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4-(Hydrazinecarbonyl)pyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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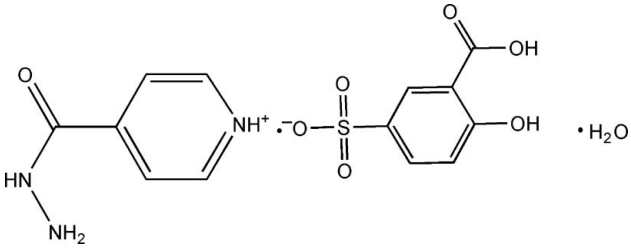
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.130; data-to-parameter ratio = 15.0.

In the crystal structure of the title compound, $C_6H_8N_3O^+\cdot C_7H_5O_6S^-\cdot H_2O$, cations, anions and water molecules are linked by a number of C/N/O—H···O and N—H···N hydrogen bonds into a three-dimensional network.

Related literature

The author has recently determined the crystal structures of two closely related compounds (Xie 2007*a*,*b*).



Experimental

Crystal data

$C_6H_8N_3O^+\cdot C_7H_5O_6S^-\cdot H_2O$
M_r = 373.34
Orthorhombic, *Pbca*
a = 13.7628 (8) Å
b = 13.0656 (8) Å
c = 16.9752 (10) Å
V = 3052.5 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 299 (2) K
0.30 × 0.20 × 0.04 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.927, T_{max} = 0.990
33729 measured reflections
3747 independent reflections
2727 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.130
S = 1.06
3747 reflections
250 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O8	0.93	2.48	3.389 (3)	166
C4—H4···O8^{i}	0.93	2.50	3.321 (3)	148
N2—H2A···O8	0.855 (10)	2.030 (12)	2.865 (3)	165 (2)
N3—H3A···N1^{i}	0.862 (10)	1.923 (11)	2.780 (3)	173 (3)
O8—H8B···O1^{ii}	0.832 (10)	1.990 (11)	2.819 (3)	174 (3)
O3—H3B···O7^{iii}	0.823 (10)	1.769 (11)	2.589 (2)	174 (4)
O4—H4A···O2	0.821 (10)	1.886 (18)	2.629 (3)	150 (3)
O4—H4A···O5^{iv}	0.821 (10)	2.39 (3)	2.921 (2)	123 (3)
C3—H3···O6^{ii}	0.93	2.54	3.262 (3)	135
N1—H1A···O6	0.864 (10)	2.256 (19)	2.984 (3)	142 (2)
N1—H1B···O5^{v}	0.861 (10)	2.545 (17)	3.309 (3)	148 (2)
O8—H8A···O5^{vi}	0.826 (10)	2.093 (11)	2.916 (3)	175 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2389).

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  doi:10.1107/S1600536807023124

supplementary materials

Acta Cryst. (2007). E**63**, o2956 [**doi:10.1107/S1600536807023124**]

4-(Hydrazinecarbonyl)pyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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Comment

As part of our continuing studies on the inter-ion and intra-associative H-bonding interactions of organic superstructures (Xie, 2007*a*, b)), we report herein the crystal structure of (I) formed by isonicid and sulfosalicylic acid.

In (I) (Fig.1), like the earlier reported structure (Xie, 2007*a*), the acid H atom is released from the sulfonic group to pyridine N atom forming the stechiometrical 1:1 organic salt with one water solvent molecule incorporated into the selected asymmetric unit.

In the supramolecular structure, the molecules are linked by a combination of C (or N, O)–H···O and N–H···N hydrogen bonds into a three-dimensional network whose formation is readily analysed in terms of three substructures. In the first of these substructures, by a combination of the first five hydrognen bonds listed in table 1 the 4-(Hydrazinecarbonyl)pyridinium cations and water molecules are linked into a two-dimensional network running parallel to the (101) direction (Fig.2). The second substructure is formed by linking of the sulphonate anions *via* three O–H···O hydrogen bonds, *i.e.* O3–H3B···O7^{iii}, O4–H4A···O2 and O4–H4A···O5^{iv}, [symmetry codes as in Table 1] so forming another two-dimensional framework running parallel to the (101) direction (Fig.3). The third substructure is the combination of the last four hydrogen bonds in Tabel 1 which link the adjacent (101) planes into a three-dimensional network (Fig.4).

There are two aromatic π–π stacking interactions in the structure of (I), which serve to reinforce the adjacent (101) sheets. The phenyl ring in the molecule at (*x*,*y*,*z*) and the pyridine ring in the molecule at (1/2 − *x*,1 − *y*,-1/2 + *z*), which lie in the different (101) sheets, are almost parallel, with a dihedral angle between the two rings of only 3.53 (1)°, an interplanar spacing of 3.243 (1) Å, and ring-centroid separation of 3.615 (1) Å *PLATON* (Spek,2003).

Experimental

All reagents and solvents were used as obtained without further purification. Equivalent molar amounts of isonicid and sulfosalicylic acid were dissolved in 95% methanol (10 ml). The mixture was stirred for ten minutes at ambient temperature and then filtered. The resulting colourless solution was kept in air for two days. colourless crystals of (I) suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of the solution at the bottom of the vessel.

Refinement

H atoms bonded to C atoms were placed in calculated positions with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). All the other H atoms were located from the difference maps with the constraints of N—H = 0.86 (1) Å, U_{iso}(H) = 1.2U_{eq}(N); O—H = 0.82 (1) Å, H—H = 1.39 (1) Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

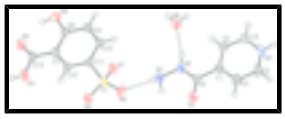

Fig. 1. Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Inter-ion and intermolecular hydrogen bonding are shown as dashed lines.

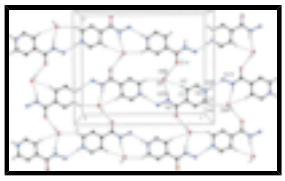

Fig. 2. Part of the crystal structure of (I), showing the formation of the (101) sheet generated by the hydrogen bonds between the cations and water solvent molecules. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms and intermolecular hydrogen bonding not involved in the motif have been omitted. Atoms marked with a hash(#) or a dollar sign($) are at the symmetry positions (1/2 + *x*, *y*, 3/2 − *z*) and (1/2 − *x*, 1 − *y*, 1/2 + *z*), respectively.

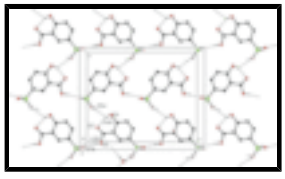

Fig. 3. Part of the crystal structure of (I), showing the formation of the (101) sheet generated by the hydrogen bonds between the anions. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms and intermolecular hydrogen bonds not involved in the motif have been omitted. Atoms marked with a hash(#) or a dollar sign($) are at the symmetry positions (1/2 + *x*, *y*, 1/2 − *z*) and (*x*, 3/2 − *y*, −1/2 + *z*), respectively.

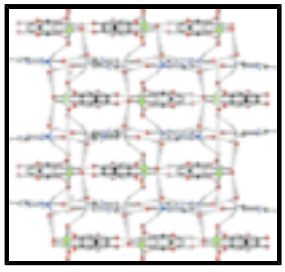

Fig. 4. Part of the crystal structure of (I), showing the formation of the three-dimensional network generated by the hydrogen bonds. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms and intermolecular hydrogen bonds not involved in the motif have been omitted.

4-(Hydrazinecarbonyl)pyridinium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

Crystal data

$C_6H_8N_3O^+·C_7H_5O_6S^-·H_2O$	F_{000} = 1552
M_r = 373.34	D_x = 1.625 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2943 reflections
a = 13.7628 (8) Å	θ = 2.8–21.4°
b = 13.0656 (8) Å	μ = 0.27 mm^{-1}
c = 16.9752 (10) Å	*T* = 299 (2) K
V = 3052.5 (3) Å^3	Plate, colourless
Z = 8	0.30 × 0.20 × 0.04 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3747 independent reflections
Radiation source: fine focus sealed Siemens Mo tube	2727 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.075
T = 299(2) K	θ_{max} = 28.3°
0.3° wide ω exposures scans	θ_{min} = 2.4°

Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -18 \rightarrow 18$
$T_{min} = 0.927$, $T_{max} = 0.990$	$k = -17 \rightarrow 17$
33729 measured reflections	$l = -22 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 1.8424P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
3747 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
250 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.17378 (17)	0.51847 (17)	0.82574 (12)	0.0254 (5)
C2	0.27410 (17)	0.52771 (19)	0.83228 (13)	0.0312 (5)
H2	0.3121	0.5368	0.7875	0.037*
C3	0.31671 (19)	0.52328 (19)	0.90534 (14)	0.0354 (6)
H3	0.3838	0.5285	0.9101	0.042*
C4	0.16537 (19)	0.5029 (2)	0.96546 (14)	0.0392 (6)
H4	0.1292	0.4949	1.0113	0.047*
C5	0.11965 (18)	0.5060 (2)	0.89398 (14)	0.0339 (6)
H5	0.0524	0.4997	0.8911	0.041*
C6	0.11982 (17)	0.51932 (17)	0.74783 (13)	0.0266 (5)
C7	0.15251 (16)	0.71604 (18)	0.26384 (13)	0.0267 (5)
C8	0.24789 (16)	0.72193 (17)	0.29228 (13)	0.0271 (5)

C9	0.26353 (16)	0.73103 (18)	0.37378 (14)	0.0287 (5)
H9	0.3267	0.7349	0.3931	0.034*
C10	0.18697 (17)	0.73430 (17)	0.42491 (13)	0.0279 (5)
H10	0.1981	0.7406	0.4787	0.033*
C11	0.09111 (16)	0.72820 (17)	0.39610 (12)	0.0243 (5)
C12	0.07484 (16)	0.71956 (18)	0.31632 (13)	0.0269 (5)
H12	0.0115	0.7161	0.2974	0.032*
C13	0.13520 (18)	0.7073 (2)	0.17783 (13)	0.0329 (6)
N1	0.13200 (16)	0.51270 (19)	0.60756 (12)	0.0363 (5)
H1A	0.0923 (16)	0.5630 (15)	0.6003 (17)	0.044*
H1B	0.0998 (18)	0.4563 (13)	0.6098 (17)	0.044*
N2	0.17413 (14)	0.52155 (17)	0.68322 (11)	0.0312 (5)
H2A	0.2359 (8)	0.528 (2)	0.6823 (15)	0.037*
N3	0.26167 (17)	0.51140 (17)	0.96953 (11)	0.0358 (5)
H3A	0.2938 (18)	0.509 (2)	1.0131 (10)	0.043*
O1	0.03087 (13)	0.51570 (15)	0.74565 (10)	0.0406 (5)
O2	0.20020 (14)	0.70257 (19)	0.12983 (10)	0.0564 (6)
O3	0.04337 (14)	0.7035 (2)	0.15867 (10)	0.0533 (6)
H3B	0.036 (3)	0.695 (3)	0.1110 (7)	0.080*
O4	0.32670 (13)	0.71925 (15)	0.24516 (10)	0.0408 (5)
H4A	0.306 (2)	0.715 (3)	0.2000 (9)	0.061*
O5	−0.09471 (12)	0.73591 (16)	0.41419 (10)	0.0439 (5)
O6	−0.00170 (13)	0.63684 (15)	0.50742 (11)	0.0458 (5)
O7	0.00528 (12)	0.82175 (14)	0.51056 (9)	0.0366 (4)
O8	0.37530 (13)	0.56058 (16)	0.65203 (11)	0.0428 (5)
H8A	0.381 (2)	0.6196 (12)	0.6353 (18)	0.064*
H8B	0.4214 (16)	0.543 (2)	0.6807 (16)	0.064*
S1	−0.00779 (4)	0.73054 (5)	0.46210 (3)	0.02779 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0319 (12)	0.0238 (11)	0.0204 (11)	0.0015 (9)	−0.0018 (9)	−0.0019 (9)
C2	0.0328 (13)	0.0360 (14)	0.0246 (11)	−0.0057 (11)	0.0009 (10)	0.0011 (10)
C3	0.0353 (14)	0.0395 (15)	0.0313 (13)	−0.0032 (11)	−0.0056 (11)	0.0002 (11)
C4	0.0418 (16)	0.0542 (17)	0.0216 (12)	0.0109 (13)	0.0049 (11)	0.0042 (11)
C5	0.0298 (13)	0.0473 (16)	0.0247 (12)	0.0072 (11)	0.0025 (10)	0.0034 (11)
C6	0.0281 (13)	0.0297 (12)	0.0219 (11)	−0.0009 (9)	−0.0009 (9)	0.0006 (9)
C7	0.0267 (12)	0.0320 (13)	0.0215 (11)	0.0002 (9)	−0.0001 (9)	0.0032 (9)
C8	0.0258 (11)	0.0261 (12)	0.0293 (12)	−0.0010 (9)	0.0013 (10)	0.0031 (10)
C9	0.0232 (11)	0.0293 (12)	0.0336 (12)	0.0002 (10)	−0.0057 (9)	0.0003 (10)
C10	0.0332 (12)	0.0288 (12)	0.0216 (11)	−0.0012 (10)	−0.0043 (9)	−0.0005 (9)
C11	0.0271 (11)	0.0258 (12)	0.0200 (10)	0.0007 (9)	0.0000 (9)	0.0032 (9)
C12	0.0252 (11)	0.0332 (13)	0.0225 (11)	0.0005 (9)	−0.0030 (9)	0.0033 (10)
C13	0.0316 (13)	0.0459 (15)	0.0211 (11)	0.0023 (11)	0.0004 (10)	0.0036 (10)
N1	0.0335 (12)	0.0554 (15)	0.0201 (10)	−0.0043 (10)	−0.0038 (9)	−0.0007 (10)
N2	0.0255 (10)	0.0505 (13)	0.0177 (9)	−0.0053 (9)	−0.0023 (8)	0.0015 (9)
N3	0.0487 (14)	0.0391 (12)	0.0197 (10)	0.0066 (10)	−0.0087 (9)	−0.0008 (9)

O1	0.0267 (9)	0.0676 (13)	0.0275 (9)	−0.0010 (8)	−0.0006 (7)	−0.0022 (9)
O2	0.0362 (11)	0.1076 (18)	0.0252 (9)	−0.0048 (11)	0.0060 (8)	−0.0027 (11)
O3	0.0332 (10)	0.1089 (18)	0.0178 (9)	0.0039 (11)	−0.0022 (8)	0.0001 (10)
O4	0.0276 (9)	0.0624 (13)	0.0323 (9)	−0.0007 (8)	0.0049 (8)	−0.0030 (9)
O5	0.0254 (9)	0.0791 (14)	0.0274 (9)	−0.0032 (9)	−0.0039 (7)	−0.0009 (9)
O6	0.0473 (11)	0.0475 (12)	0.0425 (11)	−0.0055 (9)	0.0058 (9)	0.0184 (9)
O7	0.0392 (10)	0.0483 (11)	0.0224 (8)	0.0025 (8)	−0.0005 (7)	−0.0048 (8)
O8	0.0297 (10)	0.0618 (14)	0.0369 (11)	−0.0034 (9)	−0.0004 (8)	0.0022 (9)
S1	0.0253 (3)	0.0402 (4)	0.0178 (3)	−0.0019 (2)	−0.0011 (2)	0.0033 (2)

Geometric parameters (Å, °)

C1—C5	1.387 (3)	C10—C11	1.409 (3)
C1—C2	1.390 (3)	C10—H10	0.9300
C1—C6	1.517 (3)	C11—C12	1.377 (3)
C2—C3	1.373 (3)	C11—S1	1.763 (2)
C2—H2	0.9300	C12—H12	0.9300
C3—N3	1.336 (3)	C13—O2	1.212 (3)
C3—H3	0.9300	C13—O3	1.306 (3)
C4—N3	1.332 (3)	N1—N2	1.414 (3)
C4—C5	1.367 (3)	N1—H1A	0.864 (10)
C4—H4	0.9300	N1—H1B	0.861 (10)
C5—H5	0.9300	N2—H2A	0.855 (10)
C6—O1	1.226 (3)	N3—H3A	0.862 (10)
C6—N2	1.328 (3)	O3—H3B	0.823 (10)
C7—C12	1.392 (3)	O4—H4A	0.821 (10)
C7—C8	1.401 (3)	O5—S1	1.4482 (17)
C7—C13	1.484 (3)	O6—S1	1.4484 (18)
C8—O4	1.348 (3)	O7—S1	1.4593 (18)
C8—C9	1.405 (3)	O8—H8A	0.826 (10)
C9—C10	1.366 (3)	O8—H8B	0.832 (10)
C9—H9	0.9300		
C5—C1—C2	118.5 (2)	C12—C11—C10	119.9 (2)
C5—C1—C6	117.8 (2)	C12—C11—S1	120.04 (17)
C2—C1—C6	123.7 (2)	C10—C11—S1	120.09 (17)
C3—C2—C1	119.5 (2)	C11—C12—C7	120.5 (2)
C3—C2—H2	120.2	C11—C12—H12	119.8
C1—C2—H2	120.2	C7—C12—H12	119.8
N3—C3—C2	120.0 (2)	O2—C13—O3	123.0 (2)
N3—C3—H3	120.0	O2—C13—C7	123.2 (2)
C2—C3—H3	120.0	O3—C13—C7	113.8 (2)
N3—C4—C5	120.1 (2)	N2—N1—H1A	109.1 (19)
N3—C4—H4	119.9	N2—N1—H1B	103.9 (19)
C5—C4—H4	119.9	H1A—N1—H1B	109 (3)
C4—C5—C1	119.8 (2)	C6—N2—N1	121.2 (2)
C4—C5—H5	120.1	C6—N2—H2A	125.3 (18)
C1—C5—H5	120.1	N1—N2—H2A	113.5 (18)
O1—C6—N2	122.6 (2)	C4—N3—C3	122.1 (2)
O1—C6—C1	121.0 (2)	C4—N3—H3A	123.5 (19)

N2—C6—C1	116.4 (2)	C3—N3—H3A	114.4 (19)
C12—C7—C8	119.8 (2)	C13—O3—H3B	112 (3)
C12—C7—C13	120.6 (2)	C8—O4—H4A	106 (2)
C8—C7—C13	119.6 (2)	S1—O6—H1A	140.0 (7)
O4—C8—C7	123.2 (2)	H2A—O8—H8A	112 (2)
O4—C8—C9	117.6 (2)	H2A—O8—H8B	121 (2)
C7—C8—C9	119.2 (2)	H8A—O8—H8B	112.5 (17)
C10—C9—C8	120.7 (2)	O5—S1—O6	112.77 (12)
C10—C9—H9	119.7	O5—S1—O7	112.27 (11)
C8—C9—H9	119.7	O6—S1—O7	112.56 (11)
C9—C10—C11	120.0 (2)	O5—S1—C11	106.37 (10)
C9—C10—H10	120.0	O6—S1—C11	106.15 (11)
C11—C10—H10	120.0	O7—S1—C11	106.09 (10)
C5—C1—C2—C3	0.6 (4)	S1—C11—C12—C7	−178.99 (18)
C6—C1—C2—C3	−178.2 (2)	C8—C7—C12—C11	−0.4 (3)
C1—C2—C3—N3	−0.8 (4)	C13—C7—C12—C11	−179.6 (2)
N3—C4—C5—C1	−0.3 (4)	C12—C7—C13—O2	−179.0 (3)
C2—C1—C5—C4	0.0 (4)	C8—C7—C13—O2	1.8 (4)
C6—C1—C5—C4	178.8 (2)	C12—C7—C13—O3	−0.1 (3)
C5—C1—C6—O1	4.6 (3)	C8—C7—C13—O3	−179.3 (2)
C2—C1—C6—O1	−176.6 (2)	O1—C6—N2—N1	−4.4 (4)
C5—C1—C6—N2	−173.8 (2)	C1—C6—N2—N1	173.9 (2)
C2—C1—C6—N2	5.1 (3)	C5—C4—N3—C3	0.1 (4)
C12—C7—C8—O4	−179.9 (2)	C2—C3—N3—C4	0.4 (4)
C13—C7—C8—O4	−0.6 (4)	H1A—O6—S1—O5	−174.7 (10)
C12—C7—C8—C9	0.2 (3)	H1A—O6—S1—O7	−46.4 (10)
C13—C7—C8—C9	179.5 (2)	H1A—O6—S1—C11	69.2 (10)
O4—C8—C9—C10	179.9 (2)	C12—C11—S1—O5	−7.5 (2)
C7—C8—C9—C10	−0.1 (3)	C10—C11—S1—O5	173.08 (19)
C8—C9—C10—C11	0.2 (3)	C12—C11—S1—O6	112.9 (2)
C9—C10—C11—C12	−0.4 (3)	C10—C11—S1—O6	−66.6 (2)
C9—C10—C11—S1	179.08 (18)	C12—C11—S1—O7	−127.18 (19)
C10—C11—C12—C7	0.5 (3)	C10—C11—S1—O7	53.4 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O8	0.93	2.48	3.389 (3)	166
C4—H4···O8^{i}	0.93	2.50	3.321 (3)	148
N2—H2A···O8	0.855 (10)	2.030 (12)	2.865 (3)	165 (2)
N3—H3A···N1^{i}	0.862 (10)	1.923 (11)	2.780 (3)	173 (3)
O8—H8B···O1^{ii}	0.832 (10)	1.990 (11)	2.819 (3)	174 (3)
O3—H3B···O7^{iii}	0.823 (10)	1.769 (11)	2.589 (2)	174 (4)
O4—H4A···O2	0.821 (10)	1.886 (18)	2.629 (3)	150 (3)
O4—H4A···O5^{iv}	0.821 (10)	2.39 (3)	2.921 (2)	123 (3)
C3—H3···O6^{ii}	0.93	2.54	3.262 (3)	135
N1—H1A···O6	0.864 (10)	2.256 (19)	2.984 (3)	142 (2)

N1—H1B···O5^{v}	0.861 (10)	2.545 (17)	3.309 (3)	148 (2)
O8—H8A···O5^{vi}	0.826 (10)	2.093 (11)	2.916 (3)	175 (3)

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

Fig. 1

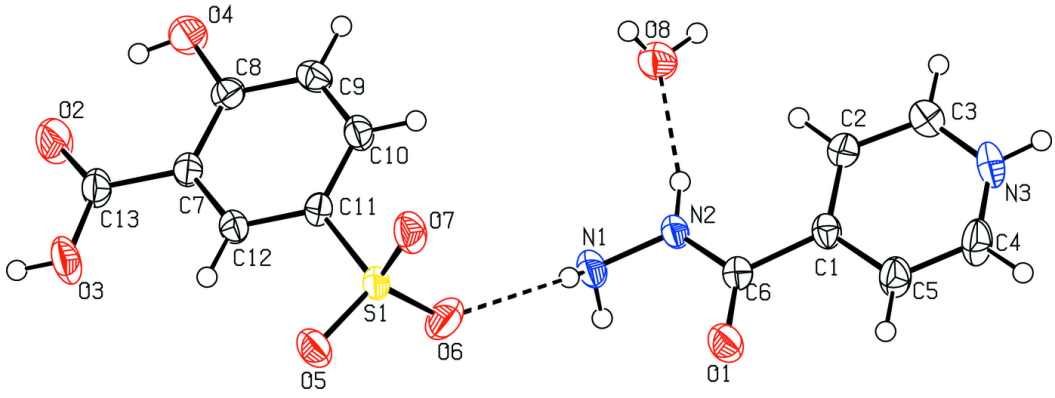
O4
C8
C9
O2
C10
C13
C7
C11
O7
C12
O3
S1
O6
O5
O8
N1
N2
C2
C3
N3
C6
C1
C4
C5
O1

Fig. 2

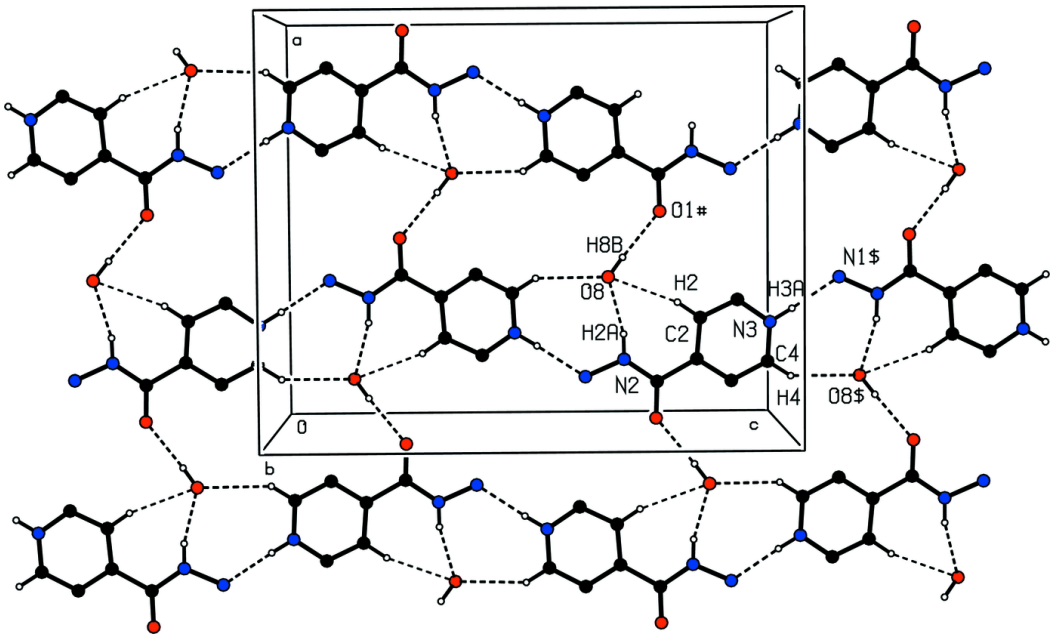

Fig. 3

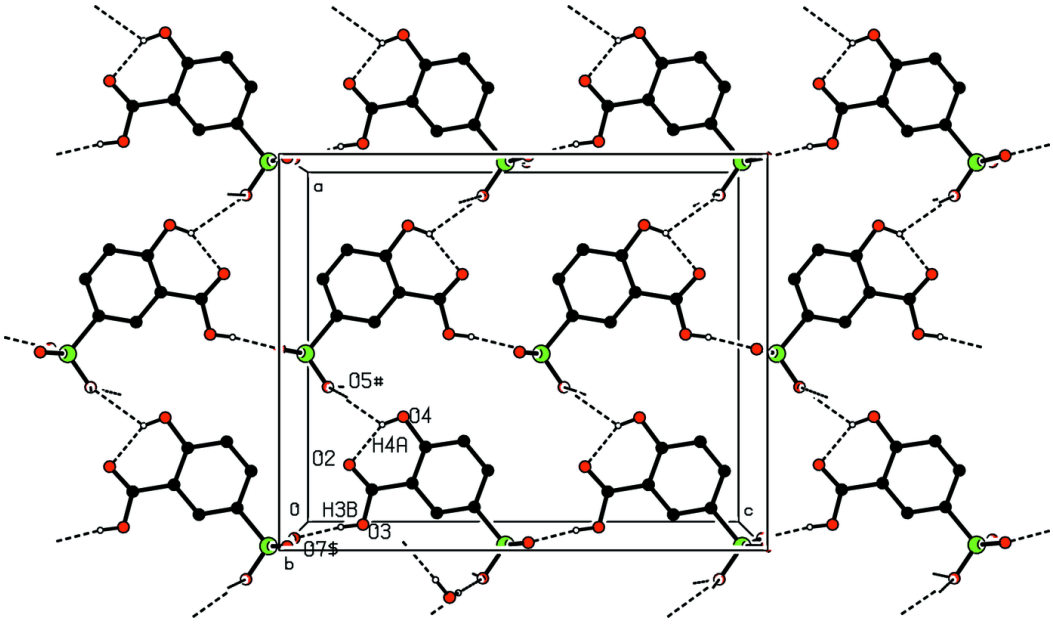

Fig. 4