Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methyl-*N*-{4-[(5-methyl-1,2-oxazol-3-yl)sulfamoyl]phenyl}benzenesulfonamide

Muhammad Sohail,[a] Muhammad Nadeem Asghar,[a] M. Nawaz Tahir,[b]* Muhammad Shafique[c] and Muhammad Ashfaq[d]

[a]Forman Christian College (A Chartered University), Ferozepur Road, Lahore 54600, Pakistan, [b]University of Sargodha, Department of Physics, Sargodha, Pakistan, [c]Department of Chemistry, GC University, Lahore 54000, Pakistan, and [d]University of Gujrat, Department of Chemistry, Gujrat, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

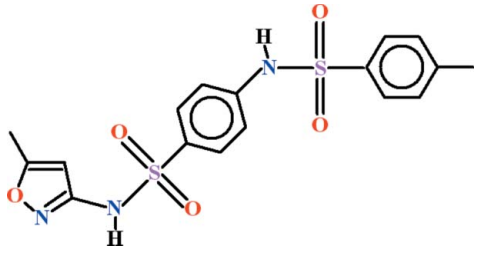
Received 2 February 2012; accepted 6 February 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.141; data-to-parameter ratio = 18.8.

In the title compound, $C_{17}H_{17}N_3O_5S_2$, the dihedral angle between the two benzene rings is 81.27 (8)° and the heterocyclic ring is oriented at 9.1 (2) and 76.01 (9)° with respect to these rings. Molecules are connected *via* N—H···N and N—H···O hydrogen bonds, generating an $R_2^2(8)$ motif, into chains running along the [001] direction. There is also an intramolecular C—H···O hydrogen bond completing an $S(6)$ ring motif. The polymeric chains are interlinked through intermolecular C—H···O hydrogen bonds.

Related literature

For a related crystal structure, see: Ashfaq *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{17}N_3O_5S_2$
M_r = 407.46
Monoclinic, $P2_1/c$
a = 10.6294 (6) Å
b = 12.2394 (7) Å
c = 14.9673 (11) Å
β = 106.863 (2)°
V = 1863.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 296 K
0.35 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.915, T_{max} = 0.938
17943 measured reflections
4629 independent reflections
2488 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.141
S = 1.02
4629 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3^{i}	0.86	2.04	2.859 (3)	159
N2—H2A···O1^{ii}	0.86	2.39	2.979 (3)	127
C2—H2···O4^{iii}	0.93	2.42	3.208 (4)	143
C13—H13···O2	0.93	2.49	3.134 (3)	126

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. The authors also acknowledge the technical support provided by Syed Muhammad Hussain Rizvi of Bana International, Karachi, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2455).

References

Ashfaq, M., Khan, I. U., Arshad, M. N., Ahmad, H. & Asghar, M. N. (2010). *Acta Cryst.* E**66**, o299.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2012). E**68**, o693 [doi:10.1107/S1600536812005260]

4-Methyl-*N*-{4-[(5-methyl-1,2-oxazol-3-yl)sulfamoyl]phenyl}benzenesulfonamide

Muhammad Sohail, Muhammad Nadeem Asghar, M. Nawaz Tahir, Muhammad Shafique and Muhammad Ashfaq

S1. Comment

The title compound (Fig. 1) has been synthesized as a part of the series of new sulfonamide derivatives. The aim of our research work is to find the potential sulfonamide derivatives possesing anti-microbial activity. The crystal structures of a similar compound, *N*-[4-(*p*-toluenesulfonamido)phenylsulfonyl]acetamide (Ashfaq *et al.*, 2010) has already been reported.

In (I), the phenyl rings A (C1–C6), B (C8—C13) and the heterocyclic five- membered ring C (C14/C15/C16/O5/N3) are planar with r. m. s. deviation of 0.0068 Å, 0.0031 Å and 0.0058 Å, respectively. The dihedral angles between A/B, A/C and B/C are 81.27 (8)°, 9.12 (20)° and 76.01 (9)°, respectively. There exist intramolecular hydrogen bond of C—H···O type (Table 1, Fig. 1) forming an S(6) ring motif (Bernstein *et al.*, 1995). There exist intermolecular hydrogen bonds of N—H···N and N—H···O types (Table 1, Fig. 2) due to which the molecules are connected from the ends to form one-dimensional polymeric network along the [0 0 1] direction and complete $R_2^2(8)$ ring motifs. The polymeric chains are interlinked through intermolecular hydrogen bond of C—H···O type (Table 1, Fig. 2).

S2. Experimental

Equimolar amount of 4-amino-*N*-(5-methyl-4,5-dihydro-1,2-oxazol-3-yl)benzenesulfonamide and *p*-toluenesulfonyl chloride was dissolved in 20 ml distilled water. The pH was adjusted to 8–9 using Na_2CO_3 (1 *M*) and the solution was stirred at room temperature for 6 h. The progress of reaction was monitored by the consumption of suspended *p*-toluenesulfonyl chloride. On completion, pH was adjusted to 2–3 using HCl (2 *N*). The precipitate formed was filtered, washed with distilled water and recrystallized from methanol to afford colorless prisms (m.p. 403 K).

S3. Refinement

The H-atoms were positioned geometrically (N–H = 0.86 Å, C–H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, N), where x = 1.5 for methyl groups and x = 1.2 for all H-atoms.

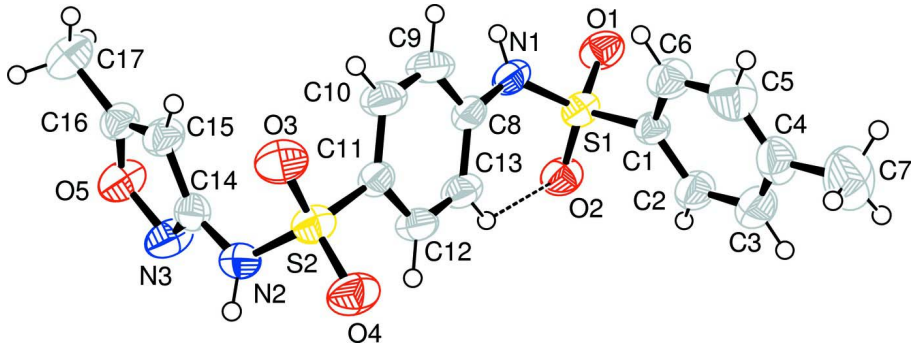


Figure 1

View of the title molecule with displacement ellipsoids drawn at the 50% probability level. H-atoms are shown as small circles of arbitrary radii. The dotted line represents an intramolecular C-H···O hydrogen bond

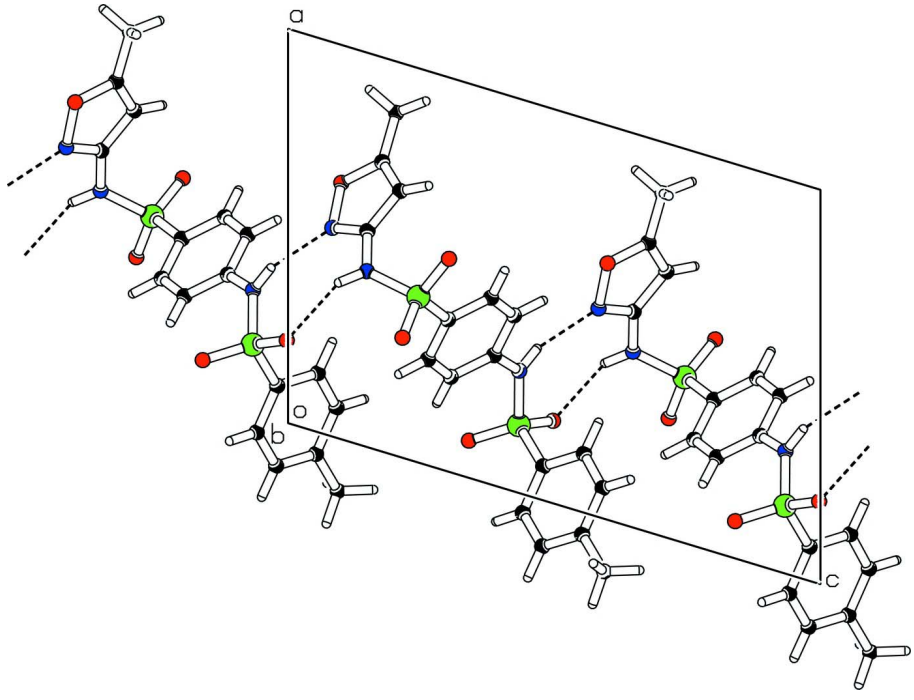


Figure 2

The partial packing (*PLATON*; Spek, 2009) which shows that molecules form polymeric chains extending along [0 0 1] direction.

4-Methyl-*N*-{4-[(5-methyl-1,2-oxazol-3- yl)sulfamoyl]phenyl}benzenesulfonamide

Crystal data

$C_{17}H_{17}N_3O_5S_2$
$M_r = 407.46$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.6294$ (6) Å
$b = 12.2394$ (7) Å
$c = 14.9673$ (11) Å
$\beta = 106.863$ (2)°
$V = 1863.5$ (2) Å^3
$Z = 4$
$F(000) = 848$
$D_x = 1.452$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2488 reflections
$\theta = 2.2$–28.3°
$\mu = 0.32$ mm^{-1}

T = 296 K
Prism, colorless

0.35 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.50 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.915, T_{max} = 0.938

17943 measured reflections
4629 independent reflections
2488 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −14→13
k = −14→16
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.141
S = 1.02
4629 reflections
246 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.1435P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > \sigma(F^2)$ 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	0.17178 (7)	0.12476 (6)	0.43330 (5)	0.0475 (3)
S2	0.42023 (7)	0.58034 (6)	0.24478 (5)	0.0485 (3)
O1	0.20899 (18)	0.03512 (15)	0.49755 (15)	0.0596 (8)
O2	0.09435 (18)	0.10311 (16)	0.33965 (14)	0.0575 (7)
O3	0.54004 (19)	0.62547 (15)	0.30218 (14)	0.0594 (7)
O4	0.30436 (19)	0.64578 (16)	0.21489 (15)	0.0642 (8)
O5	0.65024 (19)	0.33654 (16)	0.10010 (15)	0.0618 (8)
N1	0.3101 (2)	0.18092 (19)	0.43406 (16)	0.0519 (8)
N2	0.4456 (2)	0.53685 (18)	0.14776 (16)	0.0486 (8)
N3	0.5291 (2)	0.3918 (2)	0.08307 (18)	0.0605 (9)
C1	0.0863 (2)	0.2224 (2)	0.47933 (18)	0.0398 (8)
C2	−0.0473 (3)	0.2308 (3)	0.4409 (2)	0.0573 (11)
C3	−0.1174 (3)	0.3048 (3)	0.4774 (2)	0.0684 (14)
C4	−0.0567 (3)	0.3690 (3)	0.5522 (2)	0.0615 (12)

C5	0.0766 (4)	0.3572 (3)	0.5909 (3)	0.0703 (14)
C6	0.1495 (3)	0.2850 (3)	0.5556 (2)	0.0592 (11)
C7	−0.1339 (4)	0.4484 (3)	0.5932 (3)	0.1003 (19)
C8	0.3303 (2)	0.2762 (2)	0.38676 (19)	0.0440 (9)
C9	0.4465 (3)	0.3330 (3)	0.4242 (2)	0.0607 (11)
C10	0.4738 (3)	0.4247 (3)	0.3811 (2)	0.0578 (11)
C11	0.3859 (2)	0.4623 (2)	0.30027 (18)	0.0427 (9)
C12	0.2695 (3)	0.4061 (2)	0.2627 (2)	0.0509 (10)
C13	0.2425 (3)	0.3132 (2)	0.3054 (2)	0.0513 (10)
C14	0.5480 (3)	0.4644 (2)	0.14888 (19)	0.0430 (9)
C15	0.6744 (3)	0.4591 (2)	0.2104 (2)	0.0498 (10)
C16	0.7342 (3)	0.3799 (2)	0.1768 (2)	0.0482 (10)
C17	0.8701 (3)	0.3364 (3)	0.2031 (2)	0.0661 (11)
H1	0.37992	0.14872	0.46739	0.0623*
H2	−0.09040	0.18700	0.39052	0.0687*
H2A	0.39496	0.55907	0.09507	0.0583*
H3	−0.20773	0.31110	0.45045	0.0821*
H5	0.11898	0.39923	0.64258	0.0842*
H6	0.23972	0.27863	0.58283	0.0707*
H7A	−0.22555	0.42985	0.57205	0.1503*
H7B	−0.12163	0.52121	0.57344	0.1503*
H7C	−0.10358	0.44443	0.66009	0.1503*
H9	0.50638	0.30849	0.47898	0.0729*
H10	0.55227	0.46190	0.40663	0.0696*
H12	0.20926	0.43125	0.20833	0.0610*
H13	0.16469	0.27516	0.27928	0.0614*
H15	0.70953	0.50155	0.26337	0.0597*
H17A	0.90803	0.34876	0.15310	0.0992*
H17B	0.86837	0.25935	0.21492	0.0992*
H17C	0.92184	0.37272	0.25840	0.0992*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0381 (4)	0.0495 (4)	0.0522 (5)	0.0024 (3)	0.0088 (3)	−0.0024 (4)
S2	0.0440 (4)	0.0468 (4)	0.0504 (5)	0.0060 (3)	0.0071 (3)	−0.0020 (3)
O1	0.0506 (12)	0.0490 (12)	0.0743 (15)	0.0042 (10)	0.0104 (10)	0.0135 (11)
O2	0.0497 (11)	0.0649 (13)	0.0521 (13)	0.0017 (10)	0.0054 (10)	−0.0180 (10)
O3	0.0567 (12)	0.0535 (12)	0.0586 (14)	−0.0064 (10)	0.0019 (11)	−0.0103 (10)
O4	0.0588 (13)	0.0586 (13)	0.0694 (15)	0.0221 (11)	0.0095 (11)	0.0017 (11)
O5	0.0484 (12)	0.0645 (13)	0.0666 (15)	0.0060 (11)	0.0075 (11)	−0.0149 (11)
N1	0.0332 (12)	0.0610 (15)	0.0591 (16)	0.0086 (11)	0.0097 (11)	0.0108 (13)
N2	0.0456 (13)	0.0547 (14)	0.0425 (14)	0.0071 (12)	0.0083 (11)	0.0061 (11)
N3	0.0435 (14)	0.0665 (17)	0.0629 (18)	0.0073 (13)	0.0018 (13)	−0.0123 (14)
C1	0.0350 (14)	0.0425 (15)	0.0391 (15)	−0.0024 (12)	0.0063 (12)	−0.0003 (12)
C2	0.0443 (16)	0.074 (2)	0.0498 (19)	0.0014 (16)	0.0076 (14)	−0.0161 (16)
C3	0.0527 (19)	0.087 (3)	0.065 (2)	0.0168 (18)	0.0165 (17)	−0.005 (2)
C4	0.073 (2)	0.058 (2)	0.062 (2)	0.0090 (18)	0.0330 (19)	0.0019 (17)

C5	0.082 (3)	0.063 (2)	0.065 (2)	−0.014 (2)	0.020 (2)	−0.0241 (18)
C6	0.0465 (16)	0.066 (2)	0.059 (2)	−0.0070 (16)	0.0059 (15)	−0.0122 (17)
C7	0.128 (4)	0.084 (3)	0.105 (3)	0.030 (3)	0.059 (3)	−0.007 (2)
C8	0.0335 (14)	0.0518 (17)	0.0465 (17)	0.0084 (14)	0.0113 (13)	−0.0003 (14)
C9	0.0451 (17)	0.071 (2)	0.053 (2)	−0.0002 (16)	−0.0063 (15)	0.0160 (17)
C10	0.0416 (16)	0.068 (2)	0.054 (2)	−0.0052 (16)	−0.0018 (14)	0.0076 (17)
C11	0.0353 (14)	0.0511 (16)	0.0409 (16)	0.0056 (13)	0.0098 (12)	−0.0021 (13)
C12	0.0399 (16)	0.0602 (19)	0.0451 (17)	0.0064 (15)	0.0007 (14)	0.0041 (15)
C13	0.0353 (14)	0.061 (2)	0.0507 (18)	−0.0007 (14)	0.0017 (13)	−0.0019 (16)
C14	0.0414 (16)	0.0438 (16)	0.0438 (16)	−0.0055 (14)	0.0126 (13)	0.0034 (14)
C15	0.0392 (15)	0.0574 (19)	0.0480 (17)	−0.0066 (14)	0.0052 (14)	−0.0071 (15)
C16	0.0384 (15)	0.0499 (17)	0.0537 (19)	−0.0048 (14)	0.0094 (14)	0.0042 (15)
C17	0.0455 (17)	0.067 (2)	0.083 (2)	0.0075 (16)	0.0141 (17)	−0.0025 (18)

Geometric parameters (Å, º)

S1—O1	1.437 (2)	C8—C9	1.386 (4)
S1—O2	1.429 (2)	C9—C10	1.367 (5)
S1—N1	1.620 (2)	C10—C11	1.376 (4)
S1—C1	1.758 (3)	C11—C12	1.384 (4)
S2—O3	1.425 (2)	C12—C13	1.375 (4)
S2—O4	1.428 (2)	C14—C15	1.393 (4)
S2—N2	1.641 (2)	C15—C16	1.335 (4)
S2—C11	1.757 (3)	C16—C17	1.482 (5)
O5—N3	1.411 (3)	C2—H2	0.9300
O5—C16	1.342 (4)	C3—H3	0.9300
N1—C8	1.413 (3)	C5—H5	0.9300
N2—C14	1.400 (4)	C6—H6	0.9300
N3—C14	1.298 (4)	C7—H7A	0.9600
N1—H1	0.8600	C7—H7B	0.9600
N2—H2A	0.8600	C7—H7C	0.9600
C1—C2	1.373 (4)	C9—H9	0.9300
C1—C6	1.377 (4)	C10—H10	0.9300
C2—C3	1.382 (5)	C12—H12	0.9300
C3—C4	1.367 (4)	C13—H13	0.9300
C4—C7	1.512 (5)	C15—H15	0.9300
C4—C5	1.374 (5)	C17—H17A	0.9600
C5—C6	1.378 (5)	C17—H17B	0.9600
C8—C13	1.378 (4)	C17—H17C	0.9600
O1—S1—O2	118.90 (12)	C8—C13—C12	120.2 (3)
O1—S1—N1	104.26 (12)	N2—C14—N3	118.4 (3)
O1—S1—C1	109.27 (12)	N2—C14—C15	129.4 (2)
O2—S1—N1	110.41 (12)	N3—C14—C15	112.2 (3)
O2—S1—C1	107.11 (12)	C14—C15—C16	105.0 (3)
N1—S1—C1	106.26 (12)	O5—C16—C17	116.1 (2)
O3—S2—O4	120.68 (12)	C15—C16—C17	134.0 (3)
O3—S2—N2	108.17 (12)	O5—C16—C15	109.8 (3)

O3—S2—C11	107.80 (12)	C1—C2—H2	120.00
O4—S2—N2	104.65 (12)	C3—C2—H2	120.00
O4—S2—C11	109.32 (12)	C2—C3—H3	119.00
N2—S2—C11	105.17 (12)	C4—C3—H3	119.00
N3—O5—C16	108.1 (2)	C4—C5—H5	119.00
S1—N1—C8	128.05 (18)	C6—C5—H5	119.00
S2—N2—C14	121.44 (19)	C1—C6—H6	121.00
O5—N3—C14	105.0 (2)	C5—C6—H6	121.00
C8—N1—H1	116.00	C4—C7—H7A	109.00
S1—N1—H1	116.00	C4—C7—H7B	109.00
S2—N2—H2A	119.00	C4—C7—H7C	109.00
C14—N2—H2A	119.00	H7A—C7—H7B	109.00
S1—C1—C6	121.3 (2)	H7A—C7—H7C	109.00
C2—C1—C6	120.2 (3)	H7B—C7—H7C	110.00
S1—C1—C2	118.4 (2)	C8—C9—H9	120.00
C1—C2—C3	119.6 (3)	C10—C9—H9	120.00
C2—C3—C4	121.3 (3)	C9—C10—H10	120.00
C3—C4—C5	118.0 (3)	C11—C10—H10	120.00
C3—C4—C7	121.3 (3)	C11—C12—H12	120.00
C5—C4—C7	120.7 (3)	C13—C12—H12	120.00
C4—C5—C6	122.1 (4)	C8—C13—H13	120.00
C1—C6—C5	118.8 (3)	C12—C13—H13	120.00
N1—C8—C9	117.3 (2)	C14—C15—H15	128.00
N1—C8—C13	123.5 (2)	C16—C15—H15	128.00
C9—C8—C13	119.2 (3)	C16—C17—H17A	110.00
C8—C9—C10	120.5 (3)	C16—C17—H17B	109.00
C9—C10—C11	120.4 (3)	C16—C17—H17C	109.00
S2—C11—C12	120.0 (2)	H17A—C17—H17B	109.00
C10—C11—C12	119.3 (3)	H17A—C17—H17C	110.00
S2—C11—C10	120.6 (2)	H17B—C17—H17C	109.00
C11—C12—C13	120.3 (3)		

O1—S1—N1—C8	−176.4 (2)	O5—N3—C14—C15	−1.4 (3)
O2—S1—N1—C8	54.8 (3)	S1—C1—C2—C3	178.3 (2)
C1—S1—N1—C8	−61.0 (3)	C6—C1—C2—C3	2.0 (5)
O1—S1—C1—C2	−106.2 (2)	S1—C1—C6—C5	−177.5 (3)
O1—S1—C1—C6	70.1 (3)	C2—C1—C6—C5	−1.3 (5)
O2—S1—C1—C2	23.9 (3)	C1—C2—C3—C4	−1.0 (5)
O2—S1—C1—C6	−159.9 (2)	C2—C3—C4—C5	−0.6 (5)
N1—S1—C1—C2	141.9 (2)	C2—C3—C4—C7	−178.8 (3)
N1—S1—C1—C6	−41.9 (3)	C3—C4—C5—C6	1.2 (6)
O3—S2—N2—C14	53.7 (2)	C7—C4—C5—C6	179.5 (3)
O4—S2—N2—C14	−176.5 (2)	C4—C5—C6—C1	−0.3 (5)
C11—S2—N2—C14	−61.3 (2)	N1—C8—C9—C10	178.7 (3)
O3—S2—C11—C10	−4.6 (3)	C13—C8—C9—C10	0.1 (5)
O3—S2—C11—C12	175.4 (2)	N1—C8—C13—C12	−179.3 (3)
O4—S2—C11—C10	−137.5 (2)	C9—C8—C13—C12	−0.8 (4)
O4—S2—C11—C12	42.5 (3)	C8—C9—C10—C11	0.4 (5)

N2—S2—C11—C10	110.6 (2)	C9—C10—C11—S2	179.8 (2)
N2—S2—C11—C12	−69.4 (2)	C9—C10—C11—C12	−0.2 (4)
C16—O5—N3—C14	0.7 (3)	S2—C11—C12—C13	179.5 (2)
N3—O5—C16—C15	0.4 (3)	C10—C11—C12—C13	−0.5 (4)
N3—O5—C16—C17	−176.7 (2)	C11—C12—C13—C8	1.0 (4)
S1—N1—C8—C9	154.9 (2)	N2—C14—C15—C16	−176.3 (3)
S1—N1—C8—C13	−26.6 (4)	N3—C14—C15—C16	1.6 (3)
S2—N2—C14—N3	145.2 (2)	C14—C15—C16—O5	−1.1 (3)
S2—N2—C14—C15	−37.0 (4)	C14—C15—C16—C17	175.2 (3)
O5—N3—C14—N2	176.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.86	2.04	2.859 (3)	159
N2—H2*A*···O1^{ii}	0.86	2.39	2.979 (3)	127
C2—H2···O4^{iii}	0.93	2.42	3.208 (4)	143
C13—H13···O2	0.93	2.49	3.134 (3)	126

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