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2,3-Bis(benzylthio)-6-methylquinoxaline

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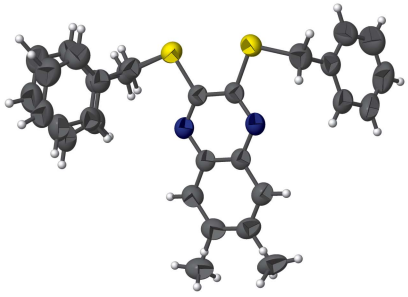
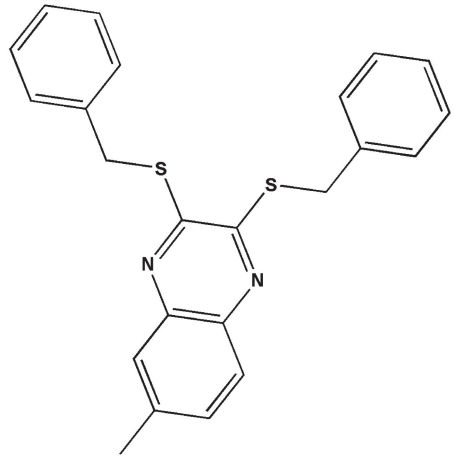
In the title compound, $C_{23}H_{20}N_2S_2$, the mean planes of the phenyl rings are twisted with respect to the mean plane of the quinoxaline ring system by 73.8 (8) and 72.2 (8)°. A weak intramolecular C—H···N interactions is observed. The methyl group attached to the quinoxaline ring system is disordered over two sets of sites on the benzene ring having occupancies 0.531 (7) and 0.469 (7), respectively. One of the phenyl rings is disordered over two sets of sites having occupancies 0.649 (7) and 0.351 (10), respectively. In the crystal, π–π stacking interactions occur.

3D view



Chemical scheme



Structure description

Quinoxalines exhibit various biological activities including antiviral (Fonseca *et al.*, 2004), antibacterial (El-Sabbagh *et al.*, 2009), anti-inflammatory (Wagle *et al.*, 2008), anti-protozoal (Hui *et al.*, 2006), anticancer (Carta *et al.*, 2006) and antituberculosis (Ancizu *et al.*, 2010) activities. Additionally, they are used in the agricultural field as fungicides, herbicides and insecticides (Kurasawa *et al.*, 1988). Quinoxaline moieties are also present in the structures of various antibiotics such as echinomycin, levomycin, and actinoleutin, which are known to inhibit the growth of gram-positive bacteria and are active against various transplantable tumors (Kim *et al.*, 2004). In this work, we report the synthesis and structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The mean planes of the pendant phenyl rings of the benzylthio groups are twisted with respect to the mean plane of the quinoxaline ring system by 73.8 (8)° (C17–C22) and 72.2 (8)° (C10–C15). The benzylthio moieties are attached to the ring in adjacent locations [S—C—C—S = −2.2 (2)°], avoiding steric repulsion. An intramolecular C—H···N hydrogen bond

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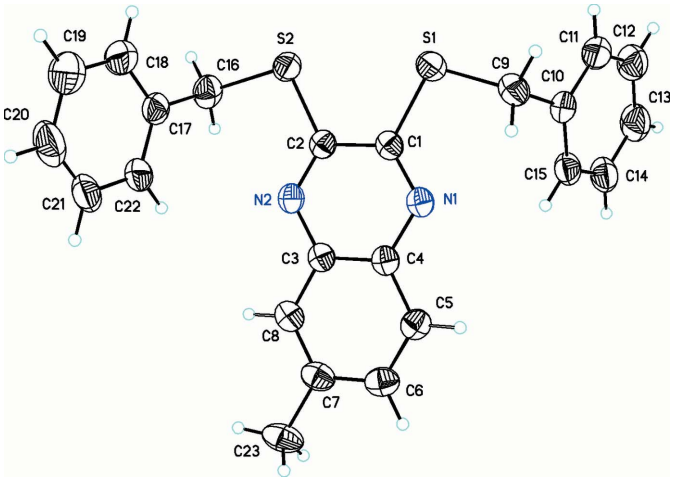

Figure 1
The molecular structure of the title compound showing 30% probability displacement ellipsoids. Atom C23, [0.531 (7) occupancy] methyl group is shown bonded to C7, whereas minor occupancy atom C23*A*, [0.469 (7) occupancy] has been omitted for clarity. Only atoms C9—C15 [occupancy 0.649 (7)] of the disordered phenyl ring of the the benzylthio ring system are shown for clarity.

occurs. (Table 1). The crystal packing (Fig. 2) features weak π–π stacking interactions involving the quinoxaline moiety [intercentroid distance, $Cg1\cdots Cg2^{ii}$ = 3.7254 (13), $Cg1\cdots Cg3^{ii}$ = 3.7254 (13) Å; symmetry code: (ii) = $1-x, 1-y, 1-z$; *Cg*1, *Cg*2 and *Cg*3 are the centroids of the N1/C1/C2/N2/C3/C4, C3–C8 and C3/C4/C5/C6*A*/C7*A*/C8 rings, respectively].

Synthesis and crystallization

To a solution of 6-methyl-1,4-dihydroquinoxaline-2,3-dithione 0.3 g (1.44 mmol) in DMF (20 ml), were added 0.47 g (3.61 mmol) of potassium carbonate and 0.1 mmol of tetra-*n*-butyl ammonium bromide (TBAB). After stirring for 10 min, 0.4 ml (3.46 mmol) of benzyl chloride was added, then the mixture was allowed to stir at room temperature for 12 h. After filtration, DMF was evaporated under reduced pressure and the residue obtained was dissolved in dichloromethane. The organic phase was then dried over Na_2SO_4 and concentrated. The mixture obtained was chromatographed on a silica gel column [eluent: hexane/ethyl acetate (3/1)]. The compound formed pale-yellow columnar crystals in 30% yield and was recrystallized from a solvent mixture (ethyl acetate–hexane: 1/3).

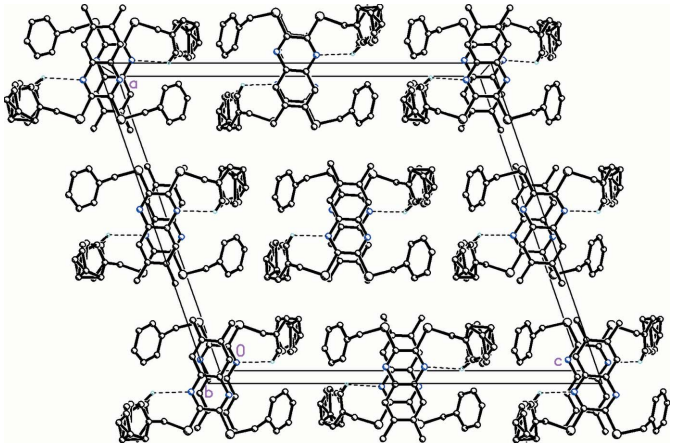

Figure 2
Packing of the title compound viewed along the *b* axis. The weak C15—H15···N1 intramolecular interactions (Table 1) are drawn as dashed lines. Hydrogen atoms not involved in the packing are removed for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···N1	0.93	2.73	3.348 (5)	125

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{20}N_2S_2$
M_r	388.53
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	22.5053 (6), 7.3510 (2), 26.1729 (7)
β (°)	109.146 (3)
V (Å^3)	4090.4 (2)
Z	8
Radiation type	Cu *K*α
μ (mm^{-1})	2.42
Crystal size (mm)	0.4 × 0.14 × 0.06
Data collection	
Diffractometer	Rigaku, Oxford diffraction
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.664, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7343, 3878, 3252
R_{int}	0.016
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.055, 0.168, 1.08
No. of reflections	3878
No. of parameters	296
No. of restraints	216
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, −0.27

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*b*), *SHELXL* (Sheldrick, 2015*a*), *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The methyl group is disordered each over atomic sites on C6 and C7 of the quinoxaline ring [occupancies C23: 0.531 (7) and C23*A*: 0.469 (7)]. Idealized disordered Me groups were refined as rotating groups. The phenyl ring on one of the benzylthio moieties (C9–C15) is disordered over two sets of atomic sites having occupancies 0.649 (7) and 0.351 (10).

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171258 [https://doi.org/10.1107/S2414314617012585]

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(I)

Crystal data

$C_{23}H_{20}N_2S_2$
M_r = 388.53
Monoclinic, *C*2/*c*
a = 22.5053 (6) Å
b = 7.3510 (2) Å
c = 26.1729 (7) Å
β = 109.146 (3)°
V = 4090.4 (2) Å^3
Z = 8
F(000) = 1632
D_x = 1.262 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 3411 reflections
θ = 4.2–71.4°
μ = 2.42 mm^{-1}
T = 293 K
Plate, colourless
0.4 × 0.14 × 0.06 mm

Data collection

Rigaku, Oxford diffraction diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min} = 0.664, T_{max} = 1.000
7343 measured reflections
3878 independent reflections
3252 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 71.3°, θ_{min} = 3.6°
h = −27→25
k = −8→5
l = −32→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.168
S = 1.08
3878 reflections
296 parameters
216 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0962P)^2 + 2.177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All H atoms were placed in calculated positions and refined using the riding model with C—H bond lengths of 0.93 Å (CH), 0.97 Å (CH_2) or 0.96 Å (CH_3). Isotropic displacement parameters were set to 1.2 (CH) or 1.5 (CH_3) times U_{eq} of the parent atom.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.33518 (3)	0.82695 (9)	0.39063 (3)	0.0642 (2)	
S2	0.33006 (3)	0.70876 (9)	0.50202 (3)	0.0626 (2)	
N1	0.46013 (10)	0.8150 (2)	0.43418 (8)	0.0520 (4)	
N2	0.45531 (10)	0.6941 (3)	0.53453 (8)	0.0530 (5)	
C1	0.40706 (11)	0.7898 (3)	0.44286 (9)	0.0501 (5)	
C2	0.40456 (11)	0.7310 (3)	0.49446 (9)	0.0501 (5)	
C3	0.51165 (11)	0.7182 (3)	0.52615 (9)	0.0500 (5)	
C4	0.51428 (11)	0.7804 (3)	0.47631 (9)	0.0507 (5)	
C5	0.57320 (12)	0.8071 (3)	0.46956 (11)	0.0591 (6)	
H5A	0.5752	0.8498	0.4367	0.071*	0.531 (7)
H5B	0.5752	0.8498	0.4367	0.071*	0.469 (7)
C6	0.62759 (13)	0.7707 (3)	0.51099 (12)	0.0645 (6)	0.531 (7)
H6	0.6663	0.7864	0.5060	0.077*	0.531 (7)
C6A	0.62759 (13)	0.7707 (3)	0.51099 (12)	0.0645 (6)	0.469 (7)
C7	0.62480 (13)	0.7098 (4)	0.56094 (12)	0.0650 (7)	0.531 (7)
C7A	0.62480 (13)	0.7098 (4)	0.56094 (12)	0.0650 (7)	0.469 (7)
H7A	0.6618	0.6874	0.5892	0.078*	0.469 (7)
C8	0.56820 (13)	0.6831 (3)	0.56825 (10)	0.0600 (6)	
H8A	0.5669	0.6412	0.6014	0.072*	0.531 (7)
H8B	0.5669	0.6412	0.6014	0.072*	0.469 (7)
C9	0.3589 (7)	0.875 (3)	0.3360 (6)	0.066 (3)	0.649 (10)
H9A	0.3276	0.9542	0.3121	0.080*	0.649 (10)
H9B	0.3977	0.9438	0.3491	0.080*	0.649 (10)
C9A	0.3660 (14)	0.879 (5)	0.3300 (11)	0.057 (2)	0.351 (10)
H9AA	0.3369	0.9571	0.3035	0.068*	0.351 (10)
H9AB	0.4069	0.9371	0.3426	0.068*	0.351 (10)
C10	0.3703 (2)	0.7144 (5)	0.3010 (2)	0.0628 (12)	0.649 (10)
C11	0.31740 (19)	0.6550 (7)	0.2597 (2)	0.0774 (13)	0.649 (10)
H11	0.2796	0.7175	0.2522	0.093*	0.649 (10)
C12	0.3211 (2)	0.5021 (8)	0.2296 (2)	0.0916 (16)	0.649 (10)
H12	0.2857	0.4624	0.2020	0.110*	0.649 (10)
C13	0.3776 (3)	0.4087 (5)	0.2409 (2)	0.0944 (16)	0.649 (10)
H13	0.3800	0.3064	0.2207	0.113*	0.649 (10)
C14	0.4305 (3)	0.4681 (7)	0.2822 (2)	0.0813 (15)	0.649 (10)
H14	0.4683	0.4056	0.2897	0.098*	0.649 (10)
C15	0.4268 (2)	0.6209 (8)	0.3123 (2)	0.0682 (13)	0.649 (10)
H15	0.4622	0.6607	0.3399	0.082*	0.649 (10)
C10A	0.3697 (5)	0.7061 (11)	0.3080 (4)	0.0661 (19)	0.351 (10)
C11A	0.3235 (4)	0.5893 (15)	0.2767 (4)	0.089 (2)	0.351 (10)
H11A	0.2814	0.6126	0.2717	0.107*	0.351 (10)
C12A	0.3403 (5)	0.4376 (14)	0.2528 (5)	0.099 (2)	0.351 (10)

H12A	0.3094	0.3595	0.2318	0.119*	0.351 (10)
C13A	0.4033 (5)	0.4028 (10)	0.2602 (4)	0.089 (2)	0.351 (10)
H13A	0.4145	0.3014	0.2442	0.107*	0.351 (10)
C14A	0.4495 (4)	0.5197 (15)	0.2916 (4)	0.081 (2)	0.351 (10)
H14A	0.4916	0.4964	0.2965	0.097*	0.351 (10)
C15A	0.4327 (4)	0.6713 (14)	0.3155 (5)	0.072 (2)	0.351 (10)
H15A	0.4636	0.7494	0.3364	0.087*	0.351 (10)
C16	0.35130 (15)	0.6469 (4)	0.57315 (11)	0.0703 (7)	
H16A	0.3154	0.5896	0.5792	0.084*	
H16B	0.3850	0.5581	0.5815	0.084*	
C17	0.37198 (13)	0.8046 (4)	0.61114 (10)	0.0647 (7)	
C18	0.32859 (17)	0.9235 (6)	0.61799 (15)	0.0986 (12)	
H18	0.2861	0.9071	0.5988	0.118*	
C19	0.3477 (2)	1.0682 (8)	0.65341 (19)	0.1274 (17)	
H19	0.3180	1.1490	0.6580	0.153*	
C20	0.4105 (2)	1.0931 (6)	0.68195 (15)	0.1080 (13)	
H20	0.4233	1.1906	0.7056	0.130*	
C21	0.45277 (18)	0.9760 (6)	0.67534 (11)	0.0920 (11)	
H21	0.4952	0.9916	0.6949	0.110*	
C22	0.43439 (14)	0.8333 (5)	0.64014 (10)	0.0750 (8)	
H22	0.4646	0.7543	0.6357	0.090*	
C23	0.6846 (3)	0.6864 (8)	0.6061 (3)	0.082 (2)	0.531 (7)
H23A	0.6759	0.6709	0.6393	0.123*	0.531 (7)
H23B	0.7105	0.7921	0.6086	0.123*	0.531 (7)
H23C	0.7063	0.5811	0.5995	0.123*	0.531 (7)
C23A	0.6940 (3)	0.7870 (8)	0.5048 (3)	0.075 (2)	0.469 (7)
H23D	0.6896	0.8223	0.4684	0.113*	0.469 (7)
H23E	0.7151	0.6717	0.5126	0.113*	0.469 (7)
H23F	0.7182	0.8770	0.5295	0.113*	0.469 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0589 (4)	0.0719 (4)	0.0572 (4)	0.0040 (3)	0.0126 (3)	−0.0033 (3)
S2	0.0587 (4)	0.0703 (4)	0.0619 (4)	−0.0067 (3)	0.0241 (3)	−0.0106 (3)
N1	0.0593 (11)	0.0463 (10)	0.0498 (10)	−0.0027 (8)	0.0172 (8)	−0.0023 (7)
N2	0.0626 (11)	0.0471 (10)	0.0507 (10)	−0.0011 (8)	0.0206 (9)	−0.0025 (7)
C1	0.0569 (12)	0.0405 (11)	0.0504 (11)	−0.0016 (9)	0.0142 (9)	−0.0087 (8)
C2	0.0567 (12)	0.0419 (11)	0.0530 (11)	−0.0017 (9)	0.0199 (10)	−0.0084 (9)
C3	0.0579 (12)	0.0395 (10)	0.0519 (11)	0.0010 (9)	0.0171 (10)	−0.0047 (8)
C4	0.0593 (13)	0.0396 (11)	0.0528 (11)	−0.0034 (9)	0.0177 (10)	−0.0059 (8)
C5	0.0632 (14)	0.0512 (13)	0.0658 (14)	−0.0068 (10)	0.0251 (11)	−0.0022 (10)
C6	0.0587 (14)	0.0511 (13)	0.0826 (17)	−0.0063 (11)	0.0218 (13)	−0.0076 (12)
C6A	0.0587 (14)	0.0511 (13)	0.0826 (17)	−0.0063 (11)	0.0218 (13)	−0.0076 (12)
C7	0.0579 (14)	0.0538 (14)	0.0730 (16)	0.0044 (11)	0.0075 (12)	−0.0039 (11)
C7A	0.0579 (14)	0.0538 (14)	0.0730 (16)	0.0044 (11)	0.0075 (12)	−0.0039 (11)
C8	0.0665 (15)	0.0514 (13)	0.0570 (13)	0.0018 (11)	0.0135 (11)	−0.0009 (10)
C9	0.069 (4)	0.067 (3)	0.058 (5)	0.006 (3)	0.013 (3)	0.004 (4)

C9A	0.066 (5)	0.070 (4)	0.041 (4)	−0.002 (4)	0.027 (3)	0.014 (3)
C10	0.069 (2)	0.074 (2)	0.051 (2)	0.000 (2)	0.0270 (18)	0.0056 (18)
C11	0.073 (2)	0.099 (3)	0.065 (3)	−0.008 (2)	0.028 (2)	−0.006 (2)
C12	0.094 (3)	0.112 (4)	0.069 (3)	−0.018 (3)	0.026 (2)	−0.021 (3)
C13	0.112 (4)	0.105 (3)	0.070 (3)	0.003 (3)	0.035 (3)	−0.018 (3)
C14	0.096 (3)	0.091 (3)	0.057 (3)	0.015 (3)	0.026 (3)	−0.002 (3)
C15	0.078 (3)	0.076 (3)	0.051 (2)	0.014 (2)	0.0222 (19)	0.010 (2)
C10A	0.070 (3)	0.078 (3)	0.052 (3)	0.000 (3)	0.022 (3)	0.008 (3)
C11A	0.083 (4)	0.097 (4)	0.083 (4)	−0.007 (4)	0.021 (4)	−0.009 (4)
C12A	0.101 (4)	0.104 (4)	0.085 (4)	−0.002 (4)	0.021 (4)	−0.020 (4)
C13A	0.100 (5)	0.097 (4)	0.069 (5)	0.006 (4)	0.025 (4)	−0.019 (4)
C14A	0.098 (4)	0.087 (4)	0.061 (4)	0.003 (4)	0.031 (4)	−0.003 (4)
C15A	0.087 (4)	0.076 (4)	0.056 (3)	0.008 (3)	0.028 (3)	0.014 (3)
C16	0.0798 (17)	0.0707 (16)	0.0676 (15)	−0.0162 (14)	0.0339 (13)	0.0022 (13)
C17	0.0684 (15)	0.0785 (17)	0.0527 (13)	−0.0109 (13)	0.0275 (12)	0.0012 (11)
C18	0.0750 (19)	0.133 (3)	0.089 (2)	−0.010 (2)	0.0285 (17)	−0.039 (2)
C19	0.114 (3)	0.150 (4)	0.116 (3)	0.011 (3)	0.034 (3)	−0.063 (3)
C20	0.128 (3)	0.119 (3)	0.0693 (19)	−0.026 (3)	0.022 (2)	−0.035 (2)
C21	0.091 (2)	0.133 (3)	0.0492 (14)	−0.027 (2)	0.0189 (14)	−0.0104 (17)
C22	0.0727 (17)	0.104 (2)	0.0478 (13)	−0.0045 (15)	0.0195 (12)	0.0048 (13)
C23	0.055 (3)	0.064 (3)	0.105 (5)	0.016 (2)	−0.003 (3)	−0.006 (3)
C23A	0.062 (3)	0.055 (3)	0.105 (5)	−0.006 (2)	0.023 (3)	0.001 (3)

Geometric parameters (Å, º)

S1—C1	1.763 (2)	C12—C13	1.3900
S1—C9	1.719 (14)	C13—H13	0.9300
S1—C9A	1.97 (2)	C13—C14	1.3900
S2—C2	1.759 (2)	C14—H14	0.9300
S2—C16	1.821 (3)	C14—C15	1.3900
N1—C1	1.300 (3)	C15—H15	0.9300
N1—C4	1.373 (3)	C10A—C11A	1.3900
N2—C2	1.301 (3)	C10A—C15A	1.3900
N2—C3	1.367 (3)	C11A—H11A	0.9300
C1—C2	1.437 (3)	C11A—C12A	1.3900
C3—C4	1.402 (3)	C12A—H12A	0.9300
C3—C8	1.407 (3)	C12A—C13A	1.3900
C4—C5	1.408 (3)	C13A—H13A	0.9300
C5—H5A	0.9300	C13A—C14A	1.3900
C5—H5B	0.9300	C14A—H14A	0.9300
C5—C6	1.369 (4)	C14A—C15A	1.3900
C5—C6A	1.369 (4)	C15A—H15A	0.9300
C6—H6	0.9300	C16—H16A	0.9700
C6—C7	1.403 (4)	C16—H16B	0.9700
C6A—C7A	1.403 (4)	C16—C17	1.499 (4)
C6A—C23A	1.560 (7)	C17—C18	1.365 (5)
C7—C8	1.363 (4)	C17—C22	1.376 (4)
C7—C23	1.482 (6)	C18—H18	0.9300

C7A—H7A	0.9300	C18—C19	1.384 (6)
C7A—C8	1.363 (4)	C19—H19	0.9300
C8—H8A	0.9300	C19—C20	1.377 (6)
C8—H8B	0.9300	C20—H20	0.9300
C9—H9A	0.9700	C20—C21	1.336 (6)
C9—H9B	0.9700	C21—H21	0.9300
C9—C10	1.563 (19)	C21—C22	1.367 (5)
C9A—H9AA	0.9700	C22—H22	0.9300
C9A—H9AB	0.9700	C23—H23A	0.9600
C9A—C10A	1.41 (4)	C23—H23B	0.9600
C10—C11	1.3900	C23—H23C	0.9600
C10—C15	1.3900	C23A—H23D	0.9600
C11—H11	0.9300	C23A—H23E	0.9600
C11—C12	1.3900	C23A—H23F	0.9600
C12—H12	0.9300		

C1—S1—C9A	100.3 (9)	C12—C13—C14	120.0
C9—S1—C1	102.7 (5)	C14—C13—H13	120.0
C2—S2—C16	101.41 (13)	C13—C14—H14	120.0
C1—N1—C4	117.2 (2)	C15—C14—C13	120.0
C2—N2—C3	117.3 (2)	C15—C14—H14	120.0
N1—C1—S1	120.29 (18)	C10—C15—H15	120.0
N1—C1—C2	121.9 (2)	C14—C15—C10	120.0
C2—C1—S1	117.81 (18)	C14—C15—H15	120.0
N2—C2—S2	120.46 (18)	C11A—C10A—C9A	131.7 (14)
N2—C2—C1	121.7 (2)	C11A—C10A—C15A	120.0
C1—C2—S2	117.79 (18)	C15A—C10A—C9A	107.7 (14)
N2—C3—C4	121.1 (2)	C10A—C11A—H11A	120.0
N2—C3—C8	119.9 (2)	C10A—C11A—C12A	120.0
C4—C3—C8	119.0 (2)	C12A—C11A—H11A	120.0
N1—C4—C3	120.7 (2)	C11A—C12A—H12A	120.0
N1—C4—C5	119.9 (2)	C13A—C12A—C11A	120.0
C3—C4—C5	119.4 (2)	C13A—C12A—H12A	120.0
C4—C5—H5A	119.7	C12A—C13A—H13A	120.0
C4—C5—H5B	119.7	C12A—C13A—C14A	120.0
C6—C5—C4	120.5 (2)	C14A—C13A—H13A	120.0
C6—C5—H5A	119.7	C13A—C14A—H14A	120.0
C6A—C5—C4	120.5 (2)	C15A—C14A—C13A	120.0
C6A—C5—H5B	119.7	C15A—C14A—H14A	120.0
C5—C6—H6	120.0	C10A—C15A—H15A	120.0
C5—C6—C7	119.9 (3)	C14A—C15A—C10A	120.0
C7—C6—H6	120.0	C14A—C15A—H15A	120.0
C5—C6A—C7A	119.9 (3)	S2—C16—H16A	108.8
C5—C6A—C23A	122.7 (4)	S2—C16—H16B	108.8
C7A—C6A—C23A	117.3 (4)	H16A—C16—H16B	107.7
C6—C7—C23	118.3 (4)	C17—C16—S2	113.9 (2)
C8—C7—C6	120.4 (2)	C17—C16—H16A	108.8
C8—C7—C23	121.2 (4)	C17—C16—H16B	108.8

C6A—C7A—H7A	119.8	C18—C17—C16	120.2 (3)
C8—C7A—C6A	120.4 (2)	C18—C17—C22	118.3 (3)
C8—C7A—H7A	119.8	C22—C17—C16	121.6 (3)
C3—C8—H8A	119.7	C17—C18—H18	119.9
C3—C8—H8B	119.7	C17—C18—C19	120.1 (4)
C7—C8—C3	120.7 (2)	C19—C18—H18	119.9
C7—C8—H8A	119.7	C18—C19—H19	119.9
C7A—C8—C3	120.7 (2)	C20—C19—C18	120.2 (4)
C7A—C8—H8B	119.7	C20—C19—H19	119.9
S1—C9—H9A	107.5	C19—C20—H20	120.3
S1—C9—H9B	107.5	C21—C20—C19	119.5 (4)
H9A—C9—H9B	107.0	C21—C20—H20	120.3
C10—C9—S1	119.2 (12)	C20—C21—H21	119.7
C10—C9—H9A	107.5	C20—C21—C22	120.7 (3)
C10—C9—H9B	107.5	C22—C21—H21	119.7
S1—C9A—H9AA	111.0	C17—C22—H22	119.4
S1—C9A—H9AB	111.0	C21—C22—C17	121.2 (3)
H9AA—C9A—H9AB	109.0	C21—C22—H22	119.4
C10A—C9A—S1	103.8 (18)	C7—C23—H23A	109.5
C10A—C9A—H9AA	111.0	C7—C23—H23B	109.5
C10A—C9A—H9AB	111.0	C7—C23—H23C	109.5
C11—C10—C9	115.4 (7)	H23A—C23—H23B	109.5
C11—C10—C15	120.0	H23A—C23—H23C	109.5
C15—C10—C9	124.3 (7)	H23B—C23—H23C	109.5
C10—C11—H11	120.0	C6A—C23A—H23D	109.5
C10—C11—C12	120.0	C6A—C23A—H23E	109.5
C12—C11—H11	120.0	C6A—C23A—H23F	109.5
C11—C12—H12	120.0	H23D—C23A—H23E	109.5
C13—C12—C11	120.0	H23D—C23A—H23F	109.5
C13—C12—H12	120.0	H23E—C23A—H23F	109.5
C12—C13—H13	120.0		

S1—C1—C2—S2	−2.2 (2)	C6—C7—C8—C3	−0.8 (4)
S1—C1—C2—N2	177.44 (17)	C6A—C7A—C8—C3	−0.8 (4)
S1—C9—C10—C11	86.6 (11)	C8—C3—C4—N1	179.6 (2)
S1—C9—C10—C15	−86.9 (11)	C8—C3—C4—C5	−0.3 (3)
S1—C9A—C10A—C11A	74 (2)	C9—S1—C1—N1	4.8 (7)
S1—C9A—C10A—C15A	−115.1 (12)	C9—S1—C1—C2	−175.0 (7)
S2—C16—C17—C18	76.2 (3)	C9—C10—C11—C12	−173.8 (8)
S2—C16—C17—C22	−104.2 (3)	C9—C10—C15—C14	173.2 (8)
N1—C1—C2—S2	177.94 (16)	C9A—S1—C1—N1	5.1 (12)
N1—C1—C2—N2	−2.4 (3)	C9A—S1—C1—C2	−174.7 (12)
N1—C4—C5—C6	−179.1 (2)	C9A—C10A—C11A—C12A	169.6 (18)
N1—C4—C5—C6A	−179.1 (2)	C9A—C10A—C15A—C14A	−171.9 (14)
N2—C3—C4—N1	−1.4 (3)	C10—C11—C12—C13	0.0
N2—C3—C4—C5	178.71 (19)	C11—C10—C15—C14	0.0
N2—C3—C8—C7	−178.7 (2)	C11—C12—C13—C14	0.0
N2—C3—C8—C7A	−178.7 (2)	C12—C13—C14—C15	0.0

C1—S1—C9—C10	86.3 (10)	C13—C14—C15—C10	0.0
C1—N1—C4—C3	0.8 (3)	C15—C10—C11—C12	0.0
C1—N1—C4—C5	−179.3 (2)	C10A—C11A—C12A—C13A	0.0
C2—S2—C16—C17	78.6 (2)	C11A—C10A—C15A—C14A	0.0
C2—N2—C3—C4	0.1 (3)	C11A—C12A—C13A—C14A	0.0
C2—N2—C3—C8	179.1 (2)	C12A—C13A—C14A—C15A	0.0
C3—N2—C2—S2	−178.60 (15)	C13A—C14A—C15A—C10A	0.0
C3—N2—C2—C1	1.7 (3)	C15A—C10A—C11A—C12A	0.0
C3—C4—C5—C6	0.8 (4)	C16—S2—C2—N2	3.6 (2)
C3—C4—C5—C6A	0.8 (4)	C16—S2—C2—C1	−176.71 (18)
C4—N1—C1—S1	−178.86 (15)	C16—C17—C18—C19	179.5 (4)
C4—N1—C1—C2	1.0 (3)	C16—C17—C22—C21	−179.0 (3)
C4—C3—C8—C7	0.3 (4)	C17—C18—C19—C20	0.0 (8)
C4—C3—C8—C7A	0.3 (4)	C18—C17—C22—C21	0.6 (5)
C4—C5—C6—C7	−1.3 (4)	C18—C19—C20—C21	−0.3 (8)
C4—C5—C6A—C7A	−1.3 (4)	C19—C20—C21—C22	0.8 (6)
C4—C5—C6A—C23A	176.4 (3)	C20—C21—C22—C17	−0.9 (5)
C5—C6—C7—C8	1.3 (4)	C22—C17—C18—C19	−0.1 (6)
C5—C6—C7—C23	−175.1 (3)	C23—C7—C8—C3	175.4 (3)
C5—C6A—C7A—C8	1.3 (4)	C23A—C6A—C7A—C8	−176.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···N1	0.93	2.73	3.348 (5)	125