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

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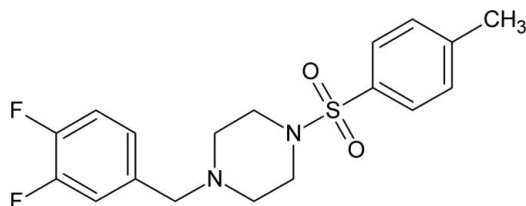
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In the title compound, $C_{18}H_{20}F_2N_2O_2S$, the central piperazine ring adopts a chair conformation. The dihedral angle between the two benzene rings is 40.20°, whereas those between the piperazine ring (considering the best fit plane through 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 C—H···O and C—H···F interactions.

## Related literature

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



## Experimental

### Crystal data

| | |
|---|---|
| $C_{18}H_{20}F_2N_2O_2S$ | $b$ = 36.0404 (8) Å |
| $M_r$ = 366.42 | $c$ = 7.6093 (2) Å |
| Monoclinic, $P2_1/c$ | $\beta$ = 99.728 (2)° |
| $a$ = 6.6680 (2) Å | $V$ = 1802.35 (8) Å$^3$ |
| $Z$ = 4 | $T$ = 298 K |
| Mo $K\alpha$ radiation | $0.28 \times 0.24 \times 0.20$ mm |
| $\mu$ = 0.21 mm$^{-1}$ | |

### Data collection

| | |
|---|---|
| Bruker APEXII diffractometer | 2434 independent reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) $T_{min}$ = 0.943, $T_{max}$ = 0.959 | 1910 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.025 |
| 9583 measured reflections | $\theta_{max}$ = 22.8° |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.045 | 227 parameters |
| $wR(F^2)$ = 0.114 | H-atom parameters constrained |
| $S$ = 1.02 | $\Delta\rho_{max}$ = 0.19 e Å$^{-3}$ |
| 2434 reflections | $\Delta\rho_{min}$ = −0.25 e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3···O1$^i$ | 0.93 | 2.67 | 3.380 (4) | 134 |
| C7—H7$A$···O1$^{ii}$ | 0.96 | 2.66 | 3.400 (4) | 134 |
| C10—H10$B$···F1$^{iii}$ | 0.97 | 2.66 | 3.585 (3) | 160 |

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

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*.

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

## References

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# supporting information

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

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### S1. 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 *P*2$_1$/*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)°, 76.86° and 30.97 (2)° respectively in (I), 1-(2,4-dichlorobenzyl)-4-[(4-methyl-phenyl)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)° and 2.44 (13)° in I, 74.36° and 68.29 (3)° in II, and 69.4 (2)° and 75.98 (2)° in III.

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

### S2. 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.

### S3. 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 CH$_3$.

Crystals were small and very weakly diffracting, with no significant data obtained beyond $\theta$ = 22.8° hence the low values of sin($\theta/\lambda$). However the structure solved and refined satisfactorily and gave acceptable residuals and su values.
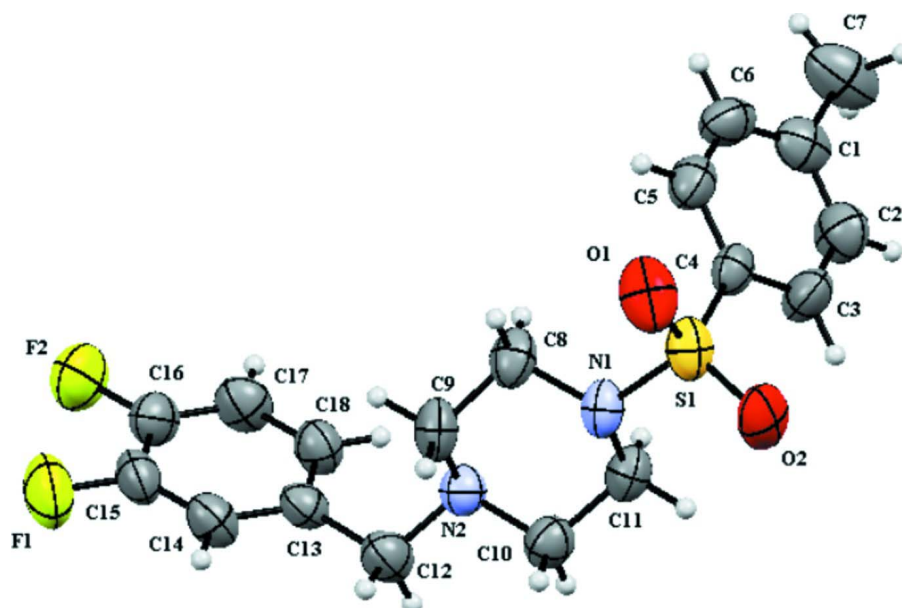
**Figure 1**

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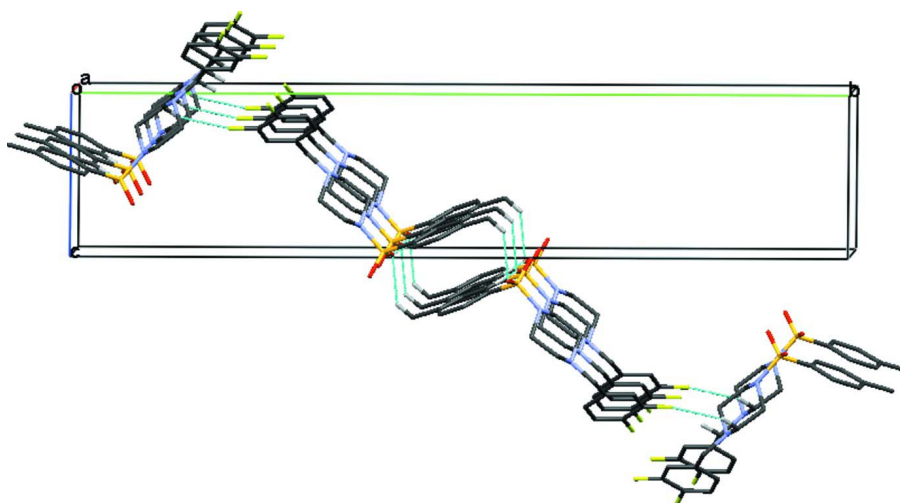


**Figure 2**

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*

| | |
|---|---|
| $C_{18}H_{20}F_2N_2O_2S$ | $c = 7.6093$ (2) Å |
| $M_r = 366.42$ | $\beta = 99.728$ (2)° |
| Monoclinic, $P2_1/c$ | $V = 1802.35$ (8) Å$^3$ |
| Hall symbol: -P 2ybc | $Z = 4$ |
| $a = 6.6680$ (2) Å | $F(000) = 768$ |
| $b = 36.0404$ (8) Å | prism |

$D_x = 1.350$ Mg m$^{-3}$

Melting point: 501 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 227 reflections

$\theta = 2.3$–$22.8°$

$\mu = 0.21$ mm$^{-1}$

$T = 298$ K

Prism, colourless

$0.28 \times 0.24 \times 0.20$ mm

*Data collection*

Bruker APEXII
  diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 1.03 pixels mm$^{-1}$

$\varphi$ and $\omega$ 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 $I > 2\sigma(I)$

$R_{int} = 0.025$

$\theta_{max} = 22.8°$, $\theta_{min} = 2.3°$

$h = -7 \rightarrow 7$

$k = -39 \rightarrow 37$

$l = -7 \rightarrow 8$

*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 $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.028$

$\Delta\rho_{max} = 0.19$ e Å$^{-3}$

$\Delta\rho_{min} = -0.25$ 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 (Å$^2$)*

|    | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|----|-----|-----|-----|---------------------|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)

| 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 (Å, º)*

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
|---|---|---|---|---|
| C3—H3⋯O1[i] | 0.93 | 2.67 | 3.380 (4) | 134 |
| C7—H7*A*⋯O1[ii] | 0.96 | 2.66 | 3.400 (4) | 134 |
| C10—H10*B*⋯F1[iii] | 0.97 | 2.66 | 3.585 (3) | 160 |

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