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(*Z*)-1-[(2*E*)-3,4-Diphenyl-2,3-dihydro-1,3-thiazol-2-ylidene]-2-[1-(4-hydroxyphenyl)ethylidene]hydrazinium bromide including an unknown solvate

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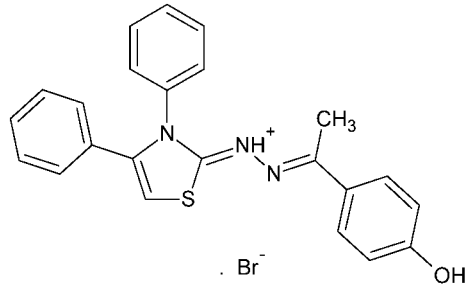
Key indicators: single-crystal X-ray study; T = 220 K; mean σ(C–C) = 0.007 Å; R factor = 0.058; wR factor = 0.157; data-to-parameter ratio = 19.6.

In the title compound, $C_{23}H_{20}N_3OS^+\cdot Br^-$, the dihydrothiazole ring (r.m.s. deviation = 0.015 Å) is twisted with respect to each of the C- and N-bound phenyl rings and the hydroxybenzene ring, making dihedral angles of 76.0 (2), 71.2 (2) and 9.8 (2)°, respectively. In the crystal, inversion-related molecules are linked by association of the bromide ions with the cations *via* N—H···Br and O—H···Br hydrogen-bonding interactions. These molecules run in channels parallel to the *a* axis through face-to-face π–π stacking interactions between the hydroxybenzene rings [centroid–centroid distances = 3.785 (3) Å] which, in turn, are connected into layers parallel to (110) by weak C—H···π interactions. A small region of electron density well removed from the main molecule and appearing disordered over a center of symmetry was removed with *PLATON* SQUEEZE [Spek (2009). *Acta Cryst.* D**65**, 148–15] following unsuccessful attempts to model it as plausible solvent molecule. The nature of the solvent was not known and hence, this is not taken into account when calculating M_r and related data.

Related literature

For general medicinal and industrial applications of five-membered *S*,*N*-heterocycles thiazolines, see: Abhinit *et al.* (2009). For chemical and diverse medicinal properties of thiazoles, see: Sreedevi *et al.* (2013); Milne (2000); De Souza & De Almeida (2003); Lednicer *et al.* (1990); Rehman *et al.* (2005); Knadler *et al.* (1986). For a similar structure, see: Mague *et al.* (2014).



Experimental

Crystal data

$C_{23}H_{20}N_3OS^+\cdot Br^-$
M_r = 466.39
Triclinic, $P\overline{1}$
a = 7.5987 (12) Å
b = 12.3017 (19) Å
c = 13.786 (2) Å
α = 68.0760 (17)°
β = 88.1540 (18)°
γ = 72.6540 (18)°
V = 1136.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.92 mm^{-1}
T = 220 K
0.17 × 0.17 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.56, T_{max} = 0.80
11044 measured reflections
5146 independent reflections
3398 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.157
S = 1.01
5146 reflections
263 parameters
73 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

*Cg*4 is the centroid of the C18–C23 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···Br1^{i}	0.83	2.50	3.328 (4)	178
N2—H2···Br1^{ii}	0.91	2.88	3.570 (3)	134
C5—H5···*Cg*4^{iii}	0.94	2.76	3.610 (5)	152

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

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5311).

References

Abhinit, M., Ghodke, M. & Pratima, N. A. (2009). *Int. J. Pharm. Pharm. Sci.* **1**, 47–64.

Bruker (2013). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

De Souza, M. V. N. & De Almeida, M. V. (2003). *Quim. Nova*, **26**, 366–372.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Knadler, M. P., Bergstrom, R. F., Callaghan, J. T. & Rubin, A. (1986). *Drug Metab. Dispos.* **14**, 175–182.

Lednicer, D., Mitscher, L. A. G. I. & George, G. I. (1990). *The Organic Chemistry of Drug Synthesis*, Vol. 4, pp. 95–97. New York: Wiley.

Mague, J. T., Mohamed, S. K., Akkurt, M., Abd El-Alaziz, A. T. & Albayati, M. R. (2014). *Acta Cryst.* E**70**, o328–o329.

Milne, G. W. A. (2000). In *Ashgate Handbook of Antineoplastic Agents*. London: Wiley.

Rehman, M. Z., Anwar, C. J. & Ahmad, S. (2005). *Bull. Korean Chem. Soc.* **26**, 1771–1775.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Sreedevi, M., Prasad, A. R. G., Spoorthy, Y. N. & Ravindranath, L. R. K. R. (2013). *Adv. Pharm. Bull.* **3**, 227–230.

supporting information

Acta Cryst. (2014). E**70**, o647–o648 [doi:10.1107/S1600536814010125]

(*Z*)-1-[(2*E*)-3,4-Diphenyl-2,3-dihydro-1,3-thiazol-2-ylidene]-2-[1-(4-hydroxyphenyl)ethylidene]hydrazinium bromide including an unknown solvate

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S1. Structural commentary

Synthesis of five-membered *S*,*N*-heterocycles thiazolines has received intensive interest from chemists and biologists due to their wide spectrum of medicinal and industrial applications (Abhinit *et al.*, 2009). Thiazoles are stable and non-carcinogenic aromatic compounds with relatively small size (Sreedevi *et al.*, 2013). Many biologically active products, such as Bleomycin and Tiazofurin (antineoplastic agents) (Milne, 2000), Ritonavir (anti-HIV drug) (De Souza & De Almeida, 2003), Fanetizole and Meloxicam (anti-inflammatory agents) (Lednicer *et al.*, 1990; Rehman *et al.*, 2005), Nizatidine (antiulcer agent) (Knadler *et al.*, 1986) and penicillin (antibiotic) are some examples of thiazole-bearing compounds.

In the title molecule (I), shown in Fig. 1, the 5-membered heterocycle (S1/N1/C1–C3) is planar to within 0.013 (3) Å for N1 and the phenyl rings C4–C9 and C10–C15 make dihedral angles with it of 76.0 (2)° and 71.2 (2)°, respectively. The dihedral angle between the ring C18–C23 and the heterocycle (S1/N1/C1–C3) is 9.8 (2)°. The N1–C3–N2–N3, C3–N2–N3–C18, N2–N3–C16–C18 torsion angles are 173.6 (4), 166.3 (4) and -177.1 (3)°, respectively. All bond lengths and bond angles in (I) are normal and are comparable with those found in a similar structure (Mague *et al.*, 2014).

In the crystal, inversion-related molecules are linked by association of the bromide ions with the cations *via* N—H···Br and O—H···Br hydrogen bonding interactions (Table 1, Fig. 2). These molecules run in channels parallel to the *a* axis through the face-to-face π—π stacking interactions [centroid-to-centroid distances = 3.785 (3) Å] between the hydroxyl-benzene rings: these are connected into layers parallel to (110) by weak C5—H5···Cg(C18–C23) interactions, Table 1.

S2. Synthesis and crystallization

The title compound was prepared according to our reported method (Mague *et al.*, 2014). The crude product has been crystallized from ethanol to afford colorless crystals suitable for X-ray diffraction (m.p.: 533 – 535 K).

S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H= 0.94–0.97 Å, N–H = 0.91 Å and O–H = 0.83 Å, and with U_{iso}(H)= 1.2U_{eq}(C,*N*) and 1.5 U_{eq}(O). A small region of electron density well–removed from the main molecule and appearing disordered over a center of symmetry was removed with *PLATON SQUEEZE* following unsuccessful attempts to model it as plausible lattice solvent (Spek, 2009).

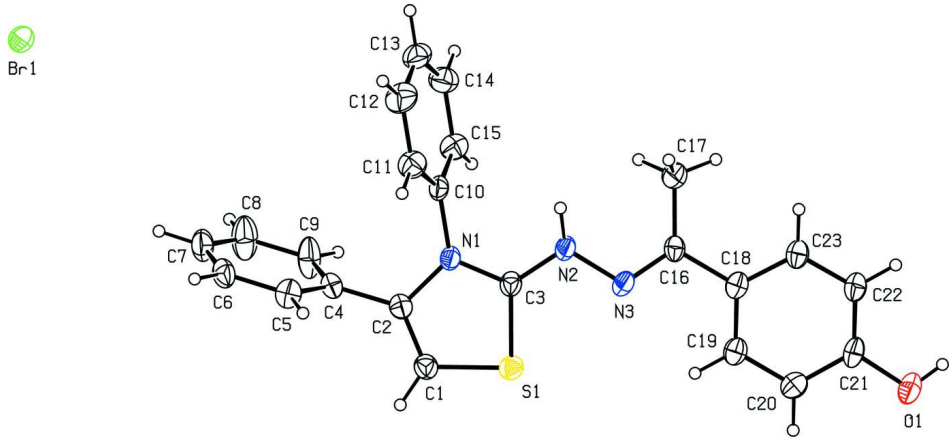

Figure 1

Perspective view of the asymmetric unit with 30% probability displacement ellipsoids.

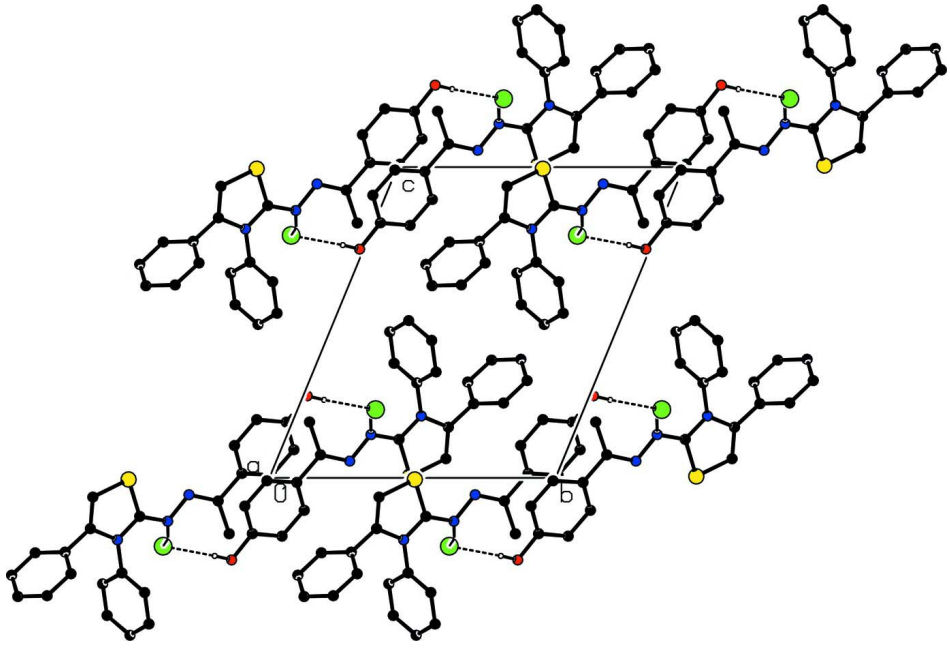

Figure 2

Packing viewed down the *a* axis and showing O—H···Br interactions.

(*Z*)-1-[(2*E*)-3,4-Diphenyl-2,3-dihydro-1,3-thiazol-2-ylidene]-2-[1-(4-hydroxyphenyl)ethylidene]hydrazinium bromide

Crystal data

$C_{23}H_{20}N_3OS^+\cdot Br^-$
M_r = 466.39
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.5987 (12) Å
b = 12.3017 (19) Å
c = 13.786 (2) Å
α = 68.0760 (17)°
β = 88.1540 (18)°
γ = 72.6540 (18)°
V = 1136.6 (3) Å^3
Z = 2
$F(000)$ = 476
D_x = 1.363 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4151 reflections

θ = 2.8–26.7°
μ = 1.92 mm^{-1}
T = 220 K

Block, colourless
0.17 × 0.17 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3660 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.56, T_{max} = 0.80

11044 measured reflections
5146 independent reflections
3398 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −9→9
k = −15→15
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.157
S = 1.01
5146 reflections
263 parameters
73 restraints

Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0867P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å) while those attached to nitrogen were placed in locations derived from a difference map and their coordinates adjusted to give N—H = 0.91 Å. That attached to oxygen was placed in an idealized position and the C—C—O—H torsion angle refined (AFIX 147)·All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. A small region of electron density well removed from the main molecule and appearing disordered over a center of symmetry was removed with *PLATON SQUEEZE* following unsuccessful attempts to model it as plausible lattice solvent (Spek, 2014).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.24831 (13)	0.51039 (10)	0.99502 (8)	0.0418 (3)
O1	−0.1920 (4)	1.0140 (3)	1.2638 (2)	0.0599 (11)
N1	0.1776 (4)	0.5582 (3)	0.8008 (2)	0.0376 (10)
N2	−0.0083 (4)	0.7072 (3)	0.8605 (2)	0.0427 (11)
N3	−0.0284 (5)	0.7434 (3)	0.9459 (2)	0.0434 (11)
C1	0.3784 (5)	0.4108 (4)	0.9384 (3)	0.0433 (12)
C2	0.3282 (5)	0.4476 (4)	0.8368 (3)	0.0399 (12)
C3	0.1253 (5)	0.6024 (4)	0.8761 (3)	0.0393 (12)
C4	0.4141 (5)	0.3930 (4)	0.7614 (3)	0.0398 (12)
C5	0.3820 (6)	0.2897 (4)	0.7589 (3)	0.0480 (16)

C6	0.4610 (6)	0.2396 (4)	0.6870 (4)	0.0510 (16)
C7	0.5711 (7)	0.2920 (5)	0.6183 (4)	0.0604 (17)
C8	0.6055 (8)	0.3930 (5)	0.6209 (5)	0.085 (3)
C9	0.5280 (7)	0.4447 (5)	0.6915 (4)	0.070 (2)
C10	0.0904 (5)	0.6216 (4)	0.6942 (3)	0.0389 (12)
C11	−0.0203 (6)	0.5700 (4)	0.6591 (4)	0.0543 (17)
C12	−0.1016 (7)	0.6310 (5)	0.5574 (4)	0.0689 (19)
C13	−0.0764 (6)	0.7396 (5)	0.4938 (4)	0.0608 (18)
C14	0.0333 (6)	0.7896 (5)	0.5299 (4)	0.0576 (17)
C15	0.1188 (6)	0.7291 (4)	0.6313 (3)	0.0495 (14)
C16	−0.1282 (5)	0.8544 (4)	0.9258 (3)	0.0380 (12)
C17	−0.2232 (6)	0.9401 (4)	0.8202 (3)	0.0478 (14)
C18	−0.1445 (5)	0.8977 (4)	1.0145 (3)	0.0388 (12)
C19	−0.0230 (6)	0.8316 (4)	1.1041 (3)	0.0443 (12)
C20	−0.0409 (6)	0.8719 (4)	1.1875 (3)	0.0480 (16)
C21	−0.1813 (6)	0.9791 (4)	1.1794 (3)	0.0446 (14)
C22	−0.2998 (6)	1.0452 (4)	1.0906 (3)	0.0470 (14)
C23	−0.2808 (6)	1.0045 (4)	1.0093 (3)	0.0451 (14)
Br1	0.46263 (6)	0.27288 (4)	0.21975 (3)	0.0504 (2)
H1	0.47420	0.33840	0.97570	0.0520*
H1O	−0.27870	1.07870	1.25100	0.0900*
H2	−0.09160	0.73360	0.80430	0.0510*
H5	0.30560	0.25280	0.80650	0.0570*
H6	0.43800	0.16900	0.68600	0.0620*
H7	0.62360	0.25870	0.56900	0.0730*
H8	0.68370	0.42830	0.57370	0.1020*
H9	0.55280	0.51490	0.69200	0.0830*
H11	−0.03950	0.49580	0.70320	0.0650*
H12	−0.17560	0.59700	0.53150	0.0830*
H13	−0.13440	0.78040	0.42500	0.0730*
H14	0.05050	0.86450	0.48600	0.0690*
H15	0.19550	0.76220	0.65630	0.0590*
H17A	−0.26820	1.02330	0.81860	0.0720*
H17B	−0.32660	0.91560	0.80600	0.0720*
H17C	−0.13670	0.93690	0.76730	0.0720*
H19	0.07160	0.75970	1.10900	0.0530*
H20	0.04110	0.82700	1.24860	0.0580*
H22	−0.39340	1.11780	1.08500	0.0570*
H23	−0.36270	1.05060	0.94830	0.0540*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0397 (6)	0.0478 (6)	0.0404 (5)	−0.0129 (5)	0.0012 (4)	−0.0197 (5)
O1	0.068 (2)	0.069 (2)	0.0568 (19)	−0.0195 (17)	0.0135 (15)	−0.0413 (17)
N1	0.0332 (17)	0.0438 (19)	0.0401 (17)	−0.0070 (14)	0.0016 (13)	−0.0244 (15)
N2	0.0413 (19)	0.050 (2)	0.0405 (18)	−0.0047 (15)	−0.0006 (14)	−0.0282 (16)
N3	0.050 (2)	0.050 (2)	0.0363 (17)	−0.0139 (17)	0.0061 (14)	−0.0244 (16)

C1	0.038 (2)	0.045 (2)	0.047 (2)	−0.0093 (18)	0.0020 (17)	−0.0202 (19)
C2	0.036 (2)	0.040 (2)	0.046 (2)	−0.0114 (17)	0.0024 (16)	−0.0192 (18)
C3	0.036 (2)	0.044 (2)	0.044 (2)	−0.0112 (17)	0.0021 (16)	−0.0243 (18)
C4	0.035 (2)	0.036 (2)	0.049 (2)	−0.0077 (17)	0.0045 (16)	−0.0193 (18)
C5	0.047 (2)	0.052 (3)	0.057 (3)	−0.026 (2)	0.0103 (19)	−0.026 (2)
C6	0.049 (3)	0.045 (2)	0.067 (3)	−0.009 (2)	−0.001 (2)	−0.034 (2)
C7	0.059 (3)	0.058 (3)	0.068 (3)	−0.008 (2)	0.018 (2)	−0.037 (3)
C8	0.092 (4)	0.073 (4)	0.114 (5)	−0.043 (3)	0.065 (4)	−0.054 (4)
C9	0.076 (4)	0.059 (3)	0.104 (4)	−0.038 (3)	0.050 (3)	−0.054 (3)
C10	0.033 (2)	0.046 (2)	0.042 (2)	−0.0056 (17)	0.0046 (16)	−0.0266 (18)
C11	0.052 (3)	0.060 (3)	0.055 (3)	−0.020 (2)	0.000 (2)	−0.024 (2)
C12	0.060 (3)	0.090 (4)	0.070 (3)	−0.024 (3)	−0.013 (2)	−0.043 (3)
C13	0.045 (3)	0.085 (4)	0.044 (2)	−0.006 (2)	−0.0011 (19)	−0.026 (2)
C14	0.049 (3)	0.062 (3)	0.050 (3)	−0.011 (2)	0.003 (2)	−0.013 (2)
C15	0.044 (2)	0.060 (3)	0.047 (2)	−0.020 (2)	0.0041 (18)	−0.020 (2)
C16	0.031 (2)	0.043 (2)	0.045 (2)	−0.0111 (17)	0.0097 (16)	−0.0230 (18)
C17	0.051 (3)	0.049 (2)	0.048 (2)	−0.016 (2)	0.0018 (18)	−0.023 (2)
C18	0.038 (2)	0.046 (2)	0.043 (2)	−0.0223 (18)	0.0144 (16)	−0.0223 (18)
C19	0.047 (2)	0.048 (2)	0.048 (2)	−0.0208 (19)	0.0112 (18)	−0.025 (2)
C20	0.050 (3)	0.055 (3)	0.044 (2)	−0.022 (2)	0.0069 (18)	−0.020 (2)
C21	0.049 (2)	0.053 (3)	0.050 (2)	−0.026 (2)	0.0232 (19)	−0.033 (2)
C22	0.043 (2)	0.055 (3)	0.052 (2)	−0.015 (2)	0.0135 (18)	−0.031 (2)
C23	0.041 (2)	0.052 (3)	0.051 (2)	−0.0170 (19)	0.0138 (18)	−0.028 (2)
Br1	0.0562 (3)	0.0514 (3)	0.0488 (3)	−0.0152 (2)	−0.0025 (2)	−0.0252 (2)

Geometric parameters (Å, º)

S1—C1	1.741 (5)	C16—C18	1.494 (6)
S1—C3	1.710 (4)	C18—C23	1.388 (7)
O1—C21	1.375 (5)	C18—C19	1.384 (6)
O1—H1O	0.8300	C19—C20	1.401 (6)
N1—C3	1.341 (5)	C20—C21	1.396 (7)
N1—C10	1.451 (5)	C21—C22	1.365 (6)
N1—C2	1.418 (6)	C22—C23	1.376 (6)
N2—C3	1.329 (6)	C1—H1	0.9400
N2—N3	1.395 (4)	C5—H5	0.9400
N3—C16	1.277 (6)	C6—H6	0.9400
N2—H2	0.9100	C7—H7	0.9400
C1—C2	1.331 (5)	C8—H8	0.9400
C2—C4	1.474 (6)	C9—H9	0.9400
C4—C9	1.378 (7)	C11—H11	0.9400
C4—C5	1.376 (7)	C12—H12	0.9400
C5—C6	1.386 (7)	C13—H13	0.9400
C6—C7	1.352 (7)	C14—H14	0.9400
C7—C8	1.357 (9)	C15—H15	0.9400
C8—C9	1.379 (9)	C17—H17A	0.9700
C10—C11	1.385 (7)	C17—H17B	0.9700
C10—C15	1.360 (6)	C17—H17C	0.9700

C11—C12	1.380 (7)	C19—H19	0.9400
C12—C13	1.363 (8)	C20—H20	0.9400
C13—C14	1.372 (8)	C22—H22	0.9400
C14—C15	1.387 (6)	C23—H23	0.9400
C16—C17	1.490 (6)		

C1—S1—C3	89.3 (2)	O1—C21—C20	116.9 (4)
C21—O1—H1O	109.00	C20—C21—C22	120.5 (4)
C2—N1—C10	125.3 (3)	C21—C22—C23	119.3 (5)
C3—N1—C10	122.2 (4)	C18—C23—C22	122.1 (4)
C2—N1—C3	112.5 (3)	S1—C1—H1	124.00
N3—N2—C3	114.7 (3)	C2—C1—H1	123.00
N2—N3—C16	115.3 (3)	C4—C5—H5	120.00
C3—N2—H2	115.00	C6—C5—H5	120.00
N3—N2—H2	128.00	C5—C6—H6	120.00
S1—C1—C2	113.1 (4)	C7—C6—H6	120.00
N1—C2—C1	111.8 (4)	C6—C7—H7	120.00
N1—C2—C4	119.4 (3)	C8—C7—H7	120.00
C1—C2—C4	128.7 (4)	C7—C8—H8	119.00
S1—C3—N1	113.3 (3)	C9—C8—H8	119.00
N1—C3—N2	123.7 (3)	C4—C9—H9	120.00
S1—C3—N2	123.0 (3)	C8—C9—H9	120.00
C5—C4—C9	118.5 (4)	C10—C11—H11	121.00
C2—C4—C5	120.9 (4)	C12—C11—H11	121.00
C2—C4—C9	120.6 (5)	C11—C12—H12	119.00
C4—C5—C6	120.7 (4)	C13—C12—H12	119.00
C5—C6—C7	120.1 (5)	C12—C13—H13	120.00
C6—C7—C8	119.7 (5)	C14—C13—H13	120.00
C7—C8—C9	121.2 (6)	C13—C14—H14	120.00
C4—C9—C8	119.8 (6)	C15—C14—H14	120.00
C11—C10—C15	121.6 (4)	C10—C15—H15	120.00
N1—C10—C11	118.6 (4)	C14—C15—H15	120.00
N1—C10—C15	119.8 (4)	C16—C17—H17A	109.00
C10—C11—C12	117.9 (5)	C16—C17—H17B	109.00
C11—C12—C13	121.2 (5)	C16—C17—H17C	109.00
C12—C13—C14	120.1 (5)	H17A—C17—H17B	110.00
C13—C14—C15	119.8 (5)	H17A—C17—H17C	110.00
C10—C15—C14	119.4 (4)	H17B—C17—H17C	109.00
C17—C16—C18	120.0 (4)	C18—C19—H19	120.00
N3—C16—C18	116.5 (3)	C20—C19—H19	120.00
N3—C16—C17	123.5 (4)	C19—C20—H20	120.00
C16—C18—C19	120.4 (4)	C21—C20—H20	120.00
C16—C18—C23	121.1 (4)	C21—C22—H22	120.00
C19—C18—C23	118.5 (4)	C23—C22—H22	120.00
C18—C19—C20	120.0 (4)	C18—C23—H23	119.00
C19—C20—C21	119.6 (4)	C22—C23—H23	119.00
O1—C21—C22	122.6 (4)		

C3—S1—C1—C2	0.0 (4)	C2—C4—C9—C8	−179.3 (5)
C1—S1—C3—N1	1.4 (3)	C5—C4—C9—C8	0.4 (7)
C1—S1—C3—N2	−178.5 (4)	C4—C5—C6—C7	0.1 (7)
C3—N1—C2—C1	2.3 (5)	C5—C6—C7—C8	0.7 (8)
C3—N1—C2—C4	−174.3 (4)	C6—C7—C8—C9	−1.0 (9)
C10—N1—C2—C1	−179.8 (4)	C7—C8—C9—C4	0.4 (9)
C10—N1—C2—C4	3.6 (6)	N1—C10—C11—C12	−179.7 (4)
C2—N1—C3—S1	−2.4 (4)	C15—C10—C11—C12	0.2 (7)
C2—N1—C3—N2	177.5 (4)	N1—C10—C15—C14	−179.4 (4)
C10—N1—C3—S1	179.6 (3)	C11—C10—C15—C14	0.8 (7)
C10—N1—C3—N2	−0.5 (6)	C10—C11—C12—C13	−1.0 (8)
C2—N1—C10—C11	72.5 (5)	C11—C12—C13—C14	0.9 (9)
C2—N1—C10—C15	−107.4 (5)	C12—C13—C14—C15	0.1 (8)
C3—N1—C10—C11	−109.8 (5)	C13—C14—C15—C10	−0.9 (8)
C3—N1—C10—C15	70.3 (5)	N3—C16—C18—C19	15.2 (6)
C3—N2—N3—C16	166.3 (4)	N3—C16—C18—C23	−164.8 (4)
N3—N2—C3—S1	6.3 (5)	C17—C16—C18—C19	−163.8 (4)
N3—N2—C3—N1	−173.6 (4)	C17—C16—C18—C23	16.2 (6)
N2—N3—C16—C17	1.9 (6)	C16—C18—C19—C20	−179.1 (4)
N2—N3—C16—C18	−177.1 (3)	C23—C18—C19—C20	0.9 (7)
S1—C1—C2—N1	−1.3 (5)	C16—C18—C23—C22	179.2 (4)
S1—C1—C2—C4	175.0 (4)	C19—C18—C23—C22	−0.9 (7)
N1—C2—C4—C5	−105.2 (5)	C18—C19—C20—C21	−0.2 (7)
N1—C2—C4—C9	74.5 (6)	C19—C20—C21—O1	180.0 (4)
C1—C2—C4—C5	78.8 (6)	C19—C20—C21—C22	−0.6 (7)
C1—C2—C4—C9	−101.5 (6)	O1—C21—C22—C23	−179.9 (4)
C2—C4—C5—C6	179.1 (4)	C20—C21—C22—C23	0.6 (7)
C9—C4—C5—C6	−0.6 (7)	C21—C22—C23—C18	0.1 (7)

Hydrogen-bond geometry (Å, º)

Cg4 is the centroid of the C18–C23 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···Br1^{i}	0.83	2.50	3.328 (4)	178
N2—H2···Br1^{ii}	0.91	2.88	3.570 (3)	134
C5—H5···*Cg*4^{iii}	0.94	2.76	3.610 (5)	152

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