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Ethyl 2-acetamidomethyl-5-methoxy-1-(phenylsulfonyl)indole-3-carboxylate

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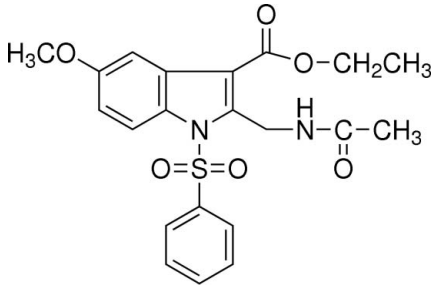
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.132; data-to-parameter ratio = 26.4.

In the title compound, $C_{21}H_{22}N_2O_6S$, the dihedral angle between the sulfonyl-bound phenyl ring and the indole ring system is 79.4 (1)°. The crystal packing is controlled by intra- and intermolecular N—H···O, C—H···O and C—H···π interactions, in addition to van der Waals forces.

Related literature

For medicinal properties of indoles, see: Kgokong *et al.* (2005); Mor *et al.* (2003); Tiwari *et al.* (2006). For related structures, see: Palani *et al.* (2007*a*,*b*).



Experimental

Crystal data

$C_{21}H_{22}N_2O_6S$
M_r = 430.47
Monoclinic, $P2_1/n$
a = 12.6551 (5) Å
b = 10.2166 (3) Å
c = 16.0960 (6) Å
β = 102.738 (2)°
V = 2029.87 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 293 (2) K
0.24 × 0.22 × 0.19 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: none
28118 measured reflections
7225 independent reflections
5514 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.132
S = 1.03
7225 reflections
274 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N17—H17···O5	0.86	2.38	2.852 (2)	115
N17—H17···O3^{i}	0.86	2.58	3.402 (2)	161
C6—H6···O1	0.93	2.37	2.917 (2)	117
C7—H7···O1^{ii}	0.93	2.51	3.416 (2)	164
C9—H9···O4	0.93	2.46	2.989 (2)	116
C16—H16*B*···O2	0.97	2.11	2.904 (2)	138
C23—H23*B*···O4^{iii}	0.96	2.53	3.267 (2)	134
C13—H13···*Cg*^{iv}	0.93	2.79	3.647 (2)	155

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2467).

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supplementary materials

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Ethyl 2-acetamidomethyl-5-methoxy-1-(phenylsulfonyl)indole-3-carboxylate

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Comment

The indole ring system is present in a number of natural products. The indole derivatives show important medicinal properties such as anti-bacterial (Tiwari *et al.*, 2006), anti-malarial (Kgokong *et al.*, 2005), cytoprotective and radical scavenging activities (Mor *et al.*, 2003). In view of the above importance, the crystal structure determination of the title compound was undertaken.

The C—C and C—N bond lengths in the indole ring system are comparable with those observed for related indole derivatives (Palani *et al.*, 2007*a*,b). The indole ring system is planar, with a maximum deviation of 0.021 (1) Å for atom C2. The sum of the bond angle around N1 [359.9 °] indicates sp^2 hybridization. The methoxy group is coplanar with the indole ring system [C23—O6—C8—C9 = 4.2 (2)°]. The phenyl ring of the phenylsulfonyl group is oriented at an angle of 79.4 (1)° to the indole ring system.

Atom S1 has a distorted tetrahedral geometry. The widening of the bond angle O1—S1—O2 [119.96 (6)°] and narrowing of the bond angle N1—S1—C10 [104.29 (5)°] are due to the electon withdrawing character of the phenylsulfonyl group.

The carboxyethyl group at C3 assumes an extended conformation as can be seen from the torsion angles C3—C20—O5—C21 [−179.19 (11)°] and C20—O5—C21—C22 [178.86 (16)°]. The C2—C16—N17—C18 torsion angle of −132.72 (13)° describes the conformation of the acetamido group.

The molecular and crystal structures are stabilized by C—H···O and N—H···O hydrogen bonds (Table 1 and Fig. 2). In addition, C—H···π intermolecular interactions involving the pyrrole (centroid *Cg*) ring is observed,

Experimental

Ethyl-1-phenylsulfonyl-5-methoxy-2-bromomethylindole-3-carboxylate (0.2 g, 0.44 mmol) was dissolved in dry CH_3CN (10 ml). To this $ZnBr_2$ (0.2 g, 0.88 mmol) was added and the reaction mixture was refluxed for 24 h. Then it was quenched with ice water (50 ml) containing few drops of concentrated HCl, extracted with $CHCl_3$ (3 × 5 ml) and dried (Na_2SO_4). The solvent was removed under vacuo and the crude product was recrystallized from methanol.

Refinement

H atoms were positioned geometrically and were treated as riding on their parent atoms, with N—H = 0.82 Å, C—H = 0.93–0.98 Å and U_{iso}(H) = 1.5U_{eq}(C_{methyl}) or 1.2U_{eq}(C). The displacement parameters of atom C22 were restrained to approximate isotropic behaviour.

Figures

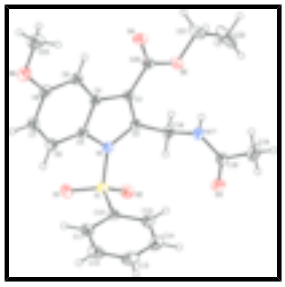

Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

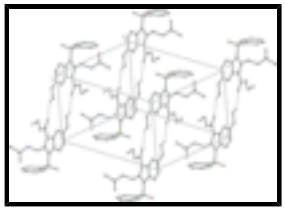

Fig. 2. View of the C–H···O hydrogen-bonded (dashed lines) dimers in the title compound.

Ethyl 2-acetamidomethyl-5-methoxy-1-(phenylsulfonyl)indole-3-carboxylate

Crystal data

$C_{21}H_{22}N_2O_6S$	F_{000} = 904
M_r = 430.47	D_x = 1.409 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 16928 reflections
a = 12.6551 (5) Å	θ = 1.9–28.8º
b = 10.2166 (3) Å	μ = 0.20 mm^{-1}
c = 16.0960 (6) Å	T = 293 (2) K
β = 102.738 (2)º	Black, colourless
V = 2029.87 (13) Å^3	0.24 × 0.22 × 0.19 mm
Z = 4	

Data collection

Bruker Kappa APEXII CCD diffractometer	5514 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.026
Monochromator: graphite	θ_{max} = 33.3º
T = 293(2) K	θ_{min} = 1.9º
ω scans	h = −19→18
Absorption correction: none	k = −8→15
28118 measured reflections	l = −21→23
7225 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.132$	$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 0.3747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
7225 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
274 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
S1	0.25606 (2)	0.24106 (3)	0.033869 (19)	0.03081 (8)
O1	0.23696 (9)	0.26356 (9)	0.11639 (6)	0.0431 (2)
O2	0.22673 (9)	0.33777 (9)	−0.03060 (6)	0.0431 (2)
O3	0.29175 (9)	0.26840 (10)	−0.23564 (8)	0.0490 (3)
O4	−0.00500 (9)	−0.24044 (10)	−0.14390 (7)	0.0479 (3)
O5	0.00232 (8)	−0.06558 (9)	−0.22619 (6)	0.0390 (2)
O6	0.12859 (10)	−0.34650 (10)	0.17262 (7)	0.0523 (3)
N1	0.18728 (8)	0.10353 (9)	−0.00187 (6)	0.02924 (19)
C2	0.13543 (9)	0.06821 (10)	−0.08556 (7)	0.0270 (2)
C3	0.09319 (9)	−0.05521 (11)	−0.08273 (7)	0.0280 (2)
C4	0.12180 (9)	−0.10222 (11)	0.00367 (7)	0.0285 (2)
C5	0.17982 (9)	−0.00283 (11)	0.05311 (7)	0.0294 (2)
C6	0.21941 (11)	−0.01788 (13)	0.14057 (8)	0.0375 (3)
H6	0.2576	0.0488	0.1735	0.045*
C7	0.19976 (13)	−0.13540 (13)	0.17626 (8)	0.0415 (3)
H7	0.2258	−0.1482	0.2344	0.050*
C8	0.14182 (12)	−0.23589 (12)	0.12755 (9)	0.0377 (3)

C9	0.10138 (11)	−0.22145 (12)	0.04093 (8)	0.0341 (2)
H9	0.0622	−0.2880	0.0086	0.041*
C10	0.39255 (10)	0.19783 (11)	0.04459 (8)	0.0319 (2)
C11	0.45391 (12)	0.17032 (14)	0.12542 (9)	0.0427 (3)
H11	0.4230	0.1728	0.1727	0.051*
C12	0.56195 (13)	0.13917 (18)	0.13380 (11)	0.0537 (4)
H12	0.6045	0.1207	0.1874	0.064*
C13	0.60697 (13)	0.13532 (17)	0.06364 (12)	0.0557 (4)
H13	0.6799	0.1145	0.0702	0.067*
C14	0.54543 (13)	0.16196 (17)	−0.01633 (12)	0.0522 (4)
H14	0.5768	0.1582	−0.0634	0.063*
C15	0.43683 (11)	0.19438 (15)	−0.02690 (9)	0.0412 (3)
H15	0.3948	0.2133	−0.0806	0.049*
C16	0.13167 (10)	0.15243 (12)	−0.16280 (7)	0.0330 (2)
H16A	0.0567	0.1669	−0.1915	0.040*
H16B	0.1638	0.2369	−0.1450	0.040*
N17	0.18908 (10)	0.09269 (11)	−0.22197 (7)	0.0383 (2)
H17	0.1767	0.0117	−0.2350	0.046*
C18	0.26035 (11)	0.15747 (13)	−0.25727 (8)	0.0367 (3)
C19	0.29745 (18)	0.08422 (18)	−0.32656 (12)	0.0623 (5)
H19A	0.2728	0.1288	−0.3798	0.094*
H19B	0.2681	−0.0028	−0.3307	0.094*
H19C	0.3751	0.0798	−0.3135	0.094*
C20	0.02614 (9)	−0.13084 (12)	−0.15252 (8)	0.0322 (2)
C21	−0.06499 (15)	−0.13493 (17)	−0.29710 (10)	0.0551 (4)
H21A	−0.1335	−0.1590	−0.2837	0.066*
H21B	−0.0289	−0.2140	−0.3095	0.066*
C22	−0.0834 (3)	−0.0456 (2)	−0.37100 (13)	0.0939 (9)
H22A	−0.1142	0.0348	−0.3565	0.141*
H22B	−0.1322	−0.0858	−0.4182	0.141*
H22C	−0.0156	−0.0278	−0.3863	0.141*
C23	0.07613 (17)	−0.45528 (16)	0.12610 (13)	0.0608 (4)
H23A	0.0031	−0.4318	0.0992	0.091*
H23B	0.0752	−0.5273	0.1642	0.091*
H23C	0.1146	−0.4803	0.0834	0.091*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03425 (15)	0.02395 (13)	0.03383 (15)	−0.00155 (10)	0.00665 (11)	−0.00387 (10)
O1	0.0520 (6)	0.0387 (5)	0.0412 (5)	−0.0023 (4)	0.0158 (4)	−0.0135 (4)
O2	0.0515 (6)	0.0258 (4)	0.0474 (5)	−0.0009 (4)	0.0013 (4)	0.0030 (4)
O3	0.0505 (6)	0.0425 (5)	0.0569 (6)	−0.0135 (4)	0.0180 (5)	−0.0045 (4)
O4	0.0529 (6)	0.0373 (5)	0.0516 (6)	−0.0164 (4)	0.0073 (5)	−0.0051 (4)
O5	0.0396 (5)	0.0370 (4)	0.0358 (4)	−0.0025 (4)	−0.0018 (4)	−0.0048 (4)
O6	0.0732 (8)	0.0365 (5)	0.0481 (6)	−0.0079 (5)	0.0151 (5)	0.0126 (4)
N1	0.0324 (5)	0.0257 (4)	0.0294 (4)	−0.0047 (3)	0.0065 (4)	−0.0010 (3)
C2	0.0255 (5)	0.0275 (5)	0.0285 (5)	0.0010 (4)	0.0066 (4)	−0.0010 (4)

C3	0.0261 (5)	0.0274 (5)	0.0308 (5)	−0.0007 (4)	0.0072 (4)	−0.0021 (4)
C4	0.0280 (5)	0.0271 (5)	0.0323 (5)	−0.0004 (4)	0.0108 (4)	−0.0012 (4)
C5	0.0319 (5)	0.0271 (5)	0.0311 (5)	−0.0011 (4)	0.0105 (4)	0.0002 (4)
C6	0.0472 (7)	0.0354 (6)	0.0300 (5)	−0.0054 (5)	0.0083 (5)	−0.0015 (4)
C7	0.0548 (8)	0.0386 (6)	0.0321 (6)	−0.0012 (6)	0.0115 (6)	0.0044 (5)
C8	0.0450 (7)	0.0309 (5)	0.0406 (6)	−0.0003 (5)	0.0168 (5)	0.0068 (5)
C9	0.0376 (6)	0.0278 (5)	0.0388 (6)	−0.0025 (4)	0.0129 (5)	0.0003 (4)
C10	0.0314 (5)	0.0289 (5)	0.0345 (5)	−0.0047 (4)	0.0053 (4)	−0.0016 (4)
C11	0.0423 (7)	0.0461 (7)	0.0361 (6)	−0.0036 (6)	0.0012 (5)	−0.0015 (5)
C12	0.0417 (7)	0.0566 (9)	0.0550 (9)	0.0006 (7)	−0.0061 (7)	0.0011 (7)
C13	0.0344 (7)	0.0511 (9)	0.0800 (12)	0.0006 (6)	0.0093 (7)	0.0022 (8)
C14	0.0445 (8)	0.0532 (9)	0.0645 (10)	0.0001 (7)	0.0243 (7)	0.0039 (7)
C15	0.0399 (7)	0.0449 (7)	0.0400 (6)	−0.0030 (5)	0.0113 (5)	0.0031 (5)
C16	0.0372 (6)	0.0302 (5)	0.0318 (5)	0.0013 (4)	0.0081 (5)	0.0025 (4)
N17	0.0488 (6)	0.0335 (5)	0.0364 (5)	−0.0082 (4)	0.0173 (5)	−0.0035 (4)
C18	0.0364 (6)	0.0387 (6)	0.0360 (6)	−0.0020 (5)	0.0098 (5)	0.0028 (5)
C19	0.0832 (13)	0.0533 (9)	0.0647 (10)	−0.0059 (9)	0.0468 (10)	−0.0048 (8)
C20	0.0270 (5)	0.0322 (5)	0.0374 (6)	−0.0014 (4)	0.0072 (4)	−0.0057 (4)
C21	0.0553 (9)	0.0518 (8)	0.0471 (8)	−0.0011 (7)	−0.0128 (7)	−0.0141 (7)
C22	0.146 (2)	0.0566 (11)	0.0529 (10)	0.0219 (13)	−0.0351 (12)	−0.0046 (9)
C23	0.0755 (12)	0.0346 (7)	0.0720 (11)	−0.0107 (7)	0.0155 (9)	0.0103 (7)

Geometric parameters (Å, °)

S1—O1	1.4203 (10)	C11—C12	1.381 (2)
S1—O2	1.4216 (10)	C11—H11	0.93
S1—N1	1.6858 (10)	C12—C13	1.373 (3)
S1—C10	1.7542 (13)	C12—H12	0.93
O3—C18	1.2257 (16)	C13—C14	1.377 (3)
O4—C20	1.2052 (15)	C13—H13	0.93
O5—C20	1.3356 (16)	C14—C15	1.387 (2)
O5—C21	1.4497 (16)	C14—H14	0.93
O6—C8	1.3728 (15)	C15—H15	0.93
O6—C23	1.420 (2)	C16—N17	1.4534 (16)
N1—C2	1.4092 (14)	C16—H16A	0.97
N1—C5	1.4176 (14)	C16—H16B	0.97
C2—C3	1.3742 (15)	N17—C18	1.3417 (16)
C2—C16	1.5041 (15)	N17—H17	0.86
C3—C4	1.4401 (16)	C18—C19	1.502 (2)
C3—C20	1.4692 (16)	C19—H19A	0.96
C4—C5	1.3949 (16)	C19—H19B	0.96
C4—C9	1.4066 (16)	C19—H19C	0.96
C5—C6	1.3948 (17)	C21—C22	1.476 (3)
C6—C7	1.3771 (18)	C21—H21A	0.97
C6—H6	0.93	C21—H21B	0.97
C7—C8	1.397 (2)	C22—H22A	0.96
C7—H7	0.93	C22—H22B	0.96
C8—C9	1.3831 (19)	C22—H22C	0.96
C9—H9	0.93	C23—H23A	0.96

C10—C15	1.3869 (18)	C23—H23B	0.96
C10—C11	1.3890 (18)	C23—H23C	0.96
O1—S1—O2	119.96 (6)	C14—C13—H13	119.6
O1—S1—N1	105.81 (5)	C13—C14—C15	120.19 (15)
O2—S1—N1	107.35 (5)	C13—C14—H14	119.9
O1—S1—C10	108.40 (6)	C15—C14—H14	119.9
O2—S1—C10	109.86 (6)	C10—C15—C14	118.35 (14)
N1—S1—C10	104.29 (5)	C10—C15—H15	120.8
C20—O5—C21	115.68 (11)	C14—C15—H15	120.8
C8—O6—C23	117.57 (12)	N17—C16—C2	111.85 (10)
C2—N1—C5	108.62 (9)	N17—C16—H16A	109.2
C2—N1—S1	129.51 (8)	C2—C16—H16A	109.2
C5—N1—S1	121.76 (8)	N17—C16—H16B	109.2
C3—C2—N1	107.81 (9)	C2—C16—H16B	109.2
C3—C2—C16	127.64 (10)	H16A—C16—H16B	107.9
N1—C2—C16	124.53 (10)	C18—N17—C16	123.38 (11)
C2—C3—C4	108.74 (10)	C18—N17—H17	118.3
C2—C3—C20	128.35 (10)	C16—N17—H17	118.3
C4—C3—C20	122.88 (10)	O3—C18—N17	122.81 (13)
C5—C4—C9	120.68 (11)	O3—C18—C19	122.46 (13)
C5—C4—C3	107.26 (10)	N17—C18—C19	114.72 (12)
C9—C4—C3	132.06 (11)	C18—C19—H19A	109.5
C6—C5—C4	121.48 (11)	C18—C19—H19B	109.5
C6—C5—N1	130.99 (11)	H19A—C19—H19B	109.5
C4—C5—N1	107.52 (10)	C18—C19—H19C	109.5
C7—C6—C5	117.35 (12)	H19A—C19—H19C	109.5
C7—C6—H6	121.3	H19B—C19—H19C	109.5
C5—C6—H6	121.3	O4—C20—O5	123.41 (12)
C6—C7—C8	121.81 (12)	O4—C20—C3	123.29 (12)
C6—C7—H7	119.1	O5—C20—C3	113.30 (10)
C8—C7—H7	119.1	O5—C21—C22	107.04 (15)
O6—C8—C9	124.01 (12)	O5—C21—H21A	110.3
O6—C8—C7	114.73 (12)	C22—C21—H21A	110.3
C9—C8—C7	121.26 (11)	O5—C21—H21B	110.3
C8—C9—C4	117.40 (11)	C22—C21—H21B	110.3
C8—C9—H9	121.3	H21A—C21—H21B	108.6
C4—C9—H9	121.3	C21—C22—H22A	109.5
C15—C10—C11	121.82 (12)	C21—C22—H22B	109.5
C15—C10—S1	119.61 (10)	H22A—C22—H22B	109.5
C11—C10—S1	118.56 (10)	C21—C22—H22C	109.5
C12—C11—C10	118.37 (14)	H22A—C22—H22C	109.5
C12—C11—H11	120.8	H22B—C22—H22C	109.5
C10—C11—H11	120.8	O6—C23—H23A	109.5
C13—C12—C11	120.50 (15)	O6—C23—H23B	109.5
C13—C12—H12	119.7	H23A—C23—H23B	109.5
C11—C12—H12	119.8	O6—C23—H23C	109.5
C12—C13—C14	120.77 (15)	H23A—C23—H23C	109.5
C12—C13—H13	119.6	H23B—C23—H23C	109.5

O1—S1—N1—C2	147.04 (10)	C6—C7—C8—C9	−0.1 (2)
O2—S1—N1—C2	17.82 (12)	O6—C8—C9—C4	−179.87 (12)
C10—S1—N1—C2	−98.72 (11)	C7—C8—C9—C4	0.6 (2)
O1—S1—N1—C5	−37.20 (11)	C5—C4—C9—C8	−0.59 (18)
O2—S1—N1—C5	−166.41 (9)	C3—C4—C9—C8	179.49 (12)
C10—S1—N1—C5	77.05 (10)	O1—S1—C10—C15	−168.10 (10)
C5—N1—C2—C3	2.07 (12)	O2—S1—C10—C15	−35.28 (12)
S1—N1—C2—C3	178.27 (8)	N1—S1—C10—C15	79.50 (11)
C5—N1—C2—C16	−176.42 (10)	O1—S1—C10—C11	10.68 (12)
S1—N1—C2—C16	−0.22 (17)	O2—S1—C10—C11	143.50 (10)
N1—C2—C3—C4	−2.20 (12)	N1—S1—C10—C11	−101.72 (11)
C16—C2—C3—C4	176.23 (11)	C15—C10—C11—C12	0.2 (2)
N1—C2—C3—C20	175.70 (11)	S1—C10—C11—C12	−178.58 (12)
C16—C2—C3—C20	−5.87 (19)	C10—C11—C12—C13	−0.2 (2)
C2—C3—C4—C5	1.51 (12)	C11—C12—C13—C14	−0.2 (3)
C20—C3—C4—C5	−176.53 (10)	C12—C13—C14—C15	0.6 (3)
C2—C3—C4—C9	−178.56 (12)	C11—C10—C15—C14	0.2 (2)
C20—C3—C4—C9	3.40 (19)	S1—C10—C15—C14	178.96 (12)
C9—C4—C5—C6	0.01 (18)	C13—C14—C15—C10	−0.6 (2)
C3—C4—C5—C6	179.95 (11)	C3—C2—C16—N17	−62.75 (15)
C9—C4—C5—N1	179.85 (10)	N1—C2—C16—N17	115.43 (12)
C3—C4—C5—N1	−0.21 (12)	C2—C16—N17—C18	−132.72 (13)
C2—N1—C5—C6	178.69 (13)	C16—N17—C18—O3	8.1 (2)
S1—N1—C5—C6	2.14 (18)	C16—N17—C18—C19	−170.97 (14)
C2—N1—C5—C4	−1.13 (12)	C21—O5—C20—O4	0.19 (19)
S1—N1—C5—C4	−177.68 (8)	C21—O5—C20—C3	−179.19 (11)
C4—C5—C6—C7	0.53 (19)	C2—C3—C20—O4	178.17 (12)
N1—C5—C6—C7	−179.26 (12)	C4—C3—C20—O4	−4.20 (18)
C5—C6—C7—C8	−0.5 (2)	C2—C3—C20—O5	−2.44 (17)
C23—O6—C8—C9	4.2 (2)	C4—C3—C20—O5	175.19 (10)
C23—O6—C8—C7	−176.27 (15)	C20—O5—C21—C22	178.86 (16)
C6—C7—C8—O6	−179.63 (14)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N17—H17···O5	0.86	2.38	2.852 (2)	115
N17—H17···O3^{i}	0.86	2.58	3.402 (2)	161
C6—H6···O1	0.93	2.37	2.917 (2)	117
C7—H7···O1^{ii}	0.93	2.51	3.416 (2)	164
C9—H9···O4	0.93	2.46	2.989 (2)	116
C16—H16B···O2	0.97	2.11	2.904 (2)	138
C23—H23B···O4^{iii}	0.96	2.53	3.267 (2)	134
C13—H13···Cg^{iv}	0.93	2.79	3.647 (2)	155

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

Fig. 1

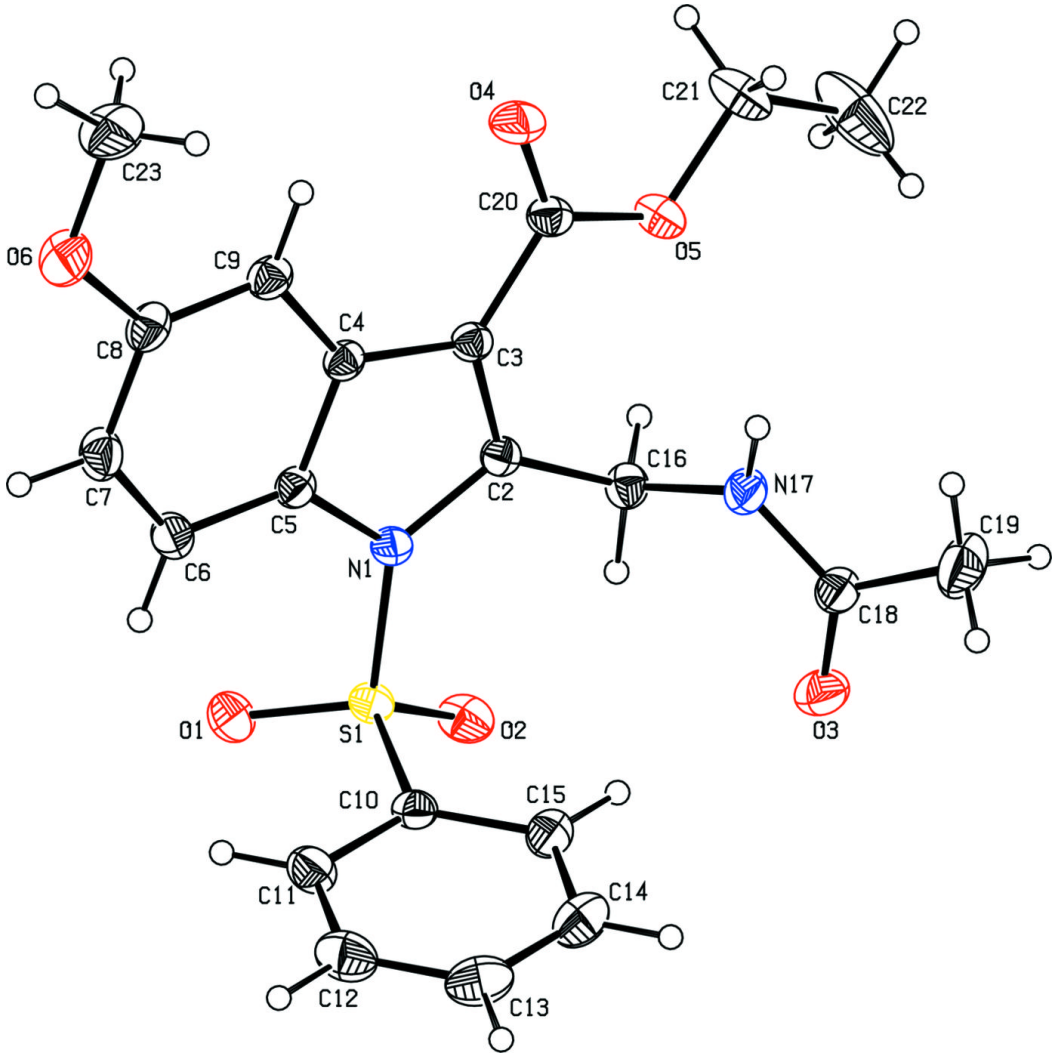
O4
C21
C22
C23
C20
O6
C9
O5
C4
C8
C3
C16
N17
C7
C5
C2
C19
C6
N1
C18
O1
S1
O2
O3
C10
C15
C11
C14
C12
C13

Fig. 2