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(*Z*)-2-(2-Aminothiazol-3-ium-4-yl)-2-[2-(*tert*-butoxycarbonyl)isopropoxyimino]-acetate monohydrate

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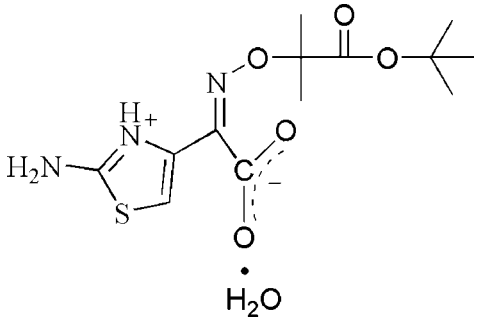
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.041; wR factor = 0.091; data-to-parameter ratio = 12.1.

In the title compound, $C_{13}H_{19}N_3O_5S\cdot H_2O$, the amino group is coplanar with the thiazole ring. The dihedral angle between the thiazole ring and the adjacent carboxylate group is 86.9 (1)°. The *tert*-butyl group is disordered over two positions, with occupancies of 0.63 (4) and 0.37 (4). O—H···O and N—H···O hydrogen bonds link the molecules into a two-dimensional network parallel to the (001) plane. The thiazole rings of inversion-related molecules are stacked with their centroids separated by a distance of 3.5387 (10) Å, indicating π–π interactions.

Related literature

For synthesis, see: Furlenmeier *et al.* (1987). For general background, see: Johnson (1999); Lynch *et al.* (1999); Powers *et al.* (2001); Toplak *et al.* (2003). For related structures, see: Laurent *et al.* (1981); Yoshida *et al.* (1989).



Experimental

Crystal data

$C_{13}H_{19}N_3O_5S\cdot H_2O$
M_r = 347.39
Orthorhombic, *Pbca*
a = 12.7918 (17) Å
b = 12.2489 (15) Å
c = 22.595 (3) Å
V = 3540.2 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 223 (2) K
0.80 × 0.80 × 0.57 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.847, T_{max} = 0.888
31871 measured reflections
3232 independent reflections
3096 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.091
S = 1.08
3232 reflections
268 parameters
22 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O5	0.88 (3)	1.85 (3)	2.726 (2)	179 (3)
O6—H6B···O2	0.81 (3)	1.93 (3)	2.745 (2)	176 (3)
N2—H2A···O5^{i}	0.90 (2)	1.81 (2)	2.656 (2)	156 (2)
N3—H3A···O6^{ii}	0.89 (2)	1.85 (2)	2.736 (2)	174 (2)
N3—H3B···O5^{i}	0.87 (2)	2.41 (2)	3.077 (2)	134 (2)
N3—H3B···O1^{i}	0.87 (2)	2.59 (2)	3.360 (2)	149 (2)

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

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2412).

References

Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Furlenmeier, A., Hofheinz, W. & Hubschw, E. (1987). US Patent No. 4 652 651.
Jacobson, R. (1998). Private communication to the Rigaku Corporation, Tokyo, Japan.
Johnson, D. K. (1999). *Anal. Chim. Acta*, **399**, 161–172.
Laurent, G., Parmentier, C., Evrard, G. & Durant, F. (1981). *Acta Cryst.* B**37**, 974–976.
Lynch, D. E., Nicholls, L. J., Smith, G., Byriel, K. A. & Kennard, C. H. L. (1999). *Acta Cryst.* B**55**, 758–766.
Powers, R. A., Caselli, E., Focia, P. J., Prati, F. & Shoichet, B. K. (2001). *Biochemistry*, **40**, 9207–9214.
Rigaku (2001). *CrystalClear*. Version 1.3. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *CrystalStructure*. Version 3.6.0. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Toplak, R., Lah, N., Volmajer, J., Leban, I. & Majcen Le Maréchal, A. (2003). *Acta Cryst.* C**59**, o502–o505.
Yoshida, A., Moroi, R., Arimoto, M. & Furukawa, M. (1989). *Anal. Sci.* **5**, 785–786.

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supplementary materials

Acta Cryst. (2007). E**63**, o3582 [**doi:10.1107/S1600536807034939**]

(*Z*)-2-(2-Aminothiazol-3-ium-4-yl)-2-[2-(*tert*-butoxycarbonyl)isopropoxyimino]acetate monohydrate

X.-W. Cheng

Comment

2-Aminothiazole compounds have been extensively studied because of their biological and industrial applications (Lynch *et al.*, 1999; Toplak *et al.*, 2003). A search of the Cambridge Structural Database (CSD, Version 5.28 of May 2007) reveals that there are 127 crystal structures containing the 2-aminothiazole moiety. The title compound is a very important intermediate of ceftazidime, which is among the most important cephalosporin antibiotics (Powers *et al.*, 2001). Crystal structures of some cephalosporin intermediates which contain a 2-aminothiazole group have been reported (Yoshida *et al.*, 1989; Laurent *et al.*, 1981). The title compound can give a reactive intermediate by reaction with diethylenetriamine-N,*N*,*N*',*N*'',*N*''- pentaacetic acid (DTPA), further, which can be used to prepare a protein-chelator conjugate (Johnson, 1999). We report here the crystal structure of the title compound.

The thiazole ring is planar to within ±0.006 (1) Å. The amino group is coplanar with the thiazole ring, with atom N3 deviating from the thiazole plane by −0.021 (2) Å. The O1/N1/C1/C2/C5/C6/C10 plane is twisted away from the thiazole plane by 21.92 (8)°. The *tert*-butyl group is disordered over two positions, with occupancies of 0.63 (4) and 0.37 (4). The carboxylate plane (C1/C5/O4/O5) is nearly perpendicular to the thiazole ring (dihedral angle 86.9 (1)°).

The crystal structure is stabilized by intermolecular O—H···O and N—H···O hydrogen bonds (Table 1) involving the O atoms of the water molecules and carboxylate groups. These hydrogen bonds link the molecules into a two-dimensional network parallel to the (001) plane (Fig. 2). The thiazole rings of the inversion-related molecules at (*x*, *y*, *z*) and (1 − *x*, 1 − *y*, 1 − *z*) are stacked with their centroids separated by a distance of 3.5387 (10) Å, indicating π-π interactions.

Experimental

The title compound was prepared according to the literature method (Furlenmeier *et al.*, 1987). Crystals suitable for X-ray analysis were obtained by slow evaporation of a ethanol solution at room temperature (m.p. 471–473 K).

Refinement

The *tert*-butyl group is disordered over two positions, with refined occupations 0.63 (4) and 0.37 (4). The C—C distances of the *tert*-butyl groups were restrained to 1.53 (1) Å, and the C—O and C···C distances involving disordered C-atoms were restrained to be equal. O– and N-bound H atoms were located from a difference Fourier map, and refined freely. C-bound H atoms were positioned geometrically (C—H = 0.94 or 0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Figures

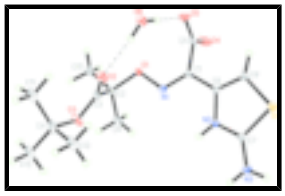

Fig. 1. Molecular structure of the title compound, showing 20% probability displacement ellipsoids and the atomic numbering. Only one disorder component is shown.

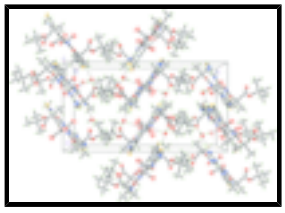

Fig. 2. The crystal packing of the title compound, viewed approximately down the *a* axis. Dashed lines indicate intermolecular hydrogen bonds. Only one disorder component is shown.

(*Z*)-2-(2-Aminothiazol-3-ium-4-yl)-2-[2-(*tert*-butoxycarbonyl)- isopropoxyimino]acetate monohydrate

Crystal data

$C_{13}H_{19}N_3O_5S·H_2O$	F_{000} = 1472
M_r = 347.39	D_x = 1.304 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71070 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 31871 reflections
a = 12.7918 (17) Å	θ = 3.2–25.4º
b = 12.2489 (15) Å	μ = 0.21 mm^{-1}
c = 22.595 (3) Å	*T* = 223 (2) K
V = 3540.2 (8) Å^3	Block, colourless
Z = 8	0.80 × 0.80 × 0.57 mm

Data collection

Rigaku Mercury diffractometer	3232 independent reflections
Radiation source: fine-focus sealed tube	3096 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 223(2) K	θ_{max} = 25.4º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (Jacobson, 1998)	*h* = −15→15
T_{min} = 0.847, T_{max} = 0.888	*k* = −14→14
31871 measured reflections	*l* = −27→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 2.4239P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
3232 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
268 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
22 restraints	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0151 (7)

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}	Occ. (<1)
S1	0.46180 (4)	0.52078 (4)	0.40564 (2)	0.03825 (17)	
O1	0.41053 (8)	0.12570 (9)	0.56784 (5)	0.0286 (3)	
O2	0.47558 (11)	0.23610 (12)	0.66636 (6)	0.0455 (4)	
O3	0.61809 (11)	0.13114 (11)	0.67241 (6)	0.0466 (4)	
O4	0.24960 (11)	0.16967 (14)	0.45102 (7)	0.0585 (4)	
O5	0.21461 (9)	0.25993 (12)	0.53369 (6)	0.0448 (4)	
O6	0.29085 (12)	0.33757 (12)	0.63821 (7)	0.0406 (3)	
N1	0.45637 (10)	0.20940 (11)	0.53363 (6)	0.0268 (3)	
N2	0.53804 (11)	0.35198 (12)	0.45411 (6)	0.0276 (3)	
N3	0.66501 (12)	0.46234 (15)	0.40943 (8)	0.0377 (4)	
C1	0.38961 (12)	0.25548 (14)	0.49967 (7)	0.0263 (4)	
C2	0.49082 (13)	0.07540 (14)	0.60427 (8)	0.0290 (4)	
C3	0.52641 (13)	0.15890 (14)	0.65053 (8)	0.0297 (4)	
C5	0.27385 (13)	0.22507 (14)	0.49359 (8)	0.0314 (4)	
C6	0.43082 (12)	0.34460 (14)	0.46353 (7)	0.0271 (4)	
C7	0.56742 (13)	0.43966 (14)	0.42388 (7)	0.0291 (4)	
C8	0.37851 (14)	0.42879 (15)	0.43978 (8)	0.0360 (4)	
H8	0.3055	0.4369	0.4415	0.043*	
C9	0.58029 (15)	0.03195 (17)	0.56715 (9)	0.0412 (5)	
H9A	0.5534	−0.0193	0.5382	0.062*	
H9B	0.6303	−0.0048	0.5926	0.062*	

H9C	0.6144	0.0921	0.5470	0.062*	
C10	0.43324 (17)	−0.01592 (17)	0.63619 (10)	0.0488 (6)	
H10A	0.3749	0.0144	0.6581	0.073*	
H10B	0.4806	−0.0521	0.6633	0.073*	
H10C	0.4075	−0.0683	0.6075	0.073*	
C4	0.6558 (15)	0.1863 (12)	0.7277 (6)	0.043 (4)	0.37 (4)
C11	0.5784 (18)	0.1947 (19)	0.7785 (11)	0.065 (4)	0.37 (4)
H11A	0.5607	0.1221	0.7924	0.098*	0.37 (4)
H11B	0.5156	0.2314	0.7650	0.098*	0.37 (4)
H11C	0.6095	0.2361	0.8106	0.098*	0.37 (4)
C12	0.695 (2)	0.2988 (16)	0.7095 (11)	0.067 (5)	0.37 (4)
H12A	0.7427	0.2916	0.6764	0.100*	0.37 (4)
H12B	0.7307	0.3327	0.7425	0.100*	0.37 (4)
H12C	0.6360	0.3438	0.6978	0.100*	0.37 (4)
C13	0.7481 (17)	0.1146 (17)	0.7456 (11)	0.070 (4)	0.37 (4)
H13A	0.7230	0.0425	0.7561	0.106*	0.37 (4)
H13B	0.7834	0.1469	0.7793	0.106*	0.37 (4)
H13C	0.7966	0.1089	0.7127	0.106*	0.37 (4)
C4'	0.6727 (10)	0.1936 (8)	0.7204 (4)	0.043 (2)	0.63 (4)
C11'	0.6069 (13)	0.1748 (14)	0.7744 (6)	0.072 (3)	0.63 (4)
H11D	0.5892	0.0979	0.7772	0.108*	0.63 (4)
H11E	0.5433	0.2176	0.7715	0.108*	0.63 (4)
H11F	0.6456	0.1966	0.8093	0.108*	0.63 (4)
C12'	0.6832 (13)	0.3121 (8)	0.7044 (6)	0.063 (3)	0.63 (4)
H12D	0.7190	0.3186	0.6667	0.095*	0.63 (4)
H12E	0.7231	0.3495	0.7347	0.095*	0.63 (4)
H12F	0.6143	0.3447	0.7013	0.095*	0.63 (4)
C13'	0.7772 (12)	0.1372 (13)	0.7235 (9)	0.088 (4)	0.63 (4)
H13D	0.7667	0.0594	0.7289	0.132*	0.63 (4)
H13E	0.8168	0.1660	0.7566	0.132*	0.63 (4)
H13F	0.8154	0.1499	0.6871	0.132*	0.63 (4)
H6A	0.267 (2)	0.312 (2)	0.6048 (12)	0.069 (9)*	
H6B	0.346 (2)	0.306 (2)	0.6449 (12)	0.069 (9)*	
H2A	0.5873 (19)	0.3049 (19)	0.4660 (10)	0.054 (7)*	
H3A	0.6783 (17)	0.5257 (19)	0.3913 (10)	0.046 (6)*	
H3B	0.7138 (18)	0.4203 (19)	0.4232 (10)	0.052 (7)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0322 (3)	0.0349 (3)	0.0477 (3)	0.00080 (19)	−0.0030 (2)	0.0154 (2)
O1	0.0212 (6)	0.0325 (6)	0.0321 (6)	−0.0040 (5)	−0.0045 (5)	0.0102 (5)
O2	0.0443 (8)	0.0477 (8)	0.0444 (8)	0.0147 (7)	−0.0090 (6)	−0.0099 (6)
O3	0.0436 (8)	0.0431 (8)	0.0530 (8)	0.0132 (6)	−0.0279 (7)	−0.0152 (7)
O4	0.0320 (7)	0.0720 (11)	0.0715 (10)	−0.0050 (7)	−0.0118 (8)	−0.0226 (9)
O5	0.0222 (6)	0.0611 (9)	0.0511 (8)	−0.0062 (6)	0.0044 (6)	−0.0019 (7)
O6	0.0370 (8)	0.0379 (8)	0.0470 (9)	0.0070 (6)	0.0045 (7)	0.0071 (7)
N1	0.0218 (7)	0.0297 (7)	0.0289 (7)	−0.0033 (6)	0.0001 (6)	0.0049 (6)

N2	0.0204 (7)	0.0297 (8)	0.0327 (8)	0.0001 (6)	−0.0001 (6)	0.0063 (6)
N3	0.0270 (8)	0.0373 (9)	0.0488 (10)	−0.0034 (7)	0.0050 (7)	0.0137 (8)
C1	0.0204 (8)	0.0294 (8)	0.0291 (8)	−0.0001 (7)	−0.0005 (7)	0.0012 (7)
C2	0.0249 (8)	0.0294 (9)	0.0328 (9)	0.0004 (7)	−0.0070 (7)	0.0055 (7)
C3	0.0292 (9)	0.0310 (9)	0.0289 (9)	0.0022 (7)	−0.0036 (7)	0.0055 (7)
C5	0.0233 (9)	0.0297 (9)	0.0410 (10)	−0.0020 (7)	−0.0066 (8)	0.0096 (8)
C6	0.0198 (8)	0.0334 (9)	0.0283 (9)	−0.0018 (7)	−0.0017 (7)	0.0026 (7)
C7	0.0281 (9)	0.0300 (9)	0.0293 (9)	−0.0014 (7)	0.0003 (7)	0.0016 (7)
C8	0.0224 (8)	0.0398 (10)	0.0458 (11)	0.0000 (8)	−0.0026 (8)	0.0105 (8)
C9	0.0357 (10)	0.0489 (12)	0.0390 (11)	0.0130 (9)	−0.0100 (9)	−0.0074 (9)
C10	0.0429 (11)	0.0425 (12)	0.0608 (14)	−0.0079 (10)	−0.0133 (10)	0.0226 (10)
C4	0.045 (6)	0.032 (6)	0.051 (8)	0.002 (4)	−0.024 (5)	−0.005 (4)
C11	0.089 (9)	0.070 (6)	0.036 (5)	0.016 (7)	−0.008 (6)	−0.004 (4)
C12	0.077 (9)	0.075 (10)	0.049 (7)	−0.004 (7)	−0.023 (6)	0.017 (6)
C13	0.069 (8)	0.075 (7)	0.068 (9)	0.027 (6)	−0.042 (6)	−0.025 (6)
C4'	0.048 (4)	0.044 (5)	0.037 (3)	0.000 (3)	−0.022 (3)	−0.007 (3)
C11'	0.090 (6)	0.091 (7)	0.036 (4)	−0.025 (5)	−0.021 (4)	0.008 (5)
C12'	0.079 (5)	0.047 (4)	0.064 (6)	−0.023 (4)	−0.035 (4)	0.000 (3)
C13'	0.069 (6)	0.093 (6)	0.102 (8)	0.028 (5)	−0.061 (5)	−0.039 (6)

Geometric parameters (Å, °)

S1—C7	1.7270 (18)	C9—H9C	0.97
S1—C8	1.7319 (18)	C10—H10A	0.97
O1—N1	1.4116 (17)	C10—H10B	0.97
O1—C2	1.4532 (19)	C10—H10C	0.97
O2—C3	1.202 (2)	C4—C13	1.526 (9)
O3—C3	1.317 (2)	C4—C12	1.523 (9)
O3—C4'	1.499 (5)	C4—C11	1.520 (9)
O3—C4	1.501 (7)	C11—H11A	0.97
O4—C5	1.217 (2)	C11—H11B	0.97
O5—C5	1.256 (2)	C11—H11C	0.97
O6—H6A	0.88 (3)	C12—H12A	0.97
O6—H6B	0.81 (3)	C12—H12B	0.97
N1—C1	1.279 (2)	C12—H12C	0.97
N2—C7	1.327 (2)	C13—H13A	0.97
N2—C6	1.391 (2)	C13—H13B	0.97
N2—H2A	0.90 (2)	C13—H13C	0.97
N3—C7	1.320 (2)	C4'—C12'	1.502 (7)
N3—H3A	0.89 (2)	C4'—C11'	1.500 (7)
N3—H3B	0.87 (2)	C4'—C13'	1.507 (7)
C1—C6	1.462 (2)	C11'—H11D	0.97
C1—C5	1.533 (2)	C11'—H11E	0.97
C2—C9	1.516 (3)	C11'—H11F	0.97
C2—C10	1.521 (3)	C12'—H12D	0.97
C2—C3	1.532 (2)	C12'—H12E	0.97
C6—C8	1.341 (2)	C12'—H12F	0.97
C8—H8	0.94	C13'—H13D	0.97
C9—H9A	0.97	C13'—H13E	0.97

C9—H9B	0.97	C13'—H13F	0.97
C7—S1—C8	90.04 (8)	O3—C4—C13	102.1 (11)
N1—O1—C2	108.93 (11)	O3—C4—C12	106.7 (14)
C3—O3—C4'	123.6 (5)	C13—C4—C12	109.8 (7)
C3—O3—C4	118.9 (7)	O3—C4—C11	116.8 (16)
H6A—O6—H6B	107 (3)	C13—C4—C11	110.1 (7)
C1—N1—O1	111.81 (13)	C12—C4—C11	110.9 (7)
C7—N2—C6	114.24 (15)	C4—C11—H11A	109.5
C7—N2—H2A	118.4 (15)	C4—C11—H11B	109.5
C6—N2—H2A	127.3 (15)	H11A—C11—H11B	109.5
C7—N3—H3A	118.4 (14)	C4—C11—H11C	109.5
C7—N3—H3B	117.8 (15)	H11A—C11—H11C	109.5
H3A—N3—H3B	123 (2)	H11B—C11—H11C	109.5
N1—C1—C6	115.08 (14)	C4—C12—H12A	109.5
N1—C1—C5	126.26 (15)	C4—C12—H12B	109.5
C6—C1—C5	118.66 (14)	H12A—C12—H12B	109.5
O1—C2—C9	111.67 (14)	C4—C12—H12C	109.5
O1—C2—C10	103.77 (13)	H12A—C12—H12C	109.5
C9—C2—C10	111.70 (17)	H12B—C12—H12C	109.5
O1—C2—C3	108.27 (13)	C4—C13—H13A	109.5
C9—C2—C3	112.81 (15)	C4—C13—H13B	109.5
C10—C2—C3	108.15 (15)	H13A—C13—H13B	109.5
O2—C3—O3	124.96 (17)	C4—C13—H13C	109.5
O2—C3—C2	124.58 (16)	H13A—C13—H13C	109.5
O3—C3—C2	110.39 (15)	H13B—C13—H13C	109.5
O4—C5—O5	127.28 (16)	O3—C4'—C12'	111.2 (7)
O4—C5—C1	116.90 (16)	O3—C4'—C11'	104.4 (10)
O5—C5—C1	115.81 (15)	C12'—C4'—C11'	113.3 (5)
C8—C6—N2	112.38 (15)	O3—C4'—C13'	102.3 (7)
C8—C6—C1	128.16 (15)	C12'—C4'—C13'	112.0 (6)
N2—C6—C1	119.32 (15)	C11'—C4'—C13'	112.9 (5)
N3—C7—N2	124.44 (17)	C4'—C11'—H11D	109.5
N3—C7—S1	124.03 (14)	C4'—C11'—H11E	109.5
N2—C7—S1	111.53 (12)	H11D—C11'—H11E	109.5
C6—C8—S1	111.81 (13)	C4'—C11'—H11F	109.5
C6—C8—H8	124.1	H11D—C11'—H11F	109.5
S1—C8—H8	124.1	H11E—C11'—H11F	109.5
C2—C9—H9A	109.5	C4'—C12'—H12D	109.5
C2—C9—H9B	109.5	C4'—C12'—H12E	109.5
H9A—C9—H9B	109.5	H12D—C12'—H12E	109.5
C2—C9—H9C	109.5	C4'—C12'—H12F	109.5
H9A—C9—H9C	109.5	H12D—C12'—H12F	109.5
H9B—C9—H9C	109.5	H12E—C12'—H12F	109.5
C2—C10—H10A	109.5	C4'—C13'—H13D	109.5
C2—C10—H10B	109.5	C4'—C13'—H13E	109.5
H10A—C10—H10B	109.5	H13D—C13'—H13E	109.5
C2—C10—H10C	109.5	C4'—C13'—H13F	109.5
H10A—C10—H10C	109.5	H13D—C13'—H13F	109.5
H10B—C10—H10C	109.5	H13E—C13'—H13F	109.5

C2—O1—N1—C1	178.74 (14)	C7—N2—C6—C8	0.0 (2)
O1—N1—C1—C6	178.92 (13)	C7—N2—C6—C1	−175.93 (15)
O1—N1—C1—C5	−1.7 (2)	N1—C1—C6—C8	−155.94 (19)
N1—O1—C2—C9	−56.78 (17)	C5—C1—C6—C8	24.6 (3)
N1—O1—C2—C10	−177.25 (14)	N1—C1—C6—N2	19.3 (2)
N1—O1—C2—C3	68.00 (16)	C5—C1—C6—N2	−160.16 (16)
C4'—O3—C3—O2	−0.5 (7)	C6—N2—C7—N3	−179.26 (17)
C4—O3—C3—O2	11.0 (10)	C6—N2—C7—S1	0.70 (19)
C4'—O3—C3—C2	−177.5 (7)	C8—S1—C7—N3	179.04 (17)
C4—O3—C3—C2	−166.0 (9)	C8—S1—C7—N2	−0.91 (14)
O1—C2—C3—O2	21.9 (2)	N2—C6—C8—S1	−0.7 (2)
C9—C2—C3—O2	146.04 (18)	C1—C6—C8—S1	174.79 (15)
C10—C2—C3—O2	−89.9 (2)	C7—S1—C8—C6	0.92 (15)
O1—C2—C3—O3	−161.07 (14)	C3—O3—C4—C13	167.3 (10)
C9—C2—C3—O3	−37.0 (2)	C3—O3—C4—C12	−77.5 (12)
C10—C2—C3—O3	87.09 (18)	C3—O3—C4—C11	47.2 (13)
N1—C1—C5—O4	−100.4 (2)	C3—O3—C4'—C12'	−53.7 (12)
C6—C1—C5—O4	78.9 (2)	C3—O3—C4'—C11'	68.8 (10)
N1—C1—C5—O5	79.1 (2)	C3—O3—C4'—C13'	−173.4 (9)
C6—C1—C5—O5	−101.53 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6A···O5	0.88 (3)	1.85 (3)	2.726 (2)	179 (3)
O6—H6B···O2	0.81 (3)	1.93 (3)	2.745 (2)	176 (3)
N2—H2A···O5^{i}	0.90 (2)	1.81 (2)	2.656 (2)	156 (2)
N3—H3A···O6^{ii}	0.89 (2)	1.85 (2)	2.736 (2)	174 (2)
N3—H3B···O5^{i}	0.87 (2)	2.41 (2)	3.077 (2)	134 (2)
N3—H3B···O1^{i}	0.87 (2)	2.59 (2)	3.360 (2)	149 (2)

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

Fig. 1

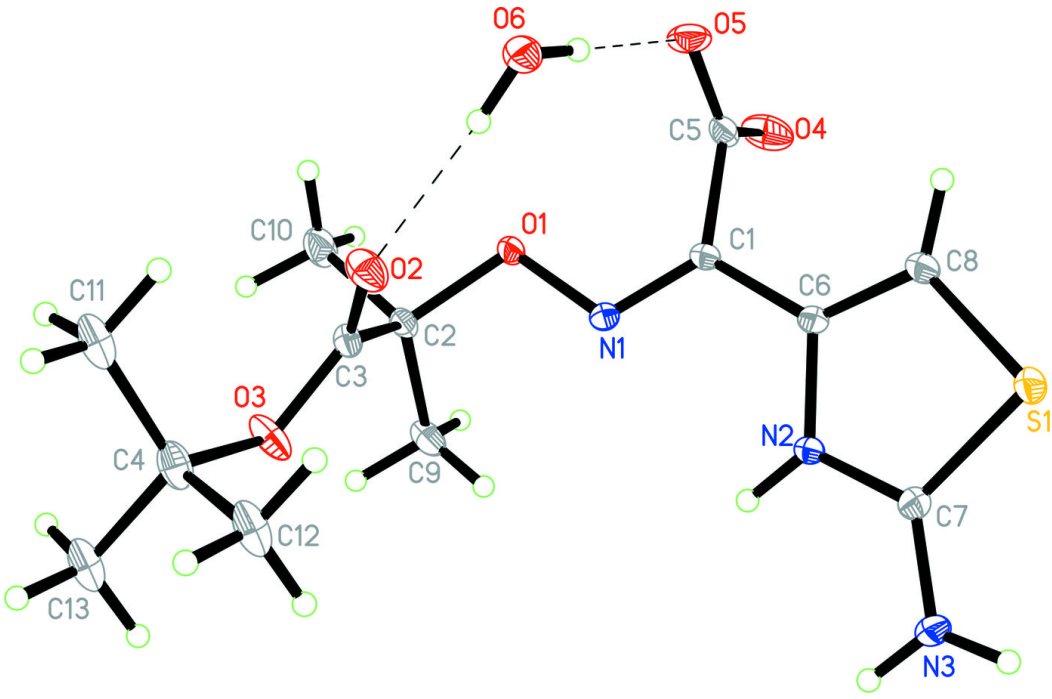
O6
O5
C5
O4
C10
O1
C1
O2
C8
C11
C6
C2
N1
C3
O3
S1
N2
C4
C9
C7
C12
C13
N3

Fig. 2