

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N-[2-(5-Bromo-2-morpholin-4-ylpyrimidin-4-ylsulfanyl)-4-methoxyphenyl]-2,4,6-trimethylbenzenesulfonamide

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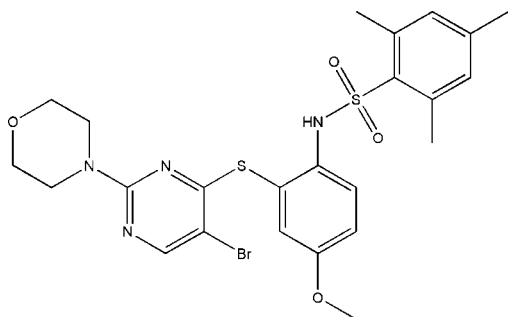
Received 25 September 2012; accepted 27 September 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.046; wR factor = 0.105; data-to-parameter ratio = 15.6.

In the title compound, $\text{C}_{24}\text{H}_{27}\text{BrN}_4\text{O}_4\text{S}_2$, the molecule is twisted at the sulfonyl S atom with a $\text{C}-\text{S}(\text{O}_2)-\text{N}(\text{H})-\text{C}$ torsion angle of $62.6(3)^\circ$. The benzene rings bridged by the sulfonamide group are tilted to each other by a dihedral angle of $60.6(1)^\circ$. The dihedral angle between the sulfur-bridged pyrimidine and benzene rings is $62.7(1)^\circ$. The morpholine ring adopts a chair conformation. The molecular conformation is stabilized by a weak intramolecular $\pi-\pi$ stacking interaction between the pyrimidine and the 2,4,6-trimethylbenzene rings [centroid-centroid distance = $3.793(2)$ Å]. In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into a chain along the b axis.

Related literature

For related structures of sulfonamides, see: Rodrigues *et al.* (2011); Akkurt *et al.* (2011); Kant *et al.* (2012). For bond-length data, see: Allen *et al.* (1987). For ring conformations, see: Duax & Norton (1975).



Experimental

Crystal data

$\text{C}_{24}\text{H}_{27}\text{BrN}_4\text{O}_4\text{S}_2$
 $M_r = 579.53$
 Monoclinic, $P2_1/n$
 $a = 10.2583(4)$ Å
 $b = 17.4727(6)$ Å
 $c = 14.4375(7)$ Å
 $\beta = 97.199(4)^\circ$
 $V = 2567.38(18)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.80$ mm⁻¹
 $T = 293$ K
 $0.3 \times 0.2 \times 0.2$ mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
 Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
 $T_{\min} = 0.526$, $T_{\max} = 0.697$
 19056 measured reflections
 5023 independent reflections
 3359 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.105$
 $S = 1.02$
 5023 reflections
 321 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.31$ e Å⁻³
 $\Delta\rho_{\min} = -0.39$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| $\text{N1}-\text{H1}\cdots\text{O25}^i$ | 0.86 | 2.09 | 2.890 (4) | 155 |

 Symmetry code: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

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).

MK acknowledges the help of Bahubali College of Engineering, Shravanabelagola for his research work. RK acknowledges the Department of Science & Technology for the single-crystal X-ray diffractometer sanctioned as a National Facility under project No. SR/S2/CMP-47/2003.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5200).

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supporting information

Acta Cryst. (2012). E68, o3061 [doi:10.1107/S1600536812040792]

***N*-[2-(5-Bromo-2-morpholin-4-ylpyrimidin-4-ylsulfanyl)-4-methoxy-phenyl]-2,4,6-trimethylbenzenesulfonamide**

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S1. Comment

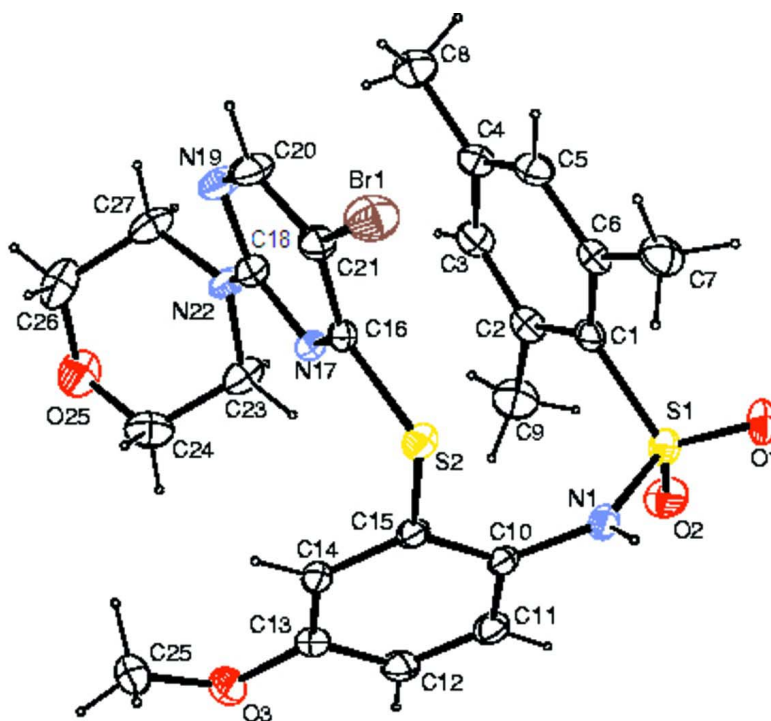
Bond lengths and angles in the title compound (Fig. 1) have normal values (Allen *et al.*, 1987) and are comparable with the similar crystal structures (Rodrigues *et al.*, 2011; Akkurt *et al.*, 2011; Kant *et al.*, 2012). The molecule is twisted at the S atom with the C2—S1—N1—C10 torsion angle of 62.6 (3)°. The morpholine ring is exhibiting chair conformation (asymmetry parameters are: [$\Delta C2(N22—C27) = 2.51$; $\Delta Cs(C24—C27) = 0.92$] (Duax & Norton, 1975). The benzene C1—C6 and C10—C15 rings are tilted relative to each other by 60.6 (1)° and the dihedral angle between the sulfur bridged pyrimidine and benzene rings is 62.7 (1)°. The molecular conformation is stabilized by a weak intramolecular π – π stacking interaction between the pyrimidine C16/N17/C18/N19/C20/C21 ring (centroid Cg1) and the 2,4,6-trimethyl benzene C1—C6 ring (centroid Cg2) [$Cg1 \cdots Cg2$ 3.793 (2) Å, perpendicular distance of Cg1 on the C1—C6 ring 3.5103 (13) Å and perpendicular distance of Cg2 on the C16/N17/C18/N19/C20/C21 ring 3.3905 (12) Å]. In the crystal, molecules are linked into chains by N1—H1 \cdots O25 hydrogen bonds (Table 1 and Fig. 2).

S2. Experimental

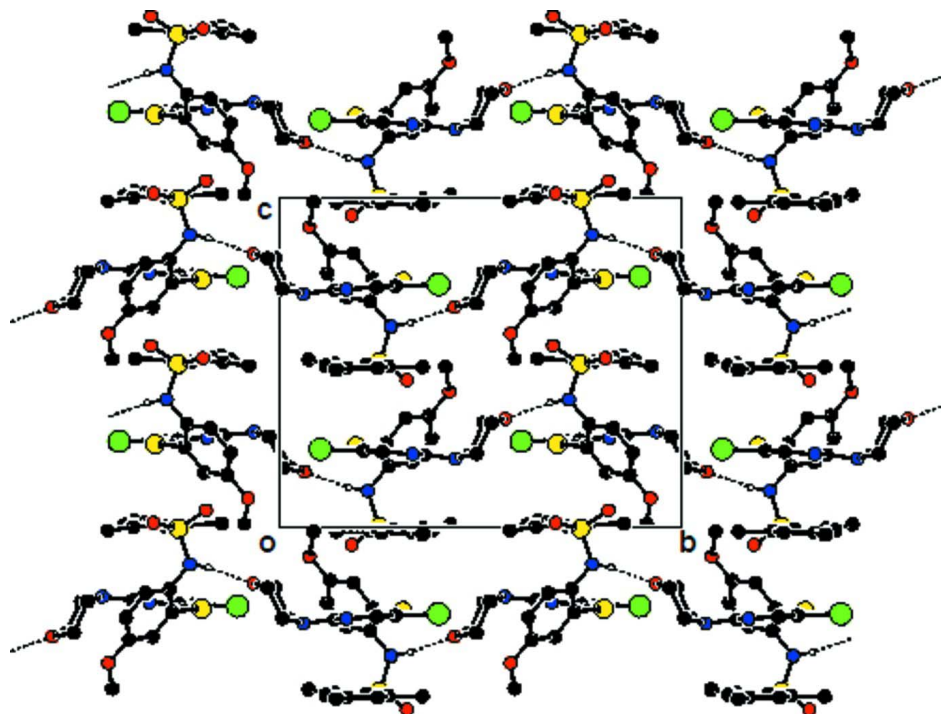
The reaction of *N*-[2-(5-bromo-2-morpholin-4-yl-pyrimidin-4-ylsulfanyl)-4-methoxy-phenyl]-2,4,6-trimethyl-benzene-sulfonamide (5.29 g, 0.01 mol) with morpholine (0.88 g, 0.01 mol) were carried out in the presence of triethylamine and the reaction mixture was allowed to stir at room temperature for 6–7 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 83%, m.p. 454–456 K).

S3. Refinement

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

**Figure 1**

ORTEP view of the molecule with the atom-labeling scheme. The displacement ellipsoids are drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

**Figure 2**

A molecular packing view of the title compound down the *a* axis, showing intermolecular interactions (dashed lines). For clarity, H atoms not involved in the hydrogen bonds have been omitted.

N*-[2-(5-Bromo-2-morpholin-4-ylpyrimidin-4-ylsulfanyl)-4-methoxyphenyl]-2,4,6-trimethylbenzenesulfonamideCrystal data*C₂₄H₂₇BrN₄O₄S₂ $M_r = 579.53$ Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

 $a = 10.2583$ (4) Å $b = 17.4727$ (6) Å $c = 14.4375$ (7) Å $\beta = 97.199$ (4)° $V = 2567.38$ (18) Å³ $Z = 4$ $F(000) = 1192$ $D_x = 1.499$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6670 reflections

 $\theta = 3.7$ – 29.0 ° $\mu = 1.80$ mm⁻¹ $T = 293$ K

Block, brown

 $0.3 \times 0.2 \times 0.2$ mm*Data collection*Oxford Diffraction Xcalibur Sapphire3
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 16.1049 pixels mm⁻¹ ω scan

Absorption correction: multi-scan

(CrysAlis PRO; Oxford Diffraction, 2010)

 $T_{\min} = 0.526$, $T_{\max} = 0.697$

19056 measured reflections

5023 independent reflections

3359 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.045$ $\theta_{\max} = 26.0$ °, $\theta_{\min} = 3.7$ ° $h = -12$ → 12 $k = -21$ → 21 $l = -17$ → 17 *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.046$ $wR(F^2) = 0.105$ $S = 1.02$

5023 reflections

321 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 1.6315P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.31$ e Å⁻³ $\Delta\rho_{\min} = -0.39$ e Å⁻³

Extinction correction: SHELXL,

 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0057 (4)

*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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|---------------|----------------------------------|
| Br1 | 1.02664 (4) | 0.10295 (2) | 0.23807 (3) | 0.07706 (19) |
| S1 | 0.50455 (9) | 0.24940 (6) | 0.00299 (6) | 0.0566 (3) |
| S2 | 0.74901 (8) | 0.19238 (5) | 0.24649 (6) | 0.0472 (2) |
| N1 | 0.5008 (2) | 0.22120 (16) | 0.11087 (18) | 0.0487 (7) |
| H1 | 0.4848 | 0.1739 | 0.1215 | 0.058* |
| O1 | 0.4808 (3) | 0.18139 (17) | -0.05220 (17) | 0.0788 (8) |
| O2 | 0.4152 (2) | 0.31164 (17) | -0.01409 (18) | 0.0774 (8) |
| O3 | 0.5639 (3) | 0.42389 (15) | 0.41145 (19) | 0.0704 (7) |
| C1 | 0.6672 (3) | 0.28269 (18) | -0.0041 (2) | 0.0430 (8) |
| C2 | 0.6972 (4) | 0.36148 (19) | -0.0014 (2) | 0.0508 (9) |
| C3 | 0.8256 (4) | 0.3831 (2) | -0.0079 (2) | 0.0562 (9) |
| H3 | 0.8455 | 0.4350 | -0.0071 | 0.067* |
| C4 | 0.9252 (3) | 0.3316 (2) | -0.0154 (2) | 0.0535 (9) |
| C5 | 0.8941 (3) | 0.2553 (2) | -0.0154 (2) | 0.0527 (9) |
| H5 | 0.9608 | 0.2197 | -0.0187 | 0.063* |
| C6 | 0.7666 (3) | 0.22861 (18) | -0.0106 (2) | 0.0460 (8) |
| C7 | 0.7498 (4) | 0.14289 (19) | -0.0125 (3) | 0.0681 (11) |
| H7A | 0.7078 | 0.1274 | -0.0727 | 0.102* |
| H7B | 0.6966 | 0.1278 | 0.0346 | 0.102* |
| H7C | 0.8344 | 0.1188 | -0.0005 | 0.102* |
| C8 | 1.0642 (4) | 0.3581 (3) | -0.0207 (3) | 0.0791 (12) |
| H8A | 1.0826 | 0.3555 | -0.0842 | 0.119* |
| H8B | 1.1244 | 0.3257 | 0.0176 | 0.119* |
| H8C | 1.0740 | 0.4100 | 0.0011 | 0.119* |
| C9 | 0.6004 (4) | 0.4257 (2) | 0.0093 (3) | 0.0787 (13) |
| H9A | 0.5321 | 0.4249 | -0.0427 | 0.118* |
| H9B | 0.6453 | 0.4739 | 0.0110 | 0.118* |
| H9C | 0.5625 | 0.4187 | 0.0662 | 0.118* |
| C10 | 0.5231 (3) | 0.27276 (18) | 0.1873 (2) | 0.0412 (7) |
| C11 | 0.4332 (3) | 0.3308 (2) | 0.1984 (2) | 0.0532 (9) |
| H11 | 0.3594 | 0.3360 | 0.1544 | 0.064* |
| C12 | 0.4508 (3) | 0.3801 (2) | 0.2724 (3) | 0.0553 (9) |
| H12 | 0.3902 | 0.4191 | 0.2774 | 0.066* |
| C13 | 0.5583 (3) | 0.3723 (2) | 0.3399 (2) | 0.0503 (8) |
| C14 | 0.6476 (3) | 0.31466 (18) | 0.3324 (2) | 0.0446 (8) |
| H14 | 0.7183 | 0.3082 | 0.3787 | 0.054* |
| C15 | 0.6321 (3) | 0.26588 (18) | 0.2552 (2) | 0.0409 (7) |
| C16 | 0.8899 (3) | 0.24701 (19) | 0.2337 (2) | 0.0404 (7) |
| N17 | 0.8793 (2) | 0.32166 (15) | 0.22635 (17) | 0.0414 (6) |
| C18 | 0.9896 (3) | 0.3618 (2) | 0.2209 (2) | 0.0490 (8) |
| N19 | 1.1113 (3) | 0.33241 (18) | 0.2232 (2) | 0.0611 (8) |
| C20 | 1.1185 (3) | 0.2570 (2) | 0.2294 (3) | 0.0614 (10) |
| H20 | 1.2006 | 0.2341 | 0.2313 | 0.074* |
| C21 | 1.0110 (3) | 0.2104 (2) | 0.2331 (2) | 0.0504 (8) |
| N22 | 0.9747 (3) | 0.43869 (16) | 0.2097 (2) | 0.0575 (8) |

| | | | | |
|------|------------|--------------|------------|-------------|
| C23 | 0.8513 (3) | 0.4755 (2) | 0.2241 (3) | 0.0623 (10) |
| H23A | 0.7806 | 0.4382 | 0.2173 | 0.075* |
| H23B | 0.8303 | 0.5154 | 0.1780 | 0.075* |
| C24 | 0.8650 (4) | 0.5089 (2) | 0.3196 (3) | 0.0726 (12) |
| H24A | 0.7834 | 0.5335 | 0.3300 | 0.087* |
| H24B | 0.8829 | 0.4685 | 0.3655 | 0.087* |
| O25 | 0.9689 (3) | 0.56335 (15) | 0.3307 (2) | 0.0848 (9) |
| C25 | 0.6630 (4) | 0.4143 (2) | 0.4887 (3) | 0.0773 (12) |
| H25A | 0.6544 | 0.3647 | 0.5158 | 0.116* |
| H25B | 0.6535 | 0.4531 | 0.5345 | 0.116* |
| H25C | 0.7479 | 0.4187 | 0.4679 | 0.116* |
| C26 | 1.0905 (4) | 0.5289 (2) | 0.3180 (3) | 0.0808 (14) |
| H26A | 1.1128 | 0.4909 | 0.3663 | 0.097* |
| H26B | 1.1589 | 0.5676 | 0.3241 | 0.097* |
| C27 | 1.0850 (3) | 0.4917 (2) | 0.2245 (3) | 0.0679 (11) |
| H27A | 1.0756 | 0.5306 | 0.1761 | 0.082* |
| H27B | 1.1663 | 0.4643 | 0.2204 | 0.082* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Br1 | 0.0695 (3) | 0.0623 (3) | 0.1013 (4) | 0.0199 (2) | 0.0181 (2) | 0.0000 (2) |
| S1 | 0.0426 (5) | 0.0840 (7) | 0.0398 (5) | -0.0032 (5) | -0.0080 (4) | -0.0043 (5) |
| S2 | 0.0379 (4) | 0.0491 (5) | 0.0532 (5) | -0.0001 (4) | 0.0004 (4) | -0.0006 (4) |
| N1 | 0.0435 (16) | 0.0588 (17) | 0.0423 (16) | -0.0127 (14) | -0.0004 (12) | -0.0017 (14) |
| O1 | 0.0723 (18) | 0.108 (2) | 0.0522 (16) | -0.0252 (16) | -0.0088 (13) | -0.0267 (16) |
| O2 | 0.0485 (15) | 0.118 (2) | 0.0611 (17) | 0.0205 (15) | -0.0109 (12) | 0.0180 (16) |
| O3 | 0.0646 (17) | 0.0829 (18) | 0.0653 (18) | 0.0025 (14) | 0.0142 (14) | -0.0251 (15) |
| C1 | 0.0422 (18) | 0.056 (2) | 0.0294 (16) | 0.0062 (16) | 0.0000 (14) | -0.0014 (15) |
| C2 | 0.062 (2) | 0.048 (2) | 0.043 (2) | 0.0115 (17) | 0.0059 (17) | 0.0018 (16) |
| C3 | 0.072 (3) | 0.046 (2) | 0.053 (2) | -0.0036 (19) | 0.0172 (19) | 0.0023 (17) |
| C4 | 0.056 (2) | 0.062 (2) | 0.045 (2) | -0.0007 (19) | 0.0162 (16) | 0.0007 (18) |
| C5 | 0.053 (2) | 0.054 (2) | 0.052 (2) | 0.0127 (17) | 0.0136 (17) | -0.0006 (17) |
| C6 | 0.057 (2) | 0.0443 (18) | 0.0370 (18) | 0.0048 (16) | 0.0079 (15) | -0.0056 (15) |
| C7 | 0.080 (3) | 0.050 (2) | 0.078 (3) | 0.002 (2) | 0.024 (2) | -0.011 (2) |
| C8 | 0.068 (3) | 0.090 (3) | 0.083 (3) | -0.013 (2) | 0.024 (2) | -0.002 (2) |
| C9 | 0.079 (3) | 0.061 (2) | 0.097 (3) | 0.027 (2) | 0.014 (2) | 0.000 (2) |
| C10 | 0.0296 (16) | 0.0559 (19) | 0.0381 (17) | -0.0055 (15) | 0.0044 (13) | 0.0027 (16) |
| C11 | 0.0321 (18) | 0.072 (2) | 0.054 (2) | 0.0021 (17) | 0.0027 (15) | 0.006 (2) |
| C12 | 0.040 (2) | 0.067 (2) | 0.061 (2) | 0.0101 (17) | 0.0152 (17) | -0.003 (2) |
| C13 | 0.043 (2) | 0.061 (2) | 0.049 (2) | -0.0048 (17) | 0.0149 (16) | -0.0064 (18) |
| C14 | 0.0362 (17) | 0.062 (2) | 0.0356 (18) | -0.0064 (16) | 0.0027 (14) | 0.0004 (16) |
| C15 | 0.0289 (16) | 0.0535 (19) | 0.0403 (18) | -0.0021 (14) | 0.0043 (13) | 0.0047 (15) |
| C16 | 0.0340 (17) | 0.056 (2) | 0.0294 (16) | 0.0019 (15) | -0.0008 (12) | -0.0041 (15) |
| N17 | 0.0294 (14) | 0.0520 (17) | 0.0424 (15) | 0.0012 (12) | 0.0025 (11) | -0.0056 (13) |
| C18 | 0.0378 (19) | 0.058 (2) | 0.050 (2) | 0.0022 (17) | 0.0043 (15) | -0.0052 (17) |
| N19 | 0.0327 (16) | 0.068 (2) | 0.084 (2) | 0.0034 (15) | 0.0117 (15) | -0.0023 (18) |
| C20 | 0.0334 (19) | 0.074 (3) | 0.079 (3) | 0.0102 (19) | 0.0130 (18) | -0.001 (2) |

| | | | | | | |
|-----|-------------|-------------|-----------|--------------|--------------|--------------|
| C21 | 0.0423 (19) | 0.058 (2) | 0.051 (2) | 0.0100 (17) | 0.0057 (15) | -0.0047 (17) |
| N22 | 0.0324 (15) | 0.0558 (18) | 0.085 (2) | -0.0048 (14) | 0.0119 (14) | -0.0099 (16) |
| C23 | 0.041 (2) | 0.049 (2) | 0.096 (3) | 0.0003 (17) | 0.007 (2) | 0.002 (2) |
| C24 | 0.078 (3) | 0.054 (2) | 0.092 (3) | 0.013 (2) | 0.033 (2) | 0.010 (2) |
| O25 | 0.081 (2) | 0.0571 (17) | 0.113 (3) | 0.0073 (16) | -0.0002 (18) | -0.0187 (16) |
| C25 | 0.079 (3) | 0.100 (3) | 0.055 (2) | -0.021 (2) | 0.014 (2) | -0.026 (2) |
| C26 | 0.065 (3) | 0.057 (2) | 0.112 (4) | -0.005 (2) | -0.022 (3) | 0.001 (3) |
| C27 | 0.040 (2) | 0.061 (2) | 0.104 (3) | -0.0081 (18) | 0.014 (2) | 0.008 (2) |

Geometric parameters (Å, °)

| | | | |
|----------|-------------|-------------|-----------|
| Br1—C21 | 1.885 (3) | C11—C12 | 1.368 (5) |
| S1—O2 | 1.424 (3) | C11—H11 | 0.9300 |
| S1—O1 | 1.434 (3) | C12—C13 | 1.384 (5) |
| S1—N1 | 1.639 (3) | C12—H12 | 0.9300 |
| S1—C1 | 1.782 (3) | C13—C14 | 1.376 (4) |
| S2—C16 | 1.761 (3) | C14—C15 | 1.396 (4) |
| S2—C15 | 1.772 (3) | C14—H14 | 0.9300 |
| N1—C10 | 1.421 (4) | C16—N17 | 1.312 (4) |
| N1—H1 | 0.8600 | C16—C21 | 1.399 (4) |
| O3—C13 | 1.367 (4) | N17—C18 | 1.342 (4) |
| O3—C25 | 1.421 (5) | C18—N19 | 1.347 (4) |
| C1—C6 | 1.402 (4) | C18—N22 | 1.359 (4) |
| C1—C2 | 1.410 (4) | N19—C20 | 1.322 (4) |
| C2—C3 | 1.385 (5) | C20—C21 | 1.377 (5) |
| C2—C9 | 1.519 (5) | C20—H20 | 0.9300 |
| C3—C4 | 1.375 (5) | N22—C27 | 1.457 (4) |
| C3—H3 | 0.9300 | N22—C23 | 1.458 (4) |
| C4—C5 | 1.371 (5) | C23—C24 | 1.487 (5) |
| C4—C8 | 1.511 (5) | C23—H23A | 0.9700 |
| C5—C6 | 1.398 (5) | C23—H23B | 0.9700 |
| C5—H5 | 0.9300 | C24—O25 | 1.423 (5) |
| C6—C7 | 1.508 (4) | C24—H24A | 0.9700 |
| C7—H7A | 0.9600 | C24—H24B | 0.9700 |
| C7—H7B | 0.9600 | O25—C26 | 1.417 (5) |
| C7—H7C | 0.9600 | C25—H25A | 0.9600 |
| C8—H8A | 0.9600 | C25—H25B | 0.9600 |
| C8—H8B | 0.9600 | C25—H25C | 0.9600 |
| C8—H8C | 0.9600 | C26—C27 | 1.493 (6) |
| C9—H9A | 0.9600 | C26—H26A | 0.9700 |
| C9—H9B | 0.9600 | C26—H26B | 0.9700 |
| C9—H9C | 0.9600 | C27—H27A | 0.9700 |
| C10—C11 | 1.393 (4) | C27—H27B | 0.9700 |
| C10—C15 | 1.396 (4) | | |
| O2—S1—O1 | 118.40 (17) | O3—C13—C12 | 115.0 (3) |
| O2—S1—N1 | 107.62 (16) | C14—C13—C12 | 119.8 (3) |
| O1—S1—N1 | 104.85 (16) | C13—C14—C15 | 120.0 (3) |

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|-------------|-------------|---------------|-----------|
| O2—S1—C1 | 109.14 (16) | C13—C14—H14 | 120.0 |
| O1—S1—C1 | 109.49 (16) | C15—C14—H14 | 120.0 |
| N1—S1—C1 | 106.67 (13) | C14—C15—C10 | 120.6 (3) |
| C16—S2—C15 | 100.73 (15) | C14—C15—S2 | 119.2 (2) |
| C10—N1—S1 | 121.8 (2) | C10—C15—S2 | 120.1 (2) |
| C10—N1—H1 | 119.1 | N17—C16—C21 | 121.2 (3) |
| S1—N1—H1 | 119.1 | N17—C16—S2 | 119.1 (2) |
| C13—O3—C25 | 118.3 (3) | C21—C16—S2 | 119.6 (3) |
| C6—C1—C2 | 120.1 (3) | C16—N17—C18 | 117.6 (3) |
| C6—C1—S1 | 118.6 (2) | N17—C18—N19 | 125.8 (3) |
| C2—C1—S1 | 121.3 (2) | N17—C18—N22 | 116.2 (3) |
| C3—C2—C1 | 118.0 (3) | N19—C18—N22 | 118.1 (3) |
| C3—C2—C9 | 116.5 (3) | C20—N19—C18 | 115.2 (3) |
| C1—C2—C9 | 125.5 (3) | N19—C20—C21 | 123.6 (3) |
| C4—C3—C2 | 123.3 (3) | N19—C20—H20 | 118.2 |
| C4—C3—H3 | 118.3 | C21—C20—H20 | 118.2 |
| C2—C3—H3 | 118.3 | C20—C21—C16 | 116.5 (3) |
| C5—C4—C3 | 117.4 (3) | C20—C21—Br1 | 121.7 (3) |
| C5—C4—C8 | 121.3 (3) | C16—C21—Br1 | 121.8 (3) |
| C3—C4—C8 | 121.3 (3) | C18—N22—C27 | 122.5 (3) |
| C4—C5—C6 | 122.9 (3) | C18—N22—C23 | 120.3 (3) |
| C4—C5—H5 | 118.6 | C27—N22—C23 | 111.8 (3) |
| C6—C5—H5 | 118.6 | N22—C23—C24 | 108.8 (3) |
| C5—C6—C1 | 118.1 (3) | N22—C23—H23A | 109.9 |
| C5—C6—C7 | 115.8 (3) | C24—C23—H23A | 109.9 |
| C1—C6—C7 | 126.0 (3) | N22—C23—H23B | 109.9 |
| C6—C7—H7A | 109.5 | C24—C23—H23B | 109.9 |
| C6—C7—H7B | 109.5 | H23A—C23—H23B | 108.3 |
| H7A—C7—H7B | 109.5 | O25—C24—C23 | 110.5 (3) |
| C6—C7—H7C | 109.5 | O25—C24—H24A | 109.6 |
| H7A—C7—H7C | 109.5 | C23—C24—H24A | 109.6 |
| H7B—C7—H7C | 109.5 | O25—C24—H24B | 109.6 |
| C4—C8—H8A | 109.5 | C23—C24—H24B | 109.6 |
| C4—C8—H8B | 109.5 | H24A—C24—H24B | 108.1 |
| H8A—C8—H8B | 109.5 | C26—O25—C24 | 111.1 (3) |
| C4—C8—H8C | 109.5 | O3—C25—H25A | 109.5 |
| H8A—C8—H8C | 109.5 | O3—C25—H25B | 109.5 |
| H8B—C8—H8C | 109.5 | H25A—C25—H25B | 109.5 |
| C2—C9—H9A | 109.5 | O3—C25—H25C | 109.5 |
| C2—C9—H9B | 109.5 | H25A—C25—H25C | 109.5 |
| H9A—C9—H9B | 109.5 | H25B—C25—H25C | 109.5 |
| C2—C9—H9C | 109.5 | O25—C26—C27 | 111.6 (3) |
| H9A—C9—H9C | 109.5 | O25—C26—H26A | 109.3 |
| H9B—C9—H9C | 109.5 | C27—C26—H26A | 109.3 |
| C11—C10—C15 | 117.7 (3) | O25—C26—H26B | 109.3 |
| C11—C10—N1 | 120.4 (3) | C27—C26—H26B | 109.3 |
| C15—C10—N1 | 121.9 (3) | H26A—C26—H26B | 108.0 |
| C12—C11—C10 | 121.6 (3) | N22—C27—C26 | 110.5 (3) |

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| C12—C11—H11 | 119.2 | N22—C27—H27A | 109.6 |
| C10—C11—H11 | 119.2 | C26—C27—H27A | 109.6 |
| C11—C12—C13 | 120.2 (3) | N22—C27—H27B | 109.6 |
| C11—C12—H12 | 119.9 | C26—C27—H27B | 109.6 |
| C13—C12—H12 | 119.9 | H27A—C27—H27B | 108.1 |
| O3—C13—C14 | 125.2 (3) | | |
| O2—S1—N1—C10 | -54.4 (3) | C13—C14—C15—C10 | -3.0 (5) |
| O1—S1—N1—C10 | 178.7 (2) | C13—C14—C15—S2 | 179.5 (2) |
| C1—S1—N1—C10 | 62.6 (3) | C11—C10—C15—C14 | 1.5 (4) |
| O2—S1—C1—C6 | -165.8 (2) | N1—C10—C15—C14 | -176.3 (3) |
| O1—S1—C1—C6 | -34.8 (3) | C11—C10—C15—S2 | 179.0 (2) |
| N1—S1—C1—C6 | 78.2 (3) | N1—C10—C15—S2 | 1.2 (4) |
| O2—S1—C1—C2 | 15.5 (3) | C16—S2—C15—C14 | -65.8 (3) |
| O1—S1—C1—C2 | 146.6 (3) | C16—S2—C15—C10 | 116.7 (3) |
| N1—S1—C1—C2 | -100.5 (3) | C15—S2—C16—N17 | -4.9 (3) |
| C6—C1—C2—C3 | 1.8 (5) | C15—S2—C16—C21 | 174.0 (3) |
| S1—C1—C2—C3 | -179.6 (2) | C21—C16—N17—C18 | -1.8 (4) |
| C6—C1—C2—C9 | -177.5 (3) | S2—C16—N17—C18 | 177.1 (2) |
| S1—C1—C2—C9 | 1.2 (5) | C16—N17—C18—N19 | -0.7 (5) |
| C1—C2—C3—C4 | -1.0 (5) | C16—N17—C18—N22 | 177.5 (3) |
| C9—C2—C3—C4 | 178.3 (3) | N17—C18—N19—C20 | 1.6 (5) |
| C2—C3—C4—C5 | -0.7 (5) | N22—C18—N19—C20 | -176.6 (3) |
| C2—C3—C4—C8 | -179.0 (3) | C18—N19—C20—C21 | 0.1 (6) |
| C3—C4—C5—C6 | 1.8 (5) | N19—C20—C21—C16 | -2.4 (5) |
| C8—C4—C5—C6 | 180.0 (3) | N19—C20—C21—Br1 | 178.1 (3) |
| C4—C5—C6—C1 | -1.0 (5) | N17—C16—C21—C20 | 3.3 (5) |
| C4—C5—C6—C7 | 179.3 (3) | S2—C16—C21—C20 | -175.6 (3) |
| C2—C1—C6—C5 | -0.8 (5) | N17—C16—C21—Br1 | -177.2 (2) |
| S1—C1—C6—C5 | -179.5 (2) | S2—C16—C21—Br1 | 3.9 (4) |
| C2—C1—C6—C7 | 178.9 (3) | N17—C18—N22—C27 | 165.2 (3) |
| S1—C1—C6—C7 | 0.2 (4) | N19—C18—N22—C27 | -16.4 (5) |
| S1—N1—C10—C11 | 67.5 (4) | N17—C18—N22—C23 | 13.2 (5) |
| S1—N1—C10—C15 | -114.8 (3) | N19—C18—N22—C23 | -168.4 (3) |
| C15—C10—C11—C12 | 0.7 (5) | C18—N22—C23—C24 | 98.4 (4) |
| N1—C10—C11—C12 | 178.5 (3) | C27—N22—C23—C24 | -56.4 (4) |
| C10—C11—C12—C13 | -1.4 (5) | N22—C23—C24—O25 | 59.2 (4) |
| C25—O3—C13—C14 | -5.5 (5) | C23—C24—O25—C26 | -60.5 (4) |
| C25—O3—C13—C12 | 173.0 (3) | C24—O25—C26—C27 | 57.3 (5) |
| C11—C12—C13—O3 | -178.6 (3) | C18—N22—C27—C26 | -100.5 (4) |
| C11—C12—C13—C14 | -0.1 (5) | C23—N22—C27—C26 | 53.6 (4) |
| O3—C13—C14—C15 | -179.3 (3) | O25—C26—C27—N22 | -53.4 (4) |
| C12—C13—C14—C15 | 2.3 (5) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------|-------|-------------|-------------|---------------|
|---------------|-------|-------------|-------------|---------------|

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|---------------------------------|------|------|-----------|-----|
| N1—H1 \cdots O25 ⁱ | 0.86 | 2.09 | 2.890 (4) | 155 |
|---------------------------------|------|------|-----------|-----|

Symmetry code: (i) $-x+3/2, y-1/2, -z+1/2$.