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2-(4-Methylphenyl)-1-phenylsulfonyl-3-nitro-1,2-dihydroquinoline

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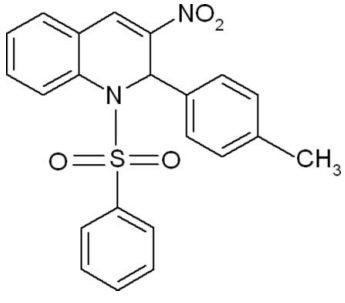
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.151; data-to-parameter ratio = 20.9.

In the title compound, $C_{22}H_{18}N_2O_4S$, the dihedral angle between the phenylsulfonyl ring and the methylphenyl ring is 67.78 (7)°. In the crystal, molecules are linked by weak intermolecular C—H···O interactions into a zigzag chain along the [101] direction.

Related literature

For the biological activity of quinoline derivatives, see: Franck *et al.* (2004); Zouhiri *et al.* (2005); Paul *et al.* (1969). For a related structure, see: Xu *et al.* (2011).



Experimental

Crystal data

$C_{22}H_{18}N_2O_4S$ M_r = 406.44
Monoclinic, $P2_1/n$
a = 9.7349 (5) Å
b = 17.0241 (9) Å
c = 12.1068 (6) Å
β = 90.240 (2)°
V = 2006.42 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 295 K
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.945, T_{max} = 0.955
26473 measured reflections
5485 independent reflections
3224 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.151
S = 1.03
5485 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O4^{i}	0.93	2.60	3.418 (4)	148

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2758).

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supporting information

Acta Cryst. (2011). E**67**, o2225 [doi:10.1107/S1600536811030455]

2-(4-Methylphenyl)-1-phenylsulfonyl-3-nitro-1,2-dihydroquinoline

J. Kanchanadevi, G. Anbalagan, V. Saravanan, A. K. Mohanakrishnan and V. Manivannan

S1. Comment

The quinoline and its derivatives have received much scientific attention during recent years, because of their wide spectrum of pharmacological activities (Franck *et al.*, 2004; Zouhiri *et al.*, 2005). In addition, the nitroquinoline derivatives possess a potent mutagenic, carcinogenic and carcinostatic agent (Paul *et al.*, 1969).

The geometric parameters of the title molecule (Fig. 1) agree well with a reported similar structure (Xu *et al.*, 2011). The phenylsulfonly ring and the methylphenyl ring are oriented at an angle of 67.78 (7)°. The sum of bond angles around N1 [352.34 (13)°] and N2 [359.95 (2)°] indicates the sp^2 hybridization state of atoms N1 and N2 in the molecule. The crystal packing is controlled by a weak intermolecular C—H···O interaction.

S2. Experimental

To a solution of N-(2-formylphenyl) benzenesulfonamide (0.50 g, 1.91 mmol) in dry benzene (20 ml), DABACO (0.10 g, 0.95 mmol) and 1-methyl-4-(2-nitrovinyl)benzene (0.41 g, 2.29 mmol) were added. The reaction mixture was stirred at reflux condition for 24 hrs under N_2 atmosphere. The reaction mass was quenched with ice water (50 ml), extracted with chloroform (3 × 10 ml) and dried (Na_2SO_4). The solvent was removed under reduced pressure. Then the column chromatographic purification of crude product afforded pure dihydro nitroquinoline 18 as pale yellow solid with a yield of 82% and a melting point of 451 K.

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for C—H, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

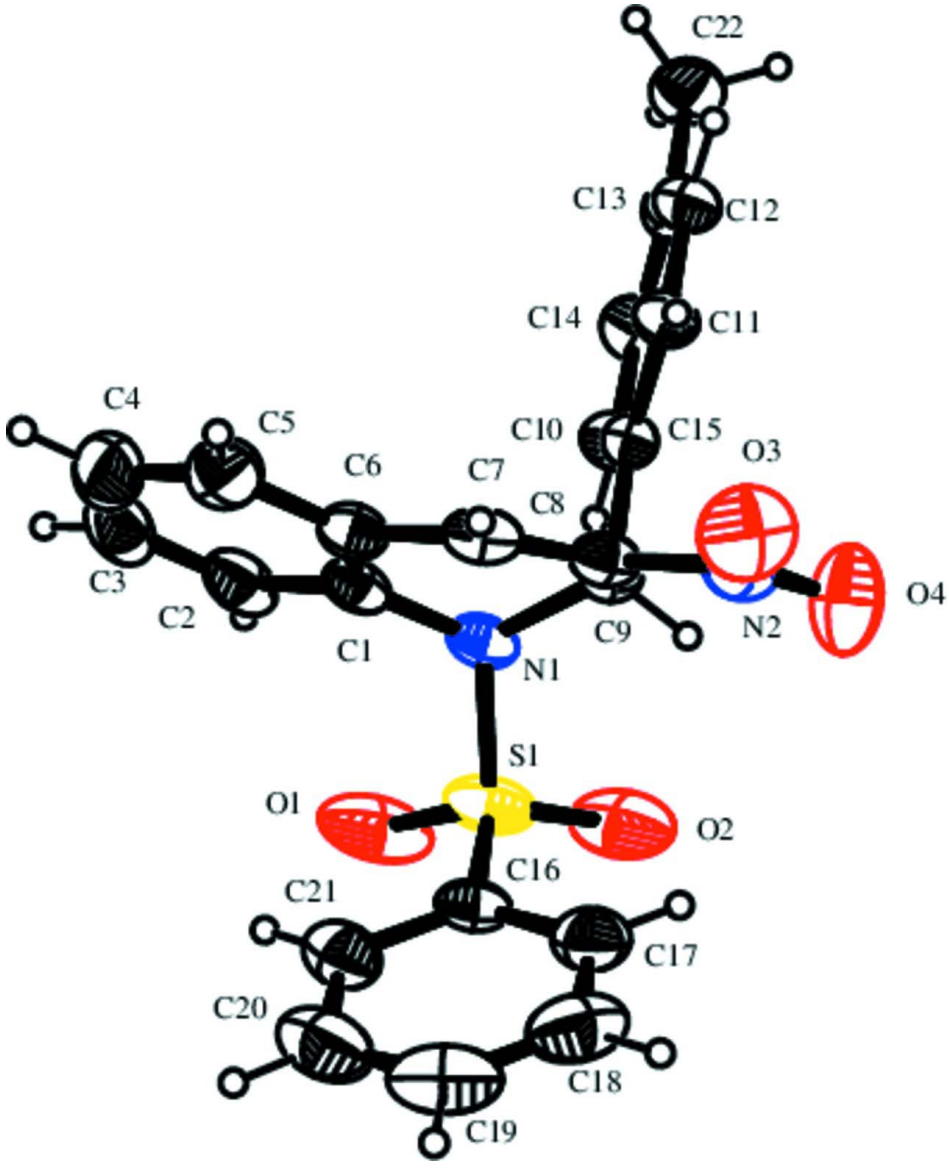

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

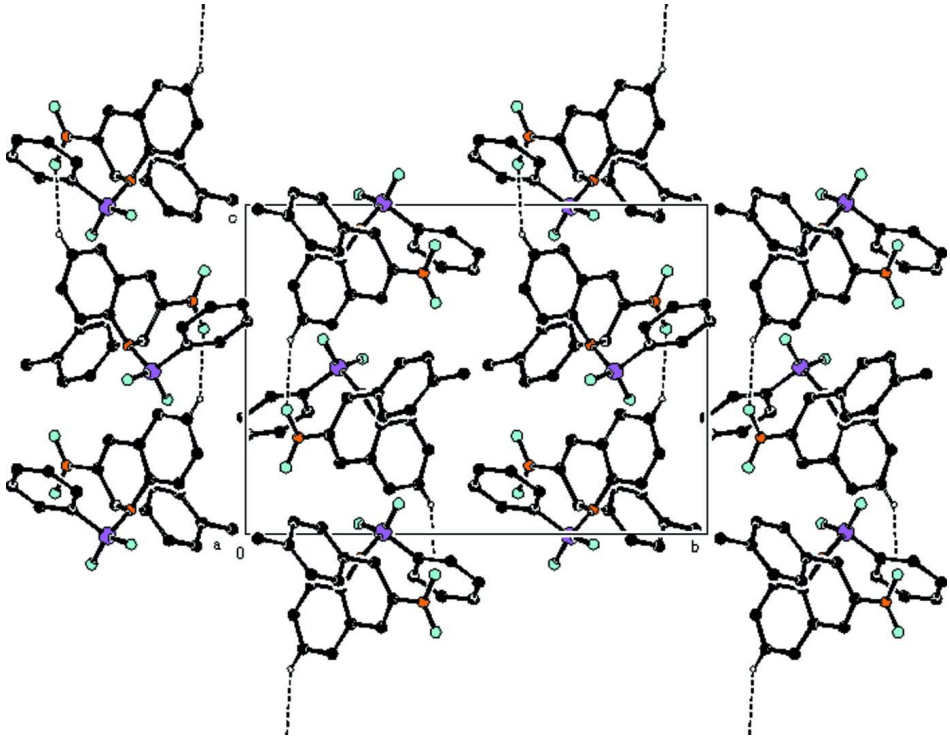

Figure 2

The packing of the title compound, viewed down the *a* axis. The C—H···O hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{22}H_{18}N_2O_4S$
$M_r = 406.44$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.7349\ (5)$ Å
$b = 17.0241\ (9)$ Å
$c = 12.1068\ (6)$ Å
$\beta = 90.240\ (2)°$
$V = 2006.42\ (18)$ Å^3
$Z = 4$
$F(000) = 848$
$D_x = 1.346$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5485 reflections
$\theta = 2.1–29.4°$
$\mu = 0.19$ mm^{-1}
$T = 295$ K
Block, pale yellow
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.945$, $T_{max} = 0.955$
26473 measured reflections
5485 independent reflections
3224 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 29.3°$, $\theta_{min} = 2.1°$
$h = -13\rightarrow7$
$k = -23\rightarrow23$
$l = -14\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.151$
$S = 1.03$
5485 reflections
263 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
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 0.3469P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.19131 (16)	0.20602 (10)	0.83358 (16)	0.0572 (4)
C2	0.1021 (2)	0.14330 (13)	0.8465 (2)	0.0782 (6)
H2	0.0747	0.1278	0.9168	0.094*
C3	0.0545 (2)	0.10423 (15)	0.7552 (3)	0.0984 (9)
H3	−0.0059	0.0624	0.7640	0.118*
C4	0.0945 (3)	0.12577 (17)	0.6509 (3)	0.1007 (9)
H4	0.0622	0.0981	0.5898	0.121*
C5	0.1819 (2)	0.18787 (15)	0.6368 (2)	0.0822 (6)
H5	0.2078	0.2028	0.5660	0.099*
C6	0.23211 (18)	0.22870 (11)	0.72767 (15)	0.0580 (4)
C7	0.32475 (19)	0.29435 (10)	0.71606 (15)	0.0583 (5)
H7	0.3352	0.3188	0.6479	0.070*
C8	0.39412 (17)	0.31926 (10)	0.80240 (15)	0.0551 (4)
C9	0.38459 (17)	0.27927 (10)	0.91304 (14)	0.0534 (4)
H9	0.4006	0.3186	0.9707	0.064*
C10	0.48831 (16)	0.21338 (10)	0.92830 (13)	0.0483 (4)
C11	0.59619 (17)	0.20168 (11)	0.85758 (14)	0.0562 (4)
H11	0.6054	0.2337	0.7958	0.067*
C12	0.69139 (18)	0.14296 (12)	0.87689 (16)	0.0639 (5)
H12	0.7646	0.1368	0.8285	0.077*
C13	0.68006 (18)	0.09341 (11)	0.96638 (15)	0.0588 (4)
C14	0.5720 (2)	0.10586 (12)	1.03651 (17)	0.0709 (5)
H14	0.5621	0.0734	1.0977	0.085*
C15	0.4780 (2)	0.16477 (12)	1.01928 (16)	0.0671 (5)
H15	0.4068	0.1720	1.0693	0.080*
C16	0.06971 (19)	0.37453 (12)	0.92595 (15)	0.0646 (5)
C17	0.1392 (2)	0.44441 (15)	0.9176 (2)	0.0860 (7)
H17	0.2226	0.4515	0.9540	0.103*
C18	0.0829 (4)	0.50453 (16)	0.8536 (3)	0.1066 (9)
H18	0.1291	0.5521	0.8465	0.128*
C19	−0.0370 (4)	0.4936 (2)	0.8029 (3)	0.1156 (11)
H19	−0.0737	0.5344	0.7610	0.139*
C20	−0.1077 (3)	0.4253 (2)	0.8102 (2)	0.1116 (10)
H20	−0.1919	0.4195	0.7746	0.134*

C21	−0.0529 (2)	0.36413 (16)	0.8715 (2)	0.0861 (7)
H21	−0.0988	0.3163	0.8757	0.103*
C22	0.7804 (2)	0.02762 (14)	0.9861 (2)	0.0873 (7)
H22A	0.8684	0.0491	1.0056	0.131*
H22B	0.7889	−0.0032	0.9201	0.131*
H22C	0.7480	−0.0050	1.0451	0.131*
N1	0.24454 (14)	0.24821 (9)	0.92602 (12)	0.0584 (4)
N2	0.48784 (19)	0.38510 (10)	0.79296 (19)	0.0773 (5)
O1	0.02787 (19)	0.24655 (12)	1.03159 (17)	0.1265 (8)
O2	0.2199 (2)	0.33166 (15)	1.09148 (12)	0.1231 (8)
O3	0.5112 (2)	0.41204 (10)	0.70211 (16)	0.1096 (6)
O4	0.5403 (2)	0.41024 (12)	0.8764 (2)	0.1219 (7)
S1	0.13716 (6)	0.29822 (4)	1.00593 (4)	0.0809 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0441 (8)	0.0530 (10)	0.0747 (12)	0.0120 (7)	0.0062 (8)	0.0164 (9)
C2	0.0526 (10)	0.0659 (13)	0.1161 (18)	0.0055 (9)	0.0055 (11)	0.0266 (13)
C3	0.0614 (13)	0.0625 (14)	0.171 (3)	0.0024 (11)	−0.0212 (17)	0.0103 (18)
C4	0.0879 (17)	0.0826 (18)	0.131 (3)	0.0143 (14)	−0.0380 (17)	−0.0154 (17)
C5	0.0858 (15)	0.0804 (16)	0.0801 (15)	0.0196 (13)	−0.0177 (12)	−0.0004 (12)
C6	0.0548 (9)	0.0569 (10)	0.0622 (11)	0.0153 (8)	0.0004 (8)	0.0097 (9)
C7	0.0646 (10)	0.0564 (10)	0.0541 (10)	0.0179 (8)	0.0164 (8)	0.0176 (8)
C8	0.0548 (9)	0.0469 (9)	0.0638 (11)	0.0081 (7)	0.0159 (8)	0.0115 (8)
C9	0.0556 (9)	0.0530 (10)	0.0517 (9)	0.0065 (7)	0.0101 (7)	0.0039 (7)
C10	0.0486 (8)	0.0493 (9)	0.0469 (9)	0.0009 (7)	0.0006 (7)	0.0010 (7)
C11	0.0541 (9)	0.0612 (11)	0.0534 (10)	0.0070 (8)	0.0056 (7)	0.0073 (8)
C12	0.0552 (9)	0.0707 (12)	0.0658 (11)	0.0123 (9)	0.0033 (8)	0.0006 (10)
C13	0.0575 (10)	0.0541 (10)	0.0645 (11)	0.0066 (8)	−0.0135 (8)	−0.0024 (9)
C14	0.0784 (12)	0.0683 (13)	0.0661 (12)	0.0075 (10)	−0.0006 (10)	0.0229 (10)
C15	0.0688 (11)	0.0702 (12)	0.0623 (11)	0.0096 (9)	0.0140 (9)	0.0164 (9)
C16	0.0582 (10)	0.0726 (13)	0.0632 (11)	0.0162 (9)	0.0233 (9)	−0.0002 (9)
C17	0.0782 (13)	0.0806 (16)	0.0993 (17)	0.0089 (12)	0.0215 (12)	−0.0109 (13)
C18	0.128 (2)	0.0684 (16)	0.124 (2)	0.0191 (17)	0.041 (2)	0.0056 (16)
C19	0.134 (3)	0.112 (3)	0.100 (2)	0.055 (2)	0.030 (2)	0.0151 (19)
C20	0.0854 (17)	0.151 (3)	0.099 (2)	0.042 (2)	−0.0056 (15)	0.000 (2)
C21	0.0668 (13)	0.0997 (18)	0.0919 (16)	0.0098 (12)	0.0120 (12)	−0.0023 (14)
C22	0.0885 (15)	0.0745 (15)	0.0986 (16)	0.0267 (12)	−0.0167 (13)	0.0054 (12)
N1	0.0523 (7)	0.0649 (10)	0.0581 (9)	0.0116 (7)	0.0170 (6)	0.0135 (7)
N2	0.0770 (11)	0.0546 (10)	0.1004 (14)	0.0011 (8)	0.0181 (10)	0.0176 (10)
O1	0.1073 (12)	0.1217 (14)	0.1512 (17)	0.0298 (11)	0.0902 (12)	0.0615 (13)
O2	0.1292 (15)	0.192 (2)	0.0477 (8)	0.0691 (15)	0.0026 (9)	−0.0158 (11)
O3	0.1342 (15)	0.0769 (11)	0.1182 (14)	−0.0176 (10)	0.0390 (11)	0.0365 (10)
O4	0.1345 (16)	0.1048 (15)	0.1263 (16)	−0.0521 (13)	−0.0165 (13)	0.0139 (13)
S1	0.0799 (3)	0.1018 (5)	0.0615 (3)	0.0312 (3)	0.0356 (3)	0.0208 (3)

Geometric parameters (Å, º)

C1—C2	1.386 (3)	C13—C14	1.371 (3)
C1—C6	1.398 (2)	C13—C22	1.505 (3)
C1—N1	1.425 (2)	C14—C15	1.373 (3)
C2—C3	1.369 (4)	C14—H14	0.9300
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.373 (4)	C16—C17	1.373 (3)
C3—H3	0.9300	C16—C21	1.373 (3)
C4—C5	1.368 (4)	C16—S1	1.747 (2)
C4—H4	0.9300	C17—C18	1.394 (4)
C5—C6	1.389 (3)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.330 (5)
C6—C7	1.443 (3)	C18—H18	0.9300
C7—C8	1.312 (3)	C19—C20	1.355 (5)
C7—H7	0.9300	C19—H19	0.9300
C8—N2	1.450 (3)	C20—C21	1.384 (4)
C8—C9	1.506 (2)	C20—H20	0.9300
C9—N1	1.471 (2)	C21—H21	0.9300
C9—C10	1.520 (2)	C22—H22A	0.9600
C9—H9	0.9800	C22—H22B	0.9600
C10—C11	1.372 (2)	C22—H22C	0.9600
C10—C15	1.382 (2)	N1—S1	1.6620 (14)
C11—C12	1.382 (2)	N2—O4	1.208 (2)
C11—H11	0.9300	N2—O3	1.214 (2)
C12—C13	1.378 (3)	O1—S1	1.4159 (19)
C12—H12	0.9300	O2—S1	1.428 (2)
C2—C1—C6	119.8 (2)	C13—C14—C15	122.10 (18)
C2—C1—N1	121.69 (19)	C13—C14—H14	119.0
C6—C1—N1	118.49 (16)	C15—C14—H14	119.0
C3—C2—C1	119.5 (2)	C14—C15—C10	120.53 (17)
C3—C2—H2	120.2	C14—C15—H15	119.7
C1—C2—H2	120.2	C10—C15—H15	119.7
C2—C3—C4	121.1 (2)	C17—C16—C21	120.3 (2)
C2—C3—H3	119.4	C17—C16—S1	120.10 (18)
C4—C3—H3	119.4	C21—C16—S1	119.64 (18)
C5—C4—C3	120.0 (3)	C16—C17—C18	119.0 (3)
C5—C4—H4	120.0	C16—C17—H17	120.5
C3—C4—H4	120.0	C18—C17—H17	120.5
C4—C5—C6	120.3 (3)	C19—C18—C17	119.8 (3)
C4—C5—H5	119.8	C19—C18—H18	120.1
C6—C5—H5	119.8	C17—C18—H18	120.1
C5—C6—C1	119.2 (2)	C18—C19—C20	122.3 (3)
C5—C6—C7	121.89 (19)	C18—C19—H19	118.8
C1—C6—C7	118.89 (18)	C20—C19—H19	118.8
C8—C7—C6	119.48 (16)	C19—C20—C21	119.1 (3)
C8—C7—H7	120.3	C19—C20—H20	120.5

C6—C7—H7	120.3	C21—C20—H20	120.5
C7—C8—N2	120.58 (17)	C16—C21—C20	119.5 (3)
C7—C8—C9	121.95 (16)	C16—C21—H21	120.2
N2—C8—C9	117.43 (18)	C20—C21—H21	120.2
N1—C9—C8	108.54 (14)	C13—C22—H22A	109.5
N1—C9—C10	109.71 (13)	C13—C22—H22B	109.5
C8—C9—C10	113.48 (13)	H22A—C22—H22B	109.5
N1—C9—H9	108.3	C13—C22—H22C	109.5
C8—C9—H9	108.3	H22A—C22—H22C	109.5
C10—C9—H9	108.3	H22B—C22—H22C	109.5
C11—C10—C15	117.95 (16)	C1—N1—C9	115.55 (13)
C11—C10—C9	122.75 (15)	C1—N1—S1	119.18 (11)
C15—C10—C9	119.24 (15)	C9—N1—S1	117.61 (13)
C10—C11—C12	120.91 (17)	O4—N2—O3	122.9 (2)
C10—C11—H11	119.5	O4—N2—C8	118.15 (19)
C12—C11—H11	119.5	O3—N2—C8	118.9 (2)
C13—C12—C11	121.32 (17)	O1—S1—O2	120.72 (13)
C13—C12—H12	119.3	O1—S1—N1	106.53 (10)
C11—C12—H12	119.3	O2—S1—N1	105.78 (9)
C14—C13—C12	117.16 (17)	O1—S1—C16	107.62 (11)
C14—C13—C22	121.08 (19)	O2—S1—C16	108.37 (12)
C12—C13—C22	121.75 (19)	N1—S1—C16	107.11 (8)

C6—C1—C2—C3	−0.1 (3)	C21—C16—C17—C18	0.4 (3)
N1—C1—C2—C3	−179.51 (17)	S1—C16—C17—C18	−179.70 (17)
C1—C2—C3—C4	0.5 (3)	C16—C17—C18—C19	0.6 (4)
C2—C3—C4—C5	−0.9 (4)	C17—C18—C19—C20	−0.4 (4)
C3—C4—C5—C6	0.9 (3)	C18—C19—C20—C21	−0.8 (5)
C4—C5—C6—C1	−0.6 (3)	C17—C16—C21—C20	−1.6 (3)
C4—C5—C6—C7	179.81 (19)	S1—C16—C21—C20	178.51 (18)
C2—C1—C6—C5	0.2 (3)	C19—C20—C21—C16	1.8 (4)
N1—C1—C6—C5	179.58 (15)	C2—C1—N1—C9	147.01 (16)
C2—C1—C6—C7	179.81 (15)	C6—C1—N1—C9	−32.4 (2)
N1—C1—C6—C7	−0.8 (2)	C2—C1—N1—S1	−64.2 (2)
C5—C6—C7—C8	−164.16 (17)	C6—C1—N1—S1	116.43 (15)
C1—C6—C7—C8	16.2 (2)	C8—C9—N1—C1	46.92 (18)
C6—C7—C8—N2	−179.99 (15)	C10—C9—N1—C1	−77.58 (17)
C6—C7—C8—C9	2.5 (2)	C8—C9—N1—S1	−102.38 (15)
C7—C8—C9—N1	−33.2 (2)	C10—C9—N1—S1	133.12 (12)
N2—C8—C9—N1	149.26 (15)	C7—C8—N2—O4	173.7 (2)
C7—C8—C9—C10	89.0 (2)	C9—C8—N2—O4	−8.7 (3)
N2—C8—C9—C10	−88.50 (19)	C7—C8—N2—O3	−7.0 (3)
N1—C9—C10—C11	133.39 (17)	C9—C8—N2—O3	170.59 (17)
C8—C9—C10—C11	11.8 (2)	C1—N1—S1—O1	48.87 (16)
N1—C9—C10—C15	−49.3 (2)	C9—N1—S1—O1	−162.97 (14)
C8—C9—C10—C15	−170.91 (17)	C1—N1—S1—O2	178.48 (15)
C15—C10—C11—C12	0.1 (3)	C9—N1—S1—O2	−33.35 (16)
C9—C10—C11—C12	177.40 (17)	C1—N1—S1—C16	−66.07 (15)

C10—C11—C12—C13	1.2 (3)	C9—N1—S1—C16	82.10 (14)
C11—C12—C13—C14	−1.3 (3)	C17—C16—S1—O1	159.82 (17)
C11—C12—C13—C22	177.92 (18)	C21—C16—S1—O1	−20.30 (19)
C12—C13—C14—C15	0.2 (3)	C17—C16—S1—O2	27.73 (18)
C22—C13—C14—C15	−179.0 (2)	C21—C16—S1—O2	−152.39 (16)
C13—C14—C15—C10	1.0 (3)	C17—C16—S1—N1	−85.98 (17)
C11—C10—C15—C14	−1.1 (3)	C21—C16—S1—N1	93.90 (16)
C9—C10—C15—C14	−178.56 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O4^{i}	0.93	2.60	3.418 (4)	148

Symmetry code: (i) $x-1/2, -y+1/2, z-1/2$.