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N-[4-(Benzylsulfamoyl)phenyl]acetamide

Peter John,[a] Waqar Ahmad,[a] Islam Ullah Khan,[a]‡ Shahzad Sharif[a] and Edward R. T. Tiekink[b]*

[a]Materials Chemistry Laboratory, Department of Chemistry, Government College University, Lahore 54000, Pakistan, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: edward.tiekink@gmail.com

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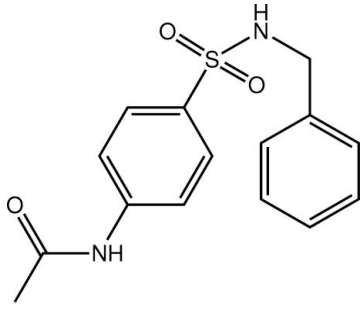
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.124; data-to-parameter ratio = 18.2.

A folded conformation is found for the title compound, $C_{15}H_{16}N_2O_3S$, whereby the benzene rings come into close proximity [centroid–centroid distance = 4.0357 (12) Å and the dihedral angle between them = 24.37 (10)°]. The amide group is coplanar with the benzene ring to which it is bound [C—C—N—C torsion angle = 11.1 (3)°]. In the crystal packing, two-dimensional arrays in the (101) plane are formed *via* N—H···O hydrogen bonding.

Related literature

For background to the pharmacological uses of sulfonamides, see: Beate *et al.* (1998); Kazmierski *et al.* (2004). For related structures, see: Khan *et al.* (2010); Sharif *et al.* (2010).



Experimental

Crystal data

$C_{15}H_{16}N_2O_3S$
M_r = 304.37
Monoclinic, $P2_1/n$
a = 9.0646 (9) Å
b = 13.6888 (14) Å
c = 12.1651 (12) Å
β = 98.635 (5)°
V = 1492.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 293 K
0.19 × 0.09 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.868, T_{max} = 0.948
13777 measured reflections
3577 independent reflections
2689 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 1.02
3577 reflections
197 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O3^{i}	0.89 (2)	2.00 (2)	2.877 (2)	168 (2)
N2—H2n···O2^{ii}	0.90 (2)	2.03 (2)	2.921 (2)	172 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: JJ2043).

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‡ Additional correspondence author, e-mail: iuklodhi@yahoo.com.

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N-[4-(Benzylsulfamoyl)phenyl]acetamide

Peter John, Waqar Ahmad, Islam Ullah Khan, Shahzad Sharif and Edward R. T. Tiekink

S1. Comment

Sulfonamide drugs are used, for example, as inhibitors of HIV infection (Kazmierski *et al.*, 2004) and as anti-hypertensive drugs (Beate *et al.*, 1998). In connection with on-going structural studies of sulfonamides (Khan *et al.*, 2010; Sharif *et al.*, 2010), the crystal and molecular structure of the title compound, $C_{15}H_{16}N_2O_3S$, was investigated.

The molecule of $C_{15}H_{16}N_2O_3S$ has a folded conformation with the benzene ring of the benzyl group somewhat orientated over the S-bound benzene ring. The rings are approximately parallel, forming a dihedral angle of 24.37 (10) °; the distance between the ring centroids is 4.0357 (12) Å. The amide group is essentially co-planar with the ring to which it is bound as seen in the C10–C11–N2–C14 torsion angle of 11.1 (3) °.

The crystal packing is dominated by N–H···O hydrogen bonds whereby the N1–H atom forms a hydrogen bond to the amide-carbonyl, and the amide N2–H forms a contact with the S-bound O2 atom, Table 1. The former leads to centrosymmetric aggregates and these are connected by the latter into a 2-D array in the (1 0 1) plane, Fig. 2.

S2. Experimental

To 4-acetamidobenzenesulfonyl chloride (498 mg, 2.14 mmol) in distilled water (10 ml) was added benzylamine (234 ml, 2.14 mmol), the reaction mixture was stirred at room temperature while maintaining the pH of the reaction mixture at 8 using 3% sodium carbonate. The progress of the reaction was monitored by TLC. After consumption of all the reactants, the precipitates were filtered, dried and crystallized from methanol to yield colourless crystals.

S3. Refinement

The C-bound H atoms were geometrically placed (C–H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2–1.5U_{eq}(C). The N-bound H atom was refined with the distance restraint N–H = 0.88±0.01 Å, and with U_{iso}(H) = 1.2U_{eq}(N).

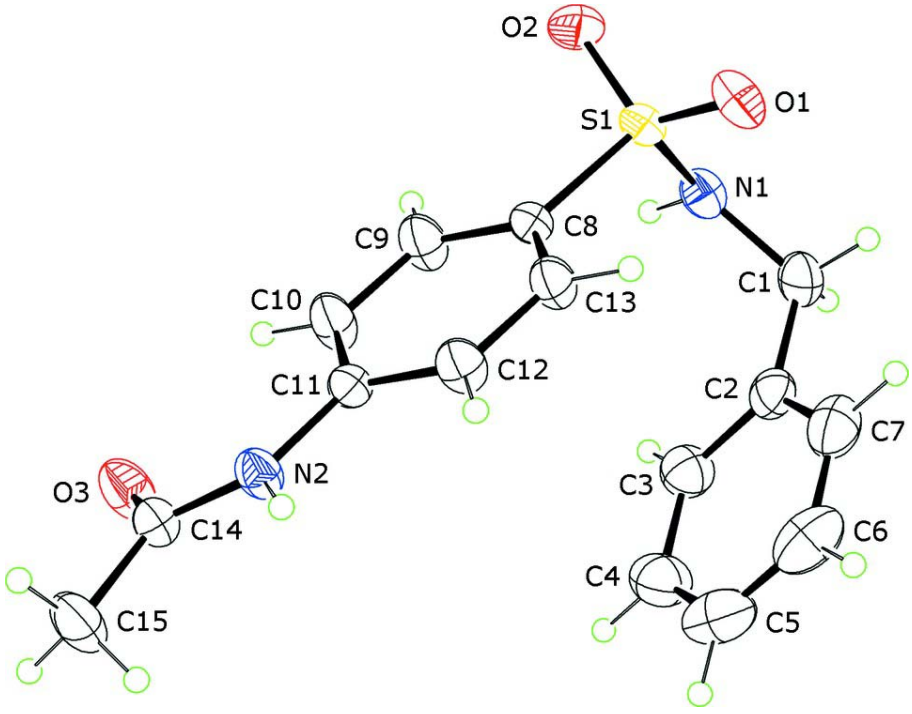

Figure 1

The molecular structure of $C_{15}H_{16}N_2O_3S$ showing the atom-labelling scheme and displacement ellipsoids at the 35% probability level.

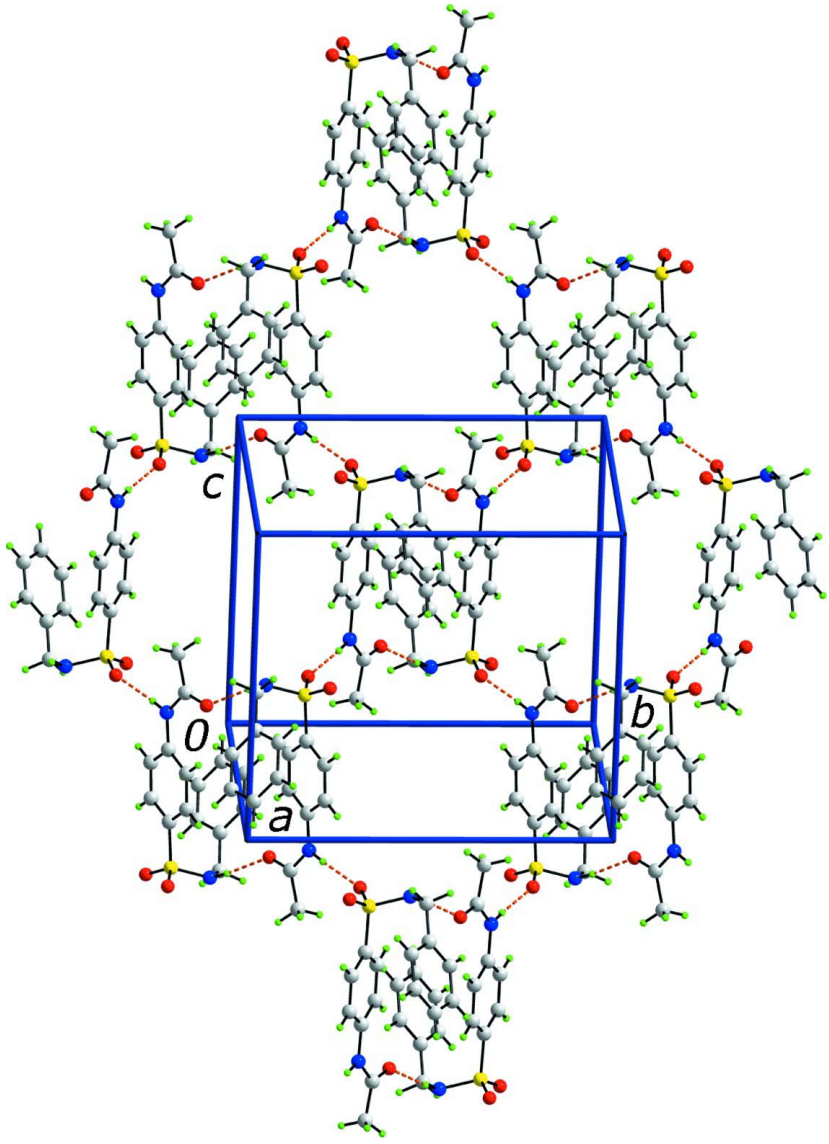

Figure 2

A view of the supramolecular 2-D array in the (1 0 1) plane mediated by N–H···O hydrogen bonding (orange dashed lines) in $C_{15}H_{16}N_2O_3S$. Colour code: S, yellow; O, red; N, blue; C, grey; and H, green.

N-[4-(Benzylsulfamoyl)phenyl]acetamide

Crystal data

$C_{15}H_{16}N_2O_3S$
M_r = 304.37
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 9.0646 (9) Å
b = 13.6888 (14) Å
c = 12.1651 (12) Å
β = 98.635 (5)°
V = 1492.4 (3) Å^3
Z = 4
$F(000)$ = 640
D_x = 1.355 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4154 reflections
θ = 2.6–27.9°
μ = 0.23 mm^{-1}
T = 293 K
Prism, colourless
0.19 × 0.09 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.868, T_{max} = 0.948
13777 measured reflections
3577 independent reflections
2689 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 28.0°, θ_{min} = 2.3°
h = −11→11
k = −18→17
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 1.02
3577 reflections
197 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 0.3076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.11090 (5)	0.33181 (3)	0.82483 (3)	0.03999 (15)
O1	0.21873 (16)	0.27094 (10)	0.88809 (10)	0.0536 (4)
O2	−0.04454 (15)	0.31532 (11)	0.82667 (12)	0.0594 (4)
O3	0.02478 (16)	0.40834 (11)	0.26180 (11)	0.0596 (4)
N1	0.14186 (17)	0.44201 (11)	0.86867 (12)	0.0448 (4)
H1N	0.0786 (18)	0.4846 (12)	0.8311 (15)	0.054*
N2	0.20419 (16)	0.31175 (10)	0.35277 (11)	0.0399 (3)
H2N	0.2876 (15)	0.2778 (12)	0.3473 (16)	0.048*
C1	0.2944 (2)	0.47687 (16)	0.90443 (16)	0.0559 (5)
H1A	0.3409	0.4347	0.9638	0.067*
H1B	0.2888	0.5418	0.9355	0.067*
C2	0.3944 (2)	0.48133 (13)	0.81674 (15)	0.0464 (4)
C3	0.3606 (2)	0.54229 (14)	0.72574 (17)	0.0532 (5)
H3	0.2748	0.5805	0.7184	0.064*
C4	0.4533 (3)	0.54678 (16)	0.6461 (2)	0.0661 (6)

H4	0.4295	0.5880	0.5852	0.079*
C5	0.5799 (3)	0.49141 (18)	0.6555 (2)	0.0732 (7)
H5	0.6416	0.4945	0.6011	0.088*
C6	0.6154 (3)	0.43158 (18)	0.7452 (2)	0.0745 (7)
H6	0.7021	0.3943	0.7523	0.089*
C7	0.5230 (2)	0.42612 (15)	0.8254 (2)	0.0611 (6)
H7	0.5477	0.3848	0.8860	0.073*
C8	0.13636 (18)	0.32476 (11)	0.68406 (13)	0.0354 (3)
C9	0.0308 (2)	0.36444 (16)	0.60359 (15)	0.0499 (5)
H9	−0.0539	0.3934	0.6238	0.060*
C10	0.0494 (2)	0.36167 (15)	0.49303 (15)	0.0496 (5)
H10	−0.0223	0.3888	0.4390	0.059*
C11	0.17580 (18)	0.31823 (11)	0.46307 (13)	0.0343 (3)
C12	0.2803 (2)	0.27757 (14)	0.54465 (14)	0.0436 (4)
H12	0.3647	0.2477	0.5250	0.052*
C13	0.26102 (19)	0.28078 (13)	0.65483 (14)	0.0426 (4)
H13	0.3321	0.2533	0.7091	0.051*
C14	0.1335 (2)	0.35627 (13)	0.26110 (14)	0.0418 (4)
C15	0.1978 (3)	0.33645 (17)	0.15660 (16)	0.0605 (6)
H15A	0.1635	0.2741	0.1270	0.091*
H15B	0.3048	0.3360	0.1730	0.091*
H15C	0.1664	0.3865	0.1029	0.091*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0444 (3)	0.0476 (3)	0.0295 (2)	−0.00397 (18)	0.01067 (17)	0.00348 (17)
O1	0.0718 (10)	0.0527 (7)	0.0358 (6)	0.0085 (6)	0.0066 (6)	0.0080 (6)
O2	0.0492 (8)	0.0830 (10)	0.0502 (8)	−0.0168 (7)	0.0209 (6)	0.0030 (7)
O3	0.0599 (9)	0.0774 (10)	0.0420 (7)	0.0218 (7)	0.0096 (6)	0.0121 (7)
N1	0.0510 (9)	0.0497 (9)	0.0341 (7)	0.0033 (7)	0.0079 (6)	−0.0005 (6)
N2	0.0407 (8)	0.0491 (8)	0.0312 (7)	0.0066 (6)	0.0094 (6)	−0.0011 (6)
C1	0.0667 (13)	0.0620 (12)	0.0363 (9)	−0.0135 (10)	−0.0015 (9)	−0.0055 (9)
C2	0.0470 (10)	0.0429 (9)	0.0467 (10)	−0.0085 (8)	−0.0014 (8)	−0.0028 (8)
C3	0.0547 (12)	0.0492 (10)	0.0555 (11)	0.0010 (8)	0.0081 (9)	0.0034 (9)
C4	0.0772 (16)	0.0596 (13)	0.0634 (14)	−0.0104 (11)	0.0167 (12)	0.0071 (11)
C5	0.0672 (15)	0.0670 (14)	0.0917 (18)	−0.0175 (12)	0.0319 (14)	−0.0142 (13)
C6	0.0467 (13)	0.0666 (14)	0.109 (2)	−0.0009 (10)	0.0096 (13)	−0.0133 (14)
C7	0.0554 (13)	0.0516 (11)	0.0706 (14)	−0.0016 (9)	−0.0091 (11)	0.0039 (10)
C8	0.0362 (9)	0.0418 (8)	0.0290 (7)	−0.0043 (6)	0.0079 (6)	0.0004 (6)
C9	0.0395 (10)	0.0759 (13)	0.0357 (9)	0.0162 (9)	0.0105 (7)	0.0016 (9)
C10	0.0420 (10)	0.0736 (12)	0.0329 (9)	0.0161 (9)	0.0050 (7)	0.0031 (9)
C11	0.0351 (8)	0.0379 (8)	0.0305 (7)	−0.0024 (6)	0.0074 (6)	−0.0015 (6)
C12	0.0397 (9)	0.0541 (10)	0.0383 (9)	0.0122 (8)	0.0098 (7)	0.0001 (8)
C13	0.0408 (10)	0.0523 (10)	0.0341 (8)	0.0080 (8)	0.0038 (7)	0.0044 (7)
C14	0.0461 (10)	0.0468 (9)	0.0327 (8)	−0.0030 (8)	0.0063 (7)	−0.0006 (7)
C15	0.0711 (14)	0.0797 (15)	0.0328 (9)	0.0057 (11)	0.0145 (9)	0.0024 (9)

Geometric parameters (Å, º)

S1—O1	1.4199 (13)	C5—C6	1.363 (4)
S1—O2	1.4304 (14)	C5—H5	0.9300
S1—N1	1.6105 (16)	C6—C7	1.380 (3)
S1—C8	1.7647 (16)	C6—H6	0.9300
O3—C14	1.217 (2)	C7—H7	0.9300
N1—C1	1.466 (2)	C8—C9	1.374 (2)
N1—H1N	0.893 (9)	C8—C13	1.373 (2)
N2—C14	1.346 (2)	C9—C10	1.381 (2)
N2—C11	1.4064 (19)	C9—H9	0.9300
N2—H2N	0.899 (9)	C10—C11	1.387 (2)
C1—C2	1.501 (3)	C10—H10	0.9300
C1—H1A	0.9700	C11—C12	1.382 (2)
C1—H1B	0.9700	C12—C13	1.378 (2)
C2—C7	1.380 (3)	C12—H12	0.9300
C2—C3	1.383 (3)	C13—H13	0.9300
C3—C4	1.376 (3)	C14—C15	1.501 (2)
C3—H3	0.9300	C15—H15A	0.9600
C4—C5	1.366 (3)	C15—H15B	0.9600
C4—H4	0.9300	C15—H15C	0.9600
O1—S1—O2	119.90 (9)	C7—C6—H6	119.9
O1—S1—N1	107.38 (8)	C2—C7—C6	120.8 (2)
O2—S1—N1	105.41 (9)	C2—C7—H7	119.6
O1—S1—C8	108.31 (8)	C6—C7—H7	119.6
O2—S1—C8	106.21 (8)	C9—C8—C13	120.05 (15)
N1—S1—C8	109.33 (8)	C9—C8—S1	119.43 (13)
C1—N1—S1	120.86 (14)	C13—C8—S1	120.52 (13)
C1—N1—H1N	116.3 (13)	C8—C9—C10	120.62 (16)
S1—N1—H1N	112.0 (13)	C8—C9—H9	119.7
C14—N2—C11	129.01 (14)	C10—C9—H9	119.7
C14—N2—H2N	118.3 (13)	C9—C10—C11	119.62 (16)
C11—N2—H2N	112.4 (13)	C9—C10—H10	120.2
N1—C1—C2	116.46 (15)	C11—C10—H10	120.2
N1—C1—H1A	108.2	C12—C11—C10	119.21 (15)
C2—C1—H1A	108.2	C12—C11—N2	117.12 (14)
N1—C1—H1B	108.2	C10—C11—N2	123.66 (15)
C2—C1—H1B	108.2	C13—C12—C11	120.82 (15)
H1A—C1—H1B	107.3	C13—C12—H12	119.6
C7—C2—C3	118.3 (2)	C11—C12—H12	119.6
C7—C2—C1	121.10 (19)	C8—C13—C12	119.68 (16)
C3—C2—C1	120.57 (18)	C8—C13—H13	120.2
C4—C3—C2	120.4 (2)	C12—C13—H13	120.2
C4—C3—H3	119.8	O3—C14—N2	123.00 (16)
C2—C3—H3	119.8	O3—C14—C15	121.99 (17)
C5—C4—C3	120.7 (2)	N2—C14—C15	115.01 (16)
C5—C4—H4	119.7	C14—C15—H15A	109.5

C3—C4—H4	119.7	C14—C15—H15B	109.5
C6—C5—C4	119.7 (2)	H15A—C15—H15B	109.5
C6—C5—H5	120.2	C14—C15—H15C	109.5
C4—C5—H5	120.2	H15A—C15—H15C	109.5
C5—C6—C7	120.2 (2)	H15B—C15—H15C	109.5
C5—C6—H6	119.9		

O1—S1—N1—C1	35.74 (15)	O1—S1—C8—C13	−11.08 (17)
O2—S1—N1—C1	164.65 (14)	O2—S1—C8—C13	−141.10 (15)
C8—S1—N1—C1	−81.56 (15)	N1—S1—C8—C13	105.63 (15)
S1—N1—C1—C2	64.4 (2)	C13—C8—C9—C10	−0.8 (3)
N1—C1—C2—C7	−118.2 (2)	S1—C8—C9—C10	178.69 (16)
N1—C1—C2—C3	62.7 (2)	C8—C9—C10—C11	0.1 (3)
C7—C2—C3—C4	0.4 (3)	C9—C10—C11—C12	0.6 (3)
C1—C2—C3—C4	179.41 (19)	C9—C10—C11—N2	179.85 (18)
C2—C3—C4—C5	−0.1 (3)	C14—N2—C11—C12	−169.65 (17)
C3—C4—C5—C6	−0.5 (4)	C14—N2—C11—C10	11.1 (3)
C4—C5—C6—C7	0.7 (4)	C10—C11—C12—C13	−0.8 (3)
C3—C2—C7—C6	−0.1 (3)	N2—C11—C12—C13	179.98 (16)
C1—C2—C7—C6	−179.14 (19)	C9—C8—C13—C12	0.6 (3)
C5—C6—C7—C2	−0.5 (3)	S1—C8—C13—C12	−178.81 (14)
O1—S1—C8—C9	169.47 (15)	C11—C12—C13—C8	0.1 (3)
O2—S1—C8—C9	39.45 (17)	C11—N2—C14—O3	−3.2 (3)
N1—S1—C8—C9	−73.82 (16)	C11—N2—C14—C15	177.27 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1n···O3^{i}	0.89 (2)	2.00 (2)	2.877 (2)	168 (2)
N2—H2n···O2^{ii}	0.90 (2)	2.03 (2)	2.921 (2)	172 (2)

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