Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4-(3-Chloro-2,2-dimethylpropanamido)-benzenesulfonamide

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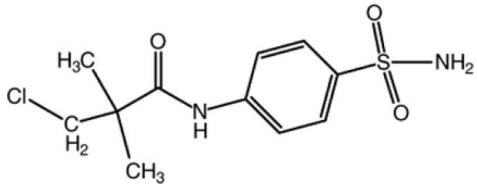
Received 8 November 2012; accepted 14 November 2012

Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.084; $wR$ factor = 0.231; data-to-parameter ratio = 24.2.

In the title compound, $C_{11}H_{15}ClN_2O_3S$, the 3-chloro-2,2-dimethylpropanamide and sulfonamide substituents are arranged on opposite sides of the benzene ring plane. In the crystal, molecules are linked by N—H···O and C—H···O hydrogen bonds, forming a three-dimensional network.

## Related literature

For the antibacterial, antimicrobial and antiglaucoma activity of sulfonamides and their derivatives and for their physical properties and pharmacological applications, see: Poulsen *et al.* (2005); Supuran & Scozzafava (2000). For related structures, see: Akkurt *et al.* (2010); Idemudia *et al.* (2012); Asiri *et al.* (2012). For the synthesis, see: Türkmen *et al.* (2011).



## Experimental

### Crystal data

$C_{11}H_{15}ClN_2O_3S$
$M_r$ = 290.77
Monoclinic, $P2_1/c$
$a$ = 20.4359 (11) Å
$b$ = 7.2437 (4) Å
$c$ = 9.4693 (5) Å
$\beta$ = 98.222 (3)°
$V$ = 1387.35 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.43 mm$^{-1}$
$T$ = 294 K
0.31 × 0.14 × 0.13 mm

### Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: refined from $\Delta F$ (*XABS2*; Parkin *et al.*, 1995)
$T_{min}$ = 0.931, $T_{max}$ = 0.946
4240 measured reflections
4240 independent reflections
2054 reflections with $I > 2\sigma(I)$

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.231
$S$ = 1.02
4240 reflections
175 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···O2$^{i}$ | 0.88 (3) | 2.57 (5) | 3.035 (4) | 114 (4) |
| N1—H1*N*···O1$^{ii}$ | 0.88 (3) | 2.21 (4) | 3.043 (5) | 160 (5) |
| N1—H2*N*···O1$^{iii}$ | 0.88 (2) | 2.10 (4) | 2.921 (4) | 155 (5) |
| N2—H3*N*···O3$^{iv}$ | 0.91 (6) | 2.16 (6) | 3.063 (5) | 173 (5) |
| C11—H11*B*···O3$^{iv}$ | 0.97 | 2.44 | 3.391 (5) | 166 |

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

The authors thank the Unit of Scientific Research Projects of Harran University, Turkey for a research grant (HUBAK project Nos. 874 and 1136).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5282).

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# supporting information

*Acta Cryst.* (2012). E**68**, o3430 [doi:10.1107/S1600536812046806]

## 4-(3-Chloro-2,2-dimethylpropanamido)benzenesulfonamide

**Şerife Pınar Yalçın, Mehmet Akkurt, Mustafa Durgun, Baki Türkkan and Hasan Türkmen**

### S1. Comment

Sulfonamides are of interest because of their unique biological properties. They are known inhibitors of the carbonic anhydrase enzyme, currently used for the treatment of glaucoma in clinical medicine (Poulsen *et al.*, 2005; Supuran & Scozzafava, 2000). The design and development of new sulfanilamide derivatives can help determine any structural requirements for improved biological activity. In this study, we have prepared and determined the crystal structure of 4-(3-Chloro-2,2-dimethylpropanoylamino)-benzenesulfonamide (I).

In Fig. 1, the molecular structure of the title compound is not planar. In the 3-chloro-2,2-dimethylpropanamide moiety of (I), the N2—C7—C8—C9, N2—C7—C8—C10 and N2—C7—C8—C11 torsion angles are 178.6 (4), 57.2 (5) and -59.4 (5) °, respectively. The values of the bond lengths and bond angles in (I) are within the normal range and are comparable to those previously reported for the related structures (Akkurt *et al.*, 2010; Idemudia *et al.*, 2012; Asiri *et al.*, 2012). The crystal structure is stabilized by intermolecular N—H···O and C—H···O hydrogen bonds (Table 1 and Fig. 2).

### S2. Experimental

Nucleophilic acyl substitution of 3-chloro-2,2-dimethyl-propanoylchloride with sulfanilamide gave the title compound as described previously (Türkmen *et al.*, 2011). Crystals suitable for X-ray diffraction studies were grown by slow evaporation of an ethanol, chloroform, dichloromethane (4/3/3 *v*/*v*) solution of the product.

### S3. Refinement

The H atoms on the NH and $NH_2$ groups were located from a difference Fourier map and refined with distance restraints of N—H = 0.88 (1) Å for the $NH_2$, with $U_{iso}$(H) = 1.2$U_{eq}$(N). The remaining H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined as riding with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C). The high R factor, low ratio of observed to unique reflections and relatively high su values indicate that the crystals were of rather poor quality and did not diffract strongly.

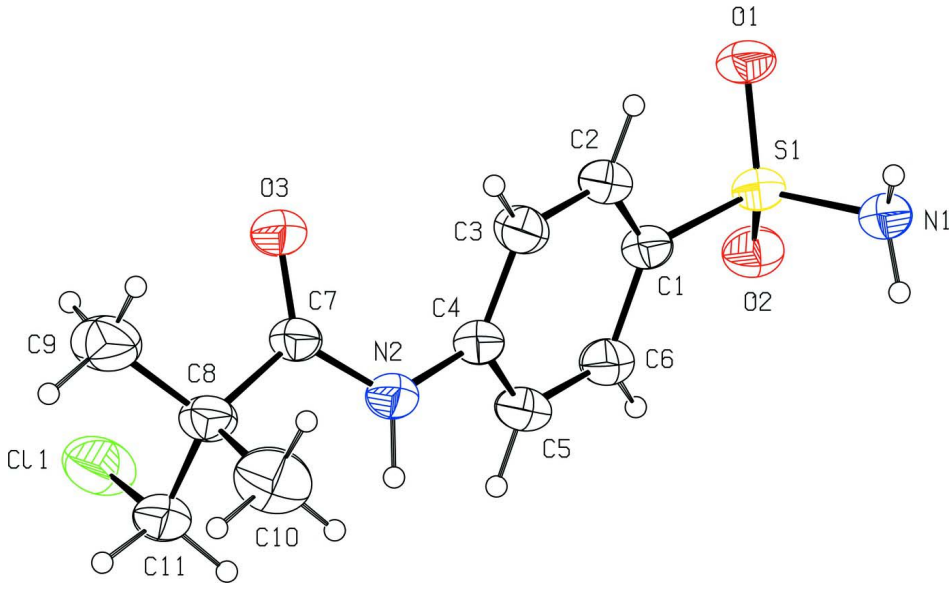


**Figure 1**

The title molecule with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

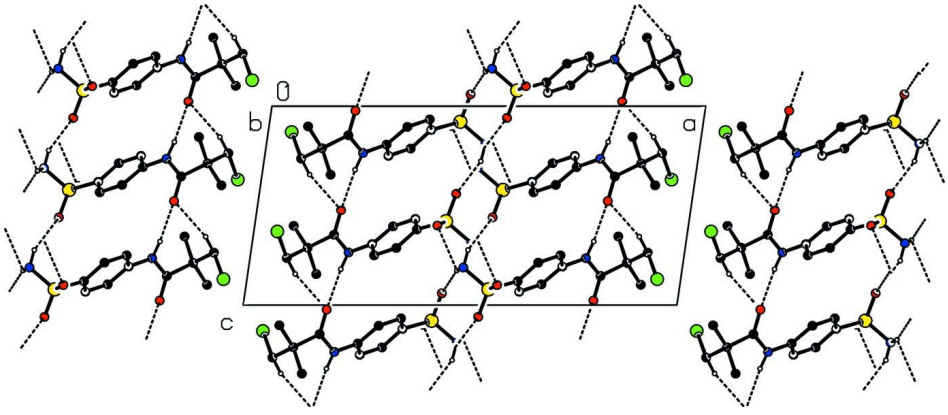


**Figure 2**

Packing of the title compound viewed along the *b* axis with N—H···O and C—H···O hydrogen bonds drawn as dashed lines. H atoms not involved in hydrogen bonding are omitted for clarity.

### 4-(3-Chloro-2,2-dimethylpropanamido)benzenesulfonamide

*Crystal data*

$C_{11}H_{15}ClN_2O_3S$
$M_r = 290.77$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 20.4359\ (11)$ Å
$b = 7.2437\ (4)$ Å
$c = 9.4693\ (5)$ Å
$\beta = 98.222\ (3)°$
$V = 1387.35\ (13)$ Å$^3$
$Z = 4$

$F(000) = 608$
$D_x = 1.392$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5710 reflections
$\theta = 2.5–30.5°$
$\mu = 0.43$ mm$^{-1}$
$T = 294$ K
Needle, white
0.31 × 0.14 × 0.13 mm

*Data collection*

Rigaku R-AXIS RAPID-S diffractometer
Radiation source: Sealed Tube
Graphite Monochromator monochromator
Detector resolution: 10.0000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: part of the refinement model ($\Delta F$)
(*XABS2*; Parkin *et al.*, 1995)
$T_{min}$ = 0.931, $T_{max}$ = 0.946
4240 measured reflections
4240 independent reflections
2054 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.000
$\theta_{max}$ = 30.6°, $\theta_{min}$ = 3.0°
$h$ = −29→28
$k$ = 0→10
$l$ = 0→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.231
$S$ = 1.02
4240 reflections
175 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0751P)^2 + 1.0033P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

*Special details*

**Experimental**. Absorption correction: (XABS2; Parkin *et al.*, 1995) Cubic fit to sin(theta)/lambda - 24 parameters

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.05415 (8) | 0.1450 (2) | 0.13028 (15) | 0.1040 (6) |
| S1 | 0.43958 (5) | −0.22940 (14) | 0.07872 (10) | 0.0540 (3) |
| O1 | 0.45415 (14) | −0.1736 (4) | −0.0593 (3) | 0.0634 (10) |
| O2 | 0.42131 (15) | −0.4163 (4) | 0.1004 (3) | 0.0684 (11) |
| O3 | 0.19397 (15) | 0.3907 (4) | 0.0227 (3) | 0.0689 (10) |
| N1 | 0.50493 (18) | −0.1856 (5) | 0.1885 (3) | 0.0592 (11) |
| N2 | 0.22555 (18) | 0.2516 (5) | 0.2354 (4) | 0.0640 (13) |
| C1 | 0.37522 (19) | −0.0863 (6) | 0.1199 (4) | 0.0550 (14) |
| C2 | 0.3682 (2) | 0.0917 (6) | 0.0669 (4) | 0.0603 (14) |
| C3 | 0.3193 (2) | 0.2057 (6) | 0.1041 (4) | 0.0628 (17) |
| C4 | 0.2770 (2) | 0.1406 (6) | 0.1935 (4) | 0.0579 (14) |
| C5 | 0.2852 (2) | −0.0344 (7) | 0.2500 (4) | 0.0691 (17) |
| C6 | 0.3339 (2) | −0.1493 (7) | 0.2132 (4) | 0.0675 (16) |
| C7 | 0.1859 (2) | 0.3629 (6) | 0.1465 (4) | 0.0563 (14) |

| | | | | |
|---|---|---|---|---|
| C8 | 0.1294 (2) | 0.4544 (6) | 0.2119 (4) | 0.0643 (16) |
| C9 | 0.0901 (3) | 0.5785 (8) | 0.1019 (6) | 0.102 (3) |
| C10 | 0.1581 (3) | 0.5664 (8) | 0.3447 (6) | 0.102 (3) |
| C11 | 0.0849 (2) | 0.3082 (7) | 0.2637 (5) | 0.0727 (18) |
| H1N | 0.519 (3) | −0.074 (3) | 0.174 (6) | 0.1230* |
| H2 | 0.39660 | 0.13480 | 0.00580 | 0.0720* |
| H2N | 0.500 (3) | −0.209 (8) | 0.277 (2) | 0.1230* |
| H3 | 0.31500 | 0.32570 | 0.06900 | 0.0750* |
| H3N | 0.213 (3) | 0.216 (8) | 0.320 (6) | 0.1230* |
| H5 | 0.25770 | −0.07550 | 0.31350 | 0.0830* |
| H6 | 0.33890 | −0.26790 | 0.25080 | 0.0810* |
| H9A | 0.11770 | 0.67740 | 0.07780 | 0.1520* |
| H9B | 0.05290 | 0.62860 | 0.14050 | 0.1520* |
| H9C | 0.07470 | 0.50810 | 0.01780 | 0.1520* |
| H10A | 0.18810 | 0.65780 | 0.31830 | 0.1530* |
| H10B | 0.18120 | 0.48500 | 0.41480 | 0.1530* |
| H10C | 0.12270 | 0.62620 | 0.38370 | 0.1530* |
| H11A | 0.04780 | 0.36890 | 0.29760 | 0.0870* |
| H11B | 0.10950 | 0.24310 | 0.34380 | 0.0870* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.1001 (11) | 0.1304 (13) | 0.0862 (9) | −0.0399 (9) | 0.0299 (8) | −0.0167 (8) |
| S1 | 0.0632 (6) | 0.0599 (6) | 0.0404 (5) | −0.0007 (5) | 0.0126 (4) | 0.0005 (4) |
| O1 | 0.079 (2) | 0.0732 (19) | 0.0411 (14) | 0.0032 (15) | 0.0195 (13) | −0.0002 (12) |
| O2 | 0.083 (2) | 0.0627 (18) | 0.0608 (17) | −0.0105 (15) | 0.0144 (15) | −0.0004 (14) |
| O3 | 0.0708 (19) | 0.090 (2) | 0.0481 (15) | 0.0074 (16) | 0.0166 (13) | 0.0051 (14) |
| N1 | 0.063 (2) | 0.068 (2) | 0.0475 (18) | −0.0015 (17) | 0.0115 (16) | 0.0033 (16) |
| N2 | 0.063 (2) | 0.084 (3) | 0.0473 (18) | 0.0104 (19) | 0.0163 (16) | 0.0035 (18) |
| C1 | 0.058 (2) | 0.066 (3) | 0.0420 (19) | −0.0019 (19) | 0.0104 (16) | 0.0019 (17) |
| C2 | 0.061 (2) | 0.070 (3) | 0.053 (2) | −0.001 (2) | 0.0190 (19) | 0.008 (2) |
| C3 | 0.063 (3) | 0.065 (3) | 0.064 (3) | 0.003 (2) | 0.021 (2) | 0.008 (2) |
| C4 | 0.056 (2) | 0.075 (3) | 0.044 (2) | 0.001 (2) | 0.0119 (17) | 0.0023 (19) |
| C5 | 0.067 (3) | 0.086 (3) | 0.059 (3) | 0.003 (2) | 0.025 (2) | 0.015 (2) |
| C6 | 0.067 (3) | 0.079 (3) | 0.059 (2) | 0.008 (2) | 0.018 (2) | 0.017 (2) |
| C7 | 0.058 (2) | 0.069 (3) | 0.044 (2) | −0.003 (2) | 0.0143 (17) | 0.0006 (18) |
| C8 | 0.074 (3) | 0.070 (3) | 0.053 (2) | 0.008 (2) | 0.023 (2) | 0.002 (2) |
| C9 | 0.113 (5) | 0.104 (4) | 0.098 (4) | 0.042 (4) | 0.048 (3) | 0.032 (3) |
| C10 | 0.125 (5) | 0.090 (4) | 0.097 (4) | −0.007 (3) | 0.035 (4) | −0.030 (3) |
| C11 | 0.073 (3) | 0.095 (4) | 0.054 (2) | 0.008 (3) | 0.023 (2) | 0.002 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C11 | 1.778 (5) | C7—C8 | 1.536 (6) |
| S1—O1 | 1.439 (3) | C8—C9 | 1.516 (7) |
| S1—O2 | 1.427 (3) | C8—C10 | 1.540 (7) |
| S1—N1 | 1.602 (4) | C8—C11 | 1.522 (6) |

| | | | |
|---|---|---|---|
| S1—C1 | 1.762 (4) | C2—H2 | 0.9300 |
| O3—C7 | 1.224 (5) | C3—H3 | 0.9300 |
| N2—C4 | 1.424 (6) | C5—H5 | 0.9300 |
| N2—C7 | 1.349 (5) | C6—H6 | 0.9300 |
| N1—H1N | 0.88 (3) | C9—H9A | 0.9600 |
| N1—H2N | 0.88 (2) | C9—H9B | 0.9600 |
| N2—H3N | 0.91 (6) | C9—H9C | 0.9600 |
| C1—C2 | 1.384 (6) | C10—H10A | 0.9600 |
| C1—C6 | 1.384 (6) | C10—H10B | 0.9600 |
| C2—C3 | 1.380 (6) | C10—H10C | 0.9600 |
| C3—C4 | 1.377 (6) | C11—H11A | 0.9700 |
| C4—C5 | 1.377 (6) | C11—H11B | 0.9700 |
| C5—C6 | 1.380 (6) | | |

| | | | |
|---|---|---|---|
| O1—S1—O2 | 119.30 (17) | C9—C8—C10 | 110.6 (4) |
| O1—S1—N1 | 105.79 (17) | C9—C8—C11 | 110.6 (4) |
| O1—S1—C1 | 107.08 (18) | Cl1—C11—C8 | 113.6 (3) |
| O2—S1—N1 | 107.79 (18) | C1—C2—H2 | 120.00 |
| O2—S1—C1 | 107.90 (19) | C3—C2—H2 | 120.00 |
| N1—S1—C1 | 108.62 (19) | C2—C3—H3 | 120.00 |
| C4—N2—C7 | 124.4 (4) | C4—C3—H3 | 120.00 |
| H1N—N1—H2N | 115 (5) | C4—C5—H5 | 120.00 |
| S1—N1—H1N | 110 (4) | C6—C5—H5 | 120.00 |
| S1—N1—H2N | 113 (4) | C1—C6—H6 | 120.00 |
| C4—N2—H3N | 113 (4) | C5—C6—H6 | 120.00 |
| C7—N2—H3N | 120 (4) | C8—C9—H9A | 110.00 |
| S1—C1—C2 | 120.7 (3) | C8—C9—H9B | 109.00 |
| C2—C1—C6 | 119.9 (4) | C8—C9—H9C | 109.00 |
| S1—C1—C6 | 119.4 (3) | H9A—C9—H9B | 109.00 |
| C1—C2—C3 | 120.4 (4) | H9A—C9—H9C | 109.00 |
| C2—C3—C4 | 119.6 (4) | H9B—C9—H9C | 109.00 |
| N2—C4—C3 | 122.1 (4) | C8—C10—H10A | 109.00 |
| N2—C4—C5 | 117.7 (4) | C8—C10—H10B | 109.00 |
| C3—C4—C5 | 120.1 (4) | C8—C10—H10C | 109.00 |
| C4—C5—C6 | 120.6 (4) | H10A—C10—H10B | 110.00 |
| C1—C6—C5 | 119.4 (4) | H10A—C10—H10C | 109.00 |
| O3—C7—C8 | 121.8 (4) | H10B—C10—H10C | 110.00 |
| N2—C7—C8 | 115.2 (3) | Cl1—C11—H11A | 109.00 |
| O3—C7—N2 | 123.0 (4) | Cl1—C11—H11B | 109.00 |
| C10—C8—C11 | 106.2 (4) | C8—C11—H11A | 109.00 |
| C7—C8—C11 | 110.4 (4) | C8—C11—H11B | 109.00 |
| C7—C8—C9 | 109.5 (4) | H11A—C11—H11B | 108.00 |
| C7—C8—C10 | 109.6 (4) | | |

| | | | |
|---|---|---|---|
| O1—S1—C1—C2 | −29.3 (4) | C2—C3—C4—N2 | −179.9 (4) |
| O1—S1—C1—C6 | 154.6 (3) | C2—C3—C4—C5 | 2.7 (6) |
| O2—S1—C1—C2 | −158.9 (3) | N2—C4—C5—C6 | 179.7 (4) |
| O2—S1—C1—C6 | 25.0 (4) | C3—C4—C5—C6 | −2.8 (6) |

| | | | |
|---|---|---|---|
| N1—S1—C1—C2 | 84.5 (4) | C4—C5—C6—C1 | 0.8 (6) |
| N1—S1—C1—C6 | −91.6 (4) | O3—C7—C8—C9 | −1.1 (6) |
| C7—N2—C4—C3 | 42.6 (6) | O3—C7—C8—C10 | −122.6 (4) |
| C7—N2—C4—C5 | −139.9 (4) | O3—C7—C8—C11 | 120.8 (4) |
| C4—N2—C7—O3 | −6.2 (7) | N2—C7—C8—C9 | 178.6 (4) |
| C4—N2—C7—C8 | 174.1 (4) | N2—C7—C8—C10 | 57.2 (5) |
| S1—C1—C2—C3 | −177.4 (3) | N2—C7—C8—C11 | −59.4 (5) |
| C6—C1—C2—C3 | −1.4 (6) | C7—C8—C11—Cl1 | −54.2 (4) |
| S1—C1—C6—C5 | 177.4 (3) | C9—C8—C11—Cl1 | 67.1 (4) |
| C2—C1—C6—C5 | 1.3 (6) | C10—C8—C11—Cl1 | −172.9 (3) |
| C1—C2—C3—C4 | −0.6 (6) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···O2$^{i}$ | 0.88 (3) | 2.57 (5) | 3.035 (4) | 114 (4) |
| N1—H1*N*···O1$^{ii}$ | 0.88 (3) | 2.21 (4) | 3.043 (5) | 160 (5) |
| N1—H2*N*···O1$^{iii}$ | 0.88 (2) | 2.10 (4) | 2.921 (4) | 155 (5) |
| N2—H3*N*···O3$^{iv}$ | 0.91 (6) | 2.16 (6) | 3.063 (5) | 173 (5) |
| C3—H3···O3 | 0.93 | 2.49 | 2.896 (5) | 106 |
| C6—H6···O2 | 0.93 | 2.59 | 2.936 (5) | 103 |
| C11—H11*B*···O3$^{iv}$ | 0.97 | 2.44 | 3.391 (5) | 166 |

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