Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Bromophenyl)-3-(4-hydroxyphenyl)-1,3-thiazolidin-4-one

Jasmine P. Vennila,[a] D. John Thiruvadigal,[b] Helen P. Kavitha,[c] G. Chakkaravarthi[d]* and V. Manivannan[e]

[a]Department of Physics, Panimalar Institute of Technology, Chennai 602 103, India, [b]Department of Physics, SRM University, Kattankulathur Campus, Chennai, India, [c]Department of Chemistry, SRM University, Ramapuram Campus, Chennai 600 089, India, [d]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India, and [e]Department of Research and Development, PRIST University, Vallam, Thanjavur 613 403, Tamil Nadu, India
Correspondence e-mail: chakkaravarthi_2005@yahoo.com

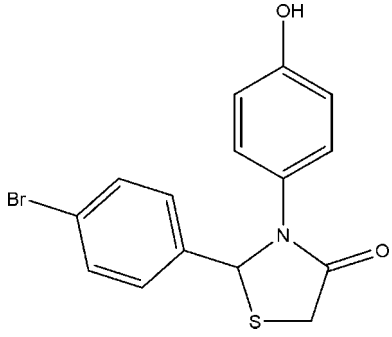
Received 25 June 2011; accepted 27 June 2011

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.087; data-to-parameter ratio = 20.0.

In the title compound, $C_{15}H_{12}BrNO_2S$, the dihedral angle between the two aromatic rings is 87.81 (8)°. The five-membered thiazolidine ring has an envelope conformation, with the S atom displaced by 0.4545 (7) Å from the mean plane of the other four ring atoms. The crystal structure exhibits O—H···O, C—H···O, C—H···Br and C—H··· π interactions.

Related literature

For the biolgical activity of thiazolidine derivatives, see: Chen *et al.* (2000); Jacop & Kutty (2004); Kalia *et al.* (2007); Vicentini *et al.* (1998); Vigorita *et al.* (1992). For bond-length data see: Allen *et al.* (1987). For related structures, see: Akkurt *et al.* (2010, 2011).



Experimental

Crystal data

$C_{15}H_{12}BrNO_2S$ M_r = 350.23
Orthorhombic, *Pbca*
a = 13.3367 (6) Å
b = 12.6292 (5) Å
c = 17.1230 (6) Å
V = 2884.1 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.00 mm^{-1}
T = 295 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.467, T_{max} = 0.586
18957 measured reflections
3617 independent reflections
2317 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.087
S = 1.02
3617 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

*Cg*2 is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.94	2.758 (2)	175
C5—H5···O2^{ii}	0.93	2.53	3.361 (3)	149
C12—H12···Br1^{iii}	0.93	2.84	3.463 (2)	125
C15—H15···*Cg*2^{iv}	0.93	2.94	3.775 (2)	150

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

The authors wish to acknowledge the SAIF, IIT, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5562).

References

Akkurt, M., Çelik, Í., Demir, H., Özkırımlı, S. & Büyükgüngör, O. (2010). *Acta Cryst.* E**66**, o1691–o1692.
Akkurt, M., Çelik, Í., Demir, H., Özkırımlı, S. & Büyükgüngör, O. (2011). *Acta Cryst.* E**67**, o914–o915.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, H. S., Li, Z. M. & Han, Y. F. (2000). *J. Agric. Food Chem.* **48**, 5312–5315.
Jacop, J. & Kutty, G. N. (2004). *Indian Drugs*, **41**, 76–79.
Kalia, R., Rao, C. M. & Kutty, N. G. (2007). *Arzneim. Forsch. (Drug Res.)*, **57**, 616–622.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Vicentini, C. B., Manfrini, M., Veronese, A. C. & Guarneri, M. (1998). *J. Heterocycl. Chem.* **35**, 29–36.
Vigorita, M. G., Basile, M., Zappala, C., Gabbrielli, G. & Pizzimenti, F. (1992). *Farmaco*, **47**, 893–906.

supporting information

Acta Cryst. (2011). E**67**, o1902 [doi:10.1107/S1600536811025281]

2-(4-Bromophenyl)-3-(4-hydroxyphenyl)-1,3-thiazolidin-4-one

Jasmine P. Vennila, D. John Thiruvadigal, Helen P. Kavitha, G. Chakkaravarthi and V. Manivannan

S1. Comment

Thiazolidine derivatives exhibit herbicidal (Chen *et al.*, 2000; Vicentini *et al.*, 1998), antineoplastic (Vigorita *et al.*, 1992), hypolipidemic (Jacop & Kutty, 2004) and anti-inflammatory (Kalia *et al.*, 2007) activities. We report here the crystal structure of the titled compound (I) (Fig. 1).

In the title compound (I), the bond lengths in the molecule are normal (Allen *et al.*, 1987) and in a good agreement with those reported previously (Akkurt *et al.*, 2010,2011). The dihedral angle between the benzene rings (C4—C9) and (C10—C15) is 87.81 (8)°. The five-membered thiazolidine ring (N1/C2/C1/S1/C3) has an envelope conformation, with the S atom displaced by 0.4545 (7) Å from the mean plane of the four other ring atoms. In the molecule, the absolute configuration at atom C3 is *R* configuration. The crystal structure exhibit weak O—H···O, C—H···O, C—H···Br and C—H··· π (Fig. 2 and Table 1) interactions. Cg2 is the centroid of C4-C9 ring.

S2. Experimental

About 5 mmol of 4-[(4-Bromobenzylidene)-amino]-phenol was taken in a round bottomed flask. To this 25 ml of dry benzene and 10 ml of mercapto acetic acid was added. The content of the flask were refluxed on the water bath for 12 hrs, cooled and poured into water. The upper organic layer was washed successively with aqueous sodium bicarbonate and water and dried with anhydrous sodium sulfate. The solvent was removed by distillation under reduced pressure. The residue on recrystallization from ethanol several times, yielded diffraction quality crystals.Yield: 62%.

S3. Refinement

The C-bound H atoms were geometrically placed (C—H = 0.93–0.98 Å) and refined as riding with U_{iso}(H) = 1.2Ueq(C) and O—H = 0.82 Å and U_{iso}(H) = 1.2Ueq(O) for OH.

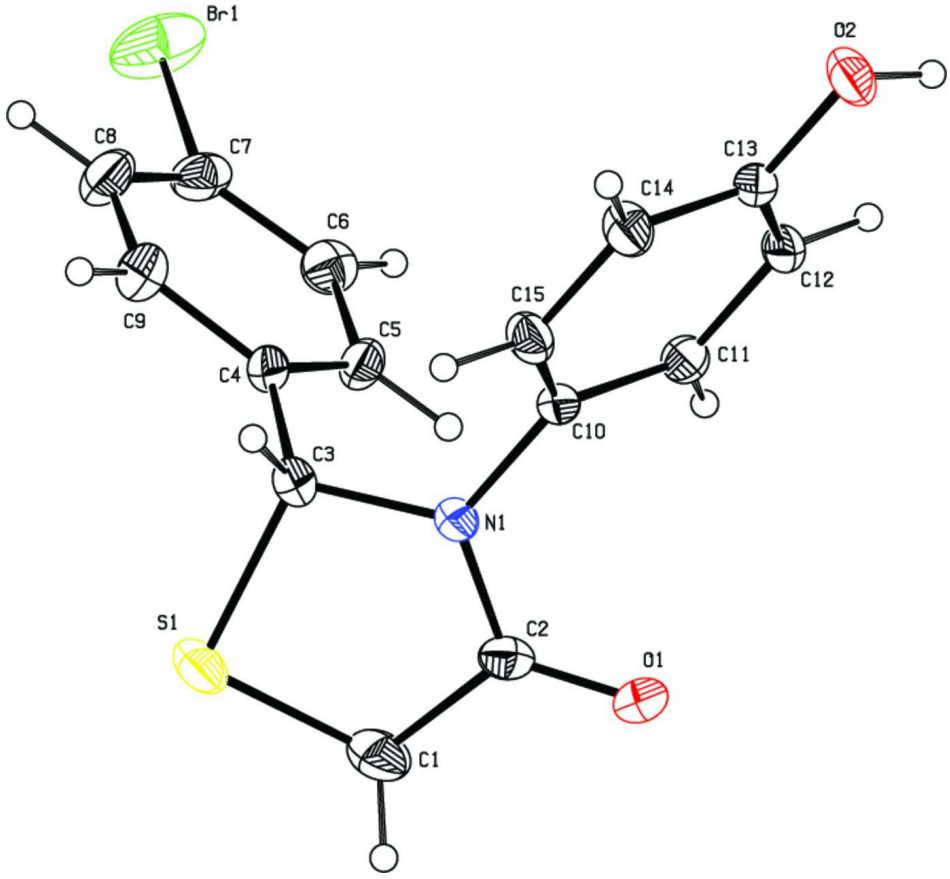


Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

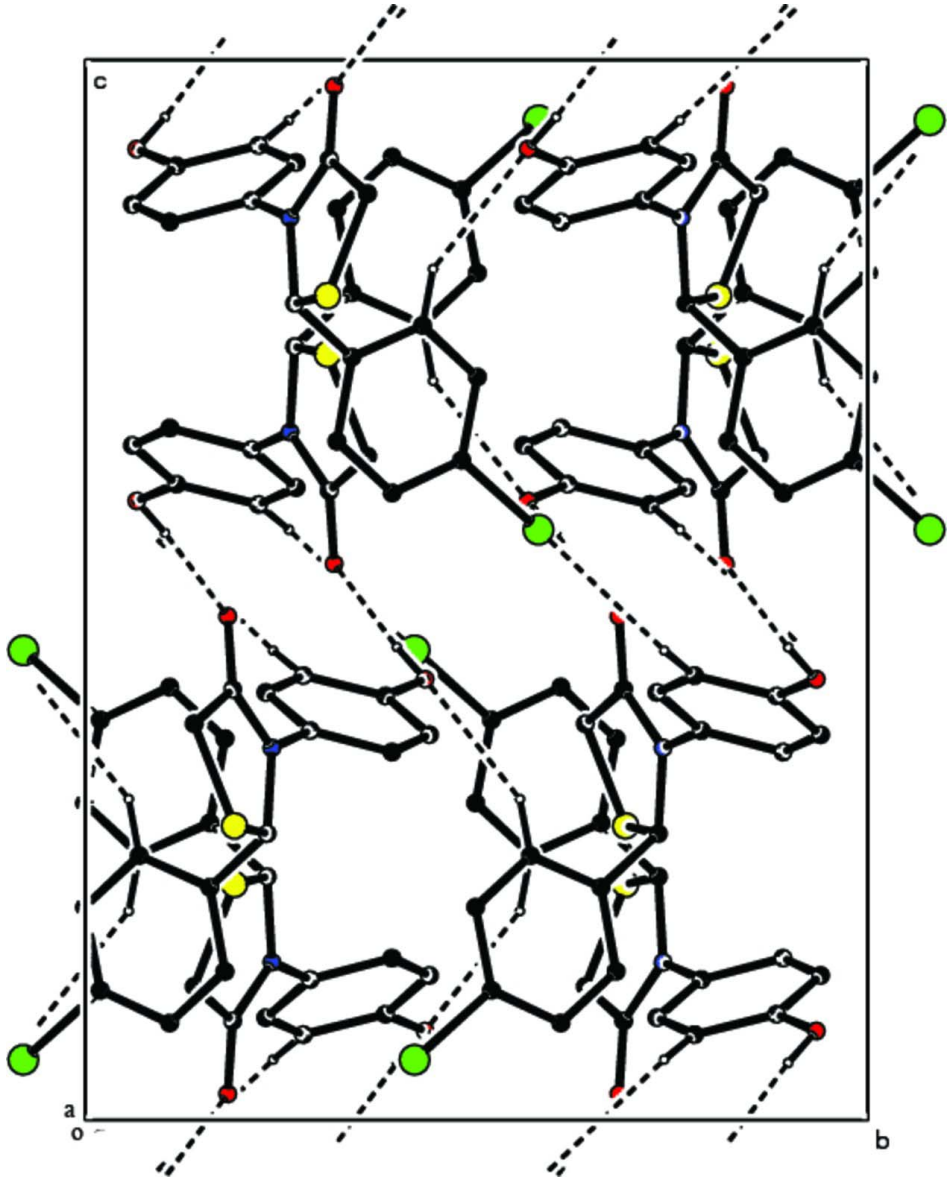


Figure 2

The packing of (I), viewed down the *a* axis. H-bonds are shown as dashed lines; H atoms not involved in hydrogen bonding have been omitted.

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$M_r = 350.23$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 13.3367\ (6)$ Å
$b = 12.6292\ (5)$ Å
$c = 17.1230\ (6)$ Å
$V = 2884.1\ (2)$ Å^3
$Z = 8$
$F(000) = 1408$
$D_x = 1.613$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4654 reflections
$\theta = 2.4$–$23.8°$
$\mu = 3.00$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.467, T_{max} = 0.586
18957 measured reflections
3617 independent reflections
2317 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 28.4°, θ_{min} = 2.4°
h = −17→16
k = −16→16
l = −16→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.087
S = 1.02
3617 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2 + 1.5996P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.63473 (19)	0.1392 (2)	0.12609 (17)	0.0510 (7)
H1A	0.6916	0.1565	0.0932	0.061*
H1B	0.6280	0.0628	0.1279	0.061*
C2	0.54086 (16)	0.18813 (18)	0.09361 (15)	0.0344 (5)
C3	0.52231 (15)	0.23237 (19)	0.22967 (13)	0.0328 (5)
H3	0.5202	0.3035	0.2525	0.039*
C4	0.46182 (16)	0.15917 (18)	0.28031 (13)	0.0316 (5)
C5	0.41708 (17)	0.06902 (18)	0.25054 (14)	0.0342 (5)
H5	0.4201	0.0555	0.1972	0.041*
C6	0.36796 (18)	−0.00109 (19)	0.29911 (15)	0.0387 (6)
H6	0.3372	−0.0612	0.2788	0.046*
C7	0.36517 (19)	0.0191 (2)	0.37752 (15)	0.0427 (6)
C8	0.4075 (2)	0.1078 (2)	0.40845 (16)	0.0515 (7)
H8	0.4044	0.1204	0.4619	0.062*
C9	0.4548 (2)	0.1784 (2)	0.35973 (15)	0.0459 (7)
H9	0.4825	0.2399	0.3804	0.055*
C10	0.39180 (15)	0.28732 (16)	0.13260 (12)	0.0262 (5)
C11	0.31686 (16)	0.23068 (17)	0.09663 (13)	0.0305 (5)
H11	0.3274	0.1603	0.0830	0.037*
C12	0.22563 (16)	0.27854 (18)	0.08068 (13)	0.0324 (5)
H12	0.1745	0.2400	0.0571	0.039*
C13	0.21067 (15)	0.38358 (18)	0.09987 (13)	0.0313 (5)
C14	0.28555 (17)	0.43972 (18)	0.13648 (15)	0.0373 (6)
H14	0.2751	0.5101	0.1502	0.045*
C15	0.37581 (17)	0.39194 (18)	0.15282 (14)	0.0351 (5)

H15	0.4263	0.4301	0.1776	0.042*
N1	0.48688 (12)	0.23846 (14)	0.14893 (10)	0.0290 (4)
O1	0.51648 (12)	0.18202 (13)	0.02472 (10)	0.0432 (4)
O2	0.12206 (12)	0.43423 (13)	0.08407 (11)	0.0472 (5)
H2	0.0887	0.3982	0.0539	0.057*
S1	0.65353 (5)	0.19057 (6)	0.22246 (4)	0.04894 (19)
Br1	0.29816 (3)	−0.07918 (3)	0.44309 (2)	0.07795 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0342 (14)	0.0612 (17)	0.0575 (18)	0.0169 (13)	0.0023 (12)	0.0021 (14)
C2	0.0277 (12)	0.0379 (12)	0.0376 (16)	0.0002 (10)	0.0076 (11)	0.0026 (11)
C3	0.0271 (11)	0.0393 (12)	0.0320 (14)	0.0020 (10)	−0.0051 (10)	−0.0013 (10)
C4	0.0285 (11)	0.0418 (13)	0.0244 (13)	0.0066 (10)	−0.0036 (9)	−0.0008 (10)
C5	0.0393 (13)	0.0402 (12)	0.0229 (12)	0.0040 (11)	−0.0011 (10)	0.0000 (11)
C6	0.0402 (14)	0.0346 (13)	0.0413 (16)	0.0070 (11)	0.0006 (11)	0.0037 (11)
C7	0.0436 (14)	0.0497 (15)	0.0349 (16)	0.0170 (12)	0.0104 (12)	0.0136 (13)
C8	0.0581 (18)	0.0711 (19)	0.0254 (14)	0.0138 (15)	0.0042 (13)	−0.0003 (14)
C9	0.0483 (15)	0.0560 (16)	0.0335 (16)	0.0013 (13)	−0.0020 (12)	−0.0098 (13)
C10	0.0226 (10)	0.0330 (11)	0.0230 (12)	0.0013 (9)	0.0013 (9)	0.0011 (9)
C11	0.0320 (12)	0.0290 (11)	0.0305 (13)	0.0008 (10)	0.0002 (10)	−0.0040 (10)
C12	0.0258 (11)	0.0405 (13)	0.0310 (13)	−0.0017 (10)	−0.0041 (9)	−0.0098 (10)
C13	0.0253 (11)	0.0421 (12)	0.0265 (13)	0.0064 (10)	−0.0012 (9)	−0.0062 (10)
C14	0.0344 (13)	0.0331 (12)	0.0442 (15)	0.0038 (10)	−0.0071 (11)	−0.0118 (11)
C15	0.0264 (11)	0.0388 (13)	0.0400 (15)	−0.0039 (10)	−0.0059 (10)	−0.0062 (11)
N1	0.0234 (9)	0.0362 (10)	0.0273 (11)	0.0037 (8)	−0.0009 (8)	0.0024 (8)
O1	0.0371 (9)	0.0622 (11)	0.0304 (11)	0.0067 (8)	0.0078 (8)	−0.0037 (8)
O2	0.0324 (9)	0.0557 (11)	0.0534 (11)	0.0145 (8)	−0.0157 (8)	−0.0223 (9)
S1	0.0268 (3)	0.0699 (5)	0.0501 (5)	0.0060 (3)	−0.0060 (3)	0.0099 (4)
Br1	0.1055 (3)	0.0617 (2)	0.0667 (3)	0.02192 (19)	0.0415 (2)	0.03136 (17)

Geometric parameters (Å, º)

C1—C2	1.503 (3)	C7—Br1	1.897 (2)
C1—S1	1.791 (3)	C8—C9	1.375 (4)
C1—H1A	0.9700	C8—H8	0.9300
C1—H1B	0.9700	C9—H9	0.9300
C2—O1	1.226 (3)	C10—C11	1.375 (3)
C2—N1	1.349 (3)	C10—C15	1.382 (3)
C3—N1	1.463 (3)	C10—N1	1.438 (3)
C3—C4	1.502 (3)	C11—C12	1.386 (3)
C3—S1	1.832 (2)	C11—H11	0.9300
C3—H3	0.9800	C12—C13	1.381 (3)
C4—C5	1.383 (3)	C12—H12	0.9300
C4—C9	1.385 (3)	C13—O2	1.371 (3)
C5—C6	1.380 (3)	C13—C14	1.376 (3)
C5—H5	0.9300	C14—C15	1.375 (3)

C6—C7	1.367 (3)	C14—H14	0.9300
C6—H6	0.9300	C15—H15	0.9300
C7—C8	1.361 (4)	O2—H2	0.8200

C2—C1—S1	107.98 (18)	C7—C8—H8	120.4
C2—C1—H1A	110.1	C9—C8—H8	120.4
S1—C1—H1A	110.1	C8—C9—C4	120.9 (2)
C2—C1—H1B	110.1	C8—C9—H9	119.6
S1—C1—H1B	110.1	C4—C9—H9	119.6
H1A—C1—H1B	108.4	C11—C10—C15	119.83 (19)
O1—C2—N1	124.3 (2)	C11—C10—N1	120.33 (19)
O1—C2—C1	123.5 (2)	C15—C10—N1	119.84 (19)
N1—C2—C1	112.2 (2)	C10—C11—C12	120.0 (2)
N1—C3—C4	113.86 (18)	C10—C11—H11	120.0
N1—C3—S1	105.06 (14)	C12—C11—H11	120.0
C4—C3—S1	111.99 (15)	C13—C12—C11	119.9 (2)
N1—C3—H3	108.6	C13—C12—H12	120.0
C4—C3—H3	108.6	C11—C12—H12	120.0
S1—C3—H3	108.6	O2—C13—C14	118.4 (2)
C5—C4—C9	118.5 (2)	O2—C13—C12	121.7 (2)
C5—C4—C3	121.7 (2)	C14—C13—C12	119.9 (2)
C9—C4—C3	119.7 (2)	C15—C14—C13	120.1 (2)
C6—C5—C4	120.7 (2)	C15—C14—H14	119.9
C6—C5—H5	119.6	C13—C14—H14	119.9
C4—C5—H5	119.6	C14—C15—C10	120.2 (2)
C7—C6—C5	119.0 (2)	C14—C15—H15	119.9
C7—C6—H6	120.5	C10—C15—H15	119.9
C5—C6—H6	120.5	C2—N1—C10	122.44 (18)
C8—C7—C6	121.6 (2)	C2—N1—C3	117.80 (18)
C8—C7—Br1	120.2 (2)	C10—N1—C3	119.42 (17)
C6—C7—Br1	118.2 (2)	C13—O2—H2	109.5
C7—C8—C9	119.2 (2)	C1—S1—C3	91.88 (11)

S1—C1—C2—O1	168.02 (19)	O2—C13—C14—C15	−179.5 (2)
S1—C1—C2—N1	−12.4 (3)	C12—C13—C14—C15	1.1 (4)
N1—C3—C4—C5	32.4 (3)	C13—C14—C15—C10	0.0 (4)
S1—C3—C4—C5	−86.6 (2)	C11—C10—C15—C14	−0.6 (3)
N1—C3—C4—C9	−151.3 (2)	N1—C10—C15—C14	179.1 (2)
S1—C3—C4—C9	89.7 (2)	O1—C2—N1—C10	2.4 (3)
C9—C4—C5—C6	−1.1 (3)	C1—C2—N1—C10	−177.1 (2)
C3—C4—C5—C6	175.3 (2)	O1—C2—N1—C3	175.7 (2)
C4—C5—C6—C7	−0.8 (3)	C1—C2—N1—C3	−3.9 (3)
C5—C6—C7—C8	1.6 (4)	C11—C10—N1—C2	52.6 (3)
C5—C6—C7—Br1	−179.47 (17)	C15—C10—N1—C2	−127.1 (2)
C6—C7—C8—C9	−0.5 (4)	C11—C10—N1—C3	−120.6 (2)
Br1—C7—C8—C9	−179.4 (2)	C15—C10—N1—C3	59.7 (3)
C7—C8—C9—C4	−1.5 (4)	C4—C3—N1—C2	−105.3 (2)
C5—C4—C9—C8	2.2 (4)	S1—C3—N1—C2	17.6 (2)

C3—C4—C9—C8	−174.2 (2)	C4—C3—N1—C10	68.2 (3)
C15—C10—C11—C12	0.1 (3)	S1—C3—N1—C10	−168.91 (15)
N1—C10—C11—C12	−179.6 (2)	C2—C1—S1—C3	18.91 (19)
C10—C11—C12—C13	1.0 (3)	N1—C3—S1—C1	−20.26 (17)
C11—C12—C13—O2	179.1 (2)	C4—C3—S1—C1	103.83 (18)
C11—C12—C13—C14	−1.6 (4)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.94	2.758 (2)	175
C5—H5···O2^{ii}	0.93	2.53	3.361 (3)	149
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Symmetry codes: (i) *x*−1/2, −*y*+1/2, −*z*; (ii) −*x*+1/2, *y*−1/2, *z*; (iii) −*x*+1/2, −*y*, *z*−1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2.