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Poly[diaqua(μ_3-2,3-dioxoindoline-5-sulfonato)-sodium]

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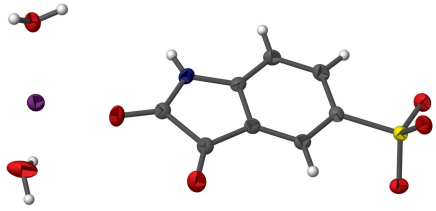
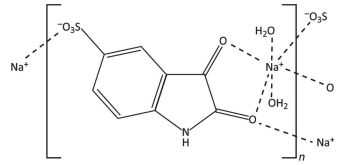
The title compound, $[Na(C_8H_4NO_5S)(H_2O)_2]_n$, is a one-dimensional coordination polymer extending along the *c* axis. It consist of isatin sulfonate molecules linking pairs of sodium cations with Na—O bonds to both carbonyl and sulfonate oxygen atoms whereby two oxygen atoms of symmetry-related carbonyl groups bridge two sodium cations. The sodium cation possesses an octahedral coordination environment, including one sulfonate and three carbonyl oxygen atoms bound in the equatorial plane, and two water molecules bound axially. The isatin moiety of the organic ligand is nearly planar, with a mean deviation from planarity of 0.038 Å. The chains of the coordination polymer are further linked into a three-dimensional network with eight distinct interactions, including one N—H···O and four O—H···O hydrogen bonds, two C—H···O interactions and one π–π interaction.

3D view



Chemical scheme



Structure description

As part of our standing project to study the crystal structures of N-H isatins, we report the crystal structure of the title compound. The asymmetric unit comprises a sodium cation, a 2,3-dioxoindoline-5-sulfonate anion and two coordinating water molecules (Fig. 1). The isatin moiety of the anion is nearly planar. The sodium cation possesses an octahedral configuration, and is coordinated by three carbonyl oxygen atoms, two water molecules, and one sulfonate oxygen atom. Two symmetry-related O1 carbonyl oxygen atoms bridge two sodium cations, with the O2 carbonyl oxygen binding to only a single sodium cation. The O5 sulfonate oxygen atom and the two water oxygen atoms (O6, O7) complete the sodium coordination environment (Fig. 2). Despite the coordination of the carbonyl oxygen atoms to the sodium cations, the C=O bonds and other metric parameters are

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O3^{i}	0.86 (1)	2.06 (1)	2.878 (2)	159 (3)
O6—H6B···O4^{ii}	0.86 (1)	2.01 (2)	2.807 (2)	153 (3)
O7—H7A···O5^{iii}	0.86 (1)	2.01 (1)	2.854 (2)	169 (2)
O7—H7B···O3^{iv}	0.86 (1)	1.94 (1)	2.780 (2)	168 (3)
N1—H1···O7^{v}	0.87 (1)	1.97 (1)	2.837 (2)	174 (2)
C6—H6···O6^{vi}	0.95	2.63	3.520 (3)	156
C7—H7···O2^{vii}	0.95	2.59	3.453 (3)	152

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

consistent with those in neutral 5-substituted isatins (Gurung *et al.*, 2016). Pairs of sodium cations are linked by the isatin molecules to form a one-dimensional coordination polymer along the *c* axis.

The sodium–isatin chains are interconnected by a series of hydrogen bonds and π–π interactions to combine into a three-dimensional network. There is an N1—H1···O7^{v} hydrogen bond between the isatin amide group and one of the water oxygen atoms. There are also two C—H···O interactions, C6—H6···O6^{vi}, between the isatin moiety and a water molecule, and C7—H7···O2^{vii}, between the isatin moiety and the

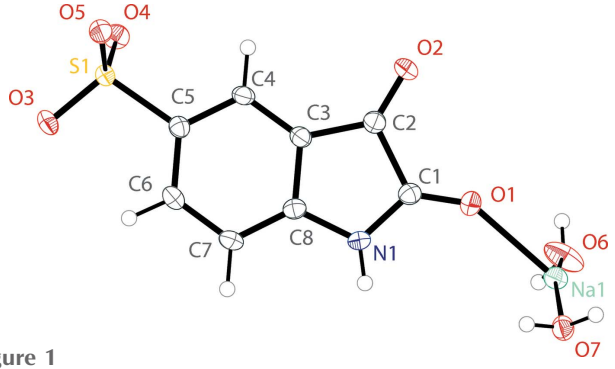


Figure 1
The asymmetric unit of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

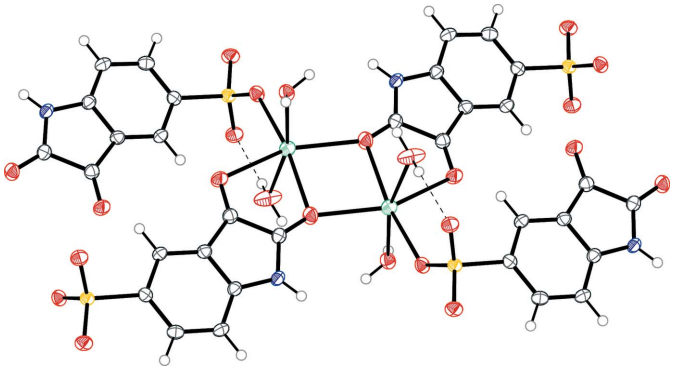


Figure 2
The coordination environment of the sodium cations in the structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen-bonding interactions are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Na(C_8H_4NO_5S)(H_2O)_2]$
M_r	285.20
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	200
a, b, c (Å)	7.4526 (17), 7.9888 (19), 10.692 (2)
α, β, γ (°)	85.916 (10), 80.181 (10), 65.237 (10)
V (Å^3)	569.6 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.35
Crystal size (mm)	0.18 × 0.15 × 0.14
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.231, 0.259
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9782, 2142, 1775
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.083, 1.06
No. of reflections	2142
No. of parameters	178
No. of restraints	5
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.41

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

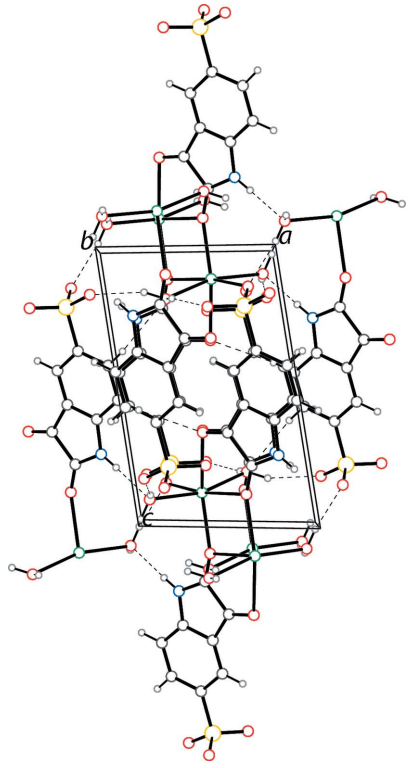


Figure 3
The crystal packing of the title compound, in a view along the *b* axis, with hydrogen bonds shown as dashed lines.

carbonyl oxygen atom of another isatin moiety (see Table 1 for symmetry codes). Both of the water molecules are involved in two O—H···O interactions to sulfonate oxygen atoms of the same chain and neighboring chains (Fig. 2). The chains are further linked between the aromatic six-membered rings in the isatin moieties, with parallel slipped π–π interactions [inter-centroid distance = 3.8314 (19) Å, interplanar distance = 3.619 (2) Å and slippage = 1.259 (4) Å]. The molecular packing of the title compound with hydrogen bonding is shown in Fig. 3.

The crystal structure of the related sodium 2-oxo-3-semi-carbazono-2,3-dihydro-1*H*-indole-5-sulfonate dihydrate, has been reported previously (Pelosi *et al.*, 2006).

Synthesis and crystallization

A commercial sample (Combi-Blocks) of sodium 2,3-dioxo-indole-5-sulfonate dihydrate was recrystallized by slow evaporation of an ethanol–water solution to yield orange blocks suitable for single-crystal X-ray diffraction analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

IUCrData (2017). **2**, x170440 [https://doi.org/10.1107/S2414314617004400]

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Crystal data

$[Na(C_8H_4NO_5S)(H_2O)_2]$
M_r = 285.20
Triclinic, $P\overline{1}$
a = 7.4526 (17) Å
b = 7.9888 (19) Å
c = 10.692 (2) Å
α = 85.916 (10)°
β = 80.181 (10)°
γ = 65.237 (10)°
V = 569.6 (2) Å^3
Z = 2
$F(000)$ = 292
D_x = 1.663 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4084 reflections
θ = 3.2–25.7°
μ = 0.35 mm^{-1}
T = 200 K
BLOCK, orange
0.18 × 0.15 × 0.14 mm

Data collection

Bruker D8 Venture CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.231, T_{max} = 0.259
9782 measured reflections
2142 independent reflections
1775 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.7°, θ_{min} = 3.1°
h = −9→9
k = −9→9
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.083
S = 1.06
2142 reflections
178 parameters
5 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 0.4169P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.62093 (12)	0.56376 (12)	1.11207 (8)	0.0228 (2)
S1	0.77858 (8)	0.88556 (7)	0.21370 (5)	0.01699 (15)
O1	0.6277 (2)	0.5579 (2)	0.89024 (14)	0.0258 (4)
O2	0.4366 (2)	0.5933 (2)	0.66757 (14)	0.0280 (4)
O3	0.9274 (2)	0.9597 (2)	0.17078 (14)	0.0247 (4)
O4	0.5735 (2)	1.0224 (2)	0.21817 (14)	0.0242 (4)
O5	0.8185 (2)	0.7209 (2)	0.14265 (13)	0.0214 (3)
O6	0.3464 (3)	0.8278 (3)	1.1862 (2)	0.0443 (5)
H6A	0.231 (2)	0.873 (4)	1.162 (3)	0.066*
H6B	0.384 (5)	0.916 (3)	1.186 (3)	0.066*
O7	0.9207 (2)	0.3007 (2)	1.09034 (14)	0.0229 (4)
H7A	0.990 (3)	0.288 (4)	1.0162 (11)	0.034*
H7B	0.911 (4)	0.1986 (19)	1.108 (2)	0.034*
N1	0.8411 (3)	0.6490 (3)	0.74783 (17)	0.0210 (4)
H1	0.918 (3)	0.656 (3)	0.7979 (17)	0.025*
C1	0.6827 (3)	0.6067 (3)	0.78595 (19)	0.0191 (5)
C2	0.5776 (3)	0.6315 (3)	0.6672 (2)	0.0203 (5)
C3	0.6918 (3)	0.7000 (3)	0.56743 (19)	0.0186 (5)
C4	0.6678 (3)	0.7541 (3)	0.44351 (19)	0.0190 (4)
H4	0.5608	0.7514	0.4077	0.023*
C5	0.8064 (3)	0.8129 (3)	0.37292 (19)	0.0177 (4)
C6	0.9651 (3)	0.8131 (3)	0.4255 (2)	0.0234 (5)
H6	1.0593	0.8509	0.3747	0.028*
C7	0.9891 (3)	0.7594 (3)	0.5508 (2)	0.0239 (5)
H7	1.0972	0.7601	0.5863	0.029*
C8	0.8495 (3)	0.7053 (3)	0.62055 (19)	0.0188 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0220 (5)	0.0256 (5)	0.0235 (5)	−0.0123 (4)	−0.0040 (3)	−0.0007 (4)
S1	0.0172 (3)	0.0175 (3)	0.0177 (3)	−0.0089 (2)	−0.0020 (2)	0.0010 (2)
O1	0.0319 (9)	0.0317 (9)	0.0193 (8)	−0.0188 (8)	−0.0061 (7)	0.0062 (7)
O2	0.0298 (9)	0.0396 (10)	0.0264 (8)	−0.0258 (8)	−0.0063 (7)	0.0036 (7)
O3	0.0255 (9)	0.0275 (9)	0.0275 (8)	−0.0182 (8)	−0.0033 (7)	0.0057 (7)
O4	0.0201 (8)	0.0217 (8)	0.0281 (8)	−0.0056 (7)	−0.0046 (6)	0.0003 (7)
O5	0.0243 (8)	0.0212 (8)	0.0197 (8)	−0.0110 (7)	−0.0006 (6)	−0.0038 (6)
O6	0.0222 (10)	0.0353 (11)	0.0768 (14)	−0.0125 (9)	−0.0070 (9)	−0.0070 (10)
O7	0.0275 (9)	0.0235 (9)	0.0204 (8)	−0.0140 (8)	−0.0016 (6)	−0.0003 (7)
N1	0.0203 (10)	0.0278 (10)	0.0191 (9)	−0.0126 (9)	−0.0077 (7)	0.0027 (8)
C1	0.0211 (12)	0.0171 (11)	0.0198 (11)	−0.0078 (10)	−0.0045 (9)	−0.0009 (9)
C2	0.0214 (12)	0.0201 (11)	0.0205 (11)	−0.0097 (10)	−0.0035 (9)	−0.0002 (9)
C3	0.0180 (11)	0.0197 (11)	0.0202 (11)	−0.0097 (9)	−0.0028 (8)	−0.0001 (9)
C4	0.0178 (11)	0.0218 (11)	0.0208 (11)	−0.0108 (10)	−0.0045 (8)	−0.0012 (9)
C5	0.0189 (11)	0.0166 (11)	0.0180 (10)	−0.0083 (9)	−0.0009 (8)	−0.0016 (8)

C6	0.0216 (12)	0.0277 (13)	0.0252 (12)	−0.0155 (11)	−0.0017 (9)	0.0014 (9)
C7	0.0190 (12)	0.0328 (13)	0.0252 (12)	−0.0151 (11)	−0.0057 (9)	0.0006 (10)
C8	0.0173 (11)	0.0188 (11)	0.0196 (11)	−0.0060 (9)	−0.0046 (8)	−0.0008 (8)

Geometric parameters (Å, º)

Na1—Na1^{i}	3.6590 (17)	O6—H6B	0.860 (5)
Na1—O1	2.3669 (17)	O7—H7A	0.857 (5)
Na1—O1^{i}	2.4309 (18)	O7—H7B	0.856 (5)
Na1—O2^{i}	2.6444 (18)	N1—H1	0.867 (5)
Na1—O5^{ii}	2.3706 (17)	N1—C1	1.351 (3)
Na1—O6	2.309 (2)	N1—C8	1.402 (3)
Na1—O7	2.3283 (19)	C1—Na1^{i}	3.113 (2)
Na1—C1^{i}	3.113 (2)	C1—C2	1.561 (3)
S1—O3	1.4596 (15)	C2—C3	1.470 (3)
S1—O4	1.4547 (16)	C3—C4	1.382 (3)
S1—O5	1.4609 (15)	C3—C8	1.406 (3)
S1—C5	1.777 (2)	C4—H4	0.9500
O1—Na1^{i}	2.4309 (18)	C4—C5	1.395 (3)
O1—C1	1.216 (2)	C5—C6	1.395 (3)
O2—Na1^{i}	2.6444 (18)	C6—H6	0.9500
O2—C2	1.210 (3)	C6—C7	1.394 (3)
O5—Na1^{iii}	2.3707 (17)	C7—H7	0.9500
O6—H6A	0.858 (5)	C7—C8	1.376 (3)
O1^{i}—Na1—Na1^{i}	39.66 (4)	S1—O5—Na1^{iii}	133.64 (9)
O1—Na1—Na1^{i}	40.95 (4)	Na1—O6—H6A	127 (2)
O1—Na1—O1^{i}	80.61 (6)	Na1—O6—H6B	109 (2)
O1—Na1—O2^{i}	145.72 (6)	H6A—O6—H6B	107 (3)
O1^{i}—Na1—O2^{i}	69.98 (5)	Na1—O7—H7A	113.6 (18)
O1—Na1—O5^{ii}	106.21 (6)	Na1—O7—H7B	115.7 (18)
O1^{i}—Na1—C1^{i}	21.08 (5)	H7A—O7—H7B	107 (3)
O1—Na1—C1^{i}	101.52 (6)	C1—N1—H1	124.4 (15)
O2^{i}—Na1—Na1^{i}	107.88 (5)	C1—N1—C8	111.27 (17)
O2^{i}—Na1—C1^{i}	49.33 (5)	C8—N1—H1	123.8 (16)
O5^{ii}—Na1—Na1^{i}	146.48 (5)	O1—C1—Na1^{i}	45.97 (11)
O5^{ii}—Na1—O1^{i}	169.43 (6)	O1—C1—N1	128.8 (2)
O5^{ii}—Na1—O2^{i}	105.59 (6)	O1—C1—C2	124.92 (19)
O5^{ii}—Na1—C1^{i}	151.73 (6)	N1—C1—Na1^{i}	168.95 (15)
O6—Na1—Na1^{i}	96.15 (6)	N1—C1—C2	106.28 (17)
O6—Na1—O1^{i}	83.70 (7)	C2—C1—Na1^{i}	79.79 (11)
O6—Na1—O1	106.17 (8)	O2—C2—C1	122.89 (19)
O6—Na1—O2^{i}	88.14 (7)	O2—C2—C3	132.4 (2)
O6—Na1—O5^{ii}	86.60 (7)	C3—C2—C1	104.67 (17)
O6—Na1—O7	164.59 (8)	C4—C3—C2	132.34 (19)
O6—Na1—C1^{i}	80.47 (7)	C4—C3—C8	121.11 (19)
O7—Na1—Na1^{i}	97.83 (5)	C8—C3—C2	106.56 (18)
O7—Na1—O1^{i}	103.12 (6)	C3—C4—H4	121.2

O7—Na1—O1	88.71 (6)	C3—C4—C5	117.57 (19)
O7—Na1—O2^{i}	81.43 (6)	C5—C4—H4	121.2
O7—Na1—O5^{ii}	85.33 (6)	C4—C5—S1	118.75 (16)
O7—Na1—C1^{i}	100.84 (6)	C6—C5—S1	120.41 (16)
C1^{i}—Na1—Na1^{i}	60.61 (5)	C6—C5—C4	120.84 (19)
O3—S1—O5	111.89 (9)	C5—C6—H6	119.2
O3—S1—C5	106.05 (9)	C7—C6—C5	121.68 (19)
O4—S1—O3	113.46 (9)	C7—C6—H6	119.2
O4—S1—O5	112.52 (9)	C6—C7—H7	121.4
O4—S1—C5	106.06 (9)	C8—C7—C6	117.12 (19)
O5—S1—C5	106.17 (9)	C8—C7—H7	121.4
Na1—O1—Na1^{i}	99.39 (6)	N1—C8—C3	111.14 (18)
C1—O1—Na1	146.85 (15)	C7—C8—N1	127.21 (19)
C1—O1—Na1^{i}	112.95 (14)	C7—C8—C3	121.65 (19)
C2—O2—Na1^{i}	107.73 (14)		
Na1—O1—C1—Na1^{i}	−166.5 (3)	N1—C1—C2—O2	175.3 (2)
Na1—O1—C1—N1	26.5 (4)	N1—C1—C2—C3	−3.0 (2)
Na1^{i}—O1—C1—N1	−166.99 (19)	C1—N1—C8—C3	−0.7 (3)
Na1^{i}—O1—C1—C2	12.7 (3)	C1—N1—C8—C7	179.6 (2)
Na1—O1—C1—C2	−153.79 (19)	C1—C2—C3—C4	−177.2 (2)
Na1^{i}—O2—C2—C1	−5.9 (2)	C1—C2—C3—C8	2.5 (2)
Na1^{i}—O2—C2—C3	171.9 (2)	C2—C3—C4—C5	−179.8 (2)
Na1^{i}—C1—C2—O2	4.8 (2)	C2—C3—C8—N1	−1.3 (2)
Na1^{i}—C1—C2—C3	−173.49 (15)	C2—C3—C8—C7	178.4 (2)
S1—C5—C6—C7	179.05 (17)	C3—C4—C5—S1	−179.40 (16)
O1—C1—C2—O2	−4.4 (3)	C3—C4—C5—C6	1.2 (3)
O1—C1—C2—C3	177.3 (2)	C4—C3—C8—N1	178.46 (19)
O2—C2—C3—C4	4.7 (4)	C4—C3—C8—C7	−1.8 (3)
O2—C2—C3—C8	−175.5 (2)	C4—C5—C6—C7	−1.6 (3)
O3—S1—O5—Na1^{iii}	−161.56 (11)	C5—S1—O5—Na1^{iii}	83.17 (13)
O3—S1—C5—C4	173.02 (16)	C5—C6—C7—C8	0.2 (3)
O3—S1—C5—C6	−7.6 (2)	C6—C7—C8—N1	−178.9 (2)
O4—S1—O5—Na1^{iii}	−32.43 (14)	C6—C7—C8—C3	1.5 (3)
O4—S1—C5—C4	52.08 (19)	C8—N1—C1—Na1^{i}	124.4 (7)
O4—S1—C5—C6	−128.54 (18)	C8—N1—C1—O1	−178.0 (2)
O5—S1—C5—C4	−67.82 (19)	C8—N1—C1—C2	2.3 (2)
O5—S1—C5—C6	111.56 (18)	C8—C3—C4—C5	0.4 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) *x*, *y*, *z*+1; (iii) *x*, *y*, *z*−1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*A*···O3^{iv}	0.86 (1)	2.06 (1)	2.878 (2)	159 (3)
O6—H6*B*···O4^{ii}	0.86 (1)	2.01 (2)	2.807 (2)	153 (3)
O7—H7*A*···O5^{v}	0.86 (1)	2.01 (1)	2.854 (2)	169 (2)
O7—H7*B*···O3^{vi}	0.86 (1)	1.94 (1)	2.780 (2)	168 (3)

N1—H1···O7^{vii}	0.87 (1)	1.97 (1)	2.837 (2)	174 (2)
C6—H6···O6^{viii}	0.95	2.63	3.520 (3)	156
C7—H7···O2^{ix}	0.95	2.59	3.453 (3)	152

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