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S-Benzyl 3-(2-bromobenzylidene)dithiocarbazate

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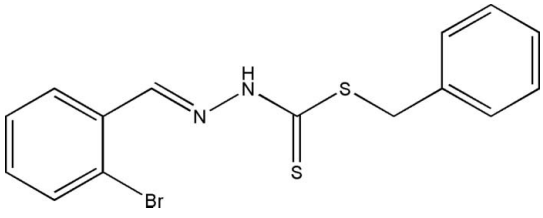
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; R factor = 0.044; wR factor = 0.122; data-to-parameter ratio = 15.0.

The title compound, $C_{15}H_{13}BrN_2S_2$, crystallizes with two independent molecules in the asymmetric unit. Both molecules display a 'C-shaped' conformation, with a *trans* configuration with respect to the C=N double bond. Intermolecular N—H···S interactions are observed.

Related literature

For related Schiff base structures, see: Qiu, Fang *et al.* (2006); Qiu, Luo, *et al.* (2006).



Experimental

Crystal data

$C_{15}H_{13}BrN_2S_2$
M_r = 365.30
Monoclinic, $P2_1/n$
a = 22.465 (6) Å
b = 5.9323 (17) Å
c = 23.668 (7) Å
β = 92.432 (5)°
V = 3151.4 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.86 mm^{-1}
T = 298 (2) K
0.12 × 0.07 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.725, T_{max} = 0.847
17549 measured reflections
5399 independent reflections
1750 reflections with $I > 2\sigma(I)$
R_{int} = 0.105

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 0.79
5399 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···S3^{i}	0.86	2.88	3.669 (5)	154
N2—H2···S1^{ii}	0.86	2.62	3.455 (5)	164

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2244).

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supplementary materials

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S-Benzyl 3-(2-bromobenzylidene)dithiocarbazate

X.-Y. Qiu and Z.-G. Luo

Comment

As an extension of our work on the structural characterization of Schiff-base compounds (Qiu, Fang *et al.*, 2006; Qiu, Luo *et al.*, 2006), we report here the crystal structure of the title compound. The asymmetric unit consists of two independent molecules (Fig. 1), both of which display a "C-shaped" conformation. In both independent molecules, all bond lengths and angles lie within normal ranges: the C7=N1 and C22=N3 bond lengths of 1.272 (7) and 1.257 (7) Å conform to the expected value for a C=N double bond. The bond lengths of 1.324 (6) and 1.338 (7) Å for C8—N2 and C23—N4, respectively, lie between the expected values for a double and single bond, because of conjugation effects in the molecule. The dihedral angle between the two benzene rings in each molecule is 107.9 (6) and 105.1 (6) ° for the two independent molecules, respectively. In the crystal, intermolecular N—H···S interactions are observed.

Experimental

The title compound was synthesized by reaction of equivalent amounts of *S*-benzyldithiocarbazate (1 mmol, 0.20 g) and 2-bromobenzaldehyde (1 mmol, 0.19 g) in ethanol (20 ml) for 1 h at 373–383 K. Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethanol solution.

Refinement

Atoms H2 and H4 were visible in a difference Fourier map, but were placed in calculated positions (N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(N). All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 or 0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C). The higher-angle diffraction data were weak, with only 1750 out of 5399 unique reflections observed ($I > 2\sigma(I)$) to θ_{max} = 25.0°, and the resulting structure is of relatively low precision.

Figures

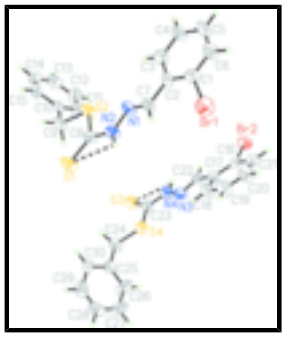


Fig. 1. The molecular structure of the title compound showing displacement ellipsoids at 30% for non-H atoms. Dashed lines denote N—H···S hydrogen bonds.

S-Benzyl 3-(2-bromobenzylidene)dithiocarbazate

Crystal data

$C_{15}H_{13}BrN_2S_2$	F_{000} = 1472
M_r = 365.30	D_x = 1.540 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3876 reflections
a = 22.465 (6) Å	θ = 4.2–25º
b = 5.9323 (17) Å	μ = 2.86 mm^{-1}
c = 23.668 (7) Å	T = 298 (2) K
β = 92.432 (5)º	Block, yellow
V = 3151.4 (16) Å^3	0.12 × 0.07 × 0.06 mm
Z = 8	

Data collection

Bruker SMART APEX CCD diffractometer	5399 independent reflections
Radiation source: fine-focus sealed tube	1750 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.105
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −26→26
T_{min} = 0.725, T_{max} = 0.847	k = −6→6
17549 measured reflections	l = −28→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.122	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.79	$(\Delta/\sigma)_{max}$ = 0.001
5399 reflections	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
361 parameters	$\Delta\rho_{min}$ = −0.31 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	0.38156 (4)	0.81077 (15)	1.06812 (3)	0.1124 (4)
Br2	0.43680 (3)	1.27449 (14)	0.61505 (4)	0.1031 (3)
C1	0.3175 (3)	0.7293 (14)	1.0175 (3)	0.077 (2)
C2	0.3203 (3)	0.5446 (11)	0.9824 (3)	0.0654 (18)
C3	0.2709 (3)	0.4962 (12)	0.9467 (3)	0.083 (2)
H3A	0.2711	0.3699	0.9234	0.099*
C4	0.2221 (3)	0.6354 (15)	0.9459 (3)	0.102 (3)
H4A	0.1900	0.6046	0.9210	0.123*
C5	0.2195 (4)	0.8175 (14)	0.9808 (3)	0.101 (3)
H5A	0.1856	0.9074	0.9811	0.122*
C6	0.2683 (4)	0.8640 (13)	1.0155 (3)	0.098 (2)
H6A	0.2679	0.9915	1.0383	0.117*
C7	0.3727 (3)	0.3955 (12)	0.9836 (3)	0.0703 (19)
H7A	0.4027	0.4135	1.0115	0.084*
C8	0.4342 (2)	−0.0640 (12)	0.9179 (2)	0.0659 (18)
C9	0.4007 (3)	−0.3370 (11)	0.8268 (3)	0.085 (2)
H9A	0.4418	−0.3170	0.8168	0.102*
H9B	0.3984	−0.4707	0.8502	0.102*
C10	0.3617 (3)	−0.3658 (12)	0.7741 (3)	0.0601 (17)
C11	0.3642 (3)	−0.2141 (12)	0.7310 (3)	0.082 (2)
H11A	0.3881	−0.0868	0.7353	0.098*
C12	0.3316 (4)	−0.2477 (14)	0.6813 (3)	0.101 (3)
H12A	0.3339	−0.1448	0.6518	0.121*
C13	0.2960 (3)	−0.4325 (18)	0.6755 (3)	0.100 (3)
H13A	0.2736	−0.4542	0.6420	0.120*
C14	0.2928 (3)	−0.5855 (13)	0.7178 (4)	0.091 (2)
H14A	0.2681	−0.7108	0.7134	0.110*
C15	0.3257 (3)	−0.5547 (12)	0.7667 (3)	0.075 (2)
H15A	0.3241	−0.6611	0.7955	0.090*
C16	0.4832 (3)	1.1731 (14)	0.6791 (3)	0.0723 (19)
C17	0.5172 (3)	0.9776 (13)	0.6768 (3)	0.075 (2)
C18	0.5487 (3)	0.9139 (13)	0.7264 (3)	0.095 (2)
H18A	0.5725	0.7855	0.7268	0.114*

C19	0.5445 (4)	1.0426 (17)	0.7755 (3)	0.109 (3)
H19A	0.5650	0.9970	0.8085	0.131*
C20	0.5111 (4)	1.2324 (16)	0.7760 (3)	0.106 (3)
H20A	0.5088	1.3171	0.8088	0.128*
C21	0.4808 (3)	1.2978 (12)	0.7275 (4)	0.092 (2)
H21A	0.4581	1.4291	0.7274	0.110*
C22	0.5213 (3)	0.8447 (12)	0.6253 (3)	0.071 (2)
H22A	0.4955	0.8756	0.5946	0.085*
C23	0.5898 (3)	0.3934 (12)	0.5621 (2)	0.0720 (19)
C24	0.6815 (3)	0.0966 (11)	0.5928 (2)	0.080 (2)
H24A	0.6555	−0.0333	0.5882	0.096*
H24B	0.6974	0.1321	0.5563	0.096*
C25	0.7320 (3)	0.0452 (14)	0.6356 (3)	0.075 (2)
C26	0.7806 (4)	0.1761 (14)	0.6396 (3)	0.127 (3)
H26A	0.7831	0.3018	0.6163	0.153*
C27	0.8270 (4)	0.1273 (18)	0.6777 (4)	0.144 (4)
H27A	0.8600	0.2217	0.6803	0.173*
C28	0.8248 (4)	−0.0578 (18)	0.7116 (3)	0.110 (3)
H28A	0.8560	−0.0904	0.7374	0.133*
C29	0.7776 (5)	−0.1902 (14)	0.7070 (3)	0.111 (3)
H29A	0.7761	−0.3192	0.7293	0.133*
C30	0.7304 (3)	−0.1405 (13)	0.6698 (3)	0.084 (2)
H30A	0.6972	−0.2341	0.6680	0.101*
N1	0.3769 (2)	0.2421 (10)	0.9464 (2)	0.0724 (15)
N2	0.4263 (2)	0.1106 (10)	0.9516 (2)	0.0770 (16)
H2	0.4532	0.1415	0.9774	0.092*
N3	0.5589 (2)	0.6892 (10)	0.6216 (2)	0.0774 (17)
N4	0.5567 (2)	0.5759 (10)	0.5714 (2)	0.0795 (17)
H4	0.5329	0.6239	0.5446	0.095*
S1	0.49163 (8)	−0.2385 (3)	0.92583 (7)	0.0950 (7)
S2	0.37642 (7)	−0.0936 (3)	0.86578 (7)	0.0773 (6)
S3	0.58178 (8)	0.2452 (3)	0.50331 (7)	0.0931 (6)
S4	0.64041 (7)	0.3345 (3)	0.61861 (7)	0.0773 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1210 (7)	0.1233 (8)	0.0901 (6)	0.0066 (6)	−0.0297 (5)	−0.0369 (5)
Br2	0.0768 (5)	0.1047 (7)	0.1263 (7)	0.0116 (5)	−0.0130 (5)	0.0037 (5)
C1	0.080 (5)	0.100 (7)	0.052 (4)	0.017 (5)	0.001 (4)	−0.007 (4)
C2	0.084 (5)	0.058 (5)	0.053 (4)	0.017 (4)	−0.006 (4)	−0.004 (4)
C3	0.083 (5)	0.091 (6)	0.072 (5)	0.005 (5)	−0.016 (4)	−0.027 (4)
C4	0.079 (6)	0.107 (7)	0.118 (7)	0.039 (5)	−0.022 (5)	−0.008 (6)
C5	0.100 (7)	0.087 (7)	0.117 (7)	0.044 (5)	−0.002 (5)	−0.019 (5)
C6	0.112 (7)	0.096 (7)	0.083 (6)	0.020 (6)	−0.004 (5)	−0.027 (5)
C7	0.074 (5)	0.065 (5)	0.071 (5)	0.007 (4)	−0.014 (4)	0.004 (4)
C8	0.051 (4)	0.082 (5)	0.064 (4)	0.013 (4)	−0.013 (3)	−0.012 (4)
C9	0.074 (5)	0.084 (5)	0.095 (5)	0.026 (4)	−0.018 (4)	−0.022 (4)

C10	0.063 (4)	0.057 (5)	0.060 (5)	0.014 (4)	−0.004 (4)	−0.002 (4)
C11	0.092 (5)	0.080 (6)	0.073 (5)	−0.024 (4)	−0.009 (4)	0.005 (5)
C12	0.129 (7)	0.091 (7)	0.082 (6)	0.004 (6)	−0.005 (5)	0.018 (5)
C13	0.097 (7)	0.128 (9)	0.071 (6)	0.023 (6)	−0.031 (5)	−0.027 (6)
C14	0.067 (5)	0.077 (6)	0.127 (7)	−0.009 (4)	−0.023 (5)	−0.012 (6)
C15	0.084 (5)	0.057 (6)	0.084 (6)	−0.001 (4)	−0.001 (4)	0.013 (4)
C16	0.062 (5)	0.069 (6)	0.085 (6)	−0.019 (4)	0.001 (4)	−0.007 (5)
C17	0.078 (5)	0.065 (6)	0.082 (6)	−0.005 (4)	−0.002 (5)	−0.012 (5)
C18	0.103 (6)	0.090 (6)	0.091 (6)	0.022 (5)	−0.018 (5)	−0.011 (5)
C19	0.124 (7)	0.122 (8)	0.079 (6)	0.014 (6)	−0.023 (5)	−0.026 (6)
C20	0.109 (7)	0.116 (8)	0.093 (7)	0.023 (6)	−0.006 (5)	−0.030 (6)
C21	0.072 (5)	0.083 (6)	0.121 (7)	0.000 (4)	0.003 (5)	−0.010 (6)
C22	0.063 (5)	0.077 (6)	0.070 (5)	−0.008 (4)	−0.014 (4)	−0.003 (4)
C23	0.075 (5)	0.078 (6)	0.061 (4)	−0.012 (4)	−0.014 (4)	−0.009 (4)
C24	0.087 (5)	0.079 (5)	0.073 (5)	0.001 (4)	−0.008 (4)	−0.013 (4)
C25	0.080 (6)	0.071 (6)	0.074 (5)	−0.003 (5)	−0.007 (4)	−0.010 (5)
C26	0.123 (7)	0.142 (8)	0.112 (7)	−0.056 (7)	−0.055 (6)	0.060 (6)
C27	0.107 (7)	0.183 (11)	0.138 (8)	−0.075 (7)	−0.055 (6)	0.060 (7)
C28	0.100 (7)	0.132 (9)	0.097 (7)	0.031 (6)	−0.026 (6)	0.006 (6)
C29	0.149 (9)	0.088 (7)	0.092 (6)	0.008 (7)	−0.028 (6)	0.021 (5)
C30	0.090 (6)	0.056 (6)	0.106 (6)	−0.011 (4)	0.004 (5)	−0.005 (5)
N1	0.072 (4)	0.071 (4)	0.072 (4)	0.026 (3)	−0.018 (3)	−0.016 (3)
N2	0.061 (4)	0.087 (5)	0.081 (4)	0.014 (3)	−0.025 (3)	−0.023 (3)
N3	0.071 (4)	0.081 (5)	0.080 (4)	0.004 (3)	−0.004 (3)	−0.010 (4)
N4	0.088 (4)	0.082 (5)	0.067 (4)	0.009 (4)	−0.021 (3)	−0.016 (4)
S1	0.0782 (13)	0.1111 (17)	0.0922 (14)	0.0329 (12)	−0.0366 (11)	−0.0305 (12)
S2	0.0734 (12)	0.0855 (14)	0.0711 (11)	0.0169 (10)	−0.0206 (9)	−0.0137 (10)
S3	0.0904 (13)	0.1104 (17)	0.0763 (12)	0.0126 (12)	−0.0227 (10)	−0.0276 (12)
S4	0.0794 (12)	0.0836 (14)	0.0674 (11)	−0.0011 (10)	−0.0161 (9)	−0.0111 (10)

Geometric parameters (Å, °)

Br1—C1	1.895 (7)	C16—C17	1.391 (8)
Br2—C16	1.901 (7)	C17—C18	1.397 (8)
C1—C6	1.363 (8)	C17—C22	1.457 (8)
C1—C2	1.379 (8)	C18—C19	1.397 (8)
C2—C3	1.396 (7)	C18—H18A	0.930
C2—C7	1.471 (8)	C19—C20	1.353 (9)
C3—C4	1.372 (8)	C19—H19A	0.930
C3—H3A	0.930	C20—C21	1.366 (9)
C4—C5	1.362 (9)	C20—H20A	0.930
C4—H4A	0.930	C21—H21A	0.930
C5—C6	1.370 (8)	C22—N3	1.257 (7)
C5—H5A	0.930	C22—H22A	0.930
C6—H6A	0.930	C23—N4	1.338 (7)
C7—N1	1.272 (7)	C23—S3	1.650 (6)
C7—H7A	0.930	C23—S4	1.752 (6)
C8—N2	1.324 (6)	C24—C25	1.520 (8)
C8—S1	1.659 (6)	C24—S4	1.808 (6)

C8—S2	1.761 (5)	C24—H24A	0.970
C9—C10	1.502 (7)	C24—H24B	0.970
C9—S2	1.810 (6)	C25—C26	1.339 (8)
C9—H9A	0.970	C25—C30	1.369 (8)
C9—H9B	0.970	C26—C27	1.381 (9)
C10—C11	1.363 (8)	C26—H26A	0.930
C10—C15	1.389 (8)	C27—C28	1.361 (10)
C11—C12	1.373 (9)	C27—H27A	0.930
C11—H11A	0.930	C28—C29	1.320 (10)
C12—C13	1.360 (9)	C28—H28A	0.930
C12—H12A	0.930	C29—C30	1.381 (9)
C13—C14	1.356 (9)	C29—H29A	0.930
C13—H13A	0.930	C30—H30A	0.930
C14—C15	1.359 (8)	N1—N2	1.359 (6)
C14—H14A	0.930	N2—H2	0.860
C15—H15A	0.930	N3—N4	1.364 (6)
C16—C21	1.366 (8)	N4—H4	0.860
C6—C1—C2	120.1 (6)	C18—C17—C22	120.6 (7)
C6—C1—Br1	117.8 (6)	C17—C18—C19	120.1 (7)
C2—C1—Br1	122.1 (6)	C17—C18—H18A	119.9
C1—C2—C3	118.2 (6)	C19—C18—H18A	119.9
C1—C2—C7	121.5 (7)	C20—C19—C18	121.2 (8)
C3—C2—C7	120.2 (6)	C20—C19—H19A	119.4
C4—C3—C2	119.9 (7)	C18—C19—H19A	119.4
C4—C3—H3A	120.0	C19—C20—C21	119.2 (8)
C2—C3—H3A	120.0	C19—C20—H20A	120.4
C5—C4—C3	121.6 (7)	C21—C20—H20A	120.4
C5—C4—H4A	119.2	C20—C21—C16	120.9 (7)
C3—C4—H4A	119.2	C20—C21—H21A	119.5
C4—C5—C6	117.9 (7)	C16—C21—H21A	119.5
C4—C5—H5A	121.0	N3—C22—C17	121.5 (7)
C6—C5—H5A	121.0	N3—C22—H22A	119.2
C1—C6—C5	122.1 (7)	C17—C22—H22A	119.2
C1—C6—H6A	119.0	N4—C23—S3	121.8 (5)
C5—C6—H6A	119.0	N4—C23—S4	112.6 (5)
N1—C7—C2	119.9 (6)	S3—C23—S4	125.6 (5)
N1—C7—H7A	120.0	C25—C24—S4	108.0 (4)
C2—C7—H7A	120.0	C25—C24—H24A	110.1
N2—C8—S1	122.9 (5)	S4—C24—H24A	110.1
N2—C8—S2	112.8 (4)	C25—C24—H24B	110.1
S1—C8—S2	124.3 (4)	S4—C24—H24B	110.1
C10—C9—S2	109.7 (4)	H24A—C24—H24B	108.4
C10—C9—H9A	109.7	C26—C25—C30	117.9 (7)
S2—C9—H9A	109.7	C26—C25—C24	120.9 (8)
C10—C9—H9B	109.7	C30—C25—C24	121.2 (7)
S2—C9—H9B	109.7	C25—C26—C27	121.0 (8)
H9A—C9—H9B	108.2	C25—C26—H26A	119.5
C11—C10—C15	118.7 (6)	C27—C26—H26A	119.5
C11—C10—C9	120.3 (7)	C28—C27—C26	120.6 (8)

C15—C10—C9	120.8 (7)	C28—C27—H27A	119.7
C10—C11—C12	120.5 (7)	C26—C27—H27A	119.7
C10—C11—H11A	119.7	C29—C28—C27	118.8 (8)
C12—C11—H11A	119.7	C29—C28—H28A	120.6
C13—C12—C11	119.5 (7)	C27—C28—H28A	120.6
C13—C12—H12A	120.2	C28—C29—C30	121.1 (8)
C11—C12—H12A	120.2	C28—C29—H29A	119.4
C14—C13—C12	121.0 (8)	C30—C29—H29A	119.4
C14—C13—H13A	119.5	C25—C30—C29	120.7 (7)
C12—C13—H13A	119.5	C25—C30—H30A	119.7
C13—C14—C15	119.6 (7)	C29—C30—H30A	119.7
C13—C14—H14A	120.2	C7—N1—N2	115.6 (5)
C15—C14—H14A	120.2	C8—N2—N1	121.6 (5)
C14—C15—C10	120.6 (6)	C8—N2—H2	119.2
C14—C15—H15A	119.7	N1—N2—H2	119.2
C10—C15—H15A	119.7	C22—N3—N4	115.0 (6)
C21—C16—C17	121.7 (7)	C23—N4—N3	122.8 (6)
C21—C16—Br2	117.2 (7)	C23—N4—H4	118.6
C17—C16—Br2	121.1 (6)	N3—N4—H4	118.6
C16—C17—C18	116.9 (7)	C8—S2—C9	102.0 (3)
C16—C17—C22	122.5 (7)	C23—S4—C24	102.8 (3)
C6—C1—C2—C3	−2.4 (10)	C18—C19—C20—C21	0.4 (13)
Br1—C1—C2—C3	179.6 (5)	C19—C20—C21—C16	0.8 (12)
C6—C1—C2—C7	−179.9 (6)	C17—C16—C21—C20	−1.1 (11)
Br1—C1—C2—C7	2.1 (9)	Br2—C16—C21—C20	177.7 (6)
C1—C2—C3—C4	2.1 (10)	C16—C17—C22—N3	169.0 (6)
C7—C2—C3—C4	179.7 (6)	C18—C17—C22—N3	−10.0 (10)
C2—C3—C4—C5	−2.3 (12)	S4—C24—C25—C26	−75.2 (8)
C3—C4—C5—C6	2.6 (13)	S4—C24—C25—C30	107.2 (6)
C2—C1—C6—C5	2.8 (11)	C30—C25—C26—C27	−1.1 (13)
Br1—C1—C6—C5	−179.1 (6)	C24—C25—C26—C27	−178.8 (7)
C4—C5—C6—C1	−2.8 (12)	C25—C26—C27—C28	1.1 (15)
C1—C2—C7—N1	−172.1 (6)	C26—C27—C28—C29	0.3 (15)
C3—C2—C7—N1	10.5 (10)	C27—C28—C29—C30	−1.6 (14)
S2—C9—C10—C11	68.9 (7)	C26—C25—C30—C29	−0.2 (11)
S2—C9—C10—C15	−115.6 (6)	C24—C25—C30—C29	177.5 (6)
C15—C10—C11—C12	0.0 (10)	C28—C29—C30—C25	1.6 (13)
C9—C10—C11—C12	175.6 (6)	C2—C7—N1—N2	−178.9 (5)
C10—C11—C12—C13	0.9 (11)	S1—C8—N2—N1	−175.6 (5)
C11—C12—C13—C14	−0.8 (12)	S2—C8—N2—N1	2.7 (8)
C12—C13—C14—C15	−0.3 (12)	C7—N1—N2—C8	175.6 (6)
C13—C14—C15—C10	1.3 (11)	C17—C22—N3—N4	178.6 (5)
C11—C10—C15—C14	−1.2 (10)	S3—C23—N4—N3	174.1 (4)
C9—C10—C15—C14	−176.7 (6)	S4—C23—N4—N3	−5.5 (8)
C21—C16—C17—C18	0.2 (10)	C22—N3—N4—C23	−173.9 (6)
Br2—C16—C17—C18	−178.5 (5)	N2—C8—S2—C9	178.8 (5)
C21—C16—C17—C22	−178.8 (6)	S1—C8—S2—C9	−2.9 (5)
Br2—C16—C17—C22	2.5 (9)	C10—C9—S2—C8	−170.6 (5)
C16—C17—C18—C19	0.9 (10)	N4—C23—S4—C24	−176.3 (5)

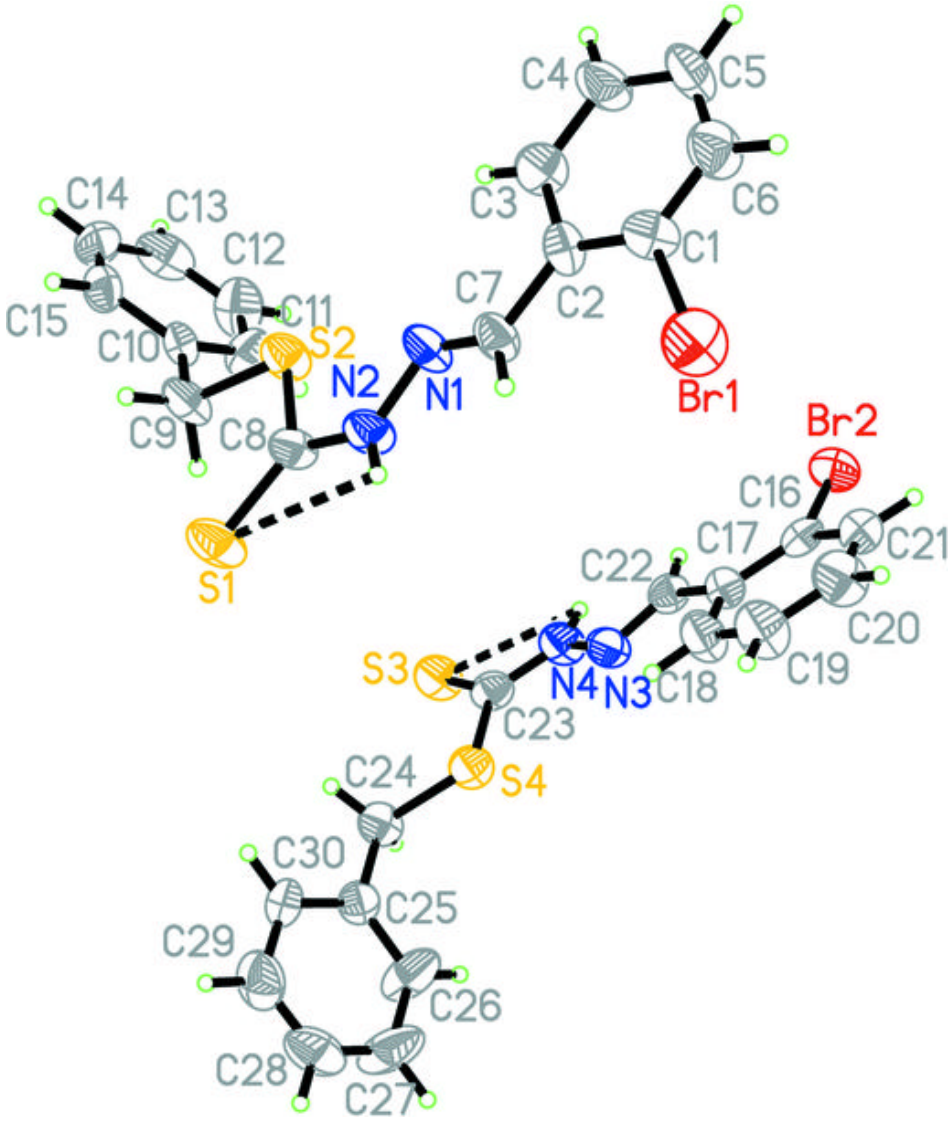
C22—C17—C18—C19	180.0 (7)	S3—C23—S4—C24	4.1 (5)
C17—C18—C19—C20	−1.2 (12)	C25—C24—S4—C23	173.6 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···S3^{i}	0.86	2.88	3.669 (5)	154
N2—H2···S1^{ii}	0.86	2.62	3.455 (5)	164

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

Fig. 1


C4
C5
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C20
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C18
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C26
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C27