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N-(4-Sulfamoylphenyl)acetamide

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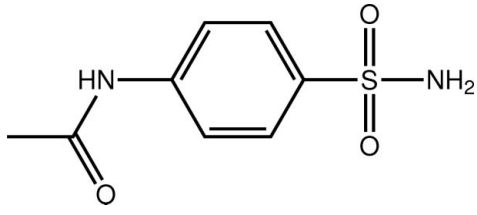
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.079; data-to-parameter ratio = 13.3.

In the title compound, $C_8H_{10}N_2O_3S$, the dihedral angle between the acetamide group and the benzene ring is 15.59 (12)° and the amino group is close to being perpendicular to the benzene ring [N—S—C_{ar}—C_{ar} (ar = aromatic) torsion angle = 109.4 (2)°]. In the crystal, molecules are linked into supramolecular tubes parallel to [001] by amine–amide N—H···O interactions and these are connected into the three-dimensional architecture by amide–sulfonamide N—H···O hydrogen bonds. The crystal studied was a racemic twin.

Related literature

For background to the biological applications of related sulfonamides, see: Croitoru *et al.* (2004); Dogruer *et al.* (2010). For related structures, see: Asiri *et al.* (2011, 2012).



Experimental

Crystal data

$C_8H_{10}N_2O_3S$
M_r = 214.24
Tetragonal, $P\bar{4}2_1c$
a = 15.2631 (4) Å
c = 8.0571 (4) Å
V = 1877.00 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 100 K
0.40 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.880, T_{max} = 0.984
3827 measured reflections
1862 independent reflections
1698 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.079
S = 1.02
1862 reflections
140 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 625 Friedel pairs
Flack parameter: 0.48 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.88 (1)	2.08 (1)	2.935 (3)	163 (3)
N1—H2···O3^{ii}	0.89 (1)	2.04 (1)	2.929 (3)	178 (3)
N2—H3···O1^{iii}	0.88 (1)	2.34 (2)	3.156 (3)	155 (2)

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6682).

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supplementary materials

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N-(4-Sulfamoylphenyl)acetamide

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Comment

The crystal and molecular structure of *N*-(4-sulfamoylphenyl)acetamide (I) is reported herein in continuation of on-going structural studies of sulfonamide derivatives (Asiri *et al.*, 2011; Asiri *et al.*, 2012), of interest owing to their biological activity, for example, to selectively inhibit COX–2 (Croitoru *et al.*, 2004) and as they exhibit anti-microbial and anti-fungal activities (Dogruer *et al.* 2010).

In (I), Fig. 1. the amide residue is twisted out of the plane of the benzene ring to which it is attached as seen in the value of the C7—N2—C4—C3 torsion angle of -166.2 (2)°, and the amino group occupies a position perpendicular to the benzene ring with the N1—S1—C1—C2 torsion angle being 109.4 (2)°.

Each of the N—H hydrogen atoms forms a hydrogen bond to an oxygen atom with the amide-O3 atom being bifurcated, Table 1. The amino-H atoms bridge the amide-O atoms to generate supramolecular tubes along the *c* axis. These are connected into the three-dimensional architecture by amide-*H*···*O*(sulfonamide) hydrogen bonds, Fig. 2 and Table 1.

Experimental

2-Acetyl chloride (0.784 g, 25 mmol) in pyridine (5 ml) was slowly added to a solution of sulfanilamide (2.00 g, 11 mmol) in pyridine (20 ml) and the reaction mixture was stirred at 258 K for 4 h under anhydrous conditions. After warming the solution to room temperature, the pyridine was removed *in vacuo* and the resulting white solid dissolved in ethyl acetate. The organic extract was washed with 3 *M* hydrochloric acid (30 ml) then with saturated sodium bicarbonate solution (30 ml) and finally with brine. Drying over magnesium sulfate and evaporation yielded a white solid which was recrystallized from ethanol to give the title compound as colourless prisms. Yield: 74%. *M*.pt: 491–492 K.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.98 Å, U_{iso}(H) = 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation. The N—H atoms were located in a difference Fourier map, and were refined with a distance restraint of N—H = 0.88±0.01 Å; their U_{iso} values were refined. Owing to poor agreement, the (7 7 0) reflection was omitted from the final cycles of refinement. The Flack (Flack, 1983) parameter was calculated from 625 Friedel pairs. The refined value, *i.e*. 0.48 (9). indicates that the crystal examined was a racemic twin.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

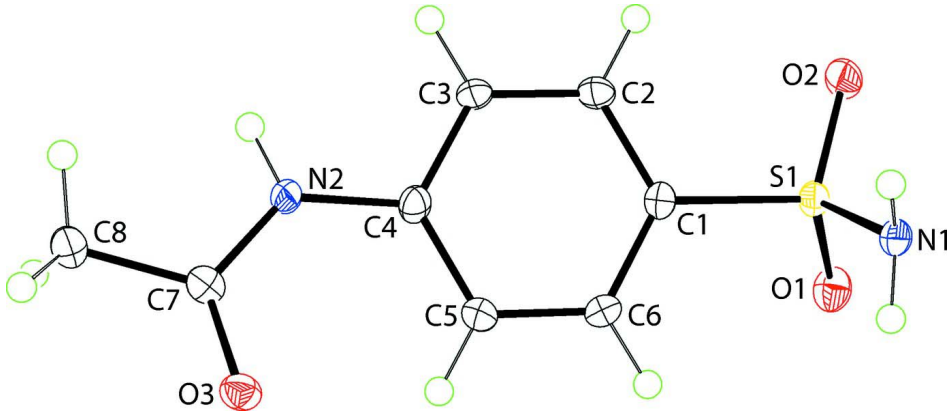

Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

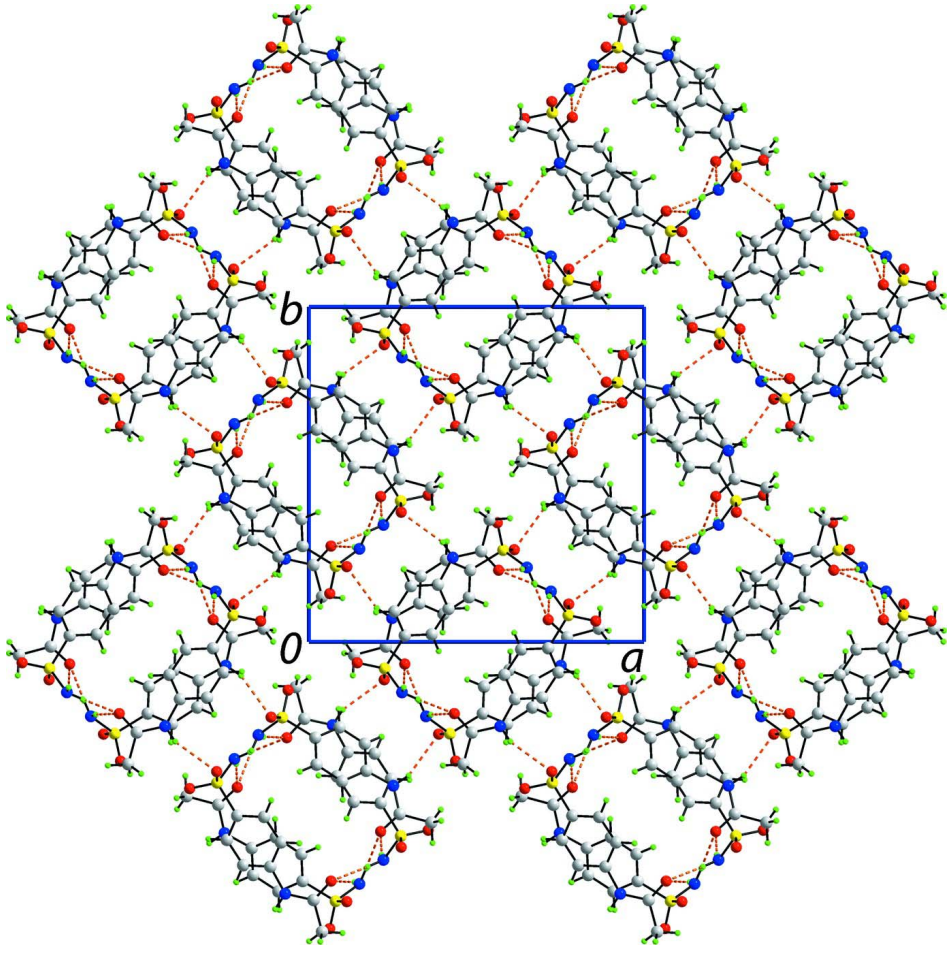

Figure 2

A view in projection down the *c* axis of the unit-cell contents of (I). The N—H···O hydrogen bonds are shown as orange dashed lines.

N-(4-Sulfamoylphenyl)acetamide

Crystal data

$C_8H_{10}N_2O_3S$
$M_r = 214.24$
Tetragonal, $P\bar{4}2_1c$
Hall symbol: P -4 2n
$a = 15.2631$ (4) Å
$c = 8.0571$ (4) Å
$V = 1877.00$ (11) Å^3
$Z = 8$
$F(000) = 896$
$D_x = 1.516$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2081 reflections
$\theta = 2.7$–$27.5°$
$\mu = 0.33$ mm^{-1}
$T = 100$ K
Prism, colourless
0.40 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.880$, $T_{max} = 0.984$
3827 measured reflections
1862 independent reflections
1698 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.7°$
$h = -12 \rightarrow 19$
$k = -18 \rightarrow 10$
$l = -10 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.079$
$S = 1.02$
1862 reflections
140 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.7254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983), 625 Friedel pairs
Flack parameter: 0.48 (9)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.42050 (3)	0.72593 (3)	0.79689 (8)	0.01459 (14)
O1	0.38712 (11)	0.72467 (12)	0.6291 (2)	0.0220 (4)
O2	0.43783 (11)	0.64415 (10)	0.8775 (2)	0.0212 (4)
O3	0.71401 (10)	1.06596 (10)	0.73297 (19)	0.0184 (4)
N1	0.34929 (12)	0.77773 (13)	0.9064 (3)	0.0165 (4)
H1	0.364 (2)	0.783 (2)	1.0119 (16)	0.038 (9)*
H2	0.329 (2)	0.8243 (14)	0.853 (4)	0.053 (11)*
N2	0.75181 (12)	0.92922 (13)	0.8186 (2)	0.0165 (4)
H3	0.7976 (12)	0.8991 (16)	0.852 (3)	0.025 (8)*
C1	0.51900 (14)	0.78616 (14)	0.7979 (3)	0.0153 (4)
C2	0.59105 (15)	0.75505 (15)	0.8838 (3)	0.0163 (5)
H2A	0.5884	0.7002	0.9394	0.020*

C3	0.66665 (15)	0.80408 (14)	0.8881 (3)	0.0164 (5)
H3A	0.7165	0.7826	0.9459	0.020*
C4	0.67072 (14)	0.88484 (15)	0.8086 (3)	0.0155 (5)
C5	0.59846 (15)	0.91651 (16)	0.7215 (4)	0.0227 (5)
H5	0.6011	0.9714	0.6662	0.027*
C6	0.52250 (16)	0.86653 (15)	0.7170 (4)	0.0226 (5)
H6	0.4727	0.8873	0.6583	0.027*
C7	0.77054 (15)	1.01386 (14)	0.7821 (3)	0.0158 (4)
C8	0.86506 (15)	1.03931 (15)	0.8005 (3)	0.0196 (5)
H8A	0.8689	1.1001	0.8392	0.029*
H8B	0.8946	1.0339	0.6930	0.029*
H8C	0.8934	1.0006	0.8813	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0124 (3)	0.0141 (3)	0.0172 (2)	−0.0010 (2)	0.0011 (2)	−0.0006 (3)
O1	0.0201 (8)	0.0260 (9)	0.0199 (8)	−0.0028 (8)	−0.0005 (7)	−0.0042 (8)
O2	0.0197 (9)	0.0116 (8)	0.0323 (9)	−0.0012 (7)	0.0006 (8)	0.0017 (7)
O3	0.0197 (8)	0.0153 (8)	0.0202 (8)	0.0024 (6)	0.0016 (7)	0.0017 (7)
N1	0.0122 (9)	0.0199 (10)	0.0176 (9)	0.0014 (8)	0.0033 (9)	0.0026 (9)
N2	0.0103 (9)	0.0147 (9)	0.0247 (10)	0.0011 (7)	0.0004 (8)	0.0038 (9)
C1	0.0129 (10)	0.0167 (10)	0.0163 (9)	−0.0010 (9)	0.0012 (10)	−0.0009 (11)
C2	0.0174 (11)	0.0119 (10)	0.0197 (11)	0.0028 (9)	0.0001 (10)	0.0017 (9)
C3	0.0138 (11)	0.0140 (11)	0.0215 (11)	0.0039 (9)	−0.0002 (10)	0.0041 (10)
C4	0.0119 (10)	0.0148 (10)	0.0197 (11)	0.0010 (8)	0.0020 (10)	−0.0012 (10)
C5	0.0167 (11)	0.0188 (11)	0.0326 (13)	−0.0003 (9)	−0.0011 (11)	0.0109 (12)
C6	0.0147 (11)	0.0237 (12)	0.0296 (12)	0.0015 (10)	−0.0034 (12)	0.0107 (12)
C7	0.0180 (11)	0.0145 (10)	0.0150 (10)	0.0012 (9)	0.0035 (10)	−0.0010 (10)
C8	0.0188 (11)	0.0186 (11)	0.0214 (11)	−0.0034 (9)	0.0003 (11)	0.0012 (11)

Geometric parameters (Å, º)

S1—O2	1.4316 (17)	C2—C3	1.376 (3)
S1—O1	1.4446 (17)	C2—H2A	0.9500
S1—N1	1.608 (2)	C3—C4	1.391 (3)
S1—C1	1.762 (2)	C3—H3A	0.9500
O3—C7	1.238 (3)	C4—C5	1.394 (3)
N1—H1	0.880 (10)	C5—C6	1.388 (3)
N1—H2	0.885 (10)	C5—H5	0.9500
N2—C7	1.355 (3)	C6—H6	0.9500
N2—C4	1.413 (3)	C7—C8	1.501 (3)
N2—H3	0.878 (10)	C8—H8A	0.9800
C1—C2	1.384 (3)	C8—H8B	0.9800
C1—C6	1.390 (3)	C8—H8C	0.9800
O2—S1—O1	118.55 (11)	C4—C3—H3A	119.7
O2—S1—N1	107.74 (11)	C3—C4—C5	120.3 (2)
O1—S1—N1	106.36 (10)	C3—C4—N2	115.9 (2)
O2—S1—C1	107.16 (10)	C5—C4—N2	123.8 (2)

O1—S1—C1	108.19 (11)	C6—C5—C4	118.9 (2)
N1—S1—C1	108.52 (11)	C6—C5—H5	120.5
S1—N1—H1	114 (2)	C4—C5—H5	120.5
S1—N1—H2	111 (2)	C5—C6—C1	120.3 (2)
H1—N1—H2	119 (3)	C5—C6—H6	119.9
C7—N2—C4	128.99 (19)	C1—C6—H6	119.9
C7—N2—H3	113.4 (18)	O3—C7—N2	122.3 (2)
C4—N2—H3	117.6 (18)	O3—C7—C8	122.33 (19)
C2—C1—C6	120.5 (2)	N2—C7—C8	115.34 (19)
C2—C1—S1	120.10 (17)	C7—C8—H8A	109.5
C6—C1—S1	119.40 (18)	C7—C8—H8B	109.5
C3—C2—C1	119.5 (2)	H8A—C8—H8B	109.5
C3—C2—H2A	120.2	C7—C8—H8C	109.5
C1—C2—H2A	120.2	H8A—C8—H8C	109.5
C2—C3—C4	120.5 (2)	H8B—C8—H8C	109.5
C2—C3—H3A	119.7		

O2—S1—C1—C2	−6.7 (2)	C2—C3—C4—N2	−179.1 (2)
O1—S1—C1—C2	−135.60 (19)	C7—N2—C4—C3	−166.2 (2)
N1—S1—C1—C2	109.4 (2)	C7—N2—C4—C5	15.6 (4)
O2—S1—C1—C6	175.7 (2)	C3—C4—C5—C6	0.5 (4)
O1—S1—C1—C6	46.8 (2)	N2—C4—C5—C6	178.6 (2)
N1—S1—C1—C6	−68.2 (2)	C4—C5—C6—C1	−0.1 (4)
C6—C1—C2—C3	−0.3 (4)	C2—C1—C6—C5	0.0 (4)
S1—C1—C2—C3	−177.88 (19)	S1—C1—C6—C5	177.6 (2)
C1—C2—C3—C4	0.7 (3)	C4—N2—C7—O3	0.5 (4)
C2—C3—C4—C5	−0.8 (4)	C4—N2—C7—C8	−177.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.88 (1)	2.08 (1)	2.935 (3)	163 (3)
N1—H2···O3^{ii}	0.89 (1)	2.04 (1)	2.929 (3)	178 (3)
N2—H3···O1^{iii}	0.88 (1)	2.34 (2)	3.156 (3)	155 (2)

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