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2-Bromo-3-ethoxy-3-[4-(methylsulfanyl)-phenyl]-1-[3-(*p*-tolyl)-4-sydnonyl]-propan-1-one

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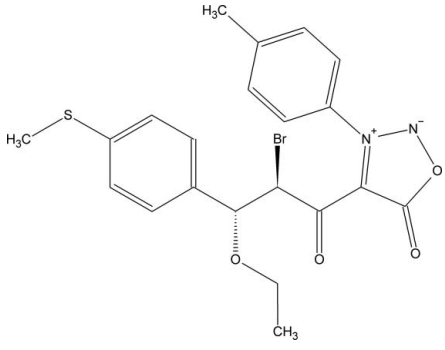
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.110; data-to-parameter ratio = 15.2.

In the title compound, $C_{21}H_{21}BrN_2O_4S$, the carbonyl group of the central propan-1-one unit is twisted by 14.7 (4)° from the plane of the cyclic sydnone group ($C_2N_2O_2$) to which it is attached, and an intramolecular C—H···O contact is formed to the exocyclic O atom of the sydnone group. Intermolecular C—H···O, C—H···S and C—H···π contacts are observed.

Related literature

For related structures see: Abdul Ajees *et al.* (2002); Balamurugan *et al.* (2006); Thamotharan *et al.* (2003). For general literature related to sydnones, see: Earl & Mackney (1935); Narla & Rao (1995); Pillai *et al.* (1993); Satyanarayana & Rao (1995); Sutherland *et al.* (1986).



Experimental

Crystal data

$C_{21}H_{21}BrN_2O_4S$
M_r = 477.37
Monoclinic, $C2/c$
a = 24.420 (3) Å
b = 12.3883 (13) Å
c = 18.3113 (19) Å
β = 127.564 (1)°
V = 4391.1 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.00 mm^{-1}
T = 292 (2) K
0.37 × 0.19 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.526, T_{max} = 0.760
21297 measured reflections
4028 independent reflections
2844 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.00
4028 reflections
265 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

Cg is the centroid of the C15–C20 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2	0.98	2.29	3.093 (4)	139
C6—H6A···Cg^{i}	0.97	2.96	3.830	150
C16—H16···S1^{ii}	0.93	2.88	3.763 (4)	159
C21—H21A···O3^{iii}	0.96	2.57	3.506 (4)	165

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1999) and *CAMERON* (Pearce & Watkin, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2231).

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supplementary materials

Acta Cryst. (2007). E**63**, o3976 [**doi:10.1107/S1600536807041931**]

2-Bromo-3-ethoxy-3-[4-(methylsulfanyl)phenyl]-1-[3-(*p*-tolyl)-4-sydnonyl]propan-1-one

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Comment

Sydnones are products of dehydration of *N*-nitroso-alpha-amino acids (Earl & Mackney, 1935). Although less toxic (Pillai *et al.*, 1993) than the latter, they remain potent porphyrinogenic (Sutherland *et al.*, 1986) and anti-inflammatory (Satyanarayana & Rao, 1995) compounds. They are also known to scavenge free radicals (Narla & Rao, 1995).

The molecular conformation of the title compound is influenced by π conjugation through the C2—C3 bond and an intramolecular C—H···O hydogen bond, resulting in near coplanarity of the atoms H4, C4, C3, C2, C1 and O2 (torsion angle C4/C3/C2/C1 = −14.7 (4)°) (Fig. 1). The crystal structure exhibits C—H···O intermolecular contacts which define dimeric units (Fig. 2 and Table 1). C—H···S contacts exist between adjacent dimers along the *b*-axis (Fig. 2 and Table 1). Intermolecular C—H···π contacts are also observed.

Experimental

2,3-Dibromo-1-(3-*p*-tolylsydnon-4-yl)-3-*p*-thiomethylphenyl-propan-1-one (0.01 mol) was dissolved in ethanol by heating and triethylamine (0.05 mol) in ethanol was added. The clear solution was stirred for 24 h then filtered. The filtrate was left to stand for a few days, then the solid was collected by filtration and recrystallized from ethanol to yield the title compound.

Refinement

H atoms were placed geometrically and refined using a riding model with C—H = 0.93–0.98 Å and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

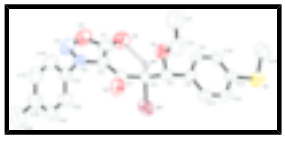

Fig. 1. The molecular structure of the title compound showing displacement ellipsoids at 50% probability for non-H atoms. The dashed line indicates an intramolecular C—H···O contact.

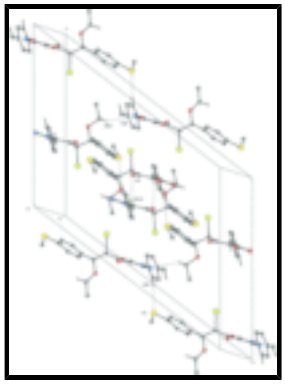

Fig. 2. Packing diagram viewed down the *b* axis. The dotted lines indicate intermolecular contacts.

2-Bromo-3-ethoxy-3-[4-(methylsulfanyl)phenyl]-1-[3-(*p*-tolyl)-4-\ sydnonyl]propan-1-one

Crystal data

$C_{21}H_{21}BrN_2O_4S$	F_{000} = 1952
M_r = 477.37	D_x = 1.444 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 398-400 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 24.420 (3) Å	Cell parameters from 1152 reflections
b = 12.3883 (13) Å	θ = 2.1–25.5º
c = 18.3113 (19) Å	μ = 2.00 mm^{-1}
β = 127.564 (1)º	*T* = 292 (2) K
V = 4391.1 (8) Å^3	Block, yellow
Z = 8	0.37 × 0.19 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer	4028 independent reflections
Radiation source: fine-focus sealed tube	2844 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 292(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −29→29
T_{min} = 0.526, T_{max} = 0.760	*k* = −14→14
21297 measured reflections	*l* = −22→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.110	$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
4028 reflections	$\Delta\rho_{max} = 0.61$ e Å^{-3}
265 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Br1	0.129744 (17)	0.37658 (3)	0.35683 (2)	0.08060 (16)
S1	0.40477 (5)	0.71008 (7)	0.60362 (7)	0.0927 (3)
O1	−0.08313 (11)	0.4536 (2)	0.36798 (17)	0.0953 (7)
O2	0.01082 (12)	0.55252 (19)	0.41210 (17)	0.0961 (7)
O3	0.09233 (9)	0.22010 (15)	0.46713 (14)	0.0724 (5)
O4	0.18750 (9)	0.39308 (14)	0.61802 (13)	0.0624 (5)
N1	−0.10169 (14)	0.3481 (3)	0.3577 (2)	0.0883 (8)
N2	−0.04712 (11)	0.2940 (2)	0.38361 (14)	0.0647 (6)
C1	−0.01380 (16)	0.4642 (3)	0.4000 (2)	0.0758 (8)
C2	0.00835 (13)	0.3559 (2)	0.40954 (18)	0.0578 (6)
C3	0.07635 (13)	0.3141 (2)	0.44795 (17)	0.0563 (6)
C4	0.12791 (13)	0.39690 (19)	0.46110 (18)	0.0559 (6)
H4	0.1112	0.4697	0.4586	0.067*
C5	0.19940 (13)	0.38213 (19)	0.55155 (18)	0.0548 (6)
H5	0.2162	0.3092	0.5546	0.066*
C6	0.24287 (16)	0.3559 (3)	0.7073 (2)	0.0831 (9)
H6A	0.2861	0.3860	0.7251	0.100*
H6B	0.2459	0.2779	0.7070	0.100*
C7	0.23095 (19)	0.3895 (3)	0.7747 (2)	0.1050 (13)
H7A	0.2643	0.3551	0.8329	0.158*
H7B	0.1853	0.3686	0.7523	0.158*
H7C	0.2356	0.4664	0.7824	0.158*
C8	0.25044 (12)	0.46434 (19)	0.56521 (16)	0.0515 (6)
C9	0.24604 (13)	0.5709 (2)	0.58355 (18)	0.0573 (6)
H9	0.2119	0.5909	0.5888	0.069*
C10	0.29095 (13)	0.6482 (2)	0.59430 (18)	0.0586 (7)

H10	0.2862	0.7197	0.6051	0.070*
C11	0.34295 (14)	0.6192 (2)	0.58894 (18)	0.0586 (7)
C12	0.34768 (14)	0.5135 (2)	0.57035 (19)	0.0658 (7)
H12	0.3821	0.4933	0.5656	0.079*
C13	0.30206 (13)	0.4374 (2)	0.55881 (18)	0.0620 (7)
H13	0.3061	0.3662	0.5464	0.074*
C14	0.39791 (19)	0.8274 (3)	0.6521 (2)	0.0859 (9)
H14A	0.4305	0.8803	0.6618	0.129*
H14B	0.4076	0.8097	0.7100	0.129*
H14C	0.3519	0.8560	0.6110	0.129*
C15	−0.05548 (12)	0.1771 (2)	0.37652 (17)	0.0617 (7)
C16	−0.07699 (15)	0.1260 (3)	0.4219 (2)	0.0737 (9)
H16	−0.0848	0.1649	0.4582	0.088*
C17	−0.08666 (15)	0.0150 (3)	0.4120 (2)	0.0773 (8)
H17	−0.1015	−0.0203	0.4419	0.093*
C18	−0.07508 (14)	−0.0435 (3)	0.35973 (18)	0.0717 (8)
C19	−0.05431 (16)	0.0108 (3)	0.31505 (19)	0.0750 (8)
H19	−0.0466	−0.0281	0.2786	0.090*
C20	−0.04448 (16)	0.1203 (2)	0.3223 (2)	0.0725 (8)
H20	−0.0306	0.1554	0.2911	0.087*
C21	−0.0857 (2)	−0.1642 (3)	0.3507 (2)	0.0961 (11)
H21A	−0.0941	−0.1889	0.3928	0.144*
H21B	−0.1246	−0.1818	0.2888	0.144*
H21C	−0.0451	−0.1989	0.3648	0.144*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0936 (3)	0.0849 (3)	0.0608 (2)	−0.01660 (16)	0.04580 (19)	−0.00885 (15)
S1	0.1017 (6)	0.0901 (6)	0.1243 (7)	−0.0290 (5)	0.0884 (6)	−0.0232 (5)
O1	0.0724 (14)	0.0963 (18)	0.1152 (18)	0.0283 (13)	0.0562 (14)	0.0039 (14)
O2	0.0999 (16)	0.0629 (15)	0.129 (2)	0.0177 (13)	0.0712 (16)	0.0076 (13)
O3	0.0580 (11)	0.0553 (12)	0.0945 (14)	0.0018 (9)	0.0417 (11)	0.0058 (10)
O4	0.0515 (10)	0.0764 (13)	0.0553 (11)	0.0026 (8)	0.0304 (9)	0.0046 (9)
N1	0.0588 (15)	0.101 (2)	0.099 (2)	0.0147 (15)	0.0451 (15)	−0.0009 (17)
N2	0.0478 (13)	0.0880 (18)	0.0532 (13)	0.0064 (12)	0.0281 (11)	−0.0032 (12)
C1	0.070 (2)	0.078 (2)	0.078 (2)	0.0163 (17)	0.0443 (17)	0.0027 (17)
C2	0.0508 (15)	0.0632 (17)	0.0536 (15)	0.0035 (12)	0.0289 (13)	−0.0003 (12)
C3	0.0546 (15)	0.0545 (17)	0.0545 (15)	0.0007 (12)	0.0306 (13)	−0.0016 (12)
C4	0.0561 (15)	0.0491 (15)	0.0582 (15)	0.0006 (11)	0.0327 (13)	−0.0013 (11)
C5	0.0538 (15)	0.0507 (15)	0.0573 (15)	0.0045 (11)	0.0325 (13)	−0.0017 (11)
C6	0.0639 (18)	0.108 (3)	0.0596 (18)	0.0037 (16)	0.0282 (16)	0.0175 (17)
C7	0.087 (2)	0.159 (4)	0.065 (2)	−0.014 (2)	0.044 (2)	0.009 (2)
C8	0.0480 (13)	0.0513 (15)	0.0514 (14)	0.0019 (11)	0.0284 (12)	−0.0024 (11)
C9	0.0535 (14)	0.0597 (16)	0.0645 (16)	0.0020 (13)	0.0389 (13)	−0.0087 (13)
C10	0.0617 (16)	0.0524 (15)	0.0620 (16)	−0.0011 (12)	0.0378 (14)	−0.0082 (12)
C11	0.0612 (16)	0.0628 (17)	0.0561 (16)	−0.0041 (13)	0.0380 (14)	−0.0048 (13)
C12	0.0649 (17)	0.0696 (19)	0.0795 (19)	0.0005 (14)	0.0525 (16)	−0.0103 (15)

C13	0.0637 (16)	0.0539 (16)	0.0721 (18)	0.0046 (13)	0.0434 (15)	−0.0078 (13)
C14	0.100 (2)	0.0644 (19)	0.093 (2)	−0.0192 (18)	0.058 (2)	−0.0040 (17)
C15	0.0443 (14)	0.081 (2)	0.0505 (15)	−0.0072 (13)	0.0240 (13)	−0.0074 (14)
C16	0.0562 (16)	0.115 (3)	0.0531 (16)	0.0031 (16)	0.0348 (14)	0.0014 (16)
C17	0.0709 (18)	0.097 (3)	0.0656 (18)	−0.0126 (17)	0.0423 (16)	0.0062 (17)
C18	0.0614 (16)	0.095 (2)	0.0432 (15)	−0.0177 (15)	0.0239 (13)	−0.0043 (15)
C19	0.085 (2)	0.083 (2)	0.0588 (17)	−0.0221 (17)	0.0447 (16)	−0.0167 (15)
C20	0.0765 (19)	0.090 (2)	0.0631 (18)	−0.0193 (16)	0.0487 (16)	−0.0108 (15)
C21	0.104 (3)	0.092 (2)	0.073 (2)	−0.032 (2)	0.044 (2)	−0.0061 (19)

Geometric parameters (Å, °)

Br1—C4	1.953 (3)	C9—C10	1.377 (4)
S1—C14	1.764 (3)	C9—H9	0.930
S1—C11	1.767 (3)	C10—C11	1.380 (4)
O1—N1	1.359 (4)	C10—H10	0.930
O1—C1	1.420 (4)	C11—C12	1.376 (3)
O2—C1	1.202 (4)	C12—C13	1.374 (4)
O3—C3	1.210 (3)	C12—H12	0.930
O4—C5	1.420 (3)	C13—H13	0.930
O4—C6	1.421 (3)	C14—H14A	0.960
N1—N2	1.296 (3)	C14—H14B	0.960
C1—C2	1.417 (4)	C14—H14C	0.960
C2—N2	1.366 (3)	C15—C20	1.370 (4)
C2—C3	1.448 (4)	C15—C16	1.377 (4)
C3—C4	1.525 (3)	C15—N2	1.457 (4)
C4—C5	1.516 (4)	C16—C17	1.388 (4)
C4—H4	0.980	C16—H16	0.930
C5—C8	1.508 (3)	C17—C18	1.360 (4)
C5—H5	0.980	C17—H17	0.930
C6—C7	1.489 (5)	C18—C19	1.373 (4)
C6—H6A	0.970	C18—C21	1.510 (5)
C6—H6B	0.970	C19—C20	1.371 (4)
C7—H7A	0.960	C19—H19	0.930
C7—H7B	0.960	C20—H20	0.930
C7—H7C	0.960	C21—H21A	0.960
C8—C13	1.376 (3)	C21—H21B	0.960
C8—C9	1.382 (3)	C21—H21C	0.960
C14—S1—C11	105.46 (14)	C10—C9—H9	119.1
N1—O1—C1	111.0 (2)	C8—C9—H9	119.1
C5—O4—C6	114.0 (2)	C9—C10—C11	119.8 (2)
N2—N1—O1	105.4 (2)	C9—C10—H10	120.1
N1—N2—C2	114.6 (3)	C11—C10—H10	120.1
N1—N2—C15	115.1 (2)	C12—C11—C10	119.0 (2)
C2—N2—C15	130.2 (2)	C12—C11—S1	116.8 (2)
O2—C1—C2	136.8 (3)	C10—C11—S1	124.2 (2)
O2—C1—O1	119.8 (3)	C13—C12—C11	120.6 (2)
C2—C1—O1	103.5 (3)	C13—C12—H12	119.7
N2—C2—C1	105.4 (2)	C11—C12—H12	119.7

N2—C2—C3	124.6 (2)	C12—C13—C8	121.3 (2)
C1—C2—C3	129.6 (3)	C12—C13—H13	119.4
O3—C3—C2	123.8 (2)	C8—C13—H13	119.4
O3—C3—C4	120.8 (2)	S1—C14—H14A	109.5
C2—C3—C4	115.3 (2)	S1—C14—H14B	109.5
C5—C4—C3	112.4 (2)	S1—C14—H14C	109.5
C5—C4—Br1	110.79 (17)	H14A—C14—H14B	109.5
C3—C4—Br1	105.53 (17)	H14A—C14—H14C	109.5
C5—C4—H4	109.3	H14B—C14—H14C	109.5
C3—C4—H4	109.3	C20—C15—C16	121.1 (3)
Br1—C4—H4	109.3	C20—C15—N2	119.8 (3)
O4—C5—C8	112.0 (2)	C16—C15—N2	119.1 (3)
O4—C5—C4	102.9 (2)	C15—C16—C17	118.2 (3)
C8—C5—C4	112.6 (2)	C15—C16—H16	120.9
O4—C5—H5	109.7	C17—C16—H16	120.9
C8—C5—H5	109.7	C18—C17—C16	121.9 (3)
C4—C5—H5	109.7	C18—C17—H17	119.1
O4—C6—C7	109.5 (3)	C16—C17—H17	119.1
O4—C6—H6A	109.8	C17—C18—C19	118.0 (3)
C7—C6—H6A	109.8	C17—C18—C21	120.6 (3)
O4—C6—H6B	109.8	C19—C18—C21	121.4 (3)
C7—C6—H6B	109.8	C20—C19—C18	122.2 (3)
H6A—C6—H6B	108.2	C20—C19—H19	118.9
C6—C7—H7A	109.5	C18—C19—H19	118.9
C6—C7—H7B	109.5	C15—C20—C19	118.6 (3)
H7A—C7—H7B	109.5	C15—C20—H20	120.7
C6—C7—H7C	109.5	C19—C20—H20	120.7
H7A—C7—H7C	109.5	C18—C21—H21A	109.5
H7B—C7—H7C	109.5	C18—C21—H21C	109.5
C13—C8—C9	117.6 (2)	H21A—C21—H21C	109.5
C13—C8—C5	122.0 (2)	C18—C21—H21B	109.5
C9—C8—C5	120.4 (2)	H21A—C21—H21B	109.5
C10—C9—C8	121.7 (2)	H21C—C21—H21B	109.5
C1—O1—N1—N2	1.5 (3)	C9—C10—C11—C12	1.8 (4)
N1—O1—C1—O2	179.3 (3)	C9—C10—C11—S1	−178.8 (2)
N1—O1—C1—C2	−0.9 (3)	C14—S1—C11—C12	−166.6 (2)
O2—C1—C2—N2	179.7 (4)	C14—S1—C11—C10	13.9 (3)
O1—C1—C2—N2	0.0 (3)	C10—C11—C12—C13	−1.1 (4)
O2—C1—C2—C3	6.3 (6)	S1—C11—C12—C13	179.4 (2)
O1—C1—C2—C3	−173.5 (3)	C11—C12—C13—C8	0.2 (4)
N2—C2—C3—O3	−5.5 (4)	C9—C8—C13—C12	0.1 (4)
C1—C2—C3—O3	166.9 (3)	C5—C8—C13—C12	179.2 (2)
N2—C2—C3—C4	173.0 (2)	C20—C15—C16—C17	0.6 (4)
C1—C2—C3—C4	−14.7 (4)	N2—C15—C16—C17	178.1 (2)
O3—C3—C4—C5	−42.9 (3)	C15—C16—C17—C18	0.4 (4)
C2—C3—C4—C5	138.6 (2)	C16—C17—C18—C19	−1.0 (5)
O3—C3—C4—Br1	77.9 (3)	C16—C17—C18—C21	179.6 (3)
C2—C3—C4—Br1	−100.6 (2)	C17—C18—C19—C20	0.6 (5)
C6—O4—C5—C8	−73.9 (3)	C21—C18—C19—C20	180.0 (3)

C6—O4—C5—C4	164.9 (2)	C16—C15—C20—C19	−1.0 (4)
C3—C4—C5—O4	−58.8 (2)	N2—C15—C20—C19	−178.4 (3)
Br1—C4—C5—O4	−176.61 (14)	C18—C19—C20—C15	0.4 (5)
C3—C4—C5—C8	−179.6 (2)	O1—N1—N2—C2	−1.5 (3)
Br1—C4—C5—C8	62.6 (2)	O1—N1—N2—C15	−178.8 (2)
C5—O4—C6—C7	169.5 (2)	C1—C2—N2—N1	1.0 (3)
O4—C5—C8—C13	136.9 (2)	C3—C2—N2—N1	174.8 (3)
C4—C5—C8—C13	−107.6 (3)	C1—C2—N2—C15	177.7 (3)
O4—C5—C8—C9	−43.9 (3)	C3—C2—N2—C15	−8.4 (4)
C4—C5—C8—C9	71.5 (3)	C20—C15—N2—N1	120.7 (3)
C13—C8—C9—C10	0.6 (4)	C16—C15—N2—N1	−56.8 (3)
C5—C8—C9—C10	−178.5 (2)	C20—C15—N2—C2	−56.1 (4)
C8—C9—C10—C11	−1.6 (4)	C16—C15—N2—C2	126.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2	0.98	2.29	3.093 (4)	139
C6—H6A···Cg^{i}	0.97	2.96	3.830	150
C16—H16···S1^{ii}	0.93	2.88	3.763 (4)	159
C21—H21A···O3^{iii}	0.96	2.57	3.506 (4)	165

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

Fig. 1

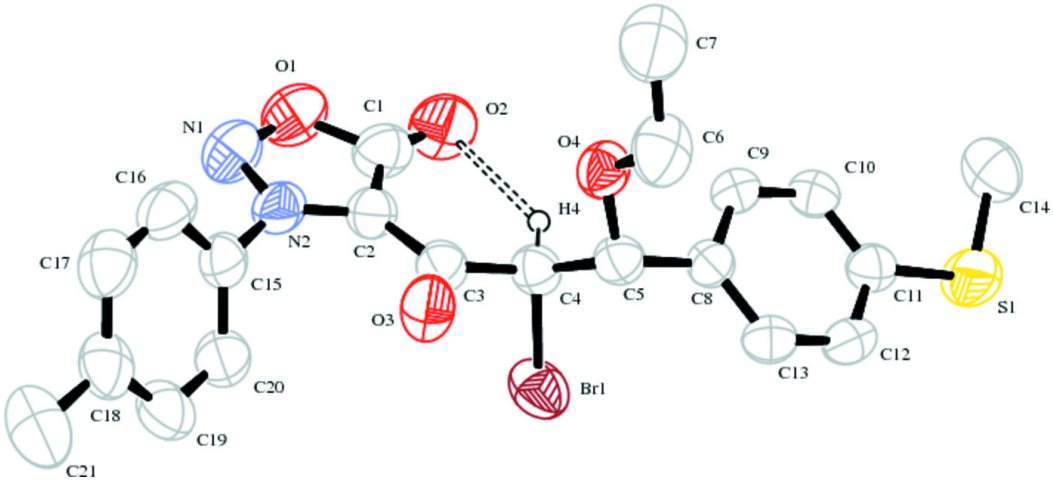
O1
C1
O2
N1
C7
O4
C6
C9
C10
C16
H4
C14
N2
C2
C17
C15
C3
C4
C5
C8
C11
S1
O3
C12
C13
Br1
C20
C18
C19
C21

Fig. 2