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Diaquabis(DL-α-lipoato-κ^2O,O')manganese(II)

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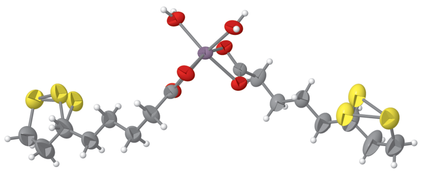
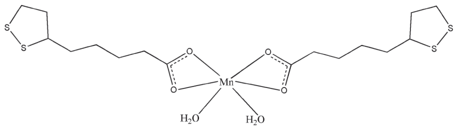
The manganese(II) coordination compound, $[Mn(C_8H_{13}S_2O_2)_2(H_2O)_2]$, with two bidentate α-lipoate ligands and two coordinating water molecules, has been structurally characterized. The cantral Mn^{II} atom lies on a crystallographic twofold rotation axis and adopts a distorted octahedral coordination environment, with carboxylate groups chelating the metal in a κ^2O,O'-binding mode. One of the sulfur atoms within the 1,2-dithiolane ring exhibits positional disorder over two sites, with refined occupancies of 0.92 and 0.08. The complex is isostructural with previously reported Zn^{II} and Cd^{II} analogues, both of which also display positional disorder in the 1,2-dithiolane ring. The molecules are linked *via* intermolecular O—H···O and C—H···S hydrogen bonds into a di-periodic supramolecular framework parallel to (100).

3D view



Chemical scheme



Structure description

α-Lipoic acid [IUPAC name: 5-(1,2-dithiolan-3-yl)pentanoic acid], also known as thioctic acid, is a naturally occurring organosulfur compound that acts as a redox-active cofactor in mitochondrial multienzyme complexes such as pyruvate dehydrogenase and α-keto-glutarate dehydrogenase (Packer *et al.*, 1995). As a result of its amphipathic nature, lipoic acid can function across various cellular compartments and participate in redox regulation (Shay *et al.*, 2009). Its antioxidant activity is attributed to its ability to scavenge reactive oxygen species (ROS), regenerate endogenous antioxidants, and chelate transition metals (Biewenga *et al.*, 1997; Solmonson & DeBerardinis, 2018). These properties make lipoic acid a promising agent for the treatment of oxidative stress-related conditions such as diabetic neuropathy and cardiovascular disorders (Ziegler *et al.*, 2006; Gorąca *et al.*, 2011). Importantly, lipoic acid forms stable complexes with metal ions through its dithiolane ring and carboxylic acid group. These metal complexes, particularly

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with transition metals, have demonstrated enhanced pharmacological properties including antioxidant, anticancer, and detoxification activities (Yan *et al.*, 2024). Chelation with Cu^{2+} and Zn^{2+} has been shown to improve its biomedical applicability, including in nanomedicine and redox modulation. Manganese (Mn), a bioactive transition metal, also exhibits notable therapeutic relevance due to its role in enzymatic activity, immune regulation, and bone formation. Mn-decorated titanium implants and manganese-based nanoparticles have shown osteogenic and immunomodulatory effects, highlighting their potential in tissue engineering and immunotherapy (Wang *et al.*, 2024; Huang *et al.*, 2023).

In this work, we report the synthesis and crystal structure of a novel Mn^{II} complex with DL-α-lipoate (abbreviated LIP). The asymmetric unit of the title compound, $[Mn(LIP)_2(H_2O)_2]$, comprises one half of the molecular unit, with the complete molecule generated by twofold rotation symmetry along the *b*-axis direction, *via* the symmetry operation $1 - x, y, \frac{1}{2} - z$. The Mn^{II} cation lies on this special position, while all other atoms, including those of the LIP ligands and water molecules, occupy general positions. The central Mn^{II} atom is six-coordinated in a distorted $[MnO_6]$ octahedral shape, defined by four oxygen atoms from two bidentate LIP ligands and two coordinating water molecules (Fig. 1). The Mn—O bond lengths span from 2.125 (2) (Mn—O1*W*) to 2.258 (2) Å (Mn—O1), with chelate-induced bite angles such as O1—Mn1—O2 = 57.76 (8)°, reflecting notable geometric strain. Notably, the title complex is isostructural with the Cd^{II} complex reported by Strasdeit *et al.* (1997). In the latter, the Cd—O bond lengths are slightly longer, ranging from 2.226 Å (Cd—O3) for the coordinating water molecule to 2.343 Å (Cd—O2) for the carboxylate oxygen atoms, consistent with the larger ionic radius of Cd^{II} compared to Mn^{II}. The S—S bond length in the disulfide ring is also similar [2.0443 (18) Å for Mn, 2.047 (3) Å for Cd], indicating structural conservation of the dithiolane moiety across the series. This distortion is further evidenced by the *cis* O—Mn—O bond angles ranging from 87.45 (8) to 108.39 (9)°, and the *trans* angles being reduced to 144.53 (8) and 162.59 (13)°. The coordination environment and geometry are closely comparable to those of the previously reported Zn^{II} analogue, $[Zn(LIP)_2(H_2O)_2]$, in which a similarly distorted octahedron is observed (Baumgartner *et al.*, 1996). The bond lengths in the Mn^{II} complex are slightly elongated, consistent with the larger ionic radius of Mn^{II} relative to Zn^{II}. The LIP ligand maintains its five-membered 1,2-dithiolane ring, but displays positional disorder of one sulfur atom. The major component (occupancy 0.92) involves an S1—S2 disulfide bridge with a bond length of 2.0443 (18) Å, whereas the minor component (occupancy 0.08) involves an alternative S2*A* position with an S1—S2*A* distance of 2.042 (12) Å. This subtle disorder suggests limited conformational flexibility in the ring, which remains geometrically intact. Similar S—S distances are observed in the Zn^{II} complex [2.025 (4) Å] and in free α-lipoic acid [2.053 (4) Å; Stroud & Carlise, 1972].

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2^{i}	0.85	1.91	2.725 (3)	159
O1*W*—H1*WB*···O1^{ii}	0.85	2.07	2.718 (3)	132
C2—H2*B*···S2*A*^{iii}	0.97	2.12	3.043 (18)	158

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

The crystal packing is consolidated by a network of classical O—H···O hydrogen bonds involving water molecules acting as donors and carboxylate oxygen atoms from adjacent symmetry-related units as acceptors. The O1*W*—H1*WA*···O2^{i} and O1*W*—H1*WB*···O1^{ii} interactions exhibit donor–acceptor distances of 2.725 (3) and 2.718 (3) Å and angles of 159 and 132°, respectively, consistent with the moderately strong hydrogen-bonding geometry typically observed in metal carboxylate systems (Table 1). In addition, a directional C—H···S hydrogen bond between a methylene hydrogen and the minor occupancy sulfur site [C2—H2*B*···S2*A*^{iii}] is present (Table 1, last entry), reinforcing the layer cohesion through weak but structurally significant interactions. These intermolecular contacts link the molecules into extended layers parallel to (100), forming a lamellar supramolecular architecture, as illustrated in Fig. 2.

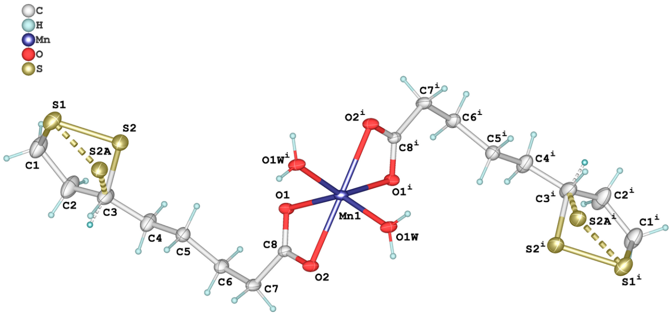

Figure 1
The molecular structure of the $[Mn(LIP)_2(H_2O)_2]$ complex showing the atom-labelling scheme and 50% probability displacement ellipsoids for non-H atoms. Hydrogen atoms are shown as spheres of arbitrary radius. [Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.]

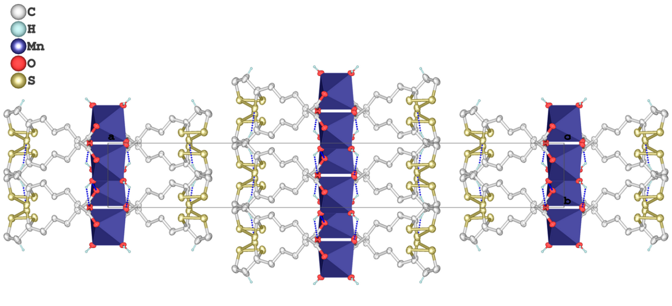

Figure 2
Crystal packing of the $[Mn(LIP)_2(H_2O)_2]$ complex viewed along the *c* axis. Intermolecular hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

Synthesis and crystallization

To an aqueous solution (2.5 ml) of $MnCl_2·4H_2O$ (0.099 g, 0.5 mmol), a sodium salt solution (2.5 ml) of DL-α-lipoic acid (0.206 g, 1 mmol) was added dropwise under constant stirring. The metal-to-ligand molar ratio was 1:2. The resulting mixture was left to stand at room temperature, and pinkish plate-shaped crystals suitable for X-ray diffraction were obtained by slow evaporation over 21 days, yield: 70%. Elemental analysis for $C_{16}H_{30}MnO_6S_4$ (M_w = 501.58): calculated (%) C, 38.31; H, 6.03; Mn, 10.95; O, 19.14; S, 25.57; found: C, 38.27; H, 5.98; Mn, 10.89; O, 19.12; S, 25.50.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One of the sulfur atoms in the 1,2-dithiolane ring, S2, is disordered over two positions, modelled as S2 and S2*A*, with site occupancies of 0.92 and 0.08, respectively. Geometric and displacement restraints or constraints were applied in the disordered 1,2-dithiolane ring: bonds S1—S2/S2*A* and C3—S2/S2*A* were restrained to have the same distance with a standard deviation of 0.02 Å, and displacement parameters for S2 and S2*A* were constrained to be identical.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Mn(C_8H_{13}O_2S_2)_2(H_2O)_2]$
M_r	501.58
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	290
a, *b*, *c* (Å)	38.4331 (13), 5.4083 (2), 11.0637 (3)
β (°)	93.566 (3)
V (Å^3)	2295.22 (13)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	8.32
Crystal size (mm)	0.30 × 0.24 × 0.08
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.419, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9876, 2214, 1795
R_{int}	0.052
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.154, 1.05
No. of reflections	2214
No. of parameters	127
No. of restraints	8
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.27

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

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Diaquabis[5-(1,2-dithiolan-3-yl)pentanoato-κ^2O,O']manganese(II)

Crystal data

$[Mn(C_8H_{13}O_2S_2)_2(H_2O)_2]$
$M_r = 501.58$
Monoclinic, $C2/c$
$a = 38.4331\ (13)$ Å
$b = 5.4083\ (2)$ Å
$c = 11.0637\ (3)$ Å
$\beta = 93.566\ (3)°$
$V = 2295.22\ (13)$ Å^3
$Z = 4$
$F(000) = 1052$
$D_x = 1.452$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 4882 reflections
$\theta = 4.6–71.2°$
$\mu = 8.32$ mm^{-1}
$T = 290$ K
Plate, pinkish
0.3 × 0.24 × 0.08 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
$T_{min} = 0.419$, $T_{max} = 1.000$
9876 measured reflections
2214 independent reflections
1795 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 71.4°$, $\theta_{min} = 2.3°$
$h = -46 \rightarrow 45$
$k = -6 \rightarrow 6$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.154$
$S = 1.05$
2214 reflections
127 parameters
8 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0936P)^2 + 1.0204P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mn1	0.500000	0.17395 (11)	0.250000	0.0400 (2)	
S1	0.71081 (4)	0.6684 (2)	0.07122 (12)	0.0889 (4)	

S2	0.66087 (3)	0.6590 (3)	0.12475 (12)	0.0818 (4)	0.92
S2A	0.6778 (4)	0.542 (3)	0.1952 (12)	0.0818 (4)	0.08
O1	0.53986 (6)	0.4747 (4)	0.28943 (18)	0.0481 (5)	
O1W	0.46681 (7)	−0.0863 (4)	0.32936 (19)	0.0521 (6)	
H1WA	0.464697	−0.113169	0.404242	0.078*	
H1WB	0.452668	−0.186774	0.293346	0.078*	
O2	0.52498 (6)	0.2365 (4)	0.43551 (19)	0.0517 (6)	
C1	0.72057 (15)	0.9590 (11)	0.1424 (5)	0.0997 (17)	
H1A	0.744854	0.960903	0.172016	0.120*	
H1B	0.717162	1.090218	0.083028	0.120*	
C3	0.67286 (13)	0.8089 (10)	0.2663 (5)	0.0857 (15)	
H3A	0.685568	0.684922	0.316278	0.103*	0.92
H3B	0.685947	0.751848	0.339876	0.103*	0.08
C4	0.64166 (12)	0.8763 (9)	0.3330 (4)	0.0795 (13)	
H4A	0.628523	0.999583	0.285669	0.095*	
H4B	0.649753	0.953975	0.408622	0.095*	
C5	0.61713 (10)	0.6719 (7)	0.3618 (4)	0.0603 (9)	
H5A	0.630382	0.538050	0.400644	0.072*	
H5B	0.606141	0.608592	0.286739	0.072*	
C6	0.58918 (10)	0.7526 (8)	0.4432 (3)	0.0599 (9)	
H6A	0.600257	0.838442	0.512319	0.072*	
H6B	0.574126	0.870293	0.399280	0.072*	
C7	0.56689 (10)	0.5489 (8)	0.4891 (3)	0.0601 (9)	
H7A	0.582235	0.427313	0.528863	0.072*	
H7B	0.552818	0.618412	0.550521	0.072*	
C8	0.54298 (8)	0.4159 (6)	0.3990 (3)	0.0420 (7)	
C2	0.69827 (16)	1.0064 (13)	0.2446 (6)	0.115 (2)	
H2A	0.713185	1.029186	0.317755	0.138*	
H2B	0.685666	1.159689	0.229112	0.138*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0538 (4)	0.0384 (4)	0.0279 (4)	0.000	0.0040 (3)	0.000
S1	0.0862 (8)	0.0991 (9)	0.0848 (8)	−0.0011 (6)	0.0323 (7)	−0.0086 (6)
S2	0.0697 (8)	0.1122 (11)	0.0638 (7)	−0.0159 (6)	0.0066 (6)	−0.0201 (6)
S2A	0.0697 (8)	0.1122 (11)	0.0638 (7)	−0.0159 (6)	0.0066 (6)	−0.0201 (6)
O1	0.0599 (13)	0.0495 (12)	0.0347 (11)	−0.0065 (10)	0.0005 (9)	0.0038 (9)
O1W	0.0740 (16)	0.0491 (12)	0.0338 (11)	−0.0126 (11)	0.0100 (10)	−0.0009 (10)
O2	0.0670 (15)	0.0548 (12)	0.0334 (11)	−0.0132 (11)	0.0037 (10)	0.0017 (10)
C1	0.087 (3)	0.102 (4)	0.116 (4)	−0.021 (3)	0.044 (3)	−0.012 (3)
C3	0.077 (3)	0.113 (4)	0.069 (3)	−0.030 (3)	0.020 (2)	−0.022 (3)
C4	0.070 (3)	0.087 (3)	0.084 (3)	−0.018 (2)	0.027 (2)	−0.023 (2)
C5	0.055 (2)	0.072 (2)	0.055 (2)	−0.0052 (17)	0.0076 (16)	−0.0035 (17)
C6	0.058 (2)	0.071 (2)	0.052 (2)	−0.0103 (18)	0.0088 (16)	−0.0134 (18)
C7	0.063 (2)	0.080 (2)	0.0375 (17)	−0.0215 (19)	0.0073 (15)	−0.0100 (17)
C8	0.0471 (16)	0.0460 (16)	0.0334 (15)	0.0020 (12)	0.0066 (12)	−0.0007 (12)
C2	0.095 (4)	0.128 (5)	0.129 (5)	−0.052 (4)	0.054 (3)	−0.048 (4)

Geometric parameters (Å, º)

Mn1—O1	2.258 (2)	C3—H3A	0.9800
Mn1—O1^{i}	2.258 (2)	C3—H3B	0.9800
Mn1—O1W^{i}	2.125 (2)	C3—C4	1.492 (6)
Mn1—O1W	2.125 (2)	C3—C2	1.477 (7)
Mn1—O2^{i}	2.237 (2)	C4—H4A	0.9700
Mn1—O2	2.237 (2)	C4—H4B	0.9700
S1—S2	2.0443 (18)	C4—C5	1.500 (6)
S1—S2A	2.042 (12)	C5—H5A	0.9700
S1—C1	1.787 (6)	C5—H5B	0.9700
S2—C3	1.797 (5)	C5—C6	1.509 (5)
S2A—C3	1.659 (14)	C6—H6A	0.9700
O1—C8	1.251 (4)	C6—H6B	0.9700
O1W—H1WA	0.8501	C6—C7	1.504 (5)
O1W—H1WB	0.8502	C7—H7A	0.9700
O2—C8	1.272 (4)	C7—H7B	0.9700
C1—H1A	0.9700	C7—C8	1.498 (5)
C1—H1B	0.9700	C2—H2A	0.9700
C1—C2	1.483 (7)	C2—H2B	0.9700

O1^{i}—Mn1—O1	87.84 (12)	C2—C3—S2A	117.1 (6)
O1W—Mn1—O1	144.53 (8)	C2—C3—H3A	106.0
O1W^{i}—Mn1—O1^{i}	144.53 (8)	C2—C3—H3B	93.0
O1W—Mn1—O1^{i}	98.02 (9)	C2—C3—C4	117.6 (5)
O1W^{i}—Mn1—O1	98.01 (9)	C3—C4—H4A	108.0
O1W—Mn1—O1W^{i}	97.07 (13)	C3—C4—H4B	108.0
O1W—Mn1—O2	87.45 (8)	C3—C4—C5	117.4 (4)
O1W—Mn1—O2^{i}	104.17 (9)	H4A—C4—H4B	107.2
O1W^{i}—Mn1—O2	104.17 (9)	C5—C4—H4A	108.0
O1W^{i}—Mn1—O2^{i}	87.45 (8)	C5—C4—H4B	108.0
O2—Mn1—O1	57.76 (8)	C4—C5—H5A	108.9
O2^{i}—Mn1—O1^{i}	57.76 (8)	C4—C5—H5B	108.9
O2—Mn1—O1^{i}	108.39 (9)	C4—C5—C6	113.2 (3)
O2^{i}—Mn1—O1	108.39 (9)	H5A—C5—H5B	107.8
O2^{i}—Mn1—O2	162.59 (13)	C6—C5—H5A	108.9
C1—S1—S2	93.99 (17)	C6—C5—H5B	108.9
C1—S1—S2A	96.9 (4)	C5—C6—H6A	108.4
C3—S2—S1	92.66 (16)	C5—C6—H6B	108.4
C3—S2A—S1	97.0 (7)	H6A—C6—H6B	107.5
C8—O1—Mn1	91.54 (19)	C7—C6—C5	115.6 (3)
Mn1—O1W—H1WA	127.7	C7—C6—H6A	108.4
Mn1—O1W—H1WB	127.8	C7—C6—H6B	108.4
H1WA—O1W—H1WB	104.5	C6—C7—H7A	107.9
C8—O2—Mn1	91.98 (18)	C6—C7—H7B	107.9
S1—C1—H1A	109.2	H7A—C7—H7B	107.2
S1—C1—H1B	109.2	C8—C7—C6	117.8 (3)
H1A—C1—H1B	107.9	C8—C7—H7A	107.9

C2—C1—S1	111.9 (4)	C8—C7—H7B	107.9
C2—C1—H1A	109.2	O1—C8—O2	118.7 (3)
C2—C1—H1B	109.2	O1—C8—C7	122.7 (3)
S2—C3—H3A	106.0	O2—C8—C7	118.5 (3)
S2A—C3—H3B	93.0	C1—C2—H2A	108.6
C4—C3—S2	111.8 (3)	C1—C2—H2B	108.6
C4—C3—S2A	124.5 (6)	C3—C2—C1	114.7 (5)
C4—C3—H3A	106.0	C3—C2—H2A	108.6
C4—C3—H3B	93.0	C3—C2—H2B	108.6
C2—C3—S2	108.7 (4)	H2A—C2—H2B	107.6
Mn1—O1—C8—O2	0.3 (3)	S2—C3—C2—C1	−29.7 (8)
Mn1—O1—C8—C7	−179.4 (3)	S2A—S1—C1—C2	−8.4 (7)
Mn1—O2—C8—O1	−0.3 (3)	S2A—C3—C4—C5	14.5 (10)
Mn1—O2—C8—C7	179.4 (3)	S2A—C3—C2—C1	12.2 (11)
S1—S2—C3—C4	171.7 (4)	C3—C4—C5—C6	172.4 (4)
S1—S2—C3—C2	40.2 (5)	C4—C3—C2—C1	−157.9 (6)
S1—S2A—C3—C4	153.7 (5)	C4—C5—C6—C7	−171.9 (4)
S1—S2A—C3—C2	−15.7 (10)	C5—C6—C7—C8	−67.3 (5)
S1—C1—C2—C3	−0.3 (8)	C6—C7—C8—O1	−3.2 (5)
S2—S1—C1—C2	24.9 (5)	C6—C7—C8—O2	177.2 (3)
S2—C3—C4—C5	57.0 (6)	C2—C3—C4—C5	−176.2 (5)

Symmetry code: (i) $-x+1, y, -z+1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2^{ii}	0.85	1.91	2.725 (3)	159
O1*W*—H1*WB*···O1^{iii}	0.85	2.07	2.718 (3)	132
C2—H2*B*···S2*A*^{iv}	0.97	2.12	3.043 (18)	158

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