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N-(2,6-Dimethylphenyl)benzenesulfonamide

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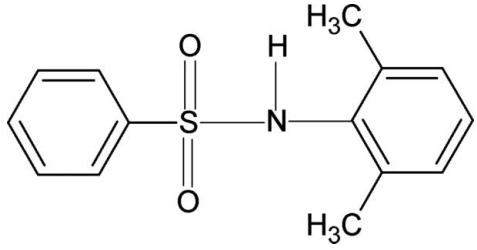
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.135; data-to-parameter ratio = 14.3.

In the crystal structure of the title compound, $C_{14}H_{15}NO_2S$, the N—H bond is *trans* to one of the S=O double bonds, similar to what is observed in *N*-(2-methylphenyl)benzenesulfonamide and other aryl sulfonamides. The two aromatic rings enclose a dihedral angle of 44.9 (1)°. The molecules are connected by intermolecular N—H···O hydrogen bonds into chains running along the *a* axis. An intermolecular C—H···O hydrogen bond is also present.

Related literature

For related literature, see: Gelbrich *et al.* (2007); Gowda *et al.* (2005, 2008); Gowda, Babitha *et al.* (2007); Gowda, Foro *et al.* (2007); Perlovich *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{15}NO_2S$
M_r = 261.33
Monoclinic, $P2_1/n$
a = 5.2133 (7) Å
b = 17.971 (2) Å
c = 14.040 (1) Å
β = 91.681 (9)°
V = 1314.8 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.13 mm^{-1}
T = 299 (2) K
0.55 × 0.35 × 0.33 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2622 measured reflections
2340 independent reflections
2197 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.134
S = 1.08
2340 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1^{i}	0.86	2.55	3.179 (2)	131
C5—H5···O2^{ii}	0.93	2.57	3.229 (3)	129

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2760).

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supporting information

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N-(2,6-Dimethylphenyl)benzenesulfonamide

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S1. Comment

As part of a study of the substituent effects on the crystal structures of *N*-(aryl)-sulfonamides, in the present work, the structure of *N*-(2,6-dimethylphenyl)-benzenesulfonamide (N26DMPBSA) has been determined (Gowda *et al.*, 2005, 2008; Gowda, Babitha *et al.* 2007; Gowda, Foro *et al.* 2007). The the N—H bond is trans to one of the S—O double bonds (Fig. 1), similar to what is observed in *N*-(2-methylphenyl)-benzenesulfonamide (N2MPBSA)(Gowda *et al.*, 2008) and other aryl sulfonamides (Perlovich *et al.*, 2006; Gelbrich *et al.*, 2007;). The two aromatic rings are rotated relative to each other by 44.9 (1)°, compared with the value of 61.5 (1)° in N2MPBSA. The other bond parameters in N26DMPBSA are similar to those observed in N2MPBSA and other *N*-(aryl)-sulfonamides (Gowda, Babitha *et al.*, 2007; Gowda, Foro *et al.* 2007; Gowda *et al.* 2008; Perlovich *et al.*, 2006; Gelbrich *et al.*, 2007). The packing diagram of N26DMPBSA *via* intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) is shown in Fig. 2.

S2. Experimental

The solution of benzene (10 cc) in chloroform (40 cc) was treated dropwise with chlorosulfonic acid (25 cc) at 0 ° C. After the initial evolution of hydrogen chloride subsided, the reaction mixture was brought to room temperature and poured into crushed ice in a beaker. The chloroform layer was separated, washed with cold water and allowed to evaporate slowly. The residual benzenesulfonylchloride was treated with 2,6-dimethylaniline in the stoichiometric ratio and boiled for ten minutes. The reaction mixture was then cooled to room temperature and added to ice cold water (100 cc). The resultant solid *N*-(2,6-dimethylphenyl)-benzenesulfonamide was filtered under suction and washed thoroughly with cold water. It was then recrystallized to constant melting point from dilute ethanol. The purity of the compound was checked and characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2005). The single crystals used in X-ray diffraction studies were grown in ethanolic solution by slow evaporation at room temperature.

S3. Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å, N—H = 0.86 Å, and were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

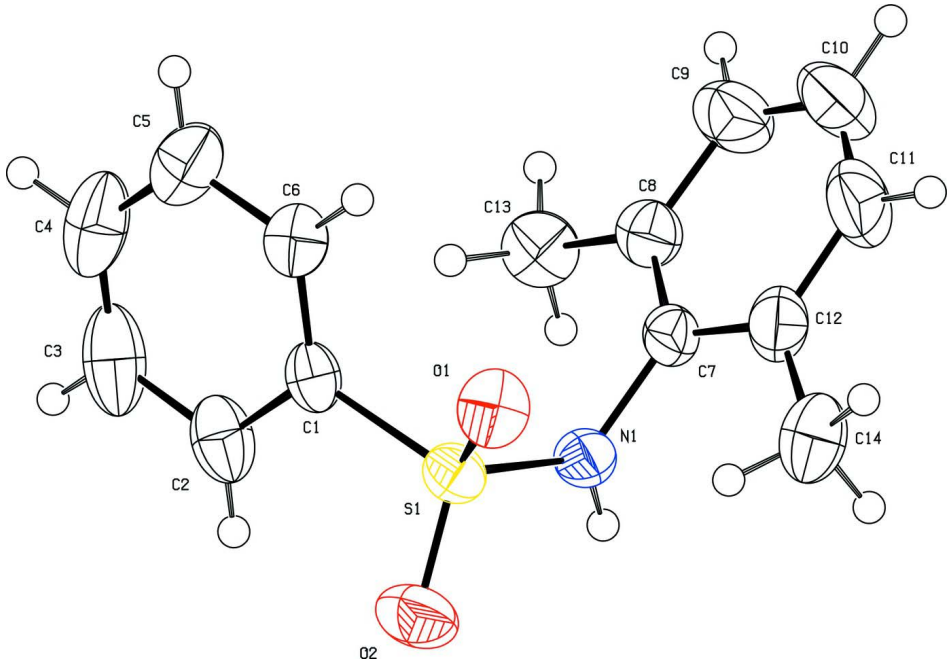

Figure 1

Molecular structure of the title compound, showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii.

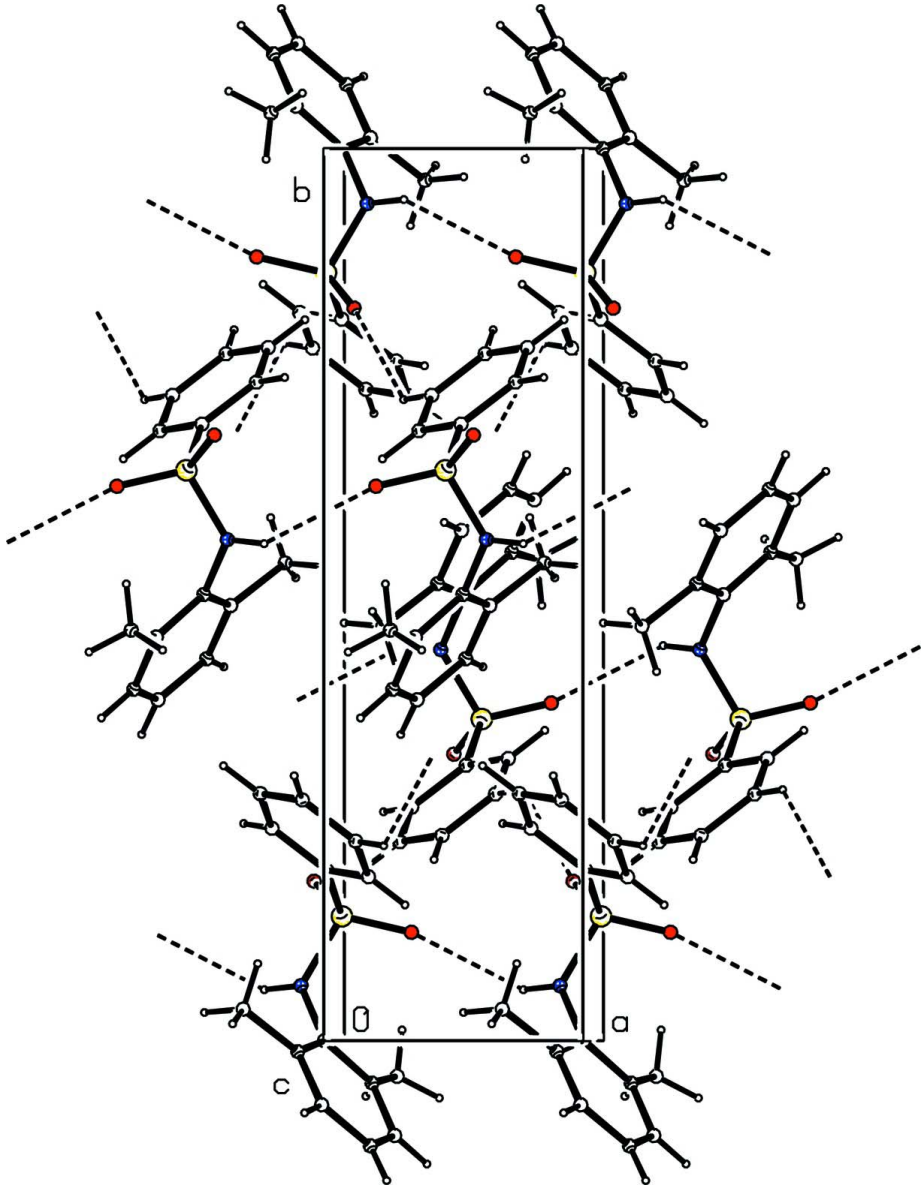

Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

N-(2,6-Dimethylphenyl)benzenesulfonamide

Crystal data

$C_{14}H_{15}NO_2S$
$M_r = 261.33$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.2133\ (7)$ Å
$b = 17.971\ (2)$ Å
$c = 14.040\ (1)$ Å
$\beta = 91.681\ (9)°$
$V = 1314.8\ (2)$ Å^3
$Z = 4$

$F(000) = 552$
$D_x = 1.320$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 4.0–19.2°$
$\mu = 2.14$ mm^{-1}
$T = 299$ K
Prism, colourless
0.55 × 0.35 × 0.33 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
2622 measured reflections
2340 independent reflections
2197 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 66.9°$, $\theta_{min} = 4.0°$
$h = -6\rightarrow1$
$k = -21\rightarrow0$
$l = -16\rightarrow16$
3 standard reflections every 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.134$
$S = 1.08$
2340 reflections
164 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
$w = 1/[\sigma^2(F_o^2) + (0.0807P)^2 + 0.6081P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0060 (9)

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 $F^2 > \sigma(F^2)$ 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}
C1	−0.0070 (4)	0.19125 (11)	0.78195 (15)	0.0359 (5)
C2	−0.2175 (4)	0.23812 (13)	0.7860 (2)	0.0518 (6)
H2	−0.3303	0.2434	0.7339	0.062*
C3	−0.2557 (5)	0.27695 (15)	0.8699 (3)	0.0677 (8)
H3	−0.3972	0.3081	0.8744	0.081*
C4	−0.0875 (6)	0.26990 (16)	0.9461 (2)	0.0666 (8)
H4	−0.1141	0.2969	1.0014	0.080*
C5	0.1186 (6)	0.22354 (15)	0.94146 (19)	0.0590 (7)
H5	0.2309	0.2186	0.9938	0.071*
C6	0.1608 (4)	0.18376 (13)	0.85885 (17)	0.0453 (5)
H6	0.3017	0.1522	0.8554	0.054*
C7	−0.0178 (4)	0.00007 (11)	0.74093 (15)	0.0373 (5)
C8	−0.1139 (4)	−0.01229 (12)	0.83144 (16)	0.0437 (5)
C9	−0.0176 (6)	−0.07186 (15)	0.8839 (2)	0.0609 (7)
H9	−0.0788	−0.0809	0.9444	0.073*

C10	0.1675 (7)	−0.11784 (16)	0.8480 (3)	0.0730 (9)
H10	0.2336	−0.1568	0.8848	0.088*
C11	0.2541 (6)	−0.10620 (14)	0.7582 (2)	0.0680 (8)
H11	0.3769	−0.1382	0.7343	0.082*
C12	0.1628 (5)	−0.04751 (13)	0.70148 (18)	0.0498 (6)
C13	−0.3213 (5)	0.03545 (14)	0.87194 (18)	0.0521 (6)
H13A	−0.4740	0.0316	0.8323	0.063*
H13B	−0.2651	0.0863	0.8741	0.063*
H13C	−0.3570	0.0189	0.9352	0.063*
C14	0.2511 (6)	−0.03980 (16)	0.6006 (2)	0.0683 (8)
H14A	0.2690	0.0120	0.5853	0.082*
H14B	0.1270	−0.0622	0.5576	0.082*
H14C	0.4135	−0.0643	0.5947	0.082*
N1	−0.1132 (3)	0.06164 (9)	0.68444 (12)	0.0371 (4)
H1N	−0.2573	0.0571	0.6536	0.044*
O1	0.3127 (3)	0.12146 (10)	0.67758 (12)	0.0478 (4)
O2	−0.0692 (4)	0.17882 (10)	0.59926 (12)	0.0576 (5)
S1	0.04474 (9)	0.13941 (3)	0.67748 (3)	0.0358 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0330 (10)	0.0277 (9)	0.0476 (11)	−0.0044 (7)	0.0082 (8)	0.0010 (8)
C2	0.0383 (11)	0.0382 (12)	0.0794 (17)	0.0005 (9)	0.0079 (11)	−0.0024 (11)
C3	0.0519 (14)	0.0440 (14)	0.109 (2)	0.0011 (11)	0.0324 (16)	−0.0178 (14)
C4	0.0731 (18)	0.0538 (15)	0.0749 (19)	−0.0173 (14)	0.0336 (15)	−0.0237 (14)
C5	0.0697 (16)	0.0576 (15)	0.0500 (14)	−0.0172 (13)	0.0086 (12)	−0.0106 (12)
C6	0.0437 (11)	0.0425 (12)	0.0500 (12)	−0.0010 (9)	0.0044 (9)	−0.0046 (9)
C7	0.0377 (10)	0.0300 (10)	0.0437 (11)	−0.0023 (8)	−0.0068 (8)	−0.0014 (8)
C8	0.0421 (11)	0.0398 (11)	0.0490 (12)	−0.0076 (9)	−0.0027 (9)	0.0031 (9)
C9	0.0698 (17)	0.0511 (14)	0.0614 (16)	−0.0060 (12)	−0.0037 (12)	0.0180 (12)
C10	0.088 (2)	0.0455 (14)	0.085 (2)	0.0092 (14)	−0.0165 (17)	0.0183 (14)
C11	0.0701 (18)	0.0419 (14)	0.091 (2)	0.0179 (13)	−0.0075 (15)	−0.0061 (14)
C12	0.0523 (13)	0.0388 (12)	0.0579 (14)	0.0040 (10)	−0.0045 (10)	−0.0108 (10)
C13	0.0489 (13)	0.0557 (14)	0.0523 (13)	−0.0057 (11)	0.0106 (10)	0.0054 (11)
C14	0.0828 (19)	0.0587 (16)	0.0638 (17)	0.0143 (14)	0.0110 (14)	−0.0211 (13)
N1	0.0333 (8)	0.0372 (9)	0.0402 (9)	−0.0016 (7)	−0.0069 (7)	0.0004 (7)
O1	0.0331 (8)	0.0539 (9)	0.0569 (10)	−0.0006 (7)	0.0104 (7)	−0.0048 (7)
O2	0.0690 (11)	0.0563 (10)	0.0473 (9)	0.0011 (8)	−0.0016 (8)	0.0193 (8)
S1	0.0351 (3)	0.0364 (3)	0.0361 (3)	−0.00027 (18)	0.0040 (2)	0.00487 (18)

Geometric parameters (Å, º)

C1—C6	1.376 (3)	C9—C10	1.377 (5)
C1—C2	1.386 (3)	C9—H9	0.9300
C1—S1	1.765 (2)	C10—C11	1.368 (5)
C2—C3	1.388 (4)	C10—H10	0.9300
C2—H2	0.9300	C11—C12	1.397 (4)

C3—C4	1.369 (5)	C11—H11	0.9300
C3—H3	0.9300	C12—C14	1.508 (4)
C4—C5	1.363 (4)	C13—H13A	0.9600
C4—H4	0.9300	C13—H13B	0.9600
C5—C6	1.386 (3)	C13—H13C	0.9600
C5—H5	0.9300	C14—H14A	0.9600
C6—H6	0.9300	C14—H14B	0.9600
C7—C8	1.397 (3)	C14—H14C	0.9600
C7—C12	1.398 (3)	N1—S1	1.6263 (17)
C7—N1	1.441 (3)	N1—H1N	0.8600
C8—C9	1.386 (3)	O1—S1	1.4334 (16)
C8—C13	1.505 (3)	O2—S1	1.4221 (17)

C6—C1—C2	120.9 (2)	C9—C10—H10	120.0
C6—C1—S1	119.41 (16)	C10—C11—C12	121.7 (3)
C2—C1—S1	119.71 (18)	C10—C11—H11	119.2
C1—C2—C3	118.3 (3)	C12—C11—H11	119.2
C1—C2—H2	120.8	C11—C12—C7	117.3 (3)
C3—C2—H2	120.8	C11—C12—C14	119.8 (2)
C4—C3—C2	120.8 (2)	C7—C12—C14	122.9 (2)
C4—C3—H3	119.6	C8—C13—H13A	109.5
C2—C3—H3	119.6	C8—C13—H13B	109.5
C5—C4—C3	120.5 (3)	H13A—C13—H13B	109.5
C5—C4—H4	119.8	C8—C13—H13C	109.5
C3—C4—H4	119.8	H13A—C13—H13C	109.5
C4—C5—C6	120.0 (3)	H13B—C13—H13C	109.5
C4—C5—H5	120.0	C12—C14—H14A	109.5
C6—C5—H5	120.0	C12—C14—H14B	109.5
C1—C6—C5	119.5 (2)	H14A—C14—H14B	109.5
C1—C6—H6	120.2	C12—C14—H14C	109.5
C5—C6—H6	120.2	H14A—C14—H14C	109.5
C8—C7—C12	121.8 (2)	H14B—C14—H14C	109.5
C8—C7—N1	119.69 (19)	C7—N1—S1	121.72 (13)
C12—C7—N1	118.5 (2)	C7—N1—H1N	119.1
C9—C8—C7	118.2 (2)	S1—N1—H1N	119.1
C9—C8—C13	119.5 (2)	O2—S1—O1	119.85 (11)
C7—C8—C13	122.3 (2)	O2—S1—N1	105.89 (10)
C10—C9—C8	121.0 (3)	O1—S1—N1	107.55 (10)
C10—C9—H9	119.5	O2—S1—C1	107.95 (11)
C8—C9—H9	119.5	O1—S1—C1	106.89 (10)
C11—C10—C9	120.0 (3)	N1—S1—C1	108.28 (9)
C11—C10—H10	120.0		

C6—C1—C2—C3	−0.4 (3)	C10—C11—C12—C14	−176.0 (3)
S1—C1—C2—C3	178.70 (18)	C8—C7—C12—C11	−3.2 (3)
C1—C2—C3—C4	0.9 (4)	N1—C7—C12—C11	179.3 (2)
C2—C3—C4—C5	−1.1 (4)	C8—C7—C12—C14	174.0 (2)
C3—C4—C5—C6	0.7 (4)	N1—C7—C12—C14	−3.5 (3)

C2—C1—C6—C5	0.1 (3)	C8—C7—N1—S1	99.9 (2)
S1—C1—C6—C5	−179.04 (18)	C12—C7—N1—S1	−82.5 (2)
C4—C5—C6—C1	−0.2 (4)	C7—N1—S1—O2	165.74 (17)
C12—C7—C8—C9	2.6 (3)	C7—N1—S1—O1	36.48 (19)
N1—C7—C8—C9	−179.8 (2)	C7—N1—S1—C1	−78.70 (18)
C12—C7—C8—C13	−175.8 (2)	C6—C1—S1—O2	−153.98 (17)
N1—C7—C8—C13	1.8 (3)	C2—C1—S1—O2	26.9 (2)
C7—C8—C9—C10	−0.1 (4)	C6—C1—S1—O1	−23.8 (2)
C13—C8—C9—C10	178.3 (3)	C2—C1—S1—O1	157.06 (17)
C8—C9—C10—C11	−1.7 (5)	C6—C1—S1—N1	91.81 (18)
C9—C10—C11—C12	1.2 (5)	C2—C1—S1—N1	−87.33 (18)
C10—C11—C12—C7	1.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.86	2.55	3.179 (2)	131
C5—H5···O2^{ii}	0.93	2.57	3.229 (3)	129

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