Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Bromo-7-methoxy-2-phenylimidazo-[2,1-*b*][1,3]benzothiazole

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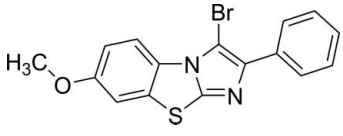
Received 3 March 2013; accepted 7 March 2013

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.070; data-to-parameter ratio = 20.5.

In the title molecule, $C_{16}H_{11}BrN_2OS$, the central imidazo-[2,1-*b*][1,3]benzothiazole tricycle is essentially planar (r.m.s. deviation = 0.021 Å). The terminal phenyl ring is twisted at 36.18 (5)° from the mean plane of the tricycle. In the crystal, pairs of eak C—H···O hydrogen bonds link molecules into centrosymmetric dimers, which are further packed into stacks along the *a* axis.

Related literature

For applications of imidazo[2,1-*b*][1,3]benzothiazoles, see: Mase *et al.* (1988); Ager *et al.* (1988); Barchéchath *et al.* (2005); Kumbhare *et al.* (2011); Yousefi *et al.* (2011); Chandak *et al.* (2013). For the crystal structures of related compounds, see: Landreau *et al.* (2002); Adib *et al.* (2008); Fun, Asik *et al.* (2011); Fun, Hemamalini *et al.* (2011).



Experimental

Crystal data

$C_{16}H_{11}BrN_2OS$
M_r = 359.24
Monoclinic, $P2_1/n$
a = 3.8346 (4) Å
b = 9.4848 (11) Å
c = 37.236 (4) Å
β = 91.810 (2)°
V = 1353.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.19 mm^{-1}
T = 100 K
0.35 × 0.15 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.402, T_{max} = 0.646
17224 measured reflections
3924 independent reflections
3578 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.070
S = 1.00
3924 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.95	2.56	3.465 (3)	158

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Ministry of Education and Science of the Russian Federation (State program No. 3.1168.2011).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5391).

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supporting information

Acta Cryst. (2013). E**69**, o531 [doi:10.1107/S1600536813006582]

3-Bromo-7-methoxy-2-phenylimidazo[2,1-*b*][1,3]benzothiazole

Alexander S. Bunev, Elena V. Sukhonosova, Dinara R. Syrazhetdinova, Vladimir E. Statsyuk, Gennady I. Ostapenko and Victor N. Khrustalev

S1. Comment

Imidazo[2,1–*b*][1,3]benzothiazoles are of great interest due to their biological properties. These compounds and their derivatives demonstrate the immunosuppressive (Mase *et al.*, 1988), antiallergic (Ager *et al.*, 1988) and anti-cancer (Kumbhare *et al.*, 2011) activities as well as the inhibition activity of apoptosis in testiculargerm cells (Chandak *et al.*, 2013) and lymphocytes (Barchéchath *et al.*, 2005). Moreover, the substituted imidazo[2,1–*b*][1,3]benzothiazoles have emerged as significant components in various diversified therapeutic applications. In particular, they are potential agents for High-Contrast PET Imaging (Yousefi *et al.*, 2011). In this work, a new halogensubstituted imidazo[2,1-*b*][1,3]benzothiazole, $C_{16}H_{11}N_2OSBr$, (**I**) was prepared by the reaction of imidazo[2,1–*b*][1,3]benzothiazole with bromine at room temperature (Figure 1), and its structure was unambiguously established by the X-ray diffraction study (Figure 2).

The bond lengths and angles within the molecule of **I** are in a good agreement with those found in the related compounds (Landreau *et al.*, 2002; Adib *et al.*, 2008; Fun, Asik *et al.*, 2011; Fun, Hemamalini *et al.*, 2011). The central imidazo[2,1–*b*][1,3]benzothiazole fragment is essentially planar (r.m.s. deviation is 0.021 Å). The methoxy group is practically coplanar to this fragment (the corresponding C6—C7—O1—C16 dihedral angle is 1.8 (3)°), and the terminal phenyl ring is twisted from it at 36.18 (5)°.

In the crystal, molecules form the centrosymmetrical dimers by the weak intermolecular C—H···O hydrogen bonds (Table 1, Figure 3). The dimers are further packed into stacks along the *a* axis.

S2. Experimental

A solution of bromine (0.51 ml, 1.6 g, 10 mmol) in dry $CHCl_3$ (10 ml) was added to a solution of 7-methoxy-2-phenyl-imidazo[2,1-*b*][1,3]benzothiazole (2.80 g, 10 mmol) in dry $CHCl_3$ (50 ml). The reaction mixture was stirred at room temperature for 3 h. The solvent was evaporated from the reaction mixture on rotavapor. The crude product was diluted with 5% solution of Na_2CO_3 in water (50 ml). The precipitate was filtered and crystallized from dimethylformamide. Yield is 89%. The single crystals of **I** were obtained by slow crystallization from dimethylformamide. *M*.p. = 447–448 K. IR (KBr), ν/cm^{-1}: 2961, 1607, 1580, 1493, 1222, 684,633. ^{1}H NMR (500 MHz, DMSO-d_6, 303 K): δ = 8.31 (d, 1H, H5, J = 9.0), 7.95–8.01 (m, 2H, H2′, H6′), 7.73 (d, 1H, H8, J = 2.8), 7.49 (t, 2H, H3′, H5′, J = 7.7), 7.38 (t, 1H, H4′, J = 7.4), 7.17 (dd, 1H, H6, J = 9.0, J = 2.6), 3.85 (s, 3H, OCH_3). Anal. Calcd. for $C_{16}H_{11}BrN_2OS$: C, 53.49; H, 3.09; N, 7.8. Found: C, 53.45; H, 3.05; N, 7.75.

S3. Refinement

All hydrogen atoms were placed in the calculated positions, with C—H = 0.95 Å (CH-groups) and 0.98 Å (CH_3-group), and refined in the riding model, with U_{iso}(H) = 1.2–1.5U_{eq}(C).

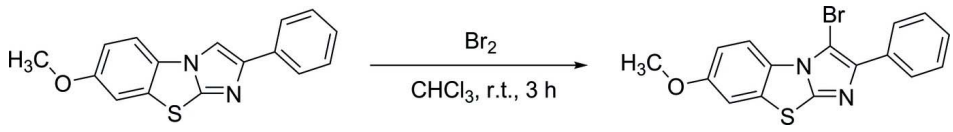

Figure 1

The reaction of imidazo[2,1-*b*][1,3]benzothiazoles with bromine.

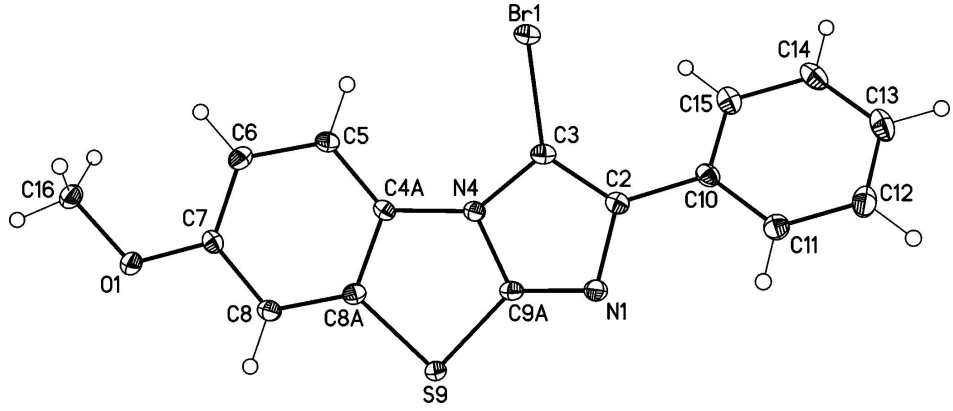

Figure 2

Molecular structure of **I**. Displacement ellipsoids are shown at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

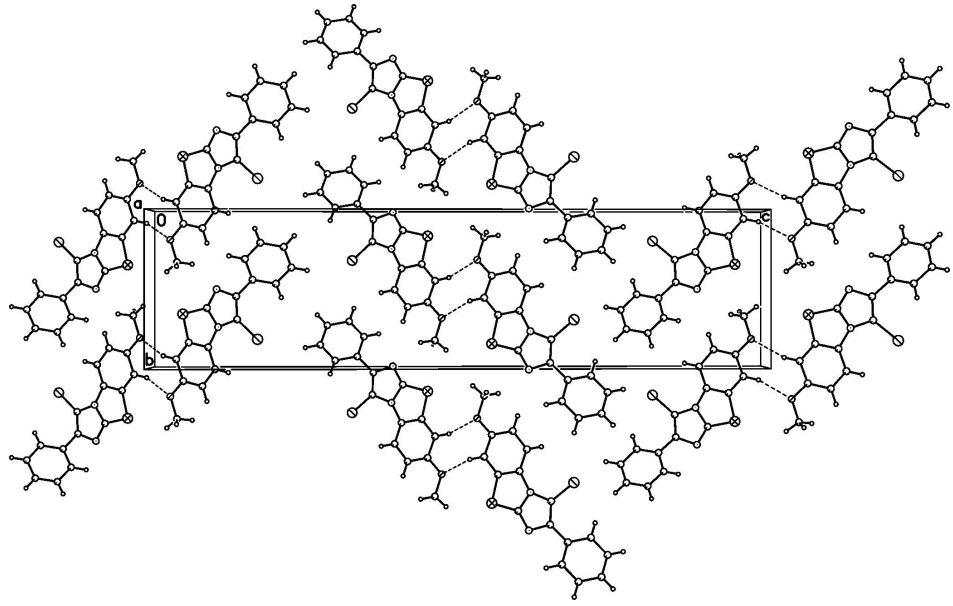

Figure 3

A portion of the crystal structure showing the packing of the H-bonded centrosymmetrical dimers of **I**. The weak intermolecular C—H···O hydrogen bonds are drawn by dashed lines.

3-Bromo-7-methoxy-2-phenylimidazo[2,1-*b*][1,3]benzothiazole

Crystal data

$C_{16}H_{11}BrN_2OS$
$M_r = 359.24$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 3.8346$ (4) Å
$b = 9.4848$ (11) Å
$c = 37.236$ (4) Å
$\beta = 91.810$ (2)°
$V = 1353.6$ (3) Å^3
$Z = 4$
$F(000) = 720$
$D_x = 1.763$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9814 reflections
$\theta = 2.2$–$30.5°$
$\mu = 3.19$ mm^{-1}
$T = 100$ K
Needle, colourless
0.35 × 0.15 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.402$, $T_{max} = 0.646$
17224 measured reflections
3924 independent reflections
3578 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.2°$
$h = -5 \rightarrow 5$
$k = -13 \rightarrow 13$
$l = -52 \rightarrow 52$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.070$
$S = 1.00$
3924 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0196P)^2 + 2.89P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.95$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	−0.02456 (5)	0.18794 (2)	0.820287 (5)	0.01435 (6)
O1	0.7765 (4)	−0.18472 (16)	0.97119 (4)	0.0169 (3)
N1	0.3136 (5)	0.49917 (19)	0.88973 (5)	0.0132 (3)
C2	0.1687 (5)	0.4553 (2)	0.85658 (5)	0.0128 (4)

C3	0.1626 (5)	0.3103 (2)	0.85500 (5)	0.0132 (4)
N4	0.3079 (4)	0.26156 (18)	0.88734 (4)	0.0114 (3)
C4A	0.4010 (5)	0.1337 (2)	0.90429 (5)	0.0108 (3)
C5	0.3563 (5)	−0.0040 (2)	0.89273 (5)	0.0122 (4)
H5	0.2447	−0.0235	0.8701	0.015*
C6	0.4774 (5)	−0.1141 (2)	0.91473 (6)	0.0140 (4)
H6	0.4476	−0.2091	0.9071	0.017*
C7	0.6429 (5)	−0.0847 (2)	0.94802 (5)	0.0123 (4)
C8	0.6842 (5)	0.0541 (2)	0.96019 (5)	0.0131 (4)
H8	0.7929	0.0739	0.9829	0.016*
C8A	0.5618 (5)	0.1615 (2)	0.93805 (5)	0.0122 (4)
S9	0.59204 (13)	0.34210 (5)	0.947997 (13)	0.01341 (10)
C9A	0.3926 (5)	0.3811 (2)	0.90637 (5)	0.0120 (4)
C10	0.0582 (5)	0.5587 (2)	0.82933 (5)	0.0130 (4)
C11	−0.0888 (5)	0.6869 (2)	0.83961 (6)	0.0154 (4)
H11	−0.1203	0.7057	0.8644	0.018*
C12	−0.1889 (6)	0.7866 (2)	0.81419 (6)	0.0192 (4)
H12	−0.2904	0.8729	0.8216	0.023*
C13	−0.1415 (6)	0.7611 (2)	0.77781 (6)	0.0198 (4)
H13	−0.2092	0.8298	0.7604	0.024*
C14	0.0052 (6)	0.6347 (3)	0.76713 (6)	0.0189 (4)
H14	0.0374	0.6168	0.7423	0.023*
C15	0.1053 (5)	0.5339 (2)	0.79261 (6)	0.0159 (4)
H15	0.2062	0.4477	0.7851	0.019*
C16	0.7532 (6)	−0.3284 (2)	0.96000 (6)	0.0161 (4)
H16A	0.8656	−0.3888	0.9783	0.024*
H16B	0.8708	−0.3400	0.9372	0.024*
H16C	0.5073	−0.3551	0.9568	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01465 (9)	0.01602 (10)	0.01221 (9)	−0.00152 (7)	−0.00252 (6)	−0.00246 (7)
O1	0.0232 (7)	0.0110 (7)	0.0161 (7)	0.0009 (6)	−0.0046 (6)	0.0000 (5)
N1	0.0148 (8)	0.0134 (8)	0.0114 (7)	−0.0011 (6)	0.0001 (6)	−0.0007 (6)
C2	0.0129 (8)	0.0144 (9)	0.0111 (8)	−0.0006 (7)	0.0002 (7)	−0.0001 (7)
C3	0.0132 (8)	0.0143 (9)	0.0121 (8)	−0.0011 (7)	−0.0012 (7)	−0.0025 (7)
N4	0.0121 (7)	0.0119 (8)	0.0102 (7)	0.0002 (6)	−0.0009 (6)	−0.0007 (6)
C4A	0.0097 (8)	0.0134 (9)	0.0091 (8)	−0.0004 (7)	−0.0005 (6)	0.0004 (7)
C5	0.0109 (8)	0.0141 (9)	0.0116 (8)	−0.0005 (7)	−0.0015 (7)	−0.0014 (7)
C6	0.0130 (9)	0.0117 (9)	0.0171 (9)	−0.0011 (7)	−0.0006 (7)	−0.0016 (7)
C7	0.0120 (8)	0.0138 (9)	0.0111 (8)	−0.0003 (7)	0.0004 (7)	0.0018 (7)
C8	0.0136 (8)	0.0149 (9)	0.0107 (8)	−0.0020 (7)	0.0001 (7)	−0.0007 (7)
C8A	0.0114 (8)	0.0125 (9)	0.0127 (8)	−0.0008 (7)	−0.0001 (7)	−0.0015 (7)
S9	0.0176 (2)	0.0104 (2)	0.0120 (2)	−0.00075 (17)	−0.00341 (17)	−0.00098 (16)
C9A	0.0124 (8)	0.0129 (9)	0.0106 (8)	−0.0018 (7)	−0.0006 (7)	−0.0020 (7)
C10	0.0109 (8)	0.0157 (9)	0.0125 (8)	−0.0019 (7)	−0.0016 (7)	0.0012 (7)
C11	0.0148 (9)	0.0150 (9)	0.0163 (9)	−0.0012 (8)	0.0001 (7)	0.0002 (7)

C12	0.0168 (10)	0.0143 (10)	0.0262 (11)	0.0000 (8)	−0.0028 (8)	0.0027 (8)
C13	0.0168 (10)	0.0213 (10)	0.0210 (10)	−0.0025 (8)	−0.0032 (8)	0.0092 (8)
C14	0.0186 (10)	0.0250 (11)	0.0130 (9)	−0.0025 (9)	−0.0020 (8)	0.0044 (8)
C15	0.0130 (8)	0.0184 (10)	0.0164 (9)	−0.0005 (7)	0.0005 (7)	0.0031 (8)
C16	0.0188 (9)	0.0112 (9)	0.0182 (9)	0.0008 (8)	−0.0022 (8)	−0.0009 (7)

Geometric parameters (Å, º)

Br1—C3	1.864 (2)	C8—H8	0.9500
O1—C7	1.371 (2)	C8A—S9	1.756 (2)
O1—C16	1.427 (2)	S9—C9A	1.746 (2)
N1—C9A	1.311 (3)	C10—C11	1.398 (3)
N1—C2	1.401 (2)	C10—C15	1.404 (3)
C2—C3	1.377 (3)	C11—C12	1.384 (3)
C2—C10	1.465 (3)	C11—H11	0.9500
C3—N4	1.390 (2)	C12—C13	1.394 (3)
N4—C9A	1.370 (3)	C12—H12	0.9500
N4—C4A	1.408 (3)	C13—C14	1.388 (3)
C4A—C5	1.385 (3)	C13—H13	0.9500
C4A—C8A	1.407 (3)	C14—C15	1.392 (3)
C5—C6	1.397 (3)	C14—H14	0.9500
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.403 (3)	C16—H16A	0.9800
C6—H6	0.9500	C16—H16B	0.9800
C7—C8	1.399 (3)	C16—H16C	0.9800
C8—C8A	1.383 (3)		
C7—O1—C16	117.30 (16)	C9A—S9—C8A	89.72 (10)
C9A—N1—C2	104.00 (17)	N1—C9A—N4	114.52 (17)
C3—C2—N1	109.89 (17)	N1—C9A—S9	133.52 (16)
C3—C2—C10	129.46 (18)	N4—C9A—S9	111.95 (15)
N1—C2—C10	120.63 (18)	C11—C10—C15	118.53 (19)
C2—C3—N4	106.81 (17)	C11—C10—C2	120.19 (18)
C2—C3—Br1	131.09 (16)	C15—C10—C2	121.25 (19)
N4—C3—Br1	121.94 (15)	C12—C11—C10	120.8 (2)
C9A—N4—C3	104.77 (17)	C12—C11—H11	119.6
C9A—N4—C4A	115.35 (16)	C10—C11—H11	119.6
C3—N4—C4A	139.80 (17)	C11—C12—C13	120.3 (2)
C5—C4A—N4	130.27 (17)	C11—C12—H12	119.9
C5—C4A—C8A	120.03 (18)	C13—C12—H12	119.9
N4—C4A—C8A	109.70 (17)	C14—C13—C12	119.7 (2)
C4A—C5—C6	119.16 (18)	C14—C13—H13	120.2
C4A—C5—H5	120.4	C12—C13—H13	120.2
C6—C5—H5	120.4	C13—C14—C15	120.2 (2)
C5—C6—C7	120.13 (19)	C13—C14—H14	119.9
C5—C6—H6	119.9	C15—C14—H14	119.9
C7—C6—H6	119.9	C14—C15—C10	120.5 (2)
O1—C7—C8	114.26 (17)	C14—C15—H15	119.8

O1—C7—C6	124.62 (18)	C10—C15—H15	119.8
C8—C7—C6	121.12 (18)	O1—C16—H16A	109.5
C8A—C8—C7	117.81 (18)	O1—C16—H16B	109.5
C8A—C8—H8	121.1	H16A—C16—H16B	109.5
C7—C8—H8	121.1	O1—C16—H16C	109.5
C8—C8A—C4A	121.72 (18)	H16A—C16—H16C	109.5
C8—C8A—S9	125.00 (16)	H16B—C16—H16C	109.5
C4A—C8A—S9	113.27 (15)		

C9A—N1—C2—C3	0.9 (2)	N4—C4A—C8A—C8	−178.98 (18)
C9A—N1—C2—C10	−177.60 (18)	C5—C4A—C8A—S9	−179.60 (15)
N1—C2—C3—N4	−0.5 (2)	N4—C4A—C8A—S9	0.2 (2)
C10—C2—C3—N4	177.8 (2)	C8—C8A—S9—C9A	178.51 (19)
N1—C2—C3—Br1	174.83 (15)	C4A—C8A—S9—C9A	−0.68 (16)
C10—C2—C3—Br1	−6.9 (4)	C2—N1—C9A—N4	−0.9 (2)
C2—C3—N4—C9A	0.0 (2)	C2—N1—C9A—S9	177.88 (18)
Br1—C3—N4—C9A	−175.90 (14)	C3—N4—C9A—N1	0.6 (2)
C2—C3—N4—C4A	−176.4 (2)	C4A—N4—C9A—N1	178.04 (18)
Br1—C3—N4—C4A	7.7 (3)	C3—N4—C9A—S9	−178.45 (14)
C9A—N4—C4A—C5	−179.7 (2)	C4A—N4—C9A—S9	−1.0 (2)
C3—N4—C4A—C5	−3.5 (4)	C8A—S9—C9A—N1	−177.9 (2)
C9A—N4—C4A—C8A	0.5 (2)	C8A—S9—C9A—N4	0.95 (15)
C3—N4—C4A—C8A	176.6 (2)	C3—C2—C10—C11	146.1 (2)
N4—C4A—C5—C6	179.2 (2)	N1—C2—C10—C11	−35.7 (3)
C8A—C4A—C5—C6	−1.0 (3)	C3—C2—C10—C15	−35.6 (3)
C4A—C5—C6—C7	−0.2 (3)	N1—C2—C10—C15	142.5 (2)
C16—O1—C7—C8	−178.10 (18)	C15—C10—C11—C12	0.6 (3)
C16—O1—C7—C6	1.8 (3)	C2—C10—C11—C12	178.9 (2)
C5—C6—C7—O1	−178.68 (19)	C10—C11—C12—C13	−0.6 (3)
C5—C6—C7—C8	1.2 (3)	C11—C12—C13—C14	0.3 (3)
O1—C7—C8—C8A	178.87 (18)	C12—C13—C14—C15	−0.1 (3)
C6—C7—C8—C8A	−1.1 (3)	C13—C14—C15—C10	0.2 (3)
C7—C8—C8A—C4A	−0.1 (3)	C11—C10—C15—C14	−0.4 (3)
C7—C8—C8A—S9	−179.27 (15)	C2—C10—C15—C14	−178.7 (2)
C5—C4A—C8A—C8	1.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.95	2.56	3.465 (3)	158

Symmetry code: (i) −*x*+2, −*y*, −*z*+2.