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# *N*-(5-Chloro-2-methoxyphenyl)benzenesulfonamide

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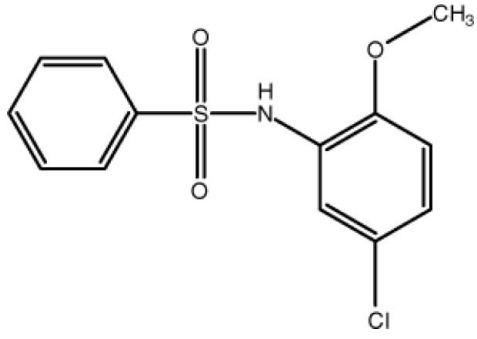
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.035; $wR$ factor = 0.096; data-to-parameter ratio = 18.8.

In the title compound, $C_{13}H_{12}ClNO_3S$, the dihedral angle between the two aromatic rings is 73.94 (9)°. An intramolecular C—H···O hydrogen bond occurs. In the crystal, intermolecular N—H···O hydrogen bonds connect the molecules to centrosymmetric dimers, forming an $R_2^2(8)$ ring motif. The packing is consolidated by C—H···O hydrogen bonds and weak $\pi$–$\pi$ interactions [centroid–centroid distances = 3.81 (3) and 3.81 (3) Å].

## Related literature

For the biological properties of sulfonamide derivatives, see: Berredjem *et al.* (2000); Lee & Lee (2002); Soledade *et al.* (2006); Xiao & Timberlake (2000). For related structures, see: Aziz-ur-Rehman *et al.* (2010*a*,*b*); Khan *et al.* (2010); Akkurt *et al.* (2010).



## Experimental

### *Crystal data*

$C_{13}H_{12}ClNO_3S$
$M_r$ = 297.76
Triclinic, $P\overline{1}$
$a$ = 8.2201 (2) Å
$b$ = 8.9395 (2) Å
$c$ = 10.5544 (2) Å
$\alpha$ = 77.206 (1)°
$\beta$ = 76.366 (1)°
$\gamma$ = 66.408 (1)°
$V$ = 683.65 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.43 mm$^{-1}$
$T$ = 296 K
0.24 × 0.16 × 0.08 mm

### *Data collection*

Bruker APEXII CCD diffractometer
12007 measured reflections
3333 independent reflections
2906 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
$S$ = 1.02
3333 reflections
177 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.828 (16) | 2.217 (16) | 3.0096 (15) | 160.2 (16) |
| C4—H4···O2$^{ii}$ | 0.93 | 2.55 | 3.368 (3) | 147 |
| C8—H8···O2 | 0.93 | 2.34 | 2.9491 (17) | 123 |
| C13—H13*B*···O2$^{iii}$ | 0.96 | 2.48 | 3.362 (3) | 153 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5375).

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# supporting information

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## *N*-(5-Chloro-2-methoxyphenyl)benzenesulfonamide

**Aziz-ur-Rehman, Shahzaman, Mehmet Akkurt, Muhammad Athar Abbasi and Islam Ullah Khan**

### S1. Comment

Sulfonamide is found in a number of synthetic as well as natural compounds. These molecules posses many biological activities *e.g.*, herbicidal, anti-malarial, anti-convulsant and anti- hypertensive (Soledade *et al.*, 2006; Xiao & Timberlake, 2000; Berredjem *et al.*, 2000; Lee & Lee, 2002). In the present paper, the structure of *N*-(5-chloro-2-methoxyphenyl) benzenesulfonamide has been determined as part of a research program involving the synthesis and biological evaluation of sulfur containing compounds.

In the title molecule (I), (Fig. 1), both sulfonamido-O atoms lie on the opposite side of the S-bound phenyl ring to the sulfonamido-N1 atom [the O1–S1–C1–C6, O2–S1–C1–C2 and N1–S1–C1–C2 torsion angles are -34.32 (13), 14.43 (13) and -101.83 (12) °, respectively]. The dihedral angle formed between the phenyl (C1–C6) and benzene (C7–C12) rings in (I) is 73.94 (9) °.

The molecules of (I) are dimerized due to the intermolecular N—H···O hydrogen bonding (Table 1, Fig. 2) producing a $R_2^2(8)$ ring motif.

In addition, there are C—H···O hydrogen bonds, as well as $\pi$-$\pi$ interactions [*Cg*1···*Cg*1(1 - *x*, -*y*, 2 - *z*) = 3.8163 (11) Å and cg2···*Cg*2(-*x*, 1 - *y*, 1 - *z*) = 3.9472 (12) Å; where *Cg*1 and *Cg*2 are centroids of the phenyl and benzene rings (C1–C6 and C7–C12), respectively], between the aromatic rings of each dimer.

### S2. Experimental

A mixture benzenesulfonyl chloride (10.0 mmol; 1.45 ml), 5-chloro-2-methoxy aniline (10.0 mmol; 1.47 g), aqueous sodium carbonate (10%; 20.0 ml) and water (25 ml) was stirred for one and half hour at room temperature. The crude mixture was washed with water and dried. The product was dissolved in methanol and recrystallized by slow evaporation of the solvent, to generate colourless crystal of *N*-(5-chloro-2-methoxyphenyl)benzenesulfonamide in 71% yield.

### S3. Refinement

The amino H atom is located in a difference Fourier map and refined freely. The remaining H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

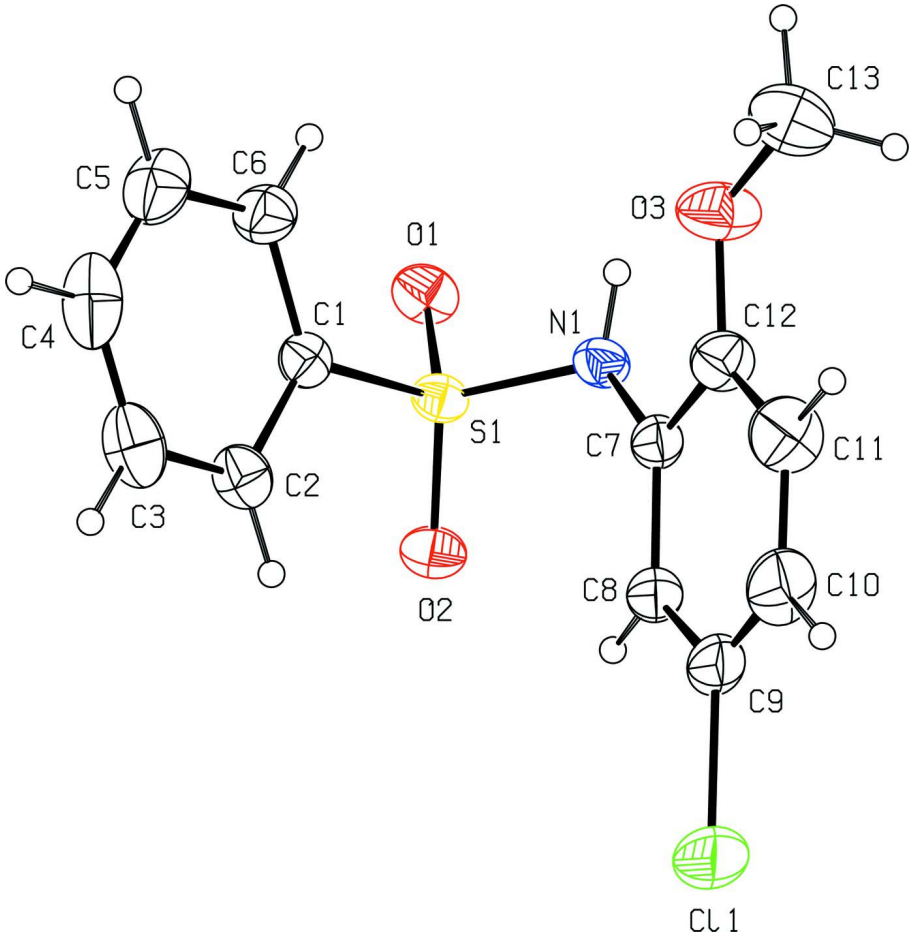


**Figure 1**

The title molecule drawn with displacement ellipsoids drawn at the 30% probability level.

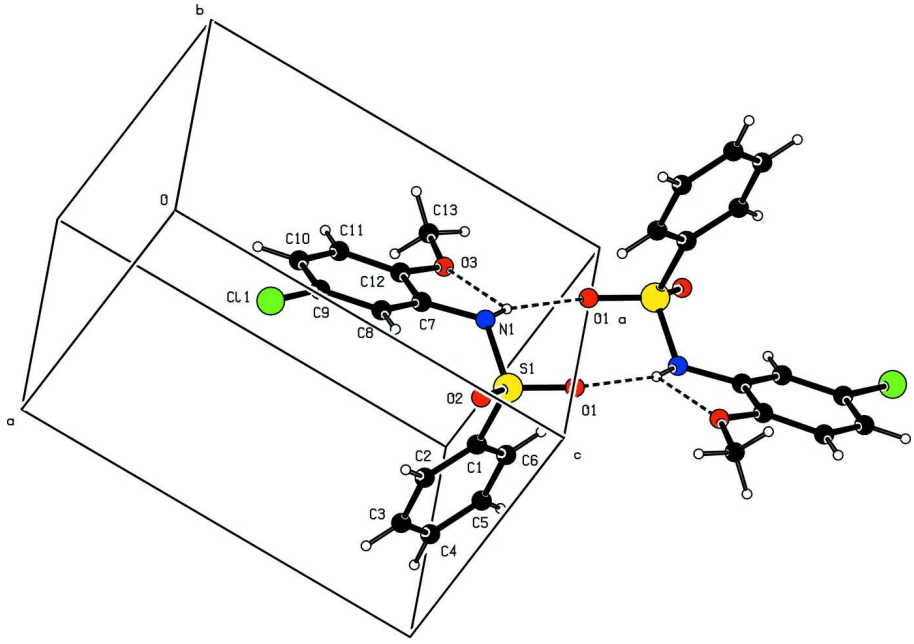


**Figure 2**

View of the dimeric N—H···O interactions between two moleculs in the unit cell.

### *N*-(5-chloro-2-methoxyphenyl)benzenesulfonamide

*Crystal data*

$C_{13}H_{12}ClNO_3S$
$M_r = 297.76$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.2201$ (2) Å
$b = 8.9395$ (2) Å
$c = 10.5544$ (2) Å
$\alpha = 77.206$ (1)°
$\beta = 76.366$ (1)°
$\gamma = 66.408$ (1)°
$V = 683.65$ (3) Å$^3$
$Z = 2$
$F(000) = 308$
$D_x = 1.446$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6946 reflections
$\theta = 2.5$–$28.2°$
$\mu = 0.43$ mm$^{-1}$
$T = 296$ K
Prism, colourless
0.24 × 0.16 × 0.08 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
12007 measured reflections
3333 independent reflections
2906 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.3°$, $\theta_{min} = 4.0°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.096$
$S = 1.02$
3333 reflections
177 parameters
1 restraint
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

$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.1401P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.27$ e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.29733 (8) | 0.24190 (8) | 0.34117 (5) | 0.0934 (2) |
| S1 | 0.14406 (4) | 0.27960 (4) | 0.88801 (3) | 0.0380 (1) |
| O1 | 0.03295 (14) | 0.31471 (13) | 1.01239 (9) | 0.0510 (3) |
| O2 | 0.13974 (14) | 0.15335 (13) | 0.82861 (10) | 0.0506 (3) |
| O3 | 0.1709 (2) | 0.71184 (16) | 0.69335 (12) | 0.0734 (5) |
| N1 | 0.08081 (16) | 0.45288 (14) | 0.78854 (10) | 0.0429 (3) |
| C1 | 0.36916 (18) | 0.23297 (16) | 0.90100 (12) | 0.0398 (4) |
| C2 | 0.5039 (2) | 0.11582 (19) | 0.83059 (15) | 0.0521 (5) |
| C3 | 0.6805 (2) | 0.0782 (2) | 0.8436 (2) | 0.0696 (6) |
| C4 | 0.7178 (3) | 0.1563 (3) | 0.9253 (2) | 0.0767 (7) |
| C5 | 0.5824 (3) | 0.2731 (3) | 0.9938 (2) | 0.0731 (7) |
| C6 | 0.4049 (2) | 0.3136 (2) | 0.98279 (16) | 0.0557 (5) |
| C7 | 0.16189 (18) | 0.47011 (17) | 0.65422 (12) | 0.0422 (4) |
| C8 | 0.1896 (2) | 0.35789 (19) | 0.57270 (13) | 0.0505 (4) |
| C9 | 0.2635 (2) | 0.3861 (2) | 0.44138 (15) | 0.0616 (5) |
| C10 | 0.3044 (3) | 0.5227 (3) | 0.39090 (16) | 0.0756 (7) |
| C11 | 0.2737 (3) | 0.6360 (3) | 0.47153 (17) | 0.0739 (7) |
| C12 | 0.2046 (2) | 0.6098 (2) | 0.60401 (14) | 0.0541 (5) |
| C13 | 0.1961 (3) | 0.8625 (3) | 0.6504 (3) | 0.0875 (9) |
| H1 | 0.058 (2) | 0.5318 (19) | 0.8273 (16) | 0.052 (4)* |
| H2 | 0.47690 | 0.06350 | 0.77580 | 0.0630* |
| H3 | 0.77380 | 0.00000 | 0.79700 | 0.0830* |
| H4 | 0.83650 | 0.12960 | 0.93410 | 0.0920* |
| H5 | 0.61010 | 0.32540 | 1.04810 | 0.0880* |
| H6 | 0.31220 | 0.39270 | 1.02900 | 0.0670* |
| H8 | 0.15940 | 0.26520 | 0.60520 | 0.0600* |
| H10 | 0.35290 | 0.53940 | 0.30240 | 0.0910* |
| H11 | 0.29940 | 0.73070 | 0.43700 | 0.0890* |
| H13A | 0.32050 | 0.84190 | 0.61440 | 0.1310* |

| | | | | |
|---|---|---|---|---|
| H13B | 0.16150 | 0.92250 | 0.72360 | 0.1310* |
| H13C | 0.12340 | 0.92620 | 0.58390 | 0.1310* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.1058 (4) | 0.0954 (4) | 0.0594 (3) | 0.0032 (3) | −0.0179 (2) | −0.0448 (3) |
| S1 | 0.0403 (2) | 0.0368 (2) | 0.0370 (2) | −0.0163 (1) | 0.0011 (1) | −0.0095 (1) |
| O1 | 0.0538 (6) | 0.0510 (6) | 0.0416 (5) | −0.0206 (5) | 0.0098 (4) | −0.0100 (4) |
| O2 | 0.0566 (6) | 0.0459 (5) | 0.0577 (6) | −0.0253 (5) | −0.0063 (5) | −0.0146 (4) |
| O3 | 0.1093 (11) | 0.0642 (8) | 0.0596 (7) | −0.0505 (8) | 0.0026 (7) | −0.0160 (6) |
| N1 | 0.0491 (6) | 0.0385 (6) | 0.0360 (5) | −0.0107 (5) | −0.0019 (4) | −0.0111 (4) |
| C1 | 0.0435 (7) | 0.0381 (6) | 0.0381 (6) | −0.0193 (5) | −0.0049 (5) | 0.0003 (5) |
| C2 | 0.0465 (8) | 0.0504 (8) | 0.0515 (8) | −0.0145 (6) | −0.0008 (6) | −0.0058 (6) |
| C3 | 0.0437 (8) | 0.0664 (11) | 0.0793 (11) | −0.0144 (8) | 0.0003 (8) | 0.0052 (9) |
| C4 | 0.0524 (10) | 0.0787 (13) | 0.0975 (14) | −0.0378 (10) | −0.0255 (10) | 0.0310 (11) |
| C5 | 0.0829 (13) | 0.0731 (12) | 0.0857 (13) | −0.0494 (11) | −0.0375 (11) | 0.0098 (10) |
| C6 | 0.0643 (9) | 0.0529 (8) | 0.0591 (9) | −0.0286 (7) | −0.0153 (7) | −0.0068 (7) |
| C7 | 0.0419 (7) | 0.0437 (7) | 0.0351 (6) | −0.0092 (5) | −0.0058 (5) | −0.0073 (5) |
| C8 | 0.0535 (8) | 0.0491 (8) | 0.0420 (7) | −0.0073 (6) | −0.0100 (6) | −0.0131 (6) |
| C9 | 0.0611 (9) | 0.0675 (10) | 0.0397 (7) | 0.0007 (8) | −0.0109 (6) | −0.0189 (7) |
| C10 | 0.0797 (12) | 0.0875 (14) | 0.0370 (7) | −0.0161 (10) | 0.0030 (7) | −0.0062 (8) |
| C11 | 0.0871 (13) | 0.0748 (12) | 0.0503 (9) | −0.0341 (10) | 0.0042 (8) | 0.0014 (8) |
| C12 | 0.0602 (9) | 0.0554 (9) | 0.0442 (7) | −0.0219 (7) | −0.0022 (6) | −0.0080 (6) |
| C13 | 0.1028 (17) | 0.0654 (12) | 0.1064 (17) | −0.0453 (12) | −0.0112 (13) | −0.0149 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C9 | 1.7424 (17) | C7—C8 | 1.380 (2) |
| S1—O1 | 1.4296 (10) | C8—C9 | 1.387 (2) |
| S1—O2 | 1.4227 (12) | C9—C10 | 1.358 (3) |
| S1—N1 | 1.6323 (12) | C10—C11 | 1.375 (3) |
| S1—C1 | 1.7588 (16) | C11—C12 | 1.386 (2) |
| O3—C12 | 1.361 (2) | C2—H2 | 0.9300 |
| O3—C13 | 1.404 (3) | C3—H3 | 0.9300 |
| N1—C7 | 1.4205 (16) | C4—H4 | 0.9300 |
| N1—H1 | 0.828 (16) | C5—H5 | 0.9300 |
| C1—C2 | 1.380 (2) | C6—H6 | 0.9300 |
| C1—C6 | 1.384 (2) | C8—H8 | 0.9300 |
| C2—C3 | 1.386 (3) | C10—H10 | 0.9300 |
| C3—C4 | 1.374 (3) | C11—H11 | 0.9300 |
| C4—C5 | 1.370 (3) | C13—H13A | 0.9600 |
| C5—C6 | 1.383 (3) | C13—H13B | 0.9600 |
| C7—C12 | 1.391 (2) | C13—H13C | 0.9600 |
| | | | |
| Cl1···C6$^{i}$ | 3.6473 (17) | C7···Cl1$^{iii}$ | 3.6152 (17) |
| Cl1···C2$^{ii}$ | 3.6292 (17) | C7···C9$^{iii}$ | 3.520 (2) |
| Cl1···C7$^{iii}$ | 3.6152 (17) | C8···C8$^{iii}$ | 3.566 (2) |

| | | | |
|---|---|---|---|
| Cl1···H2$^{ii}$ | 2.9600 | C8···O2 | 2.9491 (17) |
| Cl1···H13A$^{iv}$ | 3.0500 | C8···C9$^{iii}$ | 3.524 (2) |
| S1···H8 | 2.9900 | C9···C8$^{iii}$ | 3.524 (2) |
| O1···N1$^{v}$ | 3.0096 (15) | C9···C7$^{iii}$ | 3.520 (2) |
| O1···O1$^{v}$ | 3.0957 (15) | C13···O2$^{xi}$ | 3.362 (3) |
| O1···O3$^{v}$ | 3.1699 (16) | C3···H11$^{iv}$ | 3.0800 |
| O2···C13$^{vi}$ | 3.362 (3) | C11···H13A | 2.8100 |
| O2···C4$^{vii}$ | 3.368 (3) | C11···H13C | 2.7900 |
| O2···C8 | 2.9491 (17) | C13···H11 | 2.5800 |
| O2···C4$^{viii}$ | 3.382 (2) | H1···O3 | 2.241 (17) |
| O3···O1$^{v}$ | 3.1699 (16) | H1···O1$^{v}$ | 2.217 (16) |
| O3···N1 | 2.6284 (19) | H2···O2 | 2.5100 |
| O1···H6 | 2.7000 | H2···Cl1$^{ii}$ | 2.9600 |
| O1···H1$^{v}$ | 2.217 (16) | H4···O2$^{ix}$ | 2.5500 |
| O2···H13B$^{vi}$ | 2.4800 | H6···O1 | 2.7000 |
| O2···H4$^{vii}$ | 2.5500 | H8···S1 | 2.9900 |
| O2···H8 | 2.3400 | H8···O2 | 2.3400 |
| O2···H2 | 2.5100 | H11···C13 | 2.5800 |
| O3···H1 | 2.241 (17) | H11···H13A | 2.3700 |
| N1···O3 | 2.6284 (19) | H11···H13C | 2.3800 |
| N1···O1$^{v}$ | 3.0096 (15) | H11···C3$^{iv}$ | 3.0800 |
| C1···C3$^{viii}$ | 3.499 (2) | H13A···C11 | 2.8100 |
| C2···Cl1$^{ii}$ | 3.6292 (17) | H13A···H11 | 2.3700 |
| C3···C1$^{viii}$ | 3.499 (2) | H13A···Cl1$^{iv}$ | 3.0500 |
| C4···O2$^{ix}$ | 3.368 (3) | H13B···O2$^{xi}$ | 2.4800 |
| C4···O2$^{viii}$ | 3.382 (2) | H13C···C11 | 2.7900 |
| C6···Cl1$^{x}$ | 3.6473 (17) | H13C···H11 | 2.3800 |

| | | | |
|---|---|---|---|
| O1—S1—O2 | 118.95 (7) | C10—C11—C12 | 120.3 (2) |
| O1—S1—N1 | 105.06 (6) | C7—C12—C11 | 119.51 (16) |
| O1—S1—C1 | 109.15 (7) | O3—C12—C7 | 114.94 (13) |
| O2—S1—N1 | 108.21 (6) | O3—C12—C11 | 125.55 (17) |
| O2—S1—C1 | 107.73 (7) | C1—C2—H2 | 121.00 |
| N1—S1—C1 | 107.19 (7) | C3—C2—H2 | 121.00 |
| C12—O3—C13 | 119.30 (17) | C2—C3—H3 | 120.00 |
| S1—N1—C7 | 122.57 (10) | C4—C3—H3 | 120.00 |
| C7—N1—H1 | 115.2 (11) | C3—C4—H4 | 120.00 |
| S1—N1—H1 | 110.4 (11) | C5—C4—H4 | 120.00 |
| S1—C1—C6 | 118.85 (11) | C4—C5—H5 | 120.00 |
| S1—C1—C2 | 118.88 (12) | C6—C5—H5 | 120.00 |
| C2—C1—C6 | 122.27 (16) | C1—C6—H6 | 121.00 |
| C1—C2—C3 | 118.25 (15) | C5—C6—H6 | 121.00 |
| C2—C3—C4 | 120.09 (18) | C7—C8—H8 | 121.00 |
| C3—C4—C5 | 120.9 (2) | C9—C8—H8 | 121.00 |
| C4—C5—C6 | 120.5 (2) | C9—C10—H10 | 120.00 |
| C1—C6—C5 | 118.07 (17) | C11—C10—H10 | 120.00 |
| N1—C7—C12 | 117.82 (12) | C10—C11—H11 | 120.00 |
| N1—C7—C8 | 121.96 (13) | C12—C11—H11 | 120.00 |

| | | | |
|---|---|---|---|
| C8—C7—C12 | 120.14 (12) | O3—C13—H13A | 109.00 |
| C7—C8—C9 | 118.69 (15) | O3—C13—H13B | 109.00 |
| Cl1—C9—C8 | 117.57 (13) | O3—C13—H13C | 109.00 |
| C8—C9—C10 | 121.73 (16) | H13A—C13—H13B | 109.00 |
| Cl1—C9—C10 | 120.68 (13) | H13A—C13—H13C | 109.00 |
| C9—C10—C11 | 119.57 (17) | H13B—C13—H13C | 109.00 |
| | | | |
| O1—S1—N1—C7 | 179.00 (12) | C1—C2—C3—C4 | 0.2 (3) |
| O2—S1—N1—C7 | −52.96 (14) | C2—C3—C4—C5 | −0.7 (3) |
| C1—S1—N1—C7 | 62.98 (14) | C3—C4—C5—C6 | 0.6 (3) |
| O1—S1—C1—C2 | 144.89 (11) | C4—C5—C6—C1 | 0.0 (3) |
| O2—S1—C1—C2 | 14.43 (13) | C12—C7—C8—C9 | 1.2 (2) |
| N1—S1—C1—C2 | −101.83 (12) | N1—C7—C12—O3 | 3.1 (2) |
| O1—S1—C1—C6 | −34.32 (13) | C8—C7—C12—O3 | 179.75 (16) |
| O2—S1—C1—C6 | −164.78 (11) | C8—C7—C12—C11 | 0.5 (3) |
| N1—S1—C1—C6 | 78.96 (12) | N1—C7—C12—C11 | −176.09 (18) |
| C13—O3—C12—C7 | −175.04 (19) | N1—C7—C8—C9 | 177.65 (15) |
| C13—O3—C12—C11 | 4.1 (3) | C7—C8—C9—C10 | −1.8 (3) |
| S1—N1—C7—C12 | −135.26 (14) | C7—C8—C9—Cl1 | 179.83 (13) |
| S1—N1—C7—C8 | 48.2 (2) | C8—C9—C10—C11 | 0.6 (3) |
| C2—C1—C6—C5 | −0.4 (2) | Cl1—C9—C10—C11 | 178.93 (19) |
| C6—C1—C2—C3 | 0.3 (2) | C9—C10—C11—C12 | 1.2 (4) |
| S1—C1—C2—C3 | −178.87 (12) | C10—C11—C12—C7 | −1.7 (3) |
| S1—C1—C6—C5 | 178.76 (14) | C10—C11—C12—O3 | 179.1 (2) |

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*, −*y*+1, −*z*+2; (vi) *x*, *y*−1, *z*; (vii) *x*−1, *y*, *z*; (viii) −*x*+1, −*y*, −*z*+2; (ix) *x*+1, *y*, *z*; (x) *x*, *y*, *z*+1; (xi) *x*, *y*+1, *z*.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{v}$ | 0.828 (16) | 2.217 (16) | 3.0096 (15) | 160.2 (16) |
| C4—H4···O2$^{ix}$ | 0.93 | 2.55 | 3.368 (3) | 147 |
| C8—H8···O2 | 0.93 | 2.34 | 2.9491 (17) | 123 |
| C13—H13*B*···O2$^{xi}$ | 0.96 | 2.48 | 3.362 (3) | 153 |

Symmetry codes: (v) −*x*, −*y*+1, −*z*+2; (ix) *x*+1, *y*, *z*; (xi) *x*, *y*+1, *z*.