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# 4-(Methylsulfanyl)-2-(*p*-toluenesulfonamido)butanoic acid

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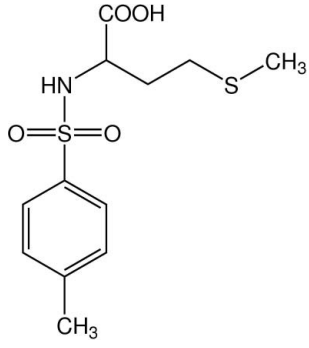
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.043; $wR$ factor = 0.120; data-to-parameter ratio = 15.0.

In the title compound, $C_{12}H_{17}NO_4S_2$, the carboxyl groups link the molecules into centrosymmetric dimers through O—H···O hydrogen bonds. An N—H···O hydrogen bond between the NH group of the L-methionine unit and a neighbouring carboxyl group, together with a complementary C—H···O contact to one O atom of the sulfonyl group, link the dimers into one-dimensional chains along the crystallographic *b* axis.

## Related literature

The title compound is closely related to the previously reported *N*-tosyl-L-glutamic acid (Zachara *et al.*, 2005).




## Experimental

### Crystal data

$C_{12}H_{17}NO_4S_2$
$M_r$ = 303.39
Monoclinic, $C2/c$
$a$ = 33.121 (7) Å
$b$ = 5.6531 (11) Å
$c$ = 17.278 (4) Å
$\beta$ = 116.62 (3)°
$V$ = 2892.2 (10) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.38 mm$^{-1}$
$T$ = 293 (2) K
0.43 × 0.28 × 0.22 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.855, $T_{max}$ = 0.922
6139 measured reflections
2689 independent reflections
2055 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
$S$ = 1.00
2689 reflections
179 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4$A$···O3$^{i}$ | 0.82 | 1.85 | 2.672 (3) | 174 |
| N1—H1···O4$^{ii}$ | 0.81 (3) | 2.62 (3) | 3.405 (3) | 163 (2) |
| C4—H4···O1$^{iii}$ | 0.98 | 2.25 | 3.165 (3) | 155 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2276).

## References

Bruker (2001). *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
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# supporting information

*Acta Cryst.* (2008). E**64**, o706 [doi:10.1107/S1600536808005035]

## 4-(Methylsulfanyl)-2-(*p*-toluenesulfonamido)butanoic acid

**Li Wang, Zheng Liu and Yong Liao Wang**

### S1. Comment

The title compound (Fig. 1) was synthesized from 4-toluenesulfonyl chloride and *L*-methionine. It is closely related to the previously reported *N*-tosyl-*L*-glutamic acid (Zachara *et al.*, 2005).

### S2. Experimental

A solution of *L*-methionine (0.005 mmol) and NaOH (0.015 mmol) in water (15 ml) was added to an ethanol solution of 4-toluenesulfonyl chloride (0.005 mmol). After stirring at 348 K for 40 min, crystals of the title compound were obtained by slow evaporation of the reaction mixture at room temperature.

### S3. Refinement

H atoms bound to C or O atoms were placed geometrically with C—H = 0.93–0.97 Å or O—H = 0.82 Å and refined as riding with $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(C/O). The H atom of the NH group was located in a difference Fourier map and refined with an isotropic displacement parameter, without restraint.

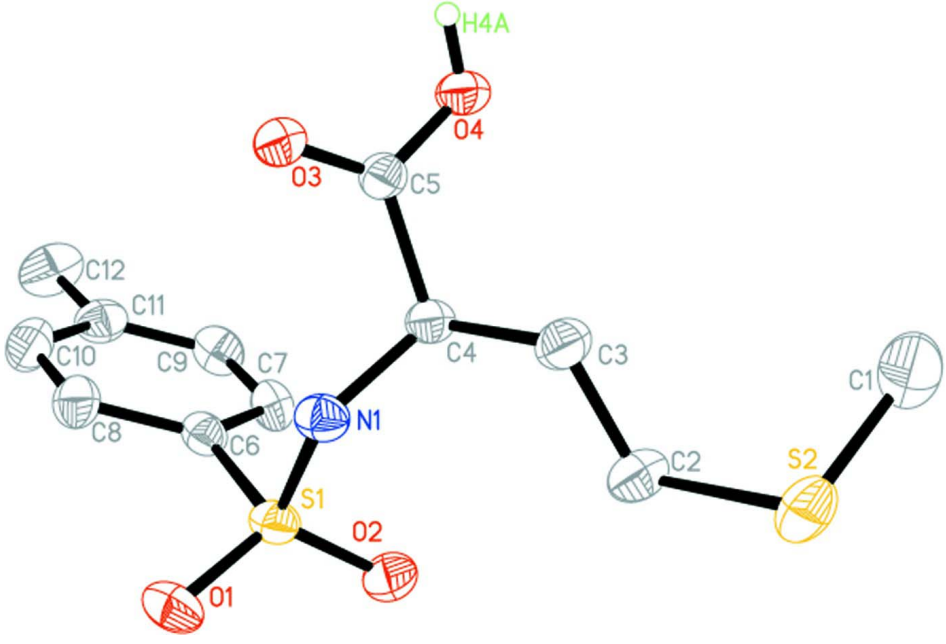


**Figure 1**

The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms. H atoms bound to C and N are omitted.

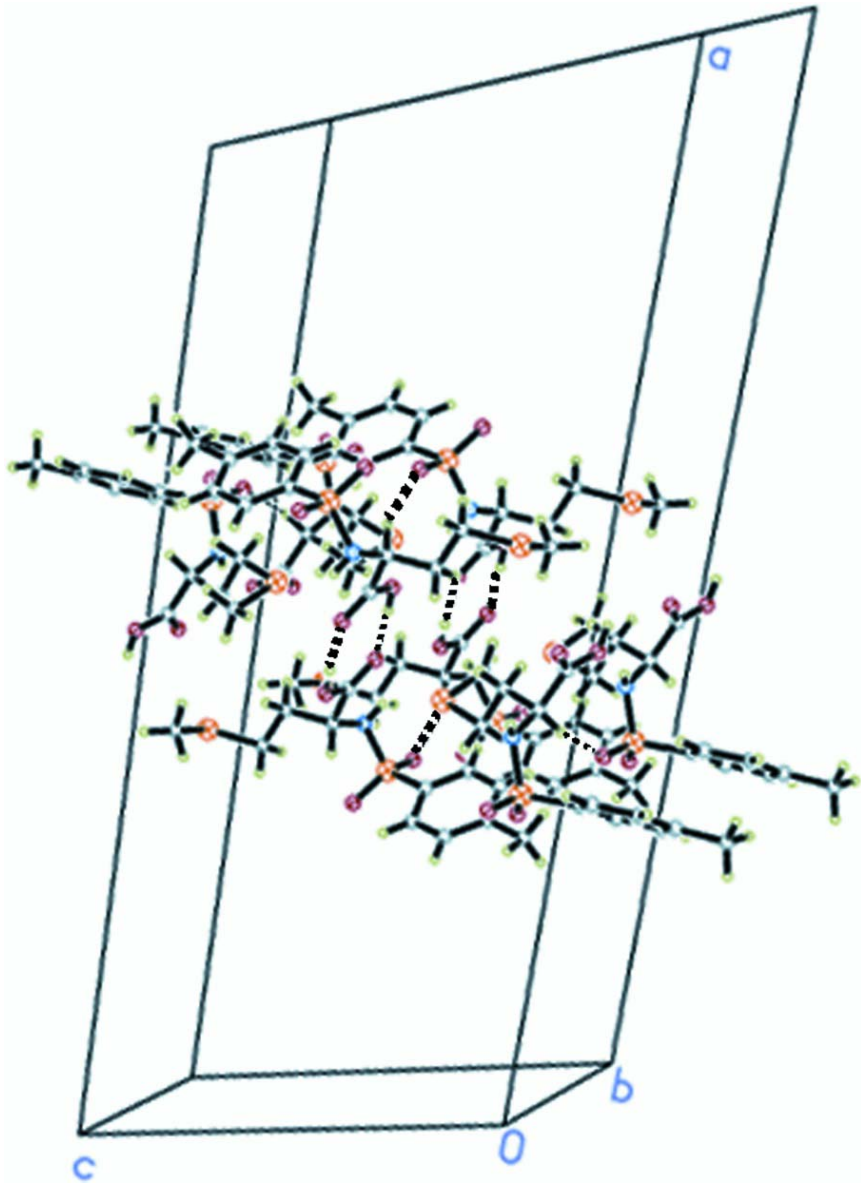


**Figure 2**

Partial packing diagram showing a hydrogen-bonded chain running along the *b* axis.

### 4-(Methylsulfanyl)-2-(*p*-toluenesulfonamido)butanoic acid

*Crystal data*

$C_{12}H_{17}NO_4S_2$
$M_r = 303.39$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 33.121\ (7)$ Å
$b = 5.6531\ (11)$ Å
$c = 17.278\ (4)$ Å
$\beta = 116.62\ (3)°$
$V = 2892.2\ (10)$ Å$^3$
$Z = 8$
$F(000) = 1280$
$D_x = 1.394$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2689 reflections
$\theta = 2.8–25.5°$
$\mu = 0.38$ mm$^{-1}$
$T = 293$ K
Block, colorless
0.43 × 0.28 × 0.22 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.855, $T_{max}$ = 0.922
6139 measured reflections
2689 independent reflections
2055 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.8°
$h$ = −40→30
$k$ = −5→6
$l$ = −17→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
$S$ = 1.00
2689 reflections
179 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 2.0643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.05669 (12) | 0.1441 (6) | −0.2992 (2) | 0.0798 (10) |
| H1A | 0.0814 | 0.0695 | −0.2516 | 0.120* |
| H1B | 0.0514 | 0.0655 | −0.3521 | 0.120* |
| H1C | 0.0300 | 0.1343 | −0.2906 | 0.120* |
| C2 | 0.09539 (9) | 0.5313 (5) | −0.19259 (17) | 0.0532 (7) |
| H2A | 0.1186 | 0.4170 | −0.1596 | 0.064* |
| H2B | 0.1098 | 0.6843 | −0.1860 | 0.064* |
| C3 | 0.06194 (8) | 0.5443 (5) | −0.15563 (16) | 0.0500 (7) |
| H3A | 0.0477 | 0.3909 | −0.1619 | 0.060* |
| H3B | 0.0385 | 0.6573 | −0.1890 | 0.060* |
| C4 | 0.08314 (7) | 0.6170 (4) | −0.05971 (14) | 0.0386 (5) |
| H4 | 0.1099 | 0.5190 | −0.0273 | 0.046* |
| C5 | 0.04899 (8) | 0.5711 (4) | −0.02597 (14) | 0.0392 (5) |
| C6 | 0.16839 (7) | 0.8595 (4) | 0.11546 (15) | 0.0405 (5) |
| C7 | 0.19182 (8) | 0.6522 (5) | 0.14801 (16) | 0.0480 (6) |

| | | | | |
|---|---|---|---|---|
| H7 | 0.1967 | 0.5472 | 0.1117 | 0.058* |
| C8 | 0.16108 (9) | 1.0154 (5) | 0.17034 (18) | 0.0512 (7) |
| H8 | 0.1452 | 1.1554 | 0.1488 | 0.061* |
| C9 | 0.20788 (9) | 0.6019 (5) | 0.23483 (18) | 0.0538 (7) |
| H9 | 0.2235 | 0.4612 | 0.2563 | 0.065* |
| C10 | 0.17754 (9) | 0.9604 (5) | 0.25668 (18) | 0.0586 (7) |
| H10 | 0.1724 | 1.0644 | 0.2930 | 0.070* |
| C11 | 0.20148 (8) | 0.7549 (5) | 0.29100 (17) | 0.0526 (7) |
| C12 | 0.22040 (10) | 0.7014 (7) | 0.38595 (19) | 0.0769 (10) |
| H12A | 0.2242 | 0.5336 | 0.3948 | 0.115* |
| H12B | 0.2000 | 0.7580 | 0.4074 | 0.115* |
| H12C | 0.2491 | 0.7783 | 0.4164 | 0.115* |
| N1 | 0.09655 (7) | 0.8649 (4) | −0.04861 (13) | 0.0429 (5) |
| H1 | 0.0819 (9) | 0.958 (5) | −0.0360 (18) | 0.051 (8)* |
| O1 | 0.15126 (6) | 1.1856 (3) | 0.00061 (12) | 0.0545 (5) |
| O2 | 0.17393 (5) | 0.7911 (3) | −0.02689 (11) | 0.0520 (5) |
| O3 | 0.02802 (6) | 0.7289 (3) | −0.01265 (11) | 0.0479 (4) |
| O4 | 0.04342 (6) | 0.3447 (3) | −0.01734 (12) | 0.0499 (5) |
| H4A | 0.0204 | 0.3249 | −0.0115 | 0.075* |
| S1 | 0.149864 (19) | 0.93464 (11) | 0.00597 (4) | 0.0414 (2) |
| S2 | 0.07010 (3) | 0.44879 (15) | −0.30518 (4) | 0.0630 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.100 (3) | 0.073 (2) | 0.069 (2) | 0.007 (2) | 0.0400 (19) | −0.0020 (17) |
| C2 | 0.0484 (14) | 0.072 (2) | 0.0443 (14) | 0.0011 (13) | 0.0249 (12) | 0.0054 (13) |
| C3 | 0.0437 (14) | 0.0659 (18) | 0.0441 (14) | −0.0064 (12) | 0.0231 (11) | −0.0046 (12) |
| C4 | 0.0380 (12) | 0.0417 (14) | 0.0382 (12) | −0.0031 (10) | 0.0190 (10) | 0.0019 (10) |
| C5 | 0.0424 (13) | 0.0435 (15) | 0.0326 (12) | −0.0045 (11) | 0.0175 (10) | −0.0006 (10) |
| C6 | 0.0353 (12) | 0.0368 (13) | 0.0474 (13) | −0.0032 (10) | 0.0167 (10) | −0.0014 (11) |
| C7 | 0.0503 (14) | 0.0377 (14) | 0.0509 (15) | 0.0017 (12) | 0.0182 (12) | −0.0033 (11) |
| C8 | 0.0529 (15) | 0.0439 (16) | 0.0607 (17) | 0.0093 (12) | 0.0290 (13) | 0.0011 (12) |
| C9 | 0.0474 (15) | 0.0459 (16) | 0.0599 (17) | 0.0045 (12) | 0.0168 (13) | 0.0079 (13) |
| C10 | 0.0564 (16) | 0.068 (2) | 0.0570 (17) | 0.0012 (14) | 0.0301 (14) | −0.0105 (14) |
| C11 | 0.0374 (13) | 0.0666 (19) | 0.0518 (15) | −0.0045 (13) | 0.0182 (11) | 0.0017 (13) |
| C12 | 0.0579 (18) | 0.116 (3) | 0.0528 (18) | 0.0025 (18) | 0.0210 (14) | 0.0104 (18) |
| N1 | 0.0386 (11) | 0.0409 (13) | 0.0508 (12) | 0.0019 (10) | 0.0214 (10) | 0.0059 (10) |
| O1 | 0.0543 (11) | 0.0385 (11) | 0.0688 (12) | −0.0036 (8) | 0.0259 (9) | 0.0097 (8) |
| O2 | 0.0434 (9) | 0.0596 (12) | 0.0605 (11) | −0.0002 (8) | 0.0300 (9) | −0.0021 (9) |
| O3 | 0.0552 (10) | 0.0449 (11) | 0.0555 (11) | −0.0038 (8) | 0.0353 (9) | −0.0017 (8) |
| O4 | 0.0556 (11) | 0.0447 (11) | 0.0633 (11) | −0.0053 (8) | 0.0391 (9) | 0.0012 (8) |
| S1 | 0.0362 (3) | 0.0394 (4) | 0.0498 (4) | −0.0030 (2) | 0.0202 (3) | 0.0023 (3) |
| S2 | 0.0773 (5) | 0.0750 (6) | 0.0407 (4) | 0.0063 (4) | 0.0300 (4) | 0.0059 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—S2 | 1.793 (4) | C6—S1 | 1.760 (3) |
| C1—H1A | 0.960 | C7—C9 | 1.378 (4) |
| C1—H1B | 0.960 | C7—H7 | 0.930 |
| C1—H1C | 0.960 | C8—C10 | 1.375 (4) |
| C2—C3 | 1.508 (3) | C8—H8 | 0.930 |
| C2—S2 | 1.801 (3) | C9—C11 | 1.385 (4) |
| C2—H2A | 0.970 | C9—H9 | 0.930 |
| C2—H2B | 0.970 | C10—C11 | 1.381 (4) |
| C3—C4 | 1.538 (3) | C10—H10 | 0.930 |
| C3—H3A | 0.970 | C11—C12 | 1.501 (4) |
| C3—H3B | 0.970 | C12—H12A | 0.960 |
| C4—N1 | 1.457 (3) | C12—H12B | 0.960 |
| C4—C5 | 1.509 (3) | C12—H12C | 0.960 |
| C4—H4 | 0.980 | N1—S1 | 1.634 (2) |
| C5—O3 | 1.214 (3) | N1—H1 | 0.81 (3) |
| C5—O4 | 1.311 (3) | O1—S1 | 1.4238 (19) |
| C6—C7 | 1.378 (4) | O2—S1 | 1.4216 (18) |
| C6—C8 | 1.393 (4) | O4—H4A | 0.820 |
| | | | |
| S2—C1—H1A | 109.5 | C9—C7—H7 | 120.3 |
| S2—C1—H1B | 109.5 | C6—C7—H7 | 120.3 |
| H1A—C1—H1B | 109.5 | C10—C8—C6 | 119.3 (3) |
| S2—C1—H1C | 109.5 | C10—C8—H8 | 120.3 |
| H1A—C1—H1C | 109.5 | C6—C8—H8 | 120.3 |
| H1B—C1—H1C | 109.5 | C7—C9—C11 | 121.9 (3) |
| C3—C2—S2 | 113.29 (18) | C7—C9—H9 | 119.1 |
| C3—C2—H2A | 108.9 | C11—C9—H9 | 119.1 |
| S2—C2—H2A | 108.9 | C8—C10—C11 | 121.9 (3) |
| C3—C2—H2B | 108.9 | C8—C10—H10 | 119.1 |
| S2—C2—H2B | 108.9 | C11—C10—H10 | 119.0 |
| H2A—C2—H2B | 107.7 | C10—C11—C9 | 117.6 (3) |
| C2—C3—C4 | 113.7 (2) | C10—C11—C12 | 121.1 (3) |
| C2—C3—H3A | 108.8 | C9—C11—C12 | 121.3 (3) |
| C4—C3—H3A | 108.8 | C11—C12—H12A | 109.5 |
| C2—C3—H3B | 108.8 | C11—C12—H12B | 109.5 |
| C4—C3—H3B | 108.8 | H12A—C12—H12B | 109.5 |
| H3A—C3—H3B | 107.7 | C11—C12—H12C | 109.5 |
| N1—C4—C5 | 110.6 (2) | H12A—C12—H12C | 109.5 |
| N1—C4—C3 | 111.3 (2) | H12B—C12—H12C | 109.5 |
| C5—C4—C3 | 108.11 (18) | C4—N1—S1 | 119.67 (17) |
| N1—C4—H4 | 108.9 | C4—N1—H1 | 119 (2) |
| C5—C4—H4 | 108.9 | S1—N1—H1 | 108 (2) |
| C3—C4—H4 | 108.9 | C5—O4—H4A | 109.5 |
| O3—C5—O4 | 125.0 (2) | O2—S1—O1 | 120.15 (11) |
| O3—C5—C4 | 122.6 (2) | O2—S1—N1 | 106.62 (12) |
| O4—C5—C4 | 112.3 (2) | O1—S1—N1 | 105.14 (11) |

| | | | |
|---|---|---|---|
| C7—C6—C8 | 119.9 (2) | O2—S1—C6 | 107.68 (11) |
| C7—C6—S1 | 120.36 (19) | O1—S1—C6 | 107.74 (12) |
| C8—C6—S1 | 119.7 (2) | N1—S1—C6 | 109.16 (11) |
| C9—C7—C6 | 119.5 (2) | C1—S2—C2 | 101.15 (15) |
| | | | |
| S2—C2—C3—C4 | −179.45 (19) | C7—C9—C11—C10 | 1.1 (4) |
| C2—C3—C4—N1 | 70.7 (3) | C7—C9—C11—C12 | −178.1 (3) |
| C2—C3—C4—C5 | −167.6 (2) | C5—C4—N1—S1 | 123.41 (19) |
| N1—C4—C5—O3 | 17.0 (3) | C3—C4—N1—S1 | −116.39 (19) |
| C3—C4—C5—O3 | −105.1 (3) | C4—N1—S1—O2 | 48.6 (2) |
| N1—C4—C5—O4 | −166.15 (18) | C4—N1—S1—O1 | 177.16 (17) |
| C3—C4—C5—O4 | 71.7 (3) | C4—N1—S1—C6 | −67.5 (2) |
| C8—C6—C7—C9 | −0.1 (4) | C7—C6—S1—O2 | −16.2 (2) |
| S1—C6—C7—C9 | 176.96 (19) | C8—C6—S1—O2 | 160.89 (19) |
| C7—C6—C8—C10 | 0.2 (4) | C7—C6—S1—O1 | −147.2 (2) |
| S1—C6—C8—C10 | −177.0 (2) | C8—C6—S1—O1 | 29.9 (2) |
| C6—C7—C9—C11 | −0.5 (4) | C7—C6—S1—N1 | 99.2 (2) |
| C6—C8—C10—C11 | 0.4 (4) | C8—C6—S1—N1 | −83.7 (2) |
| C8—C10—C11—C9 | −1.0 (4) | C3—C2—S2—C1 | −70.4 (3) |
| C8—C10—C11—C12 | 178.1 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4*A*···O3$^{i}$ | 0.82 | 1.85 | 2.672 (3) | 174 |
| N1—H1···O4$^{ii}$ | 0.81 (3) | 2.62 (3) | 3.405 (3) | 163 (2) |
| C4—H4···O1$^{iii}$ | 0.98 | 2.25 | 3.165 (3) | 155 |

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