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## 2-(Morpholinium-4-yl)ethylammonium sulfate methanol monosolvate

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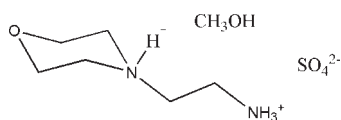
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 Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.087;  $wR$  factor = 0.286; data-to-parameter ratio = 16.3.

In the title compound,  $\text{C}_6\text{H}_{16}\text{N}_2\text{O}^{2+}\cdot\text{SO}_4^{2-}\cdot\text{CH}_3\text{OH}$ , the morpholinium ring of the dication adopts a chair conformation. The crystal structure is stabilized by an extensive three-dimensional network of intermolecular  $\text{O}-\text{H}\cdots\text{O}$ ,  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{O}-\text{H}\cdots\text{S}$  and  $\text{N}-\text{H}\cdots\text{S}$  hydrogen bonds.

### Related literature

For supramolecular compounds derived from the self-assembly of inorganic acids with organic amines, see: Xu (2010); Akhtar *et al.* (2010); Zhang & Liu (2010); Hemamalini & Fun (2010); SiMa (2010).



### Experimental

#### Crystal data

$\text{C}_6\text{H}_{16}\text{N}_2\text{O}^{2+}\cdot\text{SO}_4^{2-}\cdot\text{CH}_3\text{O}$   
 $M_r = 260.31$   
 Monoclinic,  $P2_1/c$   
 $a = 15.593$  (14) Å  
 $b = 8.573$  (8) Å  
 $c = 9.483$  (9) Å  
 $\beta = 106.395$  (11)°

$V = 1216.0$  (19) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.28$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.20 \times 0.18 \times 0.18$  mm

#### Data collection

Bruker SMART 1000 CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.946$ ,  $T_{\max} = 0.951$

5674 measured reflections  
 2462 independent reflections  
 1726 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.087$   
 $wR(F^2) = 0.286$   
 $S = 1.08$   
 2462 reflections  
 151 parameters  
 1 restraint

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.62$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.87$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$                               | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{O5}-\text{H5}\cdots\text{O4}^{\text{i}}$    | 0.82         | 1.85               | 2.659 (6)   | 172                  |
| $\text{O5}-\text{H5}\cdots\text{S1}^{\text{i}}$    | 0.82         | 2.92               | 3.636 (6)   | 147                  |
| $\text{N2}-\text{H2A}\cdots\text{O1}^{\text{ii}}$  | 0.89         | 2.07               | 2.914 (5)   | 158                  |
| $\text{N2}-\text{H2A}\cdots\text{O3}^{\text{ii}}$  | 0.89         | 2.30               | 3.001 (5)   | 135                  |
| $\text{N2}-\text{H2A}\cdots\text{S1}^{\text{ii}}$  | 0.89         | 2.68               | 3.553 (4)   | 167                  |
| $\text{N2}-\text{H2B}\cdots\text{O2}^{\text{iii}}$ | 0.89         | 2.02               | 2.898 (5)   | 168                  |
| $\text{N2}-\text{H2B}\cdots\text{O3}^{\text{iii}}$ | 0.89         | 2.45               | 3.081 (5)   | 128                  |
| $\text{N2}-\text{H2B}\cdots\text{S1}^{\text{iii}}$ | 0.89         | 2.72               | 3.567 (4)   | 160                  |
| $\text{N2}-\text{H2C}\cdots\text{O2}$              | 0.89         | 2.18               | 2.997 (5)   | 153                  |
| $\text{N2}-\text{H2C}\cdots\text{O1}$              | 0.89         | 2.23               | 2.930 (4)   | 135                  |
| $\text{N2}-\text{H2C}\cdots\text{S1}$              | 0.89         | 2.71               | 3.565 (4)   | 162                  |
| $\text{N1}-\text{H1}\cdots\text{O2}^{\text{iv}}$   | 0.90 (1)     | 2.01 (3)           | 2.837 (5)   | 152 (5)              |
| $\text{N1}-\text{H1}\cdots\text{O4}^{\text{iv}}$   | 0.90 (1)     | 2.60 (3)           | 3.382 (6)   | 146 (5)              |
| $\text{N1}-\text{H1}\cdots\text{S1}^{\text{iv}}$   | 0.90 (1)     | 2.85 (1)           | 3.738 (4)   | 172 (5)              |

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2757).

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## supporting information

*Acta Cryst.* (2010). E66, o951 [doi:10.1107/S1600536810010846]

## 2-(Morpholinium-4-yl)ethylammonium sulfate methanol monosolvate

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### S1. Comment

Self-assembly of inorganic acids with organic amines readily gives rise to hydrogen-bonded supramolecular compounds (Xu, 2010; Akhtar *et al.*, 2010; Zhang & Liu, 2010; Hemamalini & Fun, 2010; SiMa, 2010). In order to construct a similar supramolecular compound, the title compound was prepared from the reaction of 2-morpholin-4-ylethylamine with sulfuric acid in a methanol solution and its structure is reported here.

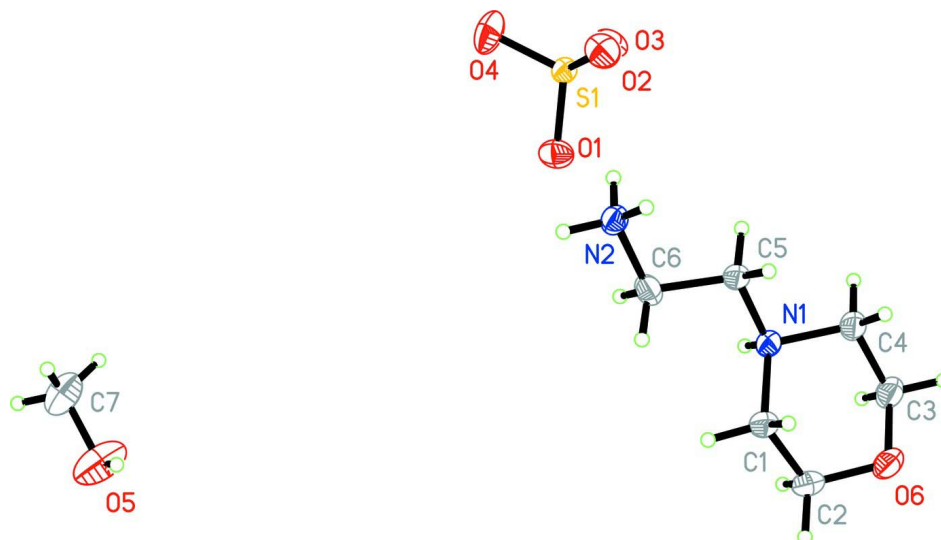
The title compound consists of a 2-morpholin-4-ylethylammonium dication, a sulfate dianion, and a methanol molecule (Fig. 1). The crystal structure is stabilized by intermolecular O–H $\cdots$ O, N–H $\cdots$ O, O–H $\cdots$ S, and N–H $\cdots$ S hydrogen bonds (Table 1, Fig. 2).

### S2. Experimental

Equimolar quantities (1.0 mmol each) of 2-morpholin-4-ylethylamine and sulfuric acid were mixed in a methanol solution. The mixture was stirred at room temperature for half an hour to give a colorless solution. After keeping the solution in air for a few days, colorless block-shaped crystals were formed.

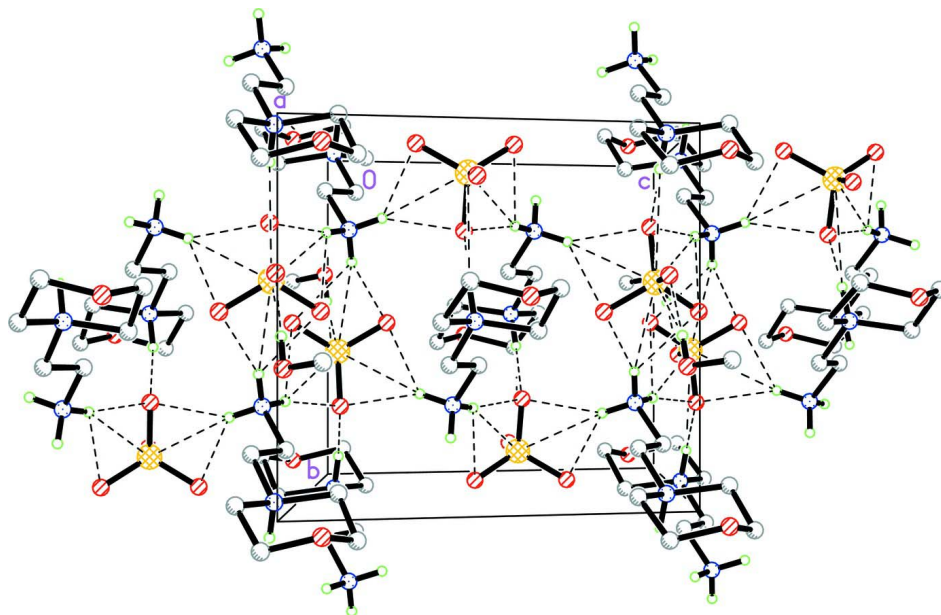
### S3. Refinement

H1 attached to N1 was located from a difference map and refined isotropically, with the N–H distance restrained to 0.90 (1) Å. Other H atoms were placed in calculated positions and constrained to ride on their parent atoms with C–H distances of 0.96–0.97 Å, N–H distances of 0.89 Å, O–H distance of 0.82 Å, and with  $U_{\text{iso}}(\text{H})$  set to  $1.2U_{\text{eq}}(\text{C}, \text{N})$  and  $1.5U_{\text{eq}}(\text{O5 and C7})$ . Crystals were small and very weakly diffracting and this is reflected in the low fraction of measured reflections and the relatively poor residuals.



**Figure 1**

The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.



**Figure 2**

Molecular packing of the title compound, viewed along the a axis. Hydrogen bonds are shown as dashed lines.

### 2-(Morpholinium-4-yl)ethylammonium sulfate methanol monosolvate

#### Crystal data

$C_6H_{16}N_2O^{2+} \cdot SO_4^{2-} \cdot CH_4O$

$M_r = 260.31$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 15.593\ (14)\ \text{\AA}$

$b = 8.573\ (8)\ \text{\AA}$

$c = 9.483\ (9)\ \text{\AA}$

$\beta = 106.395\ (11)^\circ$

$V = 1216.0\ (19)\ \text{\AA}^3$

$Z = 4$

$F(000) = 560$

$D_x = 1.422\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2104 reflections

$\theta = 2.2\text{--}27.7^\circ$   
 $\mu = 0.28\text{ mm}^{-1}$   
 $T = 298\text{ K}$

Block, colorless  
 $0.20 \times 0.18 \times 0.18\text{ mm}$

*Data collection*

Bruker SMART 1000 CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.946$ ,  $T_{\max} = 0.951$

5674 measured reflections  
 2462 independent reflections  
 1726 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$   
 $\theta_{\max} = 27.0^\circ$ ,  $\theta_{\min} = 2.7^\circ$   
 $h = -19 \rightarrow 14$   
 $k = -10 \rightarrow 10$   
 $l = -10 \rightarrow 12$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.087$   
 $wR(F^2) = 0.286$   
 $S = 1.08$   
 2462 reflections  
 151 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  
 $w = 1/[\sigma^2(F_o^2) + (0.1965P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.62\text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.87\text{ e \AA}^{-3}$

*Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 ( $\text{\AA}^2$ )*

|     | <i>x</i>     | <i>y</i>     | <i>z</i>    | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|-------------|----------------------------------|
| S1  | 0.35803 (6)  | 0.59946 (11) | 0.06772 (9) | 0.0369 (4)                       |
| O1  | 0.3987 (2)   | 0.5157 (3)   | 0.2047 (3)  | 0.0523 (8)                       |
| O2  | 0.3969 (2)   | 0.7579 (3)   | 0.0786 (3)  | 0.0557 (8)                       |
| O3  | 0.3768 (2)   | 0.5166 (4)   | -0.0531 (3) | 0.0574 (9)                       |
| O4  | 0.2617 (2)   | 0.6167 (5)   | 0.0429 (5)  | 0.0772 (11)                      |
| O5  | 0.1552 (3)   | 0.3688 (5)   | 1.0088 (7)  | 0.1071 (18)                      |
| H5  | 0.1834       | 0.4507       | 1.0182      | 0.161*                           |
| O6  | 0.9107 (2)   | 0.4451 (4)   | 0.5902 (3)  | 0.0606 (9)                       |
| N1  | 0.7246 (2)   | 0.5104 (4)   | 0.4511 (3)  | 0.0371 (7)                       |
| N2  | 0.51382 (19) | 0.7510 (4)   | 0.3894 (3)  | 0.0403 (8)                       |
| H2A | 0.5402       | 0.8420       | 0.3841      | 0.061*                           |
| H2B | 0.4754       | 0.7621       | 0.4426      | 0.061*                           |

|     |            |            |            |             |
|-----|------------|------------|------------|-------------|
| H2C | 0.4846     | 0.7192     | 0.2993     | 0.061*      |
| C1  | 0.7681 (3) | 0.5356 (5) | 0.6131 (4) | 0.0469 (10) |
| H1A | 0.7247     | 0.5183     | 0.6673     | 0.056*      |
| H1B | 0.7893     | 0.6422     | 0.6300     | 0.056*      |
| C2  | 0.8462 (3) | 0.4232 (7) | 0.6667 (5) | 0.0593 (12) |
| H2D | 0.8736     | 0.4392     | 0.7709     | 0.071*      |
| H2E | 0.8242     | 0.3168     | 0.6528     | 0.071*      |
| C3  | 0.8723 (3) | 0.4061 (6) | 0.4418 (5) | 0.0558 (12) |
| H3A | 0.8513     | 0.2991     | 0.4351     | 0.067*      |
| H3B | 0.9174     | 0.4135     | 0.3895     | 0.067*      |
| C4  | 0.7949 (3) | 0.5129 (5) | 0.3698 (4) | 0.0471 (10) |
| H4A | 0.8168     | 0.6186     | 0.3682     | 0.056*      |
| H4B | 0.7684     | 0.4801     | 0.2690     | 0.056*      |
| C5  | 0.6558 (2) | 0.6314 (5) | 0.3848 (4) | 0.0394 (8)  |
| H5A | 0.6304     | 0.6094     | 0.2810     | 0.047*      |
| H5B | 0.6841     | 0.7330     | 0.3938     | 0.047*      |
| C6  | 0.5817 (3) | 0.6351 (5) | 0.4589 (5) | 0.0497 (10) |
| H6A | 0.5542     | 0.5328     | 0.4524     | 0.060*      |
| H6B | 0.6065     | 0.6604     | 0.5621     | 0.060*      |
| C7  | 0.0750 (4) | 0.3876 (9) | 0.9066 (8) | 0.0911 (19) |
| H7A | 0.0295     | 0.3351     | 0.9386     | 0.137*      |
| H7B | 0.0778     | 0.3444     | 0.8146     | 0.137*      |
| H7C | 0.0611     | 0.4968     | 0.8944     | 0.137*      |
| H1  | 0.702 (4)  | 0.413 (3)  | 0.437 (6)  | 0.080*      |

*Atomic displacement parameters (Å<sup>2</sup>)*

|    | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$    | $U^{23}$     |
|----|-------------|-------------|-------------|--------------|-------------|--------------|
| S1 | 0.0318 (6)  | 0.0445 (6)  | 0.0335 (6)  | 0.0004 (3)   | 0.0079 (4)  | 0.0002 (3)   |
| O1 | 0.0618 (19) | 0.0560 (18) | 0.0355 (14) | -0.0019 (14) | 0.0078 (13) | 0.0054 (11)  |
| O2 | 0.068 (2)   | 0.0439 (17) | 0.0592 (18) | -0.0076 (14) | 0.0246 (14) | -0.0018 (12) |
| O3 | 0.071 (2)   | 0.065 (2)   | 0.0364 (14) | 0.0049 (15)  | 0.0159 (13) | -0.0076 (12) |
| O4 | 0.0357 (18) | 0.089 (3)   | 0.107 (3)   | 0.0122 (15)  | 0.0190 (18) | 0.005 (2)    |
| O5 | 0.070 (3)   | 0.081 (3)   | 0.143 (4)   | -0.002 (2)   | -0.016 (3)  | 0.016 (3)    |
| O6 | 0.0330 (15) | 0.092 (2)   | 0.0519 (17) | 0.0065 (15)  | 0.0046 (12) | -0.0012 (16) |
| N1 | 0.0305 (15) | 0.0446 (17) | 0.0346 (15) | -0.0036 (12) | 0.0068 (11) | -0.0012 (12) |
| N2 | 0.0317 (16) | 0.0509 (19) | 0.0376 (15) | -0.0020 (12) | 0.0085 (12) | -0.0046 (13) |
| C1 | 0.039 (2)   | 0.067 (3)   | 0.0326 (18) | 0.0013 (18)  | 0.0064 (14) | 0.0002 (16)  |
| C2 | 0.043 (2)   | 0.089 (3)   | 0.039 (2)   | 0.009 (2)    | 0.0008 (17) | 0.011 (2)    |
| C3 | 0.036 (2)   | 0.081 (3)   | 0.050 (2)   | 0.0041 (19)  | 0.0122 (17) | -0.0046 (19) |
| C4 | 0.036 (2)   | 0.068 (3)   | 0.0380 (18) | -0.0050 (18) | 0.0119 (15) | -0.0039 (16) |
| C5 | 0.0333 (18) | 0.055 (2)   | 0.0287 (16) | 0.0000 (15)  | 0.0072 (13) | -0.0001 (14) |
| C6 | 0.050 (2)   | 0.059 (2)   | 0.047 (2)   | 0.0108 (19)  | 0.0257 (17) | 0.0136 (18)  |
| C7 | 0.049 (3)   | 0.108 (5)   | 0.109 (5)   | 0.005 (3)    | 0.011 (3)   | 0.000 (4)    |

*Geometric parameters (Å, °)*

|            |             |            |           |
|------------|-------------|------------|-----------|
| S1—O3      | 1.446 (3)   | C1—H1A     | 0.9700    |
| S1—O4      | 1.461 (4)   | C1—H1B     | 0.9700    |
| S1—O1      | 1.463 (3)   | C2—H2D     | 0.9700    |
| S1—O2      | 1.479 (3)   | C2—H2E     | 0.9700    |
| O5—C7      | 1.358 (7)   | C3—C4      | 1.516 (6) |
| O5—H5      | 0.8200      | C3—H3A     | 0.9700    |
| O6—C3      | 1.405 (5)   | C3—H3B     | 0.9700    |
| O6—C2      | 1.409 (6)   | C4—H4A     | 0.9700    |
| N1—C5      | 1.497 (5)   | C4—H4B     | 0.9700    |
| N1—C4      | 1.508 (5)   | C5—C6      | 1.512 (5) |
| N1—C1      | 1.509 (5)   | C5—H5A     | 0.9700    |
| N1—H1      | 0.899 (10)  | C5—H5B     | 0.9700    |
| N2—C6      | 1.466 (5)   | C6—H6A     | 0.9700    |
| N2—H2A     | 0.8900      | C6—H6B     | 0.9700    |
| N2—H2B     | 0.8900      | C7—H7A     | 0.9600    |
| N2—H2C     | 0.8900      | C7—H7B     | 0.9600    |
| C1—C2      | 1.524 (6)   | C7—H7C     | 0.9600    |
| O3—S1—O4   | 110.5 (2)   | H2D—C2—H2E | 108.0     |
| O3—S1—O1   | 109.1 (2)   | O6—C3—C4   | 111.5 (4) |
| O4—S1—O1   | 111.2 (2)   | O6—C3—H3A  | 109.3     |
| O3—S1—O2   | 109.6 (2)   | C4—C3—H3A  | 109.3     |
| O4—S1—O2   | 107.5 (2)   | O6—C3—H3B  | 109.3     |
| O1—S1—O2   | 108.85 (17) | C4—C3—H3B  | 109.3     |
| C7—O5—H5   | 109.5       | H3A—C3—H3B | 108.0     |
| C3—O6—C2   | 108.6 (3)   | N1—C4—C3   | 111.3 (3) |
| C5—N1—C4   | 108.3 (3)   | N1—C4—H4A  | 109.4     |
| C5—N1—C1   | 113.0 (3)   | C3—C4—H4A  | 109.4     |
| C4—N1—C1   | 109.6 (3)   | N1—C4—H4B  | 109.4     |
| C5—N1—H1   | 112 (4)     | C3—C4—H4B  | 109.4     |
| C4—N1—H1   | 104 (4)     | H4A—C4—H4B | 108.0     |
| C1—N1—H1   | 109 (4)     | N1—C5—C6   | 111.7 (3) |
| C6—N2—H2A  | 109.5       | N1—C5—H5A  | 109.3     |
| C6—N2—H2B  | 109.5       | C6—C5—H5A  | 109.3     |
| H2A—N2—H2B | 109.5       | N1—C5—H5B  | 109.3     |
| C6—N2—H2C  | 109.5       | C6—C5—H5B  | 109.3     |
| H2A—N2—H2C | 109.5       | H5A—C5—H5B | 107.9     |
| H2B—N2—H2C | 109.5       | N2—C6—C5   | 110.8 (3) |
| N1—C1—C2   | 109.6 (3)   | N2—C6—H6A  | 109.5     |
| N1—C1—H1A  | 109.7       | C5—C6—H6A  | 109.5     |
| C2—C1—H1A  | 109.7       | N2—C6—H6B  | 109.5     |
| N1—C1—H1B  | 109.7       | C5—C6—H6B  | 109.5     |
| C2—C1—H1B  | 109.7       | H6A—C6—H6B | 108.1     |
| H1A—C1—H1B | 108.2       | O5—C7—H7A  | 109.5     |
| O6—C2—C1   | 111.3 (4)   | O5—C7—H7B  | 109.5     |
| O6—C2—H2D  | 109.4       | H7A—C7—H7B | 109.5     |

|           |       |            |       |
|-----------|-------|------------|-------|
| C1—C2—H2D | 109.4 | O5—C7—H7C  | 109.5 |
| O6—C2—H2E | 109.4 | H7A—C7—H7C | 109.5 |
| C1—C2—H2E | 109.4 | H7B—C7—H7C | 109.5 |

*Hydrogen-bond geometry (Å, °)*

| <i>D</i> —H... <i>A</i>    | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| O5—H5...O4 <sup>i</sup>    | 0.82        | 1.85          | 2.659 (6)             | 172                     |
| O5—H5...S1 <sup>i</sup>    | 0.82        | 2.92          | 3.636 (6)             | 147                     |
| N2—H2A...O1 <sup>ii</sup>  | 0.89        | 2.07          | 2.914 (5)             | 158                     |
| N2—H2A...O3 <sup>ii</sup>  | 0.89        | 2.30          | 3.001 (5)             | 135                     |
| N2—H2A...S1 <sup>ii</sup>  | 0.89        | 2.68          | 3.553 (4)             | 167                     |
| N2—H2B...O2 <sup>iii</sup> | 0.89        | 2.02          | 2.898 (5)             | 168                     |
| N2—H2B...O3 <sup>iii</sup> | 0.89        | 2.45          | 3.081 (5)             | 128                     |
| N2—H2B...S1 <sup>iii</sup> | 0.89        | 2.72          | 3.567 (4)             | 160                     |
| N2—H2C...O2                | 0.89        | 2.18          | 2.997 (5)             | 153                     |
| N2—H2C...O1                | 0.89        | 2.23          | 2.930 (4)             | 135                     |
| N2—H2C...S1                | 0.89        | 2.71          | 3.565 (4)             | 162                     |
| N1—H1...O2 <sup>iv</sup>   | 0.90 (1)    | 2.01 (3)      | 2.837 (5)             | 152 (5)                 |
| N1—H1...O4 <sup>iv</sup>   | 0.90 (1)    | 2.60 (3)      | 3.382 (6)             | 146 (5)                 |
| N1—H1...S1 <sup>iv</sup>   | 0.90 (1)    | 2.85 (1)      | 3.738 (4)             | 172 (5)                 |

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