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2-(5-Bromothiophen-2-yl)-1-phenyl-1*H*-phenanthro[9,10-*d*]imidazole

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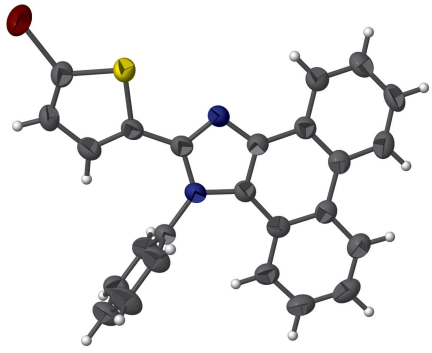
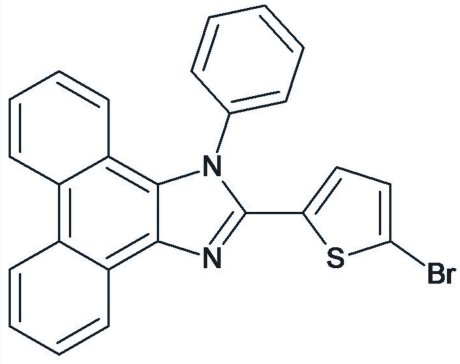
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{25}H_{15}BrN_2S$, the phenanthrene system is slightly skewed, with a dihedral angle of 8.94 (16)° between the outer benzene rings. The imidazole ring makes dihedral angles of 15.18 (16), 2.94 (15) and 88.46 (16)°, respectively, with the thiophene ring, the central benzene ring of the phenanthrene unit and the phenyl ring attached to the latter unit. In the molecule, there are two C—H···π interactions present involving the phenyl ring. In the crystal, molecules are linked by C—H···N and C—H···Br hydrogen bonds, forming zigzag chains along the *a* axis. The chains are linked by C—H···π interactions, forming a three-dimensional supramolecular structure.

3D view



Chemical scheme



Structure description

1*H*-Phenathro[9,10-*d*]imidazole derivatives act as multi-functional agents for the treatment of Alzheimer's disease (Liu *et al.*, 2014). This unit has been identified as an excellent building block for tuning carrier injection properties as well as blue emission (Wang *et al.*, 2011). Imidazole derivatives are found to have diverse activities, such as anti-inflammatory, antimicrobial (Divya *et al.*, 2013), antibacterial, anticancer, antifungal, analgesic, anti-HIV and antituberculosis (Verma *et al.*, 2013). The presence of a 5-bromothiophen-2-yl unit is found to enhance the antibacterial activity of piperazinyl quinolones (Foroumadi *et al.*, 2005) and antimicrobial activity in pyrazoline derivatives (Sasikala *et al.*, 2012).

In the title compound, illustrated in Fig. 1, the phenanthrene ring system is slightly skewed with a dihedral angle of 8.94 (16)° between the outer benzene rings. The imidazole ring makes dihedral angles of 15.18 (16), 2.94 (15) and 88.46 (16)°, respectively, with the thiophene ring, the central benzene ring (C6–C8/C13/C14/C19) of the

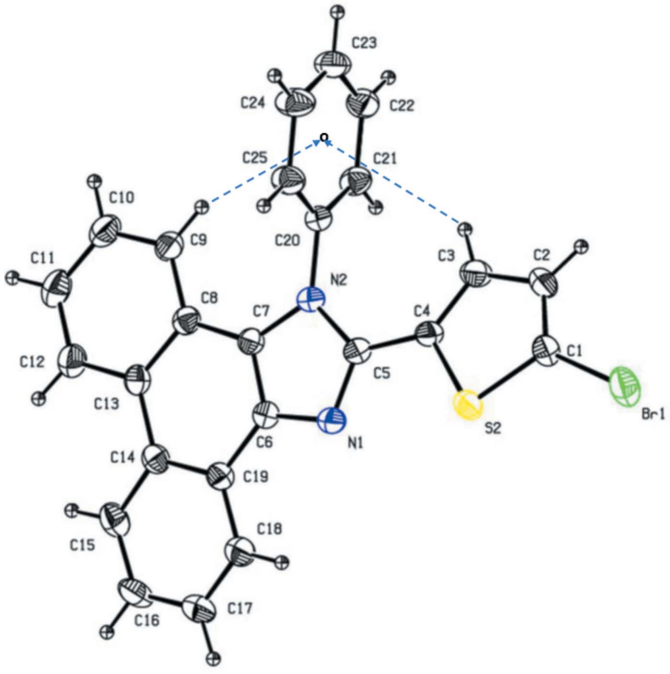


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The C—H···π interactions are shown as blue dashed arrows (see Table 1).

phenanthrene unit, and the phenyl ring (C20–C25). In the molecule, there are two C—H···π interactions present involving the phenyl ring (Table 1 and Fig. 1).

In the crystal, molecules are linked by C—H···N and C—H···Br hydrogen bonds forming zigzag chains propagating along the *a*-axis direction (Table 1 and Fig. 2). The chains are linked by C—H···π interactions, forming a three-dimensional supramolecular structure (Table 1 and Fig. 3).

Synthesis and crystallization

9,10-Phenanthrenequinone (1 equiv.), aniline (1.2 equiv.), 5-bromothiophene-2-carbaldehyde (1.5 equiv.) and ammonium

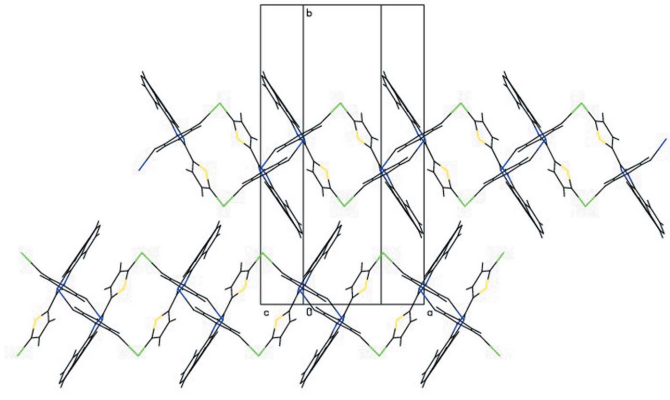


Figure 2
A partial view along the *c* axis, of the crystal packing of the title compound. The hydrogen bonds are shown as blue lines (see Table 1).

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

*Cg*1 and *Cg*2 are the centroids of the C20–C25 and C8–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···N1^{i}	0.93	2.44	3.317 (4)	157
C25—H25···Br1^{ii}	0.93	2.93	3.828 (3)	164
C3—H3···*Cg*1	0.93	2.99	3.716 (3)	136
C9—H9···*Cg*1	0.93	2.94	3.789 (3)	153
C15—H15···*Cg*2^{iii}	0.93	2.90	3.580 (4)	131

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{15}BrN_2S$
M_r	455.36
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, *b*, *c* (Å)	9.2966 (4), 23.0723 (11), 9.8089 (4)
β (°)	109.663 (1)
V (Å^3)	1981.26 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.19
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.566, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38101, 3481, 2628
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.098, 1.04
No. of reflections	3481
No. of parameters	262
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.53

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

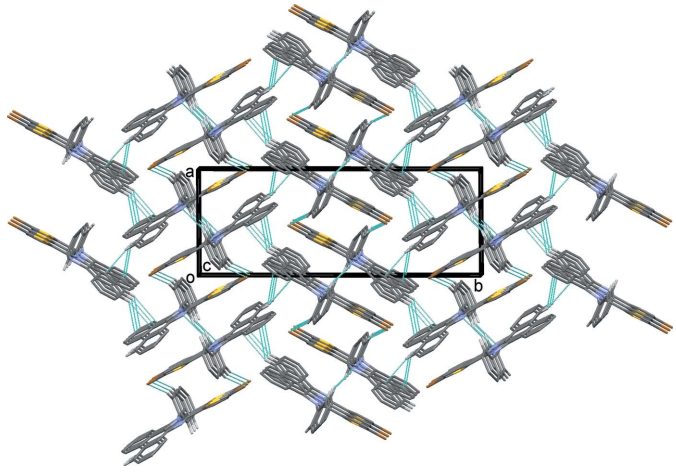


Figure 3
A view along the *c* axis, of the crystal packing of the title compound. The hydrogen bonds and C—H···π interactions are shown as dashed lines (see Table 1). For clarity, only the H atoms involved in these interactions have been included.

acetate (3.0 equiv.) in glacial acetic acid (10 ml) were refluxed for 24 h under a nitrogen atmosphere. After cooling to room temperature, the dark-yellow mixture was poured into a methanol solution with stirring. The separated solid was filtered off, washed with methanol and dried to give a white solid. A yellow powder was finally obtained after it was stirred in refluxing ethanol, subsequently filtered and dried in vacuum, yielding 2-(5-bromothiophen-2-yl)-1-phenyl-1*H*-phenanthro[9,10-*d*]imidazole. Finally, the title compound was crystallized from dimethyl sulfoxide, giving colourless block-like crystals on evaporation of the solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170089 [https://doi.org/10.1107/S241431461700089X]

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Crystal data

$C_{25}H_{15}BrN_2S$
M_r = 455.36
Monoclinic, $P2_1/n$
a = 9.2966 (4) Å
b = 23.0723 (11) Å
c = 9.8089 (4) Å
β = 109.663 (1)°
V = 1981.26 (15) Å^3
Z = 4
$F(000)$ = 920
D_x = 1.527 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5918 reflections
θ = 4.4–47.5°
μ = 2.19 mm^{-1}
T = 296 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Bruker Kappa AXEXII CCD scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.566, T_{max} = 0.746
38101 measured reflections
3481 independent reflections
2628 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −10→11
k = −27→27
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.098
S = 1.04
3481 reflections
262 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
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 1.1409P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C24	−0.0791 (4)	−0.08057 (17)	1.4777 (3)	0.0664 (10)
H24	0.015529	−0.096518	1.528863	0.080*
BR1	−0.00847 (5)	0.17241 (2)	0.93171 (4)	0.07188 (17)
S2	−0.16978 (10)	0.05218 (3)	0.89706 (8)	0.0538 (2)
N2	−0.3378 (2)	−0.06860 (10)	1.0994 (2)	0.0410 (5)
C1	−0.0987 (3)	0.11209 (12)	1.0013 (3)	0.0475 (7)
N1	−0.3613 (3)	−0.05272 (10)	0.8668 (2)	0.0442 (6)
C20	−0.2781 (3)	−0.06280 (11)	1.2546 (3)	0.0404 (6)
C6	−0.4345 (3)	−0.10315 (11)	0.8778 (3)	0.0411 (6)
C8	−0.4921 (3)	−0.16417 (12)	1.0589 (3)	0.0418 (7)
C5	−0.3052 (3)	−0.03288 (12)	1.0006 (3)	0.0418 (6)
C13	−0.5749 (3)	−0.20196 (12)	0.9446 (3)	0.0432 (7)
C7	−0.4228 (3)	−0.11464 (11)	1.0187 (3)	0.0396 (6)
C4	−0.2256 (3)	0.02220 (12)	1.0335 (3)	0.0410 (6)
C19	−0.5249 (3)	−0.13826 (12)	0.7599 (3)	0.0426 (7)
C9	−0.4840 (4)	−0.17749 (12)	1.2015 (3)	0.0492 (7)
H9	−0.432874	−0.152529	1.276629	0.059*
C2	−0.1179 (3)	0.10985 (13)	1.1311 (3)	0.0499 (7)
H2	−0.087128	0.138927	1.200569	0.060*
C14	−0.5959 (3)	−0.18781 (12)	0.7933 (3)	0.0429 (7)
C21	−0.3609 (3)	−0.03426 (13)	1.3267 (3)	0.0484 (7)
H21	−0.456502	−0.018883	1.276119	0.058*
C18	−0.5507 (3)	−0.12308 (13)	0.6154 (3)	0.0522 (7)
H18	−0.500921	−0.091129	0.594274	0.063*
C3	−0.1900 (3)	0.05827 (13)	1.1492 (3)	0.0498 (7)
H3	−0.211301	0.049664	1.233028	0.060*
C12	−0.6381 (4)	−0.25200 (13)	0.9816 (4)	0.0558 (8)
H12	−0.689606	−0.277845	0.908785	0.067*
C25	−0.1370 (3)	−0.08590 (14)	1.3285 (3)	0.0540 (8)
H25	−0.081184	−0.104828	1.279000	0.065*
C17	−0.6483 (4)	−0.15479 (14)	0.5052 (3)	0.0583 (8)
H17	−0.667786	−0.143578	0.409577	0.070*
C10	−0.5507 (4)	−0.22676 (14)	1.2310 (4)	0.0578 (8)
H10	−0.544689	−0.235002	1.325530	0.069*
C15	−0.6928 (4)	−0.21939 (14)	0.6760 (3)	0.0548 (8)
H15	−0.741404	−0.252239	0.694186	0.066*
C22	−0.2998 (4)	−0.02878 (14)	1.4756 (3)	0.0536 (8)
H22	−0.354303	−0.009112	1.525202	0.064*
C11	−0.6266 (4)	−0.26412 (14)	1.1203 (4)	0.0630 (9)
H11	−0.670272	−0.297820	1.140891	0.076*
C23	−0.1604 (4)	−0.05193 (15)	1.5505 (3)	0.0600 (9)
H23	−0.120647	−0.048303	1.650726	0.072*
C16	−0.7178 (4)	−0.20332 (15)	0.5359 (3)	0.0608 (9)
H16	−0.782361	−0.225350	0.460634	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C24	0.059 (2)	0.087 (3)	0.0433 (19)	0.0244 (19)	0.0035 (16)	−0.0002 (17)
BR1	0.1031 (3)	0.0497 (2)	0.0836 (3)	−0.01989 (18)	0.0588 (2)	−0.01601 (17)
S2	0.0765 (6)	0.0446 (4)	0.0456 (4)	−0.0110 (4)	0.0274 (4)	−0.0082 (3)
N2	0.0465 (13)	0.0412 (13)	0.0323 (12)	−0.0010 (10)	0.0091 (10)	0.0014 (10)
C1	0.0513 (17)	0.0407 (16)	0.0529 (18)	−0.0024 (13)	0.0207 (14)	−0.0059 (13)
N1	0.0505 (13)	0.0432 (13)	0.0356 (13)	−0.0054 (11)	0.0103 (11)	−0.0002 (10)
C20	0.0459 (16)	0.0388 (15)	0.0338 (15)	−0.0002 (12)	0.0098 (13)	0.0017 (11)
C6	0.0447 (16)	0.0376 (15)	0.0400 (16)	0.0003 (12)	0.0130 (13)	0.0007 (12)
C8	0.0417 (15)	0.0414 (16)	0.0432 (16)	0.0082 (12)	0.0156 (13)	0.0035 (12)
C5	0.0446 (15)	0.0412 (15)	0.0363 (16)	0.0028 (12)	0.0090 (13)	0.0029 (12)
C13	0.0438 (16)	0.0367 (15)	0.0501 (18)	0.0041 (12)	0.0170 (13)	0.0003 (13)
C7	0.0417 (15)	0.0375 (15)	0.0377 (15)	0.0059 (12)	0.0108 (12)	0.0006 (12)
C4	0.0430 (15)	0.0436 (15)	0.0333 (15)	0.0024 (12)	0.0087 (12)	0.0009 (12)
C19	0.0467 (16)	0.0411 (16)	0.0403 (16)	0.0022 (12)	0.0147 (13)	−0.0024 (12)
C9	0.0618 (19)	0.0431 (17)	0.0454 (18)	0.0076 (14)	0.0214 (15)	0.0056 (13)
C2	0.0569 (18)	0.0435 (16)	0.0478 (18)	−0.0058 (14)	0.0154 (15)	−0.0119 (14)
C14	0.0424 (15)	0.0418 (15)	0.0468 (17)	0.0041 (12)	0.0179 (13)	−0.0043 (13)
C21	0.0454 (16)	0.0545 (18)	0.0445 (17)	0.0099 (14)	0.0140 (14)	0.0053 (14)
C18	0.0617 (19)	0.0497 (18)	0.0464 (18)	−0.0052 (15)	0.0200 (15)	−0.0035 (14)
C3	0.0543 (18)	0.0558 (18)	0.0386 (17)	−0.0044 (14)	0.0150 (14)	−0.0025 (14)
C12	0.062 (2)	0.0440 (17)	0.061 (2)	−0.0049 (15)	0.0193 (16)	0.0027 (15)
C25	0.0552 (18)	0.062 (2)	0.0440 (18)	0.0158 (15)	0.0154 (15)	−0.0030 (15)
C17	0.072 (2)	0.062 (2)	0.0424 (18)	−0.0024 (17)	0.0209 (16)	−0.0116 (15)
C10	0.071 (2)	0.0533 (19)	0.056 (2)	0.0093 (16)	0.0302 (17)	0.0149 (16)
C15	0.0569 (19)	0.0488 (18)	0.064 (2)	−0.0123 (15)	0.0265 (16)	−0.0134 (15)
C22	0.064 (2)	0.0571 (19)	0.0458 (18)	0.0046 (16)	0.0258 (16)	−0.0014 (15)
C11	0.072 (2)	0.0482 (19)	0.076 (2)	−0.0021 (17)	0.0337 (19)	0.0145 (18)
C23	0.066 (2)	0.072 (2)	0.0368 (17)	0.0058 (18)	0.0105 (16)	−0.0017 (15)
C16	0.070 (2)	0.066 (2)	0.0446 (19)	−0.0132 (18)	0.0172 (16)	−0.0212 (16)

Geometric parameters (Å, º)

C24—C23	1.372 (5)	C9—C10	1.371 (4)
C24—C25	1.384 (4)	C9—H9	0.9300
C24—H24	0.9300	C2—C3	1.406 (4)
BR1—C1	1.869 (3)	C2—H2	0.9300
S2—C1	1.714 (3)	C14—C15	1.403 (4)
S2—C4	1.733 (3)	C21—C22	1.383 (4)
N2—C5	1.381 (3)	C21—H21	0.9300
N2—C7	1.399 (3)	C18—C17	1.367 (4)
N2—C20	1.441 (3)	C18—H18	0.9300
C1—C2	1.345 (4)	C3—H3	0.9300
N1—C5	1.320 (3)	C12—C11	1.358 (5)
N1—C6	1.370 (3)	C12—H12	0.9300
C20—C25	1.376 (4)	C25—H25	0.9300

C20—C21	1.376 (4)	C17—C16	1.376 (5)
C6—C7	1.375 (4)	C17—H17	0.9300
C6—C19	1.430 (4)	C10—C11	1.380 (5)
C8—C9	1.409 (4)	C10—H10	0.9300
C8—C13	1.425 (4)	C15—C16	1.366 (4)
C8—C7	1.431 (4)	C15—H15	0.9300
C5—C4	1.451 (4)	C22—C23	1.366 (4)
C13—C12	1.397 (4)	C22—H22	0.9300
C13—C14	1.468 (4)	C11—H11	0.9300
C4—C3	1.356 (4)	C23—H23	0.9300
C19—C18	1.400 (4)	C16—H16	0.9300
C19—C14	1.413 (4)		

C23—C24—C25	120.5 (3)	C3—C2—H2	124.1
C23—C24—H24	119.7	C15—C14—C19	116.8 (3)
C25—C24—H24	119.7	C15—C14—C13	123.0 (3)
C1—S2—C4	90.96 (14)	C19—C14—C13	120.1 (2)
C5—N2—C7	105.8 (2)	C20—C21—C22	119.0 (3)
C5—N2—C20	126.0 (2)	C20—C21—H21	120.5
C7—N2—C20	127.7 (2)	C22—C21—H21	120.5
C2—C1—S2	112.7 (2)	C17—C18—C19	120.6 (3)
C2—C1—BR1	126.4 (2)	C17—C18—H18	119.7
S2—C1—BR1	120.87 (17)	C19—C18—H18	119.7
C5—N1—C6	104.9 (2)	C4—C3—C2	114.0 (3)
C25—C20—C21	121.0 (3)	C4—C3—H3	123.0
C25—C20—N2	118.7 (3)	C2—C3—H3	123.0
C21—C20—N2	120.3 (2)	C11—C12—C13	122.1 (3)
N1—C6—C7	111.7 (2)	C11—C12—H12	118.9
N1—C6—C19	126.1 (2)	C13—C12—H12	118.9
C7—C6—C19	122.0 (3)	C20—C25—C24	119.0 (3)
C9—C8—C13	118.8 (3)	C20—C25—H25	120.5
C9—C8—C7	124.7 (3)	C24—C25—H25	120.5
C13—C8—C7	116.5 (2)	C18—C17—C16	119.9 (3)
N1—C5—N2	112.6 (2)	C18—C17—H17	120.1
N1—C5—C4	121.7 (2)	C16—C17—H17	120.1
N2—C5—C4	125.7 (2)	C9—C10—C11	120.0 (3)
C12—C13—C8	117.7 (3)	C9—C10—H10	120.0
C12—C13—C14	121.4 (3)	C11—C10—H10	120.0
C8—C13—C14	120.8 (3)	C16—C15—C14	122.0 (3)
C6—C7—N2	105.1 (2)	C16—C15—H15	119.0
C6—C7—C8	122.7 (2)	C14—C15—H15	119.0
N2—C7—C8	132.1 (2)	C23—C22—C21	120.7 (3)
C3—C4—C5	133.3 (3)	C23—C22—H22	119.6
C3—C4—S2	110.4 (2)	C21—C22—H22	119.6
C5—C4—S2	116.2 (2)	C12—C11—C10	120.4 (3)
C18—C19—C14	120.2 (3)	C12—C11—H11	119.8
C18—C19—C6	122.1 (3)	C10—C11—H11	119.8
C14—C19—C6	117.7 (3)	C22—C23—C24	119.8 (3)

C10—C9—C8	120.9 (3)	C22—C23—H23	120.1
C10—C9—H9	119.6	C24—C23—H23	120.1
C8—C9—H9	119.6	C15—C16—C17	120.5 (3)
C1—C2—C3	111.9 (3)	C15—C16—H16	119.7
C1—C2—H2	124.1	C17—C16—H16	119.7
C4—S2—C1—C2	−0.7 (2)	N1—C6—C19—C14	−177.7 (3)
C4—S2—C1—BR1	179.99 (18)	C7—C6—C19—C14	−3.6 (4)
C5—N2—C20—C25	−83.7 (4)	C13—C8—C9—C10	1.9 (4)
C7—N2—C20—C25	87.2 (3)	C7—C8—C9—C10	−178.3 (3)
C5—N2—C20—C21	95.8 (3)	S2—C1—C2—C3	0.8 (3)
C7—N2—C20—C21	−93.2 (3)	BR1—C1—C2—C3	180.0 (2)
C5—N1—C6—C7	−0.4 (3)	C18—C19—C14—C15	−0.9 (4)
C5—N1—C6—C19	174.3 (3)	C6—C19—C14—C15	175.6 (3)
C6—N1—C5—N2	0.4 (3)	C18—C19—C14—C13	−176.9 (3)
C6—N1—C5—C4	−176.6 (2)	C6—C19—C14—C13	−0.4 (4)
C7—N2—C5—N1	−0.3 (3)	C12—C13—C14—C15	7.1 (4)
C20—N2—C5—N1	172.2 (2)	C8—C13—C14—C15	−171.4 (3)
C7—N2—C5—C4	176.6 (3)	C12—C13—C14—C19	−177.1 (3)
C20—N2—C5—C4	−10.9 (4)	C8—C13—C14—C19	4.4 (4)
C9—C8—C13—C12	−2.9 (4)	C25—C20—C21—C22	0.3 (4)
C7—C8—C13—C12	177.2 (2)	N2—C20—C21—C22	−179.2 (3)
C9—C8—C13—C14	175.6 (3)	C14—C19—C18—C17	2.1 (4)
C7—C8—C13—C14	−4.3 (4)	C6—C19—C18—C17	−174.2 (3)
N1—C6—C7—N2	0.2 (3)	C5—C4—C3—C2	−176.5 (3)
C19—C6—C7—N2	−174.7 (2)	S2—C4—C3—C2	−0.2 (3)
N1—C6—C7—C8	178.7 (2)	C1—C2—C3—C4	−0.4 (4)
C19—C6—C7—C8	3.8 (4)	C8—C13—C12—C11	2.1 (4)
C5—N2—C7—C6	0.1 (3)	C14—C13—C12—C11	−176.4 (3)
C20—N2—C7—C6	−172.3 (2)	C21—C20—C25—C24	0.6 (5)
C5—N2—C7—C8	−178.2 (3)	N2—C20—C25—C24	−179.9 (3)
C20—N2—C7—C8	9.4 (4)	C23—C24—C25—C20	−0.9 (5)
C9—C8—C7—C6	−179.5 (3)	C19—C18—C17—C16	−2.4 (5)
C13—C8—C7—C6	0.3 (4)	C8—C9—C10—C11	0.1 (5)
C9—C8—C7—N2	−1.5 (5)	C19—C14—C15—C16	0.0 (4)
C13—C8—C7—N2	178.3 (3)	C13—C14—C15—C16	175.9 (3)
N1—C5—C4—C3	161.8 (3)	C20—C21—C22—C23	−0.9 (5)
N2—C5—C4—C3	−14.9 (5)	C13—C12—C11—C10	−0.1 (5)
N1—C5—C4—S2	−14.3 (4)	C9—C10—C11—C12	−1.0 (5)
N2—C5—C4—S2	169.0 (2)	C21—C22—C23—C24	0.5 (5)
C1—S2—C4—C3	0.5 (2)	C25—C24—C23—C22	0.4 (6)
C1—S2—C4—C5	177.5 (2)	C14—C15—C16—C17	−0.3 (5)
N1—C6—C19—C18	−1.4 (4)	C18—C17—C16—C15	1.5 (5)
C7—C6—C19—C18	172.8 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C20–C25 and C8–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···N1^{i}	0.93	2.44	3.317 (4)	157
C25—H25···Br1^{ii}	0.93	2.93	3.828 (3)	164
C3—H3···*Cg*1	0.93	2.99	3.716 (3)	136
C9—H9···*Cg*1	0.93	2.94	3.789 (3)	153
C15—H15···*Cg*2^{iii}	0.93	2.90	3.580 (4)	131

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