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Crystal structure and Hirshfeld surface analysis of 2-[(1,3-benzoxazol-2-yl)sulfanyl]-*N*-(2-methoxyphenyl)acetamide

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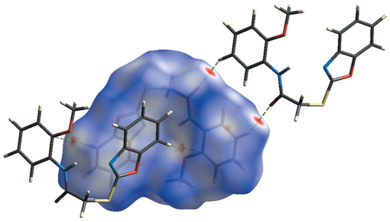
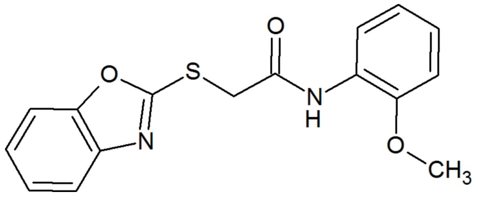
In the title compound, $C_{16}H_{14}N_2O_3S$, the 1,3-benzoxazole ring system is essentially planar (r.m.s deviation = 0.004 Å) and makes a dihedral angle of 66.16 (17)° with the benzene ring of the methoxyphenyl group. Two intramolecular N—H···O and N—H···N hydrogen bonds occur, forming *S*(5) and *S*(7) ring motifs, respectively. In the crystal, pairs of C—H···O hydrogen bonds link the molecules into inversion dimers with $R^2_2(14)$ ring motifs, stacked along the *b*-axis direction. The inversion dimers are linked by C—H···π and π–π-stacking interactions [centroid-to-centroid distances = 3.631 (2) and 3.631 (2) Å], forming a three-dimensional network. Two-dimensional fingerprint plots associated with the Hirshfeld surface show that the largest contributions to the crystal packing come from H···H (39.3%), C···H/H···C (18.0%), O···H/H···O (15.6) and S···H/H···S (10.2%) interactions.



1. Chemical context

As a part of our ongoing research on synthesis and screening of pharmacological activities of compounds with a benzoxazole ring, which is known to produce a wide range of biological activities (Aggarwal *et al.*, 2017; Gautam *et al.*, 2012), we have focused on the synthesis of 3-substituted benzoxazolone-2-thione and S-substituted benzoxazole-2-thiol derivatives. It is well known that alkylation of benzoxazolone-2-thione leads to the *S*-alkylated derivatives instead of *N*-alkylated ones (Xiang *et al.*, 2012; Rakse *et al.*, 2013; Yurttaş *et al.*, 2015). In this manner, the title compound was synthesized as a member of the target S-substituted benzoxazole-2-thiol series. The title compound is listed in the literature with registry number CASRN 331966-95-1 but corresponding scientific reference data are not available.



2. Structural commentary

In the molecular structure of the title compound (Fig. 1), the 1,3-benzoxazole ring system (N1/O1/C1–C7) is essentially

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

*Cg*3 is the centroid of the C10–C15 benzene ring of the methoxy phenyl group.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···O3	0.86	2.22	2.608 (4)	107
N2—H*N*2···N1	0.86	2.39	3.075 (4)	136
C8—H8*A*···N1	0.97	2.48	2.914 (5)	107
C11—H11···O2	0.93	2.28	2.869 (5)	121
C12—H12···O2^{i}	0.93	2.52	3.378 (6)	153
C13—H13···*Cg*3^{ii}	0.93	2.89	3.634 (5)	138

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

planar (r.m.s deviation = 0.004 Å) and makes a dihedral angle of 66.16 (17)° with the benzene ring (C10–C15) of the methoxyphenyl group. Atoms O3 and C16 deviate from the benzene ring by −0.008 (3) and 0.099 (6) Å, respectively. The torsion angle C7—S1—C8—C9 = −87.7 (3)°, S1—C8—C9—N2 = 91.6 (4)° and C8—C9—N2—C10 = −178.8 (3)°. The C7—S1 [1.740 (4) Å] and C8—S1 [1.812 (4) Å] bond lengths are comparable with those reported for three similar structures, *viz.* 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2-methylphenyl)acetamide (1.763 and 1.805 Å, respectively; Subasri *et al.*, 2014), 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2,4-dimethylphenyl)acetamide [1.7650 (14) and 1.8053 (16) Å, respectively; Choudhury *et al.*, 2017] and 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(3-methoxyphenyl) acetamide [1.7721 (17) and 1.8126 (18) Å, respectively; Choudhury *et al.*, 2017]. The two intramolecular hydrogen bonds, N2—H*N*2···O3 and N2—H*N*2···N1, form *S*(5) and *S*(7) ring motifs, respectively (Table 1, Fig. 1).

3. Supramolecular features

In the crystal, pairs of C—H···O hydrogen bonds link the molecules into inversion dimers with $R_2^2(14)$ ring motifs, stacking along the *b*-axis direction. These dimers are linked by C—H···π (Table 1, Fig. 2) and π–π-stacking interactions [Fig. 2; distances of 3.631 (2) and 3.631 (2) Å between the centroids of the five- and opposite six-membered rings of the 1,3-benzoxazole ring system of adjacent molecules], forming a three-dimensional network (Fig. 3).

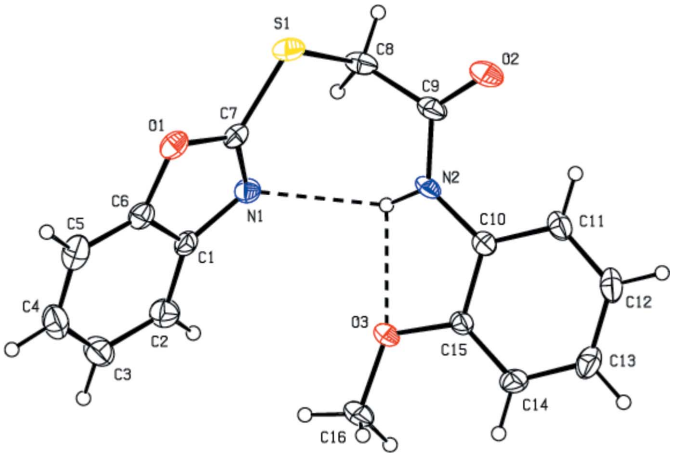


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

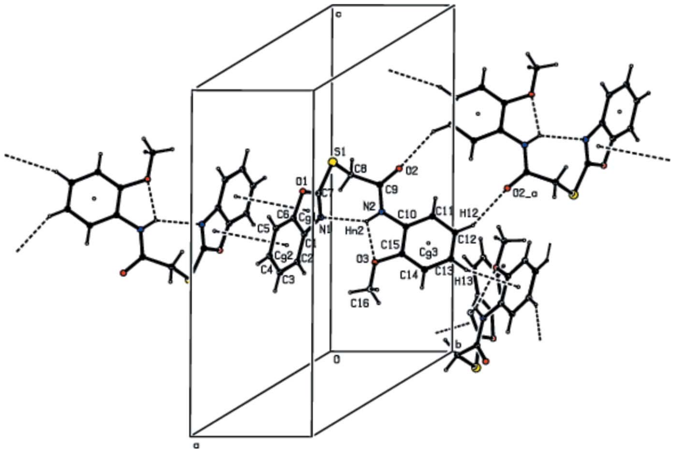


Figure 2
A packing diagram of the title compound, showing the intra- and intermolecular N—H···N and N—H···O, C—H···O hydrogen bonds, C—H···π interactions and π–π-stacking interactions (dashed lines). Symmetry code: (*a*) − *x*, 2 − *y*, 1 − *z*.

4. Hirshfeld surface analysis

In order to explore the role of weak intermolecular interactions in the crystal packing, Hirshfeld surfaces ($d_{\rm norm}$) and the related two-dimensional fingerprint plots were generated using *CrystalExplorer17.5* (Spackman & Jayatilaka, 2009; Wolff *et al.*, 2012). The three-dimensional molecular Hirshfeld surfaces were generated using a high standard surface reso-

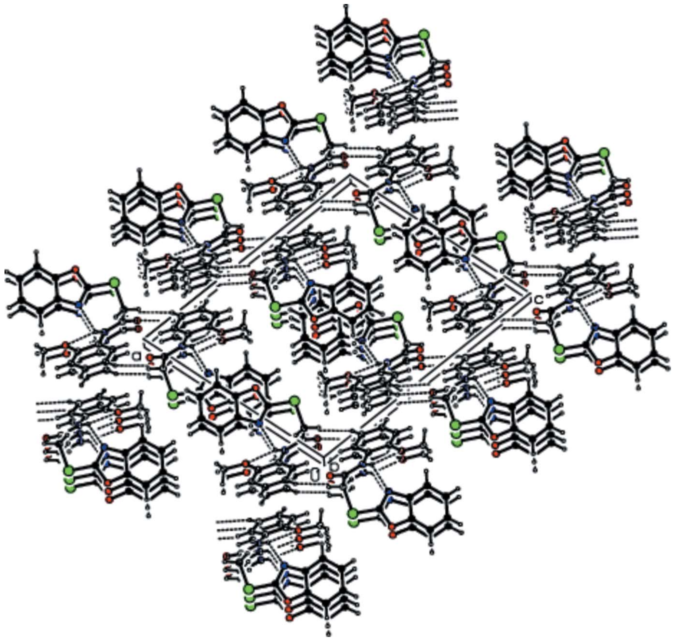


Figure 3
Packing diagram of the title compound viewed down the *b* axis.

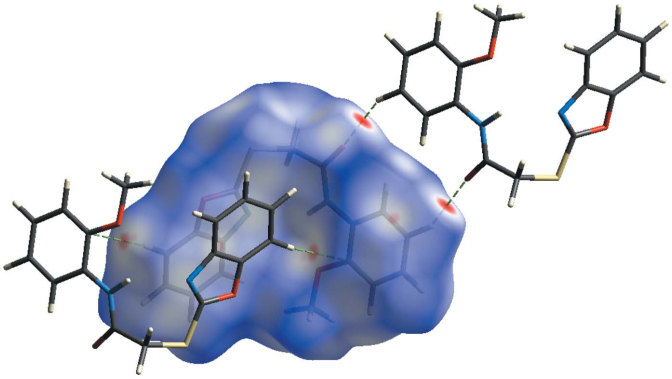


Figure 4
Hirshfeld surface mapped over $d_{\rm norm}$, showing the weak intermolecular C—H⋯O and C—H⋯C contacts.

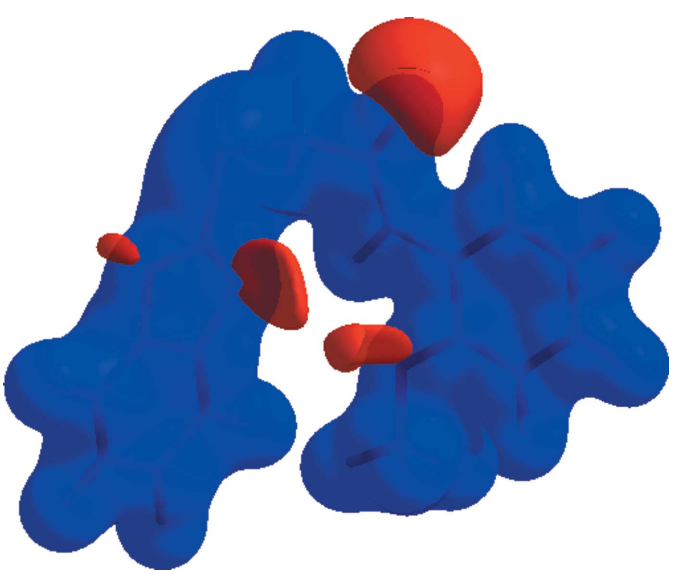


Figure 6
Hirshfeld surfaces for the title compound, mapped with shape-index.

lution over a colour scale of −0.1599 to 1.2011 a.u. for $d_{\rm norm}$ (Fig. 4). The red spots in the Hirshfeld surface represent short N⋯H/H⋯N and O⋯H/H⋯O contacts. On the shape-index surface (Fig. 5), convex blue regions represent hydrogen-donor groups and concave red regions represent hydrogen-acceptor groups. In addition, concave red regions represent C—H⋯π and π–π interactions.

The bright-red spots indicate their roles as the respective donors and/or acceptors; they also appear as blue and red regions corresponding to positive and negative potentials on the Hirshfeld surface mapped over electrostatic potential (Spackman *et al.*, 2008) shown in Fig. 6. The blue regions indicate the positive electrostatic potential (hydrogen-bond donors), while the red regions indicate the negative electrostatic potential (hydrogen-bond acceptors).

The two-dimensional fingerprint plots (Fig. 7) quantify the contributions of each type of intermolecular interaction to the Hirshfeld surface (McKinnon *et al.*, 2007). The largest contribution (39.3% of the surface) is from H⋯H contacts (Table 2), which represent van der Waals interactions, followed by C⋯H/H⋯C contacts involved in C—H⋯π interactions (18.0%). Finally, the O⋯H/H⋯O (15.6%), S⋯H/H⋯S (10.2%) and C⋯C (4.5%) contacts correspond to hydrogen bonds and π–π interactions, respectively. The

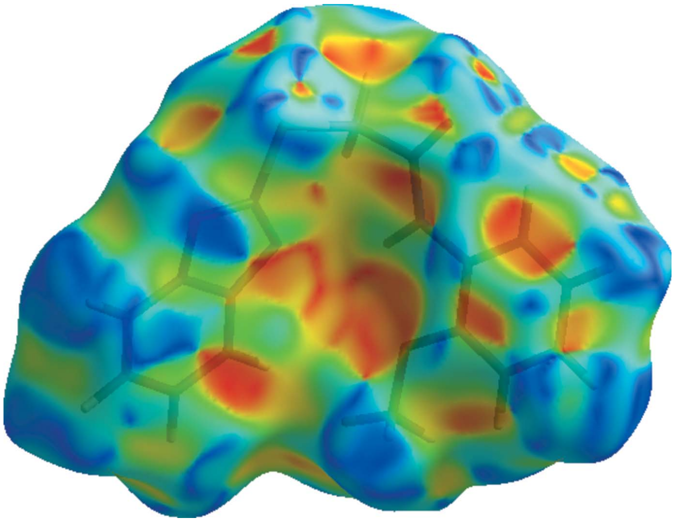
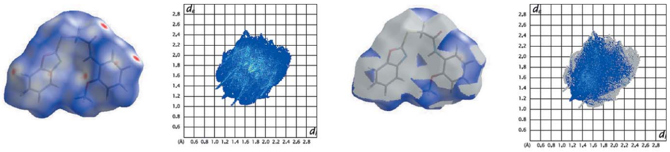
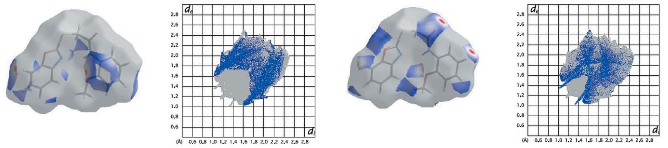


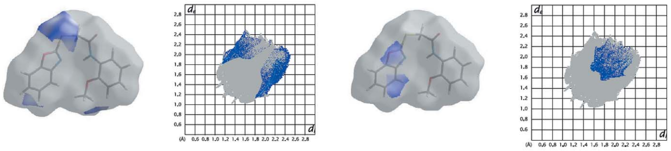
Figure 5
View of the three-dimensional Hirshfeld surface of the title compound plotted over electrostatic potential energy in the range −0.0500 to 0.0500 a.u. using the STO-3 G basis set at the Hartree–Fock level of theory. Hydrogen- bond donors and acceptors are shown as blue and red regions around the atoms corresponding to positive and negative potentials, respectively.



(a) All…All (100%) **(b) H…H (39.3%)**



(c) C…H / H…C (18.0%) **(d) O…H / H…O (15.6%)**



(e) S…H / H…S (10.2%) **(f) C…O / O…C (6.0%)**

Figure 7
Hirshfeld surfaces and two-dimensional fingerprints for the compound, showing (*a*) all interactions and those delineated into (*b*) H⋯H, (*c*) C⋯H/H⋯C, (*d*) O⋯H/H⋯O, (*e*) S⋯H/H⋯S and (*f*) C⋯O/O⋯C contacts.

Table 2
Summary of selected short interatomic contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
H5···O3	2.72	$1 - x, 1 - y, 1 - z$
S1···H2	3.10	$x, \frac{1}{2} - y, \frac{1}{2} + z$
C5···C1	3.38	$1 - x, -y, 1 - z$
H8*B*···C11	3.06	$-x, 1 - y, 1 - z$
H12···O2	2.52	$-x, 2 - y, 1 - z$
O2···H16*A*	2.74	$x, \frac{3}{2} - y, \frac{1}{2} + z$
C10···H13	3.04	$-x, -\frac{1}{2} + y, \frac{1}{2} - z$
C12···H8*A*	2.82	$x, 1 + y, z$

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surface of the title compound.

Contact	Percentage contribution
H···H	39.3
H···C/C···H	18.0
O···H/H···O	15.6
S···H/H···S	10.2
C···O/O···C	6.0
C···C	4.5
N···H/H···N	4.1
C···N/N···C	1.4
C···S/S···C	0.6
N···O/O···N	0.1

Table 4
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{14}N_2O_3S$
M_r	314.35
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	13.6670 (13), 6.8704 (6), 16.7220 (16)
β (°)	108.020 (4)
V (Å^3)	1493.1 (2)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.23
Crystal size (mm)	0.10 × 0.07 × 0.06
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
$T_{\min}$, $T_{\max}$	0.654, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23464, 3019, 2241
$R_{\rm int}$	0.092
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.627
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.092, 0.169, 1.10
No. of reflections	3019
No. of parameters	200
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.25, −0.31

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

percentage contributions to the Hirshfeld surface of the various interatomic contacts are given in Table 3.

5. Database survey

Related compounds to the title compound include 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(naphthalen-1-yl)acetamide (refcode JARPOK; Subasri *et al.*, 2017), 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(4-fluorophenyl)acetamide (JARPUQ; Subasri *et al.*, 2017), 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2-methylphenyl)acetamide (GOKWIO; Subasri *et al.*, 2014), 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(2,4-dimethylphenyl)acetamide (JAXFIA; Choudhury *et al.*, 2017), 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-*N*-(3-methoxyphenyl) acetamide (refcode: JAXFOG; Choudhury *et al.*, 2017) and 2-[(2-aminophenyl)sulfanyl]-*N*-(4-methoxyphenyl)acetamide (PAXTEP; Murtaza *et al.*, 2012).

In the crystals of JARPOK and JARPUQ, molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with $R_2^2(8)$ ring motifs. In the crystal of JARPOK, the dimers are linked by bifurcated N—H···(O,O) and C—H···O hydrogen bonds, forming layers parallel to (100). In the crystal of JARPUQ, the dimers are linked by N—H···O hydrogen bonds, also forming layers parallel to (100). The layers are linked by C—H···F hydrogen bonds, forming a three-dimensional architecture.

In the crystal of GOKWIO, molecules are linked *via* pairs of N—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif. The dimers are linked by N—H···O and C—H···O hydrogen bonds, forming sheets parallel to (100).

In the crystals of JAXFIA and JAXFOG, a pair of N—H···N hydrogen bonds links the molecules, forming inversion dimers with $R_2^2(8)$ ring motifs. In JAXFIA, the dimers are linked by N—H···O and C—H···O hydrogen bonds, enclosing $R_1^2(14)$, $R_1^2(11)$ and $R_1^2(7)$ ring motifs, forming layers parallel to the (100) plane. There is also an N—H···π interaction present within the layer. In JAXFOG, the inversion dimers are linked by N—H···O hydrogen bonds enclosing an $R_4^4(18)$ ring motif. The presence of N—H···O and C—H···O hydrogen bonds generate an $R_1^2(6)$ ring motif. The combination of these various hydrogen bonds results in the formation of layers parallel to the $(1\bar{1}1)$ plane.

In the crystal of PAXTEP, molecules are consolidated in the form of polymeric chains along [010] as a result of N—H···O hydrogen bonds, which generate $R_2^3(18)$ and $R_3^4(22)$ loops. The polymeric chains are interlinked through C—H···O interaction and complete $R_2^2(8)$ ring motifs.

6. Synthesis and crystallization

The starting materials, 2-mercaptobenzoxazole and α-chloro-*N*-(*o*-methoxyphenyl)acetamide, were synthesized according to literature methods (Maske *et al.*, 2012; Ren *et al.*, 2015). For the synthesis of the title compound, 2-mercaptobenzoxazole (1 eq) and α-chloro-*N*-(*o*-methoxyphenyl) acetamide (1 eq) were heated in acetone under reflux for 1.5 h in the presence of K_2CO_3 (1 eq). The reaction mixture was then cooled to room temperature and cold water was added until precipitation was complete. The precipitate was filtered, washed with cold water and dried. The crude product was crystallized from methanol (yield 31%); m.p. 370 K.

^{1}H NMR (DMSO-d_6, 400 MHz) δ 3.82 (3H, *s*, OCH_3), δ 4.42 (2H, *s*, CH_2), δ 6.89 (1H, *m*, Ar-H), δ 7.03–7.10 (2H, *m*, Ar-H), δ 7.31–7.38 (2H, *m*, Ar-H), δ 7.62–7.68 (2H, *m*, Ar-H), δ 7.97 (1H, *d*, J = 8.4 Hz, Ar-H), δ 9.65 (1H, *s*, NH) p.p.m. IR $\nu_{\max}$ cm^{-1}: 3295 (NH), 1675 (amide I), 1534 (amide II); MS (ESI) m/z (intensity %): 315.32 (26) $[M\text{+H}]^+$ 192.27 (100).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All H atoms were positioned with idealized geometry and refined as riding: N—H = 0.86 Å, C—H = 0.93–0.97 Å with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H atoms and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C, N) for all other H atoms. Thirty one outliers (13 1 3), $(\overline{14}\ 1\ 1)$, (8 3 12), $(\overline{7}\ 5\ 15)$, (0 3 18), (5 0 14), (14 2 5), $(\overline{12}\ 0\ 14)$, $(\overline{2}\ 4\ 17)$, (14 3 1), $(\overline{16}\ 3\ 5)$, (1 8 4), (1 4 15), (10 5 2), $(\overline{5}\ 7\ 8)$, $(\overline{16}\ 0\ 10)$, (14 2 1), $(\overline{15}\ 1\ 1)$, $(\overline{14}\ 3\ 12)$, $(\overline{15}\ 2\ 7)$, (4 1 17), (11 0 10), (15 1 2), (3 4 14), (10 2 6), $(\overline{5}\ 0\ 18)$, $(\overline{5}\ 3\ 18)$, $(\overline{1}\ 6\ 11)$, $(\overline{11}\ 5\ 2)$, (10 1 9), $(\overline{14}\ 1\ 2)$ were omitted in the final cycles of refinement.

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supporting information

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Crystal structure and Hirshfeld surface analysis of 2-[(1,3-benzoxazol-2-yl)sulfanyl]-*N*-(2-methoxyphenyl)acetamide

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Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/1* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *WinGX* (Farrugia, 2012).

2-[(1,3-Benzoxazol-2-yl)sulfanyl]-*N*-(2-methoxyphenyl)acetamide

Crystal data

$C_{16}H_{14}N_2O_3S$
$M_r = 314.35$
Monoclinic, $P2_1/c$
$a = 13.6670$ (13) Å
$b = 6.8704$ (6) Å
$c = 16.7220$ (16) Å
$\beta = 108.020$ (4)°
$V = 1493.1$ (2) Å^3
$Z = 4$
$F(000) = 656$
$D_x = 1.398$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6692 reflections
$\theta = 3.2$–26.3°
$\mu = 0.23$ mm^{-1}
$T = 296$ K
Block, colourless
0.10 × 0.07 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
$T_{min} = 0.654$, $T_{max} = 0.745$
23464 measured reflections
3019 independent reflections
2241 reflections with $I > 2\sigma(I)$
$R_{int} = 0.092$
$\theta_{max} = 26.5°$, $\theta_{min} = 3.1°$
$h = -17 \rightarrow 17$
$k = -8 \rightarrow 8$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.092$
$wR(F^2) = 0.169$
$S = 1.10$
3019 reflections
200 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 3.9251P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.4055 (3)	0.2452 (5)	0.4388 (2)	0.0301 (9)
C2	0.4121 (3)	0.1973 (6)	0.3599 (3)	0.0437 (11)
H2	0.353578	0.186794	0.313350	0.052*
C3	0.5089 (4)	0.1660 (7)	0.3535 (3)	0.0507 (12)
H3	0.515664	0.134545	0.301349	0.061*
C4	0.5962 (4)	0.1801 (6)	0.4223 (3)	0.0515 (13)
H4	0.660182	0.158127	0.415281	0.062*
C5	0.5910 (3)	0.2258 (6)	0.5012 (3)	0.0460 (11)
H5	0.649354	0.234724	0.547961	0.055*
C6	0.4940 (3)	0.2573 (5)	0.5059 (3)	0.0330 (9)
C7	0.3608 (3)	0.3093 (5)	0.5452 (2)	0.0304 (9)
C8	0.1670 (3)	0.3513 (7)	0.5515 (3)	0.0401 (10)
H8A	0.160668	0.258715	0.506432	0.048*
H8B	0.122257	0.308919	0.583244	0.048*
C9	0.1330 (3)	0.5503 (6)	0.5143 (2)	0.0368 (10)
C10	0.1249 (3)	0.7568 (6)	0.3915 (2)	0.0272 (8)
C11	0.0683 (3)	0.9111 (6)	0.4077 (2)	0.0364 (10)
H11	0.044048	0.906129	0.453818	0.044*
C12	0.0479 (3)	1.0720 (7)	0.3557 (3)	0.0438 (11)
H12	0.008978	1.173897	0.366520	0.053*
C13	0.0844 (3)	1.0826 (7)	0.2882 (3)	0.0443 (11)
H13	0.070946	1.191980	0.253773	0.053*
C14	0.1411 (3)	0.9312 (7)	0.2714 (2)	0.0380 (10)
H14	0.165837	0.938978	0.225560	0.046*
C15	0.1615 (3)	0.7687 (6)	0.3217 (2)	0.0290 (9)
C16	0.2621 (5)	0.6219 (9)	0.2449 (3)	0.078 (2)
H16A	0.209173	0.634567	0.191795	0.118*
H16B	0.301214	0.505956	0.244719	0.118*
H16C	0.306739	0.733112	0.253872	0.118*
N1	0.3202 (2)	0.2815 (5)	0.46627 (18)	0.0309 (7)
N2	0.1476 (2)	0.5848 (5)	0.43945 (19)	0.0302 (7)
HN2	0.173630	0.491051	0.418615	0.036*
O1	0.4653 (2)	0.3005 (4)	0.57658 (16)	0.0363 (7)
O2	0.0961 (3)	0.6653 (6)	0.55175 (19)	0.0687 (11)
O3	0.2163 (2)	0.6103 (4)	0.31065 (17)	0.0467 (8)
S1	0.29895 (9)	0.35394 (17)	0.62002 (6)	0.0420 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.036 (2)	0.0217 (18)	0.032 (2)	0.0038 (16)	0.0093 (17)	0.0053 (16)
C2	0.047 (3)	0.045 (3)	0.039 (2)	0.002 (2)	0.013 (2)	0.000 (2)
C3	0.059 (3)	0.046 (3)	0.058 (3)	0.006 (2)	0.033 (3)	0.001 (2)
C4	0.044 (3)	0.036 (2)	0.085 (4)	0.005 (2)	0.035 (3)	0.009 (2)
C5	0.032 (2)	0.035 (2)	0.066 (3)	−0.0031 (19)	0.007 (2)	0.009 (2)
C6	0.038 (2)	0.0217 (19)	0.039 (2)	−0.0024 (17)	0.0112 (18)	0.0046 (17)
C7	0.036 (2)	0.024 (2)	0.029 (2)	0.0016 (16)	0.0067 (17)	0.0061 (16)
C8	0.041 (2)	0.052 (3)	0.034 (2)	−0.009 (2)	0.0208 (19)	0.000 (2)
C9	0.036 (2)	0.053 (3)	0.026 (2)	−0.001 (2)	0.0156 (18)	−0.0053 (19)
C10	0.0190 (18)	0.040 (2)	0.0195 (18)	−0.0011 (16)	0.0007 (15)	−0.0058 (16)
C11	0.027 (2)	0.050 (3)	0.030 (2)	0.0069 (19)	0.0060 (17)	−0.0084 (19)
C12	0.035 (2)	0.049 (3)	0.040 (3)	0.017 (2)	0.002 (2)	−0.010 (2)
C13	0.043 (3)	0.044 (3)	0.038 (2)	0.012 (2)	0.000 (2)	0.005 (2)
C14	0.034 (2)	0.055 (3)	0.022 (2)	0.004 (2)	0.0055 (17)	0.0048 (19)
C15	0.0247 (19)	0.040 (2)	0.0224 (18)	0.0045 (17)	0.0067 (15)	−0.0009 (17)
C16	0.117 (5)	0.081 (4)	0.066 (4)	0.054 (4)	0.071 (4)	0.027 (3)
N1	0.0325 (18)	0.0342 (18)	0.0236 (17)	0.0008 (14)	0.0055 (14)	−0.0010 (14)
N2	0.0334 (18)	0.0369 (18)	0.0261 (16)	0.0024 (14)	0.0177 (14)	−0.0058 (14)
O1	0.0348 (16)	0.0358 (15)	0.0311 (15)	−0.0026 (13)	−0.0002 (12)	0.0042 (12)
O2	0.101 (3)	0.082 (3)	0.0401 (19)	0.035 (2)	0.046 (2)	0.0056 (18)
O3	0.062 (2)	0.0517 (19)	0.0380 (17)	0.0240 (16)	0.0333 (15)	0.0094 (14)
S1	0.0516 (7)	0.0517 (7)	0.0226 (5)	0.0004 (6)	0.0114 (5)	0.0050 (5)

Geometric parameters (Å, º)

C1—C6	1.375 (6)	C9—O2	1.211 (5)
C1—C2	1.389 (5)	C9—N2	1.348 (5)
C1—N1	1.401 (5)	C10—C11	1.388 (5)
C2—C3	1.377 (6)	C10—C15	1.406 (5)
C2—H2	0.9300	C10—N2	1.408 (5)
C3—C4	1.382 (7)	C11—C12	1.381 (6)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.379 (7)	C12—C13	1.370 (6)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.370 (6)	C13—C14	1.377 (6)
C5—H5	0.9300	C13—H13	0.9300
C6—O1	1.388 (5)	C14—C15	1.374 (6)
C7—N1	1.278 (5)	C14—H14	0.9300
C7—O1	1.362 (5)	C15—O3	1.366 (4)
C7—S1	1.740 (4)	C16—O3	1.426 (5)
C8—C9	1.514 (6)	C16—H16A	0.9600
C8—S1	1.812 (4)	C16—H16B	0.9600
C8—H8A	0.9700	C16—H16C	0.9600
C8—H8B	0.9700	N2—HN2	0.8600

C6—C1—C2	119.4 (4)	C11—C10—N2	124.6 (3)
C6—C1—N1	109.4 (3)	C15—C10—N2	116.7 (3)
C2—C1—N1	131.2 (4)	C12—C11—C10	120.4 (4)
C3—C2—C1	117.2 (4)	C12—C11—H11	119.8
C3—C2—H2	121.4	C10—C11—H11	119.8
C1—C2—H2	121.4	C13—C12—C11	120.4 (4)
C2—C3—C4	121.8 (4)	C13—C12—H12	119.8
C2—C3—H3	119.1	C11—C12—H12	119.8
C4—C3—H3	119.1	C12—C13—C14	120.0 (4)
C5—C4—C3	121.8 (4)	C12—C13—H13	120.0
C5—C4—H4	119.1	C14—C13—H13	120.0
C3—C4—H4	119.1	C15—C14—C13	120.6 (4)
C6—C5—C4	115.3 (4)	C15—C14—H14	119.7
C6—C5—H5	122.3	C13—C14—H14	119.7
C4—C5—H5	122.3	O3—C15—C14	125.4 (3)
C5—C6—C1	124.5 (4)	O3—C15—C10	114.6 (3)
C5—C6—O1	128.0 (4)	C14—C15—C10	120.0 (4)
C1—C6—O1	107.4 (3)	O3—C16—H16A	109.5
N1—C7—O1	117.4 (3)	O3—C16—H16B	109.5
N1—C7—S1	128.1 (3)	H16A—C16—H16B	109.5
O1—C7—S1	114.5 (3)	O3—C16—H16C	109.5
C9—C8—S1	111.7 (3)	H16A—C16—H16C	109.5
C9—C8—H8A	109.3	H16B—C16—H16C	109.5
S1—C8—H8A	109.3	C7—N1—C1	103.1 (3)
C9—C8—H8B	109.3	C9—N2—C10	127.4 (3)
S1—C8—H8B	109.3	C9—N2—HN2	116.3
H8A—C8—H8B	107.9	C10—N2—HN2	116.3
O2—C9—N2	124.7 (4)	C7—O1—C6	102.7 (3)
O2—C9—C8	120.1 (4)	C15—O3—C16	116.7 (3)
N2—C9—C8	115.2 (3)	C7—S1—C8	98.82 (18)
C11—C10—C15	118.7 (4)		

C6—C1—C2—C3	−0.6 (6)	N2—C10—C15—O3	−1.0 (5)
N1—C1—C2—C3	−178.6 (4)	C11—C10—C15—C14	0.2 (5)
C1—C2—C3—C4	0.4 (7)	N2—C10—C15—C14	179.1 (3)
C2—C3—C4—C5	0.1 (7)	O1—C7—N1—C1	1.2 (4)
C3—C4—C5—C6	−0.5 (6)	S1—C7—N1—C1	−177.6 (3)
C4—C5—C6—C1	0.3 (6)	C6—C1—N1—C7	−0.9 (4)
C4—C5—C6—O1	178.3 (4)	C2—C1—N1—C7	177.2 (4)
C2—C1—C6—C5	0.3 (6)	O2—C9—N2—C10	0.9 (7)
N1—C1—C6—C5	178.7 (4)	C8—C9—N2—C10	−178.8 (3)
C2—C1—C6—O1	−178.1 (3)	C11—C10—N2—C9	−10.6 (6)
N1—C1—C6—O1	0.3 (4)	C15—C10—N2—C9	170.5 (4)
S1—C8—C9—O2	−88.1 (5)	N1—C7—O1—C6	−1.1 (4)
S1—C8—C9—N2	91.6 (4)	S1—C7—O1—C6	177.9 (2)
C15—C10—C11—C12	0.5 (6)	C5—C6—O1—C7	−177.9 (4)
N2—C10—C11—C12	−178.3 (4)	C1—C6—O1—C7	0.4 (4)
C10—C11—C12—C13	−1.0 (6)	C14—C15—O3—C16	4.8 (6)

C11—C12—C13—C14	0.7 (7)	C10—C15—O3—C16	−175.1 (4)
C12—C13—C14—C15	0.1 (6)	N1—C7—S1—C8	−0.8 (4)
C13—C14—C15—O3	179.7 (4)	O1—C7—S1—C8	−179.7 (3)
C13—C14—C15—C10	−0.5 (6)	C9—C8—S1—C7	−87.7 (3)
C11—C10—C15—O3	−180.0 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*3 is the centroid of the C10–C15 benzene ring of the methoxy phenyl group.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···O3	0.86	2.22	2.608 (4)	107
N2—H*N*2···N1	0.86	2.39	3.075 (4)	136
C8—H8*A*···N1	0.97	2.48	2.914 (5)	107
C11—H11···O2	0.93	2.28	2.869 (5)	121
C12—H12···O2^{i}	0.93	2.52	3.378 (6)	153
C13—H13···*Cg*3^{ii}	0.93	2.89	3.634 (5)	138

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