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Bis(2-amino-3-carboxypyrazin-1-ium) sulfate dihydrate

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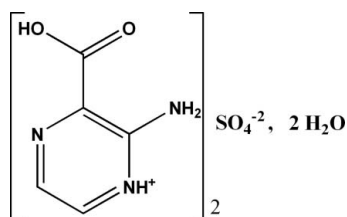
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.035; wR factor = 0.096; data-to-parameter ratio = 14.9.

The crystal structure of the title compound, $2\text{C}_5\text{H}_6\text{N}_3\text{O}_2^{+}\cdot\text{SO}_4^{2-}\cdot 2\text{H}_2\text{O}$, displays a variety of $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds in which all potential donors and acceptors are involved. In the crystal, cations and anions are interconnected, forming $R_3^3(10)$ and $R_2^2(8)$ ring motifs whereas the anions and water molecules form $R_3^3(10)$ rings, which develop in chains running along [100]. The resulting three-dimensional network exhibits undulating sheets parallel to (011), marked by the presence of $R_6^6(26)$ rings in which six cations are involved.

Related literature

For related compounds, see: Berrah *et al.* (2005*a,b*, 2011); Bouacida *et al.* (2005, 2009); Dobson & Gerkin (1996). For hydrogen-bond motifs, see: Bernstein *et al.* (1995); Etter *et al.* (1990). For similar intermolecular interactions, see: Dorn *et al.* (2005), Janiak (2000); Desiraju (2003).



Experimental

Crystal data

$2\text{C}_5\text{H}_6\text{N}_3\text{O}_2^{+}\cdot\text{SO}_4^{2-}\cdot 2\text{H}_2\text{O}$
 $M_r = 412.36$
 Monoclinic, $P2_1/a$
 $a = 7.7214$ (4) Å
 $b = 20.7043$ (14) Å
 $c = 10.6398$ (7) Å
 $\beta = 109.299$ (2)°

$V = 1605.36$ (17) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.27$ mm⁻¹
 $T = 150$ K
 $0.55 \times 0.36 \times 0.15$ mm

Data collection

Bruker APEXII diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.708$, $T_{\max} = 0.960$

13466 measured reflections
 3675 independent reflections
 3146 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.096$
 $S = 1.03$
 3675 reflections

246 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.47$ e Å⁻³
 $\Delta\rho_{\min} = -0.48$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1A}-\text{H1A1}\cdots\text{O4}$	0.88	1.92	2.7970 (18)	175
$\text{N1A}-\text{H1A2}\cdots\text{O6A}$	0.88	2.04	2.6741 (18)	128
$\text{N1A}-\text{H1A2}\cdots\text{O6B}^i$	0.88	2.30	3.0158 (18)	138
$\text{N2A}-\text{H2A}\cdots\text{O1}$	0.88	1.83	2.6915 (18)	167
$\text{N1B}-\text{H1B1}\cdots\text{O2}$	0.88	2.34	3.0827 (18)	142
$\text{N1B}-\text{H1B2}\cdots\text{O6B}$	0.88	2.08	2.7144 (19)	129
$\text{N1B}-\text{H1B2}\cdots\text{O6A}^{ii}$	0.88	2.10	2.8237 (18)	139
$\text{N2B}-\text{H2B}\cdots\text{O1W}$	0.88	1.81	2.6705 (18)	167
$\text{O5B}-\text{H5B}\cdots\text{O2W}$	0.84	1.67	2.5046 (17)	174
$\text{O5A}-\text{H5A}\cdots\text{O2}^i$	0.84	1.78	2.6192 (16)	175
$\text{O1W}-\text{H1W}\cdots\text{O3}$	0.85	1.95	2.7934 (19)	175
$\text{O1W}-\text{H2W}\cdots\text{O2}^{iii}$	0.85	2.06	2.8996 (18)	167
$\text{O1W}-\text{H2W}\cdots\text{O4}^{iii}$	0.85	2.65	3.2856 (17)	133
$\text{O2W}-\text{H3W}\cdots\text{O4}^{ii}$	0.85	1.88	2.7351 (17)	177
$\text{O2W}-\text{H4W}\cdots\text{O3}^{iv}$	0.86	1.91	2.7633 (17)	171

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

Data collection: APEX2 (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SIR2002 (Burla *et al.*, 2003); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and DIAMOND (Brandenburg & Berndt, 2001); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2656).

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supporting information

Acta Cryst. (2011). E67, o677–o678 [doi:10.1107/S1600536811005824]

Bis(2-amino-3-carboxypyrazin-1-ium) sulfate dihydrate**Fadila Berrah, Amira Ouakkaf, Sofiane Bouacida and Thierry Roisnel****S1. Comment**

Hydrogen bonds are object of several studies, that aim at elucidate their influence on crystal construction and compounds properties (Desiraju, 2003). N-heterocyclic compounds such as pyrazine and its derivatives may be interesting units to built new edifices involving original hydrogen-bonding scheme since they include a variety of potential hydrogen donors and acceptors. In this perspective and as a part of our search for new hybrid compounds based on protonated amines and imines (Berrah *et al.* 2011, 2005*a,b*; Bouacida *et al.* 2005,2009), we present here the structure of Bis (2-Amino-3-carboxypyrazin-1-ium) sulfate dihydrate.

The asymmetric units of (I) includes two symmetry- independent cations and water molecules, and one sulfate anion. Cations and anions are interconnected to form $R_3^3(10)$ and $R_2^2(8)$ ring motifs (Etter *et al.*, 1990; Bernstein *et al.*, 1995) (Fig 1). Bond lengths and angles are as expected (Berrah *et al.* 2011; Dobson & Gerkin, 1996).

The three-dimensional structure of (I), results from undulating sheets of cations dimmers parallel to (011) plane(Fig.2 and Fig.3)and sulfate-water chains extending along [100](Fig.3). An interesting hydrogen bonds network, in which all potential donors and acceptors are involved, and especially marked by the presence of $R_6^6(26)$ and $R_2^3(10)$ set-graph motifs (Etter *et al.*, 1990; Bernstein *et al.*, 1995), ensures the coherence of the structure(Fig.2 and Fig.3, table 1). This later is reinforced by the contribution of π - π , S—O \cdots π and C—O \cdots π interactions (Dorn *et al.* 2005; Janiak, 2000) (table 2,3).

S2. Experimental

The title compound was synthesized by reacting 3-amino-pyrazine 2- carboxylic acid with some excess of sulphuric acid in aqueous solution. Slow evaporation leads to well crystallized yellow needles.

S3. Refinement

All non-H atoms were refined with anisotropic atomic displacement parameters. H atoms of water molecule were located in difference Fourier maps and treated as riding on their parent oxygen atoms with O—H = 0.85, H \cdots H = 1.40 and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The remaining H atoms were localized on Fourier maps but introduced in calculated positions and treated as riding on their parent atoms (C, N or O) with C—H = 0.95 Å, O—H = 0.84 Å and N—H = 0.88 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$ and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$.

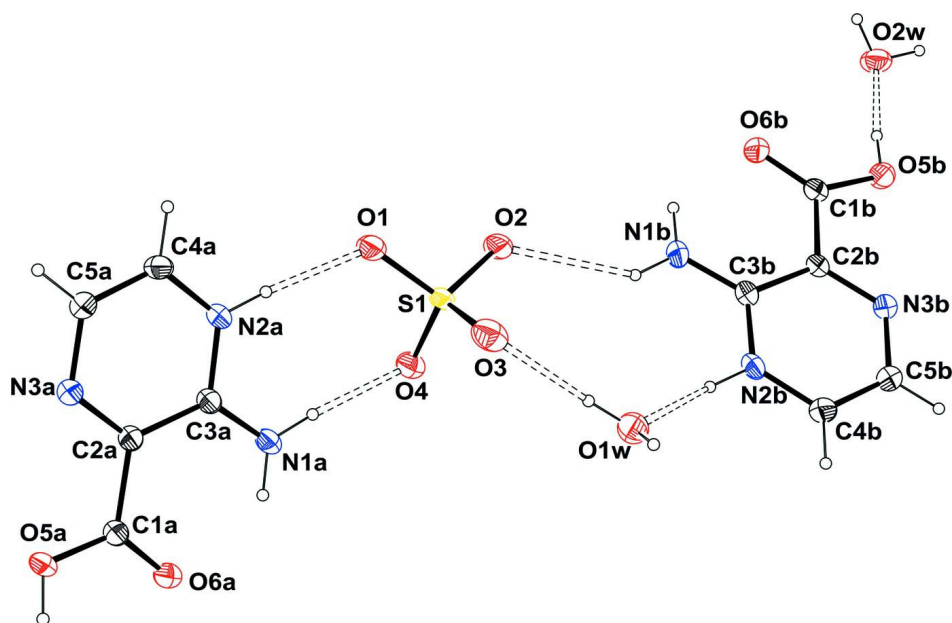


Figure 1

The asymmetric unit of the title compound with the atomic labelling scheme. Displacement are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.

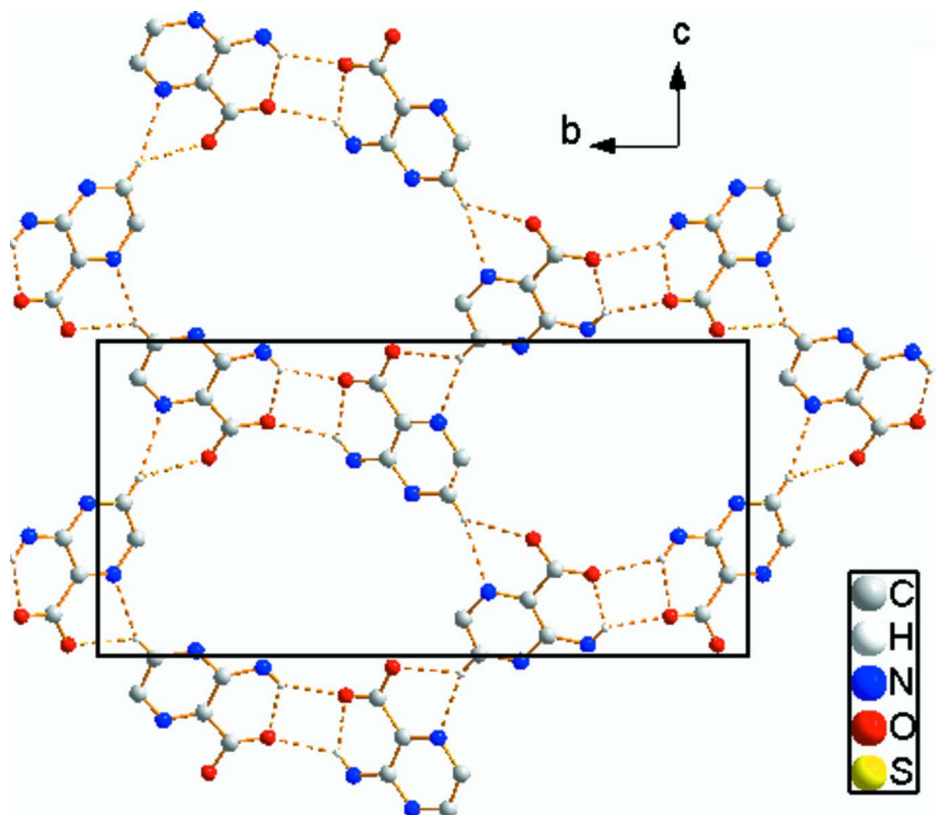
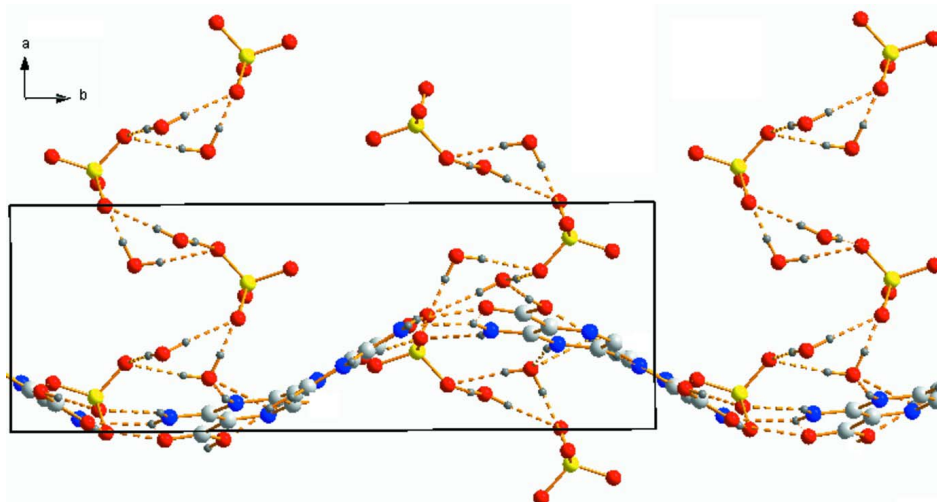


Figure 2

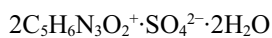
Partial packing view showing undulating sheets parallel to (011) plane and $R_6^6(26)$ rings set motif. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in H-bonds have been omitted for clarity

**Figure 3**

Partial packing view showing sulfate-water chains extending along [100] direction and undulating sheets. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in H-bonds have been omitted for clarity.

Bis(2-amino-3-carboxypyrazin-1-ium) sulfate dihydrate

Crystal data



$M_r = 412.36$

Monoclinic, $P2_1/a$

$a = 7.7214 (4) \text{ \AA}$

$b = 20.7043 (14) \text{ \AA}$

$c = 10.6398 (7) \text{ \AA}$

$\beta = 109.299 (2)^\circ$

$V = 1605.36 (17) \text{ \AA}^3$

$Z = 4$

$F(000) = 856$

$D_x = 1.706 \text{ Mg m}^{-3}$

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

Cell parameters from 5179 reflections

$\theta = 2.8\text{--}27.5^\circ$

$\mu = 0.27 \text{ mm}^{-1}$

$T = 150 \text{ K}$

Prism, yellow

$0.55 \times 0.36 \times 0.15 \text{ mm}$

Data collection

Bruker APEXII

diffractometer

Graphite monochromator

CCD rotation images, thin slices scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2002)

$T_{\min} = 0.708$, $T_{\max} = 0.960$

13466 measured reflections

3675 independent reflections

3146 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.6^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -8 \rightarrow 9$

$k = -26 \rightarrow 26$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.096$

$S = 1.03$

3675 reflections

246 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.7394P]$

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

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

$\Delta\rho_{\max} = 0.47 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.48 \text{ e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O5A	0.17659 (16)	0.04617 (6)	0.03501 (11)	0.0221 (3)
H5A	0.1515	0.0732	-0.0273	0.033*
O6A	0.03846 (18)	0.11842 (6)	0.12557 (11)	0.0258 (3)
N1A	0.0567 (2)	0.10587 (7)	0.37979 (13)	0.0231 (3)
H1A1	0.0399	0.1167	0.4549	0.028*
H1A2	0.0122	0.1303	0.3087	0.028*
N2A	0.21592 (19)	0.01604 (6)	0.48490 (13)	0.0195 (3)
H2A	0.1989	0.0288	0.5588	0.023*
N3A	0.27826 (19)	-0.02410 (6)	0.25952 (13)	0.0194 (3)
C1A	0.1266 (2)	0.06905 (7)	0.13275 (15)	0.0185 (3)
C2A	0.1875 (2)	0.02980 (7)	0.25829 (15)	0.0177 (3)
C3A	0.1485 (2)	0.05305 (7)	0.37379 (15)	0.0183 (3)
C4A	0.3079 (2)	-0.03946 (8)	0.48622 (16)	0.0207 (3)
H4A	0.3518	-0.0644	0.5654	0.025*
C5A	0.3374 (2)	-0.05941 (8)	0.37264 (16)	0.0214 (3)
H5C	0.4006	-0.0988	0.3731	0.026*
O5B	-0.03794 (19)	0.32977 (6)	1.37046 (12)	0.0273 (3)
H5B	-0.0768	0.3055	1.4185	0.041*
O6B	-0.03786 (17)	0.23824 (5)	1.25812 (11)	0.0241 (3)
N1B	0.0619 (2)	0.24559 (7)	1.03668 (14)	0.0238 (3)
H1B1	0.0821	0.2313	0.9649	0.029*
H1B2	0.0315	0.2184	1.0895	0.029*
N2B	0.12393 (19)	0.34886 (7)	0.98346 (13)	0.0205 (3)
H2B	0.1422	0.3332	0.912	0.025*
N3B	0.07073 (19)	0.39911 (6)	1.20349 (13)	0.0206 (3)
C1B	-0.0126 (2)	0.29617 (8)	1.27448 (15)	0.0196 (3)
C2B	0.0482 (2)	0.33663 (7)	1.17934 (14)	0.0178 (3)
C3B	0.0773 (2)	0.30786 (8)	1.06522 (15)	0.0187 (3)
C4B	0.1438 (2)	0.41269 (8)	1.00633 (16)	0.0227 (3)
H4B	0.1752	0.4403	0.9458	0.027*
C5B	0.1180 (2)	0.43737 (8)	1.11810 (16)	0.0233 (3)
H5D	0.1338	0.4824	1.1357	0.028*
S1	0.15317 (5)	0.131125 (18)	0.73117 (4)	0.01813 (11)
O1	0.2146 (2)	0.06509 (6)	0.71883 (12)	0.0337 (3)
O2	0.09536 (18)	0.13565 (6)	0.85065 (12)	0.0262 (3)

O3	0.30149 (17)	0.17773 (7)	0.74478 (12)	0.0306 (3)
O4	-0.00482 (16)	0.14708 (6)	0.61180 (11)	0.0236 (3)
O1W	0.23309 (17)	0.30737 (6)	0.78406 (12)	0.0262 (3)
H1W	0.2465	0.2676	0.7697	0.039*
H2W	0.3352	0.3253	0.7903	0.039*
O2W	-0.15818 (19)	0.26453 (6)	1.52193 (12)	0.0296 (3)
H3W	-0.1068	0.2285	1.5511	0.044*
H4W	-0.1653	0.2863	1.5886	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O5A	0.0332 (7)	0.0213 (6)	0.0140 (5)	0.0044 (5)	0.0109 (5)	0.0030 (4)
O6A	0.0400 (7)	0.0206 (6)	0.0184 (6)	0.0076 (5)	0.0115 (5)	0.0036 (4)
N1A	0.0340 (8)	0.0227 (7)	0.0140 (6)	0.0063 (6)	0.0100 (6)	0.0012 (5)
N2A	0.0269 (7)	0.0193 (6)	0.0128 (6)	-0.0002 (5)	0.0072 (5)	0.0001 (5)
N3A	0.0253 (7)	0.0168 (6)	0.0158 (6)	-0.0013 (5)	0.0063 (5)	-0.0003 (5)
C1A	0.0232 (8)	0.0172 (7)	0.0153 (7)	-0.0026 (6)	0.0065 (6)	-0.0007 (6)
C2A	0.0225 (8)	0.0159 (7)	0.0154 (7)	-0.0020 (6)	0.0072 (6)	-0.0008 (6)
C3A	0.0229 (8)	0.0175 (7)	0.0144 (7)	-0.0027 (6)	0.0062 (6)	-0.0007 (6)
C4A	0.0259 (8)	0.0177 (7)	0.0168 (7)	-0.0016 (6)	0.0048 (6)	0.0035 (6)
C5A	0.0279 (9)	0.0163 (7)	0.0186 (7)	0.0011 (6)	0.0056 (6)	0.0000 (6)
O5B	0.0480 (8)	0.0198 (6)	0.0201 (6)	-0.0009 (5)	0.0194 (5)	-0.0004 (5)
O6B	0.0355 (7)	0.0185 (6)	0.0193 (6)	-0.0015 (5)	0.0104 (5)	0.0003 (4)
N1B	0.0372 (8)	0.0188 (7)	0.0167 (6)	-0.0035 (6)	0.0105 (6)	-0.0037 (5)
N2B	0.0267 (7)	0.0221 (7)	0.0128 (6)	-0.0027 (5)	0.0069 (5)	-0.0024 (5)
N3B	0.0267 (7)	0.0172 (6)	0.0167 (6)	0.0005 (5)	0.0056 (5)	-0.0008 (5)
C1B	0.0231 (8)	0.0198 (8)	0.0141 (7)	0.0019 (6)	0.0039 (6)	0.0008 (6)
C2B	0.0216 (8)	0.0173 (7)	0.0127 (7)	0.0005 (6)	0.0033 (6)	0.0001 (5)
C3B	0.0203 (8)	0.0194 (7)	0.0142 (7)	-0.0010 (6)	0.0029 (6)	-0.0014 (6)
C4B	0.0276 (9)	0.0201 (8)	0.0195 (7)	-0.0035 (6)	0.0068 (6)	0.0020 (6)
C5B	0.0324 (9)	0.0177 (7)	0.0193 (7)	-0.0019 (6)	0.0077 (7)	0.0004 (6)
S1	0.0259 (2)	0.01758 (19)	0.01276 (18)	0.00290 (14)	0.00883 (15)	0.00224 (13)
O1	0.0605 (9)	0.0245 (6)	0.0186 (6)	0.0188 (6)	0.0163 (6)	0.0047 (5)
O2	0.0429 (7)	0.0230 (6)	0.0193 (6)	0.0051 (5)	0.0192 (5)	0.0035 (5)
O3	0.0291 (7)	0.0384 (7)	0.0238 (6)	-0.0067 (5)	0.0080 (5)	0.0029 (5)
O4	0.0266 (6)	0.0246 (6)	0.0179 (6)	0.0031 (5)	0.0049 (5)	0.0017 (4)
O1W	0.0294 (6)	0.0273 (6)	0.0252 (6)	-0.0009 (5)	0.0136 (5)	-0.0005 (5)
O2W	0.0460 (8)	0.0244 (6)	0.0229 (6)	0.0086 (5)	0.0174 (6)	0.0061 (5)

Geometric parameters (Å, °)

O5A—C1A	1.3116 (19)	N1B—H1B1	0.88
O5A—H5A	0.84	N1B—H1B2	0.88
O6A—C1A	1.216 (2)	N2B—C4B	1.343 (2)
N1A—C3A	1.316 (2)	N2B—C3B	1.347 (2)
N1A—H1A1	0.88	N2B—H2B	0.88
N1A—H1A2	0.88	N3B—C2B	1.319 (2)

N2A—C4A	1.349 (2)	N3B—C5B	1.344 (2)
N2A—C3A	1.360 (2)	C1B—C2B	1.503 (2)
N2A—H2A	0.88	C2B—C3B	1.435 (2)
N3A—C2A	1.315 (2)	C4B—C5B	1.368 (2)
N3A—C5A	1.352 (2)	C4B—H4B	0.95
C1A—C2A	1.500 (2)	C5B—H5D	0.95
C2A—C3A	1.442 (2)	S1—O1	1.4670 (12)
C4A—C5A	1.365 (2)	S1—O3	1.4677 (13)
C4A—H4A	0.95	S1—O4	1.4786 (12)
C5A—H5C	0.95	S1—O2	1.4831 (12)
O5B—C1B	1.3028 (19)	O1W—H1W	0.8491
O5B—H5B	0.84	O1W—H2W	0.8542
O6B—C1B	1.218 (2)	O2W—H3W	0.8543
N1B—C3B	1.321 (2)	O2W—H4W	0.8582
C1A—O5A—H5A	109.5	C4B—N2B—C3B	122.81 (14)
C3A—N1A—H1A1	120	C4B—N2B—H2B	118.6
C3A—N1A—H1A2	120	C3B—N2B—H2B	118.6
H1A1—N1A—H1A2	120	C2B—N3B—C5B	119.63 (14)
C4A—N2A—C3A	122.57 (14)	O6B—C1B—O5B	125.38 (15)
C4A—N2A—H2A	118.7	O6B—C1B—C2B	121.55 (14)
C3A—N2A—H2A	118.7	O5B—C1B—C2B	113.05 (14)
C2A—N3A—C5A	119.32 (14)	N3B—C2B—C3B	121.62 (14)
O6A—C1A—O5A	123.99 (14)	N3B—C2B—C1B	117.76 (14)
O6A—C1A—C2A	121.03 (14)	C3B—C2B—C1B	120.62 (14)
O5A—C1A—C2A	114.98 (13)	N1B—C3B—N2B	119.31 (15)
N3A—C2A—C3A	122.39 (14)	N1B—C3B—C2B	124.91 (15)
N3A—C2A—C1A	118.54 (14)	N2B—C3B—C2B	115.78 (14)
C3A—C2A—C1A	119.06 (14)	N2B—C4B—C5B	118.98 (15)
N1A—C3A—N2A	118.94 (14)	N2B—C4B—H4B	120.5
N1A—C3A—C2A	125.91 (14)	C5B—C4B—H4B	120.5
N2A—C3A—C2A	115.15 (14)	N3B—C5B—C4B	121.17 (15)
N2A—C4A—C5A	119.33 (14)	N3B—C5B—H5D	119.4
N2A—C4A—H4A	120.3	C4B—C5B—H5D	119.4
C5A—C4A—H4A	120.3	O1—S1—O3	110.91 (9)
N3A—C5A—C4A	121.21 (15)	O1—S1—O4	109.31 (7)
N3A—C5A—H5C	119.4	O3—S1—O4	109.46 (7)
C4A—C5A—H5C	119.4	O1—S1—O2	109.47 (7)
C1B—O5B—H5B	109.5	O3—S1—O2	108.66 (7)
C3B—N1B—H1B1	120	O4—S1—O2	109.00 (7)
C3B—N1B—H1B2	120	H1W—O1W—H2W	105.7
H1B1—N1B—H1B2	120	H3W—O2W—H4W	108
C5A—N3A—C2A—C3A	0.1 (2)	C5B—N3B—C2B—C3B	1.6 (2)
C5A—N3A—C2A—C1A	178.70 (14)	C5B—N3B—C2B—C1B	-177.43 (14)
O6A—C1A—C2A—N3A	178.18 (15)	O6B—C1B—C2B—N3B	179.35 (15)
O5A—C1A—C2A—N3A	-2.2 (2)	O5B—C1B—C2B—N3B	0.9 (2)
O6A—C1A—C2A—C3A	-3.2 (2)	O6B—C1B—C2B—C3B	0.3 (2)

O5A—C1A—C2A—C3A	176.41 (14)	O5B—C1B—C2B—C3B	-178.12 (14)
C4A—N2A—C3A—N1A	178.56 (15)	C4B—N2B—C3B—N1B	-179.42 (15)
C4A—N2A—C3A—C2A	-1.9 (2)	C4B—N2B—C3B—C2B	0.5 (2)
N3A—C2A—C3A—N1A	-179.04 (16)	N3B—C2B—C3B—N1B	178.17 (15)
C1A—C2A—C3A—N1A	2.4 (2)	C1B—C2B—C3B—N1B	-2.9 (2)
N3A—C2A—C3A—N2A	1.5 (2)	N3B—C2B—C3B—N2B	-1.7 (2)
C1A—C2A—C3A—N2A	-177.09 (13)	C1B—C2B—C3B—N2B	177.27 (14)
C3A—N2A—C4A—C5A	0.8 (2)	C3B—N2B—C4B—C5B	0.8 (2)
C2A—N3A—C5A—C4A	-1.4 (2)	C2B—N3B—C5B—C4B	-0.2 (3)
N2A—C4A—C5A—N3A	0.9 (2)	N2B—C4B—C5B—N3B	-1.0 (3)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1A—H1A1 \cdots O4	0.88	1.92	2.7970 (18)	175
N1A—H1A2 \cdots O6A	0.88	2.04	2.6741 (18)	128
N1A—H1A2 \cdots O6B ⁱ	0.88	2.30	3.0158 (18)	138
N2A—H2A \cdots O1	0.88	1.83	2.6915 (18)	167
N1B—H1B1 \cdots O2	0.88	2.34	3.0827 (18)	142
N1B—H1B2 \cdots O6B	0.88	2.08	2.7144 (19)	129
N1B—H1B2 \cdots O6A ⁱⁱ	0.88	2.10	2.8237 (18)	139
N2B—H2B \cdots O1W	0.88	1.81	2.6705 (18)	167
O5B—H5B \cdots O2W	0.84	1.67	2.5046 (17)	174
O5A—H5A \cdots O2 ⁱ	0.84	1.78	2.6192 (16)	175
O1W—H1W \cdots O3	0.85	1.95	2.7934 (19)	175
O1W—H2W \cdots O2 ⁱⁱⁱ	0.85	2.06	2.8996 (18)	167
O1W—H2W \cdots O4 ⁱⁱⁱ	0.85	2.65	3.2856 (17)	133
O2W—H3W \cdots O4 ⁱⁱ	0.85	1.88	2.7351 (17)	177
O2W—H4W \cdots O3 ^{iv}	0.86	1.91	2.7633 (17)	171
C4A—H4A \cdots O5B ^v	0.95	2.58	3.320 (2)	134
C4A—H4A \cdots N3B ^v	0.95	2.45	3.369 (2)	163
C4B—H4B \cdots O5A ^{vi}	0.95	2.45	3.187 (2)	134
C4B—H4B \cdots N3A ^{vi}	0.95	2.44	3.347 (2)	159
C5A—H5C \cdots O1W ^{vii}	0.95	2.55	3.175 (2)	124
C5B—H5D \cdots O1 ^{viii}	0.95	2.35	3.192 (2)	148

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