

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(2E)-4-(4-Bromophenyl)-2-{2-[(1E)-cyclopentylidene]hydrazin-1-ylidene}-3-phenyl-2,3-dihydro-1,3-thiazoleJoel T. Mague,^a Shaaban K. Mohamed,^{b,c} Mehmet Akkurt,^d Alaa A. Hassan^c and Mustafa R. Albayati^{e*}^aDepartment of Chemistry, Tulane University, New Orleans, LA 70118, USA,^bChemistry and Environmental Division, Manchester Metropolitan University, Manchester, M1 5GD, England, ^cChemistry Department, Faculty of Science, Minia University, 61519 El-Minia, Egypt, ^dDepartment of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, and ^eKirkuk University, College of Science, Department of Chemistry, Kirkuk, Iraq

Correspondence e-mail: shaabankamel@yahoo.com

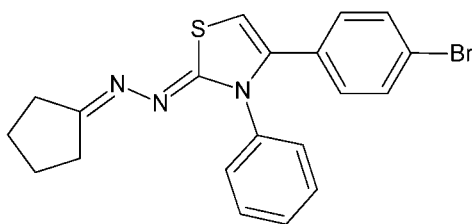
Received 9 May 2014; accepted 12 May 2014

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.030; wR factor = 0.072; data-to-parameter ratio = 14.8.

In the title compound, $\text{C}_{20}\text{H}_{18}\text{BrN}_3\text{S}$, the cyclopentane ring adopts a half-chair conformation. The 4-bromophenyl and phenyl rings make dihedral angles of 34.6 (1) and 68.52 (6)°, respectively, with the dihydrothiazole ring. In the crystal, the molecules pack in sheets approximately parallel to (101) which are formed by weak $\text{C}-\text{H}\cdots\text{Br}$ interactions

Related literature

For various medicinal applications of thiazole scaffold compounds, see: Mahajan *et al.* (2008); Abbs *et al.* (2008); Chowki *et al.* (2008); Karabasanagouda *et al.* (2008); Basavaraja *et al.* (2008); Bhusari *et al.* (2000); Basawaraj *et al.* (2005). For similar structures, see: Akkurt *et al.* (2014); Mague *et al.* (2014); Mohamed *et al.* (2013). For ring conformations, see: Cremer & Pople (1975).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{18}\text{BrN}_3\text{S}$ $M_r = 412.34$ Monoclinic, $P2_1/c$ $a = 12.5079$ (3) Å $b = 5.5728$ (1) Å $c = 25.3761$ (6) Å $\beta = 96.8480$ (11)° $V = 1756.20$ (7) Å³ $Z = 4$ Cu $K\alpha$ radiation $\mu = 4.35$ mm⁻¹ $T = 100$ K $0.10 \times 0.08 \times 0.02$ mm

Data collection

Bruker D8 VENTURE PHOTON

100 CMOS diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 2013)

 $T_{\min} = 0.80$, $T_{\max} = 0.92$

12815 measured reflections

3409 independent reflections

2960 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.033$

Refinement

 $[F^2 > 2\sigma(F^2)] = 0.030$ $wR(F^2) = 0.072$ $S = 1.06$

3409 reflections

230 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.89$ e Å⁻³ $\Delta\rho_{\min} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C}17-\text{H}17B\cdots\text{Br}1^i$	0.99	3.03	3.828 (2)	138

Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

Data collection: APEX2 (Bruker, 2013); cell refinement: SAINT (Bruker, 2013); data reduction: SAINT; program(s) used to solve structure: SHELXT (Sheldrick, 2008); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg & Putz, 2012); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

The support of NSF-MRI grant No. 1228232 for the purchase of the diffractometer is gratefully acknowledged.

Supporting information for this paper is available from the IUCr electronic archives (Reference: QM2107).

References

- Abbs, T. F., Reji, F., Devi, S. K. C., Thomas, K. K., Sreejalekshmi, K. G., Manju, S. L., Francis, M., Philip, S. K., Bharathan, A. & Rajasekharan, K. N. (2008). *Indian J. Chem. Sect. B*, **47**, 1145–1150.
- Akkurt, M., Mague, J. T., Mohamed, S. K., Hassan, A. A. & Albayati, M. R. (2014). *Acta Cryst.* **E70**, o478–o479.
- Basavaraja, K. M., Somasekhar, B. & Appalaraju, S. (2008). *Indian J. Heterocycl. Chem.* **18**, 69–72.
- Basawaraj, R., Suresh, M. & Sangapure, S. S. (2005). *Indian J. Heterocycl. Chem.* **15**, 153–156.
- Bhusari, K. P., Khedekar, P. B., Umathe, S. N., Bahekar, R. H. & Raghu, R. R. A. (2000). *Indian J. Heterocycl. Chem.* **9**, 275–278.
- Brandenburg, K. & Putz, H. (2012). *DIAMOND*, Crystal Impact GbR, Bonn, Germany.
- Bruker (2013). *APEX2*, *SAINTE*, *SADABS*, Bruker AXS, Inc., Madison, Wisconsin, USA.
- Chowki, A. A., Magdum, C. S., Ladda, P. L. & Mohite, S. K. (2008). *International Journal of Chemical Science*, **6**, 1600–1605.
- Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
- Karabasanagouda, T., Adhikari, A. V., Ramgopal, D. & Parameshwarappa, G. (2008). *Indian J. Chem. Sect. B*, **47**, 144–152.
- Mague, J. T., Mohamed, S. K., Akkurt, M., Abd El-Alaziz, A. T. & Albayati, M. R. (2014). *Acta Cryst.* **E70**, o328–o329.
- Mahajan, N. S., Pattan, S. R., Jadhav, R. L., Pimpodkar, N. V. & Manikrao, A. M. (2008). *Int. J. Chem. Sci.* **6**, 800–806.
- Mohamed, S. K., Akkurt, M., Mague, J. T., Hassan, A. A. & Albayati, M. R. (2013). *Acta Cryst.* **E69**, o1563–o1564.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2014). E70, o669 [doi:10.1107/S1600536814010897]

(2E)-4-(4-Bromophenyl)-2-{2-[(1E)-cyclopentylidene]hydrazin-1-ylidene}-3-phenyl-2,3-dihydro-1,3-thiazole

Joel T. Mague, Shaaban K. Mohamed, Mehmet Akkurt, Alaa A. Hassan and Mustafa R. Albayati

S1. Comment

The anti-microbial activities of substituted thiazoles are well established because they possess the (S—C=N) toxophoric unit (Mahajan *et al.*, 2008). Thiazoles were reported to possess anti-cancer (Abbs *et al.*, 2008), anti-tubercular (Chowki *et al.*, 2008), anti-inflammatory (Karabasanagouda *et al.*, 2008), analgesic (Basavaraja *et al.*, 2008) anthelmintic (Bhusari *et al.*, 2000) and diuretic (Basawaraj *et al.*, 2005) activities. Based on these facts and as part of our on-going study we herein report the synthesis and crystal structure of the title compound.

In the title compound (I, Fig. 1), the cyclopentane ring (C16–C20) adopts a half-chair conformation with puckering parameters of $Q(2) = 0.375(3) \text{ \AA}$, $\varphi(2) = 270.2(4)^\circ$ (Cremer & Pople, 1975). The dihydrothiazole ring (S1/N1/C7–C9) is essentially planar [max. deviations = $-0.002(2) \text{ \AA}$ for C8 and C9] and it makes dihedral angles of 34.6(1) and 68.52(6)%, respectively, with the 4-bromophenyl (C1–C6) and (C10–C15) phenyl rings. All bond lengths and angles in (I) are normal and comparable with those reported for similar structures (Mohamed *et al.*, 2013; Mague *et al.*, 2014; Akkurt *et al.*, 2014).

In the crystal, the molecules of (I) pack in sheets approximately parallel to (101) which are formed by weak C—H···Br interactions (Table 1, Fig. 2).

S2. Experimental

A mixture of 1 mmol (233 mg) of cyclopentan-1-one *N*-phenylthiosemicarbazone and 1 mmol (278 mg) of 2-bromo-1-(4-bromophenyl)ethanone in 30 ml ethanol was stirred and refluxed at 350 K. The reaction was monitored by TLC until completion. On cooling, a solid yellow product precipitated which was filtered off and recrystallized from ethanol to furnish yellow crystals, suitable for X-ray diffraction.

S3. Refinement

H-atoms were placed in calculated positions (C—H = 0.95 - 0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached carbon atoms. At the conclusion of refinement with all atoms at unit occupancy, the largest difference peak appeared in the vicinity of Br1. Refinement of this as a second component of a disorder of Br1 led to improvement in the results and a more realistic value for $U(\text{iso})$ for Br1. The geometry associated with the minor component (Br1A) suggests that there is a small amount of "whole molecule" disorder but since the refined occupancy of Br1A is only 0.02, there is not enough information from the final difference map to reliably position the remainder of the minor component.

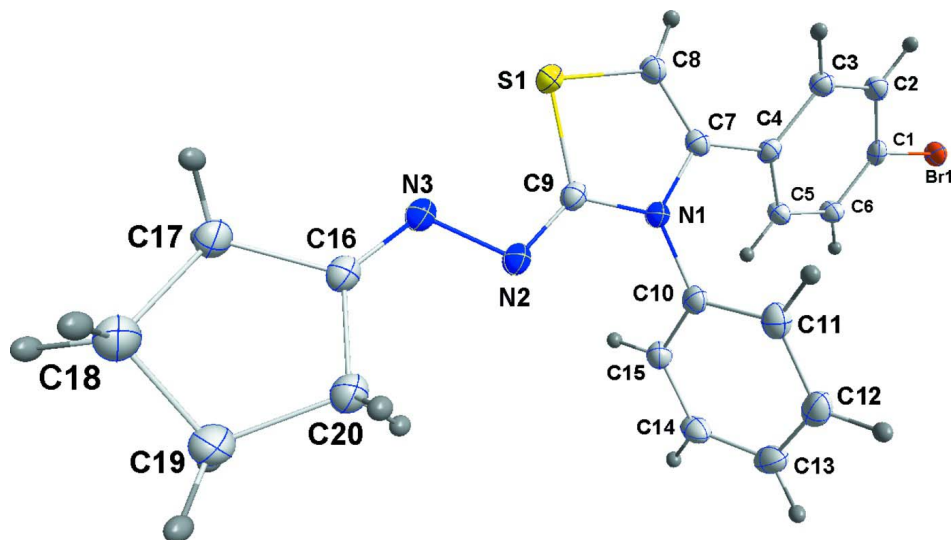


Figure 1

The title compound with 50% probability displacement ellipsoids for non-hydrogen atoms.

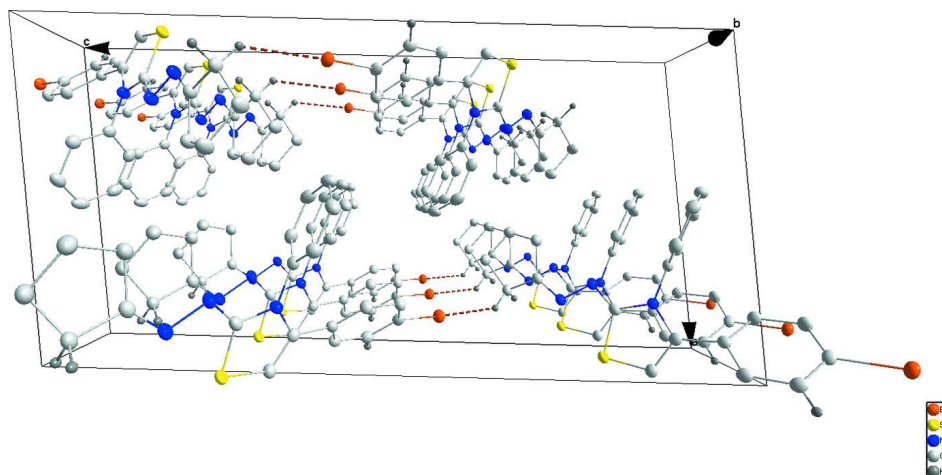


Figure 2

Packing viewed down the *b* axis with the C—H...Br interactions shown as dotted lines.

(2*E*)-4-(4-Bromophenyl)-2-{2-[(1*E*)-cyclopentylidene]hydrazin-1-ylidene}-3-phenyl-2,3-dihydro-1,3-thiazole

Crystal data

$C_{20}H_{18}BrN_3S$

$M_r = 412.34$

Monoclinic, $P2_1/c$

$a = 12.5079$ (3) Å

$b = 5.5728$ (1) Å

$c = 25.3761$ (6) Å

$\beta = 96.8480$ (11)°

$V = 1756.20$ (7) Å³

$Z = 4$

$F(000) = 840$

$D_x = 1.560$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 8908 reflections

$\theta = 3.5\text{--}72.3^\circ$

$\mu = 4.35$ mm⁻¹

$T = 100$ K

Plate, yellow

$0.10 \times 0.08 \times 0.02$ mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS
diffractometer
Radiation source: INCOATEC I μ S micro-focus
source
Mirror monochromator
Detector resolution: 10.4167 pixels mm⁻¹
 ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2013)

$T_{\min} = 0.80$, $T_{\max} = 0.92$
12815 measured reflections
3409 independent reflections
2960 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\max} = 72.3^\circ$, $\theta_{\min} = 3.5^\circ$
 $h = -14 \rightarrow 15$
 $k = -6 \rightarrow 6$
 $l = -31 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.072$
 $S = 1.06$
3409 reflections
230 parameters
1 restraint
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
 $w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 0.942P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.89 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

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. H-atoms were placed in calculated positions (C—H = 0.95 - 0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached carbon atoms. At the conclusion of refinement with all atoms at unit occupancy, the largest difference peak appeared in the vicinity of Br1. Refinement of this as a second component of a disorder of Br1 led to improvement in the results and a more realistic value for $U(\text{iso})$ for Br1. The geometry associated with the minor component (Br1A) suggests that there is a small amount of "whole molecule" disorder but since the refined occupancy of Br1A is only 0.02, there is not enough information from the final difference map to reliably position the remainder of the minor component.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Br1	0.85490 (2)	-0.31880 (7)	0.43991 (2)	0.02218 (11)	0.982 (1)
Br1A	0.8563 (12)	-0.201 (4)	0.4313 (4)	0.02218 (11)	0.0182 (11)

S1	0.94129 (4)	0.58669 (10)	0.71625 (2)	0.01954 (13)
N1	0.77696 (15)	0.4902 (3)	0.64754 (7)	0.0186 (4)
N2	0.74281 (16)	0.7923 (4)	0.70865 (8)	0.0219 (4)
N3	0.80239 (15)	0.9247 (4)	0.75009 (7)	0.0219 (4)
C1	0.85169 (18)	-0.1224 (4)	0.50103 (9)	0.0188 (4)
C2	0.91130 (18)	-0.1876 (4)	0.54836 (9)	0.0206 (5)
H2	0.9528	-0.3308	0.5507	0.025*
C3	0.90938 (18)	-0.0397 (4)	0.59242 (9)	0.0192 (4)
H3	0.9493	-0.0842	0.6252	0.023*
C4	0.84970 (17)	0.1732 (4)	0.58934 (8)	0.0173 (4)
C5	0.79033 (19)	0.2330 (4)	0.54094 (9)	0.0197 (5)
H5	0.7492	0.3767	0.5382	0.024*
C6	0.79050 (19)	0.0856 (4)	0.49681 (9)	0.0209 (5)
H6	0.7492	0.1267	0.4642	0.025*
C7	0.86033 (18)	0.3344 (4)	0.63585 (9)	0.0180 (4)
C8	0.95119 (19)	0.3650 (4)	0.66889 (9)	0.0194 (5)
H8	1.0148	0.2744	0.6666	0.023*
C9	0.80684 (18)	0.6404 (4)	0.69039 (8)	0.0183 (4)
C10	0.66773 (18)	0.4827 (4)	0.62245 (8)	0.0187 (4)
C11	0.6062 (2)	0.2806 (4)	0.62887 (9)	0.0225 (5)
H11	0.6344	0.1517	0.6508	0.027*
C12	0.5018 (2)	0.2708 (4)	0.60235 (10)	0.0265 (5)
H12	0.4580	0.1343	0.6065	0.032*
C13	0.46162 (19)	0.4581 (5)	0.57017 (10)	0.0278 (5)
H13	0.3908	0.4490	0.5520	0.033*
C14	0.5245 (2)	0.6597 (4)	0.56423 (9)	0.0254 (5)
H14	0.4968	0.7879	0.5420	0.030*
C15	0.62813 (19)	0.6735 (4)	0.59085 (9)	0.0219 (5)
H15	0.6712	0.8117	0.5874	0.026*
C16	0.74531 (18)	1.0603 (4)	0.77618 (9)	0.0202 (5)
C17	0.79575 (19)	1.2288 (4)	0.81892 (9)	0.0211 (5)
H17A	0.8308	1.3662	0.8032	0.025*
H17B	0.8499	1.1441	0.8439	0.025*
C18	0.70068 (19)	1.3126 (5)	0.84697 (10)	0.0270 (5)
H18A	0.7132	1.4763	0.8616	0.032*
H18B	0.6882	1.2020	0.8762	0.032*
C19	0.6054 (2)	1.3094 (5)	0.80314 (10)	0.0282 (5)
H19A	0.6050	1.4549	0.7807	0.034*
H19B	0.5363	1.2994	0.8184	0.034*
C20	0.62414 (19)	1.0838 (5)	0.77104 (9)	0.0248 (5)
H20A	0.5911	0.9414	0.7859	0.030*
H20B	0.5938	1.1032	0.7334	0.030*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02681 (14)	0.0192 (2)	0.02079 (13)	0.00088 (11)	0.00395 (9)	-0.00472 (11)
Br1A	0.02681 (14)	0.0192 (2)	0.02079 (13)	0.00088 (11)	0.00395 (9)	-0.00472 (11)

S1	0.0204 (3)	0.0212 (3)	0.0163 (3)	0.0003 (2)	-0.0011 (2)	-0.00170 (19)
N1	0.0182 (9)	0.0184 (9)	0.0186 (9)	0.0008 (7)	0.0001 (7)	-0.0038 (7)
N2	0.0215 (10)	0.0251 (10)	0.0185 (9)	0.0000 (8)	-0.0002 (8)	-0.0061 (8)
N3	0.0217 (10)	0.0249 (10)	0.0182 (9)	-0.0002 (8)	-0.0008 (8)	-0.0037 (8)
C1	0.0206 (11)	0.0158 (10)	0.0205 (11)	-0.0037 (9)	0.0044 (9)	-0.0035 (8)
C2	0.0203 (11)	0.0176 (10)	0.0240 (11)	0.0003 (9)	0.0029 (9)	0.0018 (9)
C3	0.0193 (11)	0.0187 (10)	0.0195 (11)	0.0000 (9)	0.0015 (9)	0.0034 (8)
C4	0.0168 (10)	0.0182 (10)	0.0167 (10)	-0.0021 (9)	0.0017 (8)	0.0008 (8)
C5	0.0225 (11)	0.0167 (10)	0.0198 (11)	0.0035 (9)	0.0017 (9)	0.0004 (8)
C6	0.0237 (12)	0.0210 (11)	0.0172 (11)	0.0020 (9)	-0.0005 (9)	0.0007 (8)
C7	0.0207 (11)	0.0160 (10)	0.0173 (10)	0.0006 (9)	0.0027 (8)	0.0021 (8)
C8	0.0221 (11)	0.0181 (10)	0.0179 (11)	0.0011 (9)	0.0020 (9)	-0.0007 (8)
C9	0.0201 (11)	0.0183 (10)	0.0157 (10)	-0.0020 (9)	-0.0012 (9)	0.0006 (8)
C10	0.0197 (11)	0.0194 (11)	0.0171 (10)	-0.0006 (9)	0.0028 (9)	-0.0041 (8)
C11	0.0264 (12)	0.0206 (11)	0.0212 (11)	-0.0027 (10)	0.0059 (9)	-0.0005 (9)
C12	0.0235 (12)	0.0260 (12)	0.0313 (13)	-0.0069 (10)	0.0089 (10)	-0.0064 (10)
C13	0.0181 (11)	0.0361 (14)	0.0286 (13)	0.0007 (11)	0.0001 (10)	-0.0095 (10)
C14	0.0250 (12)	0.0270 (12)	0.0228 (11)	0.0070 (10)	-0.0022 (10)	-0.0020 (9)
C15	0.0226 (12)	0.0196 (11)	0.0236 (11)	-0.0012 (9)	0.0028 (9)	-0.0022 (9)
C16	0.0217 (11)	0.0207 (11)	0.0176 (11)	-0.0015 (9)	0.0002 (9)	-0.0004 (8)
C17	0.0220 (11)	0.0236 (11)	0.0174 (11)	-0.0024 (9)	0.0015 (9)	-0.0029 (8)
C18	0.0245 (12)	0.0329 (13)	0.0233 (12)	0.0004 (11)	0.0024 (10)	-0.0082 (10)
C19	0.0240 (12)	0.0339 (13)	0.0264 (12)	0.0056 (11)	0.0017 (10)	-0.0062 (10)
C20	0.0221 (12)	0.0299 (13)	0.0222 (11)	-0.0009 (10)	0.0014 (9)	-0.0056 (9)

Geometric parameters (Å, °)

Br1—C1	1.903 (2)	C10—C15	1.387 (3)
Br1A—C1	1.830 (8)	C11—C12	1.397 (4)
S1—C8	1.738 (2)	C11—H11	0.9500
S1—C9	1.756 (2)	C12—C13	1.382 (4)
N1—C9	1.388 (3)	C12—H12	0.9500
N1—C7	1.415 (3)	C13—C14	1.390 (4)
N1—C10	1.437 (3)	C13—H13	0.9500
N2—C9	1.289 (3)	C14—C15	1.390 (3)
N2—N3	1.421 (3)	C14—H14	0.9500
N3—C16	1.277 (3)	C15—H15	0.9500
C1—C2	1.385 (3)	C16—C20	1.511 (3)
C1—C6	1.386 (3)	C16—C17	1.514 (3)
C2—C3	1.391 (3)	C17—C18	1.530 (3)
C2—H2	0.9500	C17—H17A	0.9900
C3—C4	1.399 (3)	C17—H17B	0.9900
C3—H3	0.9500	C18—C19	1.530 (3)
C4—C5	1.398 (3)	C18—H18A	0.9900
C4—C7	1.476 (3)	C18—H18B	0.9900
C5—C6	1.389 (3)	C19—C20	1.531 (3)
C5—H5	0.9500	C19—H19A	0.9900
C6—H6	0.9500	C19—H19B	0.9900

C7—C8	1.340 (3)	C20—H20A	0.9900
C8—H8	0.9500	C20—H20B	0.9900
C10—C11	1.384 (3)		
C8—S1—C9	90.38 (11)	C12—C11—H11	120.8
C9—N1—C7	113.44 (18)	C13—C12—C11	120.5 (2)
C9—N1—C10	121.16 (18)	C13—C12—H12	119.7
C7—N1—C10	125.08 (18)	C11—C12—H12	119.7
C9—N2—N3	108.28 (19)	C12—C13—C14	120.2 (2)
C16—N3—N2	114.49 (19)	C12—C13—H13	119.9
C2—C1—C6	121.5 (2)	C14—C13—H13	119.9
C2—C1—Br1A	134.4 (6)	C15—C14—C13	119.9 (2)
C6—C1—Br1A	102.0 (7)	C15—C14—H14	120.0
C2—C1—Br1	119.64 (17)	C13—C14—H14	120.0
C6—C1—Br1	118.90 (17)	C10—C15—C14	119.1 (2)
C1—C2—C3	118.9 (2)	C10—C15—H15	120.4
C1—C2—H2	120.6	C14—C15—H15	120.4
C3—C2—H2	120.6	N3—C16—C20	128.6 (2)
C2—C3—C4	121.2 (2)	N3—C16—C17	121.8 (2)
C2—C3—H3	119.4	C20—C16—C17	109.62 (19)
C4—C3—H3	119.4	C16—C17—C18	104.01 (19)
C5—C4—C3	118.4 (2)	C16—C17—H17A	111.0
C5—C4—C7	123.0 (2)	C18—C17—H17A	111.0
C3—C4—C7	118.35 (19)	C16—C17—H17B	111.0
C6—C5—C4	121.0 (2)	C18—C17—H17B	111.0
C6—C5—H5	119.5	H17A—C17—H17B	109.0
C4—C5—H5	119.5	C17—C18—C19	103.86 (19)
C1—C6—C5	119.1 (2)	C17—C18—H18A	111.0
C1—C6—H6	120.5	C19—C18—H18A	111.0
C5—C6—H6	120.5	C17—C18—H18B	111.0
C8—C7—N1	112.5 (2)	C19—C18—H18B	111.0
C8—C7—C4	124.5 (2)	H18A—C18—H18B	109.0
N1—C7—C4	122.84 (19)	C18—C19—C20	103.9 (2)
C7—C8—S1	113.45 (17)	C18—C19—H19A	111.0
C7—C8—H8	123.3	C20—C19—H19A	111.0
S1—C8—H8	123.3	C18—C19—H19B	111.0
N2—C9—N1	123.8 (2)	C20—C19—H19B	111.0
N2—C9—S1	125.86 (17)	H19A—C19—H19B	109.0
N1—C9—S1	110.27 (16)	C16—C20—C19	103.95 (19)
C11—C10—C15	121.8 (2)	C16—C20—H20A	111.0
C11—C10—N1	118.9 (2)	C19—C20—H20A	111.0
C15—C10—N1	119.3 (2)	C16—C20—H20B	111.0
C10—C11—C12	118.4 (2)	C19—C20—H20B	111.0
C10—C11—H11	120.8	H20A—C20—H20B	109.0
C9—N2—N3—C16	-171.4 (2)	C10—N1—C9—N2	-4.5 (3)
C6—C1—C2—C3	-0.1 (3)	C7—N1—C9—S1	0.2 (2)
Br1A—C1—C2—C3	159.7 (10)	C10—N1—C9—S1	174.06 (16)

Br1—C1—C2—C3	178.96 (16)	C8—S1—C9—N2	178.2 (2)
C1—C2—C3—C4	-0.8 (3)	C8—S1—C9—N1	-0.31 (17)
C2—C3—C4—C5	1.0 (3)	C9—N1—C10—C11	-109.5 (2)
C2—C3—C4—C7	-173.6 (2)	C7—N1—C10—C11	63.6 (3)
C3—C4—C5—C6	-0.2 (3)	C9—N1—C10—C15	73.0 (3)
C7—C4—C5—C6	174.1 (2)	C7—N1—C10—C15	-113.9 (2)
C2—C1—C6—C5	0.9 (3)	C15—C10—C11—C12	0.3 (3)
Br1A—C1—C6—C5	-164.5 (6)	N1—C10—C11—C12	-177.2 (2)
Br1—C1—C6—C5	-178.20 (17)	C10—C11—C12—C13	0.6 (3)
C4—C5—C6—C1	-0.7 (3)	C11—C12—C13—C14	-0.6 (4)
C9—N1—C7—C8	0.0 (3)	C12—C13—C14—C15	-0.2 (4)
C10—N1—C7—C8	-173.5 (2)	C11—C10—C15—C14	-1.1 (3)
C9—N1—C7—C4	-174.9 (2)	N1—C10—C15—C14	176.4 (2)
C10—N1—C7—C4	11.6 (3)	C13—C14—C15—C10	1.0 (3)
C5—C4—C7—C8	-140.5 (2)	N2—N3—C16—C20	4.6 (3)
C3—C4—C7—C8	33.8 (3)	N2—N3—C16—C17	-175.20 (19)
C5—C4—C7—N1	33.8 (3)	N3—C16—C17—C18	-168.4 (2)
C3—C4—C7—N1	-151.9 (2)	C20—C16—C17—C18	11.8 (3)
N1—C7—C8—S1	-0.3 (2)	C16—C17—C18—C19	-31.0 (2)
C4—C7—C8—S1	174.50 (17)	C17—C18—C19—C20	38.9 (3)
C9—S1—C8—C7	0.35 (18)	N3—C16—C20—C19	-167.8 (2)
N3—N2—C9—N1	-176.3 (2)	C17—C16—C20—C19	12.1 (3)
N3—N2—C9—S1	5.4 (3)	C18—C19—C20—C16	-31.2 (2)
C7—N1—C9—N2	-178.3 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C17—H17B \cdots Br1 ⁱ	0.99	3.03	3.828 (2)	138

Symmetry code: (i) *x*, $-\gamma+1/2$, *z*+1/2.