# organic compounds

# 4-[(4-Methoxybenzenesulfonamido)-methyl]cyclohexane-1-carboxylic acid

**Muhammad Ashfaq,[a] Samina Iram,[a] Mehmet Akkurt,[b]* Islam Ullah Khan,[c]‡ Ghulam Mustafa[a] and Muhammad Danish[a]**

[a]Department of Chemistry, University of Gujrat, H.H. Campus, Gujrat 50700, Pakistan, [b]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, and [c]Department of Chemistry, Government College University, Lahore 54000, Pakistan

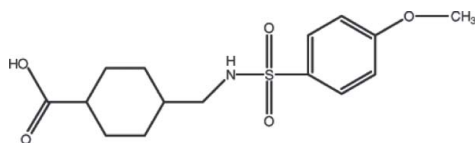Correspondence e-mail: akkurt@erciyes.edu.tr

In the title compound, $C_{15}H_{21}NO_5S$, two crystallographically independent molecules are linked into a dimer by a pair of N—H⋯O hydrogen bonds, forming an $R_2^2(8)$ ring motif. In the crystal, molecules are further linked by intermolecular O—H⋯O hydrogen bonds into a two-dimensional network parallel to (012). Additional stabilization is provided by weak intermolecular C—H⋯O hydrogen bonds.

## Related literature

For background to tranexamic acid (trans-4-(aminomethyl)-cyclohexanecarboxylic acid), see: Boylan *et al.* (1996); Khan *et al.* (2002); Nilsson (1980); Shah *et al.* (2010); Shahzadi *et al.* (2007); Svahn *et al.* (1986); Vavrova *et al.* (2005). For a related structure, see: Ashfaq *et al.* (2011). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For ring conformations, see: Cremer & Pople (1975).

## Experimental

### Crystal data

| | |
|---|---|
| $C_{15}H_{21}NO_5S$ | $\alpha = 79.736\,(3)°$ |
| $M_r = 327.40$ | $\beta = 89.813\,(3)°$ |
| Triclinic, $P\bar{1}$ | $\gamma = 75.518\,(3)°$ |
| $a = 5.9119\,(3)$ Å | $V = 1607.67\,(16)$ Å$^3$ |
| $b = 10.7223\,(7)$ Å | $Z = 4$ |
| $c = 26.6453\,(15)$ Å | Mo $K\alpha$ radiation |

| | |
|---|---|
| $\mu = 0.22$ mm$^{-1}$ | $0.25 \times 0.19 \times 0.14$ mm |
| $T$ = 296 K | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 5942 independent reflections |
| | 3973 reflections with $I > 2\sigma(I)$ |
| 25440 measured reflections | $R_{int} = 0.048$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.070$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.218$ | |
| $S = 1.03$ | |
| 5942 reflections | $\Delta\rho_{max} = 0.92$ e Å$^{-3}$ |
| 412 parameters | $\Delta\rho_{min} = -0.36$ e Å$^{-3}$ |
| 5 restraints | |

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N1—H1$N$⋯O8$^i$ | 0.83 (4) | 2.14 (3) | 2.961 (4) | 173 (3) |
| N2—H2$N$⋯O3$^{ii}$ | 0.85 (3) | 2.18 (3) | 3.024 (4) | 172 (3) |
| O4—H4$O$⋯O5$^{iii}$ | 0.83 (5) | 1.84 (5) | 2.660 (5) | 166 (6) |
| O10—H10$O$⋯O9$^{iv}$ | 0.82 (7) | 1.89 (8) | 2.631 (8) | 151 (7) |
| C16—H16$B$⋯O6$^v$ | 0.96 | 2.59 | 3.378 (7) | 139 |
| C25—H25$A$⋯O3$^{ii}$ | 0.97 | 2.54 | 3.450 (6) | 157 |

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

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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5293).

## References

Ashfaq, M., Iram, S., Akkurt, M., Khan, I. U., Mustafa, G. & Sharif, S. (2011). *Acta Cryst.* E**67**, o1563.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Boylan, J. F., Klinck, J. R., Sandier, A. N., Arellano, R., Greig, P. D., Nierenberg, H., Roger, S. L. & Glynnix, M. F. (1996). *Anesthesiology*, **85**, 1043–1048.

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Khan, M. F., Khan, M. F., Ashfaq, M. & Khan, G. M. (2002). *Pak. J. Pharm. Sci.* **15**, 55–62.

Nilsson, I. M. (1980). *J. Clin. Pathol. Suppl.* **14**, 41–47.

Shah, F. A., Ali, S. & Shahzadi, S. (2010). *J. Iran. Chem. Soc.* **7**, 59–68.

‡ Additional corresponding author, e-mail: iukhan.gcu@gmail.com.

Shahzadi, S., Ali, S., Parvez, M., Badshah, A., Ahmed, E. & Malik, A. (2007). *Russ. J. Inorg. Chem.* **52**, 386–393.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Svahn, C. M., Merenyi, F., Karlson, L., Widlund, L. & Gralls, M. (1986). *J. Med. Chem.* **29**, 448–453.

Vavrova, K., Hrabalek, A., Dolezal, P., Holas, T. & Klimentova, J. (2005). *J. Control. Release*, **104**, 41–49.

# supporting information

# 4-[(4-Methoxybenzenesulfonamido)methyl]cyclohexane-1-carboxylic acid

## Muhammad Ashfaq, Samina Iram, Mehmet Akkurt, Islam Ullah Khan, Ghulam Mustafa and Muhammad Danish

### S1. Comment

Tranexamic acid or trans-4-(aminomethyl)cyclohexanecarboxylic acid, is a synthetic amino acid used commonly for curing abnormal bleeding in a variety of diseases (Boylan *et al.*, 1996; Nilsson, 1980). A number of scientists derivatized this drug, evaluated the activity and found most derivatives were superior to the parent drug (Svahn *et al.*, 1986; Khan *et al.*, 2002; Vavrova *et al.*, 2005; Shahzadi *et al.*, 2007; Shah *et al.*, 2010). We have recently prepared a derivative of this drug and reported the crystal structure (Ashfaq *et al.*, 2011).

Fig. 1 shows the two crystallographically independent molecules in the asymmetric unit of the title compound (I). The molecules form a dimer, in which a pair of N—H⋯O hydrogen bonds generate an intermolecular $R_2^2(8)$ ring (Bernstein, *et al.*, 1995). The cyclohexane rings (C9–C14 and C24–C29) in each molecule adopt a chair configuration [the puckering parameters are $Q_T$ = 0.547 (5) Å, $\theta$ = 180.0 (5) °, $\varphi$ = 286 (35) ° and $Q_T$ = 0.561 (6) Å, $\theta$ = 3.7 (5) °, $\varphi$ = 161 (8) °, respectively] (Cremer & Pople, 1975). In the crystal, molecules are further linked by intermolecular O—H⋯O hydrogen bonds to form a two-dimensional network parallel to (012). Additional stabilization is provided by weak intermoleclar C—H⋯O hydrogen bonds (Fig. 2).

### S2. Experimental

4-Methoxybenzene sulfonyl chloride (1.32 g, 6.36 mmol) was added to a solution of tranexamic acid (1.0 g, 6.36 mmol) in distilled water (10 ml). The reaction mixture was stirred at room temperature at pH 8–9, which was adjusted by 1*M* sodium carbonate solution. After completion of the reaction which was observed by the consumption of 4-methoxy-benzene sulfonyl chloride, the pH was adjusted at 2–3 using 1 N HCl solution, which resulted in the formation of precipiates. these were filtered off and dried. The product was recrystallized using methanol.

### S3. Refinement

The H atoms of the –NH and –OH groups were located in a difference Fourier map and their positional parameters were restrained [N1—H1N = 0.83 (4), N2—H2N = 0.85 (3), O4—H4O = 0.83 (5) and O10—H10O = 0.82 (7) Å]. Their displacement parameters were refined using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(N) or 1.5$U_{eq}$(O). The other H atoms were placed in ideal positions and refined as riding with C—H = 0.93 - 0.98 Å, and $U_{iso}$ = 1.2$U_{eq}$(C) for CH and CH$_2$ groups and $U_{iso}$ = 1.5$U_{eq}$(C) for CH$_3$ group.
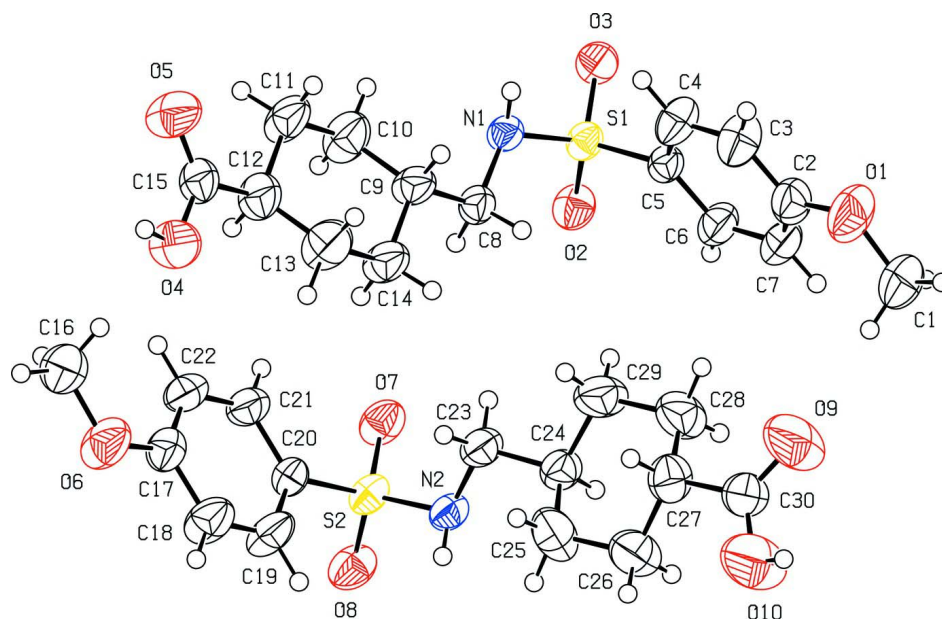
**Figure 1**

The two independent molecules in the asymmetric unit with displacement ellipsoids for non-H atoms drawn at the 50% probability level.
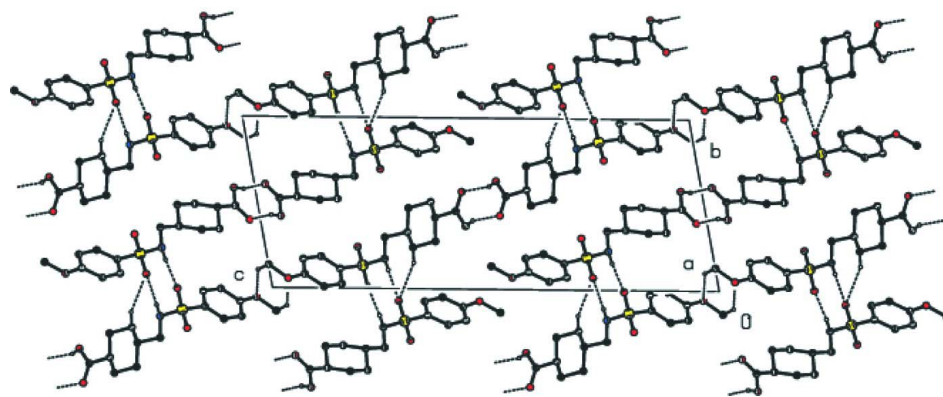


**Figure 2**

The packing and hydrogen bonding of viewed along the *a* axis. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

**4-[(4-Methoxybenzenesulfonamido)methyl]cyclohexane-1-carboxylic acid**

*Crystal data*

| | |
|---|---|
| $C_{15}H_{21}NO_5S$ | $a = 5.9119$ (3) Å |
| $M_r = 327.40$ | $b = 10.7223$ (7) Å |
| Triclinic, $P\bar{1}$ | $c = 26.6453$ (15) Å |
| Hall symbol: -P 1 | $\alpha = 79.736$ (3)° |

$\beta$ = 89.813 (3)°
$\gamma$ = 75.518 (3)°
$V$ = 1607.67 (16) Å$^3$
$Z$ = 4
$F(000)$ = 696
$D_x$ = 1.353 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 4861 reflections
$\theta$ = 2.8–24.1°
$\mu$ = 0.22 mm$^{-1}$
$T$ = 296 K
Block, colourless
0.25 × 0.19 × 0.14 mm

*Data collection*

Bruker APEXII CCD
   diffractometer
Radiation source: sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
25440 measured reflections
5942 independent reflections

3973 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 0.8°
$h = -7 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -32 \rightarrow 31$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.218
$S$ = 1.03
5942 reflections
412 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.1117P)^2 + 1.5531P]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 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 (Å$^2$)*

|    | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|----|------|------|------|------|
| S1 | 0.24030 (15) | 0.81008 (9) | 0.71667 (3) | 0.0404 (3) |
| O1 | 0.8071 (6) | 0.9302 (4) | 0.54159 (12) | 0.0852 (16) |
| O2 | 0.1613 (5) | 0.6977 (3) | 0.71162 (10) | 0.0541 (10) |
| O3 | 0.0718 (4) | 0.9282 (3) | 0.72214 (10) | 0.0522 (9) |
| O4 | 1.4245 (6) | 0.4189 (3) | 0.95284 (13) | 0.0772 (12) |
| O5 | 1.2465 (6) | 0.6045 (3) | 0.97576 (13) | 0.0827 (12) |
| N1 | 0.4128 (5) | 0.7734 (3) | 0.76697 (11) | 0.0405 (10) |
| C1 | 0.8230 (11) | 0.8647 (6) | 0.49907 (19) | 0.091 (2) |
| C2 | 0.6699 (8) | 0.8966 (4) | 0.58007 (16) | 0.0593 (16) |
| C3 | 0.6843 (8) | 0.9522 (5) | 0.62271 (17) | 0.0662 (17) |

| C4 | 0.5527 (7) | 0.9266 (4) | 0.66397 (16) | 0.0592 (16) |
|---|---|---|---|---|
| C5 | 0.4061 (6) | 0.8452 (3) | 0.66319 (13) | 0.0402 (11) |
| C6 | 0.3904 (8) | 0.7915 (4) | 0.62065 (15) | 0.0570 (16) |
| C7 | 0.5216 (9) | 0.8176 (4) | 0.57891 (16) | 0.0655 (16) |
| C8 | 0.6083 (6) | 0.6550 (4) | 0.77250 (14) | 0.0446 (12) |
| C9 | 0.7785 (7) | 0.6474 (4) | 0.81491 (16) | 0.0543 (12) |
| C10 | 0.6831 (8) | 0.6655 (5) | 0.86445 (17) | 0.0713 (19) |
| C11 | 0.8758 (8) | 0.6601 (5) | 0.90438 (17) | 0.0722 (19) |
| C12 | 1.0675 (8) | 0.5335 (5) | 0.90841 (17) | 0.0661 (17) |
| C13 | 1.1619 (8) | 0.5154 (5) | 0.85893 (18) | 0.0789 (19) |
| C14 | 0.9709 (8) | 0.5220 (4) | 0.81929 (17) | 0.0649 (17) |
| C15 | 1.2557 (7) | 0.5231 (4) | 0.94865 (16) | 0.0536 (14) |
| S2 | 0.58540 (16) | 0.13448 (10) | 0.78880 (4) | 0.0452 (3) |
| O6 | 1.2525 (6) | 0.0555 (4) | 0.96080 (12) | 0.0810 (14) |
| O7 | 0.3919 (4) | 0.2420 (3) | 0.79281 (11) | 0.0585 (10) |
| O8 | 0.5465 (5) | 0.0094 (3) | 0.78645 (11) | 0.0614 (11) |
| O9 | 1.2935 (9) | 0.5689 (4) | 0.53819 (18) | 0.126 (2) |
| O10 | 1.4743 (11) | 0.3683 (4) | 0.5428 (2) | 0.141 (2) |
| N2 | 0.7154 (5) | 0.1743 (3) | 0.73693 (11) | 0.0445 (10) |
| C16 | 1.2095 (10) | 0.1349 (5) | 0.99941 (19) | 0.0815 (19) |
| C17 | 1.0888 (8) | 0.0813 (4) | 0.92229 (15) | 0.0560 (16) |
| C18 | 1.1491 (8) | 0.0089 (5) | 0.88368 (18) | 0.0702 (16) |
| C19 | 0.9954 (7) | 0.0252 (5) | 0.84341 (16) | 0.0650 (16) |
| C20 | 0.7813 (6) | 0.1140 (4) | 0.84073 (13) | 0.0416 (11) |
| C21 | 0.7221 (7) | 0.1857 (4) | 0.87863 (15) | 0.0564 (14) |
| C22 | 0.8754 (8) | 0.1698 (4) | 0.91948 (16) | 0.0626 (16) |
| C23 | 0.7777 (8) | 0.3001 (4) | 0.72825 (15) | 0.0540 (14) |
| C24 | 0.8709 (7) | 0.3303 (4) | 0.67579 (15) | 0.0520 (12) |
| C25 | 1.1018 (9) | 0.2412 (5) | 0.6690 (2) | 0.0782 (17) |
| C26 | 1.1972 (10) | 0.2776 (5) | 0.6166 (2) | 0.088 (2) |
| C27 | 1.2156 (8) | 0.4178 (4) | 0.60792 (17) | 0.0626 (17) |
| C28 | 0.9834 (9) | 0.5085 (5) | 0.6117 (2) | 0.0756 (19) |
| C29 | 0.8827 (10) | 0.4715 (5) | 0.6639 (2) | 0.079 (2) |
| C30 | 1.3310 (8) | 0.4554 (5) | 0.55920 (18) | 0.0623 (17) |
| H1A | 0.89090 | 0.77270 | 0.51030 | 0.1370* |
| H1B | 0.91940 | 0.89960 | 0.47420 | 0.1370* |
| H1C | 0.66950 | 0.87770 | 0.48410 | 0.1370* |
| H1N | 0.441 (7) | 0.843 (3) | 0.7708 (15) | 0.0490* |
| H3 | 0.78340 | 1.00700 | 0.62340 | 0.0790* |
| H4 | 0.56250 | 0.96420 | 0.69250 | 0.0710* |
| H4O | 1.522 (8) | 0.425 (6) | 0.9742 (19) | 0.1160* |
| H6 | 0.29060 | 0.73700 | 0.61990 | 0.0680* |
| H7 | 0.50910 | 0.78150 | 0.55010 | 0.0780* |
| H8A | 0.68910 | 0.65460 | 0.74080 | 0.0540* |
| H8B | 0.54670 | 0.57810 | 0.77890 | 0.0540* |
| H9 | 0.85350 | 0.71910 | 0.80410 | 0.0660* |
| H10A | 0.60360 | 0.59760 | 0.87650 | 0.0860* |
| H10B | 0.56900 | 0.74940 | 0.86060 | 0.0860* |

| | | | |
|---|---|---|---|
| H11A | 0.94250 | 0.73440 | 0.89460 | 0.0870* |
| H11B | 0.80800 | 0.66540 | 0.93740 | 0.0870* |
| H12 | 0.99390 | 0.46160 | 0.91990 | 0.0790* |
| H13A | 1.27480 | 0.43100 | 0.86270 | 0.0950* |
| H13B | 1.24290 | 0.58260 | 0.84700 | 0.0950* |
| H14A | 1.03930 | 0.51690 | 0.78630 | 0.0780* |
| H14B | 0.90450 | 0.44750 | 0.82880 | 0.0780* |
| H2N | 0.825 (5) | 0.109 (3) | 0.7335 (15) | 0.0530* |
| H10O | 1.566 (11) | 0.400 (4) | 0.525 (3) | 0.2110* |
| H16A | 1.20210 | 0.22420 | 0.98440 | 0.1220* |
| H16B | 1.33380 | 0.10380 | 1.02520 | 0.1220* |
| H16C | 1.06370 | 0.12990 | 1.01460 | 0.1220* |
| H18 | 1.29440 | −0.05080 | 0.88530 | 0.0840* |
| H19 | 1.03580 | −0.02390 | 0.81780 | 0.0780* |
| H21 | 0.57700 | 0.24570 | 0.87680 | 0.0680* |
| H22 | 0.83410 | 0.21910 | 0.94500 | 0.0750* |
| H23A | 0.89520 | 0.29810 | 0.75390 | 0.0640* |
| H23B | 0.64060 | 0.36920 | 0.73200 | 0.0640* |
| H24 | 0.75900 | 0.31900 | 0.65100 | 0.0620* |
| H25A | 1.08620 | 0.15200 | 0.67340 | 0.0940* |
| H25B | 1.21260 | 0.24450 | 0.69520 | 0.0940* |
| H26A | 1.35020 | 0.21950 | 0.61440 | 0.1050* |
| H26B | 1.09420 | 0.26680 | 0.59030 | 0.1050* |
| H27 | 1.31590 | 0.42480 | 0.63590 | 0.0750* |
| H28A | 0.87730 | 0.50410 | 0.58470 | 0.0910* |
| H28B | 0.99900 | 0.59770 | 0.60730 | 0.0910* |
| H29A | 0.97890 | 0.48750 | 0.69030 | 0.0950* |
| H29B | 0.72660 | 0.52770 | 0.66470 | 0.0950* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0355 (5) | 0.0484 (6) | 0.0369 (5) | −0.0078 (4) | −0.0020 (4) | −0.0110 (4) |
| O1 | 0.100 (3) | 0.109 (3) | 0.055 (2) | −0.039 (2) | 0.0312 (18) | −0.0198 (19) |
| O2 | 0.0573 (16) | 0.0628 (18) | 0.0505 (16) | −0.0279 (14) | −0.0009 (13) | −0.0137 (13) |
| O3 | 0.0406 (14) | 0.0578 (17) | 0.0509 (16) | 0.0026 (12) | −0.0029 (12) | −0.0122 (13) |
| O4 | 0.067 (2) | 0.077 (2) | 0.077 (2) | 0.0080 (18) | −0.0345 (17) | −0.0229 (18) |
| O5 | 0.074 (2) | 0.086 (2) | 0.081 (2) | 0.0099 (18) | −0.0353 (18) | −0.039 (2) |
| N1 | 0.0417 (16) | 0.0421 (18) | 0.0370 (16) | −0.0065 (14) | −0.0031 (13) | −0.0113 (14) |
| C1 | 0.117 (4) | 0.097 (4) | 0.053 (3) | −0.015 (3) | 0.032 (3) | −0.015 (3) |
| C2 | 0.061 (3) | 0.065 (3) | 0.046 (2) | −0.008 (2) | 0.010 (2) | −0.006 (2) |
| C3 | 0.068 (3) | 0.090 (3) | 0.051 (3) | −0.037 (3) | 0.007 (2) | −0.016 (2) |
| C4 | 0.062 (3) | 0.081 (3) | 0.045 (2) | −0.030 (2) | 0.0037 (19) | −0.022 (2) |
| C5 | 0.0376 (18) | 0.045 (2) | 0.0357 (19) | −0.0050 (16) | −0.0032 (15) | −0.0091 (15) |
| C6 | 0.074 (3) | 0.062 (3) | 0.042 (2) | −0.025 (2) | 0.004 (2) | −0.0172 (19) |
| C7 | 0.092 (3) | 0.069 (3) | 0.042 (2) | −0.025 (3) | 0.008 (2) | −0.021 (2) |
| C8 | 0.044 (2) | 0.048 (2) | 0.038 (2) | −0.0042 (17) | −0.0018 (16) | −0.0088 (16) |
| C9 | 0.053 (2) | 0.055 (2) | 0.052 (2) | −0.0004 (19) | −0.0134 (19) | −0.0212 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.055 (3) | 0.094 (4) | 0.058 (3) | 0.000 (2) | −0.005 (2) | −0.023 (3) |
| C11 | 0.064 (3) | 0.091 (4) | 0.050 (3) | 0.014 (2) | −0.018 (2) | −0.030 (2) |
| C12 | 0.064 (3) | 0.072 (3) | 0.052 (3) | 0.003 (2) | −0.017 (2) | −0.013 (2) |
| C13 | 0.061 (3) | 0.095 (4) | 0.068 (3) | 0.013 (3) | −0.011 (2) | −0.028 (3) |
| C14 | 0.062 (3) | 0.068 (3) | 0.056 (3) | 0.010 (2) | −0.016 (2) | −0.026 (2) |
| C15 | 0.050 (2) | 0.060 (3) | 0.046 (2) | −0.007 (2) | −0.0110 (18) | −0.0071 (19) |
| S2 | 0.0432 (5) | 0.0572 (6) | 0.0409 (5) | −0.0171 (4) | 0.0084 (4) | −0.0179 (4) |
| O6 | 0.075 (2) | 0.100 (3) | 0.062 (2) | 0.0009 (19) | −0.0193 (17) | −0.0318 (19) |
| O7 | 0.0440 (15) | 0.075 (2) | 0.0540 (17) | −0.0033 (14) | 0.0048 (12) | −0.0222 (14) |
| O8 | 0.0729 (19) | 0.069 (2) | 0.0600 (18) | −0.0405 (16) | 0.0159 (15) | −0.0261 (15) |
| O9 | 0.156 (4) | 0.072 (3) | 0.127 (4) | −0.008 (3) | 0.088 (3) | 0.008 (2) |
| O10 | 0.192 (5) | 0.078 (3) | 0.140 (4) | −0.023 (3) | 0.113 (4) | −0.004 (3) |
| N2 | 0.0474 (18) | 0.0482 (19) | 0.0406 (17) | −0.0116 (15) | 0.0096 (14) | −0.0159 (14) |
| C16 | 0.101 (4) | 0.076 (3) | 0.065 (3) | −0.014 (3) | −0.024 (3) | −0.018 (3) |
| C17 | 0.062 (3) | 0.061 (3) | 0.044 (2) | −0.012 (2) | −0.0043 (19) | −0.0124 (19) |
| C18 | 0.051 (2) | 0.089 (3) | 0.063 (3) | 0.009 (2) | 0.000 (2) | −0.032 (3) |
| C19 | 0.056 (2) | 0.087 (3) | 0.053 (3) | −0.004 (2) | 0.006 (2) | −0.036 (2) |
| C20 | 0.0407 (19) | 0.048 (2) | 0.0372 (19) | −0.0119 (16) | 0.0054 (15) | −0.0102 (16) |
| C21 | 0.060 (2) | 0.055 (3) | 0.050 (2) | 0.001 (2) | −0.0001 (19) | −0.0207 (19) |
| C22 | 0.077 (3) | 0.058 (3) | 0.051 (2) | −0.003 (2) | −0.002 (2) | −0.025 (2) |
| C23 | 0.067 (3) | 0.053 (2) | 0.048 (2) | −0.020 (2) | 0.0138 (19) | −0.0184 (19) |
| C24 | 0.058 (2) | 0.052 (2) | 0.049 (2) | −0.0171 (19) | 0.0115 (18) | −0.0132 (18) |
| C25 | 0.072 (3) | 0.067 (3) | 0.077 (3) | −0.001 (2) | 0.015 (3) | 0.012 (2) |
| C26 | 0.105 (4) | 0.058 (3) | 0.088 (4) | −0.004 (3) | 0.055 (3) | −0.004 (3) |
| C27 | 0.065 (3) | 0.067 (3) | 0.058 (3) | −0.024 (2) | 0.014 (2) | −0.007 (2) |
| C28 | 0.083 (3) | 0.056 (3) | 0.083 (4) | −0.016 (2) | 0.026 (3) | −0.003 (2) |
| C29 | 0.100 (4) | 0.057 (3) | 0.084 (4) | −0.021 (3) | 0.042 (3) | −0.023 (3) |
| C30 | 0.067 (3) | 0.056 (3) | 0.065 (3) | −0.018 (2) | 0.021 (2) | −0.011 (2) |

## Geometric parameters (Å, º)

| | | | |
|---|---|---|---|
| S1—O2 | 1.424 (3) | C8—H8B | 0.9700 |
| S1—O3 | 1.432 (3) | C9—H9 | 0.9800 |
| S1—N1 | 1.616 (3) | C10—H10A | 0.9700 |
| S1—C5 | 1.766 (4) | C10—H10B | 0.9700 |
| S2—O8 | 1.428 (3) | C11—H11A | 0.9700 |
| S2—N2 | 1.622 (3) | C11—H11B | 0.9700 |
| S2—O7 | 1.426 (3) | C12—H12 | 0.9800 |
| S2—C20 | 1.755 (4) | C13—H13A | 0.9700 |
| O1—C1 | 1.427 (7) | C13—H13B | 0.9700 |
| O1—C2 | 1.359 (6) | C14—H14A | 0.9700 |
| O4—C15 | 1.287 (5) | C14—H14B | 0.9700 |
| O5—C15 | 1.220 (5) | C17—C18 | 1.390 (6) |
| O4—H4O | 0.83 (5) | C17—C22 | 1.369 (6) |
| O6—C16 | 1.432 (6) | C18—C19 | 1.367 (6) |
| O6—C17 | 1.356 (6) | C19—C20 | 1.374 (6) |
| O9—C30 | 1.211 (7) | C20—C21 | 1.369 (6) |
| O10—C30 | 1.236 (7) | C21—C22 | 1.378 (6) |

| | | | |
|---|---|---|---|
| O10—H10O | 0.82 (7) | C23—C24 | 1.512 (6) |
| N1—C8 | 1.473 (5) | C24—C29 | 1.510 (7) |
| N1—H1N | 0.83 (4) | C24—C25 | 1.489 (7) |
| N2—C23 | 1.465 (5) | C25—C26 | 1.527 (8) |
| N2—H2N | 0.85 (3) | C26—C27 | 1.511 (7) |
| C2—C3 | 1.386 (6) | C27—C28 | 1.486 (7) |
| C2—C7 | 1.367 (7) | C27—C30 | 1.503 (7) |
| C3—C4 | 1.372 (6) | C28—C29 | 1.537 (8) |
| C4—C5 | 1.378 (5) | C16—H16A | 0.9600 |
| C5—C6 | 1.373 (5) | C16—H16B | 0.9600 |
| C6—C7 | 1.382 (6) | C16—H16C | 0.9600 |
| C8—C9 | 1.493 (6) | C18—H18 | 0.9300 |
| C9—C10 | 1.459 (6) | C19—H19 | 0.9300 |
| C9—C14 | 1.515 (6) | C21—H21 | 0.9300 |
| C10—C11 | 1.545 (7) | C22—H22 | 0.9300 |
| C11—C12 | 1.523 (7) | C23—H23A | 0.9700 |
| C12—C13 | 1.456 (7) | C23—H23B | 0.9700 |
| C12—C15 | 1.518 (6) | C24—H24 | 0.9800 |
| C13—C14 | 1.529 (7) | C25—H25A | 0.9700 |
| C1—H1B | 0.9600 | C25—H25B | 0.9700 |
| C1—H1C | 0.9600 | C26—H26A | 0.9700 |
| C1—H1A | 0.9600 | C26—H26B | 0.9700 |
| C3—H3 | 0.9300 | C27—H27 | 0.9800 |
| C4—H4 | 0.9300 | C28—H28A | 0.9700 |
| C6—H6 | 0.9300 | C28—H28B | 0.9700 |
| C7—H7 | 0.9300 | C29—H29A | 0.9700 |
| C8—H8A | 0.9700 | C29—H29B | 0.9700 |
| | | | |
| S2···H25B[i] | 3.1900 | H4O···C15[iii] | 2.66 (5) |
| O3···N2[ii] | 3.024 (4) | H4O···O5[iii] | 1.84 (5) |
| O4···O5[iii] | 2.660 (5) | H6···O2 | 2.5500 |
| O5···O4[iii] | 2.660 (5) | H7···C1 | 2.5400 |
| O5···C15[iii] | 3.411 (6) | H7···H1C | 2.2100 |
| O6···C16[iv] | 3.378 (7) | H7···H1A | 2.4800 |
| O8···N1[v] | 2.961 (4) | H8A···C5 | 2.8400 |
| O9···O10[vi] | 2.631 (8) | H8A···H14A | 2.4100 |
| O9···C30[vi] | 3.412 (7) | H8B···H13B[i] | 2.5500 |
| O10···C30[vi] | 3.394 (7) | H8B···H14B | 2.4700 |
| O10···O9[vi] | 2.631 (8) | H8B···O2 | 2.7900 |
| O1···H1B[vii] | 2.7100 | H9···H13B | 2.5500 |
| O2···H29A[i] | 2.8700 | H9···H1N | 2.5400 |
| O2···H6 | 2.5500 | H9···H11A | 2.5100 |
| O2···H14A[i] | 2.7500 | H10A···H13B[i] | 2.3300 |
| O2···H8B | 2.7900 | H10A···H14B | 2.5800 |
| O3···H19[ii] | 2.6900 | H10A···H12 | 2.5500 |
| O3···H25A[ii] | 2.5400 | H10A···C13[i] | 3.0200 |
| O3···H2N[ii] | 2.18 (3) | H10A···C15[i] | 2.9700 |
| O4···H16A | 2.7400 | H10B···H1N | 2.4700 |

| | | | |
|---|---|---|---|
| O4···H4O[iii] | 2.85 (6) | H10B···N1 | 2.6100 |
| O4···H22[viii] | 2.8400 | H10B···H18[ii] | 2.5300 |
| O4···H13A | 2.5300 | H10O···O9[vi] | 1.89 (8) |
| O5···H11B | 2.6700 | H10O···H10O[vi] | 2.27 (8) |
| O5···H11A | 2.7500 | H10O···C30[vi] | 2.65 (7) |
| O5···H4O[iii] | 1.84 (5) | H10O···O10[vi] | 2.76 (6) |
| O6···H16B[iv] | 2.5900 | H11A···H13B | 2.5900 |
| O7···H21 | 2.5100 | H11A···H9 | 2.5100 |
| O7···H25B[i] | 2.8000 | H11A···O5 | 2.7500 |
| O7···H23B | 2.6200 | H11B···O5 | 2.6700 |
| O8···H1N[v] | 2.14 (3) | H11B···C16[xiii] | 2.9300 |
| O8···H4[v] | 2.6300 | H11B···H16A[xiii] | 2.5700 |
| O9···H28B | 2.5400 | H12···H14B | 2.5200 |
| O9···H1A | 2.8000 | H12···H10A | 2.5500 |
| O9···H10O[vi] | 1.89 (8) | H13A···H21[viii] | 2.2900 |
| O10···H26A | 2.4900 | H13A···O4 | 2.5300 |
| O10···H10O[vi] | 2.76 (6) | H13B···H8B[viii] | 2.5500 |
| N1···O8[ix] | 2.961 (4) | H13B···C8[viii] | 3.0800 |
| N2···O3[x] | 3.024 (4) | H13B···C10[viii] | 3.0200 |
| N1···H10B | 2.6100 | H13B···H11A | 2.5900 |
| N1···H4 | 2.8900 | H13B···H9 | 2.5500 |
| N2···H25A | 2.7500 | H13B···H10A[viii] | 2.3300 |
| C15···O5[iii] | 3.411 (6) | H14A···H8A | 2.4100 |
| C16···O6[iv] | 3.378 (7) | H14A···O2[viii] | 2.7500 |
| C30···O10[vi] | 3.394 (7) | H14B···H8B | 2.4700 |
| C30···O9[vi] | 3.412 (7) | H14B···H10A | 2.5800 |
| C1···H26B[xi] | 2.9600 | H14B···H12 | 2.5200 |
| C1···H7 | 2.5400 | H16A···O4 | 2.7400 |
| C2···H1C[xii] | 2.9900 | H16A···C22 | 2.8300 |
| C3···H26A[ii] | 3.0200 | H16A···H22 | 2.4400 |
| C4···H1N | 2.95 (4) | H16A···H11B[xiii] | 2.5700 |
| C5···H8A | 2.8400 | H16B···O6[iv] | 2.5900 |
| C6···H29B | 3.0600 | H16C···C22 | 2.6900 |
| C7···H1C | 2.6900 | H16C···H22 | 2.2200 |
| C7···H1A | 2.8500 | H16C···C17[xiv] | 2.9000 |
| C8···H13B[i] | 3.0800 | H18···H10B[x] | 2.5300 |
| C10···H13B[i] | 3.0200 | H19···O3[x] | 2.6900 |
| C10···H1N | 2.98 (4) | H19···H2N | 2.5700 |
| C13···H10A[viii] | 3.0200 | H21···O7 | 2.5100 |
| C15···H10A[viii] | 2.9700 | H21···H13A[i] | 2.2900 |
| C15···H4O[iii] | 2.66 (5) | H22···O4[i] | 2.8400 |
| C16···H22 | 2.5300 | H22···C16 | 2.5300 |
| C16···H11B[xiii] | 2.9300 | H22···H16A | 2.4400 |
| C17···H16C[xiv] | 2.9000 | H22···H16C | 2.2200 |
| C19···H2N | 3.01 (4) | H23A···C20 | 2.9500 |
| C20···H23A | 2.9500 | H23A···H25B | 2.4600 |
| C22···H16C | 2.6900 | H23A···H29A | 2.5500 |
| C22···H16A | 2.8300 | H23B···O7 | 2.6200 |

| | | | |
|---|---|---|---|
| C25···H2N | 2.81 (3) | H23B···H29B | 2.3900 |
| C30···H10O<sup>vi</sup> | 2.65 (7) | H24···H26B | 2.5700 |
| H1A···O9 | 2.8000 | H24···H27<sup>i</sup> | 2.5800 |
| H1A···C7 | 2.8500 | H25A···O3<sup>x</sup> | 2.5400 |
| H1A···H7 | 2.4800 | H25A···N2 | 2.7500 |
| H1B···O1<sup>vii</sup> | 2.7100 | H25A···H2N | 2.2900 |
| H1C···C7 | 2.6900 | H25B···S2<sup>viii</sup> | 3.1900 |
| H1C···H7 | 2.2100 | H25B···O7<sup>viii</sup> | 2.8000 |
| H1C···C2<sup>xii</sup> | 2.9900 | H25B···H23A | 2.4600 |
| H1N···O8<sup>ix</sup> | 2.14 (3) | H25B···H27 | 2.4700 |
| H1N···C4 | 2.95 (4) | H26A···O10 | 2.4900 |
| H1N···C10 | 2.98 (4) | H26A···C3<sup>x</sup> | 3.0200 |
| H1N···H4 | 2.4600 | H26B···H24 | 2.5700 |
| H1N···H9 | 2.5400 | H26B···H28A | 2.5200 |
| H1N···H10B | 2.4700 | H26B···C1<sup>xi</sup> | 2.9600 |
| H2N···C25 | 2.81 (3) | H27···H24<sup>viii</sup> | 2.5800 |
| H2N···O3<sup>x</sup> | 2.18 (3) | H27···H25B | 2.4700 |
| H2N···C19 | 3.01 (4) | H27···H29A | 2.4900 |
| H2N···H19 | 2.5700 | H28A···H26B | 2.5200 |
| H2N···H25A | 2.2900 | H28B···O9 | 2.5400 |
| H4···O8<sup>ix</sup> | 2.6300 | H29A···O2<sup>viii</sup> | 2.8700 |
| H4···N1 | 2.8900 | H29A···H23A | 2.5500 |
| H4···H1N | 2.4600 | H29A···H27 | 2.4900 |
| H4O···O4<sup>iii</sup> | 2.85 (6) | H29B···C6 | 3.0600 |
| H4O···H4O<sup>iii</sup> | 2.26 (8) | H29B···H23B | 2.3900 |
| | | | |
| O2—S1—O3 | 119.03 (18) | C13—C12—H12 | 107.00 |
| O2—S1—N1 | 108.36 (17) | C12—C13—H13B | 109.00 |
| O2—S1—C5 | 107.61 (16) | C12—C13—H13A | 109.00 |
| O3—S1—N1 | 105.26 (16) | C14—C13—H13B | 109.00 |
| O3—S1—C5 | 108.38 (16) | H13A—C13—H13B | 108.00 |
| N1—S1—C5 | 107.74 (16) | C14—C13—H13A | 109.00 |
| O8—S2—C20 | 107.74 (19) | C9—C14—H14A | 109.00 |
| N2—S2—C20 | 107.95 (17) | H14A—C14—H14B | 108.00 |
| O7—S2—N2 | 107.77 (17) | C13—C14—H14A | 109.00 |
| O7—S2—C20 | 107.64 (18) | C13—C14—H14B | 109.00 |
| O7—S2—O8 | 119.76 (18) | C9—C14—H14B | 109.00 |
| O8—S2—N2 | 105.49 (17) | O6—C17—C18 | 115.2 (4) |
| C1—O1—C2 | 117.8 (4) | O6—C17—C22 | 125.2 (4) |
| C15—O4—H4O | 107 (4) | C18—C17—C22 | 119.6 (4) |
| C16—O6—C17 | 117.8 (4) | C17—C18—C19 | 120.2 (5) |
| C30—O10—H10O | 110 (3) | C18—C19—C20 | 120.1 (4) |
| S1—N1—C8 | 118.3 (2) | S2—C20—C19 | 119.8 (3) |
| S1—N1—H1N | 106 (3) | S2—C20—C21 | 120.5 (3) |
| C8—N1—H1N | 118 (3) | C19—C20—C21 | 119.8 (4) |
| S2—N2—C23 | 118.3 (3) | C20—C21—C22 | 120.6 (4) |
| C23—N2—H2N | 115 (2) | C17—C22—C21 | 119.8 (4) |
| S2—N2—H2N | 108 (3) | N2—C23—C24 | 111.9 (3) |

| | | | |
|---|---|---|---|
| C3—C2—C7 | 119.8 (4) | C25—C24—C29 | 110.6 (4) |
| O1—C2—C7 | 125.5 (4) | C23—C24—C29 | 110.2 (4) |
| O1—C2—C3 | 114.7 (4) | C23—C24—C25 | 113.5 (4) |
| C2—C3—C4 | 120.2 (4) | C24—C25—C26 | 112.4 (4) |
| C3—C4—C5 | 120.1 (4) | C25—C26—C27 | 110.4 (4) |
| C4—C5—C6 | 119.6 (4) | C26—C27—C28 | 110.6 (4) |
| S1—C5—C4 | 120.1 (3) | C26—C27—C30 | 112.9 (4) |
| S1—C5—C6 | 120.3 (3) | C28—C27—C30 | 112.6 (4) |
| C5—C6—C7 | 120.6 (4) | C27—C28—C29 | 110.3 (4) |
| C2—C7—C6 | 119.8 (4) | C24—C29—C28 | 113.3 (4) |
| N1—C8—C9 | 112.4 (3) | O9—C30—O10 | 121.1 (5) |
| C10—C9—C14 | 111.5 (4) | O9—C30—C27 | 120.7 (5) |
| C8—C9—C14 | 109.5 (4) | O10—C30—C27 | 118.1 (5) |
| C8—C9—C10 | 117.0 (4) | O6—C16—H16A | 110.00 |
| C9—C10—C11 | 111.9 (4) | O6—C16—H16B | 109.00 |
| C10—C11—C12 | 110.6 (4) | O6—C16—H16C | 109.00 |
| C11—C12—C13 | 111.7 (4) | H16A—C16—H16B | 109.00 |
| C13—C12—C15 | 112.8 (4) | H16A—C16—H16C | 109.00 |
| C11—C12—C15 | 111.9 (4) | H16B—C16—H16C | 109.00 |
| C12—C13—C14 | 112.1 (4) | C17—C18—H18 | 120.00 |
| C9—C14—C13 | 111.6 (4) | C19—C18—H18 | 120.00 |
| O4—C15—O5 | 122.4 (4) | C18—C19—H19 | 120.00 |
| O4—C15—C12 | 114.3 (4) | C20—C19—H19 | 120.00 |
| O5—C15—C12 | 123.3 (4) | C20—C21—H21 | 120.00 |
| H1A—C1—H1B | 109.00 | C22—C21—H21 | 120.00 |
| H1A—C1—H1C | 109.00 | C17—C22—H22 | 120.00 |
| H1B—C1—H1C | 110.00 | C21—C22—H22 | 120.00 |
| O1—C1—H1B | 109.00 | N2—C23—H23A | 109.00 |
| O1—C1—H1C | 109.00 | N2—C23—H23B | 109.00 |
| O1—C1—H1A | 110.00 | C24—C23—H23A | 109.00 |
| C4—C3—H3 | 120.00 | C24—C23—H23B | 109.00 |
| C2—C3—H3 | 120.00 | H23A—C23—H23B | 108.00 |
| C5—C4—H4 | 120.00 | C23—C24—H24 | 107.00 |
| C3—C4—H4 | 120.00 | C25—C24—H24 | 107.00 |
| C7—C6—H6 | 120.00 | C29—C24—H24 | 107.00 |
| C5—C6—H6 | 120.00 | C24—C25—H25A | 109.00 |
| C2—C7—H7 | 120.00 | C24—C25—H25B | 109.00 |
| C6—C7—H7 | 120.00 | C26—C25—H25A | 109.00 |
| C9—C8—H8A | 109.00 | C26—C25—H25B | 109.00 |
| C9—C8—H8B | 109.00 | H25A—C25—H25B | 108.00 |
| H8A—C8—H8B | 108.00 | C25—C26—H26A | 110.00 |
| N1—C8—H8B | 109.00 | C25—C26—H26B | 110.00 |
| N1—C8—H8A | 109.00 | C27—C26—H26A | 110.00 |
| C10—C9—H9 | 106.00 | C27—C26—H26B | 110.00 |
| C14—C9—H9 | 106.00 | H26A—C26—H26B | 108.00 |
| C8—C9—H9 | 106.00 | C26—C27—H27 | 107.00 |
| C9—C10—H10B | 109.00 | C28—C27—H27 | 107.00 |
| C11—C10—H10A | 109.00 | C30—C27—H27 | 107.00 |

| C11—C10—H10B | 109.00 | C27—C28—H28A | 110.00 |
|---|---|---|---|
| C9—C10—H10A | 109.00 | C27—C28—H28B | 110.00 |
| H10A—C10—H10B | 108.00 | C29—C28—H28A | 110.00 |
| C12—C11—H11A | 110.00 | C29—C28—H28B | 110.00 |
| C12—C11—H11B | 110.00 | H28A—C28—H28B | 108.00 |
| H11A—C11—H11B | 108.00 | C24—C29—H29A | 109.00 |
| C10—C11—H11A | 110.00 | C24—C29—H29B | 109.00 |
| C10—C11—H11B | 110.00 | C28—C29—H29A | 109.00 |
| C15—C12—H12 | 107.00 | C28—C29—H29B | 109.00 |
| C11—C12—H12 | 107.00 | H29A—C29—H29B | 108.00 |
| | | | |
| O2—S1—N1—C8 | 51.9 (3) | C10—C9—C14—C13 | −54.1 (5) |
| O3—S1—N1—C8 | −179.8 (3) | C8—C9—C14—C13 | 174.8 (4) |
| C5—S1—N1—C8 | −64.3 (3) | C9—C10—C11—C12 | −54.7 (5) |
| O2—S1—C5—C4 | −163.4 (3) | C10—C11—C12—C13 | 54.4 (5) |
| O2—S1—C5—C6 | 16.4 (4) | C10—C11—C12—C15 | −178.1 (4) |
| O3—S1—C5—C4 | 66.7 (3) | C13—C12—C15—O5 | 130.0 (5) |
| O3—S1—C5—C6 | −113.5 (3) | C15—C12—C13—C14 | 178.3 (4) |
| N1—S1—C5—C4 | −46.8 (3) | C13—C12—C15—O4 | −51.7 (6) |
| N1—S1—C5—C6 | 133.1 (3) | C11—C12—C13—C14 | −54.7 (6) |
| C20—S2—N2—C23 | −65.3 (3) | C11—C12—C15—O4 | −178.7 (4) |
| O7—S2—C20—C19 | −173.3 (3) | C11—C12—C15—O5 | 3.0 (6) |
| O7—S2—C20—C21 | 6.8 (4) | C12—C13—C14—C9 | 54.2 (5) |
| O8—S2—C20—C19 | 56.2 (4) | O6—C17—C18—C19 | 178.8 (4) |
| O8—S2—C20—C21 | −123.7 (3) | C22—C17—C18—C19 | −0.6 (7) |
| N2—S2—C20—C19 | −57.3 (4) | O6—C17—C22—C21 | −178.9 (4) |
| N2—S2—C20—C21 | 122.9 (3) | C18—C17—C22—C21 | 0.4 (7) |
| O7—S2—N2—C23 | 50.7 (3) | C17—C18—C19—C20 | 0.5 (7) |
| O8—S2—N2—C23 | 179.7 (3) | C18—C19—C20—S2 | 179.9 (4) |
| C1—O1—C2—C3 | 172.6 (4) | C18—C19—C20—C21 | −0.3 (7) |
| C1—O1—C2—C7 | −8.9 (7) | S2—C20—C21—C22 | 180.0 (3) |
| C16—O6—C17—C18 | 174.6 (4) | C19—C20—C21—C22 | 0.1 (6) |
| C16—O6—C17—C22 | −6.1 (7) | C20—C21—C22—C17 | −0.1 (7) |
| S1—N1—C8—C9 | 168.8 (3) | N2—C23—C24—C25 | −67.8 (5) |
| S2—N2—C23—C24 | −173.2 (3) | N2—C23—C24—C29 | 167.6 (4) |
| O1—C2—C3—C4 | 179.5 (4) | C23—C24—C25—C26 | −177.4 (4) |
| C7—C2—C3—C4 | 0.9 (7) | C29—C24—C25—C26 | −52.9 (5) |
| O1—C2—C7—C6 | −179.7 (4) | C23—C24—C29—C28 | 178.2 (4) |
| C3—C2—C7—C6 | −1.3 (7) | C25—C24—C29—C28 | 51.9 (6) |
| C2—C3—C4—C5 | 0.2 (7) | C24—C25—C26—C27 | 56.8 (6) |
| C3—C4—C5—C6 | −0.9 (6) | C25—C26—C27—C28 | −58.6 (6) |
| C3—C4—C5—S1 | 179.0 (3) | C25—C26—C27—C30 | 174.2 (4) |
| S1—C5—C6—C7 | −179.3 (3) | C26—C27—C28—C29 | 57.1 (5) |
| C4—C5—C6—C7 | 0.5 (6) | C30—C27—C28—C29 | −175.6 (4) |
| C5—C6—C7—C2 | 0.6 (7) | C26—C27—C30—O9 | 155.7 (5) |
| N1—C8—C9—C10 | 50.4 (5) | C26—C27—C30—O10 | −28.1 (7) |
| N1—C8—C9—C14 | 178.6 (3) | C28—C27—C30—O9 | 29.7 (7) |

| C8—C9—C10—C11 | −178.1 (4) | C28—C27—C30—O10 | −154.2 (5) |
| C14—C9—C10—C11 | 54.7 (5) | C27—C28—C29—C24 | −54.5 (6) |

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

*Hydrogen-bond geometry (Å, °)*

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$N$···O8$^{ix}$ | 0.83 (4) | 2.14 (3) | 2.961 (4) | 173 (3) |
| N2—H2$N$···O3$^{x}$ | 0.85 (3) | 2.18 (3) | 3.024 (4) | 172 (3) |
| O4—H4$O$···O5$^{iii}$ | 0.83 (5) | 1.84 (5) | 2.660 (5) | 166 (6) |
| O10—H10$O$···O9$^{vi}$ | 0.82 (7) | 1.89 (8) | 2.631 (8) | 151 (7) |
| C6—H6···O2 | 0.93 | 2.55 | 2.918 (5) | 104 |
| C10—H10$B$···N1 | 0.97 | 2.61 | 2.945 (5) | 100 |
| C16—H16$B$···O6$^{iv}$ | 0.96 | 2.59 | 3.378 (7) | 139 |
| C21—H21···O7 | 0.93 | 2.51 | 2.890 (5) | 105 |
| C25—H25$A$···O3$^{x}$ | 0.97 | 2.54 | 3.450 (6) | 157 |

Symmetry codes: (iii) −$x$+3, −$y$+1, −$z$+2; (iv) −$x$+3, −$y$, −$z$+2; (vi) −$x$+3, −$y$+1, −$z$+1; (ix) $x$, $y$+1, $z$; (x) $x$+1, $y$−1, $z$.