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2-Amino-1-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-3-ium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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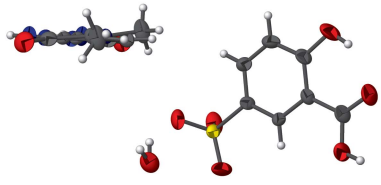
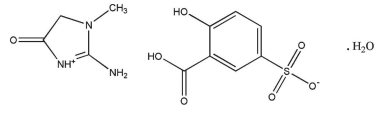
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title molecular salt, $C_4H_7N_3O^+\cdot C_7H_5O_6S^-\cdot H_2O$, contains a 5-sulfosalicylate anion, a creatininium cation and a water molecule of crystallization. The cation is protonated at the imidazole N atom and the anion is deprotonated at the sulfonic acid group. The creatininium is disordered over two sets of sites with refined site occupancies of 0.771 (3) and 0.229 (3). The benzene ring is approximately orthogonal to the disordered five-membered rings [dihedral angles of 89.7 (2) and 88.3 (8)° for the major and minor occupancy components, respectively]. In the crystal, the ions are connected through pairs of N—H···O hydrogen bonds, generating an $R_2^2(8)$ ring-motif. An intraionic O—H···O hydrogen bond generates an $S(6)$ graph-set motif. Weak C—H···O contacts link the ions and water molecule into a two-dimensional network parallel to (001). The structure was refined as a two-component twin.

3D view



Chemical scheme



Structure description

Creatine is extracted from several kinds of muscle and it is endogenously synthesized by the liver and pancreas in humans (Greenhaff *et al.*, 1993; Walker, 1979). We report herein the synthesis and the crystal structure of the title molecular salt (Fig. 1). Its geometric parameters agree well with those of reported similar structures (Thayanithi *et al.*, 2016; Jahubar Ali *et al.*, 2011).

The title compound contains a disordered creatininium cation,, with site occupancies of 0.771 (3) for the major component (C2*A*/N1*A*/C5*A*/N4*A*/C3*A*/O6*A*) and 0.229 (3) for

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···O3	0.82 (1)	2.13 (3)	2.799 (4)	139 (4)
O6—H6A···O7	0.82	1.90	2.624 (3)	146
N1A—H1A···O3^{i}	0.86	2.00	2.844 (5)	168
O2—H2A···O5^{ii}	0.82 (1)	1.99 (2)	2.780 (4)	161 (5)
N8A—H8AA···O6A^{ii}	0.86	2.07	2.917 (5)	168
N8A—H8AB···O5^{i}	0.86	1.94	2.788 (4)	170
O8—H8···O2^{iii}	0.82	1.85	2.616 (3)	155
C6A—H6AB···O4^{iv}	0.96	2.44	3.194 (7)	135

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

minor component (C2B/N1B/C5B/N4B/C3B/O6B), a 5-sulfosalicylate anion and a water molecule in the asymmetric unit. The cation is protonated at the imidizole N atom and the anion is deprotonated at the sulfonic acid group. The benzene ring (C1–C6) is orthogonal to the major [dihedral angle of 89.7 (2)°] and minor [dihedral angle of 88.3 (8)°] components of the five-membered rings. In the asymmetric unit, an intramolecular O—H···O hydrogen bond generates an S(6) graph-set motif (Fig. 2).

In the crystal, an N—H···O hydrogen bond (Table 1) links the anions and cations, generating an $R_2^2(8)$ ring-motif (Fig. 2).

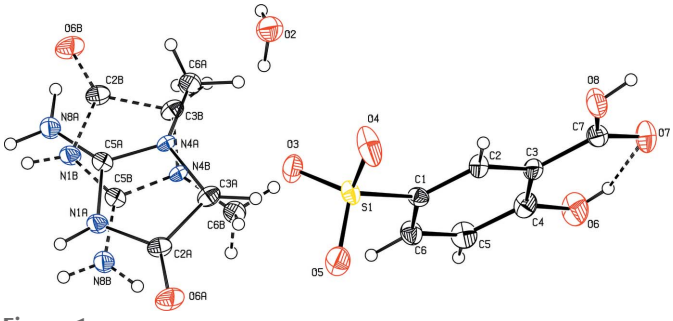


Figure 1
The molecular structure of the title molecular salt, with atom labelling and 30% probability displacement ellipsoids. The minor component in the cation is shown with dashed bonds. The intramolecular hydrogen bond in the anion is shown with a dashed line.

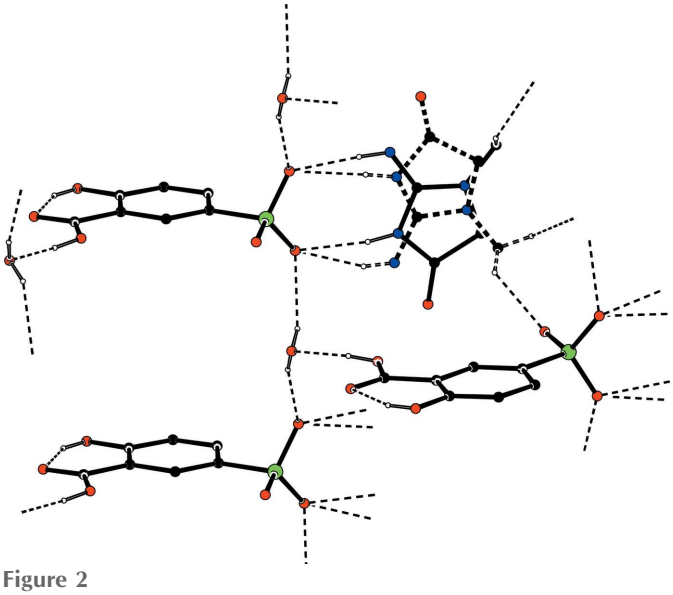


Figure 2
The partial packing of the title molecular salt, showing ring-set motifs. Hydrogen bonds are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_7N_3O^+·C_7H_5O_6S^-·H_2O$
M_r	348.31
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	7.2459 (2), 15.5638 (4), 13.0774 (3)
β (°)	90.100 (1)
V (Å^3)	1474.79 (7)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.42
Crystal size (mm)	0.15 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.587, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22225, 2905, 2798
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.620
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.129, 1.09
No. of reflections	2905
No. of parameters	245
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.31

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXT2016* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2009).

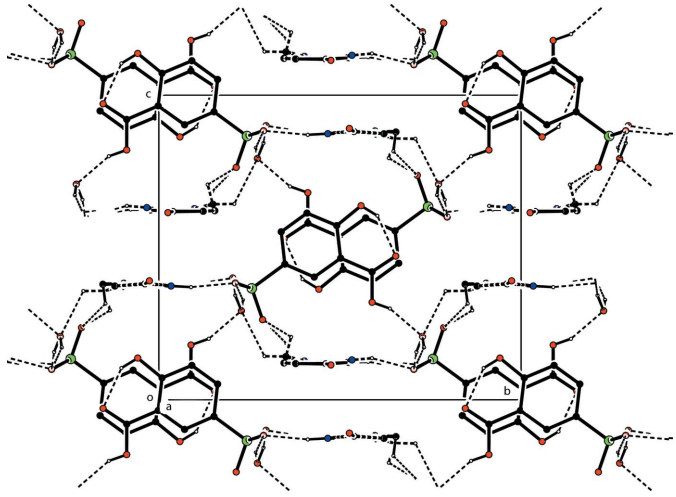


Figure 3
The crystal packing of the title molecular salt viewed along the a axis. The hydrogen bonds are shown as dashed lines. H atoms not involving in hydrogen bonds have been omitted for clarity.

The water molecule links adjacent anions through O—H···O hydrogen bonds (Table 1 and Fig. 3). Weak C—H···O contacts (Fig. 3 and Table 1) link the components into a two-dimensional network parallel to (001).

Synthesis and crystallization

The title compound was synthesized from the raw materials creatinine and 5-sulfosalicylic acid which were taken in a stoichiometric ratio and dissolved in water at ambient temperature. The solution was stirred for continuously six h to obtain a transparent homogeneous solution. The solution was filtered using Whatmann filter paper and the beaker containing the solution was covered with a perforated polythene cover. The saturated homogeneous solution was allowed to evaporate, yielding good quality crystals suitable for X-ray diffraction after three weeks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as two-component twin with twin law $\overline{1}\,0\,0\,0\,\overline{1}\,0\,0\,0\,1$. The creatinium cation is disordered over two orientations with site occupancies of 0.771 (3) and 0.229 (3). The EADP restraint in *SHELXL* (Sheldrick, 2015) was applied for the disordered atoms.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171595 [https://doi.org/10.1107/S2414314617015954]

2-Amino-1-methyl-4-oxo-4,5-dihydro-1*H*-imidazol-3-ium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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Crystal data

$C_4H_7N_3O^+·C_7H_5O_6S^-·H_2O$
M_r = 348.31
Monoclinic, $P2_1/c$
a = 7.2459 (2) Å
b = 15.5638 (4) Å
c = 13.0774 (3) Å
β = 90.100 (1)°
V = 1474.79 (7) Å^3
Z = 4
$F(000)$ = 724
D_x = 1.569 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9845 reflections
θ = 2.2–36.3°
μ = 2.42 mm^{-1}
T = 295 K
Block, colourless
0.15 × 0.15 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.587, T_{max} = 0.754
22225 measured reflections
2905 independent reflections
2798 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 72.9°, θ_{min} = 2.8°
h = −7→8
k = −19→19
l = −15→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.129
S = 1.09
2905 reflections
245 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 1.5916P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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.

Refinement. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.76216 (13)	0.74331 (4)	0.63421 (5)	0.0308 (2)	
O2	1.2464 (5)	0.77212 (16)	0.70783 (19)	0.0483 (6)	
O3	0.9162 (4)	0.79601 (15)	0.6001 (3)	0.0434 (7)	
O4	0.7878 (6)	0.71354 (15)	0.73693 (17)	0.0672 (11)	
O5	0.5909 (4)	0.78905 (16)	0.6167 (3)	0.0525 (8)	
O6	0.7490 (6)	0.44174 (15)	0.36304 (17)	0.0575 (7)	
H6A	0.750112	0.396763	0.395694	0.086*	
O7	0.7467 (5)	0.34602 (13)	0.52820 (18)	0.0512 (6)	
O8	0.7550 (6)	0.41124 (13)	0.67992 (17)	0.0506 (6)	
H8	0.772633	0.362118	0.700399	0.076*	
C1	0.7584 (5)	0.65219 (16)	0.55462 (19)	0.0269 (5)	
C2	0.7543 (5)	0.57105 (16)	0.59708 (19)	0.0288 (5)	
H2	0.754383	0.564915	0.667819	0.035*	
C3	0.7500 (5)	0.49812 (16)	0.5351 (2)	0.0303 (6)	
C4	0.7492 (7)	0.50885 (19)	0.4280 (2)	0.0369 (6)	
C5	0.7545 (6)	0.5911 (2)	0.3871 (2)	0.0407 (7)	
H5	0.757849	0.597882	0.316487	0.049*	
C6	0.7550 (6)	0.66220 (18)	0.4484 (2)	0.0357 (6)	
H6	0.752994	0.716846	0.419590	0.043*	
C7	0.7485 (7)	0.41139 (18)	0.5798 (2)	0.0363 (6)	
N1A	1.1347 (5)	1.0238 (3)	0.3774 (3)	0.0284 (7)	0.771 (3)
H1A	1.111783	1.077990	0.375202	0.034*	0.771 (3)
C2A	1.0054 (5)	0.9613 (3)	0.3817 (4)	0.0302 (7)	0.771 (3)
C3A	1.1079 (7)	0.8776 (3)	0.3811 (4)	0.0314 (8)	0.771 (3)
H3A	1.059443	0.822297	0.379979	0.038*	0.771 (3)
N4A	1.3000 (7)	0.9033 (2)	0.3826 (3)	0.0235 (7)	0.771 (3)
C5A	1.3095 (7)	0.9879 (3)	0.3770 (4)	0.0257 (8)	0.771 (3)
O6A	0.8414 (4)	0.9749 (2)	0.3856 (3)	0.0454 (7)	0.771 (3)
C6A	1.4533 (7)	0.8455 (3)	0.3792 (6)	0.0456 (14)	0.771 (3)
H6AA	1.409585	0.787429	0.384815	0.068*	0.771 (3)
H6AB	1.517571	0.852489	0.315673	0.068*	0.771 (3)
H6AC	1.535550	0.857697	0.434992	0.068*	0.771 (3)
N8A	1.4596 (6)	1.0336 (2)	0.3736 (4)	0.0362 (8)	0.771 (3)
H8AA	1.565543	1.008656	0.374992	0.043*	0.771 (3)
H8AB	1.452993	1.088636	0.369915	0.043*	0.771 (3)
N1B	1.359 (2)	1.0233 (11)	0.3762 (13)	0.0284 (7)	0.229 (3)
H1B	1.378647	1.077807	0.373429	0.034*	0.229 (3)
C2B	1.5042 (18)	0.9616 (9)	0.3808 (14)	0.0302 (7)	0.229 (3)
C3B	1.399 (3)	0.8786 (14)	0.3735 (15)	0.0314 (8)	0.229 (3)
H3B	1.447922	0.823430	0.370289	0.038*	0.229 (3)
N4B	1.210 (3)	0.9018 (9)	0.3724 (13)	0.0235 (7)	0.229 (3)
C5B	1.194 (3)	0.9897 (11)	0.3766 (14)	0.0257 (8)	0.229 (3)
O6B	1.6597 (13)	0.9739 (8)	0.3906 (12)	0.0454 (7)	0.229 (3)
C6B	1.059 (3)	0.8509 (12)	0.358 (2)	0.0456 (14)	0.229 (3)
H6BA	1.095917	0.791695	0.356864	0.068*	0.229 (3)

H6BB	0.972351	0.860018	0.412162	0.068*	0.229 (3)
H6BC	1.001645	0.865178	0.293577	0.068*	0.229 (3)
N8B	1.025 (2)	1.0332 (8)	0.3690 (14)	0.0362 (8)	0.229 (3)
H8BA	1.023308	1.088293	0.363335	0.043*	0.229 (3)
H8BB	0.923017	1.004941	0.369984	0.043*	0.229 (3)
H2A	1.340 (4)	0.768 (3)	0.672 (3)	0.054*	
H2B	1.191 (5)	0.789 (3)	0.657 (2)	0.054*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0428 (4)	0.0216 (3)	0.0280 (3)	0.0009 (4)	0.0022 (5)	−0.0013 (2)
O2	0.0439 (15)	0.0468 (12)	0.0543 (14)	0.0027 (15)	−0.0050 (17)	−0.0055 (11)
O3	0.0402 (15)	0.0318 (12)	0.0583 (18)	−0.0089 (10)	0.0060 (12)	−0.0053 (12)
O4	0.142 (3)	0.0337 (12)	0.0260 (11)	−0.0063 (18)	−0.0006 (18)	−0.0024 (9)
O5	0.0366 (14)	0.0385 (13)	0.082 (2)	0.0052 (10)	0.0110 (16)	−0.0179 (16)
O6	0.090 (2)	0.0438 (12)	0.0386 (12)	−0.0018 (18)	−0.007 (2)	−0.0200 (9)
O7	0.0671 (17)	0.0275 (10)	0.0591 (13)	−0.0055 (14)	0.0019 (18)	−0.0112 (9)
O8	0.0783 (19)	0.0285 (10)	0.0449 (12)	−0.0075 (17)	−0.013 (2)	0.0040 (9)
C1	0.0286 (14)	0.0273 (12)	0.0247 (11)	0.0052 (15)	−0.0008 (15)	−0.0021 (9)
C2	0.0339 (15)	0.0275 (12)	0.0248 (11)	−0.0037 (15)	0.0047 (16)	−0.0015 (9)
C3	0.0307 (15)	0.0262 (12)	0.0341 (13)	−0.0005 (15)	−0.0032 (17)	−0.0051 (10)
C4	0.0410 (17)	0.0368 (14)	0.0329 (13)	−0.0015 (18)	0.0039 (18)	−0.0137 (11)
C5	0.0520 (19)	0.0461 (16)	0.0239 (12)	−0.0007 (19)	0.002 (2)	−0.0032 (11)
C6	0.0460 (18)	0.0325 (14)	0.0285 (12)	−0.0022 (18)	−0.0018 (18)	0.0041 (10)
C7	0.0371 (16)	0.0292 (13)	0.0424 (14)	0.003 (2)	−0.0048 (19)	−0.0046 (11)
N1A	0.021 (2)	0.0292 (17)	0.0350 (17)	0.0047 (14)	0.0027 (18)	0.0010 (14)
C2A	0.0217 (17)	0.0411 (19)	0.0278 (16)	0.0029 (16)	0.0037 (18)	−0.0009 (14)
C3A	0.022 (2)	0.039 (2)	0.033 (2)	−0.0025 (19)	0.001 (2)	−0.0029 (17)
N4A	0.015 (2)	0.0257 (12)	0.0300 (16)	−0.0022 (17)	−0.0043 (18)	−0.0005 (11)
C5A	0.026 (2)	0.0278 (18)	0.0236 (15)	0.0034 (18)	0.003 (2)	0.0022 (14)
O6A	0.0203 (14)	0.0618 (18)	0.0543 (17)	0.0007 (14)	0.0050 (16)	0.0023 (14)
C6A	0.029 (2)	0.029 (2)	0.079 (4)	0.0078 (19)	−0.007 (3)	−0.008 (2)
N8A	0.0251 (19)	0.0283 (15)	0.055 (2)	0.0015 (14)	0.001 (2)	0.0031 (15)
N1B	0.021 (2)	0.0292 (17)	0.0350 (17)	0.0047 (14)	0.0027 (18)	0.0010 (14)
C2B	0.0217 (17)	0.0411 (19)	0.0278 (16)	0.0029 (16)	0.0037 (18)	−0.0009 (14)
C3B	0.022 (2)	0.039 (2)	0.033 (2)	−0.0025 (19)	0.001 (2)	−0.0029 (17)
N4B	0.015 (2)	0.0257 (12)	0.0300 (16)	−0.0022 (17)	−0.0043 (18)	−0.0005 (11)
C5B	0.026 (2)	0.0278 (18)	0.0236 (15)	0.0034 (18)	0.003 (2)	0.0022 (14)
O6B	0.0203 (14)	0.0618 (18)	0.0543 (17)	0.0007 (14)	0.0050 (16)	0.0023 (14)
C6B	0.029 (2)	0.029 (2)	0.079 (4)	0.0078 (19)	−0.007 (3)	−0.008 (2)
N8B	0.0251 (19)	0.0283 (15)	0.055 (2)	0.0015 (14)	0.001 (2)	0.0031 (15)

Geometric parameters (Å, º)

S1—O4	1.433 (2)	C3A—N4A	1.448 (6)
S1—O5	1.448 (3)	C3A—H3A	0.9300
S1—O3	1.456 (3)	N4A—C5A	1.321 (6)

S1—C1	1.759 (3)	N4A—C6A	1.430 (6)
O2—H2A	0.824 (10)	C5A—N8A	1.300 (7)
O2—H2B	0.819 (10)	C6A—H6AA	0.9600
O6—C4	1.347 (3)	C6A—H6AB	0.9600
O6—H6A	0.8200	C6A—H6AC	0.9600
O7—C7	1.221 (4)	N8A—H8AA	0.8600
O8—C7	1.310 (4)	N8A—H8AB	0.8600
O8—H8	0.8200	N1B—C5B	1.31 (3)
C1—C2	1.380 (3)	N1B—C2B	1.42 (2)
C1—C6	1.399 (3)	N1B—H1B	0.8600
C2—C3	1.395 (3)	C2B—O6B	1.150 (17)
C2—H2	0.9300	C2B—C3B	1.50 (2)
C3—C4	1.411 (4)	C3B—N4B	1.42 (2)
C3—C7	1.471 (4)	C3B—H3B	0.9300
C4—C5	1.387 (4)	N4B—C6B	1.36 (2)
C5—C6	1.367 (4)	N4B—C5B	1.37 (2)
C5—H5	0.9300	C5B—N8B	1.40 (2)
C6—H6	0.9300	C6B—H6BA	0.9600
N1A—C2A	1.351 (6)	C6B—H6BB	0.9600
N1A—C5A	1.384 (6)	C6B—H6BC	0.9600
N1A—H1A	0.8600	N8B—H8BA	0.8600
C2A—O6A	1.208 (5)	N8B—H8BB	0.8600
C2A—C3A	1.499 (6)		

O4—S1—O5	114.6 (2)	C5A—N4A—C6A	125.8 (5)
O4—S1—O3	111.8 (2)	C5A—N4A—C3A	108.9 (5)
O5—S1—O3	109.37 (15)	C6A—N4A—C3A	125.0 (4)
O4—S1—C1	107.21 (13)	N8A—C5A—N4A	126.2 (5)
O5—S1—C1	106.87 (18)	N8A—C5A—N1A	123.0 (4)
O3—S1—C1	106.50 (16)	N4A—C5A—N1A	110.8 (5)
H2A—O2—H2B	88 (4)	N4A—C6A—H6AA	109.5
C4—O6—H6A	109.5	N4A—C6A—H6AB	109.5
C7—O8—H8	109.5	H6AA—C6A—H6AB	109.5
C2—C1—C6	120.1 (2)	N4A—C6A—H6AC	109.5
C2—C1—S1	120.00 (19)	H6AA—C6A—H6AC	109.5
C6—C1—S1	119.9 (2)	H6AB—C6A—H6AC	109.5
C1—C2—C3	120.8 (2)	C5A—N8A—H8AA	120.0
C1—C2—H2	119.6	C5A—N8A—H8AB	120.0
C3—C2—H2	119.6	H8AA—N8A—H8AB	120.0
C2—C3—C4	118.7 (2)	C5B—N1B—C2B	113.9 (17)
C2—C3—C7	121.1 (2)	C5B—N1B—H1B	123.0
C4—C3—C7	120.2 (2)	C2B—N1B—H1B	123.0
O6—C4—C5	118.1 (3)	O6B—C2B—N1B	128.0 (16)
O6—C4—C3	122.3 (3)	O6B—C2B—C3B	130.3 (17)
C5—C4—C3	119.5 (2)	N1B—C2B—C3B	101.7 (15)
C6—C5—C4	121.4 (3)	N4B—C3B—C2B	105.8 (19)
C6—C5—H5	119.3	N4B—C3B—H3B	127.1
C4—C5—H5	119.3	C2B—C3B—H3B	127.1

C5—C6—C1	119.5 (3)	C6B—N4B—C5B	121.0 (18)
C5—C6—H6	120.3	C6B—N4B—C3B	129.0 (15)
C1—C6—H6	120.3	C5B—N4B—C3B	109.6 (19)
O7—C7—O8	123.4 (3)	N1B—C5B—N4B	109 (2)
O7—C7—C3	123.1 (3)	N1B—C5B—N8B	127.2 (15)
O8—C7—C3	113.5 (2)	N4B—C5B—N8B	123.6 (17)
C2A—N1A—C5A	110.1 (5)	N4B—C6B—H6BA	109.5
C2A—N1A—H1A	124.9	N4B—C6B—H6BB	109.5
C5A—N1A—H1A	124.9	H6BA—C6B—H6BB	109.5
O6A—C2A—N1A	123.9 (4)	N4B—C6B—H6BC	109.5
O6A—C2A—C3A	129.7 (4)	H6BA—C6B—H6BC	109.5
N1A—C2A—C3A	106.4 (4)	H6BB—C6B—H6BC	109.5
N4A—C3A—C2A	103.7 (4)	C5B—N8B—H8BA	120.0
N4A—C3A—H3A	128.2	C5B—N8B—H8BB	120.0
C2A—C3A—H3A	128.2	H8BA—N8B—H8BB	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···O3	0.82 (1)	2.13 (3)	2.799 (4)	139 (4)
O6—H6*A*···O7	0.82	1.90	2.624 (3)	146
N1*A*—H1*A*···O3^{i}	0.86	2.00	2.844 (5)	168
O2—H2*A*···O5^{ii}	0.82 (1)	1.99 (2)	2.780 (4)	161 (5)
N8*A*—H8*AA*···O6*A*^{ii}	0.86	2.07	2.917 (5)	168
N8*A*—H8*AB*···O5^{i}	0.86	1.94	2.788 (4)	170
O8—H8···O2^{iii}	0.82	1.85	2.616 (3)	155
C6*A*—H6*AB*···O4^{iv}	0.96	2.44	3.194 (7)	135

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) −*x*+2, *y*−1/2, −*z*+3/2; (iv) *x*+1, −*y*+3/2, *z*−1/2.