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2-(4-Methylphenylsulfonamido)acetic acid

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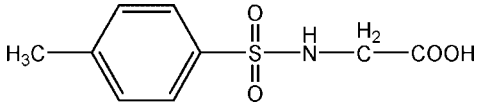
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.056; wR factor = 0.113; data-to-parameter ratio = 12.8.

In the title compound, $C_9H_{11}O_4NS$, there are two crystallographically independent molecules in the asymmetric unit. The S atoms are in a distorted tetrahedral configuration. Symmetry-related molecules are linked to form dimers *via* O—H···O hydrogen bonding, and the dimers are associated to form infinite chains *via* N—H···O hydrogen bonding. There are close C—H···O approaches of 3.342 (7) and 3.353 (7) Å between the two independent molecules.

Related literature

For the biological activity of sulfonamides, see: Yan *et al.* (2007); Patani & Lavoie (1996). For the chemistry of sulfonamides, see: Yin *et al.* (2007). For geometry, see: Lehman *et al.* (1981); Starikova *et al.* (1982); Bernstein *et al.* (1995); Etter (1990).



Experimental

Crystal data

$C_9H_{11}NO_4S$
M_r = 229.26
Monoclinic, $P2_1/c$
a = 22.3240 (19) Å
b = 5.7263 (5) Å
c = 16.5526 (14) Å
β = 109.069 (2)°
V = 1999.9 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 298 (2) K
0.27 × 0.13 × 0.11 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.919, T_{max} = 0.956
9980 measured reflections
3524 independent reflections
2969 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.114
S = 1.29
3524 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.413 (4)	S1—N1	1.625 (5)
S1—O1	1.429 (4)	S1—C5	1.769 (6)
O2—S1—O1	120.4 (3)	O2—S1—C5	107.3 (3)
O2—S1—N1	106.4 (3)	O1—S1—C5	108.6 (3)
O1—S1—N1	106.4 (3)	N1—S1—C5	107.0 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4^{i}	0.86	2.57	3.167 (6)	127
N2—H2···O8^{ii}	0.86	2.59	3.231 (7)	132
O3—H3···O4^{iii}	0.82	1.94	2.751 (6)	172
O7—H7···O8^{iv}	0.82	1.94	2.745 (7)	167
C1—H1*B*···O5^{v}	0.96	2.56	3.342 (7)	138
C10—H10*B*···O2^{vi}	0.96	2.40	3.353 (7)	170
C17—H17*B*···O6^{ii}	0.97	2.45	3.211 (6)	134

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2149).

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supplementary materials

Acta Cryst. (2007). E**63**, o3719 [**doi:10.1107/S1600536807037749**]

2-(4-Methylphenylsulfonamido)acetic acid

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Comment

The sulfonamide group is present in many bioactive compounds (Yan *et al.*, 2007; Patani & Lavoie, 1996) and may be used as a protecting group (Yin *et al.*, 2007). Many sulfonamide derivatives have been synthesized, such as sulfacetamide, sulfapyridine, sulfaguanidine, sulfathiazole, *etc*. We report here the synthesis and crystal structure of the title compound, (I).

As shown in Fig. 1, there are two crystallographically independent molecules in the asymmetric unit. Most bond lengths and angles in (I) are within normal ranges with the geometries around S atom being distorted tetrahedra (Lehman *et al.*, 1981; Starilkova *et al.*, 1982), with two O atoms, one N and C atom.

The self-related independent molecules of (I) are linked *via* O—H···O hydrogen bonds to form dimers (Fig. 2 and Table 2), which are frequently observed in carboxlic acid that can be described by a graph set of $R_2^2(8)$ (Bernstein *et al.*, 1995; Etter, 1990). Such dimers are associated *via* N—H···O hydrogen bonds to form infinite chains. In the crystal, the independent molecules are linked with each other by the C1—H1B···O5^{v} and C10—H10B···O2^{vi} hydrogen bonds.

Experimental

4-Methylbenzene-1-sulfonyl chloride (0.02 mol, 3.81 g) and 2-aminoacetic acid (0.02 mol,1.50 g) were added together at room temperature with stirring. The reaction was allowed to proceed for 8 h at room temperature. The purified product was dissovled in acetone, approximately 10 days later single crystals of (I) were formed.

Refinement

All the H atoms were placed in calculated positions and allowed to ride on their parent atoms at distances of 0.96 Å (methyl), 0.97 Å (methylene), 0.93 Å (phenyl), 0.82 Å (O—H) and 0.86 Å (N—H), with U_{iso}(H) values 1.2 times U_{eq} of the parent atoms.

Figures

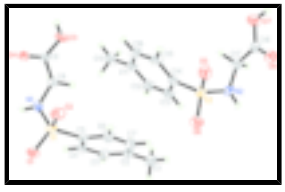

Fig. 1. The asymmetric cell unit of (I) with atom labels, showing 30% probability displacement ellipsoids. The hydrogen bond linking the two unique molecules is shown as a dashed line.

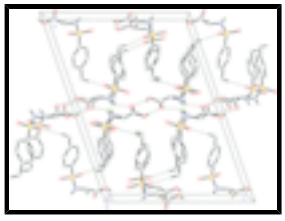

Fig. 2. The crystal packing of (I) viewed down along the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds are ommitted for clarity.

2-(4-Methylphenylsulfonamido)acetic acid

Crystal data

$C_9H_{11}NO_4S$	F_{000} = 960
M_r = 229.26	D_x = 1.523 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1978 reflections
a = 22.3240 (19) Å	θ = 2.6–24.3º
b = 5.7263 (5) Å	μ = 0.32 mm^{-1}
c = 16.5526 (14) Å	T = 298 (2) K
β = 109.069 (2)º	Rod, colourless
V = 1999.9 (3) Å^3	0.27 × 0.13 × 0.11 mm
Z = 8	

Data collection

Bruker APEX area-detector diffractometer	3524 independent reflections
Radiation source: fine-focus sealed tube	2969 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.0º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −24→26
T_{min} = 0.919, T_{max} = 0.956	k = −6→6
9980 measured reflections	l = −18→19

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-atom parameters constrained
$wR(F^2)$ = 0.114	$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 6.265P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.29	$(\Delta/\sigma)_{max}$ = 0.001
3524 reflections	$\Delta\rho_{max}$ = 0.62 e Å^{-3}
275 parameters	$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
S1	0.39781 (7)	0.4002 (3)	0.17822 (9)	0.0304 (4)
S2	0.10566 (7)	0.3305 (3)	0.28814 (10)	0.0337 (4)
O1	0.4177 (2)	0.4520 (8)	0.1064 (3)	0.0430 (12)
O2	0.3857 (2)	0.5823 (8)	0.2284 (3)	0.0448 (12)
O3	0.4516 (2)	0.2409 (9)	0.4589 (3)	0.0496 (13)
H3	0.4681	0.3220	0.5012	0.074*
O4	0.5043 (2)	0.4794 (8)	0.3988 (2)	0.0378 (11)
O5	0.1138 (2)	0.5130 (8)	0.3486 (3)	0.0471 (12)
O6	0.0937 (2)	0.3832 (9)	0.2000 (3)	0.0499 (13)
O7	0.0451 (2)	0.2317 (9)	0.5077 (3)	0.0534 (13)
H7	0.0287	0.3211	0.5331	0.080*
O8	−0.0094 (2)	0.4433 (9)	0.3949 (3)	0.0463 (12)
N1	0.4533 (2)	0.2403 (9)	0.2423 (3)	0.0324 (12)
H1	0.4873	0.2066	0.2310	0.039*
N2	0.0455 (2)	0.1782 (10)	0.2924 (3)	0.0374 (13)
H2	0.0144	0.1465	0.2470	0.045*
C1	0.1630 (3)	−0.1992 (14)	0.0510 (5)	0.056 (2)
H1A	0.1703	−0.3438	0.0821	0.083*
H1B	0.1541	−0.2304	−0.0087	0.083*
H1C	0.1276	−0.1201	0.0594	0.083*
C2	0.2204 (3)	−0.0497 (11)	0.0825 (4)	0.0383 (16)
C3	0.2776 (3)	−0.1197 (11)	0.0739 (4)	0.0374 (16)
H3A	0.2796	−0.2623	0.0481	0.045*
C4	0.3313 (3)	0.0154 (11)	0.1025 (4)	0.0364 (15)
H4	0.3688	−0.0330	0.0946	0.044*
C5	0.3288 (3)	0.2253 (11)	0.1432 (4)	0.0317 (14)
C6	0.2732 (3)	0.2982 (12)	0.1535 (4)	0.0421 (17)
H6	0.2716	0.4380	0.1813	0.050*
C7	0.2202 (3)	0.1619 (13)	0.1223 (4)	0.0447 (18)
H7A	0.1824	0.2144	0.1281	0.054*
C8	0.4430 (3)	0.1568 (11)	0.3196 (4)	0.0329 (14)

H8A	0.4616	0.0026	0.3330	0.039*
H8B	0.3978	0.1414	0.3087	0.039*
C9	0.4702 (3)	0.3116 (11)	0.3958 (4)	0.0302 (14)
C10	0.3427 (3)	−0.2626 (13)	0.3970 (4)	0.0487 (18)
H10A	0.3753	−0.1830	0.4409	0.073*
H10B	0.3564	−0.2870	0.3484	0.073*
H10C	0.3343	−0.4107	0.4182	0.073*
C11	0.2833 (3)	−0.1171 (12)	0.3709 (4)	0.0377 (16)
C12	0.2297 (3)	−0.1886 (12)	0.3062 (4)	0.0417 (16)
H12	0.2306	−0.3289	0.2784	0.050*
C13	0.1752 (3)	−0.0585 (11)	0.2820 (4)	0.0390 (16)
H13	0.1396	−0.1101	0.2383	0.047*
C14	0.1737 (3)	0.1500 (11)	0.3231 (4)	0.0324 (14)
C15	0.2263 (3)	0.2262 (12)	0.3882 (4)	0.0414 (17)
H15	0.2253	0.3654	0.4167	0.050*
C16	0.2804 (3)	0.0919 (12)	0.4102 (4)	0.0419 (16)
H16	0.3163	0.1446	0.4531	0.050*
C17	0.0465 (3)	0.0973 (12)	0.3763 (4)	0.0406 (16)
H17A	0.0894	0.0511	0.4090	0.049*
H17B	0.0197	−0.0396	0.3691	0.049*
C18	0.0242 (3)	0.2790 (12)	0.4257 (4)	0.0346 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0359 (9)	0.0317 (9)	0.0215 (8)	0.0010 (7)	0.0065 (6)	−0.0006 (6)
S2	0.0331 (9)	0.0361 (9)	0.0313 (9)	0.0002 (7)	0.0096 (7)	0.0007 (7)
O1	0.049 (3)	0.050 (3)	0.028 (2)	−0.008 (2)	0.010 (2)	0.011 (2)
O2	0.053 (3)	0.040 (3)	0.038 (3)	0.002 (2)	0.010 (2)	−0.006 (2)
O3	0.068 (3)	0.061 (3)	0.024 (2)	−0.018 (3)	0.021 (2)	0.000 (2)
O4	0.042 (3)	0.049 (3)	0.023 (2)	−0.015 (2)	0.0099 (19)	−0.005 (2)
O5	0.044 (3)	0.045 (3)	0.054 (3)	0.000 (2)	0.017 (2)	−0.009 (2)
O6	0.048 (3)	0.060 (3)	0.043 (3)	0.009 (2)	0.017 (2)	0.012 (2)
O7	0.068 (4)	0.060 (3)	0.032 (3)	0.006 (3)	0.016 (2)	0.005 (2)
O8	0.044 (3)	0.057 (3)	0.036 (3)	0.015 (3)	0.012 (2)	0.005 (2)
N1	0.027 (3)	0.043 (3)	0.030 (3)	0.001 (2)	0.013 (2)	0.000 (2)
N2	0.029 (3)	0.050 (3)	0.028 (3)	−0.002 (3)	0.003 (2)	−0.004 (2)
C1	0.051 (5)	0.060 (5)	0.047 (4)	−0.004 (4)	0.005 (4)	0.010 (4)
C2	0.040 (4)	0.035 (4)	0.035 (4)	−0.004 (3)	0.005 (3)	0.011 (3)
C3	0.042 (4)	0.029 (3)	0.034 (4)	0.004 (3)	0.002 (3)	−0.003 (3)
C4	0.030 (3)	0.044 (4)	0.033 (4)	0.005 (3)	0.007 (3)	0.001 (3)
C5	0.038 (4)	0.035 (4)	0.022 (3)	0.003 (3)	0.008 (3)	0.004 (3)
C6	0.041 (4)	0.040 (4)	0.050 (4)	0.004 (3)	0.021 (3)	−0.003 (3)
C7	0.038 (4)	0.050 (4)	0.051 (4)	0.008 (3)	0.020 (3)	0.014 (4)
C8	0.039 (4)	0.031 (3)	0.027 (3)	0.002 (3)	0.009 (3)	0.002 (3)
C9	0.025 (3)	0.042 (4)	0.020 (3)	0.007 (3)	0.004 (2)	0.004 (3)
C10	0.053 (5)	0.049 (4)	0.050 (4)	0.004 (4)	0.025 (4)	0.008 (4)
C11	0.042 (4)	0.040 (4)	0.037 (4)	0.004 (3)	0.020 (3)	0.012 (3)

C12	0.049 (4)	0.038 (4)	0.037 (4)	0.006 (3)	0.014 (3)	−0.006 (3)
C13	0.041 (4)	0.040 (4)	0.033 (4)	−0.010 (3)	0.009 (3)	−0.009 (3)
C14	0.032 (3)	0.034 (4)	0.032 (3)	−0.004 (3)	0.012 (3)	0.002 (3)
C15	0.049 (4)	0.043 (4)	0.029 (4)	−0.001 (3)	0.009 (3)	−0.010 (3)
C16	0.041 (4)	0.045 (4)	0.035 (4)	−0.004 (3)	0.004 (3)	−0.004 (3)
C17	0.037 (4)	0.041 (4)	0.041 (4)	−0.007 (3)	0.009 (3)	0.002 (3)
C18	0.030 (4)	0.043 (4)	0.030 (4)	−0.011 (3)	0.009 (3)	−0.002 (3)

Geometric parameters (Å, °)

S1—O2	1.413 (4)	C4—C5	1.388 (9)
S1—O1	1.429 (4)	C4—H4	0.9300
S1—N1	1.625 (5)	C5—C6	1.370 (8)
S1—C5	1.769 (6)	C6—C7	1.371 (9)
S2—O5	1.417 (5)	C6—H6	0.9300
S2—O6	1.427 (5)	C7—H7A	0.9300
S2—N2	1.622 (5)	C8—C9	1.499 (8)
S2—C14	1.771 (6)	C8—H8A	0.9700
O3—C9	1.308 (7)	C8—H8B	0.9700
O3—H3	0.8200	C10—C11	1.506 (9)
O4—C9	1.216 (7)	C10—H10A	0.9600
O7—C18	1.311 (7)	C10—H10B	0.9600
O7—H7	0.8200	C10—H10C	0.9600
O8—C18	1.208 (8)	C11—C16	1.373 (9)
N1—C8	1.453 (7)	C11—C12	1.382 (9)
N1—H1	0.8600	C12—C13	1.370 (9)
N2—C17	1.457 (8)	C12—H12	0.9300
N2—H2	0.8600	C13—C14	1.381 (9)
C1—C2	1.486 (9)	C13—H13	0.9300
C1—H1A	0.9600	C14—C15	1.380 (8)
C1—H1B	0.9600	C15—C16	1.377 (9)
C1—H1C	0.9600	C15—H15	0.9300
C2—C7	1.380 (10)	C16—H16	0.9300
C2—C3	1.389 (9)	C17—C18	1.506 (9)
C3—C4	1.374 (9)	C17—H17A	0.9700
C3—H3A	0.9300	C17—H17B	0.9700
O2—S1—O1	120.4 (3)	C2—C7—H7A	118.6
O2—S1—N1	106.4 (3)	N1—C8—C9	114.2 (5)
O1—S1—N1	106.4 (3)	N1—C8—H8A	108.7
O2—S1—C5	107.3 (3)	C9—C8—H8A	108.7
O1—S1—C5	108.6 (3)	N1—C8—H8B	108.7
N1—S1—C5	107.0 (3)	C9—C8—H8B	108.7
O5—S2—O6	120.3 (3)	H8A—C8—H8B	107.6
O5—S2—N2	106.4 (3)	O4—C9—O3	124.7 (6)
O6—S2—N2	106.1 (3)	O4—C9—C8	125.2 (5)
O5—S2—C14	107.5 (3)	O3—C9—C8	110.0 (5)
O6—S2—C14	108.2 (3)	C11—C10—H10A	109.5
N2—S2—C14	107.8 (3)	C11—C10—H10B	109.5
C9—O3—H3	109.5	H10A—C10—H10B	109.5

C18—O7—H7	109.5	C11—C10—H10C	109.5
C8—N1—S1	117.0 (4)	H10A—C10—H10C	109.5
C8—N1—H1	121.5	H10B—C10—H10C	109.5
S1—N1—H1	121.5	C16—C11—C12	117.6 (6)
C17—N2—S2	117.2 (4)	C16—C11—C10	121.3 (6)
C17—N2—H2	121.4	C12—C11—C10	121.1 (6)
S2—N2—H2	121.4	C13—C12—C11	121.8 (6)
C2—C1—H1A	109.5	C13—C12—H12	119.1
C2—C1—H1B	109.5	C11—C12—H12	119.1
H1A—C1—H1B	109.5	C12—C13—C14	119.2 (6)
C2—C1—H1C	109.5	C12—C13—H13	120.4
H1A—C1—H1C	109.5	C14—C13—H13	120.4
H1B—C1—H1C	109.5	C15—C14—C13	120.4 (6)
C7—C2—C3	116.7 (6)	C15—C14—S2	119.4 (5)
C7—C2—C1	122.4 (6)	C13—C14—S2	120.0 (5)
C3—C2—C1	120.9 (6)	C16—C15—C14	118.6 (6)
C4—C3—C2	122.0 (6)	C16—C15—H15	120.7
C4—C3—H3A	119.0	C14—C15—H15	120.7
C2—C3—H3A	119.0	C11—C16—C15	122.3 (6)
C3—C4—C5	119.0 (6)	C11—C16—H16	118.9
C3—C4—H4	120.5	C15—C16—H16	118.9
C5—C4—H4	120.5	N2—C17—C18	113.2 (5)
C6—C5—C4	120.4 (6)	N2—C17—H17A	108.9
C6—C5—S1	120.9 (5)	C18—C17—H17A	108.9
C4—C5—S1	118.7 (5)	N2—C17—H17B	108.9
C5—C6—C7	119.0 (6)	C18—C17—H17B	108.9
C5—C6—H6	120.5	H17A—C17—H17B	107.8
C7—C6—H6	120.5	O8—C18—O7	124.0 (6)
C6—C7—C2	122.8 (6)	O8—C18—C17	125.4 (6)
C6—C7—H7A	118.6	O7—C18—C17	110.6 (6)
O2—S1—N1—C8	52.6 (5)	S1—N1—C8—C9	−93.0 (5)
O1—S1—N1—C8	−177.8 (4)	N1—C8—C9—O4	−8.0 (9)
C5—S1—N1—C8	−61.8 (5)	N1—C8—C9—O3	171.5 (5)
O5—S2—N2—C17	−51.9 (5)	C16—C11—C12—C13	−0.6 (10)
O6—S2—N2—C17	178.9 (5)	C10—C11—C12—C13	179.8 (6)
C14—S2—N2—C17	63.2 (5)	C11—C12—C13—C14	0.1 (10)
C7—C2—C3—C4	−0.8 (9)	C12—C13—C14—C15	−0.3 (9)
C1—C2—C3—C4	−180.0 (6)	C12—C13—C14—S2	175.8 (5)
C2—C3—C4—C5	1.8 (9)	O5—S2—C14—C15	−12.0 (6)
C3—C4—C5—C6	−1.0 (9)	O6—S2—C14—C15	119.3 (5)
C3—C4—C5—S1	−179.0 (5)	N2—S2—C14—C15	−126.4 (5)
O2—S1—C5—C6	10.9 (6)	O5—S2—C14—C13	171.9 (5)
O1—S1—C5—C6	−120.8 (5)	O6—S2—C14—C13	−56.8 (6)
N1—S1—C5—C6	124.8 (5)	N2—S2—C14—C13	57.5 (6)
O2—S1—C5—C4	−171.1 (5)	C13—C14—C15—C16	1.0 (10)
O1—S1—C5—C4	57.2 (5)	S2—C14—C15—C16	−175.1 (5)
N1—S1—C5—C4	−57.3 (5)	C12—C11—C16—C15	1.3 (10)
C4—C5—C6—C7	−0.6 (9)	C10—C11—C16—C15	−179.1 (6)
S1—C5—C6—C7	177.3 (5)	C14—C15—C16—C11	−1.5 (10)

C5—C6—C7—C2	1.7 (10)	S2—N2—C17—C18	82.7 (6)
C3—C2—C7—C6	−1.0 (10)	N2—C17—C18—O8	22.6 (9)
C1—C2—C7—C6	178.2 (6)	N2—C17—C18—O7	−158.9 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4^{i}	0.86	2.57	3.167 (6)	127
N2—H2···O8^{ii}	0.86	2.59	3.231 (7)	132
O3—H3···O4^{iii}	0.82	1.94	2.751 (6)	172
O7—H7···O8^{iv}	0.82	1.94	2.745 (7)	167
C1—H1B···O5^{v}	0.96	2.56	3.342 (7)	138
C10—H10B···O2^{vi}	0.96	2.40	3.353 (7)	170
C17—H17B···O6^{ii}	0.97	2.45	3.211 (6)	134

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

Fig. 1

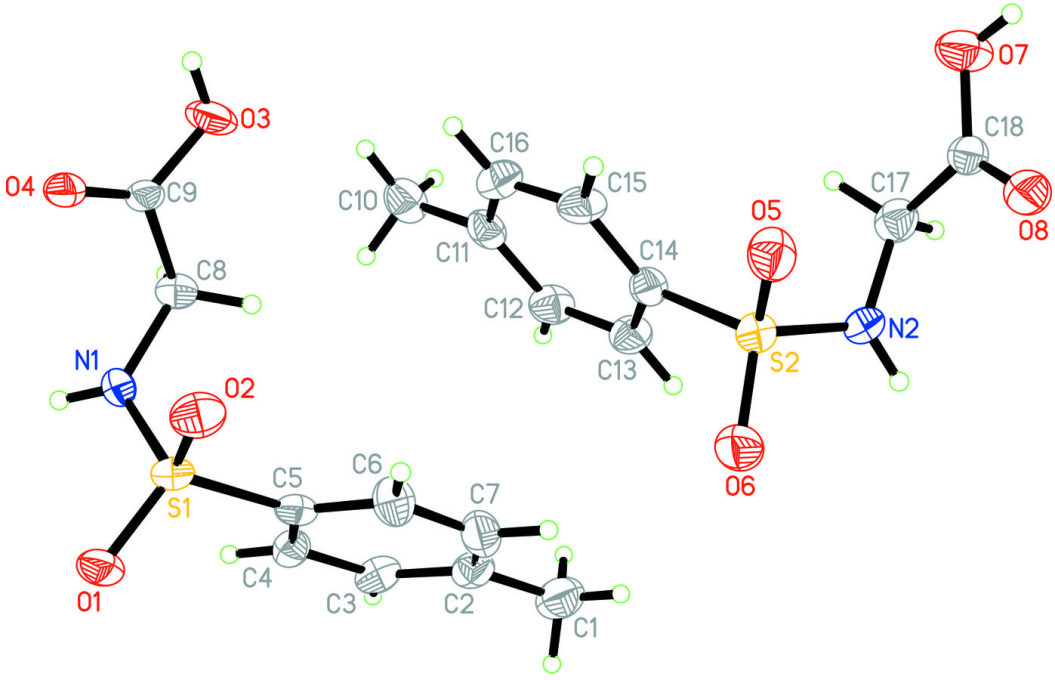
O7
O3
C18
C16
C15
O4
C9
C10
C17
O5
O8
C11
C14
C8
C12
N2
N1
C13
S2
O2
O6
C5
C6
C7
S1
C4
C3
C2
C1
O1

Fig. 2