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# (2*S*)-Methyl 2-(4-chlorobenzenesulfonamido)-4-(methylsulfanyl)butanoate

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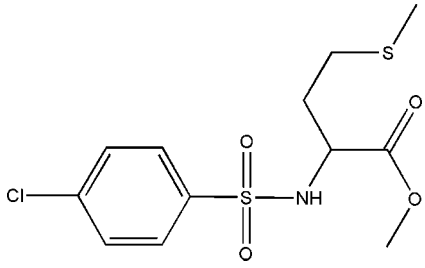
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.025; $wR$ factor = 0.062; data-to-parameter ratio = 16.5.

The enantiomerically pure title compound, $C_{12}H_{16}ClNO_4S_2$, contains a pyramidal N atom with an S—N bond length of 1.6306 (15) Å. Molecules are linked to form chains parallel to the *a* axis by classical N—H···O hydrogen bonding involving a sulfonyl O atom, supported by three weak C—H···$X$ interactions. ($X$ = S, O).

## Related literature

For the applications of esters in industry and as intermediates in the synthesis of heterocycles, see: Akhtar *et al.* (2007, 2008); Kashif *et al.* (2008); Serwar *et al.* (2009); Syed *et al.* (2009).




## Experimental

### Crystal data

$C_{12}H_{16}ClNO_4S_2$
$M_r$ = 337.83
Orthorhombic, $P2_12_12_1$
$a$ = 5.1814 (3) Å
$b$ = 12.6089 (8) Å
$c$ = 23.2137 (13) Å
$V$ = 1516.59 (16) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 4.92 mm$^{-1}$
$T$ = 100 K
0.20 × 0.12 × 0.06 mm

### Data collection

Oxford Diffraction Xcalibur Nova A diffractometer
Absorption correction: multi-scan (*CrysAlis Pro*; Oxford Diffraction, 2008)
$T_{min}$ = 0.548, $T_{max}$ = 1.000 (expected range = 0.408–0.744)
14469 measured reflections
3093 independent reflections
3027 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
$S$ = 1.04
3093 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$
Absolute structure: Flack (1983), 1250 Friedel pairs
Flack parameter: 0.005 (12)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N—H01···O3$^{i}$ | 0.81 (3) | 2.30 (3) | 3.1048 (18) | 169 (3) |
| C2—H2···O1$^{ii}$ | 1.00 | 2.66 | 3.637 (2) | 166 |
| C12—H12···O1$^{ii}$ | 0.95 | 2.37 | 3.315 (2) | 173 |
| C3—H3*B*···O3$^{iii}$ | 0.99 | 2.66 | 3.635 (2) | 170 |
| C5—H5*B*···S1$^{iv}$ | 0.98 | 2.97 | 3.892 (2) | 157 |
| C5—H5*C*···S1$^{i}$ | 0.98 | 2.88 | 3.665 (2) | 138 |

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$.

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2008); cell refinement: *CrysAlis Pro*; data reduction: *CrysAlis Pro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Siemens, 1994); 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: BT2959).

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# supporting information

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## (2*S*)-Methyl 2-(4-chlorobenzenesulfonamido)-4-(methylsulfanyl)butanoate

**Tayyaba Syed, Shahid Hameed and Peter G. Jones**

### S1. Comment

Esters have attracted widespread attention due to their applications in industry and as intermediates in the synthesis of heterocycles (Syed *et al.*, 2009; Akhtar *et al.*, 2008, 2007; Serwar *et al.*, 2009). several types of pharmacological activities have also been associated with sulfonamides (Akhtar *et al.*, 2008, Kashif *et al.*, 2008). The title compound (I), a methionine derivative, was synthesized in our laboratory as an intermediate for onward conversion to 1,3,4-oxadiazole derivatives, and here we report its structure.

Molecular dimensions of (I) may be considered normal. The nitrogen atom displays a pyramidal geometry (Syed *et al.*, 2009), lying 0.27 (1) Å out of the plane of its substituents. The molecule adopts the general shape of a thick disc (as is reflected in the short **a** axis length), with the ester group folded under the aromatic ring (C1···C11 3.374 (2) Å, C11—S2···C2—C1 - 19.3 (1)°). The molecules are connected in chains parallel to the **a** axis by the classical hydrogen bond N—H01···O3 (H···O 2.30 (3) Å), supported by the "weak" hydrogen bonds H2···O1, H12···O1 (a bifurcated system) and H5C···S1 (H···*X* 2.66, 2.37, 2.88 Å respectively). Symmetry operators for all these H bonds involve **a** axis translation.

### S2. Experimental

The title compound was synthesized by the reaction of methionine (0.02 mol) and 4-chlorobenzenesulfonyl chloride according to a reported procedure (Syed *et al.*, 2009). Recrystallization of the product from acetone/water afforded crystals suitable for X-ray analysis.

### S3. Refinement

The NH hydrogen was refined freely. Methyl H atoms were located in difference syntheses, idealized to C—H 0.98 Å and H—C—H 109.5°, and refined as rigid groups allowed to rotate but not tip. Other H atoms were placed in calculated positions and refined using a riding model with C—H 0.95 Å for aromatic H and 1.00 Å for methine CH. Hydrogen *U* values were fixed at 1.5 × *U*(eq) of the parent atom for methyl H and 1.2 × *U*(eq) of the parent atom for other H. The compound is enantiomerically pure and its absolute configuration (*S* at C2) was confirmed by the Flack (1983) parameter. Data are 99.6% complete to 2$\theta$ 145°.

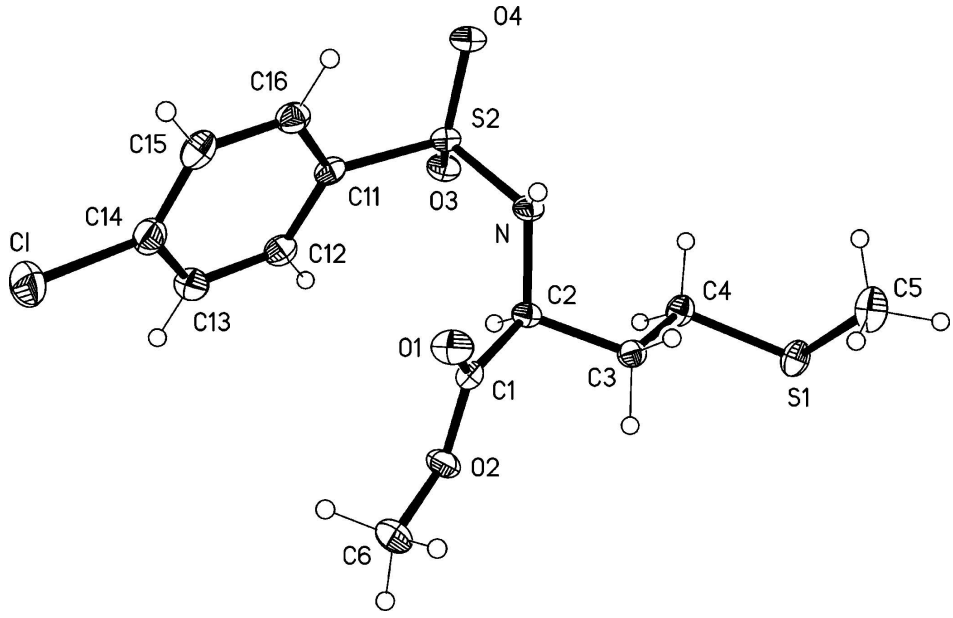


**Figure 1**

The molecule of the title compound. Ellipsoids correspond to 50% probability levels.

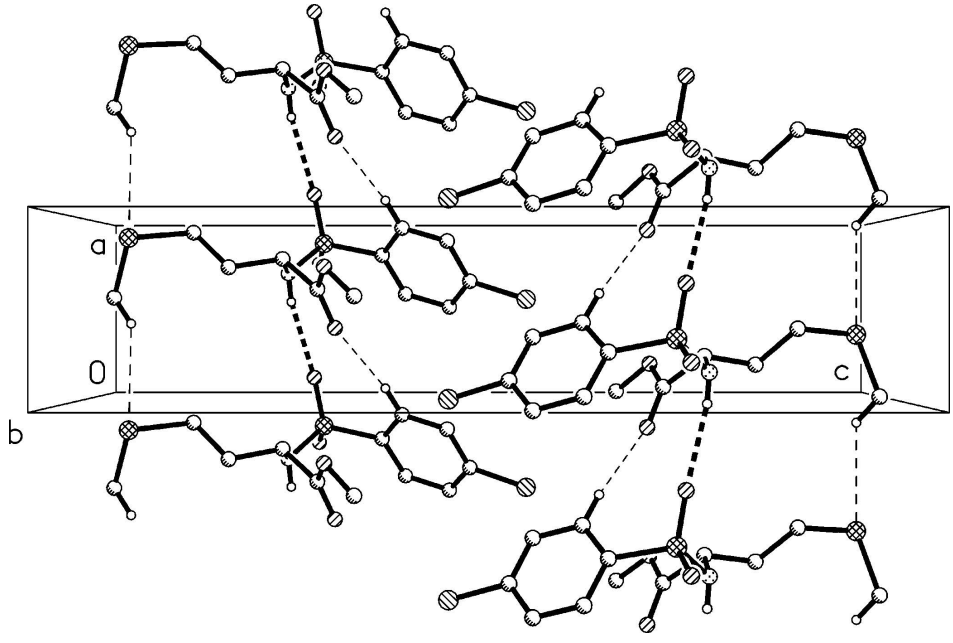


**Figure 2**

Packing diagram of the title compound, showing classical hydrogen bonds (thick dashed lines) and "weak" hydrogen bonds (thin dashed lines). H atoms not involved in these H bonds have been omitted. The interactions H2···O1 are omitted for clarity.

**(2*S*)-Methyl 2-(4-chlorobenzenesulfonamido)-4-(methylsulfanyl)butanoate**

*Crystal data*

$C_{12}H_{16}ClNO_4S_2$
$M_r = 337.83$
Orthorhombic, $P2_12_12_1$
$a = 5.1814$ (3) Å
$b = 12.6089$ (8) Å
$c = 23.2137$ (13) Å
$V = 1516.59$ (16) Å$^3$
$Z = 4$
$F(000) = 704$
$D_x = 1.480$ Mg m$^{-3}$
Melting point = 331–333 K
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 10903 reflections
$\theta = 3.5$–$75.6°$
$\mu = 4.92$ mm$^{-1}$
$T = 100$ K
Tablet, colourless
0.20 × 0.12 × 0.06 mm

*Data collection*

Oxford Diffraction Xcalibur Nova A diffractometer
Radiation source: Nova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.3543 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2008)
$T_{min} = 0.548$, $T_{max} = 1.000$
14469 measured reflections
3093 independent reflections
3027 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 75.7°$, $\theta_{min} = 3.8°$
$h = -6 \rightarrow 5$
$k = -15 \rightarrow 15$
$l = -29 \rightarrow 27$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.062$
$S = 1.04$
3093 reflections
187 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
$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.6444P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ e Å$^{-3}$
Absolute structure: Flack (1983), 1250 Friedel pairs
Absolute structure parameter: 0.005 (12)

*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 | 0.6060 (3) | 0.70856 (13) | 0.30125 (7) | 0.0157 (3) |
| C2 | 0.7658 (3) | 0.64578 (13) | 0.25767 (7) | 0.0149 (3) |
| H2 | 0.9529 | 0.6527 | 0.2676 | 0.018* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.7198 (3) | 0.69178 (13) | 0.19720 (7) | 0.0157 (3) |
| H3A | 0.5399 | 0.6770 | 0.1853 | 0.019* |
| H3B | 0.7427 | 0.7697 | 0.1984 | 0.019* |
| C4 | 0.9040 (3) | 0.64498 (13) | 0.15292 (7) | 0.0175 (3) |
| H4A | 0.8724 | 0.5677 | 0.1501 | 0.021* |
| H4B | 1.0834 | 0.6552 | 0.1665 | 0.021* |
| C5 | 0.5616 (4) | 0.65296 (18) | 0.06022 (8) | 0.0279 (4) |
| H5A | 0.5565 | 0.5761 | 0.0662 | 0.042* |
| H5B | 0.5334 | 0.6687 | 0.0194 | 0.042* |
| H5C | 0.4261 | 0.6868 | 0.0833 | 0.042* |
| C6 | 0.5679 (4) | 0.87023 (14) | 0.34955 (8) | 0.0267 (4) |
| H6A | 0.3949 | 0.8791 | 0.3332 | 0.040* |
| H6B | 0.6529 | 0.9395 | 0.3522 | 0.040* |
| H6C | 0.5541 | 0.8390 | 0.3881 | 0.040* |
| C11 | 0.7949 (3) | 0.48637 (13) | 0.37042 (7) | 0.0166 (3) |
| C12 | 0.9359 (3) | 0.56678 (13) | 0.39648 (7) | 0.0194 (3) |
| H12 | 1.0801 | 0.5972 | 0.3774 | 0.023* |
| C13 | 0.8635 (4) | 0.60215 (14) | 0.45083 (8) | 0.0230 (3) |
| H13 | 0.9576 | 0.6570 | 0.4694 | 0.028* |
| C14 | 0.6511 (4) | 0.55597 (14) | 0.47751 (7) | 0.0225 (3) |
| C15 | 0.5128 (4) | 0.47418 (15) | 0.45226 (8) | 0.0224 (4) |
| H15 | 0.3716 | 0.4425 | 0.4719 | 0.027* |
| C16 | 0.5837 (3) | 0.43950 (13) | 0.39798 (7) | 0.0192 (3) |
| H16 | 0.4898 | 0.3843 | 0.3796 | 0.023* |
| O1 | 0.4034 (3) | 0.67950 (10) | 0.32058 (5) | 0.0225 (3) |
| O2 | 0.7177 (2) | 0.80112 (10) | 0.31298 (5) | 0.0202 (3) |
| O3 | 1.1274 (2) | 0.47165 (9) | 0.28709 (5) | 0.0187 (2) |
| O4 | 0.7538 (2) | 0.34783 (10) | 0.28792 (5) | 0.0199 (3) |
| S1 | 0.87182 (9) | 0.70331 (3) | 0.081959 (17) | 0.02100 (10) |
| S2 | 0.86006 (8) | 0.45109 (3) | 0.298219 (16) | 0.01470 (9) |
| Cl | 0.55423 (10) | 0.60320 (4) | 0.54465 (2) | 0.03195 (12) |
| N | 0.6935 (3) | 0.53293 (11) | 0.25852 (6) | 0.0151 (3) |
| H01 | 0.540 (6) | 0.521 (2) | 0.2616 (12) | 0.041 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0189 (8) | 0.0141 (7) | 0.0140 (7) | 0.0002 (7) | −0.0010 (7) | 0.0023 (6) |
| C2 | 0.0149 (7) | 0.0120 (7) | 0.0176 (8) | −0.0009 (6) | −0.0006 (6) | −0.0011 (6) |
| C3 | 0.0160 (7) | 0.0143 (7) | 0.0168 (8) | 0.0003 (6) | −0.0005 (6) | 0.0005 (6) |
| C4 | 0.0157 (8) | 0.0201 (8) | 0.0168 (7) | 0.0025 (6) | 0.0004 (6) | 0.0016 (6) |
| C5 | 0.0225 (9) | 0.0396 (10) | 0.0216 (9) | 0.0020 (8) | −0.0013 (7) | 0.0023 (8) |
| C6 | 0.0365 (11) | 0.0214 (8) | 0.0223 (8) | 0.0063 (8) | 0.0019 (8) | −0.0074 (7) |
| C11 | 0.0165 (8) | 0.0140 (7) | 0.0192 (8) | 0.0022 (6) | −0.0011 (6) | 0.0035 (6) |
| C12 | 0.0187 (8) | 0.0184 (8) | 0.0212 (8) | −0.0017 (6) | 0.0012 (6) | 0.0032 (6) |
| C13 | 0.0266 (9) | 0.0195 (8) | 0.0228 (8) | −0.0008 (8) | −0.0022 (8) | −0.0008 (7) |
| C14 | 0.0259 (9) | 0.0222 (8) | 0.0194 (8) | 0.0043 (8) | 0.0005 (7) | 0.0026 (6) |
| C15 | 0.0211 (8) | 0.0249 (8) | 0.0211 (8) | −0.0006 (7) | 0.0031 (7) | 0.0068 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.0189 (8) | 0.0168 (8) | 0.0219 (8) | −0.0030 (7) | −0.0019 (7) | 0.0025 (6) |
| O1 | 0.0205 (7) | 0.0197 (6) | 0.0272 (6) | −0.0006 (5) | 0.0076 (5) | −0.0008 (5) |
| O2 | 0.0254 (6) | 0.0149 (6) | 0.0204 (6) | −0.0018 (5) | 0.0014 (5) | −0.0049 (5) |
| O3 | 0.0154 (5) | 0.0161 (5) | 0.0246 (6) | 0.0007 (5) | 0.0006 (5) | −0.0021 (4) |
| O4 | 0.0214 (6) | 0.0126 (6) | 0.0256 (6) | −0.0028 (5) | 0.0000 (5) | −0.0004 (5) |
| S1 | 0.01868 (19) | 0.0276 (2) | 0.01674 (19) | 0.00114 (18) | 0.00273 (16) | 0.00482 (15) |
| S2 | 0.01470 (18) | 0.01144 (17) | 0.01797 (18) | −0.00017 (15) | 0.00043 (15) | 0.00026 (13) |
| Cl | 0.0416 (3) | 0.0336 (2) | 0.0206 (2) | 0.0050 (2) | 0.00561 (18) | −0.00285 (18) |
| N | 0.0140 (6) | 0.0128 (6) | 0.0186 (7) | −0.0027 (5) | −0.0002 (5) | 0.0000 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.199 (2) | O4—S2 | 1.4337 (13) |
| C1—O2 | 1.331 (2) | S2—N | 1.6306 (15) |
| C1—C2 | 1.528 (2) | C2—H2 | 1.0000 |
| C2—N | 1.472 (2) | C3—H3A | 0.9900 |
| C2—C3 | 1.538 (2) | C3—H3B | 0.9900 |
| C3—C4 | 1.522 (2) | C4—H4A | 0.9900 |
| C4—S1 | 1.8117 (17) | C4—H4B | 0.9900 |
| C5—S1 | 1.800 (2) | C5—H5A | 0.9800 |
| C6—O2 | 1.443 (2) | C5—H5B | 0.9800 |
| C11—C12 | 1.388 (2) | C5—H5C | 0.9800 |
| C11—C16 | 1.398 (2) | C6—H6A | 0.9800 |
| C11—S2 | 1.7667 (18) | C6—H6B | 0.9800 |
| C12—C13 | 1.390 (2) | C6—H6C | 0.9800 |
| C13—C14 | 1.391 (3) | C12—H12 | 0.9500 |
| C14—C15 | 1.386 (3) | C13—H13 | 0.9500 |
| C14—Cl | 1.7422 (18) | C15—H15 | 0.9500 |
| C15—C16 | 1.384 (2) | C16—H16 | 0.9500 |
| O3—S2 | 1.4327 (13) | N—H01 | 0.81 (3) |
| | | | |
| O1—C1—O2 | 124.89 (16) | C2—C3—H3A | 109.2 |
| O1—C1—C2 | 124.31 (15) | C4—C3—H3B | 109.2 |
| O2—C1—C2 | 110.75 (14) | C2—C3—H3B | 109.2 |
| N—C2—C1 | 110.74 (13) | H3A—C3—H3B | 107.9 |
| N—C2—C3 | 109.73 (13) | C3—C4—H4A | 108.9 |
| C1—C2—C3 | 108.97 (13) | S1—C4—H4A | 108.9 |
| C4—C3—C2 | 111.92 (14) | C3—C4—H4B | 108.9 |
| C3—C4—S1 | 113.52 (11) | S1—C4—H4B | 108.9 |
| C12—C11—C16 | 121.41 (16) | H4A—C4—H4B | 107.7 |
| C12—C11—S2 | 119.77 (13) | S1—C5—H5A | 109.5 |
| C16—C11—S2 | 118.50 (13) | S1—C5—H5B | 109.5 |
| C11—C12—C13 | 119.20 (17) | H5A—C5—H5B | 109.5 |
| C12—C13—C14 | 118.92 (17) | S1—C5—H5C | 109.5 |
| C15—C14—C13 | 122.17 (17) | H5A—C5—H5C | 109.5 |
| C15—C14—Cl | 118.93 (14) | H5B—C5—H5C | 109.5 |
| C13—C14—Cl | 118.90 (14) | O2—C6—H6A | 109.5 |
| C16—C15—C14 | 118.88 (17) | O2—C6—H6B | 109.5 |

| | | | |
|---|---|---|---|
| C15—C16—C11 | 119.40 (16) | H6A—C6—H6B | 109.5 |
| C1—O2—C6 | 114.59 (14) | O2—C6—H6C | 109.5 |
| C5—S1—C4 | 101.18 (9) | H6A—C6—H6C | 109.5 |
| O3—S2—O4 | 120.36 (7) | H6B—C6—H6C | 109.5 |
| O3—S2—N | 107.18 (7) | C11—C12—H12 | 120.4 |
| O4—S2—N | 106.09 (7) | C13—C12—H12 | 120.4 |
| O3—S2—C11 | 108.08 (8) | C12—C13—H13 | 120.5 |
| O4—S2—C11 | 108.27 (8) | C14—C13—H13 | 120.5 |
| N—S2—C11 | 106.00 (7) | C16—C15—H15 | 120.6 |
| C2—N—S2 | 118.99 (11) | C14—C15—H15 | 120.6 |
| N—C2—H2 | 109.1 | C15—C16—H16 | 120.3 |
| C1—C2—H2 | 109.1 | C11—C16—H16 | 120.3 |
| C3—C2—H2 | 109.1 | C2—N—H01 | 115.6 (19) |
| C4—C3—H3A | 109.2 | S2—N—H01 | 110.5 (19) |

| | | | |
|---|---|---|---|
| O1—C1—C2—N | −20.6 (2) | S2—C11—C16—C15 | −173.17 (13) |
| O2—C1—C2—N | 161.73 (13) | O1—C1—O2—C6 | −3.3 (2) |
| O1—C1—C2—C3 | 100.19 (18) | C2—C1—O2—C6 | 174.33 (14) |
| O2—C1—C2—C3 | −77.48 (16) | C3—C4—S1—C5 | −69.77 (14) |
| N—C2—C3—C4 | −67.63 (17) | C12—C11—S2—O3 | 29.75 (15) |
| C1—C2—C3—C4 | 170.97 (14) | C16—C11—S2—O3 | −156.70 (13) |
| C2—C3—C4—S1 | −176.06 (11) | C12—C11—S2—O4 | 161.63 (13) |
| C16—C11—C12—C13 | −0.7 (3) | C16—C11—S2—O4 | −24.82 (15) |
| S2—C11—C12—C13 | 172.62 (13) | C12—C11—S2—N | −84.90 (15) |
| C11—C12—C13—C14 | −0.1 (3) | C16—C11—S2—N | 88.66 (14) |
| C12—C13—C14—C15 | 1.5 (3) | C1—C2—N—S2 | −94.83 (15) |
| C12—C13—C14—Cl | −177.99 (13) | C3—C2—N—S2 | 144.83 (12) |
| C13—C14—C15—C16 | −2.0 (3) | O3—S2—N—C2 | −47.30 (14) |
| Cl—C14—C15—C16 | 177.52 (14) | O4—S2—N—C2 | −177.08 (12) |
| C14—C15—C16—C11 | 1.1 (3) | C11—S2—N—C2 | 67.96 (14) |
| C12—C11—C16—C15 | 0.3 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N—H01···O3$^{i}$ | 0.81 (3) | 2.30 (3) | 3.1048 (18) | 169 (3) |
| C2—H2···O1$^{ii}$ | 1.00 | 2.66 | 3.637 (2) | 166 |
| C12—H12···O1$^{ii}$ | 0.95 | 2.37 | 3.315 (2) | 173 |
| C3—H3*B*···O3$^{iii}$ | 0.99 | 2.66 | 3.635 (2) | 170 |
| C5—H5*B*···S1$^{iv}$ | 0.98 | 2.97 | 3.892 (2) | 157 |
| C5—H5*C*···S1$^{i}$ | 0.98 | 2.88 | 3.665 (2) | 138 |

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*; (iii) −*x*+2, *y*+1/2, −*z*+1/2; (iv) *x*−1/2, −*y*+3/2, −*z*.