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# 3,5-Bis(trifluoromethyl)phenyl 4-methylbenzenesulfonate

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**Keywords:** crystal structure; tosylates; cross-coupling reactions.

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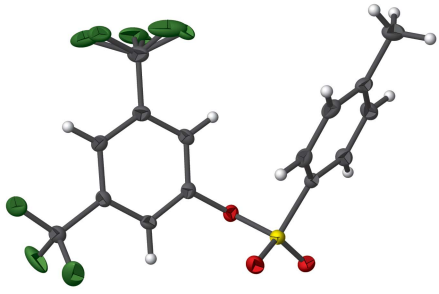
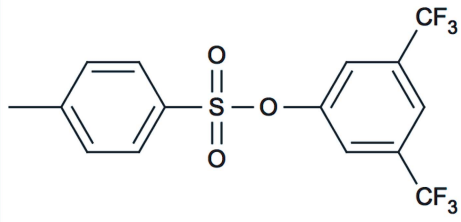
**Structural data**: full structural data are available from iucrdata.iucr.org

Molecules of the title compound, $C_{15}H_{10}F_6O_3S$, are composed of 3,5-bis(trifluoromethyl)phenyl substituted with a toluene-4-sulfonate group. The dihedral angle between two aromatic moieties is 45.10 (5)°. In the crystal, molecules are connected by weak C—H···O and C—H···F contacts. One of the trifluoromethyl groups is disordered.

**3D view**



**Chemical scheme**




## Structure description

Transition-metal-catalyzed cross-coupling reactions can be applied to aryl tosylates (Ackermann *et al.*, 2006; Zhou & Fu, 2003). We apply 4-methylbenzenesulfonates to study the reaction progress and performance using first-row metal catalysts. The high natural abundance of these non-precious transition metal elements makes them an interesting target of study (Torborg & Beller, 2009).

In the asymmetric unit of the title compound, there is one independent molecule. The molecular structure is shown in Fig. 1. In the molecular structure, the bond lengths and angles are within normal ranges (Allen *et al.*, 2002). One of the trifluoromethyl groups in the molecule is disordered with occupation factors of 0.65 and 0.35. The dihedral angle between the aromatic moieties is 45.10 (5)°.

In the crystal (Fig. 2), there are two hydrogen bonds (Table 1), both of which connect the molecules into dimers. There are also two F···$\pi$ T-shape halogen bonds to a 3,5-di(trifluoromethyl)phenyl moiety. The distances of F5$A^{i}$ and F5$B^{i}$ from the centre of a plane defined by atoms C9–C13 of the 3,5-di(trifluoromethyl)phenyl ring are 3.348 (12) and 3.256 (19) Å [symmetry code: (i) $-x$, $-y+1$, $-z+1$].

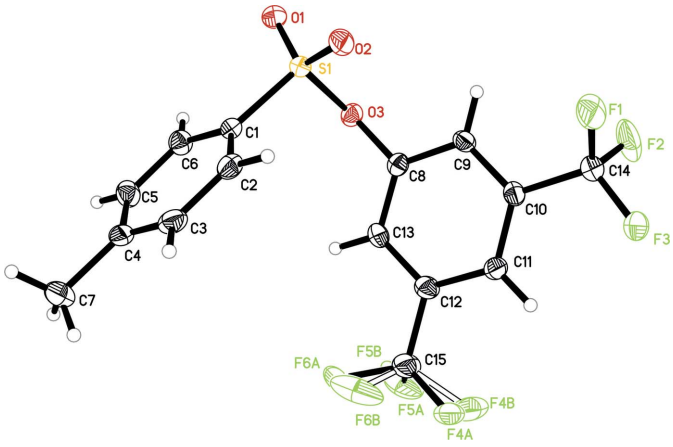



**Figure 1**
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

## Synthesis and crystallization

3,5-Di(trifluoromethyl)phenyl 4-methylbenzenesulfonate was synthesized according to a procedure described by Murai and co-workers (Murai *et al.*, 2012). The crystallization was performed in a diethyl ether solution. Diethyl ether (0.6 ml) was placed in storage reaction vials (8 ml) with silicone septa. The title compound was placed in small portions until a saturated solution was obtained. The solution was warmed, then left to stand in refrigerator (−20°C).

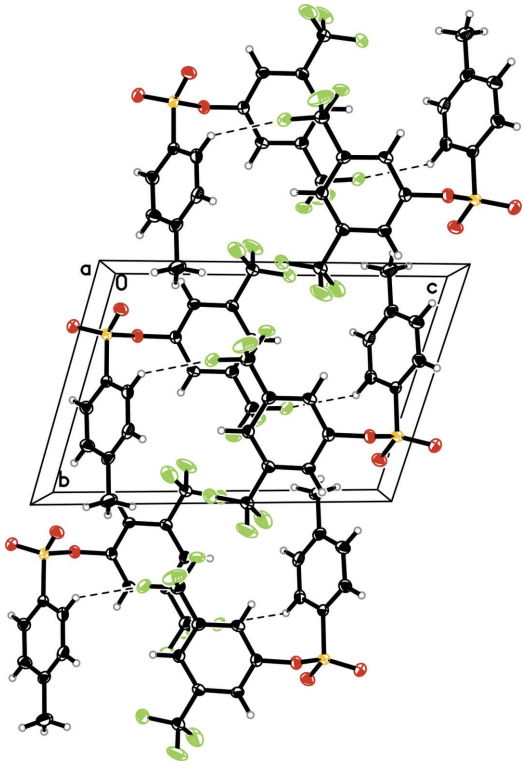



**Figure 2**
The crystal packing of the title compound, viewed along the *a* axis. Disordered fluorine atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···F4A$^{i}$ | 0.93 | 2.55 | 3.308 (3) | 139 |
| C9—H9···O1$^{ii}$ | 0.93 | 2.40 | 3.2959 (17) | 162 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{15}H_{10}F_6O_3S$ |
| $M_r$ | 384.29 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 100 |
| *a*, *b*, *c* (Å) | 8.2805 (3), 8.6053 (3), 12.2396 (4) |
| $\alpha, \beta, \gamma$ (°) | 103.519 (3), 99.935 (3), 105.188 (3) |
| *V* (Å$^3$) | 792.56 (5) |
| *Z* | 2 |
| Radiation type | Mo *K*$\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.28 |
| Crystal size (mm) | 0.4 × 0.25 × 0.24 |
| Data collection | |
| Diffractometer | Oxford Diffraction Xcalibur |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 5437, 3070, 2614 |
| $R_{int}$ | 0.013 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.616 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.030, 0.080, 1.06 |
| No. of reflections | 3070 |
| No. of parameters | 254 |
| No. of restraints | 36 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.27, −0.37 |

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2008), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *SHELXTL* (Sheldrick, 2008).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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# full crystallographic data

*IUCrData* (2017). **2**, x170981 [https://doi.org/10.1107/S2414314617009816]

## 3,5-Bis(trifluoromethyl)phenyl 4-methylbenzenesulfonate

**Aleksandra Olszowy, Dawid Siodłak and Bartosz Zarychta**

### 3,5-Bis(trifluoromethyl)phenyl 4-methylbenzenesulfonate

*Crystal data*

$C_{15}H_{10}F_6O_3S$
$M_r$ = 384.29
Triclinic, $P\overline{1}$
$a$ = 8.2805 (3) Å
$b$ = 8.6053 (3) Å
$c$ = 12.2396 (4) Å
$\alpha$ = 103.519 (3)°
$\beta$ = 99.935 (3)°
$\gamma$ = 105.188 (3)°
$V$ = 792.56 (5) Å$^3$
$Z$ = 2
$F(000)$ = 388
$D_x$ = 1.610 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5437 reflections
$\theta$ = 3.5–26.0°
$\mu$ = 0.28 mm$^{-1}$
$T$ = 100 K
Irregular, colourless
0.4 × 0.25 × 0.24 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 1024 x 1024 with blocks 2 x 2 pixels mm$^{-1}$
$\omega$–scan
5437 measured reflections
3070 independent reflections
2614 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.013
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 3.5°
$h$ = −10→10
$k$ = −6→10
$l$ = −15→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
$S$ = 1.06
3070 reflections
254 parameters
36 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.1137P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. All H atoms were found in a difference map but set to idealized positions and treated as riding with $C_{Ar}$—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) and with $C_{methyl}$—H = 0.96 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| S1 | 0.18701 (5) | 0.27629 (4) | 0.03515 (3) | 0.01913 (11) | |
| O1 | 0.07383 (14) | 0.23781 (13) | −0.07602 (9) | 0.0260 (3) | |
| O2 | 0.28474 (14) | 0.16929 (13) | 0.05977 (9) | 0.0253 (3) | |
| O3 | 0.05670 (13) | 0.27937 (12) | 0.11983 (8) | 0.0194 (2) | |
| F1 | 0.27606 (16) | −0.09183 (13) | 0.34224 (9) | 0.0447 (3) | |
| F2 | 0.03104 (14) | −0.12166 (12) | 0.38253 (10) | 0.0457 (3) | |
| F3 | 0.26421 (14) | 0.01544 (11) | 0.51597 (8) | 0.0371 (3) | |
| F4A | 0.3770 (3) | 0.6057 (3) | 0.62880 (19) | 0.0405 (6) | 0.65 |
| F5A | 0.1573 (14) | 0.6652 (12) | 0.5462 (8) | 0.0432 (17) | 0.65 |
| F6A | 0.3974 (7) | 0.7323 (6) | 0.4990 (3) | 0.0254 (6) | 0.65 |
| F5B | 0.134 (2) | 0.669 (2) | 0.5219 (14) | 0.0266 (17) | 0.35 |
| F4B | 0.2762 (7) | 0.5775 (6) | 0.6351 (4) | 0.0582 (13) | 0.35 |
| F6B | 0.3987 (15) | 0.7169 (12) | 0.5299 (7) | 0.055 (2) | 0.35 |
| C1 | 0.32014 (19) | 0.48591 (18) | 0.07914 (12) | 0.0179 (3) | |
| C2 | 0.48144 (19) | 0.53300 (19) | 0.15499 (13) | 0.0215 (3) | |
| H2 | 0.5222 | 0.4533 | 0.1802 | 0.026* | |
| C3 | 0.5807 (2) | 0.7017 (2) | 0.19247 (13) | 0.0246 (3) | |
| H3 | 0.6894 | 0.7346 | 0.2429 | 0.030* | |
| C4 | 0.5209 (2) | 0.82248 (19) | 0.15611 (13) | 0.0234 (3) | |
| C5 | 0.3587 (2) | 0.77115 (19) | 0.07913 (14) | 0.0242 (3) | |
| H5 | 0.3177 | 0.8507 | 0.0538 | 0.029* | |
| C6 | 0.2580 (2) | 0.60379 (19) | 0.03999 (13) | 0.0216 (3) | |
| H6 | 0.1503 | 0.5704 | −0.0117 | 0.026* | |
| C7 | 0.6294 (2) | 1.0054 (2) | 0.19699 (15) | 0.0336 (4) | |
| H7A | 0.6946 | 1.0293 | 0.1418 | 0.050* | |
| H7B | 0.7071 | 1.0288 | 0.2710 | 0.050* | |
| H7C | 0.5556 | 1.0747 | 0.2042 | 0.050* | |
| C8 | 0.12143 (18) | 0.28625 (18) | 0.23573 (12) | 0.0172 (3) | |
| C9 | 0.12658 (18) | 0.13922 (17) | 0.26128 (13) | 0.0183 (3) | |
| H9 | 0.0925 | 0.0376 | 0.2028 | 0.022* | |
| C10 | 0.18379 (19) | 0.14705 (18) | 0.37620 (13) | 0.0183 (3) | |
| C11 | 0.23417 (19) | 0.29824 (18) | 0.46388 (13) | 0.0193 (3) | |
| H11 | 0.2714 | 0.3021 | 0.5409 | 0.023* | |
| C12 | 0.22819 (19) | 0.44313 (18) | 0.43511 (13) | 0.0212 (3) | |
| C13 | 0.17096 (19) | 0.43894 (18) | 0.32017 (13) | 0.0196 (3) | |
| H13 | 0.1663 | 0.5364 | 0.3010 | 0.024* | |
| C14 | 0.1894 (2) | −0.01242 (19) | 0.40458 (14) | 0.0247 (3) | |
| C15 | 0.2802 (3) | 0.6082 (2) | 0.52824 (14) | 0.0308 (4) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0247 (2) | 0.01547 (19) | 0.01623 (19) | 0.00521 (15) | 0.00510 (15) | 0.00420 (14) |
| O1 | 0.0326 (6) | 0.0220 (6) | 0.0168 (5) | 0.0023 (5) | 0.0022 (5) | 0.0034 (4) |
| O2 | 0.0344 (6) | 0.0198 (5) | 0.0274 (6) | 0.0126 (5) | 0.0131 (5) | 0.0088 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O3 | 0.0201 (5) | 0.0210 (5) | 0.0170 (5) | 0.0058 (4) | 0.0030 (4) | 0.0070 (4) |
| F1 | 0.0808 (9) | 0.0347 (6) | 0.0450 (7) | 0.0411 (6) | 0.0343 (6) | 0.0212 (5) |
| F2 | 0.0434 (6) | 0.0265 (5) | 0.0610 (8) | −0.0035 (5) | 0.0023 (5) | 0.0253 (5) |
| F3 | 0.0649 (7) | 0.0238 (5) | 0.0235 (5) | 0.0183 (5) | 0.0016 (5) | 0.0105 (4) |
| F4A | 0.0712 (15) | 0.0204 (9) | 0.0191 (9) | 0.0125 (11) | −0.0070 (11) | 0.0012 (7) |
| F5A | 0.038 (3) | 0.027 (2) | 0.056 (4) | 0.0084 (15) | 0.022 (3) | −0.008 (2) |
| F6A | 0.0257 (11) | 0.0137 (9) | 0.0306 (14) | 0.0016 (8) | 0.0007 (11) | 0.0049 (10) |
| F5B | 0.034 (4) | 0.011 (2) | 0.039 (4) | 0.012 (2) | 0.017 (3) | 0.006 (3) |
| F4B | 0.116 (4) | 0.033 (2) | 0.0211 (18) | 0.039 (3) | −0.005 (3) | −0.0005 (15) |
| F6B | 0.032 (3) | 0.037 (4) | 0.070 (5) | 0.004 (3) | 0.009 (4) | −0.023 (3) |
| C1 | 0.0217 (7) | 0.0169 (7) | 0.0149 (7) | 0.0049 (6) | 0.0063 (6) | 0.0042 (6) |
| C2 | 0.0247 (8) | 0.0249 (8) | 0.0169 (7) | 0.0095 (7) | 0.0054 (6) | 0.0077 (6) |
| C3 | 0.0227 (8) | 0.0302 (8) | 0.0152 (7) | 0.0036 (7) | 0.0027 (6) | 0.0027 (6) |
| C4 | 0.0279 (8) | 0.0203 (8) | 0.0187 (8) | 0.0031 (7) | 0.0113 (6) | 0.0007 (6) |
| C5 | 0.0280 (8) | 0.0200 (8) | 0.0286 (9) | 0.0102 (7) | 0.0108 (7) | 0.0092 (7) |
| C6 | 0.0213 (8) | 0.0217 (8) | 0.0221 (8) | 0.0070 (6) | 0.0043 (6) | 0.0076 (6) |
| C7 | 0.0381 (10) | 0.0219 (8) | 0.0314 (10) | 0.0005 (7) | 0.0106 (8) | −0.0008 (7) |
| C8 | 0.0147 (7) | 0.0199 (7) | 0.0176 (7) | 0.0048 (6) | 0.0047 (6) | 0.0066 (6) |
| C9 | 0.0188 (7) | 0.0140 (7) | 0.0195 (7) | 0.0026 (6) | 0.0050 (6) | 0.0028 (6) |
| C10 | 0.0193 (7) | 0.0162 (7) | 0.0213 (8) | 0.0059 (6) | 0.0074 (6) | 0.0071 (6) |
| C11 | 0.0225 (8) | 0.0195 (7) | 0.0166 (7) | 0.0081 (6) | 0.0050 (6) | 0.0051 (6) |
| C12 | 0.0248 (8) | 0.0177 (7) | 0.0213 (8) | 0.0088 (6) | 0.0056 (6) | 0.0039 (6) |
| C13 | 0.0220 (7) | 0.0153 (7) | 0.0235 (8) | 0.0072 (6) | 0.0058 (6) | 0.0075 (6) |
| C14 | 0.0346 (9) | 0.0183 (7) | 0.0221 (8) | 0.0086 (7) | 0.0076 (7) | 0.0072 (6) |
| C15 | 0.0468 (11) | 0.0209 (9) | 0.0233 (9) | 0.0151 (9) | 0.0010 (8) | 0.0042 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.4234 (11) | C4—C5 | 1.395 (2) |
| S1—O2 | 1.4246 (11) | C4—C7 | 1.507 (2) |
| S1—O3 | 1.6208 (11) | C5—C6 | 1.382 (2) |
| S1—C1 | 1.7488 (15) | C5—H5 | 0.9300 |
| O3—C8 | 1.4089 (17) | C6—H6 | 0.9300 |
| F1—C14 | 1.3293 (19) | C7—H7A | 0.9600 |
| F2—C14 | 1.3374 (19) | C7—H7B | 0.9600 |
| F3—C14 | 1.3334 (18) | C7—H7C | 0.9600 |
| F4A—C15 | 1.356 (3) | C8—C13 | 1.378 (2) |
| F5A—C15 | 1.270 (11) | C8—C9 | 1.382 (2) |
| F6A—C15 | 1.402 (5) | C9—C10 | 1.384 (2) |
| F5B—C15 | 1.432 (19) | C9—H9 | 0.9300 |
| F4B—C15 | 1.398 (5) | C10—C11 | 1.388 (2) |
| F6B—C15 | 1.158 (10) | C10—C14 | 1.502 (2) |
| C1—C2 | 1.387 (2) | C11—C12 | 1.383 (2) |
| C1—C6 | 1.393 (2) | C11—H11 | 0.9300 |
| C2—C3 | 1.388 (2) | C12—C13 | 1.394 (2) |
| C2—H2 | 0.9300 | C12—C15 | 1.502 (2) |
| C3—C4 | 1.391 (2) | C13—H13 | 0.9300 |
| C3—H3 | 0.9300 | | |

| | | | |
|---|---|---|---|
| O1—S1—O2 | 121.19 (7) | C8—C9—C10 | 118.28 (13) |
| O1—S1—O3 | 102.31 (6) | C8—C9—H9 | 120.9 |
| O2—S1—O3 | 108.14 (6) | C10—C9—H9 | 120.9 |
| O1—S1—C1 | 110.29 (7) | C9—C10—C11 | 121.09 (13) |
| O2—S1—C1 | 110.36 (7) | C9—C10—C14 | 118.55 (13) |
| O3—S1—C1 | 102.61 (6) | C11—C10—C14 | 120.37 (13) |
| C8—O3—S1 | 117.42 (9) | C12—C11—C10 | 119.08 (14) |
| C2—C1—C6 | 121.31 (14) | C12—C11—H11 | 120.5 |
| C2—C1—S1 | 119.98 (12) | C10—C11—H11 | 120.5 |
| C6—C1—S1 | 118.66 (11) | C11—C12—C13 | 121.06 (14) |
| C1—C2—C3 | 118.59 (14) | C11—C12—C15 | 120.26 (14) |
| C1—C2—H2 | 120.7 | C13—C12—C15 | 118.67 (13) |
| C3—C2—H2 | 120.7 | C8—C13—C12 | 118.07 (13) |
| C2—C3—C4 | 121.34 (14) | C8—C13—H13 | 121.0 |
| C2—C3—H3 | 119.3 | C12—C13—H13 | 121.0 |
| C4—C3—H3 | 119.3 | F1—C14—F3 | 107.05 (13) |
| C3—C4—C5 | 118.76 (14) | F1—C14—F2 | 106.36 (13) |
| C3—C4—C7 | 121.10 (15) | F3—C14—F2 | 106.91 (12) |
| C5—C4—C7 | 120.14 (15) | F1—C14—C10 | 111.94 (13) |
| C6—C5—C4 | 120.95 (15) | F3—C14—C10 | 112.39 (13) |
| C6—C5—H5 | 119.5 | F2—C14—C10 | 111.81 (13) |
| C4—C5—H5 | 119.5 | F5A—C15—F4A | 111.0 (4) |
| C5—C6—C1 | 119.04 (14) | F6B—C15—F4B | 114.9 (5) |
| C5—C6—H6 | 120.5 | F5A—C15—F6A | 106.2 (5) |
| C1—C6—H6 | 120.5 | F4A—C15—F6A | 101.2 (2) |
| C4—C7—H7A | 109.5 | F6B—C15—F5B | 107.7 (8) |
| C4—C7—H7B | 109.5 | F4B—C15—F5B | 94.9 (7) |
| H7A—C7—H7B | 109.5 | F6B—C15—C12 | 119.4 (5) |
| C4—C7—H7C | 109.5 | F5A—C15—C12 | 115.2 (5) |
| H7A—C7—H7C | 109.5 | F4A—C15—C12 | 112.22 (16) |
| H7B—C7—H7C | 109.5 | F4B—C15—C12 | 109.2 (2) |
| C13—C8—C9 | 122.41 (13) | F6A—C15—C12 | 109.9 (2) |
| C13—C8—O3 | 118.51 (12) | F5B—C15—C12 | 107.7 (7) |
| C9—C8—O3 | 119.03 (12) | | |

| | | | |
|---|---|---|---|
| O1—S1—O3—C8 | 169.55 (10) | C14—C10—C11—C12 | 179.80 (14) |
| O2—S1—O3—C8 | 40.56 (11) | C10—C11—C12—C13 | 0.7 (2) |
| C1—S1—O3—C8 | −76.08 (11) | C10—C11—C12—C15 | 179.37 (15) |
| O1—S1—C1—C2 | −152.88 (12) | C9—C8—C13—C12 | 0.1 (2) |
| O2—S1—C1—C2 | −16.32 (15) | O3—C8—C13—C12 | 177.43 (12) |
| O3—S1—C1—C2 | 98.72 (13) | C11—C12—C13—C8 | −0.4 (2) |
| O1—S1—C1—C6 | 29.51 (14) | C15—C12—C13—C8 | −179.14 (15) |
| O2—S1—C1—C6 | 166.07 (11) | C9—C10—C14—F1 | 52.61 (19) |
| O3—S1—C1—C6 | −78.89 (12) | C11—C10—C14—F1 | −127.77 (16) |
| C6—C1—C2—C3 | 0.5 (2) | C9—C10—C14—F3 | 173.13 (13) |
| S1—C1—C2—C3 | −177.05 (11) | C11—C10—C14—F3 | −7.2 (2) |
| C1—C2—C3—C4 | 0.4 (2) | C9—C10—C14—F2 | −66.61 (18) |

| | | | |
|---|---|---|---|
| C2—C3—C4—C5 | −0.9 (2) | C11—C10—C14—F2 | 113.01 (16) |
| C2—C3—C4—C7 | −179.91 (14) | C11—C12—C15—F6B | 116.5 (6) |
| C3—C4—C5—C6 | 0.5 (2) | C13—C12—C15—F6B | −64.8 (6) |
| C7—C4—C5—C6 | 179.48 (14) | C11—C12—C15—F5A | −109.7 (5) |
| C4—C5—C6—C1 | 0.4 (2) | C13—C12—C15—F5A | 69.1 (5) |
| C2—C1—C6—C5 | −0.9 (2) | C11—C12—C15—F4A | 18.7 (3) |
| S1—C1—C6—C5 | 176.65 (12) | C13—C12—C15—F4A | −162.53 (17) |
| S1—O3—C8—C13 | 101.10 (13) | C11—C12—C15—F4B | −18.6 (3) |
| S1—O3—C8—C9 | −81.44 (14) | C13—C12—C15—F4B | 160.1 (3) |
| C13—C8—C9—C10 | 0.0 (2) | C11—C12—C15—F6A | 130.5 (3) |
| O3—C8—C9—C10 | −177.35 (12) | C13—C12—C15—F6A | −50.8 (3) |
| C8—C9—C10—C11 | 0.3 (2) | C11—C12—C15—F5B | −120.5 (7) |
| C8—C9—C10—C14 | 179.88 (13) | C13—C12—C15—F5B | 58.2 (7) |
| C9—C10—C11—C12 | −0.6 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···F4*A*$^{i}$ | 0.93 | 2.55 | 3.308 (3) | 139 |
| C9—H9···O1$^{ii}$ | 0.93 | 2.40 | 3.2959 (17) | 162 |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*, −*z*.