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1-(3,4-Difluorobenzyl)-4-(4-methylphenylsulfonyl)piperazine

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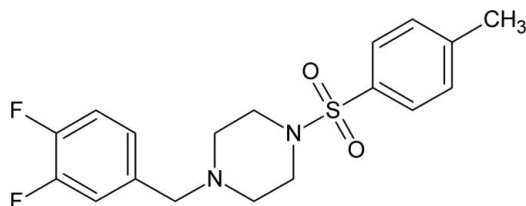
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.045; wR factor = 0.114; data-to-parameter ratio = 10.7.

In the title compound, $\text{C}_{18}\text{H}_{20}\text{F}_2\text{N}_2\text{O}_2\text{S}$, the central piperazine ring adopts a chair conformation. The dihedral angle between the two benzene rings is 40.20° , whereas those between the piperazine ring (considering the best fit plane through all the non-H atoms) and the sulfonyl-bound benzene and difluorobenzene rings are 74.96 and 86.16° , respectively. In the crystal, molecules are stacked along the a axis through weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ interactions.

Related literature

 For similar structures, see: Sreenivasa *et al.* (2013a,b,c).


Experimental

Crystal data

$\text{C}_{18}\text{H}_{20}\text{F}_2\text{N}_2\text{O}_2\text{S}$
 $M_r = 366.42$
 Monoclinic, $P2_1/c$
 $a = 6.6680$ (2) Å

$b = 36.0404$ (8) Å
 $c = 7.6093$ (2) Å
 $\beta = 99.728$ (2)°
 $V = 1802.35$ (8) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.21$ mm⁻¹

$T = 298$ K
 $0.28 \times 0.24 \times 0.20$ mm

Data collection

Bruker APEXII diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.943$, $T_{\max} = 0.959$
 9583 measured reflections

2434 independent reflections
 1910 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\text{max}} = 22.8^\circ$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.114$
 $S = 1.02$
 2434 reflections

227 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.19$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3}\cdots\text{O1}^{\text{i}}$	0.93	2.67	3.380 (4)	134
$\text{C7}-\text{H7A}\cdots\text{O1}^{\text{ii}}$	0.96	2.66	3.400 (4)	134
$\text{C10}-\text{H10B}\cdots\text{F1}^{\text{iii}}$	0.97	2.66	3.585 (3)	160

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

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: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5330).

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supplementary materials

Acta Cryst. (2013). E69, o1179 [doi:10.1107/S1600536813016462]

1-(3,4-Difluorobenzyl)-4-(4-methylphenylsulfonyl)piperazine

S. Sreenivasa, H. C. Anitha, P. A. Suchetan, B. S. Palakshamurthy, J. Savanur and J. Tonannavar

Comment

As a part of our continued efforts to study the crystal structures of *N*-(aryl)(4-tosylpiperazin-1-yl)methanone derivatives (Sreenivasa *et al.*, 2013*a,b,c*), we report herein the crystal structure of the title compound.

The title compound, Fig. 1, crystallizes in the monoclinic crystal system and $P2_1/c$ space group. The piperazine ring in the title compound adopts a chair conformation. The dihedral angle between the two benzene rings is 40.20° , compared to the observed dihedral angles of $72.2(12)^\circ$, 76.86° and $30.97(2)^\circ$ respectively in (I), 1-(2,4-dichlorobenzyl)-4-[(4-methylphenyl)sulfonyl]-piperazine (Sreenivasa *et al.*, 2013*a*), (II) 1-tosyl-4-[2-(trifluoromethyl)-benzyl]piperazine (Sreenivasa *et al.*, 2013*b*) and (III) (2,3-difluorophenyl)(4-tosylpiperazin-1-yl)methanone (Sreenivasa *et al.*, 2013*c*). Further, the dihedral angles between the piperazine ring (considering the best fit plane through all the non-hydrogen atoms) and the sulfonyl bound benzene and difluorobenzene rings are 74.96° and 86.16° respectively, compared to $74.16(2)^\circ$ and $2.44(13)^\circ$ in I, 74.36° and $68.29(3)^\circ$ in II, and $69.4(2)^\circ$ and $75.98(2)^\circ$ in III.

In the crystal structure, the molecules are stacked along the *a* axis through weak C—H \cdots O and C—H \cdots F interactions, Fig. 2.

Experimental

A mixture of 1-tosylpiperazine (0.01 mmol), potassium carbonate (0.03 mmol) and 3,4-difluorobenzyl bromide (0.01 mmol) was added to dry acetonitrile (5 ml). The mixture was stirred at 85°C for 8 h. The reaction was monitored by TLC. Solvent was removed by vacuum distillation and the crude product obtained was purified by column chromatography using 230–400 silica gel and petroleum ether/ethyl acetate as eluent.

Colourless prisms were obtained from a mixture of dichloromethane/methanol (7:3) by slow evaporation.

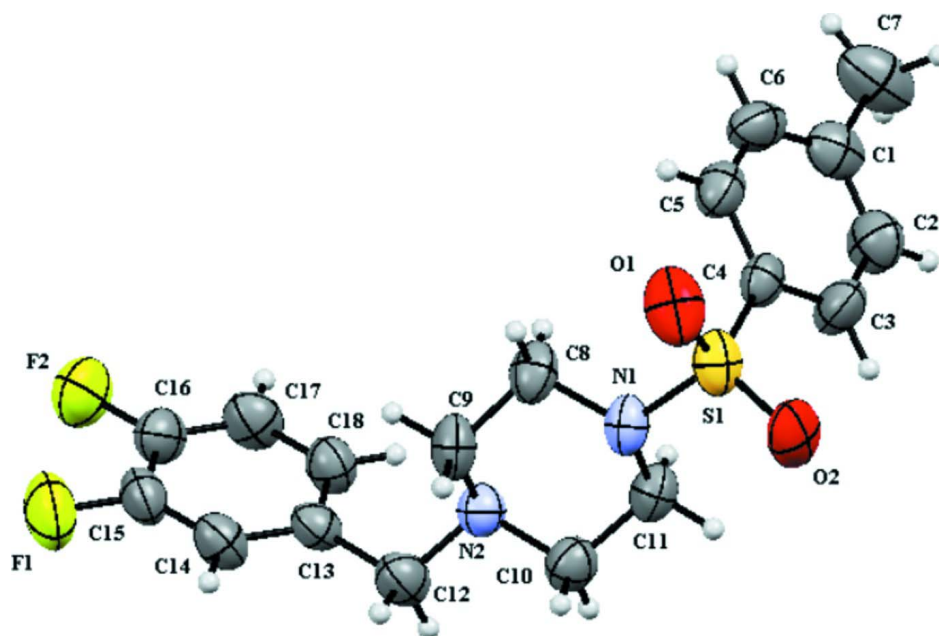
Refinement

H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 - 0.96 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 CH₃.

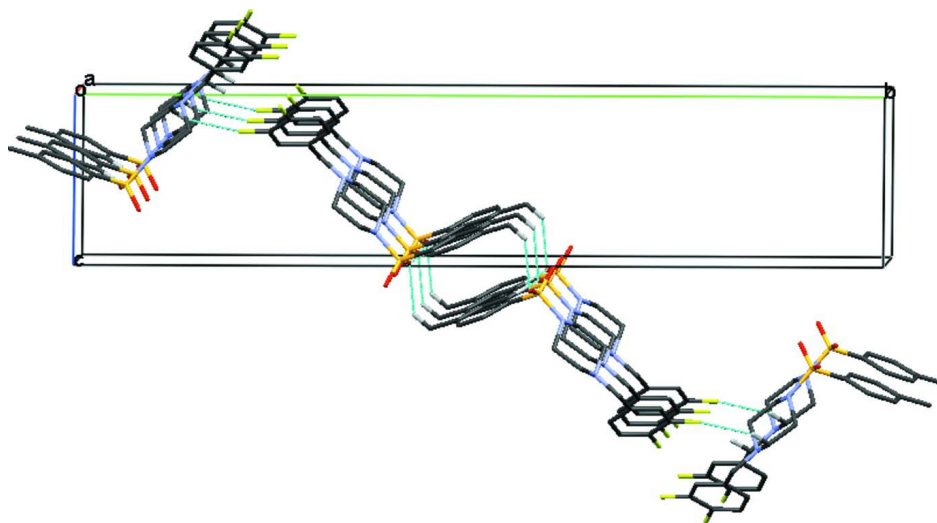
Crystals were small and very weakly diffracting, with no significant data obtained beyond $\theta = 22.8^\circ$ hence the low values of $\sin(\theta/\lambda)$. However the structure solved and refined satisfactorily and gave acceptable residuals and *su* values.

Computing details

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: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

**Figure 1**

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

**Figure 2**

A packing diagram of the title compound, showing C–H...O and C–H...F interactions (dotted lines). Hydrogen atoms not involved in hydrogen bonding are omitted.

1-(3,4-Difluorobenzyl)-4-(4-methylphenylsulfonyl)piperazine

Crystal data

$C_{18}H_{20}F_2N_2O_2S$
 $M_r = 366.42$
 Monoclinic, $P2_1/c$
 Hall symbol: $-P 2_1/c$

$a = 6.6680 (2) \text{ \AA}$
 $b = 36.0404 (8) \text{ \AA}$
 $c = 7.6093 (2) \text{ \AA}$
 $\beta = 99.728 (2)^\circ$

$V = 1802.35 (8) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 768$
 prism
 $D_x = 1.350 \text{ Mg m}^{-3}$
 Melting point: 501 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 227 reflections

$\theta = 2.3\text{--}22.8^\circ$
 $\mu = 0.21 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Prism, colourless
 $0.28 \times 0.24 \times 0.20 \text{ mm}$

Data collection

Bruker APEXII
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 1.03 pixels mm^{-1}
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.943$, $T_{\max} = 0.959$

9583 measured reflections
 2434 independent reflections
 1910 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\max} = 22.8^\circ$, $\theta_{\min} = 2.3^\circ$
 $h = -7 \rightarrow 7$
 $k = -39 \rightarrow 37$
 $l = -7 \rightarrow 8$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.114$
 $S = 1.02$
 2434 reflections
 227 parameters
 0 restraints
 32 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
 $w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.6421P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.028$
 $\Delta\rho_{\max} = 0.19 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.25 \text{ e \AA}^{-3}$

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	-0.3654 (5)	0.51803 (9)	0.7226 (4)	0.0763 (8)
C2	-0.4516 (5)	0.48860 (11)	0.7956 (4)	0.0850 (9)
H2	-0.5880	0.4901	0.8070	0.102*
C3	-0.3451 (5)	0.45692 (9)	0.8529 (4)	0.0761 (8)
H3	-0.4088	0.4376	0.9028	0.091*
C4	-0.1454 (4)	0.45409 (7)	0.8359 (3)	0.0598 (7)
C5	-0.0564 (4)	0.48283 (9)	0.7599 (4)	0.0821 (9)
H5	0.0790	0.4811	0.7455	0.099*
C6	-0.1666 (6)	0.51438 (9)	0.7045 (4)	0.0870 (9)

H6	-0.1034	0.5336	0.6535	0.104*
C7	-0.4821 (6)	0.55287 (10)	0.6662 (5)	0.1135 (13)
H7A	-0.4283	0.5729	0.7431	0.170*
H7B	-0.6229	0.5492	0.6742	0.170*
H7C	-0.4697	0.5587	0.5455	0.170*
C8	-0.2454 (4)	0.36712 (8)	0.6955 (4)	0.0737 (8)
H8A	-0.3419	0.3850	0.6347	0.088*
H8B	-0.2926	0.3592	0.8033	0.088*
C9	-0.2310 (5)	0.33415 (7)	0.5761 (4)	0.0738 (8)
H9A	-0.1406	0.3157	0.6400	0.089*
H9B	-0.3644	0.3230	0.5431	0.089*
C10	0.0484 (4)	0.36109 (8)	0.4655 (4)	0.0734 (8)
H10A	0.1008	0.3680	0.3587	0.088*
H10B	0.1392	0.3427	0.5292	0.088*
C11	0.0404 (4)	0.39451 (7)	0.5809 (4)	0.0680 (7)
H11A	0.1762	0.4046	0.6154	0.082*
H11B	-0.0443	0.4134	0.5148	0.082*
C12	-0.1536 (5)	0.31498 (8)	0.2910 (4)	0.0801 (9)
H12A	-0.0854	0.2938	0.3529	0.096*
H12B	-0.0773	0.3224	0.1990	0.096*
C13	-0.3660 (4)	0.30386 (8)	0.2051 (3)	0.0629 (7)
C14	-0.4280 (5)	0.26741 (8)	0.2015 (4)	0.0737 (8)
H14	-0.3405	0.2492	0.2572	0.088*
C15	-0.6186 (5)	0.25787 (8)	0.1158 (4)	0.0759 (8)
C16	-0.7479 (5)	0.28422 (10)	0.0346 (4)	0.0772 (8)
C17	-0.6903 (5)	0.32020 (9)	0.0356 (4)	0.0834 (9)
H17	-0.7788	0.3381	-0.0212	0.100*
C18	-0.4993 (5)	0.33006 (8)	0.1215 (4)	0.0729 (8)
H18	-0.4596	0.3548	0.1231	0.088*
N1	-0.0432 (3)	0.38434 (6)	0.7410 (3)	0.0646 (6)
N2	-0.1548 (3)	0.34542 (6)	0.4167 (3)	0.0627 (6)
O1	0.2056 (3)	0.42331 (6)	0.9324 (3)	0.0918 (7)
O2	-0.0916 (4)	0.39768 (6)	1.0463 (2)	0.0989 (7)
F1	-0.6798 (3)	0.22224 (5)	0.1108 (3)	0.1225 (8)
F2	-0.9357 (3)	0.27392 (6)	-0.0489 (3)	0.1200 (7)
S1	-0.00612 (12)	0.41390 (2)	0.90583 (9)	0.0734 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.080 (2)	0.089 (2)	0.0536 (17)	0.0093 (19)	-0.0063 (15)	-0.0117 (15)
C2	0.0544 (19)	0.114 (3)	0.086 (2)	0.001 (2)	0.0093 (16)	-0.022 (2)
C3	0.074 (2)	0.087 (2)	0.0703 (19)	-0.0205 (18)	0.0190 (15)	-0.0075 (16)
C4	0.0567 (18)	0.0677 (18)	0.0527 (15)	-0.0136 (13)	0.0024 (12)	-0.0043 (13)
C5	0.0567 (18)	0.077 (2)	0.114 (3)	-0.0079 (16)	0.0178 (17)	0.0131 (18)
C6	0.092 (3)	0.071 (2)	0.099 (2)	-0.0020 (18)	0.0179 (19)	0.0170 (17)
C7	0.128 (3)	0.116 (3)	0.082 (2)	0.047 (2)	-0.023 (2)	-0.014 (2)
C8	0.082 (2)	0.079 (2)	0.0601 (17)	-0.0242 (16)	0.0110 (15)	0.0036 (15)
C9	0.084 (2)	0.0610 (17)	0.0711 (19)	-0.0216 (15)	-0.0014 (15)	0.0047 (14)
C10	0.0626 (19)	0.076 (2)	0.0795 (19)	-0.0024 (15)	0.0056 (14)	0.0011 (16)

C11	0.0652 (18)	0.0661 (18)	0.0705 (18)	-0.0125 (14)	0.0051 (14)	0.0079 (14)
C12	0.073 (2)	0.077 (2)	0.086 (2)	0.0074 (16)	0.0020 (16)	-0.0156 (17)
C13	0.0687 (19)	0.0607 (18)	0.0582 (16)	0.0072 (15)	0.0069 (13)	-0.0111 (13)
C14	0.086 (2)	0.0618 (19)	0.0689 (18)	0.0114 (16)	0.0011 (16)	-0.0066 (14)
C15	0.093 (2)	0.0558 (19)	0.080 (2)	-0.0109 (18)	0.0167 (18)	-0.0134 (15)
C16	0.066 (2)	0.087 (2)	0.075 (2)	-0.0040 (18)	-0.0003 (15)	-0.0177 (17)
C17	0.082 (2)	0.079 (2)	0.083 (2)	0.0152 (18)	-0.0043 (17)	-0.0005 (17)
C18	0.078 (2)	0.0592 (18)	0.0782 (19)	0.0012 (15)	0.0042 (16)	-0.0011 (15)
N1	0.0693 (15)	0.0594 (13)	0.0599 (13)	-0.0137 (11)	-0.0038 (11)	0.0045 (10)
N2	0.0631 (15)	0.0628 (14)	0.0602 (13)	-0.0042 (11)	0.0047 (11)	-0.0009 (11)
O1	0.0685 (14)	0.0894 (15)	0.1015 (16)	-0.0033 (11)	-0.0311 (11)	-0.0102 (12)
O2	0.148 (2)	0.0899 (15)	0.0536 (12)	-0.0194 (13)	0.0032 (12)	0.0131 (11)
F1	0.1360 (18)	0.0734 (13)	0.154 (2)	-0.0270 (12)	0.0134 (14)	-0.0162 (12)
F2	0.0804 (14)	0.1292 (17)	0.1398 (18)	-0.0121 (11)	-0.0119 (12)	-0.0334 (13)
S1	0.0845 (6)	0.0688 (5)	0.0590 (5)	-0.0099 (4)	-0.0110 (4)	0.0051 (4)

Geometric parameters (Å, °)

C1—C6	1.362 (4)	C10—H10A	0.9700
C1—C2	1.368 (4)	C10—H10B	0.9700
C1—C7	1.501 (4)	C11—N1	1.469 (3)
C2—C3	1.376 (4)	C11—H11A	0.9700
C2—H2	0.9300	C11—H11B	0.9700
C3—C4	1.363 (4)	C12—N2	1.457 (3)
C3—H3	0.9300	C12—C13	1.510 (4)
C4—C5	1.369 (4)	C12—H12A	0.9700
C4—S1	1.754 (3)	C12—H12B	0.9700
C5—C6	1.381 (4)	C13—C14	1.376 (4)
C5—H5	0.9300	C13—C18	1.377 (4)
C6—H6	0.9300	C14—C15	1.371 (4)
C7—H7A	0.9600	C14—H14	0.9300
C7—H7B	0.9600	C15—F1	1.346 (3)
C7—H7C	0.9600	C15—C16	1.359 (4)
C8—N1	1.472 (3)	C16—C17	1.352 (4)
C8—C9	1.508 (4)	C16—F2	1.356 (3)
C8—H8A	0.9700	C17—C18	1.377 (4)
C8—H8B	0.9700	C17—H17	0.9300
C9—N2	1.450 (3)	C18—H18	0.9300
C9—H9A	0.9700	N1—S1	1.632 (2)
C9—H9B	0.9700	O1—S1	1.432 (2)
C10—N2	1.457 (3)	O2—S1	1.419 (2)
C10—C11	1.497 (4)		
C6—C1—C2	116.7 (3)	N1—C11—C10	110.0 (2)
C6—C1—C7	121.2 (3)	N1—C11—H11A	109.7
C2—C1—C7	122.1 (3)	C10—C11—H11A	109.7
C1—C2—C3	122.8 (3)	N1—C11—H11B	109.7
C1—C2—H2	118.6	C10—C11—H11B	109.7
C3—C2—H2	118.6	H11A—C11—H11B	108.2
C4—C3—C2	119.5 (3)	N2—C12—C13	112.0 (2)

C4—C3—H3	120.3	N2—C12—H12A	109.2
C2—C3—H3	120.3	C13—C12—H12A	109.2
C3—C4—C5	118.9 (3)	N2—C12—H12B	109.2
C3—C4—S1	120.5 (2)	C13—C12—H12B	109.2
C5—C4—S1	120.5 (2)	H12A—C12—H12B	107.9
C4—C5—C6	120.4 (3)	C14—C13—C18	118.5 (3)
C4—C5—H5	119.8	C14—C13—C12	121.2 (3)
C6—C5—H5	119.8	C18—C13—C12	120.2 (3)
C1—C6—C5	121.7 (3)	C15—C14—C13	120.0 (3)
C1—C6—H6	119.2	C15—C14—H14	120.0
C5—C6—H6	119.2	C13—C14—H14	120.0
C1—C7—H7A	109.5	F1—C15—C16	119.2 (3)
C1—C7—H7B	109.5	F1—C15—C14	120.3 (3)
H7A—C7—H7B	109.5	C16—C15—C14	120.5 (3)
C1—C7—H7C	109.5	C17—C16—F2	120.3 (3)
H7A—C7—H7C	109.5	C17—C16—C15	120.6 (3)
H7B—C7—H7C	109.5	F2—C16—C15	119.1 (3)
N1—C8—C9	109.0 (2)	C16—C17—C18	119.3 (3)
N1—C8—H8A	109.9	C16—C17—H17	120.3
C9—C8—H8A	109.9	C18—C17—H17	120.3
N1—C8—H8B	109.9	C17—C18—C13	121.0 (3)
C9—C8—H8B	109.9	C17—C18—H18	119.5
H8A—C8—H8B	108.3	C13—C18—H18	119.5
N2—C9—C8	110.5 (2)	C11—N1—C8	111.8 (2)
N2—C9—H9A	109.6	C11—N1—S1	116.43 (17)
C8—C9—H9A	109.6	C8—N1—S1	118.03 (18)
N2—C9—H9B	109.6	C9—N2—C12	112.3 (2)
C8—C9—H9B	109.6	C9—N2—C10	109.7 (2)
H9A—C9—H9B	108.1	C12—N2—C10	110.5 (2)
N2—C10—C11	109.7 (2)	O2—S1—O1	120.16 (13)
N2—C10—H10A	109.7	O2—S1—N1	106.38 (12)
C11—C10—H10A	109.7	O1—S1—N1	106.30 (13)
N2—C10—H10B	109.7	O2—S1—C4	108.02 (14)
C11—C10—H10B	109.7	O1—S1—C4	107.81 (12)
H10A—C10—H10B	108.2	N1—S1—C4	107.58 (11)
C6—C1—C2—C3	1.5 (5)	C14—C13—C18—C17	-0.1 (4)
C7—C1—C2—C3	-178.0 (3)	C12—C13—C18—C17	177.0 (3)
C1—C2—C3—C4	-0.6 (4)	C10—C11—N1—C8	-56.5 (3)
C2—C3—C4—C5	-0.8 (4)	C10—C11—N1—S1	163.77 (18)
C2—C3—C4—S1	-179.4 (2)	C9—C8—N1—C11	55.7 (3)
C3—C4—C5—C6	1.2 (4)	C9—C8—N1—S1	-165.23 (18)
S1—C4—C5—C6	179.8 (2)	C8—C9—N2—C12	-175.5 (2)
C2—C1—C6—C5	-1.1 (5)	C8—C9—N2—C10	61.1 (3)
C7—C1—C6—C5	178.4 (3)	C13—C12—N2—C9	70.2 (3)
C4—C5—C6—C1	-0.2 (5)	C13—C12—N2—C10	-166.9 (2)
N1—C8—C9—N2	-57.8 (3)	C11—C10—N2—C9	-60.8 (3)
N2—C10—C11—N1	58.1 (3)	C11—C10—N2—C12	174.7 (2)
N2—C12—C13—C14	-129.4 (3)	C11—N1—S1—O2	-177.66 (19)

N2—C12—C13—C18	53.5 (4)	C8—N1—S1—O2	45.1 (2)
C18—C13—C14—C15	0.0 (4)	C11—N1—S1—O1	-48.5 (2)
C12—C13—C14—C15	-177.1 (3)	C8—N1—S1—O1	174.31 (19)
C13—C14—C15—F1	179.6 (3)	C11—N1—S1—C4	66.8 (2)
C13—C14—C15—C16	-0.3 (4)	C8—N1—S1—C4	-70.4 (2)
F1—C15—C16—C17	-179.3 (3)	C3—C4—S1—O2	-28.3 (3)
C14—C15—C16—C17	0.6 (5)	C5—C4—S1—O2	153.0 (2)
F1—C15—C16—F2	0.2 (4)	C3—C4—S1—O1	-159.6 (2)
C14—C15—C16—F2	-179.9 (3)	C5—C4—S1—O1	21.8 (3)
F2—C16—C17—C18	179.8 (3)	C3—C4—S1—N1	86.1 (2)
C15—C16—C17—C18	-0.7 (5)	C5—C4—S1—N1	-92.5 (2)
C16—C17—C18—C13	0.4 (5)		

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C3—H3 \cdots O1 ⁱ	0.93	2.67	3.380 (4)	134
C7—H7A \cdots O1 ⁱⁱ	0.96	2.66	3.400 (4)	134
C10—H10B \cdots F1 ⁱⁱⁱ	0.97	2.66	3.585 (3)	160

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