# N-(2-{[5-Bromo-2-(piperidin-1-yl)-pyrimidin-4-yl]sulfanyl}-4-methoxy-phenyl)benzenesulfonamide

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The title compound, $C_{22}H_{23}BrN_4O_3S_2$, crystallizes with two molecules, $A$ and $B$, in the asymmetric unit. In one of these, the methoxy group is disordered over two sets of sites in a 0.565 (9):0.435 (9) ratio. The benzene rings bridged by the sulfonamide group are tilted relative to each other by 37.4 (1) and 56.1 (1)° in molecules $A$ and $B$, respectively, while the dihedral angles between the sulfur-bridged pyrimidine and benzene rings are 72.4 (1) and 70.2 (1)° for $A$ and $B$, respectively. The piperidine ring adopts a chair conformation in both molecules. In the crystal, inversion dimers linked by pairs of N—H$\cdots$N hydrogen bonds occur for both $A$ and $B$; the dimers are linked into [010] chains by C—H$\cdots$O hydrogen bonds. The crystal structure also features inversion-generated aromatic $\pi$–$\pi$ stacking interactions between the pyrimidine rings for both molecules [centroid–centroid distances = 3.412 (2) (molecule $A$) and 3.396 (2) Å (molecule $B$)].

## Related literature

For the biological activity of sulfonamide compounds, see: Lee *et al.* (2002); Laurence (2009). For related structures, see: Rodrigues *et al.* (2011); Akkurt *et al.* (2011); Kant *et al.* (2012); Kumar *et al.* (2012).
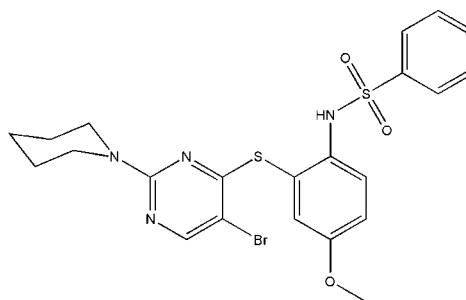
## Experimental

### Crystal data

| | |
|---|---|
| $C_{22}H_{23}BrN_4O_3S_2$ | $\gamma = 62.581\ (4)°$ |
| $M_r = 535.47$ | $V = 2405.10\ (18)$ Å$^3$ |
| Triclinic, $P\bar{1}$ | $Z = 4$ |
| $a = 13.6081\ (6)$ Å | Mo $K\alpha$ radiation |
| $b = 14.5662\ (5)$ Å | $\mu = 1.91$ mm$^{-1}$ |
| $c = 14.7502\ (7)$ Å | $T = 293$ K |
| $\alpha = 74.439\ (4)°$ | $0.30 \times 0.20 \times 0.20$ mm |
| $\beta = 69.077\ (4)°$ | |

### Data collection

| | |
|---|---|
| Oxford Diffraction Xcalibur Sapphire3 CCD diffractometer | 18681 measured reflections |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010) | 8017 independent reflections |
| | 5364 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.920$, $T_{max} = 1.000$ | $R_{int} = 0.032$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.103$ | |
| $S = 1.02$ | |
| 8017 reflections | $\Delta\rho_{max} = 0.34$ e Å$^{-3}$ |
| 601 parameters | $\Delta\rho_{min} = -0.36$ e Å$^{-3}$ |
| 35 restraints | |

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| N8$A$—H8$A\cdots$N20$A^i$ | 0.86 | 2.15 | 2.940 (4) | 152 |
| N8$B$—H8$B\cdots$N20$B^{ii}$ | 0.78 (4) | 2.28 (4) | 2.974 (5) | 149 (4) |
| C11$A$—H11$A\cdots$O1$A^{iii}$ | 0.93 | 2.47 | 3.372 (5) | 164 |
| C10$B$—H10$B\cdots$O2$B^{iv}$ | 0.93 | 2.60 | 3.278 (6) | 131 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

# organic compounds

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6971).

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# supporting information

# *N*-(2-{[5-Bromo-2-(piperidin-1-yl)pyrimidin-4-yl]sulfanyl}-4-methoxyphenyl)-benzenesulfonamide

**Mohan Kumar, L. Mallesha, M. A. Sridhar, Kamini Kapoor, Vivek K. Gupta and Rajni Kant**

### S1. Comment

The amide and sulfonamide moieties are the constituents of many biologically significant compounds. Sulfonamide compounds are well known as antimicrobial agents and are familiar in the literature for their anti-malarial, anti-convulsant, antineoplastic, antituberculosic, antidiabetic, antiobesity. and anti-hypertensive activities [Lee *et al.*, 2002]. Sulfonamides commonly named as Sulfa drugs are the medicines capable of controlling the bacterial infections[Laurence, 2009]. In view of the importance of sulfonamide, the title compound (I) is prepared and its crystal structure is reported.

  Bond lengths and angles in the title compound (Fig. 1) have normal values and are comparable with the similar crystal structures (Rodrigues *et al.*, 2011; Akkurt *et al.*, 2011; Kant *et al.*, 2012); Kumar *et al.* (2012). There are no significant differences in bond lengths and angles for molecule A & B. The molecules are twisted about the S—N bonds with (C1A—S1A—N8A—C9A) and (C1B—S1B—N8B—C9B) torsion angles of 60.5 (3) and 58.9 (4)°, respectively. The piperidine ring is in chair conformation in both the molecules. The benzene rings bridged by the sulfonamide group are tilted relative to each other by 37.4 (2) and 56.1 (1)° while the dihedral angle between the sulfur bridged pyrimidine and benzene rings is 72.4 (1) and 70.2 (1)° in molecules A and B, respectively. In one of the molecules (molecule A), methoxy group is disordered over two sets of sites in a 0.57 (1): 0.43 (1) ratio. In the crystal, molecule A is forming dimer with other molecule A by N8A—H8A ⋯N20A and molecule B is also forming dimer with molecule B by N8B—H8B ⋯N20B hydrogen bonds (Fig. 2). These dimers are further connected into chains by C10B—H10B⋯O2B and C11A—H11A⋯O1A along *a* axis (Fig. 3). In addition to these hydrogen bonds there is one intramolecular N8B—H8B⋯S2B hydrogen bond in molecule B (Table 1). The crystal structure also features π–π interactions between the pyrimidine rings in both the molecules, A & B [molecule A: centroid separation = 3.412 (2) Å, interplanar spacing = 3.401 Å and centroid shift = 0.27 Å; molecule B: centroid separation = 3.396 (2) Å, interplanar spacing = 3.322 Å and centroid shift = 0.70 Å].

### S2. Experimental

The reaction of *N*-[2-(5-bromo-2-piperidin-1-yl-pyrimidin-4-yl-sulfanyl) -4-methoxy-phenyl]-benzenesulfonamide (4.87 g, 0.01 mol) and piperidine (0.86 g, 0.01 mol) were carried out in the presence of triethylamine and the reaction mixture was allowed to stir at room temperature for 6–7 h in dry dichloromethane. The progress of the reaction was monitored by TLC. Upon completion, the solvent was removed under reduced pressure and residue was extracted with ethyl acetate. The compound was purified by successive recrystallization from methanol (yield 79%, m.p. 471–473 K) to yield colourless blocks.

### S3. Refinement

All H atoms were positioned geometrically and were treated as riding on their parent C/N atoms, with C—H distances of 0.93–0.97 Å and N—H distance of 0.86 with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).
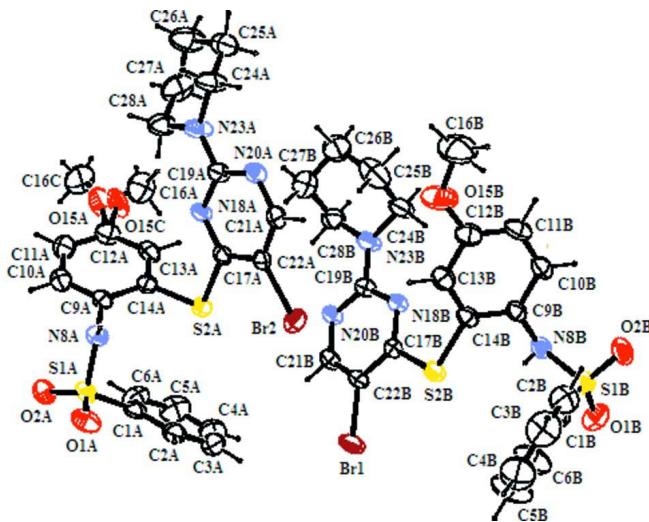
**Figure 1**

The molecular structure with displacnent ellipsoids drawn at the 40% probability level.
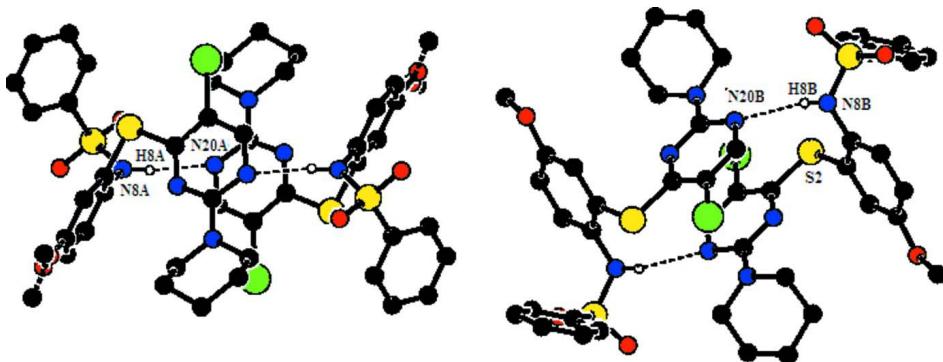


**Figure 2**

Dimer formation between the molecules.
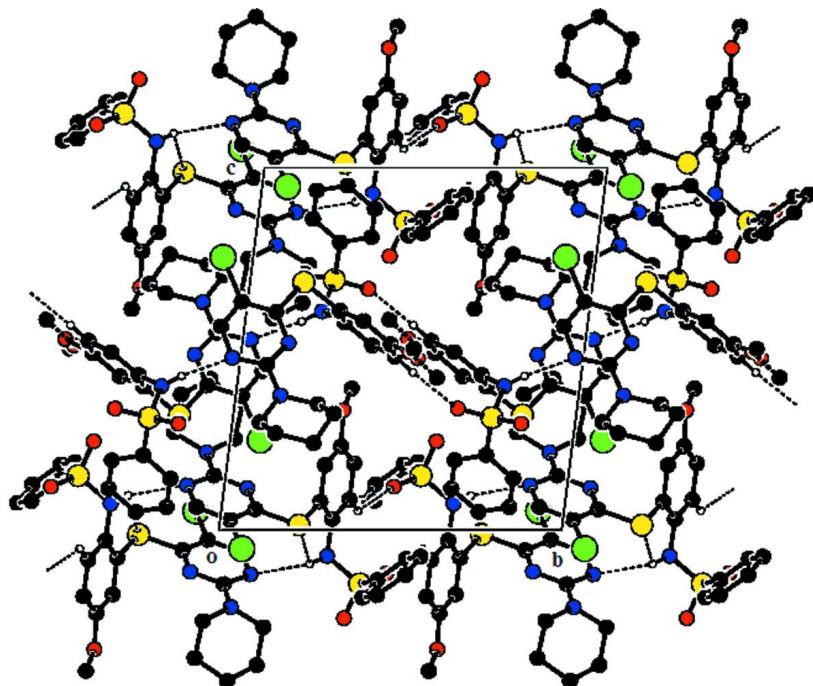
**Figure 3**

A molecular packing view of the title compound down the *a* axis, showing intermolecular interactions. For clarity, hydrogen atoms which are not involved in hydrogen bonding have been omitted.

**_N_-(2-{[5-Bromo-2-(piperidin-1-yl)pyrimidin-4-yl]sulfanyl}-4- methoxyphenyl)benzenesulfonamide**

*Crystal data*

| | |
|---|---|
| $C_{22}H_{23}BrN_4O_3S_2$ | $Z = 4$ |
| $M_r = 535.47$ | $F(000) = 1096$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.479$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 13.6081$ (6) Å | Cell parameters from 6323 reflections |
| $b = 14.5662$ (5) Å | $\theta = 3.4$–29.0° |
| $c = 14.7502$ (7) Å | $\mu = 1.91$ mm$^{-1}$ |
| $\alpha = 74.439$ (4)° | $T = 293$ K |
| $\beta = 69.077$ (4)° | Block, colourless |
| $\gamma = 62.581$ (4)° | $0.30 \times 0.20 \times 0.20$ mm |
| $V = 2405.10$ (18) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Sapphire3 CCD diffractometer | 18681 measured reflections |
| Radiation source: fine-focus sealed tube | 8017 independent reflections |
| Graphite monochromator | 5364 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 16.1049 pixels mm$^{-1}$ | $R_{int} = 0.032$ |
| $\omega$ scan | $\theta_{max} = 25.0°$, $\theta_{min} = 3.4°$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010) | $h = -16 \rightarrow 15$ |
| | $k = -17 \rightarrow 17$ |
| | $l = -17 \rightarrow 17$ |
| $T_{min} = 0.920$, $T_{max} = 1.000$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.103$ | |
| $S = 1.02$ | H atoms treated by a mixture of independent and constrained refinement |
| 8017 reflections | |
| 601 parameters | $w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 0.8571P]$ |
| 35 restraints | where $P = (F_o^2 + 2F_c^2)/3$ |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} = 0.001$ |
| | $\Delta\rho_{max} = 0.34$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.36$ e Å$^{-3}$ |

*Special details*

**Experimental**. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171. NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**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.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1A | 0.9685 (3) | 0.2480 (3) | 0.7938 (3) | 0.0560 (10) | |
| C2A | 0.8683 (5) | 0.3377 (3) | 0.8080 (3) | 0.0820 (14) | |
| H2A | 0.8638 | 0.3983 | 0.7649 | 0.098* | |
| C3A | 0.7749 (5) | 0.3370 (4) | 0.8862 (4) | 0.0990 (17) | |
| H3A | 0.7071 | 0.3970 | 0.8950 | 0.119* | |
| C4A | 0.7816 (5) | 0.2491 (5) | 0.9504 (4) | 0.0934 (16) | |
| H4A | 0.7185 | 0.2491 | 1.0031 | 0.112* | |
| C5A | 0.8809 (5) | 0.1609 (4) | 0.9373 (3) | 0.0880 (15) | |
| H5A | 0.8856 | 0.1010 | 0.9816 | 0.106* | |
| C6A | 0.9744 (4) | 0.1602 (3) | 0.8585 (3) | 0.0675 (11) | |
| H6A | 1.0416 | 0.0997 | 0.8496 | 0.081* | |
| C9A | 0.9556 (3) | 0.2902 (3) | 0.5727 (3) | 0.0503 (9) | |
| C10A | 0.9569 (4) | 0.3794 (3) | 0.5091 (3) | 0.0669 (11) | |
| H10A | 1.0235 | 0.3915 | 0.4869 | 0.080* | |
| C11A | 0.8627 (4) | 0.4495 (3) | 0.4785 (3) | 0.0740 (12) | |
| H11A | 0.8656 | 0.5081 | 0.4347 | 0.089* | |
| C12A | 0.7634 (4) | 0.4334 (3) | 0.5125 (3) | 0.0687 (12) | |
| O15A | 0.6783 (14) | 0.5178 (12) | 0.4733 (16) | 0.104 (3) | 0.565 (9) |
| C16A | 0.5841 (8) | 0.5017 (8) | 0.5000 (8) | 0.110 (4) | 0.565 (9) |
| H16D | 0.5264 | 0.5601 | 0.4733 | 0.166* | 0.565 (9) |
| H16E | 0.5567 | 0.4937 | 0.5701 | 0.166* | 0.565 (9) |

| H16F | 0.6002 | 0.4396 | 0.4763 | 0.166* | 0.565 (9) |
| O15C | 0.6630 (17) | 0.4908 (15) | 0.4905 (19) | 0.091 (4) | 0.435 (9) |
| C16C | 0.6574 (12) | 0.5800 (10) | 0.4197 (10) | 0.121 (5) | 0.435 (9) |
| H16G | 0.5825 | 0.6140 | 0.4086 | 0.182* | 0.435 (9) |
| H16H | 0.7147 | 0.5589 | 0.3596 | 0.182* | 0.435 (9) |
| H16I | 0.6711 | 0.6272 | 0.4432 | 0.182* | 0.435 (9) |
| C13A | 0.7588 (3) | 0.3452 (3) | 0.5764 (3) | 0.0617 (10) | |
| H13A | 0.6910 | 0.3350 | 0.5999 | 0.074* | |
| C14A | 0.8561 (3) | 0.2725 (3) | 0.6048 (2) | 0.0516 (9) | |
| C17A | 0.8532 (3) | 0.0872 (3) | 0.6017 (2) | 0.0447 (8) | |
| C19A | 0.8363 (3) | 0.0788 (3) | 0.4561 (3) | 0.0523 (9) | |
| C21A | 0.8764 (3) | −0.0689 (3) | 0.5619 (3) | 0.0517 (9) | |
| H21A | 0.8922 | −0.1396 | 0.5781 | 0.062* | |
| C22A | 0.8721 (3) | −0.0174 (3) | 0.6297 (2) | 0.0450 (8) | |
| C24A | 0.8154 (4) | 0.0798 (3) | 0.2969 (3) | 0.0885 (15) | |
| H24C | 0.8793 | 0.0806 | 0.2403 | 0.106* | |
| H24D | 0.8288 | 0.0075 | 0.3222 | 0.106* | |
| C25A | 0.7108 (5) | 0.1291 (4) | 0.2668 (4) | 0.0983 (16) | |
| H25A | 0.6497 | 0.1160 | 0.3198 | 0.118* | |
| H25B | 0.7220 | 0.0983 | 0.2113 | 0.118* | |
| C26A | 0.6750 (5) | 0.2438 (4) | 0.2394 (4) | 0.117 (2) | |
| H26C | 0.6004 | 0.2745 | 0.2265 | 0.140* | |
| H26D | 0.7300 | 0.2575 | 0.1801 | 0.140* | |
| C27A | 0.6684 (5) | 0.2930 (4) | 0.3207 (4) | 0.1037 (18) | |
| H27A | 0.6500 | 0.3667 | 0.3000 | 0.124* | |
| H27B | 0.6074 | 0.2860 | 0.3778 | 0.124* | |
| C28A | 0.7793 (5) | 0.2426 (3) | 0.3468 (3) | 0.0872 (15) | |
| H28C | 0.8387 | 0.2564 | 0.2922 | 0.105* | |
| H28D | 0.7716 | 0.2715 | 0.4023 | 0.105* | |
| N8A | 1.0569 (3) | 0.2203 (2) | 0.6031 (2) | 0.0560 (8) | |
| H8A | 1.1033 | 0.1651 | 0.5752 | 0.067* | |
| N18A | 0.8354 (2) | 0.1346 (2) | 0.5161 (2) | 0.0494 (7) | |
| N20A | 0.8594 (2) | −0.0238 (2) | 0.4749 (2) | 0.0527 (8) | |
| N23A | 0.8120 (3) | 0.1302 (2) | 0.3711 (3) | 0.0772 (11) | |
| O1A | 1.0816 (3) | 0.3475 (2) | 0.6652 (2) | 0.0901 (10) | |
| O2A | 1.1862 (2) | 0.1570 (2) | 0.7068 (2) | 0.0866 (9) | |
| S1A | 1.08444 (10) | 0.24479 (9) | 0.69014 (8) | 0.0652 (3) | |
| S2A | 0.85282 (9) | 0.15692 (8) | 0.68323 (7) | 0.0583 (3) | |
| Br2 | 0.89499 (4) | −0.08786 (3) | 0.75225 (3) | 0.07432 (16) | |
| C1B | 0.7248 (4) | −0.4807 (3) | 1.1382 (3) | 0.0621 (11) | |
| C2B | 0.8015 (5) | −0.5570 (4) | 1.0799 (3) | 0.0874 (14) | |
| H2B | 0.7761 | −0.5815 | 1.0444 | 0.105* | |
| C3B | 0.9179 (5) | −0.5978 (4) | 1.0742 (4) | 0.1111 (19) | |
| H3B | 0.9707 | −0.6505 | 1.0355 | 0.133* | |
| C4B | 0.9542 (5) | −0.5608 (6) | 1.1251 (5) | 0.124 (2) | |
| H4B | 1.0322 | −0.5886 | 1.1212 | 0.149* | |
| C5B | 0.8804 (6) | −0.4850 (5) | 1.1809 (5) | 0.135 (2) | |
| H5B | 0.9067 | −0.4599 | 1.2151 | 0.162* | |

| | | | |
|---|---|---|---|
| C6B | 0.7642 (4) | −0.4440 (4) | 1.1872 (5) | 0.112 (2) |
| H6B | 0.7125 | −0.3908 | 1.2256 | 0.134* |
| C9B | 0.6003 (3) | −0.3267 (2) | 0.9702 (3) | 0.0482 (9) |
| C10B | 0.5698 (3) | −0.3699 (3) | 0.9165 (3) | 0.0599 (10) |
| H10B | 0.5161 | −0.3989 | 0.9479 | 0.072* |
| C11B | 0.6192 (4) | −0.3700 (3) | 0.8163 (3) | 0.0683 (12) |
| H11B | 0.5992 | −0.3999 | 0.7810 | 0.082* |
| C12B | 0.6971 (4) | −0.3264 (3) | 0.7694 (3) | 0.0684 (11) |
| C13B | 0.7305 (3) | −0.2857 (3) | 0.8216 (3) | 0.0616 (10) |
| H13B | 0.7854 | −0.2581 | 0.7897 | 0.074* |
| C14B | 0.6820 (3) | −0.2860 (2) | 0.9222 (3) | 0.0494 (9) |
| C16B | 0.7037 (5) | −0.3354 (6) | 0.6099 (4) | 0.145 (3) |
| H16A | 0.7162 | −0.4075 | 0.6208 | 0.217* |
| H16B | 0.7405 | −0.3178 | 0.5430 | 0.217* |
| H16C | 0.6226 | −0.2928 | 0.6237 | 0.217* |
| C17B | 0.6646 (3) | −0.0985 (3) | 0.9436 (2) | 0.0434 (8) |
| C19B | 0.5571 (3) | 0.0341 (3) | 0.8500 (3) | 0.0504 (9) |
| C21B | 0.6364 (3) | 0.0740 (3) | 0.9370 (3) | 0.0531 (9) |
| H21B | 0.6486 | 0.1227 | 0.9565 | 0.064* |
| C22B | 0.6874 (3) | −0.0282 (3) | 0.9720 (2) | 0.0464 (9) |
| C24B | 0.4822 (4) | −0.0133 (3) | 0.7486 (3) | 0.0765 (13) |
| H24A | 0.4020 | 0.0083 | 0.7526 | 0.092* |
| H24B | 0.5074 | −0.0803 | 0.7881 | 0.092* |
| C25B | 0.5520 (4) | −0.0234 (5) | 0.6457 (5) | 0.114 (2) |
| H25C | 0.5402 | −0.0716 | 0.6207 | 0.137* |
| H25D | 0.6329 | −0.0516 | 0.6427 | 0.137* |
| C26B | 0.5200 (6) | 0.0801 (6) | 0.5830 (4) | 0.136 (3) |
| H26A | 0.4421 | 0.1042 | 0.5789 | 0.164* |
| H26B | 0.5714 | 0.0726 | 0.5174 | 0.164* |
| C27B | 0.5279 (5) | 0.1599 (5) | 0.6262 (4) | 0.1155 (19) |
| H27C | 0.6078 | 0.1408 | 0.6212 | 0.139* |
| H27D | 0.4998 | 0.2279 | 0.5887 | 0.139* |
| C28B | 0.4593 (4) | 0.1662 (3) | 0.7312 (3) | 0.0725 (12) |
| H28A | 0.4717 | 0.2125 | 0.7583 | 0.087* |
| H28B | 0.3780 | 0.1943 | 0.7358 | 0.087* |
| N8B | 0.5458 (3) | −0.3251 (3) | 1.0724 (3) | 0.0559 (9) |
| N18B | 0.5992 (2) | −0.0683 (2) | 0.8847 (2) | 0.0486 (7) |
| N20B | 0.5702 (2) | 0.1085 (2) | 0.8768 (2) | 0.0510 (7) |
| N23B | 0.4937 (3) | 0.0634 (3) | 0.7865 (3) | 0.0696 (10) |
| O1B | 0.5161 (2) | −0.3977 (2) | 1.2444 (2) | 0.0872 (9) |
| O2B | 0.5586 (3) | −0.5052 (2) | 1.1192 (2) | 0.0920 (10) |
| O15B | 0.7486 (3) | −0.3187 (3) | 0.6696 (3) | 0.1108 (12) |
| S1B | 0.57689 (9) | −0.43041 (8) | 1.14932 (8) | 0.0654 (3) |
| S2B | 0.72653 (8) | −0.23224 (7) | 0.98706 (7) | 0.0554 (3) |
| Br1B | 0.78611 (4) | −0.07405 (4) | 1.05211 (4) | 0.07916 (17) |
| H8B | 0.536 (3) | −0.278 (3) | 1.095 (2) | 0.043 (11)* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1A | 0.078 (3) | 0.050 (2) | 0.061 (2) | −0.029 (2) | −0.036 (2) | −0.0098 (19) |
| C2A | 0.119 (4) | 0.061 (3) | 0.065 (3) | −0.032 (3) | −0.028 (3) | −0.012 (2) |
| C3A | 0.108 (4) | 0.087 (4) | 0.083 (4) | −0.016 (3) | −0.018 (3) | −0.035 (3) |
| C4A | 0.108 (4) | 0.116 (5) | 0.071 (3) | −0.055 (4) | −0.014 (3) | −0.030 (3) |
| C5A | 0.132 (5) | 0.096 (4) | 0.068 (3) | −0.073 (4) | −0.039 (3) | 0.008 (3) |
| C6A | 0.084 (3) | 0.064 (3) | 0.073 (3) | −0.035 (2) | −0.038 (3) | −0.002 (2) |
| C9A | 0.061 (2) | 0.048 (2) | 0.053 (2) | −0.027 (2) | −0.0176 (19) | −0.0115 (17) |
| C10A | 0.073 (3) | 0.067 (3) | 0.072 (3) | −0.038 (2) | −0.027 (2) | 0.000 (2) |
| C11A | 0.088 (3) | 0.064 (3) | 0.077 (3) | −0.040 (3) | −0.031 (3) | 0.007 (2) |
| C12A | 0.071 (3) | 0.057 (3) | 0.079 (3) | −0.015 (2) | −0.034 (2) | −0.012 (2) |
| O15A | 0.091 (6) | 0.085 (8) | 0.151 (9) | −0.044 (4) | −0.048 (6) | −0.002 (6) |
| C16A | 0.115 (8) | 0.083 (6) | 0.118 (7) | −0.033 (7) | −0.022 (7) | −0.014 (5) |
| O15C | 0.057 (5) | 0.091 (9) | 0.143 (8) | −0.044 (5) | −0.046 (6) | 0.009 (6) |
| C16C | 0.127 (9) | 0.087 (8) | 0.138 (10) | −0.031 (7) | −0.088 (7) | 0.052 (7) |
| C13A | 0.062 (3) | 0.066 (3) | 0.071 (3) | −0.033 (2) | −0.018 (2) | −0.021 (2) |
| C14A | 0.065 (3) | 0.055 (2) | 0.046 (2) | −0.029 (2) | −0.0159 (19) | −0.0131 (17) |
| C17A | 0.0366 (19) | 0.054 (2) | 0.049 (2) | −0.0225 (17) | −0.0098 (16) | −0.0098 (17) |
| C19A | 0.055 (2) | 0.050 (2) | 0.058 (2) | −0.0187 (19) | −0.0240 (19) | −0.0098 (18) |
| C21A | 0.050 (2) | 0.045 (2) | 0.063 (2) | −0.0208 (18) | −0.0146 (19) | −0.0088 (19) |
| C22A | 0.042 (2) | 0.054 (2) | 0.044 (2) | −0.0265 (18) | −0.0079 (16) | −0.0058 (17) |
| C24A | 0.128 (4) | 0.069 (3) | 0.090 (3) | −0.023 (3) | −0.065 (3) | −0.024 (2) |
| C25A | 0.131 (4) | 0.109 (4) | 0.092 (4) | −0.067 (4) | −0.059 (3) | 0.002 (3) |
| C26A | 0.139 (5) | 0.092 (4) | 0.128 (5) | −0.018 (4) | −0.089 (4) | −0.010 (4) |
| C27A | 0.130 (5) | 0.061 (3) | 0.092 (4) | −0.010 (3) | −0.044 (3) | −0.001 (3) |
| C28A | 0.139 (4) | 0.062 (3) | 0.082 (3) | −0.042 (3) | −0.056 (3) | −0.004 (2) |
| N8A | 0.0604 (19) | 0.0581 (19) | 0.0576 (19) | −0.0255 (17) | −0.0184 (16) | −0.0138 (15) |
| N18A | 0.0554 (18) | 0.0496 (18) | 0.0542 (18) | −0.0231 (15) | −0.0221 (15) | −0.0100 (15) |
| N20A | 0.0557 (19) | 0.0482 (19) | 0.061 (2) | −0.0186 (16) | −0.0218 (16) | −0.0136 (15) |
| N23A | 0.122 (3) | 0.047 (2) | 0.082 (2) | −0.021 (2) | −0.065 (2) | −0.0084 (17) |
| O1A | 0.140 (3) | 0.088 (2) | 0.089 (2) | −0.082 (2) | −0.044 (2) | −0.0002 (17) |
| O2A | 0.0668 (19) | 0.102 (2) | 0.106 (2) | −0.0290 (18) | −0.0446 (17) | −0.0161 (18) |
| S1A | 0.0817 (8) | 0.0697 (7) | 0.0722 (7) | −0.0451 (6) | −0.0343 (6) | −0.0062 (5) |
| S2A | 0.0795 (7) | 0.0670 (6) | 0.0474 (5) | −0.0445 (6) | −0.0170 (5) | −0.0086 (5) |
| Br2 | 0.0983 (3) | 0.0802 (3) | 0.0506 (2) | −0.0503 (3) | −0.0176 (2) | 0.0050 (2) |
| C1B | 0.072 (3) | 0.049 (2) | 0.071 (3) | −0.021 (2) | −0.034 (2) | −0.002 (2) |
| C2B | 0.095 (4) | 0.077 (3) | 0.086 (3) | −0.028 (3) | −0.021 (3) | −0.023 (3) |
| C3B | 0.080 (4) | 0.096 (4) | 0.116 (5) | −0.007 (3) | −0.006 (3) | −0.031 (3) |
| C4B | 0.084 (4) | 0.125 (6) | 0.151 (6) | −0.025 (4) | −0.048 (4) | −0.008 (5) |
| C5B | 0.100 (5) | 0.136 (6) | 0.190 (7) | −0.012 (4) | −0.085 (5) | −0.058 (5) |
| C6B | 0.079 (4) | 0.102 (4) | 0.167 (6) | −0.004 (3) | −0.057 (4) | −0.063 (4) |
| C9B | 0.052 (2) | 0.0350 (19) | 0.063 (2) | −0.0157 (18) | −0.0234 (19) | −0.0076 (17) |
| C10B | 0.062 (3) | 0.047 (2) | 0.084 (3) | −0.024 (2) | −0.032 (2) | −0.010 (2) |
| C11B | 0.077 (3) | 0.060 (3) | 0.084 (3) | −0.018 (2) | −0.039 (3) | −0.028 (2) |
| C12B | 0.071 (3) | 0.067 (3) | 0.069 (3) | −0.019 (2) | −0.021 (2) | −0.024 (2) |
| C13B | 0.057 (2) | 0.059 (2) | 0.071 (3) | −0.022 (2) | −0.015 (2) | −0.019 (2) |

| | | | | | |
|---|---|---|---|---|---|
| C14B | 0.048 (2) | 0.0373 (19) | 0.068 (3) | −0.0122 (18) | −0.0253 (19) | −0.0123 (17) |
| C16B | 0.149 (6) | 0.198 (7) | 0.106 (5) | −0.069 (5) | −0.017 (4) | −0.073 (5) |
| C17B | 0.0405 (19) | 0.045 (2) | 0.047 (2) | −0.0164 (17) | −0.0120 (16) | −0.0099 (16) |
| C19B | 0.051 (2) | 0.054 (2) | 0.052 (2) | −0.0200 (19) | −0.0189 (18) | −0.0117 (18) |
| C21B | 0.053 (2) | 0.053 (2) | 0.066 (2) | −0.024 (2) | −0.0200 (19) | −0.0179 (19) |
| C22B | 0.046 (2) | 0.050 (2) | 0.053 (2) | −0.0206 (18) | −0.0168 (17) | −0.0153 (17) |
| C24B | 0.093 (3) | 0.074 (3) | 0.093 (3) | −0.037 (3) | −0.054 (3) | −0.013 (2) |
| C25B | 0.078 (3) | 0.153 (6) | 0.130 (5) | −0.053 (4) | 0.004 (4) | −0.080 (5) |
| C26B | 0.183 (7) | 0.218 (8) | 0.060 (3) | −0.142 (6) | 0.007 (4) | −0.038 (4) |
| C27B | 0.129 (5) | 0.151 (5) | 0.088 (4) | −0.091 (4) | −0.024 (4) | 0.008 (4) |
| C28B | 0.080 (3) | 0.072 (3) | 0.075 (3) | −0.029 (2) | −0.039 (2) | 0.000 (2) |
| N8B | 0.063 (2) | 0.044 (2) | 0.069 (2) | −0.0237 (18) | −0.0241 (18) | −0.0068 (17) |
| N18B | 0.0494 (17) | 0.0500 (18) | 0.0552 (18) | −0.0203 (15) | −0.0207 (15) | −0.0107 (14) |
| N20B | 0.0531 (18) | 0.0488 (18) | 0.0597 (19) | −0.0193 (15) | −0.0220 (15) | −0.0133 (14) |
| N23B | 0.089 (2) | 0.057 (2) | 0.085 (2) | −0.0271 (19) | −0.053 (2) | −0.0065 (18) |
| O1B | 0.082 (2) | 0.092 (2) | 0.068 (2) | −0.0320 (18) | −0.0142 (16) | 0.0052 (16) |
| O2B | 0.121 (3) | 0.0620 (18) | 0.131 (3) | −0.0573 (19) | −0.072 (2) | 0.0182 (17) |
| O15B | 0.116 (3) | 0.145 (3) | 0.080 (2) | −0.040 (2) | −0.025 (2) | −0.053 (2) |
| S1B | 0.0707 (7) | 0.0570 (6) | 0.0778 (8) | −0.0323 (6) | −0.0318 (6) | 0.0054 (5) |
| S2B | 0.0585 (6) | 0.0522 (6) | 0.0688 (6) | −0.0244 (5) | −0.0297 (5) | −0.0067 (5) |
| Br1B | 0.0961 (3) | 0.0770 (3) | 0.0988 (4) | −0.0401 (3) | −0.0633 (3) | −0.0036 (2) |

## Geometric parameters (Å, º)

| | | | |
|---|---|---|---|
| C1A—C6A | 1.364 (5) | O1A—S1A | 1.427 (3) |
| C1A—C2A | 1.383 (5) | O2A—S1A | 1.435 (3) |
| C1A—S1A | 1.753 (4) | C1B—C6B | 1.358 (6) |
| C2A—C3A | 1.380 (6) | C1B—C2B | 1.366 (6) |
| C2A—H2A | 0.9300 | C1B—S1B | 1.756 (4) |
| C3A—C4A | 1.360 (7) | C2B—C3B | 1.391 (7) |
| C3A—H3A | 0.9300 | C2B—H2B | 0.9300 |
| C4A—C5A | 1.364 (6) | C3B—C4B | 1.351 (8) |
| C4A—H4A | 0.9300 | C3B—H3B | 0.9300 |
| C5A—C6A | 1.381 (6) | C4B—C5B | 1.334 (8) |
| C5A—H5A | 0.9300 | C4B—H4B | 0.9300 |
| C6A—H6A | 0.9300 | C5B—C6B | 1.387 (7) |
| C9A—C14A | 1.386 (5) | C5B—H5B | 0.9300 |
| C9A—C10A | 1.387 (5) | C6B—H6B | 0.9300 |
| C9A—N8A | 1.429 (4) | C9B—C14B | 1.382 (5) |
| C10A—C11A | 1.360 (5) | C9B—C10B | 1.393 (5) |
| C10A—H10A | 0.9300 | C9B—N8B | 1.423 (5) |
| C11A—C12A | 1.370 (6) | C10B—C11B | 1.388 (5) |
| C11A—H11A | 0.9300 | C10B—H10B | 0.9300 |
| C12A—O15C | 1.34 (2) | C11B—C12B | 1.367 (6) |
| C12A—C13A | 1.388 (5) | C11B—H11B | 0.9300 |
| C12A—O15A | 1.404 (17) | C12B—C13B | 1.375 (5) |
| O15A—C16A | 1.311 (14) | C12B—O15B | 1.385 (5) |
| C16A—H16D | 0.9600 | C13B—C14B | 1.392 (5) |

| | | | |
|---|---|---|---|
| C16A—H16E | 0.9600 | C13B—H13B | 0.9300 |
| C16A—H16F | 0.9600 | C14B—S2B | 1.774 (4) |
| O15C—C16C | 1.421 (16) | C16B—O15B | 1.358 (6) |
| C16C—H16G | 0.9600 | C16B—H16A | 0.9600 |
| C16C—H16H | 0.9600 | C16B—H16B | 0.9600 |
| C16C—H16I | 0.9600 | C16B—H16C | 0.9600 |
| C13A—C14A | 1.385 (5) | C17B—N18B | 1.315 (4) |
| C13A—H13A | 0.9300 | C17B—C22B | 1.391 (5) |
| C14A—S2A | 1.778 (4) | C17B—S2B | 1.766 (3) |
| C17A—N18A | 1.313 (4) | C19B—N20B | 1.350 (4) |
| C17A—C22A | 1.391 (5) | C19B—N18B | 1.351 (4) |
| C17A—S2A | 1.767 (4) | C19B—N23B | 1.353 (4) |
| C19A—N23A | 1.344 (4) | C21B—N20B | 1.330 (4) |
| C19A—N18A | 1.346 (4) | C21B—C22B | 1.363 (5) |
| C19A—N20A | 1.349 (4) | C21B—H21B | 0.9300 |
| C21A—N20A | 1.324 (4) | C22B—Br1B | 1.879 (3) |
| C21A—C22A | 1.373 (5) | C24B—N23B | 1.464 (5) |
| C21A—H21A | 0.9300 | C24B—C25B | 1.478 (6) |
| C22A—Br2 | 1.879 (3) | C24B—H24A | 0.9700 |
| C24A—C25A | 1.440 (6) | C24B—H24B | 0.9700 |
| C24A—N23A | 1.451 (5) | C25B—C26B | 1.501 (8) |
| C24A—H24C | 0.9700 | C25B—H25C | 0.9700 |
| C24A—H24D | 0.9700 | C25B—H25D | 0.9700 |
| C25A—C26A | 1.490 (7) | C26B—C27B | 1.526 (7) |
| C25A—H25A | 0.9700 | C26B—H26A | 0.9700 |
| C25A—H25B | 0.9700 | C26B—H26B | 0.9700 |
| C26A—C27A | 1.511 (7) | C27B—C28B | 1.498 (6) |
| C26A—H26C | 0.9700 | C27B—H27C | 0.9700 |
| C26A—H26D | 0.9700 | C27B—H27D | 0.9700 |
| C27A—C28A | 1.485 (6) | C28B—N23B | 1.448 (5) |
| C27A—H27A | 0.9700 | C28B—H28A | 0.9700 |
| C27A—H27B | 0.9700 | C28B—H28B | 0.9700 |
| C28A—N23A | 1.461 (5) | N8B—S1B | 1.622 (3) |
| C28A—H28C | 0.9700 | N8B—H8B | 0.78 (3) |
| C28A—H28D | 0.9700 | O1B—S1B | 1.430 (3) |
| N8A—S1A | 1.621 (3) | O2B—S1B | 1.426 (3) |
| N8A—H8A | 0.8600 | | |
| | | | |
| C6A—C1A—C2A | 119.3 (4) | O2A—S1A—N8A | 105.92 (17) |
| C6A—C1A—S1A | 120.1 (3) | O1A—S1A—C1A | 106.80 (19) |
| C2A—C1A—S1A | 120.5 (3) | O2A—S1A—C1A | 108.87 (19) |
| C3A—C2A—C1A | 119.9 (4) | N8A—S1A—C1A | 105.93 (16) |
| C3A—C2A—H2A | 120.1 | C17A—S2A—C14A | 100.74 (16) |
| C1A—C2A—H2A | 120.1 | C6B—C1B—C2B | 119.3 (4) |
| C4A—C3A—C2A | 120.3 (5) | C6B—C1B—S1B | 120.4 (4) |
| C4A—C3A—H3A | 119.8 | C2B—C1B—S1B | 120.4 (4) |
| C2A—C3A—H3A | 119.8 | C1B—C2B—C3B | 119.5 (5) |
| C3A—C4A—C5A | 119.9 (5) | C1B—C2B—H2B | 120.3 |

| | | | |
|---|---|---|---|
| C3A—C4A—H4A | 120.1 | C3B—C2B—H2B | 120.3 |
| C5A—C4A—H4A | 120.1 | C4B—C3B—C2B | 119.8 (5) |
| C4A—C5A—C6A | 120.3 (5) | C4B—C3B—H3B | 120.1 |
| C4A—C5A—H5A | 119.8 | C2B—C3B—H3B | 120.1 |
| C6A—C5A—H5A | 119.8 | C5B—C4B—C3B | 121.3 (6) |
| C1A—C6A—C5A | 120.2 (4) | C5B—C4B—H4B | 119.4 |
| C1A—C6A—H6A | 119.9 | C3B—C4B—H4B | 119.4 |
| C5A—C6A—H6A | 119.9 | C4B—C5B—C6B | 119.3 (6) |
| C14A—C9A—C10A | 118.9 (4) | C4B—C5B—H5B | 120.4 |
| C14A—C9A—N8A | 122.5 (3) | C6B—C5B—H5B | 120.4 |
| C10A—C9A—N8A | 118.6 (4) | C1B—C6B—C5B | 120.8 (5) |
| C11A—C10A—C9A | 121.3 (4) | C1B—C6B—H6B | 119.6 |
| C11A—C10A—H10A | 119.3 | C5B—C6B—H6B | 119.6 |
| C9A—C10A—H10A | 119.3 | C14B—C9B—C10B | 118.7 (4) |
| C10A—C11A—C12A | 119.7 (4) | C14B—C9B—N8B | 122.2 (3) |
| C10A—C11A—H11A | 120.1 | C10B—C9B—N8B | 119.1 (3) |
| C12A—C11A—H11A | 120.1 | C11B—C10B—C9B | 120.4 (4) |
| O15C—C12A—C11A | 129.2 (7) | C11B—C10B—H10B | 119.8 |
| O15C—C12A—C13A | 110.2 (7) | C9B—C10B—H10B | 119.8 |
| C11A—C12A—C13A | 120.5 (4) | C12B—C11B—C10B | 120.1 (4) |
| O15C—C12A—O15A | 20.6 (9) | C12B—C11B—H11B | 119.9 |
| C11A—C12A—O15A | 108.8 (6) | C10B—C11B—H11B | 119.9 |
| C13A—C12A—O15A | 130.6 (6) | C11B—C12B—C13B | 120.3 (4) |
| C16A—O15A—C12A | 110.2 (11) | C11B—C12B—O15B | 125.1 (4) |
| O15A—C16A—H16D | 109.5 | C13B—C12B—O15B | 114.6 (4) |
| O15A—C16A—H16E | 109.5 | C12B—C13B—C14B | 119.9 (4) |
| H16D—C16A—H16E | 109.5 | C12B—C13B—H13B | 120.1 |
| O15A—C16A—H16F | 109.5 | C14B—C13B—H13B | 120.1 |
| H16D—C16A—H16F | 109.5 | C9B—C14B—C13B | 120.5 (3) |
| H16E—C16A—H16F | 109.5 | C9B—C14B—S2B | 120.8 (3) |
| C12A—O15C—C16C | 116.7 (13) | C13B—C14B—S2B | 118.7 (3) |
| O15C—C16C—H16G | 109.5 | O15B—C16B—H16A | 109.5 |
| O15C—C16C—H16H | 109.5 | O15B—C16B—H16B | 109.5 |
| H16G—C16C—H16H | 109.5 | H16A—C16B—H16B | 109.5 |
| O15C—C16C—H16I | 109.5 | O15B—C16B—H16C | 109.5 |
| H16G—C16C—H16I | 109.5 | H16A—C16B—H16C | 109.5 |
| H16H—C16C—H16I | 109.5 | H16B—C16B—H16C | 109.5 |
| C14A—C13A—C12A | 119.4 (4) | N18B—C17B—C22B | 121.9 (3) |
| C14A—C13A—H13A | 120.3 | N18B—C17B—S2B | 119.1 (3) |
| C12A—C13A—H13A | 120.3 | C22B—C17B—S2B | 119.0 (3) |
| C13A—C14A—C9A | 120.0 (3) | N20B—C19B—N18B | 125.0 (3) |
| C13A—C14A—S2A | 119.9 (3) | N20B—C19B—N23B | 118.3 (3) |
| C9A—C14A—S2A | 120.1 (3) | N18B—C19B—N23B | 116.7 (3) |
| N18A—C17A—C22A | 121.1 (3) | N20B—C21B—C22B | 124.1 (4) |
| N18A—C17A—S2A | 119.8 (3) | N20B—C21B—H21B | 118.0 |
| C22A—C17A—S2A | 119.2 (3) | C22B—C21B—H21B | 118.0 |
| N23A—C19A—N18A | 116.9 (3) | C21B—C22B—C17B | 116.4 (3) |
| N23A—C19A—N20A | 117.9 (3) | C21B—C22B—Br1B | 122.5 (3) |

| | | | |
|---|---|---|---|
| N18A—C19A—N20A | 125.1 (3) | C17B—C22B—Br1B | 121.0 (3) |
| N20A—C21A—C22A | 123.9 (3) | N23B—C24B—C25B | 110.5 (4) |
| N20A—C21A—H21A | 118.0 | N23B—C24B—H24A | 109.6 |
| C22A—C21A—H21A | 118.0 | C25B—C24B—H24A | 109.6 |
| C21A—C22A—C17A | 116.7 (3) | N23B—C24B—H24B | 109.6 |
| C21A—C22A—Br2 | 120.7 (3) | C25B—C24B—H24B | 109.6 |
| C17A—C22A—Br2 | 122.6 (3) | H24A—C24B—H24B | 108.1 |
| C25A—C24A—N23A | 112.9 (4) | C24B—C25B—C26B | 111.2 (4) |
| C25A—C24A—H24C | 109.0 | C24B—C25B—H25C | 109.4 |
| N23A—C24A—H24C | 109.0 | C26B—C25B—H25C | 109.4 |
| C25A—C24A—H24D | 109.0 | C24B—C25B—H25D | 109.4 |
| N23A—C24A—H24D | 109.0 | C26B—C25B—H25D | 109.4 |
| H24C—C24A—H24D | 107.8 | H25C—C25B—H25D | 108.0 |
| C24A—C25A—C26A | 112.6 (5) | C25B—C26B—C27B | 110.3 (5) |
| C24A—C25A—H25A | 109.1 | C25B—C26B—H26A | 109.6 |
| C26A—C25A—H25A | 109.1 | C27B—C26B—H26A | 109.6 |
| C24A—C25A—H25B | 109.1 | C25B—C26B—H26B | 109.6 |
| C26A—C25A—H25B | 109.1 | C27B—C26B—H26B | 109.6 |
| H25A—C25A—H25B | 107.8 | H26A—C26B—H26B | 108.1 |
| C25A—C26A—C27A | 110.5 (4) | C28B—C27B—C26B | 111.6 (4) |
| C25A—C26A—H26C | 109.6 | C28B—C27B—H27C | 109.3 |
| C27A—C26A—H26C | 109.6 | C26B—C27B—H27C | 109.3 |
| C25A—C26A—H26D | 109.6 | C28B—C27B—H27D | 109.3 |
| C27A—C26A—H26D | 109.6 | C26B—C27B—H27D | 109.3 |
| H26C—C26A—H26D | 108.1 | H27C—C27B—H27D | 108.0 |
| C28A—C27A—C26A | 110.9 (4) | N23B—C28B—C27B | 109.9 (4) |
| C28A—C27A—H27A | 109.5 | N23B—C28B—H28A | 109.7 |
| C26A—C27A—H27A | 109.5 | C27B—C28B—H28A | 109.7 |
| C28A—C27A—H27B | 109.5 | N23B—C28B—H28B | 109.7 |
| C26A—C27A—H27B | 109.5 | C27B—C28B—H28B | 109.7 |
| H27A—C27A—H27B | 108.0 | H28A—C28B—H28B | 108.2 |
| N23A—C28A—C27A | 109.9 (4) | C9B—N8B—S1B | 121.4 (3) |
| N23A—C28A—H28C | 109.7 | C9B—N8B—H8B | 116 (3) |
| C27A—C28A—H28C | 109.7 | S1B—N8B—H8B | 111 (3) |
| N23A—C28A—H28D | 109.7 | C17B—N18B—C19B | 117.3 (3) |
| C27A—C28A—H28D | 109.7 | C21B—N20B—C19B | 115.2 (3) |
| H28C—C28A—H28D | 108.2 | C19B—N23B—C28B | 122.7 (4) |
| C9A—N8A—S1A | 120.2 (2) | C19B—N23B—C24B | 121.5 (3) |
| C9A—N8A—H8A | 119.9 | C28B—N23B—C24B | 113.7 (3) |
| S1A—N8A—H8A | 119.9 | C16B—O15B—C12B | 118.7 (5) |
| C17A—N18A—C19A | 118.0 (3) | O2B—S1B—O1B | 120.6 (2) |
| C21A—N20A—C19A | 115.1 (3) | O2B—S1B—N8B | 107.80 (19) |
| C19A—N23A—C24A | 123.3 (3) | O1B—S1B—N8B | 105.81 (19) |
| C19A—N23A—C28A | 122.0 (3) | O2B—S1B—C1B | 106.8 (2) |
| C24A—N23A—C28A | 114.7 (3) | O1B—S1B—C1B | 107.7 (2) |
| O1A—S1A—O2A | 120.56 (19) | N8B—S1B—C1B | 107.61 (18) |
| O1A—S1A—N8A | 107.91 (17) | C17B—S2B—C14B | 100.68 (16) |

| | | | |
|---|---|---|---|
| C6A—C1A—C2A—C3A | −1.1 (6) | C22A—C17A—S2A—C14A | 168.4 (3) |
| S1A—C1A—C2A—C3A | 175.5 (4) | C13A—C14A—S2A—C17A | 72.9 (3) |
| C1A—C2A—C3A—C4A | 1.1 (8) | C9A—C14A—S2A—C17A | −107.4 (3) |
| C2A—C3A—C4A—C5A | −0.2 (8) | C6B—C1B—C2B—C3B | 2.0 (7) |
| C3A—C4A—C5A—C6A | −0.6 (8) | S1B—C1B—C2B—C3B | −178.3 (4) |
| C2A—C1A—C6A—C5A | 0.2 (6) | C1B—C2B—C3B—C4B | −1.0 (9) |
| S1A—C1A—C6A—C5A | −176.4 (3) | C2B—C3B—C4B—C5B | −0.3 (11) |
| C4A—C5A—C6A—C1A | 0.6 (7) | C3B—C4B—C5B—C6B | 0.5 (11) |
| C14A—C9A—C10A—C11A | 0.4 (6) | C2B—C1B—C6B—C5B | −1.8 (9) |
| N8A—C9A—C10A—C11A | −179.1 (4) | S1B—C1B—C6B—C5B | 178.4 (5) |
| C9A—C10A—C11A—C12A | 1.4 (6) | C4B—C5B—C6B—C1B | 0.6 (11) |
| C10A—C11A—C12A—O15C | −178.5 (17) | C14B—C9B—C10B—C11B | −1.3 (5) |
| C10A—C11A—C12A—C13A | −1.2 (7) | N8B—C9B—C10B—C11B | 178.3 (3) |
| C10A—C11A—C12A—O15A | 177.8 (11) | C9B—C10B—C11B—C12B | −0.8 (6) |
| O15C—C12A—O15A—C16A | 4 (5) | C10B—C11B—C12B—C13B | 2.5 (6) |
| C11A—C12A—O15A—C16A | 176.4 (14) | C10B—C11B—C12B—O15B | −177.5 (4) |
| C13A—C12A—O15A—C16A | −5 (3) | C11B—C12B—C13B—C14B | −2.0 (6) |
| C11A—C12A—O15C—C16C | 2 (3) | O15B—C12B—C13B—C14B | 178.0 (3) |
| C13A—C12A—O15C—C16C | −175.4 (18) | C10B—C9B—C14B—C13B | 1.8 (5) |
| O15A—C12A—O15C—C16C | 12 (4) | N8B—C9B—C14B—C13B | −177.8 (3) |
| O15C—C12A—C13A—C14A | 177.0 (14) | C10B—C9B—C14B—S2B | −178.7 (3) |
| C11A—C12A—C13A—C14A | −0.8 (6) | N8B—C9B—C14B—S2B | 1.7 (5) |
| O15A—C12A—C13A—C14A | −179.6 (13) | C12B—C13B—C14B—C9B | −0.1 (5) |
| C12A—C13A—C14A—C9A | 2.6 (5) | C12B—C13B—C14B—S2B | −179.6 (3) |
| C12A—C13A—C14A—S2A | −177.8 (3) | N20B—C21B—C22B—C17B | −1.8 (5) |
| C10A—C9A—C14A—C13A | −2.4 (5) | N20B—C21B—C22B—Br1B | 176.9 (3) |
| N8A—C9A—C14A—C13A | 177.1 (3) | N18B—C17B—C22B—C21B | 1.3 (5) |
| C10A—C9A—C14A—S2A | 178.0 (3) | S2B—C17B—C22B—C21B | −179.4 (3) |
| N8A—C9A—C14A—S2A | −2.5 (5) | N18B—C17B—C22B—Br1B | −177.4 (3) |
| N20A—C21A—C22A—C17A | −2.7 (5) | S2B—C17B—C22B—Br1B | 1.9 (4) |
| N20A—C21A—C22A—Br2 | 179.0 (3) | N23B—C24B—C25B—C26B | −56.1 (6) |
| N18A—C17A—C22A—C21A | 3.0 (5) | C24B—C25B—C26B—C27B | 54.2 (7) |
| S2A—C17A—C22A—C21A | −177.3 (2) | C25B—C26B—C27B—C28B | −53.4 (7) |
| N18A—C17A—C22A—Br2 | −178.7 (2) | C26B—C27B—C28B—N23B | 54.0 (6) |
| S2A—C17A—C22A—Br2 | 1.0 (4) | C14B—C9B—N8B—S1B | −107.0 (4) |
| N23A—C24A—C25A—C26A | 51.0 (6) | C10B—C9B—N8B—S1B | 73.5 (4) |
| C24A—C25A—C26A—C27A | −53.1 (7) | C22B—C17B—N18B—C19B | 1.9 (5) |
| C25A—C26A—C27A—C28A | 55.4 (7) | S2B—C17B—N18B—C19B | −177.5 (2) |
| C26A—C27A—C28A—N23A | −55.0 (6) | N20B—C19B—N18B—C17B | −5.0 (5) |
| C14A—C9A—N8A—S1A | −98.8 (4) | N23B—C19B—N18B—C17B | 177.5 (3) |
| C10A—C9A—N8A—S1A | 80.7 (4) | C22B—C21B—N20B—C19B | −0.9 (5) |
| C22A—C17A—N18A—C19A | −0.2 (5) | N18B—C19B—N20B—C21B | 4.5 (5) |
| S2A—C17A—N18A—C19A | −179.9 (3) | N23B—C19B—N20B—C21B | −178.0 (3) |
| N23A—C19A—N18A—C17A | 176.7 (3) | N20B—C19B—N23B—C28B | 12.8 (6) |
| N20A—C19A—N18A—C17A | −3.2 (5) | N18B—C19B—N23B—C28B | −169.5 (3) |
| C22A—C21A—N20A—C19A | −0.3 (5) | N20B—C19B—N23B—C24B | 175.6 (3) |
| N23A—C19A—N20A—C21A | −176.4 (3) | N18B—C19B—N23B—C24B | −6.7 (6) |
| N18A—C19A—N20A—C21A | 3.5 (5) | C27B—C28B—N23B—C19B | 106.9 (5) |

| | | | |
|---|---|---|---|
| N18A—C19A—N23A—C24A | 176.7 (4) | C27B—C28B—N23B—C24B | −57.1 (5) |
| N20A—C19A—N23A—C24A | −3.3 (6) | C25B—C24B—N23B—C19B | −105.7 (5) |
| N18A—C19A—N23A—C28A | −3.6 (6) | C25B—C24B—N23B—C28B | 58.5 (5) |
| N20A—C19A—N23A—C28A | 176.3 (4) | C11B—C12B—O15B—C16B | 14.2 (7) |
| C25A—C24A—N23A—C19A | 127.6 (5) | C13B—C12B—O15B—C16B | −165.9 (5) |
| C25A—C24A—N23A—C28A | −52.1 (6) | C9B—N8B—S1B—O2B | −55.9 (4) |
| C27A—C28A—N23A—C19A | −126.0 (4) | C9B—N8B—S1B—O1B | 173.8 (3) |
| C27A—C28A—N23A—C24A | 53.7 (6) | C9B—N8B—S1B—C1B | 58.9 (4) |
| C9A—N8A—S1A—O1A | −53.6 (3) | C6B—C1B—S1B—O2B | −160.6 (4) |
| C9A—N8A—S1A—O2A | 176.0 (3) | C2B—C1B—S1B—O2B | 19.7 (4) |
| C9A—N8A—S1A—C1A | 60.5 (3) | C6B—C1B—S1B—O1B | −29.7 (5) |
| C6A—C1A—S1A—O1A | −151.9 (3) | C2B—C1B—S1B—O1B | 150.5 (3) |
| C2A—C1A—S1A—O1A | 31.5 (4) | C6B—C1B—S1B—N8B | 83.9 (4) |
| C6A—C1A—S1A—O2A | −20.3 (4) | C2B—C1B—S1B—N8B | −95.9 (4) |
| C2A—C1A—S1A—O2A | 163.2 (3) | N18B—C17B—S2B—C14B | 4.3 (3) |
| C6A—C1A—S1A—N8A | 93.2 (3) | C22B—C17B—S2B—C14B | −175.1 (3) |
| C2A—C1A—S1A—N8A | −83.3 (3) | C9B—C14B—S2B—C17B | −109.7 (3) |
| N18A—C17A—S2A—C14A | −11.8 (3) | C13B—C14B—S2B—C17B | 69.8 (3) |

*Hydrogen-bond geometry (Å, º)*

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N8$A$—H8$A$⋯N20$A$[i] | 0.86 | 2.15 | 2.940 (4) | 152 |
| N8$B$—H8$B$⋯N20$B$[ii] | 0.78 (4) | 2.28 (4) | 2.974 (5) | 149 (4) |
| C11$A$—H11$A$⋯O1$A$[iii] | 0.93 | 2.47 | 3.372 (5) | 164 |
| C10$B$—H10$B$⋯O2$B$[iv] | 0.93 | 2.60 | 3.278 (6) | 131 |

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