# 3-Chloro-*N*-(4-sulfamoylphenyl)-propanamide

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In the title compound, $C_9H_{11}ClN_2O_3S$, the dihedral angle between the benzene ring and the amido –NHCO– plane is 15.0 (2)°. An intramolecular C—H···O hydrogen bond generates an $S(6)$ ring motif. In the crystal structure, the amino $NH_2$ group is involved in intermolecular N—H···O hydrogen bonds, which connect the molecules into a double layer structure expanding parallel to the *bc* plane. The layers are further linked by an amido N—H···O hydrogen bond. Between the layers, a weak $\pi$–$\pi$ interaction with a centroid–centroid distance of 3.7447 (12) Å is also observed.

## Related literature

For the antibacterial and pharmacological properties of sulfonamides and their derivatives, see: Albala *et al.* (1994); Mann & Keilin (1940); Maren (1976); Pastorekova *et al.* (2004); Reynolds (1996); Silverman (1992); Supuran & Scozzafava (2001, 2002); Supuran *et al.* (2003, 2004); Türkmen *et al.* (2005). For graph-set notation, see: Bernstein *et al.* (1995).
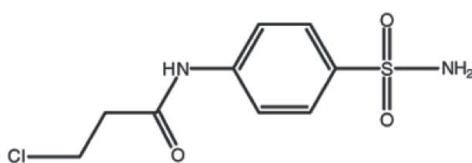


## Experimental

### Crystal data

| | |
|---|---|
| $C_9H_{11}ClN_2O_3S$ | $V$ = 1117.36 (10) Å³ |
| $M_r$ = 262.72 | $Z$ = 4 |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a$ = 7.7554 (4) Å | $\mu$ = 0.52 mm⁻¹ |
| $b$ = 14.8191 (8) Å | $T$ = 296 K |
| $c$ = 9.7482 (5) Å | 0.78 × 0.45 × 0.22 mm |
| $\beta$ = 94.181 (4)° | |

### Data collection

| | |
|---|---|
| Stoe IPDS2 diffractometer | 6023 measured reflections |
| Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002) | 2294 independent reflections |
| $T_{min}$ = 0.754, $T_{max}$ = 0.892 | 2007 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.040 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.038 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.106 | |
| $S$ = 1.08 | |
| 2294 reflections | $\Delta\rho_{max}$ = 0.28 e Å⁻³ |
| 153 parameters | $\Delta\rho_{min}$ = −0.44 e Å⁻³ |
| 2 restraints | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O1$^i$ | 0.859 (18) | 2.14 (2) | 2.926 (2) | 151 (3) |
| N1—H1$B$···O3$^{ii}$ | 0.85 (2) | 2.12 (3) | 2.923 (2) | 158 (3) |
| N2—H2$A$···O2$^{iii}$ | 0.86 | 2.13 | 2.991 (2) | 175 |
| C3—H3···O3 | 0.93 | 2.32 | 2.889 (3) | 120 |

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2555).

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# supporting information

## 3-Chloro-*N*-(4-sulfamoylphenyl)propanamide

**Mehmet Akkurt, Şerife Pınar Yalçın, Hasan Türkmen and Orhan Büyükgüngör**

### S1. Comment

Sulfanilamide is a sulfonamide antibacterial. Chemically, it is a molecule containing the sulfonamide functional group attached to an aniline. As an antibiotic, it functions by competitively inhibiting (*i.e*, by acting as a substrate analogue) enzymatic reactions involving. Inhibition of the zinc enzyme carbonic anhydrase (CA, EC 4.2.1.1) with sulfonamides may be exploited clinically for the treatment and prevention of a multitude of diseases (Pastorekova *et al.*, 2004; Supuran *et al.*, 2004; Mann & Keilin, 1940). With the early report that sulfanilamide acts as an inhibitor of CA, a great scientific adventure initiated, leading to the development of several classes of drugs based on the sulfonamide motif.

Sulfonamides and their derivatives have been the subject of investigation for many reasons. The amides are important constituent of many biologically significant compounds. The chemistry of sulfonamides is of interest as they show distinct physical, chemical and biological properties. The sulfonamide derivatives are known for their numerous pharmacological activities, antibacterial, antitumor, insulin-release stimulation and antithyroid properties (Maren, 1976). In addition, the unsubstituted aromatic/heterocyclic sulfonamides act as carbonic anhydrase inhibitors (Supuran & Scozzafava, 2001; Türkmen *et al.*, 2005; Supuran *et al.*, 2003) whereas other types of derivatives show diuretic activity (high-ceiling diuretics or thiadiazine diuretics), hypoglycemic activity and anti- cancer properties (Supuran & Scozzafava, 2002). Although sulfonamides are best known as bacteriostatic (Silverman, 1992) and antimalarial agents (Albala *et al.*, 1994), there is now a range of drugs, possessing very different pharmacological activities, in which the sulfonamide group is present (Reynolds, 1996). Due to their significant pharmacology applications and widespread use in medicine, these compounds have gained attention in bio-inorganic and metal-based drug chemistry. In this work we report the crystal structure of 3-chloro-*N*-(4-sulfamoylphenyl)propanamide.

In the title molecule (I), (Fig. 1), the S═O distances [1.4302 (14) and 1.4349 (16) Å] and the O═S═O angle [118.21 (9)°] are within the normal range as the values of the other geometric parameters of the molecule. The dihedral angle between the benzene ring and the amido –NHCO– plane is 15.0 (2)°.

The crystal structure is stabilized by N—H⋯O type hydrogen bonds (Table 1, Fig. 2). N1—H1A⋯O1 and N1—H1B⋯O3 generate the two-dimensional network (double layer structure), but N2—H2A⋯O2 links the layers into a three-dimensional network. An intramolecular hydrogen contact C3—H3⋯O3 generates a ring of graph-set motif S(6) (Bernstein *et al.*, 1995) (Table 1). Furthermore, crystal packing is influenced by weak π–π stacking interactions between nearby aromatic rings of the adjacent molecules, [*Cg*⋯*Cg*[iv] = 3.7447 (12) Å; *Cg* is the centroid of the C1–C6 ring; symmetry code: (iv) 1 - *x*, 1 - *y*, 1 - *z*].

### S2. Experimental

Sulfanilamide (2.00 g, 0.011 mol) and *N*-ethylmaleimide (NEM) (1.566 g, 0.016 mol) were stirred in tetrahydrofuran (THF) (200 ml) until most of the starting material had dissolved. 3-Chloropropanoylchloride (1.782 g, 0.014 mol) in THF was slowly added to the reaction mixture. The reaction was stirred at 258 K for 4 h under anhydrous conditions. After

warming to room temperature the white precipitate of NEM/HCl salt filtered off. The THF was removed in *vacuo* and the resulting white solid dissolved in ethyl acetate. The organic extract was washed with 3*M* hydrochloric acid (20 ml) then with saturated sodium bicarbonate solution (20 ml) and finally with brine. Drying over magnesium sulfate and evaporation yielded a white solid which was recrystallized from water to give the title compound (yield: 70%, m.p: 501–503 K).

## S3. Refinement

The H-atoms of the $NH_2$ group were located in a difference Fourier map, and were refined with distance restraints of N—H = 0.86 (2) Å; their temperature factors were freely refined. The other H-atoms were placed in calculated positions with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and were included in the refinement in the riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C, N)$.
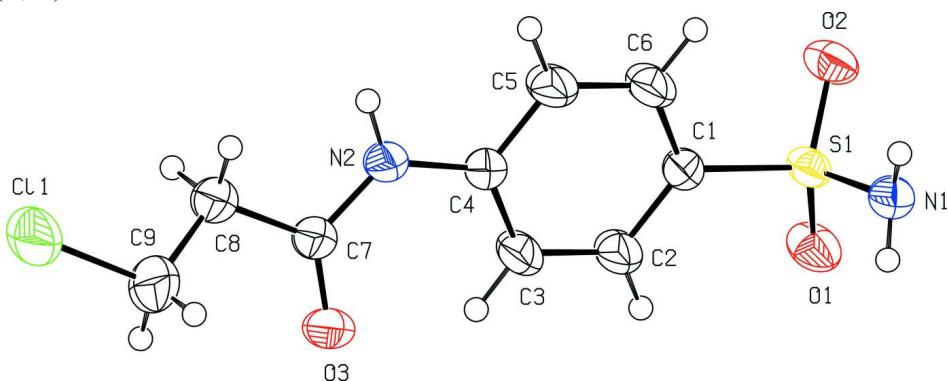


**Figure 1**

The title molecule with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.
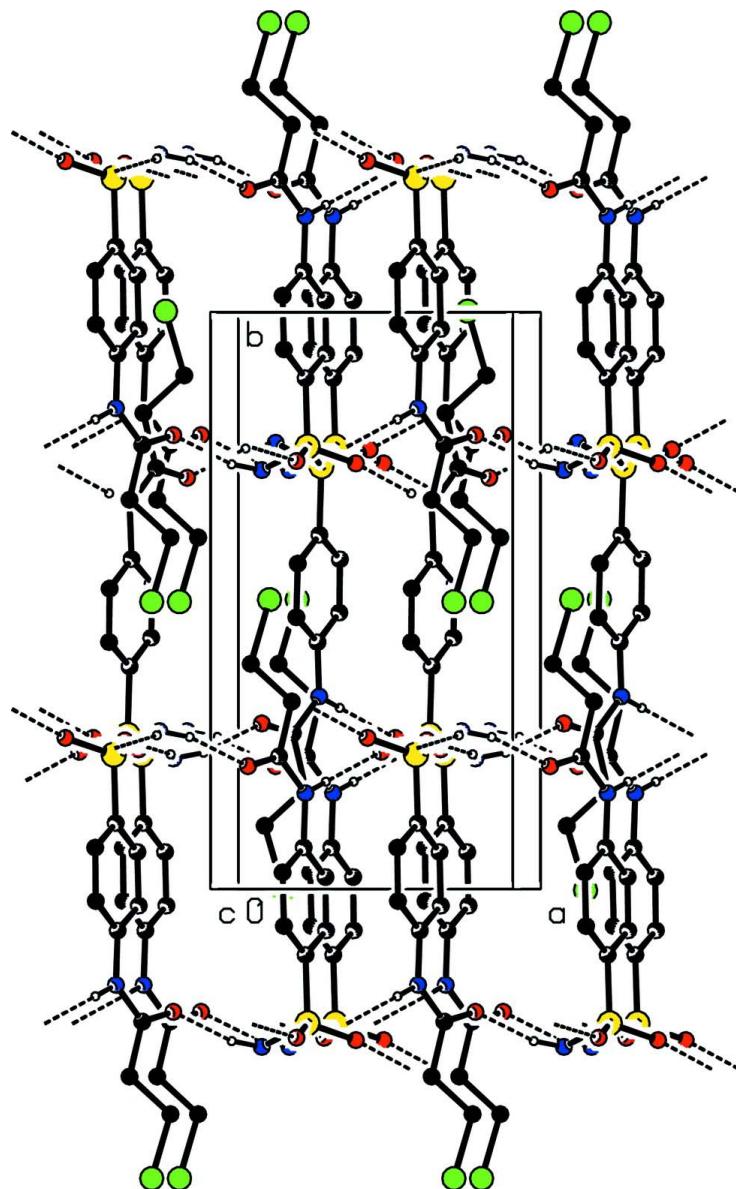
**Figure 2**

The packing of the molecules of (I) linked by of N—H···O hydrogen bonds, viewed down the *c* axis. All hydrogen atoms not involved in hydrogen bonding have been omitted for clarity. Hydrogen bonds are indicated by dotted lines.

**3-Chloro-*N*-(4-sulfamoylphenyl)propanamide**

*Crystal data*

| | |
|---|---|
| $C_9H_{11}ClN_2O_3S$ | $V = 1117.36\,(10)$ Å$^3$ |
| $M_r = 262.72$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | $F(000) = 544$ |
| Hall symbol: -P 2ybc | $D_x = 1.562$ Mg m$^{-3}$ |
| $a = 7.7554\,(4)$ Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $b = 14.8191\,(8)$ Å | Cell parameters from 8775 reflections |
| $c = 9.7482\,(5)$ Å | $\theta = 2.1–28.0°$ |
| $\beta = 94.181\,(4)°$ | $\mu = 0.52$ mm$^{-1}$ |

$T = 296$ K

Prism, colourless

$0.78 \times 0.45 \times 0.22$ mm

*Data collection*

| | |
|---|---|
| Stoe IPDS2 diffractometer | $T_{min} = 0.754$, $T_{max} = 0.892$ |
| Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus | 6023 measured reflections |
| | 2294 independent reflections |
| Plane graphite monochromator | 2007 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 6.67 pixels mm⁻¹ | $R_{int} = 0.040$ |

Stoe IPDS2 diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus

Plane graphite monochromator

Detector resolution: 6.67 pixels mm$^{-1}$

$\omega$ scans

Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)

$T_{min} = 0.754$, $T_{max} = 0.892$

6023 measured reflections

2294 independent reflections

2007 reflections with $I > 2\sigma(I)$

$R_{int} = 0.040$

$\theta_{max} = 26.5°$, $\theta_{min} = 2.5°$

$h = -8 \rightarrow 9$

$k = -16 \rightarrow 18$

$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.106$

$S = 1.08$

2294 reflections

153 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

$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.351P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.28$ e Å⁻³

$\Delta\rho_{min} = -0.44$ 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 | 0.18392 (12) | −0.00186 (4) | 0.38004 (9) | 0.0791 (3) |
| S1 | 0.31196 (6) | 0.73280 (3) | 0.40392 (4) | 0.0330 (1) |
| O1 | 0.2882 (2) | 0.75787 (10) | 0.54296 (14) | 0.0471 (5) |
| O2 | 0.4665 (2) | 0.76199 (10) | 0.34461 (15) | 0.0445 (5) |
| O3 | 0.1258 (2) | 0.28706 (10) | 0.52407 (19) | 0.0571 (6) |
| N1 | 0.1520 (2) | 0.77368 (12) | 0.31092 (18) | 0.0398 (5) |
| N2 | 0.3009 (2) | 0.33382 (11) | 0.36141 (18) | 0.0419 (5) |
| C1 | 0.3044 (2) | 0.61415 (12) | 0.39403 (17) | 0.0331 (5) |
| C2 | 0.2424 (3) | 0.56420 (15) | 0.4978 (2) | 0.0499 (7) |
| C3 | 0.2372 (4) | 0.47119 (15) | 0.4898 (2) | 0.0530 (7) |
| C4 | 0.2965 (2) | 0.42797 (13) | 0.37652 (19) | 0.0360 (5) |
| C5 | 0.3592 (3) | 0.47919 (15) | 0.2722 (2) | 0.0508 (7) |
| C6 | 0.3617 (3) | 0.57169 (15) | 0.2792 (2) | 0.0488 (7) |

| | | | |
|---|---|---|---|
| C7 | 0.2202 (3) | 0.27011 (13) | 0.4329 (2) | 0.0389 (6) |
| C8 | 0.2583 (3) | 0.17489 (14) | 0.3889 (2) | 0.0448 (6) |
| C9 | 0.1263 (4) | 0.10957 (16) | 0.4265 (4) | 0.0725 (10) |
| H1A | 0.153 (4) | 0.7665 (17) | 0.2235 (18) | 0.053 (7)* |
| H1B | 0.055 (3) | 0.7636 (17) | 0.342 (3) | 0.051 (7)* |
| H2 | 0.20340 | 0.59310 | 0.57430 | 0.0600* |
| H2A | 0.36310 | 0.31400 | 0.29840 | 0.0500* |
| H3 | 0.19400 | 0.43770 | 0.56030 | 0.0640* |
| H5 | 0.40020 | 0.45050 | 0.19620 | 0.0610* |
| H6 | 0.40150 | 0.60550 | 0.20760 | 0.0590* |
| H8A | 0.26540 | 0.17370 | 0.29000 | 0.0540* |
| H8B | 0.36990 | 0.15670 | 0.43140 | 0.0540* |
| H9A | 0.01560 | 0.12520 | 0.38000 | 0.0870* |
| H9B | 0.11490 | 0.11230 | 0.52490 | 0.0870* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.1120 (6) | 0.0337 (3) | 0.0982 (6) | −0.0094 (3) | 0.0520 (5) | −0.0065 (3) |
| S1 | 0.0424 (3) | 0.0302 (2) | 0.0276 (2) | −0.0060 (2) | 0.0106 (2) | −0.0011 (2) |
| O1 | 0.0702 (10) | 0.0434 (8) | 0.0294 (7) | −0.0105 (7) | 0.0146 (6) | −0.0057 (5) |
| O2 | 0.0459 (8) | 0.0452 (8) | 0.0440 (8) | −0.0140 (6) | 0.0142 (6) | 0.0000 (6) |
| O3 | 0.0628 (10) | 0.0383 (8) | 0.0757 (11) | −0.0035 (7) | 0.0427 (9) | −0.0018 (7) |
| N1 | 0.0471 (10) | 0.0372 (9) | 0.0367 (9) | 0.0024 (7) | 0.0131 (7) | 0.0019 (7) |
| N2 | 0.0504 (10) | 0.0315 (8) | 0.0466 (9) | 0.0014 (7) | 0.0233 (7) | −0.0011 (7) |
| C1 | 0.0382 (10) | 0.0295 (9) | 0.0323 (8) | 0.0002 (7) | 0.0075 (7) | 0.0012 (6) |
| C2 | 0.0740 (15) | 0.0352 (10) | 0.0443 (11) | 0.0005 (10) | 0.0310 (10) | 0.0001 (8) |
| C3 | 0.0814 (16) | 0.0348 (11) | 0.0473 (11) | 0.0008 (11) | 0.0354 (11) | 0.0060 (9) |
| C4 | 0.0383 (10) | 0.0315 (9) | 0.0394 (9) | 0.0021 (8) | 0.0116 (8) | 0.0022 (7) |
| C5 | 0.0732 (15) | 0.0387 (10) | 0.0447 (11) | −0.0035 (10) | 0.0323 (11) | −0.0041 (9) |
| C6 | 0.0712 (15) | 0.0377 (10) | 0.0410 (10) | −0.0061 (10) | 0.0278 (10) | 0.0009 (8) |
| C7 | 0.0385 (10) | 0.0335 (10) | 0.0461 (11) | −0.0008 (8) | 0.0126 (8) | 0.0004 (8) |
| C8 | 0.0500 (12) | 0.0344 (10) | 0.0520 (11) | −0.0010 (9) | 0.0176 (9) | −0.0027 (8) |
| C9 | 0.0714 (18) | 0.0328 (11) | 0.118 (2) | −0.0020 (12) | 0.0382 (17) | −0.0012 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C9 | 1.778 (3) | C3—C4 | 1.384 (3) |
| S1—O1 | 1.4302 (14) | C4—C5 | 1.385 (3) |
| S1—O2 | 1.4349 (16) | C5—C6 | 1.373 (3) |
| S1—N1 | 1.6012 (17) | C7—C8 | 1.510 (3) |
| S1—C1 | 1.7617 (18) | C8—C9 | 1.475 (4) |
| O3—C7 | 1.218 (3) | C2—H2 | 0.9300 |
| N2—C4 | 1.404 (3) | C3—H3 | 0.9300 |
| N2—C7 | 1.354 (3) | C5—H5 | 0.9300 |
| N1—H1A | 0.859 (18) | C6—H6 | 0.9300 |
| N1—H1B | 0.85 (2) | C8—H8A | 0.9700 |
| N2—H2A | 0.8600 | C8—H8B | 0.9700 |

| | | | |
|---|---|---|---|
| C1—C2 | 1.369 (3) | C9—H9A | 0.9700 |
| C1—C6 | 1.385 (3) | C9—H9B | 0.9700 |
| C2—C3 | 1.381 (3) | | |
| | | | |
| Cl1···N1<sup>i</sup> | 3.3993 (19) | C3···O3 | 2.889 (3) |
| Cl1···C9<sup>ii</sup> | 3.543 (3) | C7···O2<sup>vi</sup> | 3.173 (3) |
| Cl1···H9B<sup>ii</sup> | 3.0400 | C8···O2<sup>vi</sup> | 3.372 (3) |
| S1···O1<sup>iii</sup> | 3.5128 (14) | C9···Cl1<sup>ii</sup> | 3.543 (3) |
| O1···N1<sup>iv</sup> | 2.926 (2) | C7···H3 | 2.7900 |
| O1···S1<sup>iv</sup> | 3.5128 (14) | C8···H6<sup>x</sup> | 3.0400 |
| O1···O2<sup>iv</sup> | 3.171 (2) | H1A···O1<sup>iii</sup> | 2.14 (2) |
| O2···N2<sup>v</sup> | 2.992 (2) | H1A···H2<sup>iii</sup> | 2.5800 |
| O2···C8<sup>vi</sup> | 3.372 (3) | H1B···O3<sup>vii</sup> | 2.12 (3) |
| O2···O1<sup>iii</sup> | 3.171 (2) | H2···O1 | 2.5500 |
| O2···C7<sup>vi</sup> | 3.173 (3) | H2···H1A<sup>iv</sup> | 2.5800 |
| O3···N1<sup>vii</sup> | 2.923 (2) | H2A···H5 | 2.2800 |
| O3···C3 | 2.889 (3) | H2A···H8A | 2.2100 |
| O1···H6<sup>iv</sup> | 2.6900 | H2A···O2<sup>x</sup> | 2.1300 |
| O1···H1A<sup>iv</sup> | 2.14 (2) | H3···O3 | 2.3200 |
| O1···H2 | 2.5500 | H3···C7 | 2.7900 |
| O2···H8A<sup>v</sup> | 2.8600 | H5···H2A | 2.2800 |
| O2···H6 | 2.7100 | H6···O2 | 2.7100 |
| O2···H2A<sup>v</sup> | 2.1300 | H6···C8<sup>v</sup> | 3.0400 |
| O2···H8B<sup>vi</sup> | 2.7200 | H6···H8B<sup>v</sup> | 2.4300 |
| O3···H9A | 2.8800 | H6···O1<sup>iii</sup> | 2.6900 |
| O3···H9B | 2.5900 | H8A···H2A | 2.2100 |
| O3···H3 | 2.3200 | H8A···O2<sup>x</sup> | 2.8600 |
| O3···H1B<sup>vii</sup> | 2.12 (3) | H8A···O3<sup>xi</sup> | 2.8000 |
| O3···H8A<sup>viii</sup> | 2.8000 | H8B···H6<sup>x</sup> | 2.4300 |
| N1···Cl1<sup>ix</sup> | 3.3993 (19) | H8B···O2<sup>vi</sup> | 2.7200 |
| N1···O3<sup>vii</sup> | 2.923 (2) | H9A···O3 | 2.8800 |
| N1···O1<sup>iii</sup> | 2.926 (2) | H9B···O3 | 2.5900 |
| N2···O2<sup>x</sup> | 2.991 (2) | H9B···Cl1<sup>ii</sup> | 3.0400 |
| | | | |
| O1—S1—O2 | 118.21 (9) | N2—C7—C8 | 113.46 (18) |
| O1—S1—N1 | 106.87 (9) | O3—C7—C8 | 122.71 (18) |
| O1—S1—C1 | 107.76 (8) | C7—C8—C9 | 112.9 (2) |
| O2—S1—N1 | 107.05 (9) | Cl1—C9—C8 | 110.8 (2) |
| O2—S1—C1 | 107.72 (8) | C1—C2—H2 | 120.00 |
| N1—S1—C1 | 108.98 (9) | C3—C2—H2 | 120.00 |
| C4—N2—C7 | 128.58 (17) | C2—C3—H3 | 120.00 |
| S1—N1—H1A | 117 (2) | C4—C3—H3 | 120.00 |
| S1—N1—H1B | 113.8 (19) | C4—C5—H5 | 120.00 |
| H1A—N1—H1B | 114 (3) | C6—C5—H5 | 119.00 |
| C4—N2—H2A | 116.00 | C1—C6—H6 | 120.00 |
| C7—N2—H2A | 116.00 | C5—C6—H6 | 120.00 |
| S1—C1—C2 | 120.76 (14) | C7—C8—H8A | 109.00 |
| S1—C1—C6 | 119.09 (14) | C7—C8—H8B | 109.00 |

| | | | |
|---|---|---|---|
| C2—C1—C6 | 120.15 (18) | C9—C8—H8A | 109.00 |
| C1—C2—C3 | 120.56 (19) | C9—C8—H8B | 109.00 |
| C2—C3—C4 | 119.8 (2) | H8A—C8—H8B | 108.00 |
| N2—C4—C5 | 117.07 (17) | Cl1—C9—H9A | 109.00 |
| C3—C4—C5 | 119.15 (19) | Cl1—C9—H9B | 109.00 |
| N2—C4—C3 | 123.77 (18) | C8—C9—H9A | 110.00 |
| C4—C5—C6 | 121.01 (19) | C8—C9—H9B | 109.00 |
| C1—C6—C5 | 119.32 (19) | H9A—C9—H9B | 108.00 |
| O3—C7—N2 | 123.84 (18) | | |
| | | | |
| O1—S1—C1—C2 | 14.47 (18) | C2—C1—C6—C5 | −1.5 (3) |
| O2—S1—C1—C2 | 143.03 (16) | C6—C1—C2—C3 | 0.4 (3) |
| N1—S1—C1—C2 | −101.16 (17) | C1—C2—C3—C4 | 0.6 (4) |
| O1—S1—C1—C6 | −165.74 (15) | C2—C3—C4—N2 | 178.1 (2) |
| O2—S1—C1—C6 | −37.18 (17) | C2—C3—C4—C5 | −0.5 (3) |
| N1—S1—C1—C6 | 78.63 (17) | N2—C4—C5—C6 | −179.24 (19) |
| C7—N2—C4—C3 | 15.1 (3) | C3—C4—C5—C6 | −0.6 (3) |
| C7—N2—C4—C5 | −166.4 (2) | C4—C5—C6—C1 | 1.6 (3) |
| C4—N2—C7—O3 | 1.0 (3) | O3—C7—C8—C9 | 21.5 (3) |
| C4—N2—C7—C8 | −178.99 (18) | N2—C7—C8—C9 | −158.5 (2) |
| S1—C1—C2—C3 | −179.80 (19) | C7—C8—C9—Cl1 | −177.00 (18) |
| S1—C1—C6—C5 | 178.75 (17) | | |

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*, −*y*, −*z*+1; (iii) *x*, −*y*+3/2, *z*−1/2; (iv) *x*, −*y*+3/2, *z*+1/2; (v) −*x*+1, *y*+1/2, −*z*+1/2; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) −*x*, −*y*+1, −*z*+1; (viii) *x*, −*y*+1/2, *z*+1/2; (ix) *x*, *y*+1, *z*; (x) −*x*+1, *y*−1/2, −*z*+1/2; (xi) *x*, −*y*+1/2, *z*−1/2.

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N1—H1*A*···O1ⁱⁱⁱ | 0.859 (18) | 2.14 (2) | 2.926 (2) | 151 (3) |
| N1—H1*B*···O3ᵛⁱⁱ | 0.85 (2) | 2.12 (3) | 2.923 (2) | 158 (3) |
| N2—H2*A*···O2ˣ | 0.86 | 2.13 | 2.991 (2) | 175 |
| C3—H3···O3 | 0.93 | 2.32 | 2.889 (3) | 120 |

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