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N-(4-Methoxybenzyl)-3-[(1*E*)-3-oxo-3-phenylprop-1-en-1-yl]benzenesulfonamide

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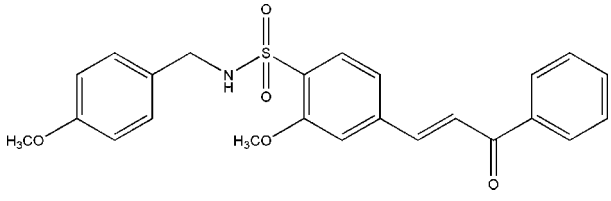
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.135; data-to-parameter ratio = 13.7.

In the title compound, $C_{24}H_{23}NO_5S$, the enone group and the two attached aromatic rings are approximately coplanar. The planes of the two methoxybenzene groups are almost perpendicular, with a dihedral angle of 82.41 (8)°. The C—S—N—C and S—N—C—C torsion angles of 62.5 (2) and 60.0 (1)°, respectively, also show the nonplanarity of the system. The amino group has an intramolecular contact to a methoxy O atom. The crystal structure is stabilized by one N—H···O and three C—H···O intermolecular hydrogen bonds.

Related literature

For related literature, see: Buchmann & Schalinatus (1962); Go *et al.* (2004); Hermoso *et al.* (2003); Hsieh *et al.* (1998); Liu *et al.* (2003); Lunardi *et al.* (2003); Nielsen *et al.* (2004); Sabzevari *et al.* (2004); da Silva *et al.* (2007); Wu *et al.* (2003).



Experimental

Crystal data

$C_{24}H_{23}NO_5S$
M_r = 437.49
Triclinic, $P\overline{1}$
a = 10.754 (1) Å
b = 10.950 (1) Å
c = 11.307 (2) Å
α = 65.020 (2)°
β = 65.64 (2)°
γ = 85.92 (2)°
V = 1090.9 (2) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 1.62 mm^{-1}
T = 299 (2) K
0.60 × 0.60 × 0.50 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
6636 measured reflections
3885 independent reflections
3564 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.135
S = 1.07
3885 reflections
284 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O3	0.83 (2)	2.59 (2)	3.060 (2)	116.7 (19)
N1—H1N···O4^{i}	0.83 (2)	2.32 (2)	3.085 (2)	154 (2)
C16—H16A···O1^{ii}	0.97	2.51	3.299 (3)	138
C23—H23C···O2^{iii}	0.96	2.45	3.204 (2)	136
C24—H24B···O2^{iv}	0.96	2.44	3.216 (3)	138

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y+2, -z$; (iii) $-x, -y+1, -z+1$; (iv) $x, y, z-1$.

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); 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: NC2043).

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supplementary materials

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N-(4-Methoxybenzyl)-3-[(1*E*)-3-oxo-3-phenylprop-1-en-1-yl]benzenesulfonamide

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Comment

Chalones, considered as the precursors of flavonoids and isoflavonoids, are abundant in edible plants, and have also been shown to display a diverse array of pharmacological activities. Thus, naturally occurring and synthetic chalones have been reported to possess many useful properties, including antiflammatory (Hsieh *et al.*, 1998), antitrypanosomal (Lunardi *et al.*, 2003), antibacterial (Nielsen *et al.*, 2004), antiviral (Wu *et al.*, 2003), anticancer (Sabzevari *et al.*, 2004), antileishmanial (Hermoso *et al.*, 2003) and antimalarial (Liu *et al.*, 2003, Go *et al.*, 2004). As part of a project to develop more effective antileishmanial compounds (da Silva *et al.*, 2007), we report here the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1) the C1—S1—N1—C16 and S1—N1—C16—C17 torsion angles of 62,5 (2)° and 160.0 (1)°, respectivily, indicate the non-planarity of the system. The planes of the two methoxybenzene are approximately perpendicular, their dihedral angle is 82.41°. The enone group with the two phenyl rings are roughly planar with maximum deviations from the mean plane of −0.361 (2) Å for atom C1 and 0.280 (2) Å for atom C4. The title compound, (I), is stabilized by one N—H···O and three C—H···O intermolecular hydrogen bonds. The amino H atom has an intramolecular contact to O3 of a methoxy group. Details of the hydrogen-bonding parameters are given in Table 1.

Experimental

The title compound (I) was prepared by the reaction of 1 equivalent of chalconesulfonyl chloride (0.50 g, 1.48 mmol) and 2 equivalent of 4- methoxybenzylamine (0.30 g, 2.19 mmol) in the presence of pyridine. The mixture was stirred at 273 K for 30 min and then overnight at room temperatur, according to the literature procedure of Buchmann & Schalinatus (1962). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from ethanol-water (95:5) solution.

Refinement

The amino H atom was located in difference map and refined freely. The C—H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.97 Å. The isotropic displacement parameters of all H atoms were set equal to $1.2U_{eq}$ (parent atom).

Figures

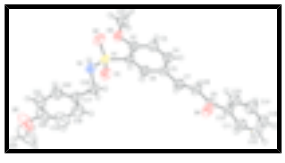

Fig. 1. Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

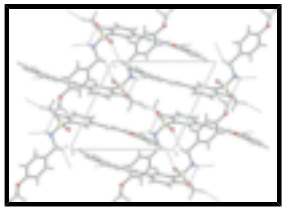

Fig. 2. Molecular packing of (I) with hydrogen bonding shown as dashed lines.

N-(4-Methoxybenzyl)-3-[(1E)-3-oxo-3-phenylprop-1-en-1- yl]benzenesulfonamide

Crystal data

$C_{24}H_{23}NO_5S$	$Z = 2$
$M_r = 437.49$	$F_{000} = 460$
Triclinic, $P\overline{1}$	$D_x = 1.332$ Mg m^{-3}
Hall symbol: -P 1	Cu $K\alpha$ radiation $\lambda = 1.54180$ Å
$a = 10.754$ (1) Å	Cell parameters from 25 reflections
$b = 10.950$ (1) Å	$\theta = 4.5$–21.2º
$c = 11.307$ (2) Å	$\mu = 1.62$ mm^{-1}
$\alpha = 65.020$ (2)º	$T = 299$ (2) K
$\beta = 65.64$ (2)º	Prism, colourless
$\gamma = 85.92$ (2)º	0.60 × 0.60 × 0.50 mm
$V = 1090.9$ (2) Å^3	

Data collection

Enraf–Nonius CAD4 diffractometer	$R_{int} = 0.019$
Radiation source: fine-focus sealed tube	$\theta_{max} = 66.9$º
Monochromator: graphite	$\theta_{min} = 4.5$º
$T = 299$(2) K	$h = -12 \rightarrow 12$
$\omega/2\theta$ scans	$k = -13 \rightarrow 7$
Absorption correction: none	$l = -13 \rightarrow 13$
6636 measured reflections	3 standard reflections
3885 independent reflections	every 120 min
3564 reflections with $I > 2\sigma(I)$	intensity decay: 1.0%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0859P)^2 + 0.2564P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.135$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.76$ e Å^{-3}

3885 reflections

284 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.38$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.035 (2)

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.15246 (17)	0.89121 (17)	0.31382 (18)	0.0399 (4)
C2	0.02059 (17)	0.82499 (17)	0.36844 (18)	0.0416 (4)
C3	−0.09074 (19)	0.89823 (19)	0.3909 (2)	0.0492 (4)
H3	−0.1793	0.8555	0.4293	0.059*
C4	−0.0703 (2)	1.03431 (19)	0.3564 (2)	0.0494 (4)
H4	−0.1461	1.0818	0.3719	0.059*
C5	0.06040 (19)	1.10280 (17)	0.29886 (19)	0.0442 (4)
C6	0.17139 (18)	1.02804 (17)	0.28016 (19)	0.0427 (4)
H6	0.2595	1.0703	0.2446	0.051*
C7	0.0846 (2)	1.24824 (18)	0.2554 (2)	0.0492 (4)
H7	0.1709	1.2815	0.2372	0.059*
C8	−0.0034 (2)	1.33693 (19)	0.2393 (2)	0.0559 (5)
H8	−0.0916	1.3059	0.2600	0.067*
C9	0.0314 (2)	1.48286 (19)	0.1900 (2)	0.0506 (4)
C10	−0.0680 (2)	1.57794 (18)	0.1533 (2)	0.0487 (4)
C11	−0.0281 (3)	1.7164 (2)	0.0892 (3)	0.0664 (6)
H11	0.0607	1.7483	0.0659	0.080*
C12	−0.1185 (3)	1.8078 (2)	0.0596 (3)	0.0765 (7)
H12	−0.0897	1.9005	0.0157	0.092*
C13	−0.2500 (3)	1.7630 (2)	0.0943 (3)	0.0716 (6)
H13	−0.3111	1.8248	0.0759	0.086*
C14	−0.2904 (3)	1.6273 (3)	0.1560 (3)	0.0774 (7)
H14	−0.3796	1.5963	0.1796	0.093*
C15	−0.1995 (2)	1.5348 (2)	0.1839 (3)	0.0672 (6)
H15	−0.2278	1.4424	0.2239	0.081*
C16	0.3357 (2)	0.8561 (2)	0.0215 (2)	0.0577 (5)
H16A	0.3999	0.9302	−0.0034	0.069*

H16B	0.2504	0.8918	0.0219	0.069*
C17	0.39353 (19)	0.80263 (19)	−0.0906 (2)	0.0515 (5)
C18	0.3629 (2)	0.8547 (3)	−0.2081 (3)	0.0734 (7)
H18	0.3024	0.9197	−0.2147	0.088*
C19	0.4199 (3)	0.8125 (3)	−0.3166 (3)	0.0842 (8)
H19	0.3989	0.8503	−0.3958	0.101*
C20	0.5076 (2)	0.7146 (3)	−0.3074 (3)	0.0678 (6)
C21	0.5397 (2)	0.6611 (3)	−0.1897 (3)	0.0636 (6)
H21	0.5992	0.5951	−0.1824	0.076*
C22	0.4836 (2)	0.7055 (2)	−0.0842 (2)	0.0578 (5)
H22	0.5066	0.6696	−0.0063	0.069*
C23	−0.1213 (2)	0.6179 (2)	0.4637 (2)	0.0558 (5)
H23A	−0.1716	0.6598	0.4067	0.067*
H23B	−0.1699	0.6171	0.5569	0.067*
H23C	−0.1120	0.5265	0.4744	0.067*
C24	0.5319 (4)	0.7055 (6)	−0.5223 (4)	0.1353 (17)
H24A	0.5530	0.8023	−0.5766	0.162*
H24B	0.4351	0.6802	−0.4862	0.162*
H24C	0.5826	0.6624	−0.5832	0.162*
N1	0.30943 (17)	0.75095 (15)	0.16603 (18)	0.0504 (4)
H1N	0.246 (3)	0.691 (2)	0.196 (3)	0.061*
O1	0.41463 (13)	0.89476 (13)	0.22650 (17)	0.0584 (4)
O2	0.27018 (14)	0.67994 (13)	0.41698 (16)	0.0575 (4)
O3	0.01235 (12)	0.69317 (12)	0.39384 (16)	0.0521 (3)
O4	0.13915 (16)	1.52652 (15)	0.1792 (2)	0.0679 (4)
O5	0.5685 (2)	0.6637 (3)	−0.4059 (2)	0.1024 (7)
S1	0.29639 (4)	0.79940 (4)	0.28704 (5)	0.04518 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0368 (8)	0.0334 (8)	0.0445 (9)	0.0023 (6)	−0.0147 (7)	−0.0145 (7)
C2	0.0389 (9)	0.0334 (8)	0.0475 (9)	0.0013 (7)	−0.0152 (7)	−0.0157 (7)
C3	0.0367 (9)	0.0430 (10)	0.0614 (11)	0.0026 (7)	−0.0162 (8)	−0.0208 (9)
C4	0.0442 (10)	0.0404 (9)	0.0609 (11)	0.0112 (7)	−0.0212 (8)	−0.0215 (8)
C5	0.0485 (10)	0.0359 (9)	0.0475 (9)	0.0050 (7)	−0.0202 (8)	−0.0175 (7)
C6	0.0413 (9)	0.0358 (9)	0.0483 (9)	0.0012 (7)	−0.0176 (7)	−0.0164 (7)
C7	0.0529 (10)	0.0390 (10)	0.0569 (10)	0.0036 (8)	−0.0233 (9)	−0.0212 (8)
C8	0.0565 (11)	0.0370 (10)	0.0745 (13)	0.0067 (8)	−0.0302 (10)	−0.0220 (9)
C9	0.0568 (11)	0.0373 (9)	0.0570 (11)	0.0056 (8)	−0.0230 (9)	−0.0208 (8)
C10	0.0597 (11)	0.0360 (9)	0.0490 (10)	0.0071 (8)	−0.0226 (8)	−0.0177 (8)
C11	0.0767 (15)	0.0391 (10)	0.0826 (15)	0.0048 (10)	−0.0406 (12)	−0.0184 (10)
C12	0.102 (2)	0.0382 (11)	0.0880 (17)	0.0159 (12)	−0.0496 (15)	−0.0180 (11)
C13	0.0833 (17)	0.0600 (14)	0.0698 (14)	0.0293 (12)	−0.0385 (13)	−0.0236 (11)
C14	0.0682 (15)	0.0638 (14)	0.0938 (18)	0.0148 (12)	−0.0417 (14)	−0.0221 (13)
C15	0.0681 (14)	0.0443 (11)	0.0858 (15)	0.0073 (10)	−0.0378 (12)	−0.0201 (11)
C16	0.0582 (12)	0.0381 (10)	0.0646 (12)	0.0034 (8)	−0.0192 (10)	−0.0178 (9)
C17	0.0433 (10)	0.0433 (10)	0.0573 (11)	−0.0011 (8)	−0.0162 (8)	−0.0162 (8)

C18	0.0591 (13)	0.0799 (16)	0.0718 (14)	0.0226 (12)	−0.0308 (11)	−0.0236 (13)
C19	0.0589 (14)	0.129 (3)	0.0641 (14)	0.0185 (15)	−0.0325 (12)	−0.0356 (15)
C20	0.0373 (10)	0.1054 (19)	0.0641 (13)	0.0027 (11)	−0.0168 (9)	−0.0431 (13)
C21	0.0517 (12)	0.0751 (15)	0.0724 (14)	0.0172 (10)	−0.0284 (10)	−0.0387 (12)
C22	0.0554 (11)	0.0616 (12)	0.0609 (12)	0.0116 (9)	−0.0286 (10)	−0.0273 (10)
C23	0.0446 (10)	0.0413 (10)	0.0700 (12)	−0.0070 (8)	−0.0177 (9)	−0.0185 (9)
C24	0.086 (2)	0.262 (6)	0.096 (2)	0.017 (3)	−0.0407 (19)	−0.107 (3)
N1	0.0443 (8)	0.0341 (8)	0.0607 (10)	−0.0014 (6)	−0.0104 (7)	−0.0203 (7)
O1	0.0387 (7)	0.0437 (7)	0.0847 (10)	−0.0025 (6)	−0.0214 (7)	−0.0241 (7)
O2	0.0539 (8)	0.0391 (7)	0.0694 (9)	0.0034 (6)	−0.0320 (7)	−0.0085 (6)
O3	0.0381 (6)	0.0334 (6)	0.0751 (9)	−0.0008 (5)	−0.0171 (6)	−0.0209 (6)
O4	0.0652 (9)	0.0451 (8)	0.1030 (12)	0.0077 (7)	−0.0435 (9)	−0.0329 (8)
O5	0.0650 (11)	0.187 (2)	0.0935 (13)	0.0307 (12)	−0.0360 (10)	−0.0943 (16)
S1	0.0343 (3)	0.0330 (3)	0.0608 (3)	0.00177 (17)	−0.0175 (2)	−0.0159 (2)

Geometric parameters (Å, °)

C1—C6	1.389 (2)	C15—H15	0.9300
C1—C2	1.401 (2)	C16—N1	1.467 (3)
C1—S1	1.7740 (17)	C16—C17	1.504 (3)
C2—O3	1.349 (2)	C16—H16A	0.9700
C2—C3	1.388 (3)	C16—H16B	0.9700
C3—C4	1.380 (3)	C17—C18	1.376 (3)
C3—H3	0.9300	C17—C22	1.386 (3)
C4—C5	1.395 (3)	C18—C19	1.382 (4)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.392 (3)	C19—C20	1.375 (4)
C5—C7	1.462 (2)	C19—H19	0.9300
C6—H6	0.9300	C20—O5	1.361 (3)
C7—C8	1.316 (3)	C20—C21	1.388 (3)
C7—H7	0.9300	C21—C22	1.371 (3)
C8—C9	1.471 (3)	C21—H21	0.9300
C8—H8	0.9300	C22—H22	0.9300
C9—O4	1.225 (2)	C23—O3	1.432 (2)
C9—C10	1.497 (3)	C23—H23A	0.9600
C10—C15	1.377 (3)	C23—H23B	0.9600
C10—C11	1.384 (3)	C23—H23C	0.9600
C11—C12	1.380 (3)	C24—O5	1.410 (4)
C11—H11	0.9300	C24—H24A	0.9600
C12—C13	1.368 (4)	C24—H24B	0.9600
C12—H12	0.9300	C24—H24C	0.9600
C13—C14	1.360 (4)	N1—S1	1.6179 (18)
C13—H13	0.9300	N1—H1N	0.83 (2)
C14—C15	1.388 (3)	O1—S1	1.4293 (13)
C14—H14	0.9300	O2—S1	1.4271 (14)
C6—C1—C2	120.57 (15)	N1—C16—H16A	109.2
C6—C1—S1	119.79 (13)	C17—C16—H16A	109.2
C2—C1—S1	119.64 (12)	N1—C16—H16B	109.2
O3—C2—C3	124.83 (15)	C17—C16—H16B	109.2

O3—C2—C1	116.54 (15)	H16A—C16—H16B	107.9
C3—C2—C1	118.63 (15)	C18—C17—C22	117.6 (2)
C4—C3—C2	120.14 (17)	C18—C17—C16	120.2 (2)
C4—C3—H3	119.9	C22—C17—C16	122.13 (19)
C2—C3—H3	119.9	C17—C18—C19	121.5 (2)
C3—C4—C5	122.10 (17)	C17—C18—H18	119.2
C3—C4—H4	118.9	C19—C18—H18	119.2
C5—C4—H4	118.9	C20—C19—C18	120.0 (2)
C6—C5—C4	117.54 (16)	C20—C19—H19	120.0
C6—C5—C7	119.63 (17)	C18—C19—H19	120.0
C4—C5—C7	122.81 (17)	O5—C20—C19	125.5 (2)
C1—C6—C5	120.97 (16)	O5—C20—C21	115.3 (2)
C1—C6—H6	119.5	C19—C20—C21	119.2 (2)
C5—C6—H6	119.5	C22—C21—C20	119.8 (2)
C8—C7—C5	126.67 (19)	C22—C21—H21	120.1
C8—C7—H7	116.7	C20—C21—H21	120.1
C5—C7—H7	116.7	C21—C22—C17	121.7 (2)
C7—C8—C9	123.05 (19)	C21—C22—H22	119.1
C7—C8—H8	118.5	C17—C22—H22	119.1
C9—C8—H8	118.5	O3—C23—H23A	109.5
O4—C9—C8	121.05 (18)	O3—C23—H23B	109.5
O4—C9—C10	120.23 (17)	H23A—C23—H23B	109.5
C8—C9—C10	118.72 (17)	O3—C23—H23C	109.5
C15—C10—C11	117.9 (2)	H23A—C23—H23C	109.5
C15—C10—C9	123.28 (17)	H23B—C23—H23C	109.5
C11—C10—C9	118.82 (19)	O5—C24—H24A	109.5
C12—C11—C10	120.8 (2)	O5—C24—H24B	109.5
C12—C11—H11	119.6	H24A—C24—H24B	109.5
C10—C11—H11	119.6	O5—C24—H24C	109.5
C13—C12—C11	120.5 (2)	H24A—C24—H24C	109.5
C13—C12—H12	119.7	H24B—C24—H24C	109.5
C11—C12—H12	119.7	C16—N1—S1	117.95 (13)
C14—C13—C12	119.4 (2)	C16—N1—H1N	112.0 (16)
C14—C13—H13	120.3	S1—N1—H1N	112.5 (16)
C12—C13—H13	120.3	C2—O3—C23	118.27 (14)
C13—C14—C15	120.5 (2)	C20—O5—C24	118.3 (3)
C13—C14—H14	119.8	O2—S1—O1	119.13 (9)
C15—C14—H14	119.8	O2—S1—N1	107.33 (9)
C10—C15—C14	120.9 (2)	O1—S1—N1	107.20 (9)
C10—C15—H15	119.6	O2—S1—C1	109.06 (9)
C14—C15—H15	119.6	O1—S1—C1	106.28 (8)
N1—C16—C17	112.19 (16)	N1—S1—C1	107.31 (9)
C6—C1—C2—O3	177.98 (16)	C9—C10—C15—C14	175.8 (2)
S1—C1—C2—O3	−1.8 (2)	C13—C14—C15—C10	1.6 (4)
C6—C1—C2—C3	−1.3 (3)	N1—C16—C17—C18	147.5 (2)
S1—C1—C2—C3	178.87 (14)	N1—C16—C17—C22	−35.6 (3)
O3—C2—C3—C4	−177.63 (18)	C22—C17—C18—C19	−0.2 (4)
C1—C2—C3—C4	1.6 (3)	C16—C17—C18—C19	176.7 (2)
C2—C3—C4—C5	−0.2 (3)	C17—C18—C19—C20	1.2 (4)

C3—C4—C5—C6	−1.5 (3)	C18—C19—C20—O5	179.1 (3)
C3—C4—C5—C7	177.04 (19)	C18—C19—C20—C21	−1.2 (4)
C2—C1—C6—C5	−0.4 (3)	O5—C20—C21—C22	−180.0 (2)
S1—C1—C6—C5	179.39 (13)	C19—C20—C21—C22	0.3 (4)
C4—C5—C6—C1	1.8 (3)	C20—C21—C22—C17	0.6 (3)
C7—C5—C6—C1	−176.81 (16)	C18—C17—C22—C21	−0.7 (3)
C6—C5—C7—C8	165.6 (2)	C16—C17—C22—C21	−177.6 (2)
C4—C5—C7—C8	−13.0 (3)	C17—C16—N1—S1	160.04 (14)
C5—C7—C8—C9	−177.75 (19)	C3—C2—O3—C23	−7.2 (3)
C7—C8—C9—O4	−9.6 (3)	C1—C2—O3—C23	173.51 (16)
C7—C8—C9—C10	170.6 (2)	C19—C20—O5—C24	−5.3 (4)
O4—C9—C10—C15	−169.4 (2)	C21—C20—O5—C24	175.0 (3)
C8—C9—C10—C15	10.4 (3)	C16—N1—S1—O2	179.58 (14)
O4—C9—C10—C11	8.6 (3)	C16—N1—S1—O1	−51.33 (17)
C8—C9—C10—C11	−171.6 (2)	C16—N1—S1—C1	62.49 (16)
C15—C10—C11—C12	1.1 (4)	C6—C1—S1—O2	127.79 (15)
C9—C10—C11—C12	−177.0 (2)	C2—C1—S1—O2	−52.39 (16)
C10—C11—C12—C13	0.6 (4)	C6—C1—S1—O1	−1.81 (17)
C11—C12—C13—C14	−1.3 (4)	C2—C1—S1—O1	178.01 (14)
C12—C13—C14—C15	0.2 (4)	C6—C1—S1—N1	−116.25 (15)
C11—C10—C15—C14	−2.2 (4)	C2—C1—S1—N1	63.57 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O3	0.83 (2)	2.59 (2)	3.060 (2)	116.7 (19)
N1—H1N···O4^{i}	0.83 (2)	2.32 (2)	3.085 (2)	154 (2)
C16—H16A···O1^{ii}	0.97	2.51	3.299 (3)	138
C23—H23C···O2^{iii}	0.96	2.45	3.204 (2)	136
C24—H24B···O2^{iv}	0.96	2.44	3.216 (3)	138

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

Fig. 1

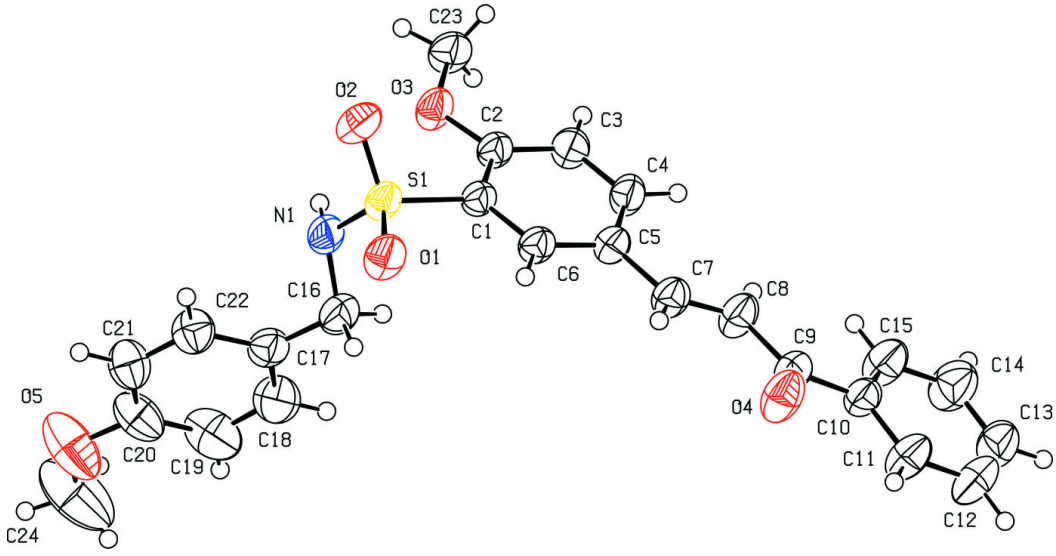
C23
O2
O3
C2
C3
C4
S1
N1
C1
O1
C5
C6
C7
C8
C16
C22
C21
C17
C9
C15
C14
O5
O4
C10
C13
C20
C19
C18
C11
C12
C24

Fig. 2