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Hydrazine-1,2-dium bis(3-carboxy-4-hydroxybenzenesulfonate) tetrahydrate

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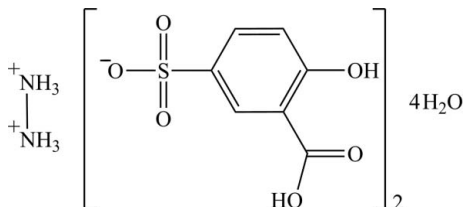
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.040; wR factor = 0.107; data-to-parameter ratio = 14.5.

Reaction of 5-sulfosalicylic acid with hydrazine hydrate at $\text{pH} = 1$ results in the formation of the title hydrated salt, $0.5\text{N}_2\text{H}_6^{2+} \cdot \text{C}_7\text{H}_5\text{O}_6\text{S}^- \cdot 2\text{H}_2\text{O}$. The hydrazinium dicationic centres lie on centres of inversion. They are located between 3-carboxy-4-hydroxybenzenesulfonate anions, forming intermolecular $\text{N} \cdots \text{O}$ hydrogen bonds with sulfonate ions and water molecules of crystallisation. Further intra- and intermolecular $\text{O} \cdots \text{O}$ hydrogen bonds are observed in the crystal structure.

Related literature

For general background on hydrogen bonding in proton-transfer compounds of 3-carboxy-4-hydroxybenzenesulfonate anions with Lewis bases, see: Smith *et al.* (2004, 2005). For recent related structures containing the 3-carboxy-4-hydroxybenzenesulfonate anion, see: Wang, Yang *et al.* (2008); Wang, Yao *et al.* (2008); Smith & Wermuth (2009); Hemamalini & Fun (2010); Yin *et al.* (2010). For related structures containing the $\text{N}_2\text{H}_6^{2+}$ hydrazinium dication, see: Starosta & Leciejewicz (2008); Klapotke *et al.* (1996).



Experimental

Crystal data

 $0.5\text{N}_2\text{H}_6^{2+} \cdot \text{C}_7\text{H}_5\text{O}_6\text{S}^- \cdot 2\text{H}_2\text{O}$ $M_r = 270.25$ Triclinic, $P\bar{1}$ $a = 7.0620$ (5) Å $b = 7.2069$ (4) Å $c = 11.5995$ (8) Å $\alpha = 78.460$ (3)° $\beta = 75.806$ (3)° $\gamma = 77.379$ (3)°
 $V = 551.77$ (6) Å³
 $Z = 2$
Mo $K\alpha$ radiation $\mu = 0.33$ mm⁻¹
 $T = 296$ K
 $0.50 \times 0.40 \times 0.30$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 1999)
 $T_{\min} = 0.823$, $T_{\max} = 0.882$ 9320 measured reflections
2711 independent reflections
2582 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.107$
 $S = 1.12$
2711 reflections
187 parameters
6 restraintsH atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.41$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.52$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|--|----------|--------------|--------------|----------------|
| $\text{O6}-\text{H6} \cdots \text{O5}$ | 0.82 | 1.88 | 2.6074 (18) | 146 |
| $\text{O7}-\text{H7A} \cdots \text{O2}^{\text{i}}$ | 0.83 (2) | 1.98 (2) | 2.8036 (15) | 177 (2) |
| $\text{O7}-\text{H7B} \cdots \text{O8}$ | 0.85 (2) | 1.84 (2) | 2.6754 (17) | 171 (2) |
| $\text{O4}-\text{H4} \cdots \text{O7}^{\text{ii}}$ | 0.79 (3) | 1.89 (3) | 2.6758 (16) | 174 (3) |
| $\text{O8}-\text{H8B} \cdots \text{O2}^{\text{iii}}$ | 0.86 (2) | 2.00 (2) | 2.8384 (16) | 165 (2) |
| $\text{O8}-\text{H8A} \cdots \text{O3}^{\text{iv}}$ | 0.87 (2) | 1.95 (2) | 2.8213 (17) | 177 (3) |
| $\text{N1}-\text{H1A} \cdots \text{O3}^{\text{v}}$ | 0.82 (2) | 1.93 (2) | 2.7493 (17) | 175.2 (19) |
| $\text{N1}-\text{H1B} \cdots \text{O7}$ | 0.94 (2) | 1.84 (2) | 2.7798 (16) | 174.5 (19) |
| $\text{N1}-\text{H1C} \cdots \text{O1}^{\text{vi}}$ | 0.91 (2) | 1.84 (2) | 2.6813 (16) | 154 (2) |

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

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2 and SAINT (Bruker, 2004); data reduction: SAINT and XPREP (Bruker, 2004); program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and Mercury (Bruno *et al.*, 2002); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2096).

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supporting information

Acta Cryst. (2011). E67, o1236–o1237 [doi:10.1107/S1600536811014231]

Hydrazine-1,2-dium bis(3-carboxy-4-hydroxybenzenesulfonate) tetrahydrate**Devipriya Selvaraju, Ranjithkumar Venkatesh and Vairam Sundararajan****S1. Comment**

5-Sulfosalicylic acid, a strong organic acid with $pK_a = 2.85$, donates its sulfonic protons to N-containing Lewis bases (Smith *et al.*, 2004, 2005) forming organic salts (Wang, Yang *et al.*, 2008; Wang, Yao *et al.*, 2008; Smith & Wermuth, 2009; Hemamalini & Fun, 2010; Yin *et al.*, 2010). Hydrazine as a diacidic base captures the H atoms of sulfonic groups from two acid molecules to form a dicationic hydrazinium salt. The molecular structure of the salt, $C_7H_5O_6S \cdot 0.5(H_6N_2) \cdot 2(H_2O)$, formed by the reaction of 5-sulfosalicylic acid with hydrazine hydrate at $pH = 1$ is shown in Fig. 1 and the various types of hydrogen bonds involved in the crystal structure are reported in Table 1.

The unit cell of the crystal structure of the title compound contains eight $(N_2H_6)^{2+}$ units located at the unit cell corners (centres of inversion) which contribute to 1/8 of the charge of each cell, two compensating 3-carboxy-4-hydroxybenzenesulfonate anions, and four isolated water molecules. The anions are held by intermolecular N—H \cdots O hydrogen bonds in all directions with the hydrazinium ions. These N \cdots O interactions fall in the range of 2.6813 (16)–2.7798 (16) Å. In addition, the intramolecular O6—H6 \cdots O5 hydrogen bond [$D\cdots A = 2.6074$ (18) Å] and intermolecular O—H \cdots O hydrogen bonds, O7—H7 \cdots O2 [$D\cdots A = 2.8036$ (15) Å] between sulfonyl O atoms and water molecules, O4—H4 \cdots O7 [$D\cdots A = 2.6758$ (16) Å] between carboxyl H atoms and isolated water molecules, and O7—H7B \cdots O8 [$D\cdots A = 2.6754$ (17) Å] between lattice water molecules, stabilize the molecular conformation and the crystal structure.

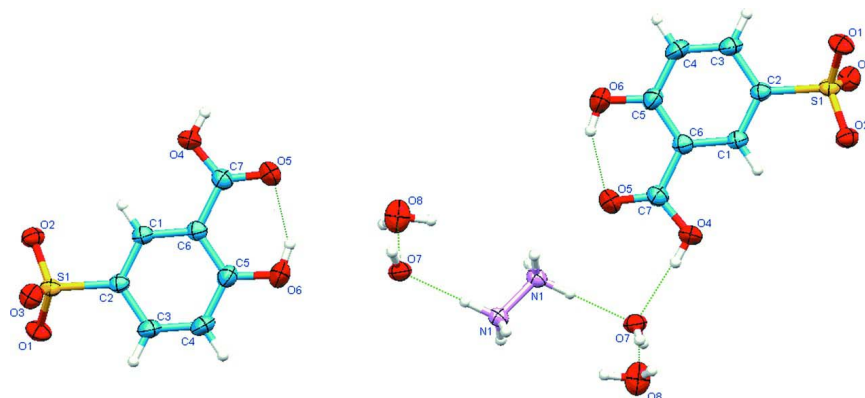
The N1—N1ⁱ distance of 1.433 (2) Å (symmetry code: (i) -x, -y, -z + 2) is in a good agreement with the values reported by Starosta & Leciejewicz (2008) and Klapotke *et al.* (1996). The hydrazinium ion has a staggered conformation due to the symmetry imposed by the centre of inversion located in the middle of the N—N bond.

S2. Experimental

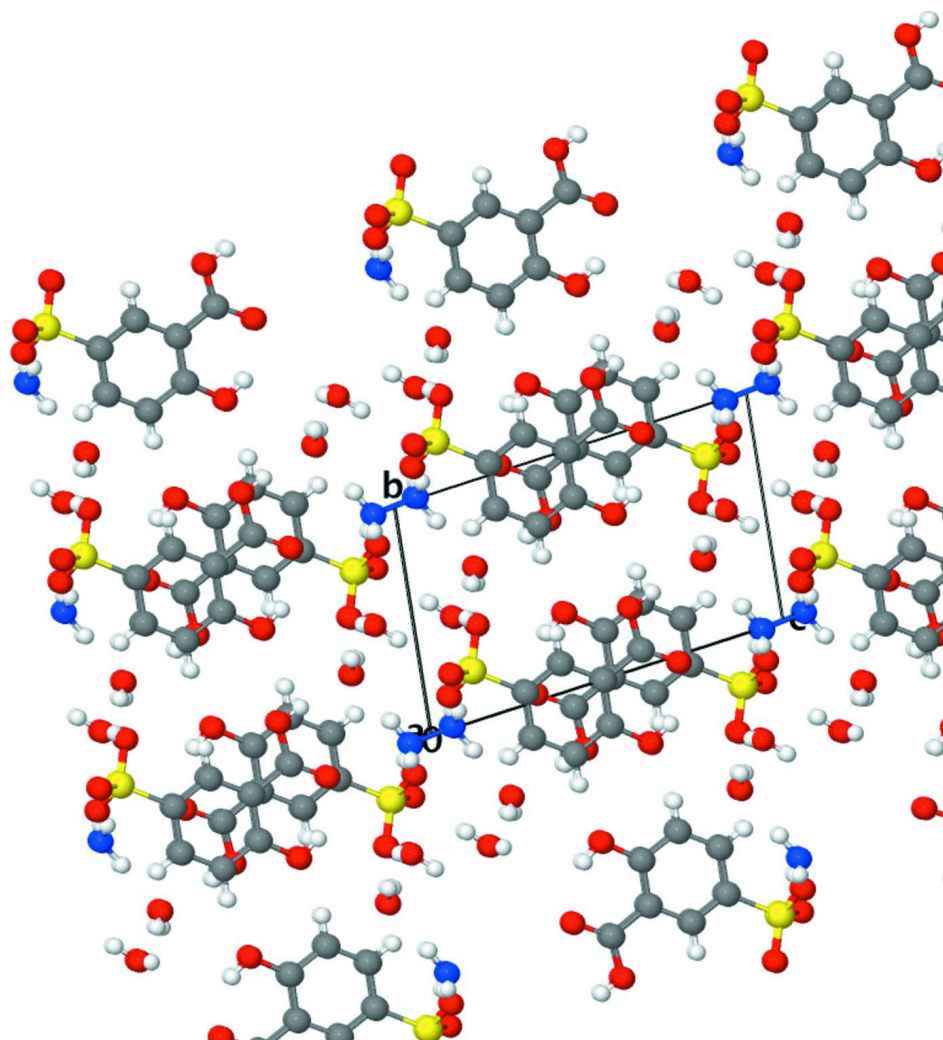
The title compound was synthesized by dissolving 5-sulfosalicylic acid dihydrate (2 mmol, 0.508 g) and hydrazine hydrate (99.98% pure; 1 mmol, 0.05 ml) in 30 ml of distilled water at $pH = 1$. The mixture was stirred for 4 h at ambient temperature and then filtered. The resulting clear solution was kept for three weeks in a wooden enclosure. Colourless prismatic crystals suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of the solvent.

S3. Refinement

All non-H atoms were refined anisotropically. H atoms bonded to C atoms were positioned geometrically with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ while H atoms bonded to N and O atoms were found in difference Fourier maps and their coordinates and thermal parameters freely refined.

**Figure 1**

View of the title compound (I), showing displacement ellipsoids at the 50% probability level. Symmetry code: 1 - x, 1 - y, 1 - z.

**Figure 2**

The packing diagram of title compound (I).

Hydrazine-1,2-dium bis(3-carboxy-4-hydroxybenzenesulfonate) tetrahydrate*Crystal data*0.5N₂H₆²⁺·C₇H₅O₆S⁻·2H₂O $M_r = 270.25$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 7.0620$ (5) Å $b = 7.2069$ (4) Å $c = 11.5995$ (8) Å $\alpha = 78.460$ (3)° $\beta = 75.806$ (3)° $\gamma = 77.379$ (3)° $V = 551.77$ (6) Å³ $Z = 2$ $F(000) = 282$ $D_x = 1.627$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6221 reflections

 $\theta = 2.5$ – 26.2 ° $\mu = 0.33$ mm⁻¹ $T = 296$ K

Block, colourless

 $0.50 \times 0.40 \times 0.30$ mm*Data collection*Bruker Kappa APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω and φ scans

Absorption correction: multi-scan

(SADABS; Bruker, 1999)

 $T_{\min} = 0.823$, $T_{\max} = 0.882$

9320 measured reflections

2711 independent reflections

2582 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.057$ $\theta_{\max} = 28.2$ °, $\theta_{\min} = 2.9$ ° $h = -9 \rightarrow 9$ $k = -9 \rightarrow 9$ $l = -13 \rightarrow 15$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.040$ $wR(F^2) = 0.107$ $S = 1.12$

2711 reflections

187 parameters

6 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.1344P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.41$ e Å⁻³ $\Delta\rho_{\min} = -0.52$ e Å⁻³Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 1.12 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å²)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|--------------|--------------|----------------------------------|
| C1 | 0.28715 (19) | 1.12543 (18) | 0.37831 (12) | 0.0277 (3) |
| H7 | 0.2576 | 1.2577 | 0.3783 | 0.033* |

| | | | | |
|-----|---------------|---------------|--------------|--------------|
| C2 | 0.36576 (19) | 1.05458 (18) | 0.27144 (12) | 0.0268 (3) |
| C3 | 0.4096 (2) | 0.8553 (2) | 0.27042 (15) | 0.0373 (3) |
| H1 | 0.4618 | 0.8079 | 0.1981 | 0.045* |
| C4 | 0.3755 (3) | 0.7304 (2) | 0.37640 (16) | 0.0434 (4) |
| H3 | 0.4049 | 0.5983 | 0.3756 | 0.052* |
| C5 | 0.2966 (2) | 0.8008 (2) | 0.48587 (14) | 0.0364 (3) |
| C6 | 0.2515 (2) | 1.00021 (19) | 0.48664 (13) | 0.0290 (3) |
| C7 | 0.1686 (2) | 1.0757 (2) | 0.60113 (13) | 0.0323 (3) |
| N1 | 0.01665 (18) | -0.00608 (18) | 0.93729 (10) | 0.0272 (3) |
| O1 | 0.59710 (15) | 1.13796 (16) | 0.06468 (10) | 0.0369 (3) |
| O7 | -0.03247 (17) | 0.36335 (14) | 0.80737 (10) | 0.0340 (3) |
| O2 | 0.40796 (15) | 1.40062 (14) | 0.17028 (9) | 0.0333 (3) |
| O8 | 0.19337 (19) | 0.5388 (2) | 0.88950 (13) | 0.0505 (3) |
| O3 | 0.24335 (15) | 1.22941 (15) | 0.07799 (10) | 0.0356 (3) |
| O4 | 0.1284 (2) | 1.26416 (17) | 0.58929 (11) | 0.0445 (3) |
| O5 | 0.1392 (2) | 0.97087 (18) | 0.69881 (10) | 0.0454 (3) |
| O6 | 0.2667 (2) | 0.67267 (18) | 0.58729 (12) | 0.0568 (4) |
| H6 | 0.2187 | 0.7301 | 0.6450 | 0.085* |
| S1 | 0.40819 (4) | 1.21604 (4) | 0.13623 (3) | 0.02543 (16) |
| H7A | -0.144 (2) | 0.430 (3) | 0.8122 (19) | 0.046 (5)* |
| H7B | 0.043 (3) | 0.425 (3) | 0.825 (2) | 0.062 (7)* |
| H4 | 0.086 (4) | 1.300 (4) | 0.653 (2) | 0.058 (7)* |
| H8B | 0.312 (3) | 0.559 (4) | 0.858 (2) | 0.069 (7)* |
| H8A | 0.208 (4) | 0.446 (3) | 0.949 (2) | 0.091 (10)* |
| H1A | -0.060 (3) | -0.070 (3) | 0.9285 (17) | 0.035 (5)* |
| H1B | -0.008 (3) | 0.118 (3) | 0.8930 (19) | 0.045 (5)* |
| H1C | 0.144 (3) | -0.067 (3) | 0.9181 (19) | 0.047 (5)* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|------------|------------|---------------|---------------|---------------|
| C1 | 0.0271 (6) | 0.0250 (6) | 0.0312 (6) | -0.0017 (5) | -0.0065 (5) | -0.0078 (5) |
| C2 | 0.0240 (6) | 0.0262 (6) | 0.0300 (6) | -0.0008 (4) | -0.0065 (5) | -0.0067 (5) |
| C3 | 0.0428 (8) | 0.0286 (7) | 0.0387 (8) | 0.0024 (6) | -0.0068 (6) | -0.0130 (6) |
| C4 | 0.0567 (10) | 0.0237 (6) | 0.0467 (9) | 0.0024 (6) | -0.0108 (8) | -0.0092 (6) |
| C5 | 0.0438 (8) | 0.0273 (7) | 0.0374 (7) | -0.0021 (6) | -0.0134 (6) | -0.0018 (6) |
| C6 | 0.0289 (6) | 0.0291 (6) | 0.0303 (6) | -0.0027 (5) | -0.0090 (5) | -0.0069 (5) |
| C7 | 0.0331 (7) | 0.0350 (7) | 0.0300 (7) | -0.0061 (5) | -0.0079 (5) | -0.0063 (5) |
| N1 | 0.0263 (6) | 0.0313 (6) | 0.0243 (6) | -0.0042 (4) | -0.0055 (4) | -0.0061 (4) |
| O1 | 0.0251 (5) | 0.0461 (6) | 0.0361 (5) | -0.0001 (4) | 0.0002 (4) | -0.0140 (5) |
| O7 | 0.0362 (6) | 0.0295 (5) | 0.0361 (5) | -0.0013 (4) | -0.0069 (4) | -0.0105 (4) |
| O2 | 0.0336 (5) | 0.0292 (5) | 0.0376 (5) | -0.0074 (4) | -0.0033 (4) | -0.0094 (4) |
| O8 | 0.0391 (7) | 0.0573 (8) | 0.0577 (8) | -0.0184 (6) | -0.0190 (6) | 0.0066 (6) |
| O3 | 0.0306 (5) | 0.0376 (5) | 0.0417 (6) | -0.0068 (4) | -0.0152 (4) | -0.0031 (4) |
| O4 | 0.0646 (8) | 0.0348 (6) | 0.0307 (6) | -0.0039 (5) | -0.0029 (5) | -0.0115 (4) |
| O5 | 0.0622 (8) | 0.0433 (6) | 0.0285 (5) | -0.0086 (5) | -0.0079 (5) | -0.0034 (5) |
| O6 | 0.0906 (11) | 0.0314 (6) | 0.0418 (7) | -0.0058 (6) | -0.0132 (7) | 0.0033 (5) |
| S1 | 0.0201 (2) | 0.0276 (2) | 0.0285 (2) | -0.00186 (12) | -0.00404 (13) | -0.00819 (13) |

Geometric parameters (Å, °)

| | | | |
|-------------|--------------|-------------------------|--------------|
| C1—C2 | 1.3775 (19) | N1—N1 ⁱ | 1.433 (2) |
| C1—C6 | 1.3954 (19) | N1—H1A | 0.82 (2) |
| C1—H7 | 0.9300 | N1—H1B | 0.94 (2) |
| C2—C3 | 1.4030 (18) | N1—H1C | 0.91 (2) |
| C2—S1 | 1.7594 (14) | O1—S1 | 1.4495 (10) |
| C3—C4 | 1.374 (2) | O7—H7A | 0.826 (15) |
| C3—H1 | 0.9300 | O7—H7B | 0.847 (15) |
| C4—C5 | 1.403 (2) | O2—S1 | 1.4610 (10) |
| C4—H3 | 0.9300 | O8—H8B | 0.859 (16) |
| C5—O6 | 1.3453 (19) | O8—H8A | 0.874 (17) |
| C5—C6 | 1.404 (2) | O3—S1 | 1.4599 (10) |
| C6—C7 | 1.473 (2) | O4—H4 | 0.79 (3) |
| C7—O5 | 1.2282 (18) | O6—H6 | 0.8200 |
| C7—O4 | 1.3115 (19) | | |
| C2—C1—C6 | 120.48 (12) | O5—C7—C6 | 122.77 (14) |
| C2—C1—H7 | 119.8 | O4—C7—C6 | 114.08 (13) |
| C6—C1—H7 | 119.8 | N1 ⁱ —N1—H1A | 108.5 (13) |
| C1—C2—C3 | 120.22 (13) | N1 ⁱ —N1—H1B | 109.8 (13) |
| C1—C2—S1 | 119.44 (10) | H1A—N1—H1B | 109.2 (19) |
| C3—C2—S1 | 120.34 (11) | N1 ⁱ —N1—H1C | 104.8 (14) |
| C4—C3—C2 | 119.94 (14) | H1A—N1—H1C | 110.6 (18) |
| C4—C3—H1 | 120.0 | H1B—N1—H1C | 113.7 (18) |
| C2—C3—H1 | 120.0 | H7A—O7—H7B | 108.4 (18) |
| C3—C4—C5 | 120.36 (13) | H8B—O8—H8A | 104 (2) |
| C3—C4—H3 | 119.8 | C7—O4—H4 | 111.4 (18) |
| C5—C4—H3 | 119.8 | C5—O6—H6 | 109.5 |
| O6—C5—C4 | 118.15 (13) | O1—S1—O3 | 112.19 (7) |
| O6—C5—C6 | 122.23 (14) | O1—S1—O2 | 112.97 (6) |
| C4—C5—C6 | 119.63 (14) | O3—S1—O2 | 110.87 (6) |
| C1—C6—C5 | 119.37 (13) | O1—S1—C2 | 107.30 (6) |
| C1—C6—C7 | 120.56 (12) | O3—S1—C2 | 106.83 (6) |
| C5—C6—C7 | 120.07 (13) | O2—S1—C2 | 106.24 (6) |
| O5—C7—O4 | 123.15 (14) | | |
| C6—C1—C2—C3 | 0.4 (2) | C4—C5—C6—C7 | 180.00 (15) |
| C6—C1—C2—S1 | 179.78 (10) | C1—C6—C7—O5 | -178.27 (14) |
| C1—C2—C3—C4 | -0.5 (2) | C5—C6—C7—O5 | 1.3 (2) |
| S1—C2—C3—C4 | -179.82 (13) | C1—C6—C7—O4 | 2.0 (2) |
| C2—C3—C4—C5 | 0.1 (3) | C5—C6—C7—O4 | -178.35 (14) |
| C3—C4—C5—O6 | -179.70 (16) | C1—C2—S1—O1 | 139.04 (11) |
| C3—C4—C5—C6 | 0.3 (3) | C3—C2—S1—O1 | -41.61 (14) |
| C2—C1—C6—C5 | 0.0 (2) | C1—C2—S1—O3 | -100.46 (12) |
| C2—C1—C6—C7 | 179.62 (12) | C3—C2—S1—O3 | 78.89 (13) |
| O6—C5—C6—C1 | 179.65 (14) | C1—C2—S1—O2 | 17.95 (13) |

| | | | |
|-------------|----------|-------------|--------------|
| C4—C5—C6—C1 | -0.4 (2) | C3—C2—S1—O2 | -162.70 (12) |
| O6—C5—C6—C7 | 0.0 (2) | | |

Symmetry code: (i) $-x, -y, -z+2$.

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|----------------------------|------------|--------------|--------------|----------------|
| O6—H6...O5 | 0.82 | 1.88 | 2.6074 (18) | 146 |
| O7—H7A...O2 ⁱⁱ | 0.83 (2) | 1.98 (2) | 2.8036 (15) | 177 (2) |
| O7—H7B...O8 | 0.85 (2) | 1.84 (2) | 2.6754 (17) | 171 (2) |
| O4—H4...O7 ⁱⁱⁱ | 0.79 (3) | 1.89 (3) | 2.6758 (16) | 174 (3) |
| O8—H8B...O2 ^{iv} | 0.86 (2) | 2.00 (2) | 2.8384 (16) | 165 (2) |
| O8—H8A...O3 ^v | 0.87 (2) | 1.95 (2) | 2.8213 (17) | 177 (3) |
| N1—H1A...O3 ^{vi} | 0.82 (2) | 1.93 (2) | 2.7493 (17) | 175.2 (19) |
| N1—H1B...O7 | 0.94 (2) | 1.84 (2) | 2.7798 (16) | 174.5 (19) |
| N1—H1C...O1 ^{vii} | 0.91 (2) | 1.84 (2) | 2.6813 (16) | 154 (2) |

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