

Tetraaquabis(2-sulfamoylbenzoato)-manganese(II)

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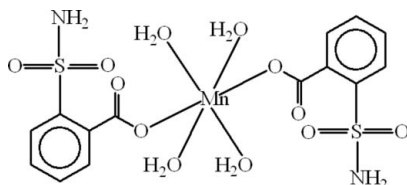
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.029; wR factor = 0.106; data-to-parameter ratio = 16.5.

In the title compound, $[\text{Mn}(\text{C}_7\text{H}_6\text{NO}_4\text{S})_2(\text{H}_2\text{O})_4]$, the Mn atom, lying on an inversion center, exhibits a distorted octahedral coordination by six O atoms, two from carboxylate groups and four from water molecules. The SO_2NH_2 group is involved in a three dimensional polymeric hydrogen bonding network along with the water molecules. π -Stacking interactions parallel to the c axis lead to a separation of 4.0050 (12) Å between the centroids of the benzene rings.

Related literature

For related literature, see: Allen (2002); Aurengzeb *et al.* (1994); Eltayeb *et al.* (2008); Hulme *et al.* (1997); Siddiqui *et al.* (2007, 2008); Tahir *et al.* (1997); Zhang & Janiak (2001).



Experimental

Crystal data

$[\text{Mn}(\text{C}_7\text{H}_6\text{NO}_4\text{S})_2(\text{H}_2\text{O})_4]$
 $M_r = 527.38$
 Monoclinic, $P2_1/c$
 $a = 15.2442$ (4) Å
 $b = 8.2835$ (2) Å
 $c = 7.9188$ (2) Å
 $\beta = 99.971$ (1)°

$V = 984.85$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.95$ mm⁻¹
 $T = 296$ (2) K
 $0.20 \times 0.15 \times 0.12$ mm

Data collection

Bruker KAPPA APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2007)
 $T_{\min} = 0.840$, $T_{\max} = 0.895$
 10903 measured reflections

2445 independent reflections
 2174 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.106$
 $S = 1.05$
 2445 reflections
 148 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.46$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------------------|-------------|------------------------|-------------|
| Mn1—O1 | 2.1194 (13) | Mn1—O6 ⁱ | 2.1628 (14) |
| Mn1—O5 | 2.2582 (14) | S1—O3 | 1.4313 (15) |
| Mn1—O6 | 2.1628 (14) | S1—O4 | 1.4352 (16) |
| Mn1—O1 ⁱ | 2.1194 (13) | S1—N1 | 1.6223 (17) |
| Mn1—O5 ⁱ | 2.2582 (14) | | |
| O1—Mn1—O5 | 93.95 (5) | O1—Mn1—O6 ⁱ | 95.36 (5) |
| O1—Mn1—O6 | 84.64 (5) | O5—Mn1—O6 | 84.27 (5) |
| O1—Mn1—O5 ⁱ | 86.05 (5) | Mn1—O1—C7 | 128.58 (11) |

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

Table 2

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|----------|-------------|-------------|---------------|
| O5—H5A \cdots O3 ⁱⁱⁱ | 0.86 | 2.02 | 2.869 (2) | 167 |
| O5—H5B \cdots O2 ⁱⁱⁱ | 0.97 | 1.83 | 2.775 (2) | 164 |
| O6—H6A \cdots O5 ⁱⁱⁱ | 0.94 | 1.85 | 2.765 (2) | 164 |
| O6—H6B \cdots N1 ^{iv} | 0.86 | 2.25 | 3.008 (2) | 148 |
| N1—H11 \cdots O2 | 0.77 (3) | 2.19 (3) | 2.799 (2) | 137 (2) |
| N1—H12 \cdots O4 ^v | 0.85 (2) | 2.50 (2) | 3.300 (2) | 157 (2) |
| C3—H3 \cdots O4 | 0.93 | 2.40 | 2.834 (3) | 108 |

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

Data collection: APEX2 (Bruker, 2007); cell refinement: APEX2; data reduction: SAINT (Bruker, 2007); 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) and PLATON (Spek, 2003); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2154).

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supporting information

Acta Cryst. (2008). E64, m1293–m1294 [doi:10.1107/S1600536808029450]

Tetraaquabis(2-sulfamoylbenzoato)manganese(II)

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S1. Comment

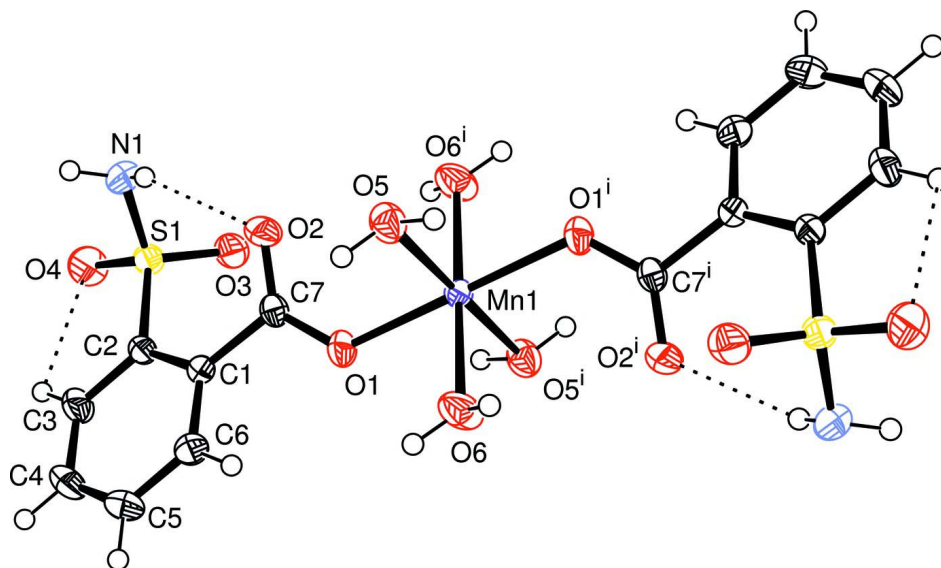
The coordination chemistry of manganese in various oxidation states and in different combinations of donor environments like nitrogen and oxygen has been extensively investigated. The manganese complexes with Schiff base ligands have attracted considerable interest in the past decades and recently, due to their importance and variety of applications in chemistry, biology, physics and advanced materials (Eltayeb *et al.*, 2008). One class of high-valent manganese complexes receiving considerable attention is of those involving carboxylic acid and Schiff base ligands (Aurengzeb *et al.*, 1994; Hulme *et al.*, 1997; Zhang *et al.*, 2001). In continuation to the synthesis of benzene sulfonamide derivatives (Siddiqui *et al.*, 2008), we are also interested in the complexation of these ligands with human friendly transition metals. The title complex (I) is being reported in this context.

The CCDC search (Allen, 2002) showed that no crystal structure has been reported of manganese with sulfamoylbenzoate. The complexation of the Mn(II) with *o*-sulfamoylbenzoate confirmed that there is no coordination of SO₂NH₂ group. The Mn(II) is hexa-coordinated (Table 1) through carboxylate group (Fig 1) and four water molecules, whereas SO₂NH₂ is involved in the three dimensional network of H-bonding (Table 2). The Title compound (I) has shown a typical coordination geometry as is seen in most of the transition metal complexes (Tahir *et al.*, 1997) with monoanionic carboxylate ligands in the aqueous media. There exists a three dimensional polymeric network due to intra as well as intermolecular H-bonding. The molecules are further stabilized due to π - π -interaction at a distance of 4.0050 (12) Å, between the centroids of the benzene ring $Cg \cdots Cg^i$ [symmetry code: $i = x, 3/2 - y, -1/2 + z$].

S2. Experimental

A suspension of (1.0 g, 5.0 mmol) *o*-sulfamoyl benzoic acid (Siddiqui *et al.*, 2007), manganese acetate tetrahydrate (0.6 g, 2.5 mmol) and sodium carbonate (0.3 g, 2.5 mmol) was subjected to reflux in aqueous methanol (50%, 50 ml) for 4 h. The volume of the reaction mixture was reduced to half on rotary evaporator (11 torr) at room temperature and its pH was adjusted to 6 using hydrochloric acid (15%). The reaction mixture was then kept in ice-bath for 2 h. The off-white crystals were filtered, washed with cold distilled water and dried at room temperature. The product was recrystallized at 313 K from aqueous methanol to obtain colorless crystals.

m.p 498–503 K.

**Figure 1**

ORTEP drawing of the title compound, $C_{14}H_{20}MnN_2O_{12}S_2$, with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii. The intramolecular H-bonds are shown by dotted lines.

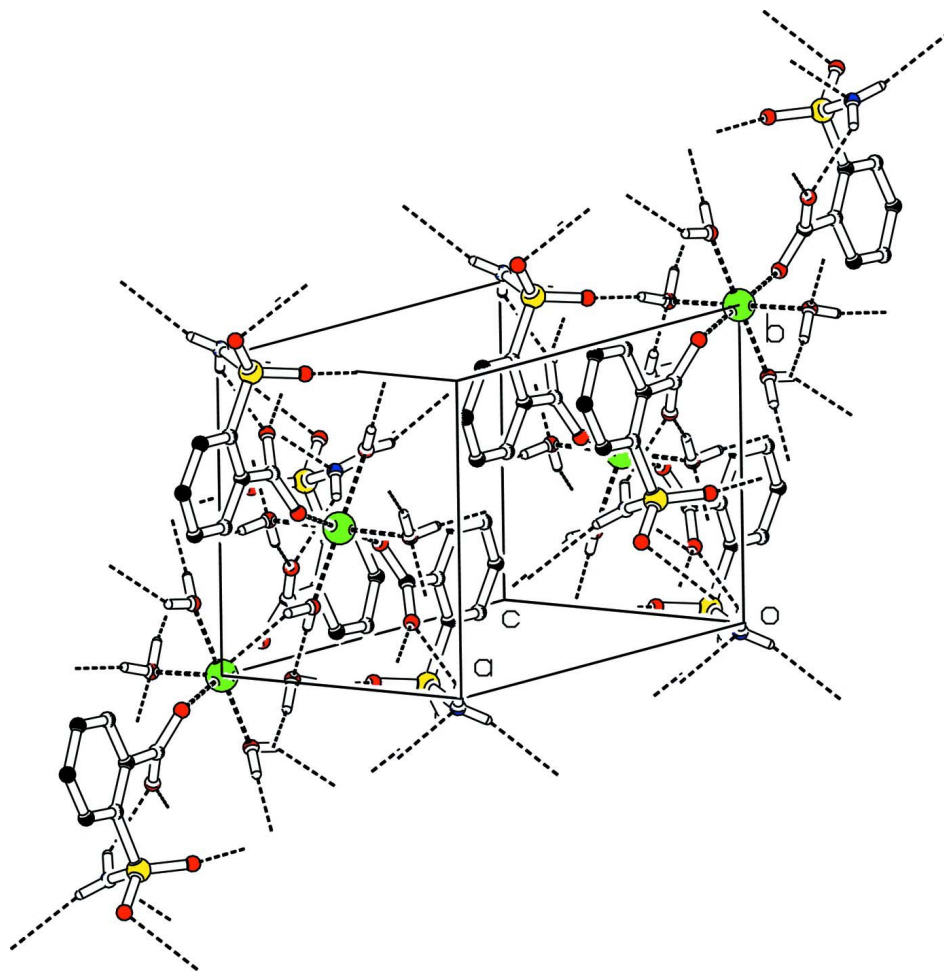


Figure 2

The packing figure (*PLATON*: Spek, 2003) which shows the three dimensional polymeric network through H-bonding. The H-atoms of benzene ring are not shown for clarity.

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Crystal data

$[\text{Mn}(\text{C}_7\text{H}_6\text{NO}_4\text{S})_2(\text{H}_2\text{O})_4]$

$M_r = 527.38$

Monoclinic, $P2_1/c$

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

$a = 15.2442\ (4)\ \text{\AA}$

$b = 8.2835\ (2)\ \text{\AA}$

$c = 7.9188\ (2)\ \text{\AA}$

$\beta = 99.971\ (1)^\circ$

$V = 984.85\ (4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 542$

$D_x = 1.778\ \text{Mg m}^{-3}$

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

Cell parameters from 2445 reflections

$\theta = 1.4\text{--}28.3^\circ$

$\mu = 0.95\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Prismatic, colourless

$0.20 \times 0.15 \times 0.12\ \text{mm}$

Data collection

Bruker KAPPA APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $7.50\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2007)

$T_{\min} = 0.840$, $T_{\max} = 0.895$

10903 measured reflections

2445 independent reflections

2174 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 1.4^\circ$

$h = -20 \rightarrow 20$

$k = -11 \rightarrow 7$

$l = -10 \rightarrow 8$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.106$

$S = 1.05$

2445 reflections

148 parameters

0 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

$w = 1/[\sigma^2(F_o^2) + (0.0727P)^2 + 0.2877P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$

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 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| Mn1 | 0.00000 | 1.00000 | 0.00000 | 0.0202 (1) |
| S1 | 0.26720 (3) | 0.44810 (6) | 0.04336 (6) | 0.0258 (1) |
| O1 | 0.13332 (8) | 0.92172 (17) | 0.01231 (17) | 0.0292 (4) |
| O2 | 0.13202 (9) | 0.68245 (19) | 0.1401 (2) | 0.0399 (4) |
| O3 | 0.19410 (10) | 0.46089 (19) | -0.09625 (18) | 0.0352 (4) |
| O4 | 0.33501 (10) | 0.33230 (18) | 0.0254 (2) | 0.0415 (5) |
| O5 | 0.00686 (10) | 0.99300 (17) | 0.28706 (18) | 0.0334 (4) |
| O6 | 0.05852 (9) | 1.23701 (17) | 0.0481 (2) | 0.0411 (5) |
| N1 | 0.22897 (12) | 0.3966 (2) | 0.2145 (2) | 0.0324 (5) |
| C1 | 0.26985 (10) | 0.7841 (2) | 0.0847 (2) | 0.0213 (4) |
| C2 | 0.31781 (10) | 0.6410 (2) | 0.0774 (2) | 0.0226 (4) |
| C3 | 0.41025 (11) | 0.6438 (3) | 0.0899 (3) | 0.0330 (5) |
| C4 | 0.45577 (12) | 0.7888 (3) | 0.1114 (3) | 0.0407 (7) |
| C5 | 0.40934 (13) | 0.9313 (3) | 0.1195 (3) | 0.0363 (6) |
| C6 | 0.31757 (12) | 0.9290 (2) | 0.1056 (2) | 0.0275 (5) |
| C7 | 0.16968 (10) | 0.7939 (2) | 0.0780 (2) | 0.0224 (4) |
| H3 | 0.44130 | 0.54792 | 0.08374 | 0.0395* |
| H4 | 0.51741 | 0.79050 | 0.12051 | 0.0488* |
| H5 | 0.43986 | 1.02886 | 0.13417 | 0.0436* |

| | | | | |
|-----|-------------|-----------|-----------|---------|
| H5A | 0.06046 | 1.01646 | 0.33453 | 0.0400* |
| H5B | -0.03444 | 1.07596 | 0.31053 | 0.0400* |
| H6 | 0.28707 | 1.02566 | 0.11038 | 0.0330* |
| H6A | 0.02784 | 1.31074 | 0.10610 | 0.0493* |
| H6B | 0.11478 | 1.24615 | 0.08246 | 0.0493* |
| H11 | 0.2043 (19) | 0.467 (4) | 0.248 (3) | 0.0389* |
| H12 | 0.2695 (16) | 0.353 (3) | 0.288 (3) | 0.0389* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|-------------|-------------|-------------|-------------|-------------|
| Mn1 | 0.0192 (2) | 0.0176 (2) | 0.0239 (2) | 0.0011 (1) | 0.0040 (1) | 0.0001 (1) |
| S1 | 0.0248 (2) | 0.0198 (3) | 0.0320 (2) | -0.0007 (2) | 0.0028 (2) | -0.0006 (2) |
| O1 | 0.0223 (6) | 0.0287 (7) | 0.0359 (7) | 0.0066 (5) | 0.0028 (5) | 0.0026 (5) |
| O2 | 0.0246 (6) | 0.0393 (8) | 0.0591 (9) | 0.0024 (6) | 0.0169 (6) | 0.0163 (7) |
| O3 | 0.0339 (7) | 0.0389 (8) | 0.0303 (7) | -0.0078 (6) | -0.0011 (5) | -0.0005 (6) |
| O4 | 0.0396 (8) | 0.0245 (7) | 0.0612 (10) | 0.0071 (6) | 0.0114 (7) | -0.0040 (7) |
| O5 | 0.0280 (7) | 0.0441 (9) | 0.0276 (7) | 0.0002 (5) | 0.0035 (5) | -0.0005 (5) |
| O6 | 0.0301 (7) | 0.0257 (7) | 0.0684 (10) | -0.0049 (6) | 0.0112 (6) | -0.0081 (7) |
| N1 | 0.0351 (9) | 0.0273 (9) | 0.0343 (8) | -0.0006 (7) | 0.0046 (7) | 0.0067 (7) |
| C1 | 0.0197 (7) | 0.0219 (8) | 0.0224 (7) | 0.0007 (6) | 0.0037 (5) | 0.0033 (6) |
| C2 | 0.0185 (7) | 0.0216 (8) | 0.0274 (8) | -0.0005 (6) | 0.0030 (6) | 0.0009 (6) |
| C3 | 0.0199 (8) | 0.0326 (10) | 0.0461 (10) | 0.0038 (7) | 0.0049 (7) | 0.0028 (8) |
| C4 | 0.0189 (8) | 0.0454 (13) | 0.0571 (13) | -0.0060 (8) | 0.0050 (8) | 0.0049 (10) |
| C5 | 0.0304 (9) | 0.0318 (11) | 0.0460 (11) | -0.0121 (8) | 0.0045 (8) | 0.0016 (9) |
| C6 | 0.0287 (8) | 0.0223 (9) | 0.0313 (9) | -0.0013 (7) | 0.0045 (7) | 0.0011 (7) |
| C7 | 0.0195 (7) | 0.0248 (8) | 0.0232 (7) | 0.0035 (6) | 0.0042 (5) | -0.0023 (6) |

Geometric parameters (Å, °)

| | | | |
|------------------------|-------------|-----------------------|-----------|
| Mn1—O1 | 2.1194 (13) | O6—H6B | 0.8600 |
| Mn1—O5 | 2.2582 (14) | N1—H11 | 0.77 (3) |
| Mn1—O6 | 2.1628 (14) | N1—H12 | 0.85 (2) |
| Mn1—O1 ⁱ | 2.1194 (13) | C1—C7 | 1.521 (2) |
| Mn1—O5 ⁱ | 2.2582 (14) | C1—C2 | 1.399 (2) |
| Mn1—O6 ⁱ | 2.1628 (14) | C1—C6 | 1.398 (2) |
| S1—O3 | 1.4313 (15) | C2—C3 | 1.396 (2) |
| S1—O4 | 1.4352 (16) | C3—C4 | 1.383 (3) |
| S1—N1 | 1.6223 (17) | C4—C5 | 1.384 (3) |
| S1—C2 | 1.7746 (17) | C5—C6 | 1.384 (3) |
| O1—C7 | 1.265 (2) | C3—H3 | 0.9300 |
| O2—C7 | 1.234 (2) | C4—H4 | 0.9300 |
| O5—H5A | 0.8600 | C5—H5 | 0.9300 |
| O5—H5B | 0.9700 | C6—H6 | 0.9300 |
| O6—H6A | 0.9400 | | |
| S1...O2 | 3.0246 (16) | O4...H6 ⁱⁱ | 2.7600 |
| S1...H6B ⁱⁱ | 2.9200 | O4...H3 | 2.4000 |

| | | | |
|-------------------------|-------------|---------------------------|-----------|
| O1...O5 | 3.202 (2) | O4...H4 ^{xi} | 2.8900 |
| O1...O6 | 2.883 (2) | O5...H6A ^v | 1.8500 |
| O1...O6 ⁱ | 3.1663 (19) | O6...H5A | 2.9100 |
| O1...O5 ⁱ | 2.989 (2) | O6...H5A ^{ix} | 2.6500 |
| O1...O3 ⁱⁱⁱ | 3.228 (2) | O6...H5B ^{ix} | 2.6500 |
| O1...O2 ^{iv} | 3.068 (2) | N1...O2 | 2.799 (2) |
| O2...O1 ⁱⁱⁱ | 3.068 (2) | N1...O6 ⁱⁱ | 3.008 (2) |
| O2...N1 | 2.799 (2) | N1...H6B ⁱⁱ | 2.2500 |
| O2...O6 ⁱ | 3.099 (2) | C6...O4 ^{viii} | 3.420 (2) |
| O2...S1 | 3.0246 (16) | C6...O3 ⁱⁱⁱ | 3.389 (2) |
| O2...O3 | 2.895 (2) | C7...O3 ⁱⁱⁱ | 3.254 (2) |
| O2...O5 ^v | 2.775 (2) | C7...O3 | 3.135 (2) |
| O3...C7 | 3.135 (2) | C3...H5 ^{xii} | 3.0300 |
| O3...O5 ^{iv} | 2.869 (2) | C6...H12 ^{iv} | 3.08 (2) |
| O3...O6 ⁱⁱ | 3.136 (2) | C7...H11 | 3.03 (3) |
| O3...C6 ^{iv} | 3.389 (2) | C7...H5B ^v | 2.9900 |
| O3...O1 ^{iv} | 3.228 (2) | H3...O4 | 2.4000 |
| O3...C7 ^{iv} | 3.254 (2) | H3...H3 ^{xi} | 2.5300 |
| O3...O2 | 2.895 (2) | H4...O4 ^{xi} | 2.8900 |
| O4...C6 ⁱⁱ | 3.420 (2) | H5...C3 ^{xiii} | 3.0300 |
| O5...O6 ^v | 2.765 (2) | H5A...H6A ^v | 2.2700 |
| O5...O1 ⁱ | 2.989 (2) | H5A...O3 ⁱⁱⁱ | 2.0200 |
| O5...O6 | 2.967 (2) | H5A...O6 ^{vi} | 2.6500 |
| O5...O6 ^{vi} | 3.055 (2) | H5B...O2 ^{vii} | 1.8300 |
| O5...O2 ^{vii} | 2.775 (2) | H5B...C7 ^{vii} | 2.9900 |
| O5...O1 | 3.202 (2) | H5B...H6A ^v | 2.2900 |
| O5...O3 ⁱⁱⁱ | 2.869 (2) | H5B...O6 ^{vi} | 2.6500 |
| O6...O5 ^{vii} | 2.765 (2) | H5B...H6A ^{vi} | 2.5500 |
| O6...O3 ^{viii} | 3.136 (2) | H6...O1 | 2.4900 |
| O6...O5 | 2.967 (2) | H6...O4 ^{viii} | 2.7600 |
| O6...O1 ⁱ | 3.1663 (19) | H6A...O5 ^{vii} | 1.8500 |
| O6...O2 ⁱ | 3.099 (2) | H6A...H5A ^{vii} | 2.2700 |
| O6...N1 ^{viii} | 3.008 (2) | H6A...H5B ^{vii} | 2.2900 |
| O6...O5 ^{ix} | 3.055 (2) | H6A...O2 ⁱ | 2.8500 |
| O6...O1 | 2.883 (2) | H6A...H5B ^{ix} | 2.5500 |
| O1...H6 | 2.4900 | H6B...S1 ^{viii} | 2.9200 |
| O1...H6B | 2.7700 | H6B...O3 ^{viii} | 2.6900 |
| O1...H11 ^{iv} | 2.68 (3) | H6B...N1 ^{viii} | 2.2500 |
| O1...H5B ⁱ | 2.7300 | H6B...H11 ^{viii} | 2.5100 |
| O2...H11 | 2.19 (3) | H11...O2 | 2.19 (3) |
| O2...H5B ^v | 1.8300 | H11...C7 | 3.03 (3) |
| O2...H6A ⁱ | 2.8500 | H11...H6B ⁱⁱ | 2.5100 |
| O3...H6B ⁱⁱ | 2.6900 | H11...O1 ⁱⁱⁱ | 2.68 (3) |
| O3...H5A ^{iv} | 2.0200 | H12...O4 ^{xiv} | 2.50 (2) |
| O4...H12 ^x | 2.50 (2) | H12...C6 ⁱⁱⁱ | 3.08 (2) |
| O1—Mn1—O5 | 93.95 (5) | Mn1—O6—H6A | 117.00 |
| O1—Mn1—O6 | 84.64 (5) | H6A—O6—H6B | 110.00 |

| | | | |
|--------------------------------------|--------------|-------------|--------------|
| O1—Mn1—O1 ⁱ | 180.00 | S1—N1—H12 | 111.1 (16) |
| O1—Mn1—O5 ⁱ | 86.05 (5) | S1—N1—H11 | 111 (2) |
| O1—Mn1—O6 ⁱ | 95.36 (5) | H11—N1—H12 | 115 (2) |
| O5—Mn1—O6 | 84.27 (5) | C2—C1—C6 | 117.85 (15) |
| O1 ⁱ —Mn1—O5 | 86.05 (5) | C2—C1—C7 | 124.92 (14) |
| O5—Mn1—O5 ⁱ | 180.00 | C6—C1—C7 | 117.19 (15) |
| O5—Mn1—O6 ⁱ | 95.73 (5) | S1—C2—C1 | 123.55 (12) |
| O1 ⁱ —Mn1—O6 | 95.36 (5) | S1—C2—C3 | 115.65 (14) |
| O5 ⁱ —Mn1—O6 | 95.73 (5) | C1—C2—C3 | 120.76 (17) |
| O6—Mn1—O6 ⁱ | 180.00 | C2—C3—C4 | 120.1 (2) |
| O1 ⁱ —Mn1—O5 ⁱ | 93.95 (5) | C3—C4—C5 | 119.80 (18) |
| O1 ⁱ —Mn1—O6 ⁱ | 84.64 (5) | C4—C5—C6 | 120.2 (2) |
| O5 ⁱ —Mn1—O6 ⁱ | 84.27 (5) | C1—C6—C5 | 121.27 (17) |
| O3—S1—O4 | 116.79 (9) | O2—C7—C1 | 118.68 (15) |
| O3—S1—N1 | 108.69 (9) | O1—C7—O2 | 126.13 (15) |
| O3—S1—C2 | 108.09 (9) | O1—C7—C1 | 115.15 (14) |
| O4—S1—N1 | 106.03 (9) | C2—C3—H3 | 120.00 |
| O4—S1—C2 | 108.37 (8) | C4—C3—H3 | 120.00 |
| N1—S1—C2 | 108.63 (8) | C3—C4—H4 | 120.00 |
| Mn1—O1—C7 | 128.58 (11) | C5—C4—H4 | 120.00 |
| H5A—O5—H5B | 111.00 | C4—C5—H5 | 120.00 |
| Mn1—O5—H5B | 105.00 | C6—C5—H5 | 120.00 |
| Mn1—O5—H5A | 108.00 | C1—C6—H6 | 119.00 |
| Mn1—O6—H6B | 120.00 | C5—C6—H6 | 119.00 |
| O5—Mn1—O1—C7 | 57.48 (15) | C7—C1—C2—S1 | 4.8 (2) |
| O6—Mn1—O1—C7 | 141.35 (15) | C7—C1—C2—C3 | -177.97 (17) |
| O5 ⁱ —Mn1—O1—C7 | -122.52 (15) | C2—C1—C6—C5 | -0.3 (2) |
| O6 ⁱ —Mn1—O1—C7 | -38.65 (15) | C7—C1—C6—C5 | 177.57 (17) |
| O3—S1—C2—C1 | 46.54 (16) | C2—C1—C7—O1 | -150.20 (16) |
| O3—S1—C2—C3 | -130.87 (15) | C2—C1—C7—O2 | 32.0 (2) |
| O4—S1—C2—C1 | 174.00 (14) | C6—C1—C7—O1 | 32.1 (2) |
| O4—S1—C2—C3 | -3.41 (17) | C6—C1—C7—O2 | -145.67 (16) |
| N1—S1—C2—C1 | -71.23 (16) | S1—C2—C3—C4 | 178.11 (17) |
| N1—S1—C2—C3 | 111.36 (16) | C1—C2—C3—C4 | 0.6 (3) |
| Mn1—O1—C7—O2 | 4.9 (3) | C2—C3—C4—C5 | -0.4 (3) |
| Mn1—O1—C7—C1 | -172.72 (10) | C3—C4—C5—C6 | -0.2 (3) |
| C6—C1—C2—S1 | -177.56 (12) | C4—C5—C6—C1 | 0.6 (3) |
| C6—C1—C2—C3 | -0.3 (2) | | |

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x, y-1, z$; (iii) $x, -y+3/2, z+1/2$; (iv) $x, -y+3/2, z-1/2$; (v) $-x, y-1/2, -z+1/2$; (vi) $x, -y+5/2, z+1/2$; (vii) $-x, y+1/2, -z+1/2$; (viii) $x, y+1, z$; (ix) $x, -y+5/2, z-1/2$; (x) $x, -y+1/2, z-1/2$; (xi) $-x+1, -y+1, -z$; (xii) $-x+1, y-1/2, -z+1/2$; (xiii) $-x+1, y+1/2, -z+1/2$; (xiv) $x, -y+1/2, z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| O5—H5A \cdots O3 ⁱⁱⁱ | 0.86 | 2.02 | 2.869 (2) | 167 |
| O5—H5B \cdots O2 ^{vii} | 0.97 | 1.83 | 2.775 (2) | 164 |

| | | | | |
|-----------------------------|----------|----------|-----------|---------|
| O6—H6A···O5 ^{vii} | 0.94 | 1.85 | 2.765 (2) | 164 |
| O6—H6B···N1 ^{viii} | 0.86 | 2.25 | 3.008 (2) | 148 |
| N1—H11···O2 | 0.77 (3) | 2.19 (3) | 2.799 (2) | 137 (2) |
| N1—H12···O4 ^{xiv} | 0.85 (2) | 2.50 (2) | 3.300 (2) | 157 (2) |
| C3—H3···O4 | 0.93 | 2.40 | 2.834 (3) | 108 |

Symmetry codes: (iii) $x, -y+3/2, z+1/2$; (vii) $-x, y+1/2, -z+1/2$; (viii) $x, y+1, z$; (xiv) $x, -y+1/2, z+1/2$.