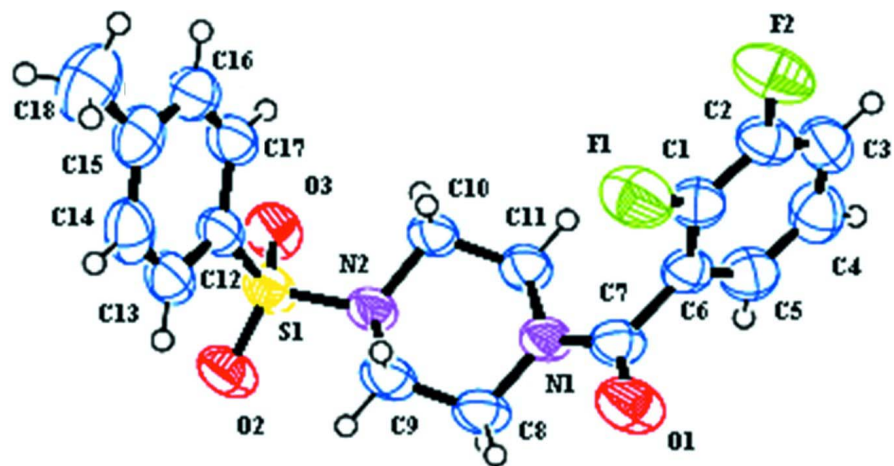


Figure 1

Molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

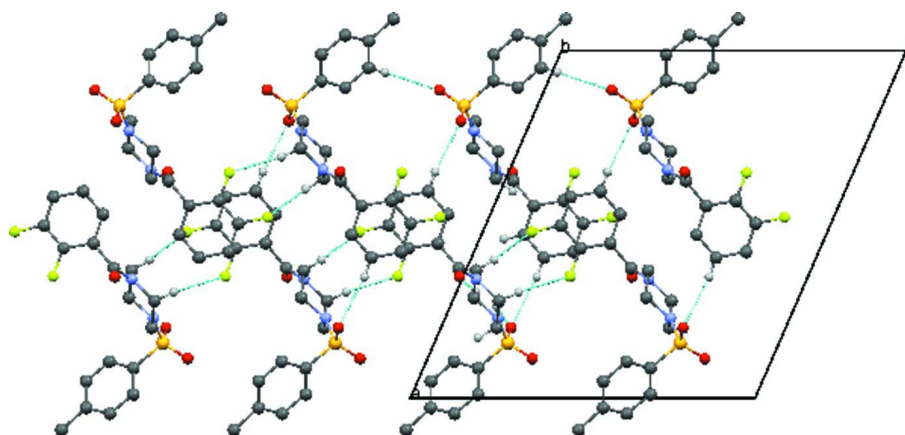


Figure 2

Molecular packing in the title compound. Hydrogen bonds are shown as dashed lines.

(2,3-Difluorophenyl)(4-tosylpiperazin-1-yl)methanone

Crystal data

$C_{18}H_{18}F_2N_2O_3S$
 $M_r = 380.40$
 Monoclinic, $P2_1/c$
 Hall symbol: -P 2ybc
 $a = 17.0456(4) \text{ \AA}$
 $b = 7.6026(1) \text{ \AA}$
 $c = 15.5113(3) \text{ \AA}$
 $\beta = 113.513(1)^\circ$
 $V = 1843.22(6) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 792$

Prism
 $D_x = 1.371 \text{ Mg m}^{-3}$
 Melting point: 457 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 2364 reflections
 $\theta = 2.6\text{--}22.4^\circ$
 $\mu = 0.22 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Prism, colourless
 $0.28 \times 0.26 \times 0.20 \text{ mm}$

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 0.95 pixels mm⁻¹
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.942$, $T_{\max} = 0.958$

11988 measured reflections
 2359 independent reflections
 1930 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\max} = 22.4^\circ$, $\theta_{\min} = 2.6^\circ$
 $h = -18 \rightarrow 15$
 $k = -8 \rightarrow 7$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.092$
 $S = 1.06$
 2359 reflections
 236 parameters
 0 restraints
 0 constraints
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.3661P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.56842 (15)	0.1855 (3)	-0.19563 (16)	0.0606 (6)
C2	0.50273 (17)	0.2154 (3)	-0.28076 (15)	0.0652 (6)
C3	0.42103 (17)	0.2278 (3)	-0.28889 (17)	0.0712 (7)
H3	0.3767	0.2486	-0.3470	0.085*
C4	0.40468 (16)	0.2091 (3)	-0.20946 (19)	0.0788 (7)
H4	0.3488	0.2165	-0.2137	0.095*
C5	0.47062 (17)	0.1794 (3)	-0.12370 (17)	0.0710 (7)
H5	0.4587	0.1672	-0.0705	0.085*
C6	0.55410 (14)	0.1675 (3)	-0.11526 (14)	0.0542 (6)
C7	0.62575 (15)	0.1198 (3)	-0.02411 (15)	0.0599 (6)
C8	0.71988 (15)	0.1996 (3)	0.13429 (14)	0.0644 (6)
H8A	0.7369	0.0777	0.1353	0.077*
H8B	0.6944	0.2135	0.1797	0.077*
C9	0.79693 (15)	0.3155 (3)	0.16094 (15)	0.0632 (6)
H9A	0.8364	0.2901	0.2249	0.076*

H9B	0.8260	0.2935	0.1195	0.076*
C10	0.71040 (13)	0.5453 (3)	0.05710 (14)	0.0574 (6)
H10A	0.7382	0.5278	0.0141	0.069*
H10B	0.6938	0.6679	0.0542	0.069*
C11	0.63270 (14)	0.4302 (3)	0.02931 (15)	0.0598 (6)
H11A	0.6015	0.4580	0.0679	0.072*
H11B	0.5954	0.4525	-0.0358	0.072*
C12	0.91357 (14)	0.6645 (3)	0.15849 (14)	0.0584 (6)
C13	0.98919 (15)	0.5691 (3)	0.19152 (16)	0.0659 (6)
H13	1.0022	0.4951	0.2431	0.079*
C14	1.04489 (16)	0.5843 (3)	0.14784 (19)	0.0746 (7)
H14	1.0952	0.5191	0.1702	0.089*
C15	1.02791 (17)	0.6943 (3)	0.07146 (18)	0.0730 (7)
C16	0.95135 (18)	0.7848 (3)	0.03828 (17)	0.0742 (7)
H16	0.9379	0.8565	-0.0143	0.089*
C17	0.89459 (16)	0.7722 (3)	0.08056 (16)	0.0659 (6)
H17	0.8437	0.8354	0.0571	0.079*
C18	1.0916 (2)	0.7155 (4)	0.0280 (2)	0.1021 (10)
H18A	1.0634	0.7612	-0.0346	0.153*
H18B	1.1165	0.6034	0.0256	0.153*
H18C	1.1357	0.7956	0.0651	0.153*
N1	0.65731 (11)	0.2441 (2)	0.04104 (11)	0.0572 (5)
N2	0.76965 (11)	0.5003 (2)	0.15333 (11)	0.0571 (5)
O1	0.65057 (13)	-0.0330 (2)	-0.01083 (11)	0.0937 (6)
O2	0.88639 (11)	0.5727 (2)	0.30408 (10)	0.0772 (5)
O3	0.79753 (10)	0.8085 (2)	0.20235 (11)	0.0740 (5)
F1	0.64895 (9)	0.1741 (2)	-0.19068 (10)	0.0971 (5)
F2	0.52079 (11)	0.2303 (2)	-0.35774 (10)	0.1029 (6)
S1	0.84155 (4)	0.64492 (7)	0.21283 (4)	0.0619 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0636 (15)	0.0573 (14)	0.0623 (15)	0.0075 (12)	0.0267 (13)	0.0050 (11)
C2	0.0869 (18)	0.0589 (15)	0.0500 (14)	0.0087 (13)	0.0274 (14)	0.0016 (10)
C3	0.0761 (18)	0.0625 (16)	0.0607 (15)	0.0060 (13)	0.0122 (13)	-0.0038 (11)
C4	0.0635 (16)	0.0821 (19)	0.087 (2)	0.0011 (14)	0.0268 (16)	-0.0009 (14)
C5	0.0809 (18)	0.0705 (16)	0.0687 (16)	0.0017 (14)	0.0372 (15)	0.0020 (12)
C6	0.0702 (15)	0.0380 (12)	0.0526 (13)	0.0016 (10)	0.0226 (11)	-0.0001 (9)
C7	0.0803 (16)	0.0451 (15)	0.0530 (13)	0.0055 (12)	0.0252 (12)	0.0038 (11)
C8	0.0877 (17)	0.0441 (13)	0.0535 (13)	0.0094 (12)	0.0198 (12)	0.0069 (10)
C9	0.0733 (15)	0.0474 (14)	0.0556 (13)	0.0164 (12)	0.0117 (12)	0.0094 (10)
C10	0.0643 (14)	0.0413 (13)	0.0549 (13)	0.0079 (11)	0.0115 (11)	0.0077 (9)
C11	0.0672 (14)	0.0435 (13)	0.0596 (13)	0.0097 (11)	0.0158 (11)	0.0037 (10)
C12	0.0631 (14)	0.0409 (12)	0.0522 (12)	-0.0002 (11)	0.0031 (11)	-0.0037 (10)
C13	0.0656 (15)	0.0497 (14)	0.0621 (14)	0.0027 (12)	0.0040 (13)	-0.0012 (11)
C14	0.0597 (15)	0.0575 (16)	0.0884 (18)	0.0001 (13)	0.0105 (14)	-0.0153 (14)
C15	0.0815 (18)	0.0529 (15)	0.0763 (17)	-0.0159 (14)	0.0227 (15)	-0.0202 (13)

C16	0.0898 (19)	0.0559 (16)	0.0635 (15)	-0.0092 (14)	0.0163 (15)	-0.0017 (12)
C17	0.0702 (15)	0.0513 (15)	0.0592 (14)	0.0028 (12)	0.0079 (13)	0.0031 (11)
C18	0.109 (2)	0.089 (2)	0.120 (2)	-0.0272 (18)	0.058 (2)	-0.0307 (18)
N1	0.0741 (12)	0.0373 (11)	0.0504 (10)	0.0061 (9)	0.0144 (9)	0.0024 (8)
N2	0.0660 (11)	0.0395 (10)	0.0518 (10)	0.0089 (9)	0.0089 (9)	0.0057 (8)
O1	0.1381 (16)	0.0460 (11)	0.0679 (10)	0.0203 (10)	0.0104 (10)	-0.0024 (8)
O2	0.0933 (12)	0.0732 (11)	0.0470 (8)	0.0107 (9)	0.0088 (8)	0.0031 (7)
O3	0.0833 (11)	0.0487 (9)	0.0760 (10)	0.0128 (8)	0.0169 (9)	-0.0088 (7)
F1	0.0793 (10)	0.1325 (14)	0.0878 (10)	0.0192 (9)	0.0422 (8)	0.0291 (9)
F2	0.1248 (13)	0.1301 (14)	0.0601 (9)	0.0342 (11)	0.0437 (9)	0.0201 (8)
S1	0.0722 (4)	0.0485 (4)	0.0499 (3)	0.0083 (3)	0.0084 (3)	-0.0018 (2)

Geometric parameters (Å, °)

C1—F1	1.347 (2)	C10—H10A	0.9700
C1—C2	1.367 (3)	C10—H10B	0.9700
C1—C6	1.369 (3)	C11—N1	1.466 (3)
C2—C3	1.351 (3)	C11—H11A	0.9700
C2—F2	1.352 (3)	C11—H11B	0.9700
C3—C4	1.375 (3)	C12—C13	1.387 (3)
C3—H3	0.9300	C12—C17	1.387 (3)
C4—C5	1.375 (3)	C12—S1	1.751 (2)
C4—H4	0.9300	C13—C14	1.374 (3)
C5—C6	1.379 (3)	C13—H13	0.9300
C5—H5	0.9300	C14—C15	1.383 (4)
C6—C7	1.498 (3)	C14—H14	0.9300
C7—O1	1.225 (3)	C15—C16	1.380 (4)
C7—N1	1.330 (3)	C15—C18	1.497 (4)
C8—N1	1.454 (3)	C16—C17	1.372 (3)
C8—C9	1.496 (3)	C16—H16	0.9300
C8—H8A	0.9700	C17—H17	0.9300
C8—H8B	0.9700	C18—H18A	0.9600
C9—N2	1.470 (3)	C18—H18B	0.9600
C9—H9A	0.9700	C18—H18C	0.9600
C9—H9B	0.9700	N2—S1	1.6311 (17)
C10—N2	1.470 (2)	O2—S1	1.4234 (15)
C10—C11	1.500 (3)	O3—S1	1.4281 (16)
F1—C1—C2	119.3 (2)	C10—C11—H11A	109.5
F1—C1—C6	119.3 (2)	N1—C11—H11B	109.5
C2—C1—C6	121.4 (2)	C10—C11—H11B	109.5
C3—C2—F2	120.1 (2)	H11A—C11—H11B	108.1
C3—C2—C1	121.2 (2)	C13—C12—C17	119.3 (2)
F2—C2—C1	118.7 (2)	C13—C12—S1	120.31 (18)
C2—C3—C4	118.6 (2)	C17—C12—S1	120.34 (18)
C2—C3—H3	120.7	C14—C13—C12	119.8 (2)
C4—C3—H3	120.7	C14—C13—H13	120.1
C3—C4—C5	120.3 (2)	C12—C13—H13	120.1

C3—C4—H4	119.9	C13—C14—C15	121.6 (2)
C5—C4—H4	119.9	C13—C14—H14	119.2
C4—C5—C6	121.1 (2)	C15—C14—H14	119.2
C4—C5—H5	119.4	C16—C15—C14	117.7 (3)
C6—C5—H5	119.4	C16—C15—C18	121.7 (3)
C1—C6—C5	117.3 (2)	C14—C15—C18	120.6 (3)
C1—C6—C7	120.6 (2)	C17—C16—C15	121.9 (2)
C5—C6—C7	121.8 (2)	C17—C16—H16	119.0
O1—C7—N1	122.5 (2)	C15—C16—H16	119.0
O1—C7—C6	119.0 (2)	C16—C17—C12	119.6 (2)
N1—C7—C6	118.36 (19)	C16—C17—H17	120.2
N1—C8—C9	110.67 (17)	C12—C17—H17	120.2
N1—C8—H8A	109.5	C15—C18—H18A	109.5
C9—C8—H8A	109.5	C15—C18—H18B	109.5
N1—C8—H8B	109.5	H18A—C18—H18B	109.5
C9—C8—H8B	109.5	C15—C18—H18C	109.5
H8A—C8—H8B	108.1	H18A—C18—H18C	109.5
N2—C9—C8	109.02 (18)	H18B—C18—H18C	109.5
N2—C9—H9A	109.9	C7—N1—C8	120.31 (17)
C8—C9—H9A	109.9	C7—N1—C11	125.61 (17)
N2—C9—H9B	109.9	C8—N1—C11	114.06 (16)
C8—C9—H9B	109.9	C9—N2—C10	111.79 (16)
H9A—C9—H9B	108.3	C9—N2—S1	117.19 (14)
N2—C10—C11	109.02 (16)	C10—N2—S1	118.30 (13)
N2—C10—H10A	109.9	O2—S1—O3	119.91 (10)
C11—C10—H10A	109.9	O2—S1—N2	106.66 (9)
N2—C10—H10B	109.9	O3—S1—N2	106.31 (9)
C11—C10—H10B	109.9	O2—S1—C12	108.06 (10)
H10A—C10—H10B	108.3	O3—S1—C12	107.97 (10)
N1—C11—C10	110.57 (17)	N2—S1—C12	107.32 (9)
N1—C11—H11A	109.5		
F1—C1—C2—C3	180.0 (2)	C15—C16—C17—C12	-0.6 (3)
C6—C1—C2—C3	-0.2 (4)	C13—C12—C17—C16	-1.0 (3)
F1—C1—C2—F2	0.8 (3)	S1—C12—C17—C16	-179.41 (17)
C6—C1—C2—F2	-179.4 (2)	O1—C7—N1—C8	-4.0 (3)
F2—C2—C3—C4	178.9 (2)	C6—C7—N1—C8	172.92 (19)
C1—C2—C3—C4	-0.2 (4)	O1—C7—N1—C11	178.1 (2)
C2—C3—C4—C5	0.4 (4)	C6—C7—N1—C11	-5.1 (3)
C3—C4—C5—C6	-0.1 (4)	C9—C8—N1—C7	127.7 (2)
F1—C1—C6—C5	-179.7 (2)	C9—C8—N1—C11	-54.1 (3)
C2—C1—C6—C5	0.5 (3)	C10—C11—N1—C7	-128.3 (2)
F1—C1—C6—C7	-5.4 (3)	C10—C11—N1—C8	53.6 (2)
C2—C1—C6—C7	174.8 (2)	C8—C9—N2—C10	-60.2 (2)
C4—C5—C6—C1	-0.3 (3)	C8—C9—N2—S1	158.59 (15)
C4—C5—C6—C7	-174.6 (2)	C11—C10—N2—C9	59.8 (2)
C1—C6—C7—O1	-76.6 (3)	C11—C10—N2—S1	-159.43 (14)
C5—C6—C7—O1	97.4 (3)	C9—N2—S1—O2	-44.59 (18)

C1—C6—C7—N1	106.4 (2)	C10—N2—S1—O2	176.77 (15)
C5—C6—C7—N1	-79.5 (3)	C9—N2—S1—O3	-173.63 (15)
N1—C8—C9—N2	55.6 (2)	C10—N2—S1—O3	47.72 (18)
N2—C10—C11—N1	-54.7 (2)	C9—N2—S1—C12	71.02 (17)
C17—C12—C13—C14	1.0 (3)	C10—N2—S1—C12	-67.62 (17)
S1—C12—C13—C14	179.43 (16)	C13—C12—S1—O2	18.83 (19)
C12—C13—C14—C15	0.5 (3)	C17—C12—S1—O2	-162.78 (17)
C13—C14—C15—C16	-2.0 (3)	C13—C12—S1—O3	149.92 (17)
C13—C14—C15—C18	176.9 (2)	C17—C12—S1—O3	-31.70 (19)
C14—C15—C16—C17	2.1 (3)	C13—C12—S1—N2	-95.85 (17)
C18—C15—C16—C17	-176.9 (2)	C17—C12—S1—N2	82.53 (18)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4 \cdots O3 ⁱ	0.93	2.58	3.495 (3)	169
C8—H8A \cdots O3 ⁱⁱ	0.97	2.34	3.255 (3)	157
C10—H10B \cdots O1 ⁱⁱⁱ	0.97	2.48	3.402 (3)	159
C8—H8B \cdots F1 ^{iv}	0.97	2.57	3.518 (3)	165
C11—H11A \cdots F2 ^{iv}	0.97	2.56	3.296 (3)	133

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, y-1, z$; (iii) $x, y+1, z$; (iv) $x, -y+1/2, z+1/2$.