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2,3-Diaminopyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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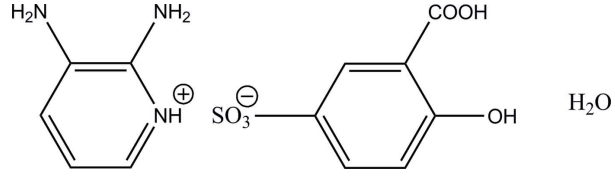
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.087; data-to-parameter ratio = 14.5.

In the title hydrated molecular salt, $C_5H_8N_3^+\cdot C_7H_5O_6S^-\cdot H_2O$, the ion pairs and water molecules are connected by N—H···O, O—H···O and C—H···O hydrogen bonds, thereby forming a three-dimensional network. There is an intramolecular O—H···O hydrogen bond in the 3-carboxy-4-hydroxybenzenesulfonate anion, which generates an S(6) ring motif.

Related literature

For background to 5-sulfosalicylic acid and related compounds, see: Marzotto *et al.* (2001); Onoda *et al.* (2001); Baskar Raj *et al.* (2003). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_5H_8N_3^+\cdot C_7H_5O_6S^-\cdot H_2O$
M_r = 345.33
Monoclinic, Cc
a = 7.0407 (7) Å
b = 15.5775 (16) Å
c = 13.6244 (12) Å
β = 101.491 (2)°
V = 1464.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 100 K
0.36 × 0.31 × 0.08 mm

Data collection

Bruker APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.910, T_{max} = 0.981
6890 measured reflections
3880 independent reflections
3645 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.03
3880 reflections
268 parameters
2 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1770 Friedel pairs
Flack parameter: −0.02 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O1W^{i}	0.91 (3)	1.95 (3)	2.806 (3)	158 (3)
N2—H1*N*2···O1^{i}	0.90 (3)	2.48 (3)	3.222 (2)	140 (2)
N2—H1*N*2···O1W^{i}	0.90 (3)	2.28 (3)	3.060 (3)	145 (2)
N2—H2*N*2···O2^{ii}	0.86 (3)	2.10 (3)	2.963 (2)	177 (3)
N3—H1*N*3···O2^{ii}	0.89 (3)	2.10 (3)	2.970 (3)	168 (3)
N3—H2*N*3···O4^{iii}	0.92 (3)	2.08 (3)	2.980 (3)	167 (3)
O1—H1*O*1···O6	1.03 (3)	1.75 (3)	2.625 (2)	141 (2)
O5—H1*O*5···O3^{iv}	0.84 (3)	1.87 (3)	2.655 (2)	155 (3)
O1*W*—H1*W*1···O3^{v}	0.89 (3)	1.94 (3)	2.757 (3)	151 (2)
O1*W*—H2*W*1···O4^{iii}	0.98 (6)	1.89 (6)	2.838 (3)	162 (4)
C7—H7···O3^{vi}	0.95 (3)	2.56 (3)	3.477 (2)	163 (2)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6457).

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§ Thomson Reuters ResearcherID: A-3561-2009.

supporting information

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2,3-Diaminopyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

Madhukar Hemamalini, Jia Hao Goh and Hoong-Kun Fun

S1. Comment

5-sulfosalicylic acid, (5-SSA), has been known for a long time to possess anti-inflammatory activity. When it forms complexes with metals, its biological activity is greatly enhanced (Marzotto *et al.*, 2001). Hydrogen-bonding patterns involving sulfonate groups in biological systems and metal complexes are of current interest (Onoda *et al.*, 2001). Such interactions can be utilized for designing supramolecular architectures (Baskar Raj *et al.*, 2003). With the aim of gaining more insight into hydrogen-bonding interactions involving 5-SSA and pyridine derivatives, we report here the molecular and supramolecular structure of the title compound.

The asymmetric unit of (I) contains a 2,3-diaminopyridinium cation, a sulfosalicylate anion and a water molecule (Fig. 1). The 2,3-di aminopyridinium cation is planar, with a maximum deviation of 0.015 (2) Å for atom C1. The dihedral angle between the pyridine (N1/C–C5) and the benzene (C6–C11) ring is 6.09 (9)°. The protonated N1 atom has lead to a slight increase in the C1—N1—C5 angle to 124. 4(2)°. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. There is an intramolecular O—H···O hydrogen bond in the 3-carboxy-4-hydroxy benzenesulfonate anion, which generates an *S*(6) (Bernstein *et al.*, 1995) ring motif.

In the crystal (Fig. 2), the ion-pairs and water molecules are connected *via* N—H···O, O—H···O and C—H···O hydrogen bonds (Table 1), forming a three-dimensional network.

S2. Experimental

Hot methanol solutions (20 ml) of 2,3-diaminopyridine (52 mg, Aldrich) and 5-sulfosalicylic acid (54. 5 mg, Merck) were mixed and warmed over a heating magnetic stirrer for 5 minutes. The resulting solution was allowed to cool slowly at room temperature. Brown plates of the title compound appeared from the mother liquor after a few days.

S3. Refinement

All hydrogen atoms were located from a difference Fourier maps and refined freely [N–H = 0.86 (3)–0.92 (3) Å; O–H = 0.90 (3)– 1.02 (3) Å and C–H = 0.91 (4)–1.06 (3) Å]. 1770 Friedel pairs were used to determine the absolute structure.

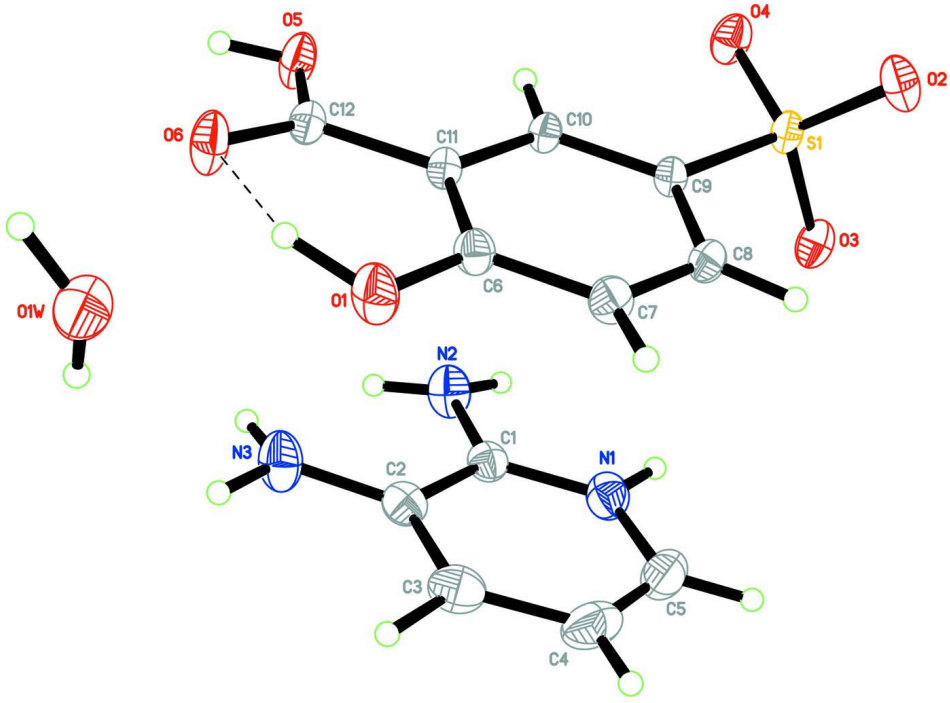

Figure 1

The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids. Intramolecular hydrogen bonds shown by dashed lines.

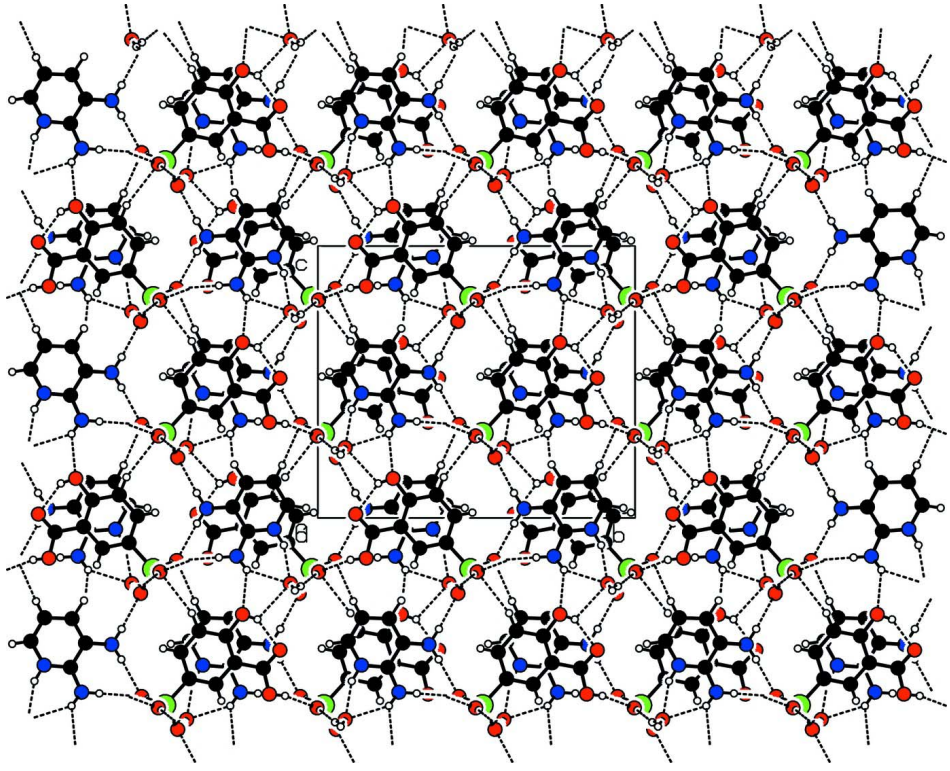

Figure 2

The crystal packing of title compound (I).

2,3-Diaminopyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

Crystal data

$C_5H_8N_3^+·C_7H_5O_6S^-·H_2O$
M_r = 345.33
Monoclinic, *Cc*
Hall symbol: C -2yc
a = 7.0407 (7) Å
b = 15.5775 (16) Å
c = 13.6244 (12) Å
β = 101.491 (2)°
V = 1464.3 (2) Å^3
Z = 4
F(000) = 720
D_x = 1.566 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3903 reflections
θ = 3.0–32.4°
μ = 0.26 mm^{-1}
T = 100 K
Plate, brown
0.36 × 0.31 × 0.08 mm

Data collection

Bruker APEXII DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.910, T_{max} = 0.981
6890 measured reflections
3880 independent reflections
3645 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 30.0°, θ_{min} = 3.0°
h = −9→9
k = −20→21
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.03
3880 reflections
268 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1770 Friedel pairs
Absolute structure parameter: −0.02 (5)

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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_{iso}*/U_{eq}
N1	0.9025 (3)	0.36254 (11)	−0.04106 (15)	0.0419 (4)
N2	0.7986 (3)	0.24446 (13)	−0.14072 (14)	0.0438 (4)
N3	0.7871 (3)	0.14977 (13)	0.03470 (16)	0.0482 (4)
C1	0.8513 (2)	0.27950 (12)	−0.04911 (15)	0.0328 (3)
C2	0.8521 (2)	0.23206 (13)	0.04046 (14)	0.0349 (4)
C3	0.9159 (3)	0.27470 (17)	0.12994 (16)	0.0465 (4)
C4	0.9699 (3)	0.36114 (19)	0.1331 (2)	0.0551 (6)
C5	0.9615 (3)	0.40443 (15)	0.0472 (2)	0.0516 (5)
S1	0.36330 (5)	0.48126 (2)	−0.18842 (3)	0.02841 (9)
O1	0.4248 (2)	0.23706 (10)	0.14554 (10)	0.0430 (3)
O2	0.2649 (2)	0.55517 (9)	−0.15649 (10)	0.0430 (3)
O3	0.5610 (2)	0.50245 (9)	−0.19835 (11)	0.0408 (3)
O4	0.2514 (2)	0.44146 (9)	−0.27754 (10)	0.0402 (3)
O5	0.2302 (2)	0.15275 (9)	−0.14779 (11)	0.0444 (3)
O6	0.2779 (3)	0.11944 (10)	0.01427 (12)	0.0484 (4)
C6	0.4112 (2)	0.28932 (11)	0.06627 (12)	0.0305 (3)
C7	0.4712 (3)	0.37427 (12)	0.08458 (13)	0.0337 (3)
C8	0.4596 (2)	0.43146 (11)	0.00715 (13)	0.0312 (3)
C9	0.3843 (2)	0.40512 (10)	−0.09102 (11)	0.0253 (3)
C10	0.3256 (2)	0.32121 (10)	−0.11074 (12)	0.0258 (3)
C11	0.3407 (2)	0.26183 (10)	−0.03244 (12)	0.0264 (3)
C12	0.2809 (2)	0.17180 (11)	−0.05209 (13)	0.0306 (3)
O1W	0.3732 (3)	0.08650 (11)	0.25895 (15)	0.0533 (4)
H3	0.930 (4)	0.2373 (19)	0.1958 (19)	0.046 (7)*
H4	1.007 (5)	0.389 (2)	0.193 (3)	0.069 (9)*
H5	1.011 (5)	0.463 (2)	0.039 (2)	0.067 (9)*
H7	0.515 (4)	0.3983 (18)	0.149 (2)	0.041 (6)*
H8	0.510 (4)	0.4874 (19)	0.021 (2)	0.043 (7)*
H10	0.271 (3)	0.3039 (15)	−0.1722 (17)	0.025 (5)*
H1N1	0.899 (5)	0.393 (2)	−0.098 (2)	0.057 (8)*
H1N2	0.820 (4)	0.277 (2)	−0.192 (2)	0.053 (8)*
H2N2	0.793 (4)	0.1894 (19)	−0.146 (2)	0.042 (6)*
H1N3	0.763 (4)	0.1187 (19)	−0.021 (2)	0.047 (7)*
H2N3	0.794 (4)	0.1179 (18)	0.092 (2)	0.044 (6)*
H1O1	0.354 (4)	0.181 (2)	0.122 (2)	0.053 (7)*
H1O5	0.203 (5)	0.100 (2)	−0.149 (2)	0.057 (8)*
H1W1	0.265 (5)	0.055 (2)	0.250 (2)	0.053 (8)*
H2W1	0.490 (8)	0.071 (4)	0.234 (4)	0.110 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0392 (8)	0.0377 (9)	0.0515 (10)	0.0004 (6)	0.0154 (7)	0.0051 (7)
N2	0.0607 (10)	0.0399 (10)	0.0340 (8)	0.0010 (7)	0.0169 (7)	0.0017 (7)
N3	0.0721 (12)	0.0387 (9)	0.0373 (9)	−0.0017 (8)	0.0194 (8)	0.0054 (8)

C1	0.0297 (7)	0.0335 (8)	0.0366 (8)	0.0024 (6)	0.0103 (6)	0.0016 (7)
C2	0.0330 (8)	0.0385 (10)	0.0352 (9)	0.0044 (6)	0.0116 (7)	0.0007 (8)
C3	0.0452 (10)	0.0592 (13)	0.0343 (10)	0.0045 (9)	0.0058 (8)	0.0009 (9)
C4	0.0444 (11)	0.0639 (15)	0.0538 (14)	−0.0043 (9)	0.0017 (9)	−0.0239 (12)
C5	0.0415 (9)	0.0405 (11)	0.0723 (15)	−0.0054 (8)	0.0105 (10)	−0.0113 (10)
S1	0.03858 (18)	0.02089 (16)	0.02544 (16)	−0.00344 (14)	0.00561 (12)	−0.00076 (14)
O1	0.0647 (9)	0.0366 (7)	0.0267 (6)	−0.0019 (6)	0.0068 (6)	0.0070 (5)
O2	0.0621 (8)	0.0302 (7)	0.0362 (7)	0.0129 (6)	0.0085 (6)	0.0010 (5)
O3	0.0469 (7)	0.0314 (6)	0.0462 (8)	−0.0108 (5)	0.0141 (6)	0.0010 (5)
O4	0.0577 (8)	0.0349 (7)	0.0264 (6)	−0.0101 (6)	0.0043 (5)	−0.0034 (5)
O5	0.0663 (9)	0.0270 (6)	0.0374 (7)	−0.0146 (6)	0.0043 (6)	−0.0016 (5)
O6	0.0745 (11)	0.0289 (7)	0.0416 (8)	−0.0115 (7)	0.0114 (7)	0.0064 (6)
C6	0.0364 (8)	0.0281 (8)	0.0275 (7)	0.0003 (6)	0.0078 (6)	0.0019 (6)
C7	0.0417 (8)	0.0323 (9)	0.0256 (8)	0.0013 (6)	0.0031 (6)	−0.0057 (6)
C8	0.0349 (7)	0.0246 (7)	0.0323 (8)	−0.0024 (6)	0.0027 (6)	−0.0067 (6)
C9	0.0303 (7)	0.0209 (6)	0.0250 (7)	−0.0012 (5)	0.0060 (5)	0.0000 (5)
C10	0.0310 (7)	0.0208 (6)	0.0257 (7)	−0.0020 (5)	0.0063 (5)	−0.0019 (5)
C11	0.0298 (7)	0.0220 (7)	0.0285 (8)	−0.0008 (5)	0.0083 (6)	0.0001 (5)
C12	0.0337 (7)	0.0245 (7)	0.0342 (8)	−0.0029 (6)	0.0084 (6)	0.0010 (6)
O1W	0.0539 (9)	0.0464 (9)	0.0617 (10)	−0.0046 (7)	0.0169 (8)	−0.0035 (8)

Geometric parameters (Å, º)

N1—C1	1.342 (3)	S1—C9	1.7640 (16)
N1—C5	1.358 (3)	O1—C6	1.341 (2)
N1—H1N1	0.91 (3)	O1—H1O1	1.02 (3)
N2—C1	1.345 (3)	O5—C12	1.315 (2)
N2—H1N2	0.90 (3)	O5—H1O5	0.84 (4)
N2—H2N2	0.86 (3)	O6—C12	1.221 (2)
N3—C2	1.358 (3)	C6—C7	1.396 (3)
N3—H1N3	0.88 (3)	C6—C11	1.404 (2)
N3—H2N3	0.92 (3)	C7—C8	1.371 (3)
C1—C2	1.426 (3)	C7—H7	0.95 (3)
C2—C3	1.382 (3)	C8—C9	1.398 (2)
C3—C4	1.397 (4)	C8—H8	0.95 (3)
C3—H3	1.06 (3)	C9—C10	1.381 (2)
C4—C5	1.342 (4)	C10—C11	1.400 (2)
C4—H4	0.91 (4)	C10—H10	0.89 (2)
C5—H5	0.99 (4)	C11—C12	1.473 (2)
S1—O4	1.4484 (14)	O1W—H1W1	0.90 (3)
S1—O2	1.4542 (14)	O1W—H2W1	0.98 (5)
S1—O3	1.4631 (14)		

C1—N1—C5	124.4 (2)	O4—S1—C9	107.04 (8)
C1—N1—H1N1	118 (2)	O2—S1—C9	106.31 (8)
C5—N1—H1N1	117 (2)	O3—S1—C9	106.41 (8)
C1—N2—H1N2	115.9 (19)	C6—O1—H1O1	108.2 (16)
C1—N2—H2N2	118.6 (18)	C12—O5—H1O5	105 (2)

H1N2—N2—H2N2	120 (3)	O1—C6—C7	117.46 (16)
C2—N3—H1N3	124.8 (18)	O1—C6—C11	122.76 (16)
C2—N3—H2N3	120.1 (18)	C7—C6—C11	119.78 (15)
H1N3—N3—H2N3	113 (3)	C8—C7—C6	120.59 (15)
N1—C1—N2	119.15 (19)	C8—C7—H7	114.7 (16)
N1—C1—C2	118.33 (18)	C6—C7—H7	124.6 (16)
N2—C1—C2	122.50 (18)	C7—C8—C9	119.90 (15)
N3—C2—C3	123.45 (19)	C7—C8—H8	119.0 (17)
N3—C2—C1	119.73 (18)	C9—C8—H8	121.1 (17)
C3—C2—C1	116.80 (19)	C10—C9—C8	120.37 (15)
C2—C3—C4	121.9 (2)	C10—C9—S1	120.87 (12)
C2—C3—H3	116.2 (16)	C8—C9—S1	118.76 (12)
C4—C3—H3	121.7 (16)	C9—C10—C11	120.19 (14)
C5—C4—C3	119.5 (2)	C9—C10—H10	121.7 (15)
C5—C4—H4	120 (2)	C11—C10—H10	118.0 (15)
C3—C4—H4	120 (2)	C10—C11—C6	119.14 (14)
C4—C5—N1	118.9 (2)	C10—C11—C12	120.99 (15)
C4—C5—H5	127.2 (19)	C6—C11—C12	119.87 (14)
N1—C5—H5	113.4 (19)	O6—C12—O5	122.81 (16)
O4—S1—O2	112.20 (9)	O6—C12—C11	123.21 (16)
O4—S1—O3	112.80 (9)	O5—C12—C11	113.97 (15)
O2—S1—O3	111.58 (9)	H1W1—O1W—H2W1	124 (4)

C5—N1—C1—N2	−178.76 (19)	O2—S1—C9—C10	129.29 (13)
C5—N1—C1—C2	2.2 (3)	O3—S1—C9—C10	−111.65 (13)
N1—C1—C2—N3	175.05 (18)	O4—S1—C9—C8	−170.06 (13)
N2—C1—C2—N3	−3.9 (3)	O2—S1—C9—C8	−49.97 (14)
N1—C1—C2—C3	−3.3 (2)	O3—S1—C9—C8	69.09 (14)
N2—C1—C2—C3	177.74 (19)	C8—C9—C10—C11	0.1 (2)
N3—C2—C3—C4	−175.7 (2)	S1—C9—C10—C11	−179.10 (11)
C1—C2—C3—C4	2.5 (3)	C9—C10—C11—C6	1.7 (2)
C2—C3—C4—C5	−0.6 (4)	C9—C10—C11—C12	−179.31 (14)
C3—C4—C5—N1	−0.7 (4)	O1—C6—C11—C10	178.04 (16)
C1—N1—C5—C4	−0.2 (3)	C7—C6—C11—C10	−2.2 (2)
O1—C6—C7—C8	−179.37 (17)	O1—C6—C11—C12	−1.0 (2)
C11—C6—C7—C8	0.8 (3)	C7—C6—C11—C12	178.81 (15)
C6—C7—C8—C9	1.0 (3)	C10—C11—C12—O6	−174.36 (18)
C7—C8—C9—C10	−1.5 (2)	C6—C11—C12—O6	4.6 (3)
C7—C8—C9—S1	177.74 (14)	C10—C11—C12—O5	5.4 (2)
O4—S1—C9—C10	9.19 (15)	C6—C11—C12—O5	−175.63 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O1*W*^{i}	0.91 (3)	1.95 (3)	2.806 (3)	158 (3)
N2—H1*N*2···O1^{i}	0.90 (3)	2.48 (3)	3.222 (2)	140 (2)
N2—H1*N*2···O1*W*^{i}	0.90 (3)	2.28 (3)	3.060 (3)	145 (2)
N2—H2*N*2···O2^{ii}	0.86 (3)	2.10 (3)	2.963 (2)	177 (3)

N3—H1*N*3···O2^{ii}	0.89 (3)	2.10 (3)	2.970 (3)	168 (3)
N3—H2*N*3···O4^{iii}	0.92 (3)	2.08 (3)	2.980 (3)	167 (3)
O1—H1*O*1···O6	1.03 (3)	1.75 (3)	2.625 (2)	141 (2)
O5—H1*O*5···O3^{iv}	0.84 (3)	1.87 (3)	2.655 (2)	155 (3)
O1*W*—H1*W*1···O3^{v}	0.89 (3)	1.94 (3)	2.757 (3)	151 (2)
O1*W*—H2*W*1···O4^{iii}	0.98 (6)	1.89 (6)	2.838 (3)	162 (4)
C7—H7···O3^{vi}	0.95 (3)	2.56 (3)	3.477 (2)	163 (2)

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