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Crystal structures of (*S*)-3-{1-[(4-chlorophenyl)-sulfonyl]piperidin-2-yl}pyridine, (*S*)-3-[1-(4-methylphenyl)piperidin-2-yl]pyridine, (*S*)-3-{1-[(4-methoxyphenyl)sulfonyl]piperidin-2-yl}pyridine and (*S*)-3-{1-[(3,4-dimethylphenyl)sulfonyl]piperidin-2-yl}pyridine

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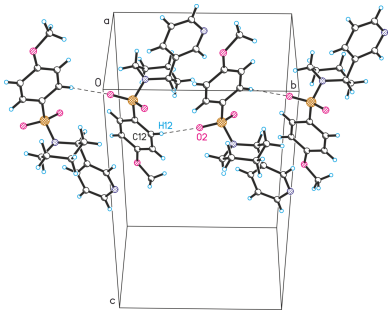
In the presence of trimethylamine, new compounds were obtained by arylsulfonylation of 3-(piperidin-2-yl)pyridine (the alkaloid anabasine), namely: (*S*)-3-{1-[(4-chlorophenyl)sulfonyl]piperidin-2-yl}pyridine, $C_{16}H_{17}ClN_2O_2S$ (**1**); (*S*)-3-[1-(4-methylphenyl)piperidin-2-yl]pyridine, $C_{17}H_{20}N_2O_2S$ (**2**); (*S*)-3-{1-[(4-methoxyphenyl)sulfonyl]piperidin-2-yl}pyridine, $C_{17}H_{20}N_2O_3S$ (**3**); and (*S*)-3-{1-[(3,4-dimethylphenyl)sulfonyl]piperidin-2-yl}pyridine, $C_{18}H_{22}N_2O_2S$ (**4**). In the crystal structures, the spatial arrangement of the pyridine and piperidine rings around the Csp^2—C* bond, as well as the orientation of the benzene ring of the arylsulfonyl group relative to the anabasine moiety, are analyzed.

1. Chemical context

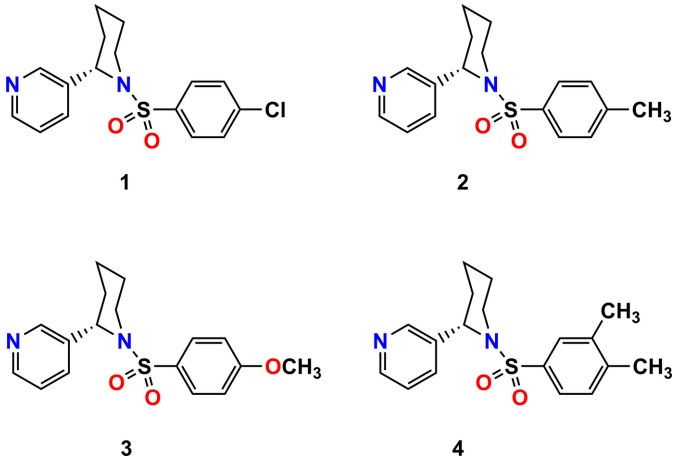
Alkaloids are natural organic compounds containing nitrogen atoms that are synthesized by plants. They play an important role in pharmacology, toxicology, and medicinal chemistry (Dewick, 2009; Daly, 2005).

Anabasine ($C_{10}H_{14}N_2$) is a natural alkaloid with a pyridine–piperidine structure, primarily found in *Anabasis aphylla* L. (Ujváry, 2010). Pharmacological studies have shown that anabasine exhibits a stimulating effect at low doses, whereas at high doses it produces strong toxic effects. High concentrations may lead to paralysis of the nervous system, depression of the respiratory center, and death (Kuete, 2014). For this reason, anabasine is classified as a toxic alkaloid and its use is restricted. Historically, anabasine was used as an insecticide in agriculture; however, due to its high toxicity, it is not widely applied in practice today (Amtaghri *et al.*, 2025).

In addition to being isolated from plants, synthetic methods for obtaining anabasine have also been developed (Felpin *et al.*, 2000). Numerous reactions have been carried out based on anabasine, most of which are focused on the synthesis of N-derivatives (Kulakov, 2010; Slyn'ko *et al.*, 2013; Bakbardina *et al.*, 2006). Although the main objective of these studies has been the synthesis of new biologically active compounds, particular emphasis has been placed on obtaining less toxic and biologically selective derivatives (Mukusheva *et al.*, 2022; Artyushin *et al.*, 2016).



Arylsulfonylation reactions are typically carried out at room temperature in various solvents in the presence of triethylamine or sodium hydroxide. According to the literature, the reaction time varies, mainly depending on the reactivity of the reagents involved. Structural studies of the synthesized arylsulfonyl products using X-ray crystallographic analysis have provided interesting and distinctive results (Abdireymov *et al.*, 2011; Okmanov *et al.*, 2022, 2023).



2. Structural commentary

The asymmetric unit of all the structures consists of a single molecule (Fig. 1). In the anabasine fragment, the piperidine rings adopt a chair conformation, and the spatial orientation

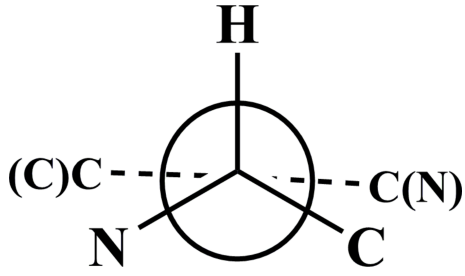


Figure 2
The spatial arrangement of the pyridine and piperidine rings in *N*-arylsulfonyl anabasine (**1**–**4**)

of the pyridine ring relative to it is observed to be axial. In structures **1**–**4**, the relative arrangement of the pyridine and piperidine rings around the Csp^2—C* bond differs slightly. This can be explained by the values of the N1′—C*—C—C torsion angles. The torsion angle values are 34.0 (4)° for **1**, 31.3 (4)° for **2**, 25.2 (5)° for **3**, and 28.4 (5)° for **4**. According to literature sources, in anabasine derivatives with various substituents, these torsion angles range from 17 to 82° (Kulakov *et al.*, 2010; Wojciechowska-Nowak *et al.*, 2007).

When comparing the N(pyridine)···N(piperidine) distances in the anabasine fragment, it is observed that they are very similar: 4.799 (4) Å for **1**, 4.819 (4) Å for **2**, 4.833 (5) Å for **3**, and 4.832 (4) Å for **4**. In other anabasine derivatives, depending on the spatial arrangement of the piperidine and pyridine rings, the N···N distances have been reported to range from 4.29 to 4.86 Å (Wojciechowska-Nowak *et al.*, 2007).

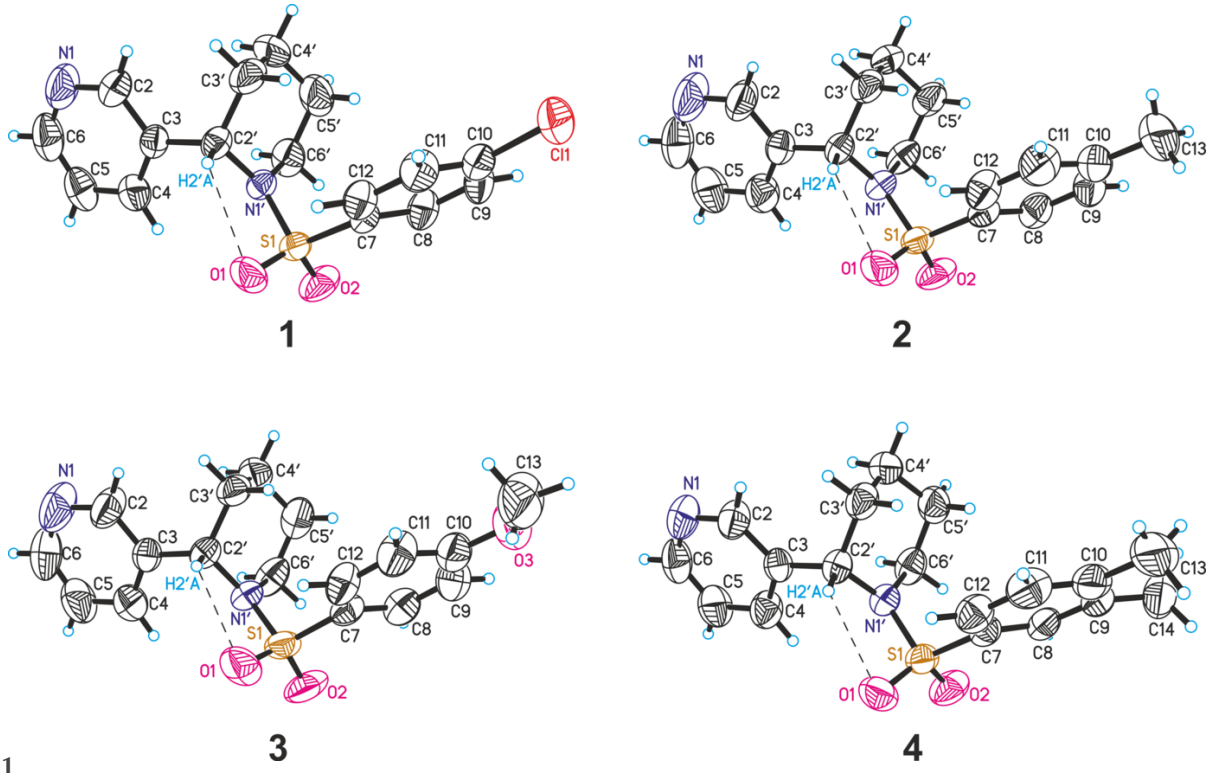


Figure 1
The molecular structures of the title compounds drawn at 50% probability ellipsoids.

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O2^{i}	0.93	2.58	3.383 (4)	145
C3′—H3′B···Cl1^{ii}	0.97	2.98	3.923 (4)	163
C8—H8···Cl1^{iii}	0.93	2.97	3.807 (3)	150
C2′—H2′A···O1	0.98	2.38	2.880 (4)	111

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

Table 2
Hydrogen-bond geometry (Å, °) for **2**.

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O2^{i}	0.93	2.62	3.474 (4)	152
C5′—H5′A···O1^{ii}	0.97	2.51	3.369 (4)	147
C2′—H2′A···O1	0.98	2.37	2.884 (4)	112

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

Table 3
Hydrogen-bond geometry (Å, °) for **3**.

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O2^{i}	0.93	2.47	3.252 (5)	142
C5′—H5′A···O1^{ii}	0.97	2.49	3.298 (5)	140
C2′—H2′A···O1	0.98	2.37	2.880 (5)	111

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

Table 4
Hydrogen-bond geometry (Å, °) for **4**.

D—H···A	D—H	H···A	D···A	D—H···A
C5′—H5′A···O1^{i}	0.97	2.60	3.462 (5)	148
C5—H5···O1^{ii}	0.93	2.64	3.384 (5)	138
C2′—H2′A···O1	0.98	2.39	2.892 (4)	111

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

In studies by Wojciechowska-Nowak *et al.* on the structures of salts of anabasine derivatives, four conformations were proposed based on the arrangement of the piperidine and pyridine rings. The N-arylsulfonyl anabasine derivatives **1**–**4** studied here differ from the proposed conformations (Fig. 2).

The position of the arylsulfonyl group relative to the piperidine ring in structures (around the N1—S1 and S1—C7 bonds) is nearly identical. The mutual arrangement of the piperidine and benzene rings was analyzed using the C2′—N1′—S1—O1 and O1—S1—C7—C12 torsion angles, which are 34.8 (2) and −24.4 (3)° for **1**, 33.7 (2) and −31.5 (3)° for **2**, 37.2 (4) and −24.0 (4)° for **3**, and 35.6 (3) and −32.3 (3)° for **4**, respectively. In all structures, such an arrangement of groups can be explained by the presence of intramolecular hydrogen bonding.

The mutual arrangement of planar aromatic rings relative to the six-membered saturated heterocycle in compounds **2**–**4** is nearly identical. The nature of intermolecular van der Waals contacts in these structures is also similar, indicating the formation of isostructural crystals in the packing (space group $P2_12_12_1$) with identical unit-cell parameters (Table 5).

It was established that in the crystal structures, the similar arrangement of the piperidine ring and the benzene ring connected via the sulfonyl group is due to intermolecular interactions. Substituents on the benzene ring (Cl, CH_3, OCH_3) do not significantly affect the mutual arrangement of the rings.

3. Supramolecular features

The analysis of intermolecular interactions in all studied structures revealed only weak hydrogen bonding, which plays a key role in consolidating the crystal packing (Tables 1–4, Figs. 3–6).

A consistent intramolecular C—H···O hydrogen bond was observed to consolidate the molecular conformation in the solid state. This interaction involves the piperidine ring via the asymmetric carbon atom and the oxygen atom of the SO_2 group (C2′—H2′A···O1).

In the crystal structure of compound **1**, an infinite ribbon is formed along the *c*-axis direction, driven by donor–acceptor interactions between the oxygen atom of the SO_2 group and the chlorine atom at the C10 position [Cl···O distance = 3.127 (2) Å; symmetry operation: $\frac{3}{2}-x, 2-y, -\frac{1}{2}+z$; Fig. 3). These ribbons are further interconnected along the *a*-axis direction through intermolecular C12—H12···O2 hydrogen

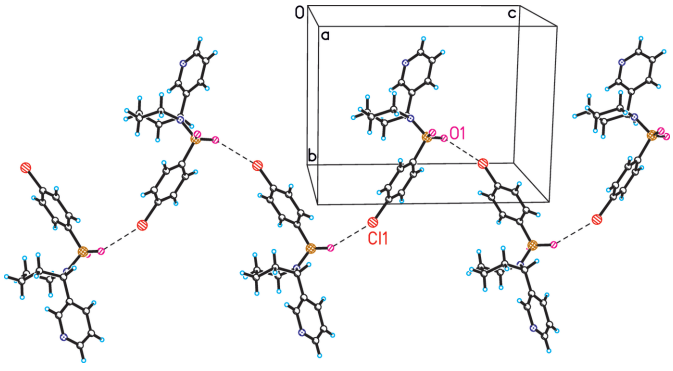


Figure 3
Observed intermolecular O1···Cl1 contacts in the crystal structure of **1** (the molecules are linked along the *c*-axis direction).

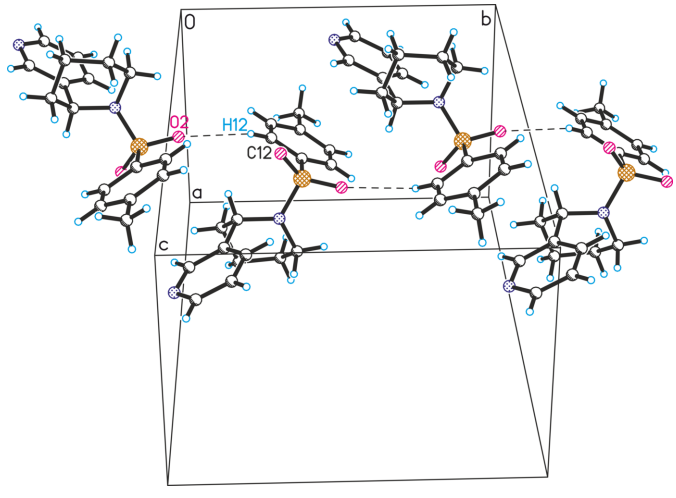


Figure 4
Observed intermolecular C12—H12···O2 interactions in the crystal structure of **2** (the molecules are linked along the *b*-axis direction).

Table 5
Experimental details.

	1	**2**	**3**	**4**
Crystal data				
Chemical formula	$C_{16}H_{17}ClN_2O_2S$	$C_{17}H_{20}N_2O_2S$	$C_{17}H_{20}N_2O_3S$	$C_{18}H_{22}N_2O_2S$
M_r	336.83	316.41	332.41	330.43
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
Temperature (K)	294	297	297	295
a, b, c (Å)	10.694 (2), 10.715 (2), 14.110 (3)	7.8933 (16), 11.408 (2), 18.195 (4)	7.9758 (16), 11.131 (2), 18.754 (4)	7.9087 (16), 11.737 (2), 18.117 (4)
V (Å^3)	1616.8 (6)	1638.5 (6)	1664.9 (6)	1681.6 (6)
Z	4	4	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	3.37	1.82	1.87	1.80
Crystal size (mm)	0.50 × 0.45 × 0.30	0.45 × 0.30 × 0.25	0.30 × 0.25 × 0.25	0.45 × 0.25 × 0.22
Data collection				
Diffractometer	Bruker D8 VENTURE dual wavelength Mo/Cu	Xcalibur, Ruby	Xcalibur, Ruby	Xcalibur, Ruby
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.32, 0.43	0.79, 1.00	0.78, 1.00	0.88, 1.00
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	50181, 3234, 3222	11987, 3372, 3194	12142, 3427, 2899	12220, 3428, 2886
R_{int}	0.029	0.033	0.048	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.630	0.629	0.630
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.102, 1.06	0.051, 0.123, 1.12	0.054, 0.133, 1.10	0.045, 0.111, 1.07
No. of reflections	3234	3372	3427	3428
No. of parameters	199	200	209	210
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.44	0.33, −0.63	0.23, −0.53	0.21, −0.34
Absolute structure	Flack x determined using 1346 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1275 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1030 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1007 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.094 (3)	0.005 (8)	−0.014 (15)	0.011 (14)

Computer programs: *APEX5* and *SAINT* (Bruker, 2012), *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*), *XP* in *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2020), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

bonds. Additionally, the chlorine atom participates in weak C–H···Cl (C3′—H3′*B*···Cl1 and C8—H8···Cl1) hydrogen bonding interactions.

In the crystal structures of compounds **2** and **3**, similar intermolecular hydrogen bonding patterns are observed, where molecules are linked along the *b*-axis direction via

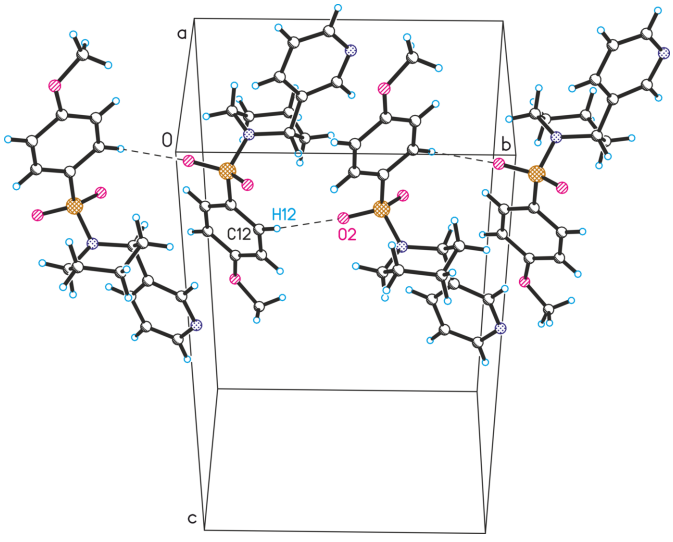


Figure 5
Observed intermolecular C12—H12···O2 interactions in the crystal structure of **3** (the molecules are linked along the *b*-axis direction).

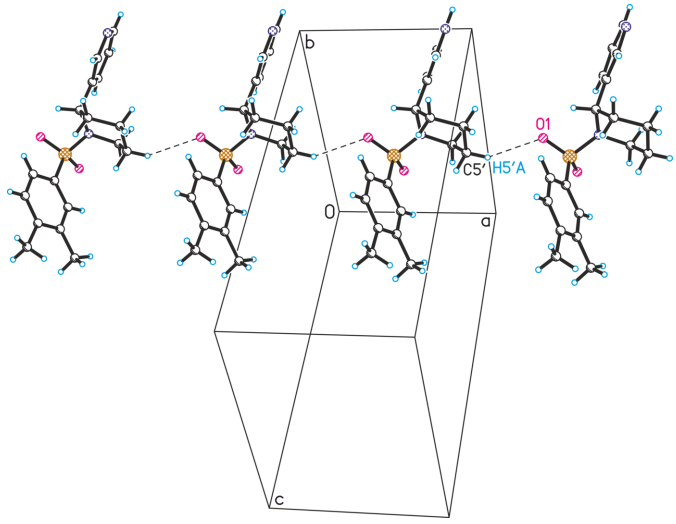


Figure 6
Observed intermolecular C5′—H5′*A*···O1 interactions in the crystal structure of **4** (the molecules are linked along the *a*-axis direction).

C12—H12···O2 interactions (Figs. 4 and 5). The resulting chains are further consolidated by C5′—H5′*A*···O1 hydrogen bonds. In the crystal structure of **4**, this type of interaction leads to the formation of molecular chains along the *a*-axis direction (Fig. 6). In contrast to the previous structures, the chains in structure **4** are interconnected via intermolecular C5—H5···O1 hydrogen bonds.

4. Database survey

A search of anabasine derivatives in the Cambridge Structural Database (CSD, updated to November 2025; Groom *et al.*, 2016) yielded 37 results. Of them, 13 are N-derivatives of anabasin alkaloids.

The axial orientation of the pyridine ring is observed in the crystal structures of *N*-ethyl-2-(pyridin-3-yl)piperidine-1-carbothioamide (ATUGAZ; Nurkenov *et al.*, 2016) and 2-(pyridin-3-yl)-*N*-[2-(vinyloxy)ethyl]piperidine-1-carbothiamide (QELPON; Ibraev *et al.*, 2006).

Structurally similar compounds in terms of the orientation of the pyridine ring relative to the piperidine ring and the distance between the nitrogen atoms are *N*-(anabasinyl-1-carbonothioyl)-2-furamide (FUSKUA; Kulakov *et al.*, 2009) and 2-(pyridin-3-yl)-*N*-[2-(vinyloxy)ethyl]piperidine-1-carbothiamide (QELPON; Ibraev *et al.*, 2006).

5. Synthesis and crystallization

(*S*)-3-{1-[(4-Chlorophenyl)sulfonyl]piperidin-2-yl}pyridine (**1**), (*S*)-3-[1-(4-methylphenyl)piperidin-2-yl]pyridine (**2**), (*S*)-3-{1-[(4-methoxyphenyl)sulfonyl]piperidin-2-yl}pyridine (**3**), and (*S*)-3-{1-[(3,4-dimethylphenyl)sulfonyl]piperidin-2-yl} pyridine (**4**) were synthesized according to the reported method (Olimova *et al.*, 2025). Colourless single crystals of the compounds, suitable for X-ray diffraction analysis, were successfully obtained from ethanol.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. All hydrogen atoms were found in difference maps and then freely refined with isotropic shift parameters, resulting in C—H distances of 0.97 Å for CH_2, 0.96 Å for CH_3 and 0.93 Å for C_{ar}.

Funding information

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supporting information

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Crystal structures of (*S*)-3-{1-[(4-chlorophenyl)sulfonyl]piperidin-2-yl}pyridine, (*S*)-3-[1-(4-methylphenyl)piperidin-2-yl]pyridine, (*S*)-3-{1-[(4-methoxyphenyl)-sulfonyl]piperidin-2-yl}pyridine and (*S*)-3-{1-[(3,4-dimethylphenyl)sulfonyl]-piperidin-2-yl}pyridine

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Computing details

(*S*)-3-{1-[(4-Chlorophenyl)sulfonyl]piperidin-2-yl}pyridine (1)

Crystal data

$C_{16}H_{17}ClN_2O_2S$
M_r = 336.83
Orthorhombic, $P2_12_12_1$
a = 10.694 (2) Å
b = 10.715 (2) Å
c = 14.110 (3) Å
V = 1616.8 (6) Å^3
Z = 4
$F(000)$ = 704
D_x = 1.384 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9773 reflections
θ = 4.1–74.2°
μ = 3.37 mm^{-1}
T = 294 K
Prism, colourless
0.50 × 0.45 × 0.30 mm

Data collection

Bruker D8 VENTURE dual wavelength Mo/Cu diffractometer
Radiation source: microfocus sealed X-ray tube, INCOATEC IμS
Detector resolution: 7.39 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.32, T_{max} = 0.43
50181 measured reflections
3234 independent reflections
3222 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 74.4°, θ_{min} = 5.2°
h = −13→13
k = −13→13
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.102
S = 1.06
3234 reflections
199 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 0.4484P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Absolute structure: Flack *x* determined using 1346 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.094 (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}
S1	0.78885 (6)	0.66179 (6)	0.48625 (4)	0.04518 (19)
Cl1	0.82268 (11)	1.15407 (11)	0.25168 (8)	0.0926 (4)
O1	0.7158 (3)	0.6849 (2)	0.56915 (13)	0.0642 (6)
O2	0.9117 (2)	0.6108 (2)	0.4948 (2)	0.0731 (7)
N1	0.3482 (4)	0.3020 (4)	0.4288 (3)	0.0849 (11)
N1′	0.7089 (2)	0.5681 (2)	0.41990 (15)	0.0406 (5)
C2	0.4014 (3)	0.4113 (4)	0.4065 (3)	0.0643 (9)
H2	0.359882	0.463138	0.364013	0.077*
C3	0.5152 (3)	0.4518 (3)	0.4432 (2)	0.0457 (6)
C4	0.5723 (4)	0.3748 (3)	0.5077 (2)	0.0620 (8)
H4	0.646868	0.398968	0.536173	0.074*
C5	0.5184 (5)	0.2607 (4)	0.5303 (3)	0.0776 (11)
H5	0.557477	0.206614	0.572456	0.093*
C6	0.4083 (5)	0.2297 (4)	0.4899 (4)	0.0817 (13)
H6	0.372584	0.153400	0.505841	0.098*
C2′	0.5711 (2)	0.5783 (3)	0.4172 (2)	0.0450 (6)
H2′A	0.545691	0.638507	0.465762	0.054*
C3′	0.5304 (4)	0.6293 (4)	0.3211 (3)	0.0808 (13)
H3′A	0.557074	0.715537	0.315568	0.097*
H3′B	0.439910	0.627501	0.317113	0.097*
C4′	0.5852 (5)	0.5542 (6)	0.2392 (3)	0.0984 (18)
H4′A	0.554452	0.469097	0.241802	0.118*
H4′B	0.559108	0.590475	0.179400	0.118*
C5′	0.7247 (5)	0.5543 (5)	0.2453 (3)	0.0894 (14)
H5′A	0.755575	0.638741	0.237147	0.107*
H5′B	0.758889	0.503317	0.194713	0.107*
C6′	0.7677 (3)	0.5041 (3)	0.3396 (2)	0.0599 (8)
H6′A	0.748388	0.415765	0.342963	0.072*
H6′B	0.857766	0.513171	0.344197	0.072*
C7	0.8030 (2)	0.8051 (2)	0.42494 (19)	0.0424 (5)
C8	0.9004 (3)	0.8207 (3)	0.3612 (3)	0.0574 (8)
H8	0.960987	0.759082	0.354115	0.069*
C9	0.9062 (4)	0.9289 (4)	0.3083 (3)	0.0680 (9)
H9	0.970115	0.940354	0.264489	0.082*
C10	0.8171 (3)	1.0196 (3)	0.3209 (2)	0.0587 (8)

C11	0.7225 (3)	1.0061 (3)	0.3849 (3)	0.0596 (7)
H11	0.663730	1.069156	0.393154	0.071*
C12	0.7150 (3)	0.8969 (3)	0.4374 (2)	0.0522 (6)
H12	0.650597	0.885872	0.480863	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0438 (3)	0.0471 (3)	0.0446 (3)	−0.0057 (3)	−0.0095 (3)	0.0027 (3)
Cl1	0.0952 (8)	0.0797 (6)	0.1027 (8)	−0.0302 (6)	−0.0210 (6)	0.0445 (6)
O1	0.0915 (16)	0.0653 (13)	0.0358 (9)	−0.0170 (13)	0.0048 (11)	−0.0063 (9)
O2	0.0457 (11)	0.0698 (14)	0.104 (2)	0.0008 (10)	−0.0306 (13)	0.0130 (14)
N1	0.080 (2)	0.079 (2)	0.096 (2)	−0.0393 (18)	0.008 (2)	−0.007 (2)
N1′	0.0352 (10)	0.0437 (11)	0.0430 (10)	−0.0005 (9)	0.0010 (9)	−0.0058 (9)
C2	0.0530 (17)	0.067 (2)	0.073 (2)	−0.0170 (16)	−0.0035 (16)	0.0014 (17)
C3	0.0430 (13)	0.0475 (14)	0.0467 (13)	−0.0068 (11)	0.0072 (11)	−0.0054 (11)
C4	0.0677 (19)	0.0587 (17)	0.0595 (18)	−0.0078 (14)	0.0022 (15)	0.0091 (15)
C5	0.099 (3)	0.062 (2)	0.072 (2)	−0.007 (2)	0.017 (2)	0.0197 (19)
C6	0.102 (3)	0.061 (2)	0.082 (3)	−0.027 (2)	0.030 (2)	−0.001 (2)
C2′	0.0352 (12)	0.0430 (13)	0.0568 (15)	−0.0002 (10)	−0.0013 (11)	0.0011 (12)
C3′	0.060 (2)	0.076 (2)	0.106 (3)	−0.0196 (18)	−0.034 (2)	0.042 (2)
C4′	0.114 (4)	0.135 (4)	0.0460 (18)	−0.056 (3)	−0.025 (2)	0.022 (2)
C5′	0.115 (3)	0.107 (3)	0.0457 (17)	−0.044 (3)	0.015 (2)	−0.0083 (19)
C6′	0.0606 (19)	0.0631 (18)	0.0559 (16)	−0.0027 (15)	0.0172 (14)	−0.0162 (14)
C7	0.0364 (12)	0.0451 (12)	0.0457 (12)	−0.0089 (10)	−0.0044 (10)	0.0014 (10)
C8	0.0390 (13)	0.0601 (18)	0.0731 (19)	−0.0042 (13)	0.0102 (13)	0.0010 (15)
C9	0.0545 (18)	0.078 (2)	0.071 (2)	−0.0210 (17)	0.0160 (16)	0.0097 (18)
C10	0.0556 (18)	0.0560 (16)	0.0646 (18)	−0.0188 (14)	−0.0127 (14)	0.0121 (14)
C11	0.0514 (17)	0.0506 (15)	0.077 (2)	0.0018 (14)	−0.0025 (16)	0.0047 (15)
C12	0.0436 (13)	0.0533 (15)	0.0597 (16)	−0.0031 (12)	0.0055 (13)	−0.0002 (12)

Geometric parameters (Å, º)

S1—O2	1.428 (2)	C3′—H3′A	0.9700
S1—O1	1.428 (2)	C3′—H3′B	0.9700
S1—N1′	1.617 (2)	C4′—C5′	1.494 (8)
S1—C7	1.769 (3)	C4′—H4′A	0.9700
Cl1—C10	1.741 (3)	C4′—H4′B	0.9700
N1—C6	1.326 (7)	C5′—C6′	1.507 (6)
N1—C2	1.339 (5)	C5′—H5′A	0.9700
N1′—C6′	1.466 (3)	C5′—H5′B	0.9700
N1′—C2′	1.478 (3)	C6′—H6′A	0.9700
C2—C3	1.392 (4)	C6′—H6′B	0.9700
C2—H2	0.9300	C7—C12	1.372 (4)
C3—C4	1.371 (5)	C7—C8	1.387 (4)
C3—C2′	1.526 (4)	C8—C9	1.380 (5)
C4—C5	1.389 (5)	C8—H8	0.9300
C4—H4	0.9300	C9—C10	1.373 (6)

C5—C6	1.350 (7)	C9—H9	0.9300
C5—H5	0.9300	C10—C11	1.364 (5)
C6—H6	0.9300	C11—C12	1.387 (4)
C2′—C3′	1.525 (5)	C11—H11	0.9300
C2′—H2′A	0.9800	C12—H12	0.9300
C3′—C4′	1.525 (8)		

O2—S1—O1	120.04 (18)	C5′—C4′—C3′	109.8 (3)
O2—S1—N1′	107.32 (14)	C5′—C4′—H4′A	109.7
O1—S1—N1′	107.00 (14)	C3′—C4′—H4′A	109.7
O2—S1—C7	107.15 (14)	C5′—C4′—H4′B	109.7
O1—S1—C7	107.28 (14)	C3′—C4′—H4′B	109.7
N1′—S1—C7	107.51 (12)	H4′A—C4′—H4′B	108.2
C6—N1—C2	117.2 (4)	C4′—C5′—C6′	110.8 (3)
C6′—N1′—C2′	116.2 (2)	C4′—C5′—H5′A	109.5
C6′—N1′—S1	120.7 (2)	C6′—C5′—H5′A	109.5
C2′—N1′—S1	119.75 (18)	C4′—C5′—H5′B	109.5
N1—C2—C3	123.8 (4)	C6′—C5′—H5′B	109.5
N1—C2—H2	118.1	H5′A—C5′—H5′B	108.1
C3—C2—H2	118.1	N1′—C6′—C5′	112.6 (3)
C4—C3—C2	116.6 (3)	N1′—C6′—H6′A	109.1
C4—C3—C2′	121.3 (3)	C5′—C6′—H6′A	109.1
C2—C3—C2′	122.0 (3)	N1′—C6′—H6′B	109.1
C3—C4—C5	119.8 (4)	C5′—C6′—H6′B	109.1
C3—C4—H4	120.1	H6′A—C6′—H6′B	107.8
C5—C4—H4	120.1	C12—C7—C8	120.8 (3)
C6—C5—C4	118.8 (4)	C12—C7—S1	120.1 (2)
C6—C5—H5	120.6	C8—C7—S1	119.1 (2)
C4—C5—H5	120.6	C9—C8—C7	119.0 (3)
N1—C6—C5	123.7 (4)	C9—C8—H8	120.5
N1—C6—H6	118.2	C7—C8—H8	120.5
C5—C6—H6	118.2	C10—C9—C8	119.6 (3)
N1′—C2′—C3′	109.5 (3)	C10—C9—H9	120.2
N1′—C2′—C3	108.6 (2)	C8—C9—H9	120.2
C3′—C2′—C3	114.9 (3)	C11—C10—C9	121.7 (3)
N1′—C2′—H2′A	107.9	C11—C10—Cl1	119.0 (3)
C3′—C2′—H2′A	107.9	C9—C10—Cl1	119.3 (3)
C3—C2′—H2′A	107.9	C10—C11—C12	119.1 (3)
C2′—C3′—C4′	112.0 (3)	C10—C11—H11	120.5
C2′—C3′—H3′A	109.2	C12—C11—H11	120.5
C4′—C3′—H3′A	109.2	C7—C12—C11	119.8 (3)
C2′—C3′—H3′B	109.2	C7—C12—H12	120.1
C4′—C3′—H3′B	109.2	C11—C12—H12	120.1
H3′A—C3′—H3′B	107.9		

O2—S1—N1′—C6′	−36.4 (3)	C3—C2′—C3′—C4′	−69.6 (4)
O1—S1—N1′—C6′	−166.5 (2)	C2′—C3′—C4′—C5′	−57.9 (5)
C7—S1—N1′—C6′	78.6 (3)	C3′—C4′—C5′—C6′	56.6 (5)

O2—S1—N1′—C2′	164.8 (2)	C2′—N1′—C6′—C5′	50.8 (4)
O1—S1—N1′—C2′	34.8 (2)	S1—N1′—C6′—C5′	−108.7 (3)
C7—S1—N1′—C2′	−80.2 (2)	C4′—C5′—C6′—N1′	−52.9 (5)
C6—N1—C2—C3	0.4 (6)	O2—S1—C7—C12	−154.5 (2)
N1—C2—C3—C4	−1.8 (5)	O1—S1—C7—C12	−24.4 (3)
N1—C2—C3—C2′	−178.9 (3)	N1′—S1—C7—C12	90.4 (2)
C2—C3—C4—C5	2.4 (5)	O2—S1—C7—C8	28.5 (3)
C2′—C3—C4—C5	179.6 (3)	O1—S1—C7—C8	158.6 (2)
C3—C4—C5—C6	−1.9 (6)	N1′—S1—C7—C8	−86.6 (3)
C2—N1—C6—C5	0.2 (7)	C12—C7—C8—C9	−1.6 (5)
C4—C5—C6—N1	0.5 (7)	S1—C7—C8—C9	175.4 (3)
C6′—N1′—C2′—C3′	−49.9 (4)	C7—C8—C9—C10	1.1 (5)
S1—N1′—C2′—C3′	109.8 (3)	C8—C9—C10—C11	0.3 (5)
C6′—N1′—C2′—C3	76.3 (3)	C8—C9—C10—Cl1	−178.3 (3)
S1—N1′—C2′—C3	−124.0 (2)	C9—C10—C11—C12	−1.1 (5)
C4—C3—C2′—N1′	34.0 (4)	Cl1—C10—C11—C12	177.4 (3)
C2—C3—C2′—N1′	−149.0 (3)	C8—C7—C12—C11	0.8 (5)
C4—C3—C2′—C3′	157.0 (3)	S1—C7—C12—C11	−176.2 (2)
C2—C3—C2′—C3′	−26.0 (4)	C10—C11—C12—C7	0.6 (5)
N1′—C2′—C3′—C4′	52.9 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O2^{i}	0.93	2.58	3.383 (4)	145
C3′—H3′*B*···Cl1^{ii}	0.97	2.98	3.923 (4)	163
C8—H8···Cl1^{iii}	0.93	2.97	3.807 (3)	150
C2′—H2′*A*···O1	0.98	2.38	2.880 (4)	111

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) −*x*+2, *y*−1/2, −*z*+1/2.

(*S*)-3-[1-(4-Methylphenyl)piperidin-2-yl]pyridine (2)

Crystal data

$C_{17}H_{20}N_2O_2S$
M_r = 316.41
Orthorhombic, $P2_12_12_1$
a = 7.8933 (16) Å
b = 11.408 (2) Å
c = 18.195 (4) Å
V = 1638.5 (6) Å^3
Z = 4
F(000) = 672
D_x = 1.283 Mg m^{-3}
Cu *Kα* radiation, λ = 1.54184 Å
Cell parameters from 7339 reflections
θ = 4.6–75.5°
μ = 1.82 mm^{-1}
T = 297 K
Prism, colourless
0.45 × 0.30 × 0.25 mm

Data collection

Xcalibur, Ruby diffractometer
Radiation source: Enhance (Cu) X-ray Source
Detector resolution: 10.25 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.79, T_{max} = 1.00
11987 measured reflections
3372 independent reflections
3194 reflections with $I > 2\sigma(I)$

R_{int} = 0.033
θ_{max} = 76.1°, θ_{min} = 4.6°
h = −6→9
k = −13→14
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.123
S = 1.12
3372 reflections
200 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2 + 0.0529P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}
Absolute structure: Flack x determined using 1275 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.005 (8)

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}
S1	0.55288 (8)	0.37284 (6)	0.27853 (4)	0.0502 (2)
O1	0.4044 (3)	0.3086 (3)	0.29892 (14)	0.0721 (7)
O2	0.5731 (4)	0.4921 (2)	0.30207 (14)	0.0760 (7)
N1	0.8626 (7)	−0.0151 (4)	0.4744 (2)	0.1120 (15)
N1′	0.7130 (3)	0.30057 (18)	0.31083 (13)	0.0457 (5)
C2	0.8256 (7)	0.0261 (4)	0.4078 (2)	0.0849 (12)
H2	0.852141	−0.021362	0.367817	0.102*
C3	0.7515 (3)	0.1328 (3)	0.39290 (15)	0.0527 (6)
C4	0.7098 (6)	0.2002 (4)	0.4530 (2)	0.0784 (10)
H4	0.657245	0.272468	0.446699	0.094*
C5	0.7469 (7)	0.1593 (5)	0.5232 (2)	0.0969 (15)
H5	0.719813	0.203753	0.564383	0.116*
C6	0.8237 (7)	0.0529 (5)	0.5304 (3)	0.1011 (16)
H6	0.850092	0.026908	0.577437	0.121*
C2′	0.7089 (3)	0.1711 (2)	0.31480 (15)	0.0453 (5)
H2′A	0.592381	0.146268	0.304605	0.054*
C3′	0.8224 (4)	0.1185 (2)	0.25495 (17)	0.0606 (7)
H3′A	0.827492	0.034133	0.261322	0.073*
H3′B	0.772751	0.134164	0.207184	0.073*
C4′	1.0008 (4)	0.1681 (3)	0.2570 (2)	0.0681 (8)
H4′A	1.054458	0.147950	0.303297	0.082*
H4′B	1.067557	0.134495	0.217513	0.082*
C5′	0.9938 (4)	0.3002 (3)	0.2487 (2)	0.0693 (9)

H5′A	1.107324	0.332288	0.251852	0.083*
H5′B	0.947808	0.320006	0.200815	0.083*
C6′	0.8839 (4)	0.3532 (2)	0.3083 (2)	0.0596 (7)
H6′A	0.938763	0.342307	0.355476	0.072*
H6′B	0.873433	0.436851	0.299725	0.072*
C7	0.5649 (3)	0.3733 (2)	0.18179 (14)	0.0481 (5)
C8	0.6399 (4)	0.4666 (3)	0.1460 (2)	0.0626 (7)
H8	0.681949	0.529831	0.172646	0.075*
C9	0.6520 (6)	0.4652 (4)	0.0700 (2)	0.0819 (11)
H9	0.703039	0.527751	0.045869	0.098*
C10	0.5884 (5)	0.3708 (4)	0.02895 (19)	0.0784 (10)
C11	0.5151 (6)	0.2779 (4)	0.0668 (2)	0.0793 (11)
H11	0.473604	0.213963	0.040632	0.095*
C12	0.5027 (5)	0.2787 (3)	0.14224 (18)	0.0625 (7)
H12	0.452790	0.215910	0.166656	0.075*
C13	0.5936 (8)	0.3691 (6)	−0.0544 (2)	0.127 (2)
H13A	0.667796	0.429881	−0.071637	0.190*
H13B	0.481636	0.382083	−0.073425	0.190*
H13C	0.634474	0.294420	−0.070964	0.190*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0479 (3)	0.0526 (3)	0.0501 (3)	0.0144 (3)	−0.0047 (2)	−0.0035 (3)
O1	0.0437 (10)	0.1059 (19)	0.0667 (13)	0.0080 (11)	0.0036 (9)	0.0118 (12)
O2	0.0981 (18)	0.0566 (12)	0.0733 (13)	0.0353 (13)	−0.0174 (13)	−0.0188 (10)
N1	0.149 (4)	0.102 (3)	0.085 (3)	0.018 (3)	−0.024 (3)	0.037 (2)
N1′	0.0442 (10)	0.0379 (10)	0.0550 (11)	0.0017 (8)	−0.0103 (9)	−0.0008 (9)
C2	0.117 (3)	0.067 (2)	0.070 (2)	0.016 (2)	−0.006 (2)	0.0198 (18)
C3	0.0557 (14)	0.0492 (14)	0.0533 (13)	−0.0067 (11)	−0.0059 (11)	0.0056 (12)
C4	0.099 (3)	0.080 (2)	0.0566 (18)	0.004 (2)	−0.0004 (18)	0.0021 (17)
C5	0.120 (4)	0.117 (4)	0.0541 (19)	−0.014 (3)	0.002 (2)	−0.003 (2)
C6	0.115 (4)	0.118 (4)	0.070 (3)	−0.024 (3)	−0.027 (2)	0.036 (3)
C2′	0.0486 (12)	0.0361 (11)	0.0512 (13)	−0.0043 (9)	−0.0080 (10)	0.0012 (10)
C3′	0.0848 (19)	0.0404 (12)	0.0565 (14)	0.0077 (13)	−0.0022 (14)	−0.0022 (12)
C4′	0.0637 (16)	0.0616 (16)	0.079 (2)	0.0210 (14)	0.0109 (15)	0.0129 (15)
C5′	0.0460 (13)	0.0626 (17)	0.099 (2)	0.0015 (12)	0.0014 (14)	0.0232 (17)
C6′	0.0530 (14)	0.0388 (12)	0.087 (2)	−0.0075 (11)	−0.0178 (14)	0.0043 (12)
C7	0.0443 (12)	0.0464 (12)	0.0536 (13)	0.0084 (11)	−0.0065 (10)	0.0012 (11)
C8	0.0639 (17)	0.0525 (15)	0.0714 (18)	−0.0007 (13)	−0.0036 (15)	0.0082 (14)
C9	0.082 (2)	0.087 (3)	0.077 (2)	0.011 (2)	0.0118 (19)	0.030 (2)
C10	0.087 (2)	0.094 (3)	0.0540 (16)	0.029 (2)	0.0010 (15)	0.0079 (18)
C11	0.101 (3)	0.075 (2)	0.0610 (18)	0.013 (2)	−0.0191 (18)	−0.0132 (17)
C12	0.0765 (19)	0.0513 (14)	0.0596 (16)	−0.0014 (14)	−0.0153 (14)	0.0005 (13)
C13	0.146 (5)	0.179 (6)	0.056 (2)	0.054 (5)	0.010 (3)	0.012 (3)

Geometric parameters (Å, º)

S1—O1	1.431 (2)	C4′—C5′	1.516 (4)
S1—O2	1.436 (2)	C4′—H4′A	0.9700
S1—N1′	1.620 (2)	C4′—H4′B	0.9700
S1—C7	1.763 (3)	C5′—C6′	1.515 (5)
N1—C6	1.316 (7)	C5′—H5′A	0.9700
N1—C2	1.333 (5)	C5′—H5′B	0.9700
N1′—C6′	1.477 (3)	C6′—H6′A	0.9700
N1′—C2′	1.479 (3)	C6′—H6′B	0.9700
C2—C3	1.378 (5)	C7—C8	1.381 (4)
C2—H2	0.9300	C7—C12	1.387 (4)
C3—C4	1.376 (5)	C8—C9	1.386 (6)
C3—C2′	1.524 (4)	C8—H8	0.9300
C4—C5	1.390 (6)	C9—C10	1.404 (6)
C4—H4	0.9300	C9—H9	0.9300
C5—C6	1.364 (8)	C10—C11	1.391 (6)
C5—H5	0.9300	C10—C13	1.518 (5)
C6—H6	0.9300	C11—C12	1.376 (5)
C2′—C3′	1.533 (4)	C11—H11	0.9300
C2′—H2′A	0.9800	C12—H12	0.9300
C3′—C4′	1.518 (5)	C13—H13A	0.9600
C3′—H3′A	0.9700	C13—H13B	0.9600
C3′—H3′B	0.9700	C13—H13C	0.9600
O1—S1—O2	119.94 (17)	C5′—C4′—H4′B	109.8
O1—S1—N1′	106.52 (13)	C3′—C4′—H4′B	109.8
O2—S1—N1′	106.71 (13)	H4′A—C4′—H4′B	108.2
O1—S1—C7	107.73 (14)	C6′—C5′—C4′	110.3 (3)
O2—S1—C7	106.80 (15)	C6′—C5′—H5′A	109.6
N1′—S1—C7	108.78 (12)	C4′—C5′—H5′A	109.6
C6—N1—C2	116.4 (4)	C6′—C5′—H5′B	109.6
C6′—N1′—C2′	115.3 (2)	C4′—C5′—H5′B	109.6
C6′—N1′—S1	119.61 (18)	H5′A—C5′—H5′B	108.1
C2′—N1′—S1	120.58 (18)	N1′—C6′—C5′	112.5 (2)
N1—C2—C3	125.7 (4)	N1′—C6′—H6′A	109.1
N1—C2—H2	117.2	C5′—C6′—H6′A	109.1
C3—C2—H2	117.2	N1′—C6′—H6′B	109.1
C4—C3—C2	116.1 (3)	C5′—C6′—H6′B	109.1
C4—C3—C2′	121.8 (3)	H6′A—C6′—H6′B	107.8
C2—C3—C2′	122.0 (3)	C8—C7—C12	120.5 (3)
C3—C4—C5	119.5 (4)	C8—C7—S1	119.7 (2)
C3—C4—H4	120.3	C12—C7—S1	119.8 (2)
C5—C4—H4	120.3	C7—C8—C9	119.4 (3)
C6—C5—C4	118.7 (4)	C7—C8—H8	120.3
C6—C5—H5	120.6	C9—C8—H8	120.3
C4—C5—H5	120.6	C8—C9—C10	121.0 (4)
N1—C6—C5	123.7 (4)	C8—C9—H9	119.5

N1—C6—H6	118.2	C10—C9—H9	119.5
C5—C6—H6	118.2	C11—C10—C9	118.1 (3)
N1′—C2′—C3	109.1 (2)	C11—C10—C13	119.8 (4)
N1′—C2′—C3′	110.1 (2)	C9—C10—C13	122.2 (4)
C3—C2′—C3′	114.9 (2)	C12—C11—C10	121.2 (4)
N1′—C2′—H2′A	107.5	C12—C11—H11	119.4
C3—C2′—H2′A	107.5	C10—C11—H11	119.4
C3′—C2′—H2′A	107.5	C11—C12—C7	119.8 (3)
C4′—C3′—C2′	112.2 (2)	C11—C12—H12	120.1
C4′—C3′—H3′A	109.2	C7—C12—H12	120.1
C2′—C3′—H3′A	109.2	C10—C13—H13A	109.5
C4′—C3′—H3′B	109.2	C10—C13—H13B	109.5
C2′—C3′—H3′B	109.2	H13A—C13—H13B	109.5
H3′A—C3′—H3′B	107.9	C10—C13—H13C	109.5
C5′—C4′—C3′	109.5 (2)	H13A—C13—H13C	109.5
C5′—C4′—H4′A	109.8	H13B—C13—H13C	109.5
C3′—C4′—H4′A	109.8		

O1—S1—N1′—C6′	−171.2 (2)	C3—C2′—C3′—C4′	−70.5 (3)
O2—S1—N1′—C6′	−41.9 (3)	C2′—C3′—C4′—C5′	−57.7 (4)
C7—S1—N1′—C6′	73.0 (2)	C3′—C4′—C5′—C6′	57.1 (4)
O1—S1—N1′—C2′	33.7 (2)	C2′—N1′—C6′—C5′	51.9 (3)
O2—S1—N1′—C2′	162.9 (2)	S1—N1′—C6′—C5′	−104.5 (3)
C7—S1—N1′—C2′	−82.2 (2)	C4′—C5′—C6′—N1′	−54.2 (4)
C6—N1—C2—C3	0.2 (9)	O1—S1—C7—C8	150.1 (2)
N1—C2—C3—C4	−1.5 (7)	O2—S1—C7—C8	20.0 (3)
N1—C2—C3—C2′	−178.1 (4)	N1′—S1—C7—C8	−94.8 (2)
C2—C3—C4—C5	1.3 (6)	O1—S1—C7—C12	−31.5 (3)
C2′—C3—C4—C5	178.0 (4)	O2—S1—C7—C12	−161.6 (2)
C3—C4—C5—C6	−0.1 (7)	N1′—S1—C7—C12	83.6 (2)
C2—N1—C6—C5	1.2 (9)	C12—C7—C8—C9	0.3 (5)
C4—C5—C6—N1	−1.2 (9)	S1—C7—C8—C9	178.7 (3)
C6′—N1′—C2′—C3	76.8 (3)	C7—C8—C9—C10	0.4 (6)
S1—N1′—C2′—C3	−127.1 (2)	C8—C9—C10—C11	−0.9 (6)
C6′—N1′—C2′—C3′	−50.2 (3)	C8—C9—C10—C13	177.5 (4)
S1—N1′—C2′—C3′	106.0 (2)	C9—C10—C11—C12	0.9 (6)
C4—C3—C2′—N1′	31.3 (4)	C13—C10—C11—C12	−177.6 (4)
C2—C3—C2′—N1′	−152.3 (3)	C10—C11—C12—C7	−0.3 (6)
C4—C3—C2′—C3′	155.4 (3)	C8—C7—C12—C11	−0.3 (5)
C2—C3—C2′—C3′	−28.1 (4)	S1—C7—C12—C11	−178.7 (3)
N1′—C2′—C3′—C4′	53.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O2^{i}	0.93	2.62	3.474 (4)	152

C5′—H5′*A*···O1^{ii}	0.97	2.51	3.369 (4)	147
C2′—H2′*A*···O1	0.98	2.37	2.884 (4)	112

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

(*S*)-3-{1-[(4-Methoxyphenyl)sulfonyl]piperidin-2-yl}pyridine (3)

Crystal data

$C_{17}H_{20}N_2O_3S$
M_r = 332.41
Orthorhombic, $P2_12_12_1$
a = 7.9758 (16) Å
b = 11.131 (2) Å
c = 18.754 (4) Å
V = 1664.9 (6) Å^3
Z = 4
F(000) = 704
D_x = 1.326 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 3974 reflections
θ = 4.6–75.4°
μ = 1.87 mm^{-1}
T = 297 K
Prism, colorless
0.30 × 0.25 × 0.25 mm

Data collection

Xcalibur, Ruby diffractometer
Radiation source: Enhance (Cu) X-ray Source
Detector resolution: 10.25 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.78, T_{max} = 1.00
12142 measured reflections
3427 independent reflections
2899 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 76.0°, θ_{min} = 4.6°
h = −9→9
k = −13→12
l = −16→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.133
S = 1.10
3427 reflections
209 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}
Absolute structure: Flack *x* determined using 1030 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.014 (15)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.46400 (12)	0.61342 (10)	0.28240 (5)	0.0586 (3)
O1	0.6090 (3)	0.6847 (4)	0.29802 (18)	0.0831 (10)
O2	0.4573 (5)	0.4897 (3)	0.30408 (18)	0.0914 (12)

O3	0.3669 (6)	0.6134 (4)	−0.02843 (18)	0.0992 (12)
N1	0.1744 (9)	1.0089 (4)	0.4792 (3)	0.1096 (19)
N1′	0.3076 (4)	0.6794 (3)	0.32116 (16)	0.0484 (7)
C2	0.2009 (9)	0.9644 (5)	0.4140 (3)	0.0853 (16)
H2	0.171996	1.012250	0.375206	0.102*
C3	0.2682 (4)	0.8523 (3)	0.39991 (19)	0.0505 (8)
C4	0.3119 (7)	0.7844 (5)	0.4577 (2)	0.0783 (13)
H4	0.360841	0.709297	0.451587	0.094*
C5	0.2817 (9)	0.8299 (6)	0.5265 (3)	0.0959 (19)
H5	0.308423	0.784710	0.566621	0.115*
C6	0.2137 (9)	0.9398 (6)	0.5333 (3)	0.098 (2)
H6	0.193347	0.968466	0.579069	0.118*
C2′	0.2998 (4)	0.8114 (3)	0.32333 (19)	0.0474 (8)
H2′A	0.409873	0.842128	0.308922	0.057*
C3′	0.1712 (6)	0.8573 (4)	0.2696 (2)	0.0635 (10)
H3′A	0.160356	0.943672	0.274506	0.076*
H3′B	0.210472	0.840398	0.221716	0.076*
C4′	0.0021 (5)	0.7995 (5)	0.2804 (3)	0.0758 (13)
H4′A	−0.075740	0.828800	0.244638	0.091*
H4′B	−0.041450	0.820735	0.327007	0.091*
C5′	0.0179 (5)	0.6647 (5)	0.2745 (3)	0.0803 (14)
H5′A	−0.090207	0.627923	0.283817	0.096*
H5′B	0.051468	0.643487	0.226458	0.096*
C6′	0.1448 (5)	0.6170 (4)	0.3267 (3)	0.0680 (11)
H6′A	0.101579	0.626174	0.374716	0.082*
H6′B	0.161359	0.531918	0.318011	0.082*
C7	0.4342 (4)	0.6160 (4)	0.1891 (2)	0.0527 (8)
C8	0.3478 (6)	0.5245 (4)	0.1551 (2)	0.0629 (10)
H8	0.303865	0.461422	0.181689	0.076*
C9	0.3268 (7)	0.5258 (4)	0.0837 (3)	0.0723 (12)
H9	0.269326	0.463568	0.061386	0.087*
C10	0.3910 (6)	0.6203 (4)	0.0433 (2)	0.0707 (11)
C11	0.4770 (7)	0.7131 (4)	0.0767 (2)	0.0754 (13)
H11	0.520194	0.776552	0.050174	0.091*
C12	0.4977 (6)	0.7099 (4)	0.1497 (2)	0.0645 (11)
H12	0.554942	0.771753	0.172491	0.077*
C13	0.4504 (13)	0.6978 (6)	−0.0724 (3)	0.126 (3)
H13A	0.428234	0.679622	−0.121564	0.189*
H13B	0.568898	0.693693	−0.063780	0.189*
H13C	0.410630	0.777137	−0.061717	0.189*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0518 (4)	0.0659 (6)	0.0579 (4)	0.0238 (4)	0.0040 (4)	0.0017 (5)
O1	0.0406 (14)	0.132 (3)	0.076 (2)	0.0124 (16)	−0.0029 (13)	−0.0161 (19)
O2	0.127 (3)	0.068 (2)	0.078 (2)	0.055 (2)	0.016 (2)	0.0145 (16)
O3	0.139 (4)	0.100 (3)	0.0585 (17)	0.005 (3)	−0.005 (2)	−0.005 (2)

N1	0.171 (6)	0.083 (3)	0.074 (3)	0.009 (4)	0.028 (3)	−0.023 (3)
N1′	0.0449 (15)	0.0412 (15)	0.0591 (17)	0.0035 (12)	0.0085 (13)	0.0000 (13)
C2	0.130 (5)	0.060 (3)	0.065 (3)	0.014 (3)	0.015 (3)	−0.010 (2)
C3	0.0511 (18)	0.049 (2)	0.0517 (17)	−0.0082 (15)	0.0032 (14)	−0.0040 (15)
C4	0.095 (3)	0.079 (3)	0.061 (2)	0.008 (3)	−0.012 (2)	−0.003 (2)
C5	0.126 (5)	0.107 (5)	0.055 (2)	−0.014 (4)	−0.014 (3)	0.002 (3)
C6	0.125 (5)	0.099 (4)	0.069 (3)	−0.037 (4)	0.024 (3)	−0.027 (3)
C2′	0.0460 (17)	0.0416 (18)	0.0546 (19)	−0.0007 (14)	0.0090 (14)	−0.0014 (15)
C3′	0.086 (3)	0.052 (2)	0.0524 (19)	0.0177 (19)	0.0015 (18)	0.0036 (16)
C4′	0.058 (2)	0.099 (3)	0.070 (2)	0.030 (2)	−0.011 (2)	−0.022 (3)
C5′	0.0406 (18)	0.092 (3)	0.108 (4)	−0.0055 (19)	0.004 (2)	−0.041 (3)
C6′	0.065 (2)	0.0450 (19)	0.094 (3)	−0.0125 (19)	0.028 (2)	−0.007 (2)
C7	0.052 (2)	0.0500 (19)	0.0566 (17)	0.0104 (16)	0.0106 (14)	−0.0024 (17)
C8	0.062 (2)	0.053 (2)	0.074 (3)	−0.0044 (18)	0.0116 (19)	−0.0008 (19)
C9	0.078 (3)	0.065 (3)	0.074 (3)	−0.010 (2)	0.000 (2)	−0.011 (2)
C10	0.086 (3)	0.068 (3)	0.058 (2)	0.013 (3)	0.004 (2)	−0.007 (2)
C11	0.105 (4)	0.056 (2)	0.066 (2)	−0.003 (2)	0.021 (3)	0.004 (2)
C12	0.081 (3)	0.048 (2)	0.064 (2)	−0.007 (2)	0.013 (2)	−0.0084 (18)
C13	0.215 (9)	0.103 (4)	0.061 (3)	0.023 (5)	0.019 (4)	0.009 (3)

Geometric parameters (Å, º)

S1—O1	1.433 (4)	C3′—H3′B	0.9700
S1—O2	1.437 (4)	C4′—C5′	1.510 (7)
S1—N1′	1.620 (3)	C4′—H4′A	0.9700
S1—C7	1.765 (4)	C4′—H4′B	0.9700
O3—C10	1.360 (5)	C5′—C6′	1.504 (7)
O3—C13	1.416 (8)	C5′—H5′A	0.9700
N1—C6	1.311 (8)	C5′—H5′B	0.9700
N1—C2	1.337 (6)	C6′—H6′A	0.9700
N1′—C2′	1.471 (4)	C6′—H6′B	0.9700
N1′—C6′	1.477 (5)	C7—C12	1.377 (6)
C2—C3	1.384 (6)	C7—C8	1.386 (6)
C2—H2	0.9300	C8—C9	1.349 (7)
C3—C4	1.365 (6)	C8—H8	0.9300
C3—C2′	1.528 (5)	C9—C10	1.394 (7)
C4—C5	1.408 (7)	C9—H9	0.9300
C4—H4	0.9300	C10—C11	1.389 (7)
C5—C6	1.344 (9)	C11—C12	1.380 (6)
C5—H5	0.9300	C11—H11	0.9300
C6—H6	0.9300	C12—H12	0.9300
C2′—C3′	1.525 (5)	C13—H13A	0.9600
C2′—H2′A	0.9800	C13—H13B	0.9600
C3′—C4′	1.508 (7)	C13—H13C	0.9600
C3′—H3′A	0.9700		
O1—S1—O2	120.2 (2)	C5′—C4′—H4′A	109.7
O1—S1—N1′	106.19 (18)	C3′—C4′—H4′B	109.7

O2—S1—N1′	106.21 (19)	C5′—C4′—H4′B	109.7
O1—S1—C7	107.59 (19)	H4′A—C4′—H4′B	108.2
O2—S1—C7	106.9 (2)	C6′—C5′—C4′	111.1 (4)
N1′—S1—C7	109.47 (17)	C6′—C5′—H5′A	109.4
C10—O3—C13	118.1 (5)	C4′—C5′—H5′A	109.4
C6—N1—C2	116.9 (5)	C6′—C5′—H5′B	109.4
C2′—N1′—C6′	115.5 (3)	C4′—C5′—H5′B	109.4
C2′—N1′—S1	119.9 (2)	H5′A—C5′—H5′B	108.0
C6′—N1′—S1	119.7 (3)	N1′—C6′—C5′	112.3 (4)
N1—C2—C3	124.7 (5)	N1′—C6′—H6′A	109.1
N1—C2—H2	117.6	C5′—C6′—H6′A	109.1
C3—C2—H2	117.6	N1′—C6′—H6′B	109.1
C4—C3—C2	116.5 (4)	C5′—C6′—H6′B	109.1
C4—C3—C2′	122.6 (4)	H6′A—C6′—H6′B	107.9
C2—C3—C2′	120.8 (4)	C12—C7—C8	119.5 (4)
C3—C4—C5	119.0 (5)	C12—C7—S1	119.7 (3)
C3—C4—H4	120.5	C8—C7—S1	120.8 (3)
C5—C4—H4	120.5	C9—C8—C7	120.7 (4)
C6—C5—C4	118.9 (6)	C9—C8—H8	119.6
C6—C5—H5	120.5	C7—C8—H8	119.6
C4—C5—H5	120.5	C8—C9—C10	120.1 (4)
N1—C6—C5	123.8 (5)	C8—C9—H9	119.9
N1—C6—H6	118.1	C10—C9—H9	119.9
C5—C6—H6	118.1	O3—C10—C11	123.9 (5)
N1′—C2′—C3′	110.1 (3)	O3—C10—C9	116.3 (5)
N1′—C2′—C3	109.3 (3)	C11—C10—C9	119.8 (4)
C3′—C2′—C3	114.2 (3)	C12—C11—C10	119.2 (4)
N1′—C2′—H2′A	107.7	C12—C11—H11	120.4
C3′—C2′—H2′A	107.7	C10—C11—H11	120.4
C3—C2′—H2′A	107.7	C7—C12—C11	120.6 (4)
C4′—C3′—C2′	111.8 (3)	C7—C12—H12	119.7
C4′—C3′—H3′A	109.3	C11—C12—H12	119.7
C2′—C3′—H3′A	109.3	O3—C13—H13A	109.5
C4′—C3′—H3′B	109.3	O3—C13—H13B	109.5
C2′—C3′—H3′B	109.3	H13A—C13—H13B	109.5
H3′A—C3′—H3′B	107.9	O3—C13—H13C	109.5
C3′—C4′—C5′	109.8 (3)	H13A—C13—H13C	109.5
C3′—C4′—H4′A	109.7	H13B—C13—H13C	109.5

O1—S1—N1′—C2′	37.2 (4)	C2′—C3′—C4′—C5′	−57.7 (5)
O2—S1—N1′—C2′	166.2 (3)	C3′—C4′—C5′—C6′	56.3 (5)
C7—S1—N1′—C2′	−78.7 (3)	C2′—N1′—C6′—C5′	50.9 (5)
O1—S1—N1′—C6′	−168.7 (3)	S1—N1′—C6′—C5′	−104.3 (4)
O2—S1—N1′—C6′	−39.7 (4)	C4′—C5′—C6′—N1′	−52.4 (5)
C7—S1—N1′—C6′	75.4 (3)	O1—S1—C7—C12	−24.0 (4)
C6—N1—C2—C3	−0.9 (11)	O2—S1—C7—C12	−154.3 (3)
N1—C2—C3—C4	−0.9 (9)	N1′—S1—C7—C12	91.0 (3)
N1—C2—C3—C2′	−177.6 (6)	O1—S1—C7—C8	155.9 (3)

C2—C3—C4—C5	1.9 (8)	O2—S1—C7—C8	25.6 (4)
C2′—C3—C4—C5	178.6 (5)	N1′—S1—C7—C8	−89.1 (3)
C3—C4—C5—C6	−1.2 (9)	C12—C7—C8—C9	0.7 (6)
C2—N1—C6—C5	1.7 (11)	S1—C7—C8—C9	−179.2 (4)
C4—C5—C6—N1	−0.6 (11)	C7—C8—C9—C10	−0.5 (8)
C6′—N1′—C2′—C3′	−50.7 (4)	C13—O3—C10—C11	7.6 (8)
S1—N1′—C2′—C3′	104.4 (3)	C13—O3—C10—C9	−171.0 (6)
C6′—N1′—C2′—C3	75.5 (4)	C8—C9—C10—O3	178.8 (5)
S1—N1′—C2′—C3	−129.4 (3)	C8—C9—C10—C11	0.1 (8)
C4—C3—C2′—N1′	25.2 (5)	O3—C10—C11—C12	−178.5 (5)
C2—C3—C2′—N1′	−158.3 (4)	C9—C10—C11—C12	0.1 (8)
C4—C3—C2′—C3′	149.1 (4)	C8—C7—C12—C11	−0.5 (6)
C2—C3—C2′—C3′	−34.4 (6)	S1—C7—C12—C11	179.4 (4)
N1′—C2′—C3′—C4′	54.0 (4)	C10—C11—C12—C7	0.1 (7)
C3—C2′—C3′—C4′	−69.4 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O2^{i}	0.93	2.47	3.252 (5)	142
C5′—H5′*A*···O1^{ii}	0.97	2.49	3.298 (5)	140
C2′—H2′*A*···O1	0.98	2.37	2.880 (5)	111

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

(*S*)-3-{1-[(3,4-Dimethylphenyl)sulfonyl]piperidin-2-yl}pyridine (4)

Crystal data

$C_{18}H_{22}N_2O_2S$
M_r = 330.43
Orthorhombic, $P2_12_12_1$
a = 7.9087 (16) Å
b = 11.737 (2) Å
c = 18.117 (4) Å
V = 1681.6 (6) Å^3
Z = 4
F(000) = 704
D_x = 1.305 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 3960 reflections
θ = 3.8–75.1°
μ = 1.80 mm^{-1}
T = 295 K
Prism, colourless
0.45 × 0.25 × 0.22 mm

Data collection

Xcalibur, Ruby diffractometer
Radiation source: Enhance (Cu) X-ray Source
Detector resolution: 10.25 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.88, T_{max} = 1.00
12220 measured reflections
3428 independent reflections
2886 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 76.2°, θ_{min} = 4.5°
h = −9→9
k = −14→14
l = −22→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.111
S = 1.07
3428 reflections

210 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Absolute structure: Flack *x* determined using 1007 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.011 (14)

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}
S1	0.44287 (11)	0.14787 (7)	0.28526 (4)	0.0513 (2)
O1	0.5899 (3)	0.2085 (3)	0.30954 (14)	0.0713 (8)
O2	0.4152 (4)	0.0330 (2)	0.30906 (14)	0.0738 (8)
N1	0.1338 (6)	0.5418 (3)	0.4672 (2)	0.0802 (11)
N1′	0.2807 (3)	0.2215 (2)	0.31248 (14)	0.0459 (6)
C2	0.1745 (6)	0.4979 (3)	0.4014 (2)	0.0648 (10)
H2	0.157045	0.543351	0.360070	0.078*
C3	0.2404 (4)	0.3903 (3)	0.39001 (17)	0.0471 (7)
C4	0.2700 (6)	0.3259 (3)	0.45187 (19)	0.0660 (10)
H4	0.318057	0.253834	0.447733	0.079*
C5	0.2273 (6)	0.3694 (4)	0.5209 (2)	0.0775 (12)
H5	0.244599	0.326389	0.563353	0.093*
C6	0.1599 (6)	0.4756 (4)	0.5252 (2)	0.0762 (13)
H6	0.130429	0.503421	0.571493	0.091*
C2′	0.2876 (4)	0.3471 (3)	0.31322 (16)	0.0458 (7)
H2′A	0.404956	0.369480	0.303765	0.055*
C3′	0.1791 (6)	0.3954 (3)	0.25051 (18)	0.0601 (9)
H3′A	0.175535	0.477799	0.254520	0.072*
H3′B	0.230610	0.376342	0.203524	0.072*
C4′	0.0008 (5)	0.3491 (4)	0.2525 (2)	0.0687 (10)
H4′B	−0.054026	0.372414	0.297957	0.082*
H4′A	−0.063361	0.379805	0.211468	0.082*
C5′	0.0037 (5)	0.2213 (4)	0.2479 (2)	0.0685 (11)
H5′B	0.050165	0.198218	0.200642	0.082*
H5′A	−0.110794	0.192194	0.251255	0.082*
C6′	0.1102 (5)	0.1715 (3)	0.3099 (2)	0.0585 (9)
H6′A	0.053836	0.184907	0.356662	0.070*
H6′B	0.119525	0.089753	0.303072	0.070*
C7	0.4458 (4)	0.1468 (3)	0.18773 (16)	0.0478 (6)
C8	0.3742 (5)	0.0569 (3)	0.1500 (2)	0.0536 (8)

H8	0.326167	−0.003003	0.176245	0.064*
C9	0.3728 (5)	0.0547 (4)	0.0731 (2)	0.0662 (11)
C10	0.4447 (6)	0.1471 (4)	0.03484 (19)	0.0725 (11)
C11	0.5126 (6)	0.2369 (4)	0.0740 (2)	0.0727 (12)
H11	0.558208	0.298156	0.048268	0.087*
C12	0.5152 (5)	0.2386 (3)	0.1501 (2)	0.0609 (9)
H12	0.562128	0.299646	0.175608	0.073*
C13	0.4524 (9)	0.1493 (6)	−0.0490 (2)	0.117 (2)
H13A	0.465980	0.226429	−0.065598	0.176*
H13B	0.349504	0.118467	−0.068832	0.176*
H13C	0.546474	0.104368	−0.065538	0.176*
C14	0.2982 (7)	−0.0467 (5)	0.0344 (3)	0.1006 (17)
H14A	0.242833	−0.094837	0.069736	0.151*
H14B	0.386563	−0.088725	0.010278	0.151*
H14C	0.217586	−0.021386	−0.001693	0.151*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0538 (4)	0.0543 (4)	0.0457 (3)	0.0128 (4)	−0.0003 (4)	0.0025 (3)
O1	0.0490 (16)	0.103 (2)	0.0614 (14)	0.0111 (14)	−0.0086 (11)	−0.0105 (14)
O2	0.099 (2)	0.0579 (15)	0.0644 (14)	0.0281 (15)	0.0088 (15)	0.0157 (12)
N1	0.099 (3)	0.072 (2)	0.070 (2)	0.005 (2)	0.0139 (19)	−0.0233 (19)
N1′	0.0470 (15)	0.0423 (14)	0.0484 (13)	−0.0004 (12)	0.0055 (11)	−0.0010 (11)
C2	0.083 (3)	0.054 (2)	0.057 (2)	0.0003 (19)	0.0050 (19)	−0.0065 (17)
C3	0.0486 (18)	0.0468 (17)	0.0457 (16)	−0.0090 (13)	0.0018 (14)	−0.0031 (13)
C4	0.086 (3)	0.063 (2)	0.0494 (18)	0.003 (2)	0.0042 (18)	−0.0026 (16)
C5	0.096 (3)	0.091 (3)	0.0453 (18)	−0.005 (3)	0.0028 (19)	−0.005 (2)
C6	0.079 (3)	0.091 (3)	0.059 (2)	−0.014 (2)	0.012 (2)	−0.028 (2)
C2′	0.0528 (18)	0.0396 (15)	0.0449 (13)	−0.0040 (14)	0.0076 (13)	0.0001 (13)
C3′	0.085 (3)	0.0494 (19)	0.0461 (19)	0.0083 (17)	0.0047 (17)	0.0002 (14)
C4′	0.070 (2)	0.076 (3)	0.060 (2)	0.021 (2)	−0.0114 (16)	−0.011 (2)
C5′	0.051 (2)	0.079 (3)	0.076 (2)	−0.0010 (18)	−0.0030 (17)	−0.024 (2)
C6′	0.057 (2)	0.0468 (18)	0.071 (2)	−0.0100 (14)	0.0121 (17)	−0.0071 (15)
C7	0.0470 (16)	0.0500 (16)	0.0463 (13)	0.0116 (17)	0.0035 (13)	−0.0027 (13)
C8	0.0516 (19)	0.0476 (18)	0.0615 (18)	0.0099 (14)	0.0050 (15)	−0.0060 (15)
C9	0.055 (2)	0.079 (3)	0.064 (2)	0.025 (2)	−0.0063 (18)	−0.021 (2)
C10	0.076 (3)	0.094 (3)	0.0475 (16)	0.035 (3)	0.0031 (18)	0.000 (2)
C11	0.083 (3)	0.077 (3)	0.058 (2)	0.016 (2)	0.0150 (19)	0.017 (2)
C12	0.067 (3)	0.056 (2)	0.0602 (19)	0.0046 (17)	0.0099 (17)	0.0030 (17)
C13	0.131 (5)	0.174 (6)	0.046 (2)	0.070 (5)	0.002 (3)	0.002 (3)
C14	0.086 (4)	0.115 (4)	0.100 (3)	0.016 (3)	−0.012 (3)	−0.056 (3)

Geometric parameters (Å, º)

S1—O1	1.432 (3)	C4′—H4′A	0.9700
S1—O2	1.432 (3)	C5′—C6′	1.521 (6)
S1—N1′	1.623 (3)	C5′—H5′B	0.9700

S1—C7	1.767 (3)	C5′—H5′A	0.9700
N1—C6	1.322 (6)	C6′—H6′A	0.9700
N1—C2	1.339 (5)	C6′—H6′B	0.9700
N1′—C6′	1.472 (4)	C7—C8	1.378 (5)
N1′—C2′	1.475 (4)	C7—C12	1.387 (5)
C2—C3	1.381 (5)	C8—C9	1.394 (5)
C2—H2	0.9300	C8—H8	0.9300
C3—C4	1.372 (5)	C9—C10	1.407 (6)
C3—C2′	1.527 (4)	C9—C14	1.503 (6)
C4—C5	1.392 (5)	C10—C11	1.379 (7)
C4—H4	0.9300	C10—C13	1.520 (5)
C5—C6	1.359 (7)	C11—C12	1.380 (5)
C5—H5	0.9300	C11—H11	0.9300
C6—H6	0.9300	C12—H12	0.9300
C2′—C3′	1.532 (5)	C13—H13A	0.9600
C2′—H2′A	0.9800	C13—H13B	0.9600
C3′—C4′	1.511 (6)	C13—H13C	0.9600
C3′—H3′A	0.9700	C14—H14A	0.9600
C3′—H3′B	0.9700	C14—H14B	0.9600
C4′—C5′	1.502 (6)	C14—H14C	0.9600
C4′—H4′B	0.9700		

O1—S1—O2	119.96 (19)	C4′—C5′—C6′	110.6 (3)
O1—S1—N1′	106.46 (15)	C4′—C5′—H5′B	109.5
O2—S1—N1′	106.79 (17)	C6′—C5′—H5′B	109.5
O1—S1—C7	107.46 (17)	C4′—C5′—H5′A	109.5
O2—S1—C7	107.23 (16)	C6′—C5′—H5′A	109.5
N1′—S1—C7	108.54 (14)	H5′B—C5′—H5′A	108.1
C6—N1—C2	116.3 (4)	N1′—C6′—C5′	112.2 (3)
C6′—N1′—C2′	115.6 (3)	N1′—C6′—H6′A	109.2
C6′—N1′—S1	120.2 (2)	C5′—C6′—H6′A	109.2
C2′—N1′—S1	120.4 (2)	N1′—C6′—H6′B	109.2
N1—C2—C3	125.2 (4)	C5′—C6′—H6′B	109.2
N1—C2—H2	117.4	H6′A—C6′—H6′B	107.9
C3—C2—H2	117.4	C8—C7—C12	120.9 (3)
C4—C3—C2	116.5 (3)	C8—C7—S1	119.7 (3)
C4—C3—C2′	121.3 (3)	C12—C7—S1	119.4 (3)
C2—C3—C2′	122.2 (3)	C7—C8—C9	120.9 (4)
C3—C4—C5	119.3 (4)	C7—C8—H8	119.6
C3—C4—H4	120.3	C9—C8—H8	119.6
C5—C4—H4	120.3	C8—C9—C10	118.4 (4)
C6—C5—C4	118.9 (4)	C8—C9—C14	119.0 (5)
C6—C5—H5	120.6	C10—C9—C14	122.6 (4)
C4—C5—H5	120.6	C11—C10—C9	119.5 (3)
N1—C6—C5	123.7 (4)	C11—C10—C13	119.0 (5)
N1—C6—H6	118.1	C9—C10—C13	121.4 (5)
C5—C6—H6	118.1	C10—C11—C12	122.1 (4)
N1′—C2′—C3	109.4 (2)	C10—C11—H11	119.0

N1′—C2′—C3′	110.0 (3)	C12—C11—H11	119.0
C3—C2′—C3′	114.5 (3)	C11—C12—C7	118.3 (4)
N1′—C2′—H2′A	107.5	C11—C12—H12	120.9
C3—C2′—H2′A	107.5	C7—C12—H12	120.9
C3′—C2′—H2′A	107.5	C10—C13—H13A	109.5
C4′—C3′—C2′	111.8 (3)	C10—C13—H13B	109.5
C4′—C3′—H3′A	109.3	H13A—C13—H13B	109.5
C2′—C3′—H3′A	109.3	C10—C13—H13C	109.5
C4′—C3′—H3′B	109.3	H13A—C13—H13C	109.5
C2′—C3′—H3′B	109.3	H13B—C13—H13C	109.5
H3′A—C3′—H3′B	107.9	C9—C14—H14A	109.5
C5′—C4′—C3′	110.1 (3)	C9—C14—H14B	109.5
C5′—C4′—H4′B	109.6	H14A—C14—H14B	109.5
C3′—C4′—H4′B	109.6	C9—C14—H14C	109.5
C5′—C4′—H4′A	109.6	H14A—C14—H14C	109.5
C3′—C4′—H4′A	109.6	H14B—C14—H14C	109.5
H4′B—C4′—H4′A	108.2		

O1—S1—N1′—C6′	−167.4 (3)	C2′—C3′—C4′—C5′	−57.8 (4)
O2—S1—N1′—C6′	−38.2 (3)	C3′—C4′—C5′—C6′	56.9 (4)
C7—S1—N1′—C6′	77.2 (3)	C2′—N1′—C6′—C5′	51.4 (4)
O1—S1—N1′—C2′	35.6 (3)	S1—N1′—C6′—C5′	−106.6 (3)
O2—S1—N1′—C2′	164.9 (2)	C4′—C5′—C6′—N1′	−53.3 (4)
C7—S1—N1′—C2′	−79.8 (3)	O1—S1—C7—C8	150.0 (3)
C6—N1—C2—C3	0.1 (7)	O2—S1—C7—C8	19.8 (3)
N1—C2—C3—C4	−1.9 (7)	N1′—S1—C7—C8	−95.3 (3)
N1—C2—C3—C2′	−178.6 (4)	O1—S1—C7—C12	−32.2 (3)
C2—C3—C4—C5	2.3 (6)	O2—S1—C7—C12	−162.5 (3)
C2′—C3—C4—C5	179.0 (4)	N1′—S1—C7—C12	82.5 (3)
C3—C4—C5—C6	−1.1 (7)	C12—C7—C8—C9	1.4 (5)
C2—N1—C6—C5	1.4 (7)	S1—C7—C8—C9	179.1 (3)
C4—C5—C6—N1	−0.9 (8)	C7—C8—C9—C10	−0.7 (5)
C6′—N1′—C2′—C3	76.0 (4)	C7—C8—C9—C14	178.1 (4)
S1—N1′—C2′—C3	−126.1 (2)	C8—C9—C10—C11	−0.5 (6)
C6′—N1′—C2′—C3′	−50.6 (4)	C14—C9—C10—C11	−179.3 (4)
S1—N1′—C2′—C3′	107.3 (3)	C8—C9—C10—C13	178.3 (4)
C4—C3—C2′—N1′	28.4 (5)	C14—C9—C10—C13	−0.5 (7)
C2—C3—C2′—N1′	−155.1 (3)	C9—C10—C11—C12	1.0 (7)
C4—C3—C2′—C3′	152.5 (4)	C13—C10—C11—C12	−177.7 (4)
C2—C3—C2′—C3′	−31.0 (5)	C10—C11—C12—C7	−0.4 (6)
N1′—C2′—C3′—C4′	53.3 (4)	C8—C7—C12—C11	−0.9 (6)
C3—C2′—C3′—C4′	−70.3 (4)	S1—C7—C12—C11	−178.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5′—H5′*A*···O1^{i}	0.97	2.60	3.462 (5)	148

C5—H5···O1^{ii}	0.93	2.64	3.384 (5)	138
C2′—H2′*A*···O1	0.98	2.39	2.892 (4)	111

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