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Crystal structures of arylsulfonylation products of 2-alkyl-5-substituted-1*H*-benzimidazoles

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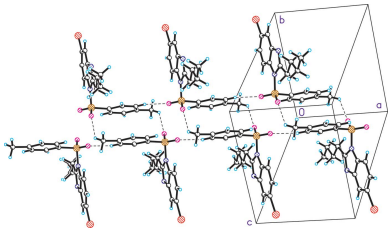
Mixed crystals of 1-(4-chlorophenylsulfonyl)-2,5-dimethyl-1*H*-benzimidazole and 1-(4-chlorophenylsulfonyl)-2,6-dimethyl-1*H*-benzimidazole (ratio 0.707:0.293; two molecules in the asymmetric unit), $0.707C_{15}H_{13}ClN_2O_2S\cdot 0.293C_{15}H_{13}ClN_2O_2S$, (**I**), and of 2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-5-chloro-1*H*-benzimidazole and 2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-6-chloro-1*H*-benzimidazole [ratio 0.731 (2):0.269 (2); one molecule in the asymmetric unit], $0.731C_{21}H_{25}ClN_2O_2S\cdot 0.269C_{21}H_{25}ClN_2O_2S$, (**II**), were obtained from the arylsulfonylation reaction of the corresponding 2-alkylbenzimidazoles. In addition, two products were obtained from the reaction of 2-*n*-butyl-5-chloro-1*H*-benzimidazole with 4-methylbenzenesulfonyl chloride. These reaction products were separated by column chromatography and the crystal structure of one of the products, 2-*n*-butyl-5-chloro-1-(4-methylphenylsulfonyl)-1*H*-benzimidazole (one molecule in the asymmetric unit), $C_{18}H_{19}ClN_2O_2S$, (**III**), was determined. In the crystal structures of (**I**)–(**III**), there is a difference in the arrangement of the planar benzimidazole and arylsulfonyl fragments. The formation of weak C—H···O hydrogen-bonding interactions is characteristic of all three crystal structures.

1. Chemical context

Benzimidazole derivatives are an important class of heteroaromatic compounds because of their biological and pharmaceutical activities (Keri *et al.*, 2015). The benzimidazole entity has seven positions for substitution of various moieties. The literature describes most biologically active compounds based on benzimidazole derivatives bearing functional groups in positions 1, 2 and/or 5 (or 6) (Bansal & Silakari, 2012). A large number of benzimidazole derivatives have been found to exhibit antibacterial (Elnima *et al.*, 1981), antiviral (Townsend *et al.*, 1995), antifungal (Desai & Desai, 2006), antidiabetic, antiasthmatic (Ramanatham *et al.*, 2008), anti-HIV (Li *et al.*, 2009), anticonvulsant (Bhrigu *et al.*, 2012), antihypertensive (Jain *et al.*, 2013), and antidepressant (Mathew *et al.*, 2016) activities.

In addition, among derivatives of arylsulfonylbenzimidazoles, substances with a variety of biological activities have been reported, such as inhibition of HBV (Li *et al.*, 2007), acting on the NPY Y5 receptor (Tamura *et al.*, 2012), and as antimicrobial and antitubercular (Ranjith *et al.*, 2013), anti-inflammatory and analgesic agents (Gaba *et al.*, 2010).

The synthesis of arylsulfonylbenzimidazoles has therefore attracted the attention of organic chemists. The preparation of an individual substance of this class involves the aryl-



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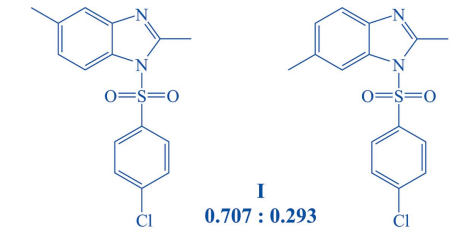
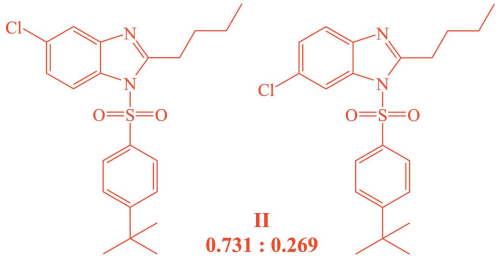
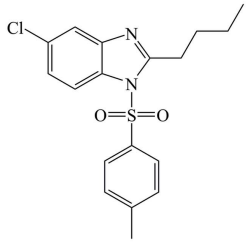
sulfonylation of benzimidazole (Abdireimov *et al.*, 2010), either by an intramolecular Csp^2—H amidation using *N*-iodosuccinimide (Alam *et al.*, 2018), the rearrangement of 7-sulfonamidobenzoxazole with $ZnCl_2$ or $Zn(NO_3)_2$ (Tanakit *et al.*, 2012), or the intramolecular amidation of *N*-tosyl-*o*-phenylenediamine derivatives (for obtaining 1,2-disubstituted benzimidazoles) (Maiti & Mal, 2015; Hu *et al.*, 2017). The above reactions produce a variety of arylsulfonyl-benzimidazole derivatives but there are other conditions that produce two derivatives such as the amination of *N*′′-aryl-*N*′-tosyl/*N*′-methylsulfonylamidines derivatives (Alla *et al.*, 2013). The main reason for two-product formation is the content of the functional group in the phenyl fragment of the starting compound.

In the arylsulfonylation reaction of 2,5-dimethyl-1*H*-benzimidazole and 2-*n*-butyl-5-chloro-1*H*-benzimidazole, the formation of two products was likewise observed, which can be explained by the tautomerism of benzimidazoles. During the arylsulfonylation reaction of benzimidazole derivatives, the acidic proton of benzimidazole is in equilibrium between positions 1 and 3, and consequently, two isomers are formed (Ranjith *et al.*, 2013).







In the reaction of 2,5-dimethyl-1*H*-benzimidazole with 4-chlorobenzenesulfonyl chloride in the presence of triethylamine, two products were formed (Fig. 1). After purification of the reaction mixture, the single crystals of the two corresponding components were subjected to structure analysis by

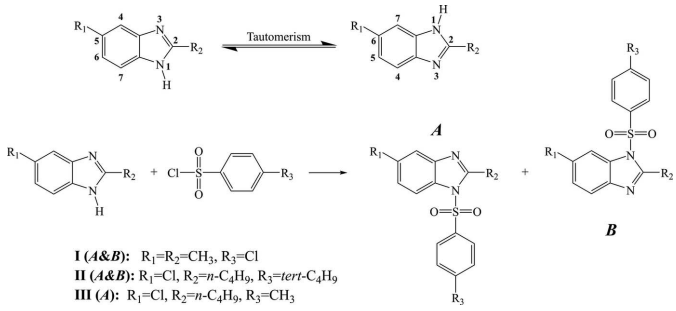


Figure 1
Reaction scheme for the synthesis of the 2-alkyl-5(6)-substituted 1-(phenylsulfonyl)-1*H*-benzimidazoles.

X-ray diffraction, showing that mixed crystals of 1-(4-chlorophenylsulfonyl)-2,5-dimethyl-1*H*-benzimidazole and 1-(4-chlorophenylsulfonyl)-2,6-dimethyl-1*H*-benzimidazole (**I**) were obtained. Likewise, mixed crystals of 2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-5-chloro-1*H*-benzimidazole and 2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-6-chloro-1*H*-benzimidazole (**II**) were obtained from the reaction of 2-*n*-butyl-5-chloro-1*H*-benzimidazole and 4-*tert*-butylbenzenesulfonil chloride. In addition, arylsulfonylation of 2-*n*-butyl-5-chloro-1*H*-benzimidazole with 4-methylbenzenesulfonyl chloride also gave two products. To study the structural features, the latter mixture of products was separated using column chromatography. From the separated products, single crystals of 2-*n*-butyl-5-chloro-1-(4-methylphenylsulfonyl)-1*H*-benzimidazole (**III**) were grown.

2. Structural commentary

The asymmetric unit of crystal (**I**) consists of two molecules: *A* and *B* (Fig. 2). Molecule *A* corresponds to 1-(4-chlorophenylsulfonyl)-2,5-dimethyl-1*H*-benzimidazole, and for *B* the allocated molecules are 1-(4-chlorophenylsulfonyl)-2,6-dimethyl-1*H*-benzimidazole and 1-(4-chlorophenylsulfonyl)-2,5-dimethyl-1*H*-benzimidazole in the ratio 0.555 (10):0.445 (10) (overall *A*:*B* ratio in the crystal of 0.707:0.293). Hence, (**I**) can be considered as a mixed crystal of the two latter molecules.

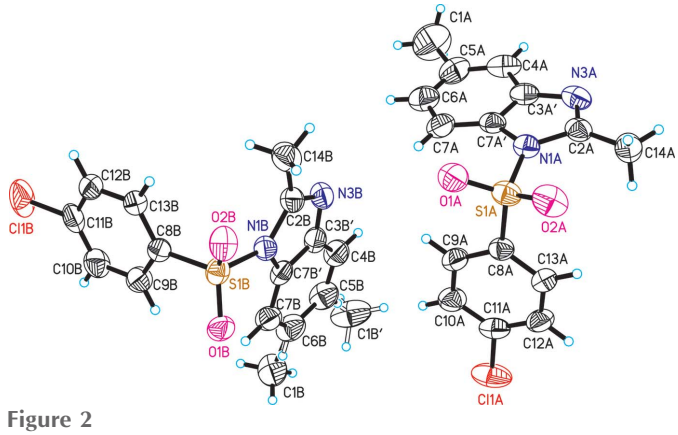


Figure 2
The asymmetric unit of (**I**) with atom labeling. Displacement ellipsoids represent 30% probability levels.

Table 1
Selected torsion angles (°) for (**I**).

O2*A*—S1*A*—N1*A*—C2*A*	22.7 (5)	O2*B*—S1*B*—N1*B*—C2*B*	−25.1 (5)
O2*A*—S1*A*—C8*A*—C13*A*	−25.6 (5)	O2*B*—S1*B*—C8*B*—C13*B*	18.8 (4)

Table 2
Selected torsion angles (°) for (**II**).

O2—S1—N1—C2	−44.7 (2)	O2—S1—C8—C13	−9.6 (2)

Table 3
Selected torsion angles (°) for (**III**).

O2—S1—N1—C2	17.4 (2)	O2—S1—C8—C13	−48.5 (2)

Crystal (**II**) is a mixed crystal of 2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-5-chloro-1*H*-benzimidazole and of 2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-6-chloro-1*H*-benzimidazole in the ratio of 0.731 (2):0.269 (2), that differ in the position of the chloro substituent. Here, only one molecule is present in the asymmetric unit (Fig. 3).

The asymmetric unit of crystal (**III**) likewise comprises one molecule, 2-*n*-butyl-5-chloro-1-(4-methylphenylsulfonyl)-1*H*-benzimidazole (Fig. 4).

The molecules of (**I**)–(**III**) consist of two flat fragments, *viz*. benzimidazole (N1/C2/N3/C3*A*/C4–C7/C7*A*) and benzene (C8–C13). The angles between the fragments are 83.4 (1)° for (**I*A***), 79.3 (1)° for (**I*B***), 87.1 (1)° for (**II**), and 86.6 (1)° for (**III**). These values do not differ significantly from the previously reported structures of related benzimidazole derivatives (Abdireymov *et al.*, 2011). However, the orientation of the entities along the N1—S1 and S1—C8 bonds is different (Tables 1, 2 and 3).

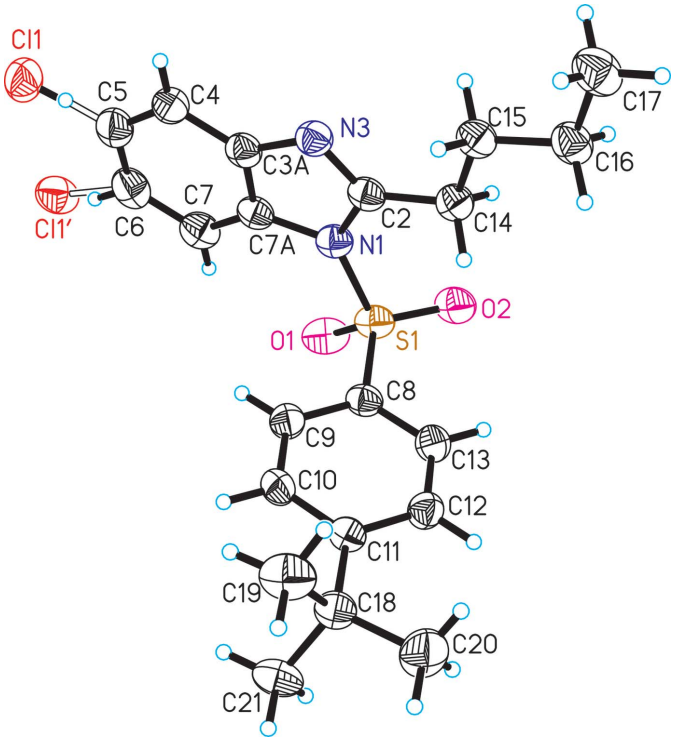


Figure 3
The asymmetric unit of (**II**) with atom labeling. Displacement ellipsoids represent the 30% probability level.

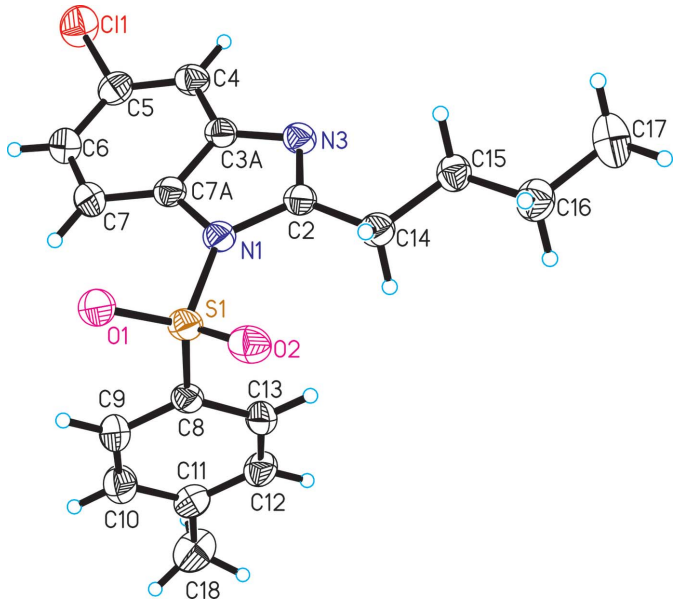


Figure 4
The molecular structure of (**III**) with atom labeling. Displacement ellipsoids represent the 30% probability level.

3. Supramolecular features

In the crystal packing of (**I**), two *A* molecules form a centrosymmetric dimer by weak C14*A*—H14*C*···O1*A* hydrogen bonds. A Cl···Cl interaction between these dimers [Cl1*A*···Cl1*A*(2 − *x*, 1 − *y*, 1 − *z*) = 3.304 (3) Å, 0.20 Å less than the sum of the the van der Waals radii] links the molecules into chains running parallel to the *b* axis. Molecules of *B* are linked by C4*B*—H4*BA*···Cl1 hydrogen bonds, which also form chains extending in the same direction (Table 4, Fig. 5). Intermolecular C—H···π interactions between these chains consolidate the crystal structure [C12*A*—H12*A*···*Cg*1:

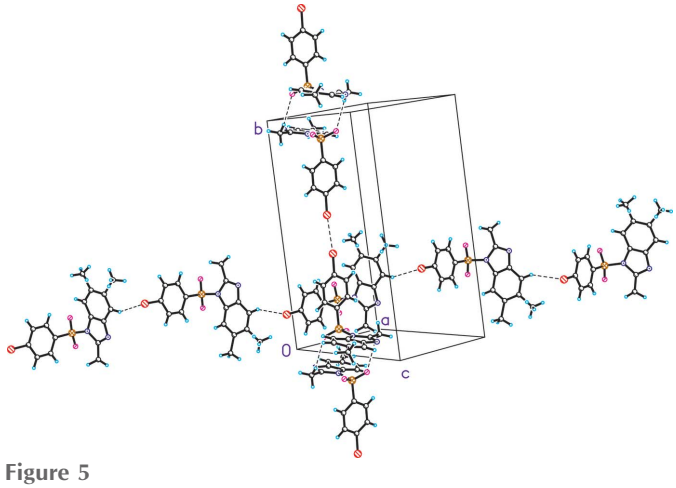


Figure 5
The observed hydrogen bond and Cl1*A*···Cl1*A* interactions in the crystal structure of (**I**).

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

D—H···A	D—H	H···A	D···A	D—H···A
C14A—H14C···O1A^{i}	0.96	2.59	3.271 (6)	128
C4B—H4BA···Cl1B^{ii}	0.93	2.95	3.800 (6)	153

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

Table 5
Hydrogen-bond geometry (Å, °) for (**II**).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O2^{i}	0.93	2.67	3.595 (3)	176

Symmetry code: (i) $x-1, y, z$.

Table 6
Hydrogen-bond geometry (Å, °) for (**III**).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···O1^{i}	0.93	2.55	3.467 (3)	170
C18—H18D···O2^{ii}	0.96	2.46	3.199 (4)	133

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

H···$Cg1$ = 2.85 Å; C12A—H···$Cg1$ = 3.549 (7) Å; C12A—H···$Cg1$ = 133° (symmetry code for $Cg1$: $1+x, y, z$; $Cg1$ is the centroid of the C3B'/C4B--C7B/C7B' benzene ring); C10B—H10B···$Cg2$: H···$Cg2$ = 2.81 Å; C10B—H···$Cg2$ = 3.558 (6) Å; C10B—H···$Cg2$ = 139° (symmetry code for the $Cg2$ centroid: $-1+x, \frac{1}{2}-y, -\frac{1}{2}+z$; $Cg2$ is centroid of the C3A'/C4A–C7A/C7A' benzene ring)].

In the crystal packing of (**II**), the formation of a centrosymmetric dimer as the result of an intermolecular C—H···π bond is also observed [C4—H4A···$Cg3$: H···$Cg3$ = 2.71 Å; C4—H···$Cg3$ = 3.590 (4) Å; C4—H···$Cg3$ = 158° (symmetry code for $Cg3$: $-x, 1-y, 1-z$; $Cg3$ is centroid of the C8–C13 benzene ring)]. These dimers are linked into chains running parallel to the a axis by Cl···Cl interactions [Cl1···Cl1($-x, 2-y, 2-z$) = 3.435 (3) Å, 0.06 Å less than the sum of the van der Waals radii] and a weak intermolecular C10—H10A···O2 hydrogen bond (Table 5, Fig. 6). Similar C—H···π and C—H···O interactions were observed in the previously studied mixed crystal of 2-*n*-butyl-6-chloro-1-(2,4-dimethylbenzenesulfonyl)-1*H*-benzimidazole and 2-*n*-butyl-5-chloro-1-(2,4-dimethylbenzenesulfonyl)-1*H*-benzimidazole (Abdireymov *et al.*, 2011).

In the crystal packing of (**III**), only weak hydrogen bonds of the type C—H···O are observed. Chains parallel to the a axis are formed through intermolecular C12—H12A···O1 interactions. Further C18—H18D···O2 hydrogen bonds between the formed chains consolidate the packing (Table 6, Fig. 7). Interactions such as Cl···Cl and C—H···π are not observed in (**III**).

Halogen–halogen bonds such as the Cl···Cl interactions observed in the crystals of (**I**) and (**II**) have been studied by various methods, with the characteristics of such interactions described in the literature (Hathwar *et al.*, 2010; Bui *et al.*, 2009).

4. Database survey

A search in the Cambridge database (version 2022.1.0; Groom *et al.*, 2016) showed that 1-arylsulfonyl-1*H*-benzimidazoles with one or more substituents in positions 2, 4, 5, 6 resulted in 21 hits. Of these, five are 1-arylsulfonyl-2-alkyl(aryl)-1*H*-benzimidazole derivatives. The most similar structures are 6-chloro-2-methyl-1-[(4-methylphenyl)sulfonyl]-1*H*-benzimidazole (MEZDAY; Alla *et al.*, 2013), and the mixed crystals of 2-*n*-butyl-6-chloro-1-(2,4-dimethylbenzenesulfonyl)-1*H*-benzimidazole and 2-*n*-butyl-5-chloro-1-(2,4-dimethylbenzenesulfonyl)-1*H*-benzimidazole (OCEVEZ; Abdireymov *et al.*, 2011).

5. Synthesis and crystallization

The title compounds were synthesized according to a previously reported procedure (Abdireimov *et al.*, 2010). After purification of the corresponding reaction mixtures, single crystals for X-ray diffraction analysis were obtained by evaporation of ethanol solutions at room temperature.

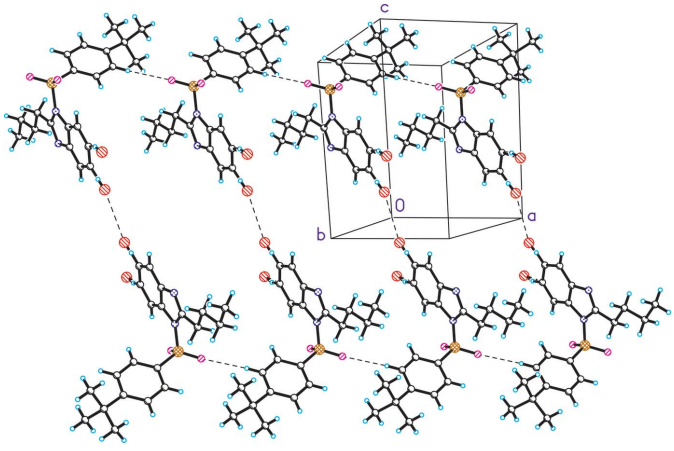


Figure 6
The observed hydrogen bond and Cl1···Cl1 interactions in the crystal structure of (**II**).

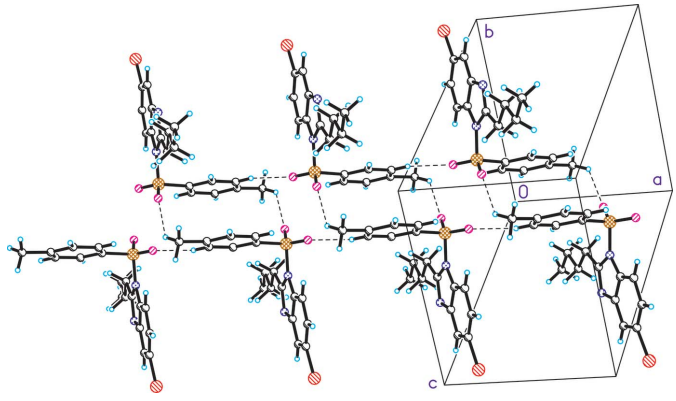


Figure 7
The observed hydrogen bond in the crystal structure of (**III**).

Table 7
Experimental details.

	(**I**)	(**II**)	(**III**)
Crystal data			
Chemical formula	0.707$C_{15}H_{13}ClN_2O_2S$·-0.293$C_{15}H_{13}ClN_2O_2S$	0.731$C_{21}H_{25}ClN_2O_2S$·-0.269$C_{21}H_{25}ClN_2O_2S$	$C_{18}H_{19}ClN_2O_2S$
M_r	320.78	404.94	362.86
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	296	296	297
a, b, c (Å)	9.837 (2), 19.674 (4), 16.046 (3)	8.2990 (17), 11.644 (2), 12.279 (3)	8.1491 (16), 10.039 (2), 12.485 (3)
α, β, γ (°)	90, 101.91 (3), 90	115.85 (3), 99.03 (3), 94.96 (3)	112.23 (3), 105.49 (3), 96.02 (3)
V (Å^3)	3038.6 (11)	1038.5 (4)	886.5 (4)
Z	8	2	2
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	3.56	2.71	3.11
Crystal size (mm)	0.60 × 0.40 × 0.30	0.36 × 0.20 × 0.20	0.40 × 0.34 × 0.28
Data collection			
Diffractometer	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)
T_{min}, T_{max}	0.482, 1.000	0.842, 1.000	0.394, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13759, 5354, 2629	7093, 4179, 3244	8070, 3662, 3088
R_{int}	0.071	0.029	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596	0.630	0.631
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.190, 1.00	0.050, 0.152, 1.05	0.047, 0.151, 1.06
No. of reflections	5354	4179	3662
No. of parameters	394	258	219
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.30	0.31, −0.30	0.62, −0.57

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *SHELXTL* and *XP* in *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

The reaction products of 2-*n*-butyl-5-chloro-1*H*-benzimidazole with 4-methylbenzenesulfonyl chloride were separated by column chromatography in a benzene:acetone (10:1 *v*:*v*) system. Colorless crystals of (**III**) for X-ray analysis were obtained by slow evaporation of an ethanol solution.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 7. In the crystal structure of (**I**), the C1*B* site in the (**I*B***) molecule is disordered over two positions (C1*B* and C1*B*′). The site occupancy factors refined to a ratio of 0.555 (10):0.445 (10). In the crystal structure of (**II**), the Cl site is disordered over two positions (Cl1 and Cl1′), with refined site occupation factors of 0.731 (2):0.269 (2) for the major and minor components. All H atoms bound to C atoms were placed geometrically (with C—H distances of 0.97 Å for CH_2, 0.96 Å for CH_3 and 0.93 Å for C_{ar}) and included in the refinement in a riding-motion approximation with U_{iso}(H) = 1.2U_{eq}(C) [U_{iso} = 1.5U_{eq}(C) for methyl H atoms].

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Crystal structures of arylsulfonylation products of 2-alkyl-5-substituted-1*H*-benzimidazoles

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Computing details

For all structures, data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

1-(4-Chlorophenylsulfonyl)-2,5-dimethyl-1*H*-benzimidazole–\ 1-(4-chlorophenylsulfonyl)-2,6-dimethyl-1*H*-benzimidazole (0.707/0.293) (I)

Crystal data

$0.707C_{15}H_{13}ClN_2O_2S{\cdot}0.293C_{15}H_{13}ClN_2O_2S$
M_r = 320.78
Monoclinic, $P2_1/c$
a = 9.837 (2) Å
b = 19.674 (4) Å
c = 16.046 (3) Å
β = 101.91 (3)°
V = 3038.6 (11) Å^3
Z = 8
$F(000)$ = 1328
D_x = 1.402 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 1714 reflections
θ = 3.6–43.7°
μ = 3.56 mm^{-1}
T = 296 K
Prizmatic, colorless
0.60 × 0.40 × 0.30 mm

Data collection

Xcalibur, Ruby diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.2576 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.482, T_{max} = 1.000
13759 measured reflections
5354 independent reflections
2629 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 66.8°, θ_{min} = 3.6°
h = −11→11
k = −23→23
l = −19→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.190
S = 1.00
5354 reflections
394 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.092P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1A	0.98039 (16)	0.10855 (7)	0.48596 (8)	0.0759 (4)	
O1A	0.8450 (4)	0.08551 (18)	0.4479 (2)	0.0963 (12)	
O2A	1.0979 (5)	0.08877 (19)	0.4541 (2)	0.1020 (13)	
Cl1A	0.9719 (2)	0.42170 (7)	0.52959 (10)	0.1301 (8)	
N1A	1.0069 (4)	0.08135 (18)	0.5868 (2)	0.0695 (11)	
N3A	1.1128 (6)	0.0524 (2)	0.7190 (3)	0.0839 (13)	
C1A	0.6646 (9)	0.0576 (4)	0.8265 (5)	0.178 (4)	
H1AA	0.568434	0.062899	0.799769	0.268*	
H1AB	0.689313	0.090950	0.870784	0.268*	
H1AC	0.679452	0.012922	0.850632	0.268*	
C2A	1.1341 (6)	0.0658 (2)	0.6431 (3)	0.0754 (14)	
C3A′	0.9698 (7)	0.0613 (2)	0.7144 (4)	0.0804 (15)	
C4A	0.8939 (9)	0.0536 (3)	0.7809 (4)	0.103 (2)	
H4AA	0.936901	0.039950	0.835433	0.124*	
C5A	0.7550 (9)	0.0675 (3)	0.7599 (5)	0.103 (2)	
C6A	0.6906 (8)	0.0861 (3)	0.6798 (5)	0.111 (2)	
H6AA	0.595586	0.094593	0.668762	0.133*	
C7A	0.7607 (7)	0.0927 (3)	0.6149 (4)	0.0916 (17)	
H7AA	0.715480	0.105605	0.560447	0.110*	
C7A′	0.9013 (6)	0.0793 (2)	0.6338 (3)	0.0706 (13)	
C8A	0.9767 (5)	0.1967 (2)	0.4957 (3)	0.0648 (12)	
C9A	0.8527 (6)	0.2297 (2)	0.4937 (3)	0.0809 (15)	
H9AA	0.770588	0.204821	0.485164	0.097*	
C10A	0.8489 (6)	0.2996 (3)	0.5042 (3)	0.0888 (16)	
H10A	0.765648	0.322211	0.503487	0.107*	
C11A	0.9722 (8)	0.3343 (3)	0.5156 (3)	0.0836 (16)	
C12A	1.0956 (7)	0.3026 (3)	0.5166 (3)	0.0895 (17)	
H12A	1.177596	0.327482	0.523920	0.107*	
C13A	1.0973 (6)	0.2332 (3)	0.5065 (3)	0.0821 (15)	
H13A	1.180961	0.210991	0.507059	0.099*	
C14A	1.2700 (6)	0.0651 (3)	0.6187 (4)	0.0952 (17)	
H14A	1.340001	0.050644	0.666258	0.143*	
H14B	1.291553	0.109979	0.601750	0.143*	
H14C	1.267197	0.034256	0.571991	0.143*	

S1B	0.27801 (13)	0.20178 (7)	0.24317 (7)	0.0697 (4)	
O1B	0.3041 (4)	0.26502 (18)	0.20548 (19)	0.0845 (11)	
O2B	0.3156 (4)	0.13910 (19)	0.2109 (2)	0.0880 (11)	
Cl1B	−0.34000 (16)	0.19051 (12)	0.27275 (11)	0.1444 (9)	
N1B	0.3639 (4)	0.2062 (2)	0.3441 (2)	0.0664 (10)	
N3B	0.4687 (4)	0.1754 (3)	0.4773 (3)	0.0825 (13)	
C1B	0.3389 (12)	0.4565 (5)	0.4256 (7)	0.121 (5)	0.555 (10)
H1BA	0.380443	0.483598	0.473870	0.182*	0.555 (10)
H1BB	0.239668	0.457241	0.419044	0.182*	0.555 (10)
H1BC	0.363827	0.474586	0.375207	0.182*	0.555 (10)
C1B′	0.5215 (19)	0.4175 (7)	0.5827 (8)	0.148 (8)	0.445 (10)
H1BD	0.615790	0.406184	0.608341	0.222*	0.445 (10)
H1BE	0.468026	0.421590	0.626136	0.222*	0.445 (10)
H1BF	0.519539	0.459796	0.552680	0.222*	0.445 (10)
C2B	0.4156 (5)	0.1531 (3)	0.4014 (3)	0.0745 (14)	
C3B′	0.4514 (5)	0.2458 (3)	0.4737 (3)	0.0742 (14)	
C4B	0.4894 (6)	0.2945 (4)	0.5384 (3)	0.0910 (17)	
H4BA	0.534228	0.281439	0.592826	0.109*	
C5B	0.4594 (7)	0.3612 (4)	0.5200 (4)	0.102 (2)	
H5BA	0.484947	0.393493	0.562622	0.122*	0.555 (10)
C6B	0.3917 (7)	0.3823 (3)	0.4394 (4)	0.103 (2)	
H6BA	0.370651	0.428069	0.429278	0.123*	0.445 (10)
C7B	0.3553 (6)	0.3353 (3)	0.3738 (3)	0.0843 (16)	
H7BA	0.311950	0.348838	0.319236	0.101*	
C7B′	0.3864 (5)	0.2667 (3)	0.3930 (3)	0.0692 (13)	
C8B	0.1024 (5)	0.1986 (2)	0.2501 (2)	0.0597 (11)	
C9B	0.0312 (6)	0.2576 (3)	0.2556 (3)	0.0797 (15)	
H9BA	0.075341	0.299434	0.255486	0.096*	
C10B	−0.1040 (7)	0.2546 (3)	0.2612 (4)	0.0916 (17)	
H10B	−0.153441	0.294480	0.264433	0.110*	
C11B	−0.1681 (6)	0.1931 (4)	0.2621 (3)	0.0870 (17)	
C12B	−0.0993 (6)	0.1337 (3)	0.2560 (3)	0.0829 (15)	
H12B	−0.144353	0.092187	0.256028	0.099*	
C13B	0.0385 (5)	0.1365 (2)	0.2499 (3)	0.0678 (13)	
H13B	0.087610	0.096660	0.245649	0.081*	
C14B	0.4104 (7)	0.0798 (3)	0.3785 (4)	0.1045 (19)	
H14D	0.453652	0.053565	0.427283	0.157*	
H14E	0.458839	0.072588	0.333116	0.157*	
H14F	0.315348	0.065870	0.360439	0.157*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0993 (11)	0.0590 (7)	0.0667 (8)	0.0013 (7)	0.0111 (7)	−0.0035 (6)
O1A	0.110 (3)	0.071 (2)	0.092 (2)	−0.016 (2)	−0.015 (2)	−0.0091 (18)
O2A	0.133 (4)	0.094 (3)	0.089 (2)	0.029 (3)	0.045 (2)	−0.006 (2)
Cl1A	0.223 (2)	0.0559 (8)	0.1053 (11)	−0.0132 (11)	0.0190 (12)	0.0026 (7)
N1A	0.081 (3)	0.059 (2)	0.068 (2)	0.000 (2)	0.014 (2)	0.0017 (19)

N3A	0.113 (4)	0.063 (3)	0.067 (3)	0.000 (3)	−0.001 (3)	0.003 (2)
C1A	0.192 (10)	0.200 (10)	0.163 (7)	−0.015 (8)	0.081 (7)	−0.007 (6)
C2A	0.087 (4)	0.051 (3)	0.083 (4)	−0.001 (3)	0.006 (3)	−0.003 (2)
C3A′	0.104 (5)	0.050 (3)	0.088 (4)	−0.005 (3)	0.024 (4)	−0.002 (3)
C4A	0.153 (7)	0.069 (4)	0.092 (4)	−0.014 (4)	0.036 (5)	0.006 (3)
C5A	0.114 (6)	0.094 (5)	0.112 (5)	−0.019 (4)	0.051 (5)	−0.010 (4)
C6A	0.119 (6)	0.072 (4)	0.142 (6)	−0.015 (4)	0.027 (5)	0.001 (4)
C7A	0.091 (5)	0.078 (4)	0.109 (4)	−0.017 (3)	0.029 (4)	0.007 (3)
C7A′	0.087 (4)	0.048 (2)	0.074 (3)	−0.007 (3)	0.011 (3)	0.002 (2)
C8A	0.075 (3)	0.062 (3)	0.057 (3)	−0.003 (3)	0.012 (2)	0.003 (2)
C9A	0.078 (4)	0.062 (3)	0.104 (4)	−0.009 (3)	0.023 (3)	0.008 (3)
C10A	0.093 (4)	0.067 (3)	0.114 (4)	0.009 (3)	0.038 (3)	0.011 (3)
C11A	0.122 (5)	0.056 (3)	0.073 (3)	−0.009 (3)	0.021 (3)	0.007 (2)
C12A	0.091 (4)	0.078 (4)	0.093 (4)	−0.032 (4)	0.006 (3)	0.013 (3)
C13A	0.072 (4)	0.078 (4)	0.099 (4)	−0.007 (3)	0.022 (3)	0.017 (3)
C14A	0.082 (4)	0.084 (4)	0.115 (4)	0.001 (3)	0.010 (3)	−0.003 (3)
S1B	0.0610 (8)	0.0857 (9)	0.0641 (7)	−0.0045 (7)	0.0167 (6)	−0.0066 (7)
O1B	0.086 (3)	0.101 (3)	0.067 (2)	−0.022 (2)	0.0169 (18)	0.0136 (18)
O2B	0.075 (2)	0.106 (3)	0.086 (2)	0.011 (2)	0.0232 (19)	−0.024 (2)
Cl1B	0.0531 (9)	0.257 (3)	0.1239 (13)	0.0122 (12)	0.0199 (8)	0.0576 (14)
N1B	0.061 (2)	0.071 (3)	0.066 (2)	0.001 (2)	0.0108 (19)	0.002 (2)
N3B	0.070 (3)	0.096 (4)	0.077 (3)	0.001 (3)	0.004 (2)	0.009 (3)
C1B	0.130 (11)	0.073 (8)	0.147 (10)	−0.005 (7)	−0.004 (8)	−0.036 (7)
C1B′	0.25 (2)	0.110 (12)	0.090 (10)	−0.073 (13)	0.046 (12)	−0.033 (9)
C2B	0.063 (3)	0.077 (3)	0.085 (4)	0.007 (3)	0.018 (3)	0.007 (3)
C3B′	0.061 (3)	0.099 (4)	0.062 (3)	−0.008 (3)	0.012 (3)	0.002 (3)
C4B	0.090 (4)	0.118 (5)	0.062 (3)	−0.023 (4)	0.010 (3)	0.000 (3)
C5B	0.119 (6)	0.100 (5)	0.086 (4)	−0.027 (4)	0.020 (4)	−0.021 (4)
C6B	0.119 (5)	0.101 (5)	0.087 (4)	−0.032 (4)	0.020 (4)	−0.014 (4)
C7B	0.091 (4)	0.082 (4)	0.079 (3)	−0.016 (3)	0.014 (3)	0.002 (3)
C7B′	0.057 (3)	0.081 (3)	0.071 (3)	−0.015 (3)	0.018 (3)	−0.004 (3)
C8B	0.063 (3)	0.065 (3)	0.053 (2)	−0.001 (2)	0.015 (2)	−0.002 (2)
C9B	0.074 (4)	0.069 (3)	0.098 (4)	0.009 (3)	0.021 (3)	0.003 (3)
C10B	0.072 (4)	0.094 (5)	0.109 (4)	0.025 (3)	0.020 (3)	0.007 (4)
C11B	0.057 (3)	0.137 (6)	0.064 (3)	0.011 (4)	0.006 (2)	0.027 (3)
C12B	0.068 (4)	0.097 (4)	0.080 (3)	−0.013 (3)	0.008 (3)	0.019 (3)
C13B	0.065 (3)	0.067 (3)	0.069 (3)	−0.001 (3)	0.008 (2)	0.003 (2)
C14B	0.104 (5)	0.084 (4)	0.118 (5)	0.011 (4)	0.006 (4)	0.003 (4)

Geometric parameters (Å, º)

S1A—O2A	1.412 (4)	S1B—C8B	1.755 (5)
S1A—O1A	1.420 (4)	Cl1B—C11B	1.735 (6)
S1A—N1A	1.673 (4)	N1B—C2B	1.414 (6)
S1A—C8A	1.743 (5)	N1B—C7B′	1.419 (6)
Cl1A—C11A	1.734 (5)	N3B—C2B	1.297 (6)
N1A—C7A′	1.403 (6)	N3B—C3B′	1.394 (7)
N1A—C2A	1.418 (6)	C1B—C6B	1.549 (12)

N3A—C2A	1.305 (6)	C1B—H1BA	0.9600
N3A—C3A′	1.404 (7)	C1B—H1BB	0.9600
C1A—C5A	1.537 (9)	C1B—H1BC	0.9600
C1A—H1AA	0.9600	C1B′—C5B	1.536 (13)
C1A—H1AB	0.9600	C1B′—H1BD	0.9600
C1A—H1AC	0.9600	C1B′—H1BE	0.9600
C2A—C14A	1.469 (7)	C1B′—H1BF	0.9600
C3A′—C7A′	1.376 (7)	C2B—C14B	1.487 (7)
C3A′—C4A	1.431 (8)	C3B′—C7B′	1.384 (6)
C4A—C5A	1.366 (9)	C3B′—C4B	1.405 (7)
C4A—H4AA	0.9300	C4B—C5B	1.364 (8)
C5A—C6A	1.361 (9)	C4B—H4BA	0.9300
C6A—C7A	1.369 (8)	C5B—C6B	1.390 (8)
C6A—H6AA	0.9300	C5B—H5BA	0.9300
C7A—C7A′	1.379 (7)	C6B—C7B	1.391 (7)
C7A—H7AA	0.9300	C6B—H6BA	0.9300
C8A—C13A	1.367 (7)	C7B—C7B′	1.404 (7)
C8A—C9A	1.376 (7)	C7B—H7BA	0.9300
C9A—C10A	1.388 (7)	C8B—C9B	1.368 (6)
C9A—H9AA	0.9300	C8B—C13B	1.374 (6)
C10A—C11A	1.370 (8)	C9B—C10B	1.353 (7)
C10A—H10A	0.9300	C9B—H9BA	0.9300
C11A—C12A	1.362 (7)	C10B—C11B	1.366 (8)
C12A—C13A	1.375 (7)	C10B—H10B	0.9300
C12A—H12A	0.9300	C11B—C12B	1.363 (7)
C13A—H13A	0.9300	C12B—C13B	1.380 (7)
C14A—H14A	0.9600	C12B—H12B	0.9300
C14A—H14B	0.9600	C13B—H13B	0.9300
C14A—H14C	0.9600	C14B—H14D	0.9600
S1B—O2B	1.416 (3)	C14B—H14E	0.9600
S1B—O1B	1.430 (3)	C14B—H14F	0.9600
S1B—N1B	1.667 (4)		

O2A—S1A—O1A	121.4 (2)	N1B—S1B—C8B	104.37 (19)
O2A—S1A—N1A	106.7 (2)	C2B—N1B—C7B′	105.4 (4)
O1A—S1A—N1A	105.0 (2)	C2B—N1B—S1B	129.5 (4)
O2A—S1A—C8A	109.9 (3)	C7B′—N1B—S1B	124.8 (3)
O1A—S1A—C8A	108.8 (2)	C2B—N3B—C3B′	106.0 (4)
N1A—S1A—C8A	103.5 (2)	C6B—C1B—H1BA	109.5
C7A′—N1A—C2A	107.8 (4)	C6B—C1B—H1BB	109.5
C7A′—N1A—S1A	122.9 (4)	H1BA—C1B—H1BB	109.5
C2A—N1A—S1A	128.8 (4)	C6B—C1B—H1BC	109.5
C2A—N3A—C3A′	106.1 (5)	H1BA—C1B—H1BC	109.5
C5A—C1A—H1AA	109.5	H1BB—C1B—H1BC	109.5
C5A—C1A—H1AB	109.5	C5B—C1B′—H1BD	109.5
H1AA—C1A—H1AB	109.5	C5B—C1B′—H1BE	109.5
C5A—C1A—H1AC	109.5	H1BD—C1B′—H1BE	109.5
H1AA—C1A—H1AC	109.5	C5B—C1B′—H1BF	109.5

H1AB—C1A—H1AC	109.5	H1BD—C1B′—H1BF	109.5
N3A—C2A—N1A	110.3 (5)	H1BE—C1B′—H1BF	109.5
N3A—C2A—C14A	125.3 (5)	N3B—C2B—N1B	112.5 (5)
N1A—C2A—C14A	124.4 (5)	N3B—C2B—C14B	123.1 (5)
C7A′—C3A′—N3A	111.9 (5)	N1B—C2B—C14B	124.4 (5)
C7A′—C3A′—C4A	119.9 (6)	C7B′—C3B′—N3B	111.3 (5)
N3A—C3A′—C4A	128.2 (6)	C7B′—C3B′—C4B	119.3 (6)
C5A—C4A—C3A′	116.4 (6)	N3B—C3B′—C4B	129.4 (5)
C5A—C4A—H4AA	121.8	C5B—C4B—C3B′	118.9 (5)
C3A′—C4A—H4AA	121.8	C5B—C4B—H4BA	120.5
C6A—C5A—C4A	122.2 (7)	C3B′—C4B—H4BA	120.5
C6A—C5A—C1A	117.9 (8)	C4B—C5B—C6B	122.0 (6)
C4A—C5A—C1A	119.8 (8)	C4B—C5B—C1B′	120.9 (8)
C5A—C6A—C7A	122.4 (7)	C6B—C5B—C1B′	116.3 (8)
C5A—C6A—H6AA	118.8	C4B—C5B—H5BA	119.0
C7A—C6A—H6AA	118.8	C6B—C5B—H5BA	119.0
C6A—C7A—C7A′	117.0 (6)	C5B—C6B—C7B	120.2 (6)
C6A—C7A—H7AA	121.5	C5B—C6B—C1B	119.8 (6)
C7A′—C7A—H7AA	121.5	C7B—C6B—C1B	119.4 (7)
C3A′—C7A′—C7A	122.0 (6)	C5B—C6B—H6BA	119.9
C3A′—C7A′—N1A	103.8 (5)	C7B—C6B—H6BA	119.9
C7A—C7A′—N1A	134.1 (5)	C6B—C7B—C7B′	117.6 (5)
C13A—C8A—C9A	119.9 (5)	C6B—C7B—H7BA	121.2
C13A—C8A—S1A	120.0 (4)	C7B′—C7B—H7BA	121.2
C9A—C8A—S1A	120.1 (4)	C3B′—C7B′—C7B	122.0 (5)
C8A—C9A—C10A	120.7 (5)	C3B′—C7B′—N1B	104.9 (5)
C8A—C9A—H9AA	119.7	C7B—C7B′—N1B	133.1 (5)
C10A—C9A—H9AA	119.7	C9B—C8B—C13B	121.0 (5)
C11A—C10A—C9A	117.7 (5)	C9B—C8B—S1B	119.8 (4)
C11A—C10A—H10A	121.2	C13B—C8B—S1B	119.1 (4)
C9A—C10A—H10A	121.2	C10B—C9B—C8B	119.3 (5)
C12A—C11A—C10A	122.4 (5)	C10B—C9B—H9BA	120.3
C12A—C11A—Cl1A	118.6 (5)	C8B—C9B—H9BA	120.3
C10A—C11A—Cl1A	119.0 (5)	C9B—C10B—C11B	120.1 (6)
C11A—C12A—C13A	119.1 (5)	C9B—C10B—H10B	119.9
C11A—C12A—H12A	120.5	C11B—C10B—H10B	119.9
C13A—C12A—H12A	120.5	C12B—C11B—C10B	121.4 (5)
C8A—C13A—C12A	120.3 (6)	C12B—C11B—Cl1B	119.4 (5)
C8A—C13A—H13A	119.8	C10B—C11B—Cl1B	119.2 (5)
C12A—C13A—H13A	119.8	C11B—C12B—C13B	118.8 (5)
C2A—C14A—H14A	109.5	C11B—C12B—H12B	120.6
C2A—C14A—H14B	109.5	C13B—C12B—H12B	120.6
H14A—C14A—H14B	109.5	C8B—C13B—C12B	119.3 (5)
C2A—C14A—H14C	109.5	C8B—C13B—H13B	120.3
H14A—C14A—H14C	109.5	C12B—C13B—H13B	120.3
H14B—C14A—H14C	109.5	C2B—C14B—H14D	109.5
O2B—S1B—O1B	121.4 (2)	C2B—C14B—H14E	109.5
O2B—S1B—N1B	106.4 (2)	H14D—C14B—H14E	109.5

O1B—S1B—N1B	105.5 (2)	C2B—C14B—H14F	109.5
O2B—S1B—C8B	109.1 (2)	H14D—C14B—H14F	109.5
O1B—S1B—C8B	108.9 (2)	H14E—C14B—H14F	109.5
O2A—S1A—N1A—C7A′	−166.7 (4)	O1B—S1B—N1B—C2B	−155.2 (4)
O1A—S1A—N1A—C7A′	−36.6 (4)	C8B—S1B—N1B—C2B	90.1 (4)
C8A—S1A—N1A—C7A′	77.4 (4)	O2B—S1B—N1B—C7B′	162.2 (4)
O2A—S1A—N1A—C2A	22.7 (5)	O1B—S1B—N1B—C7B′	32.1 (4)
O1A—S1A—N1A—C2A	152.7 (4)	C8B—S1B—N1B—C7B′	−82.6 (4)
C8A—S1A—N1A—C2A	−93.3 (4)	C3B′—N3B—C2B—N1B	1.2 (6)
C3A′—N3A—C2A—N1A	−1.9 (5)	C3B′—N3B—C2B—C14B	−178.7 (5)
C3A′—N3A—C2A—C14A	178.1 (5)	C7B′—N1B—C2B—N3B	−1.6 (5)
C7A′—N1A—C2A—N3A	2.1 (5)	S1B—N1B—C2B—N3B	−175.4 (3)
S1A—N1A—C2A—N3A	173.9 (3)	C7B′—N1B—C2B—C14B	178.3 (5)
C7A′—N1A—C2A—C14A	−177.8 (4)	S1B—N1B—C2B—C14B	4.5 (7)
S1A—N1A—C2A—C14A	−6.0 (7)	C2B—N3B—C3B′—C7B′	−0.4 (6)
C2A—N3A—C3A′—C7A′	1.0 (6)	C2B—N3B—C3B′—C4B	179.5 (5)
C2A—N3A—C3A′—C4A	−179.1 (5)	C7B′—C3B′—C4B—C5B	0.9 (8)
C7A′—C3A′—C4A—C5A	−2.3 (8)	N3B—C3B′—C4B—C5B	−178.9 (6)
N3A—C3A′—C4A—C5A	177.9 (5)	C3B′—C4B—C5B—C6B	0.4 (10)
C3A′—C4A—C5A—C6A	1.5 (10)	C3B′—C4B—C5B—C1B′	−168.7 (9)
C3A′—C4A—C5A—C1A	177.4 (5)	C4B—C5B—C6B—C7B	−1.6 (10)
C4A—C5A—C6A—C7A	−0.5 (10)	C1B′—C5B—C6B—C7B	167.9 (9)
C1A—C5A—C6A—C7A	−176.5 (6)	C4B—C5B—C6B—C1B	170.1 (8)
C5A—C6A—C7A—C7A′	0.3 (9)	C5B—C6B—C7B—C7B′	1.5 (9)
N3A—C3A′—C7A′—C7A	−178.0 (5)	C1B—C6B—C7B—C7B′	−170.2 (7)
C4A—C3A′—C7A′—C7A	2.2 (7)	N3B—C3B′—C7B′—C7B	178.9 (5)
N3A—C3A′—C7A′—N1A	0.3 (5)	C4B—C3B′—C7B′—C7B	−0.9 (8)
C4A—C3A′—C7A′—N1A	−179.6 (4)	N3B—C3B′—C7B′—N1B	−0.6 (6)
C6A—C7A—C7A′—C3A′	−1.1 (8)	C4B—C3B′—C7B′—N1B	179.6 (4)
C6A—C7A—C7A′—N1A	−178.8 (5)	C6B—C7B—C7B′—C3B′	−0.3 (8)
C2A—N1A—C7A′—C3A′	−1.4 (5)	C6B—C7B—C7B′—N1B	179.0 (5)
S1A—N1A—C7A′—C3A′	−173.7 (3)	C2B—N1B—C7B′—C3B′	1.2 (5)
C2A—N1A—C7A′—C7A	176.6 (5)	S1B—N1B—C7B′—C3B′	175.4 (3)
S1A—N1A—C7A′—C7A	4.2 (8)	C2B—N1B—C7B′—C7B	−178.2 (5)
O2A—S1A—C8A—C13A	−25.6 (5)	S1B—N1B—C7B′—C7B	−4.0 (8)
O1A—S1A—C8A—C13A	−160.7 (4)	O2B—S1B—C8B—C9B	−161.2 (4)
N1A—S1A—C8A—C13A	88.0 (4)	O1B—S1B—C8B—C9B	−26.8 (4)
O2A—S1A—C8A—C9A	155.2 (4)	N1B—S1B—C8B—C9B	85.5 (4)
O1A—S1A—C8A—C9A	20.1 (5)	O2B—S1B—C8B—C13B	18.8 (4)
N1A—S1A—C8A—C9A	−91.1 (4)	O1B—S1B—C8B—C13B	153.2 (3)
C13A—C8A—C9A—C10A	−1.3 (7)	N1B—S1B—C8B—C13B	−94.6 (4)
S1A—C8A—C9A—C10A	177.9 (4)	C13B—C8B—C9B—C10B	0.2 (7)
C8A—C9A—C10A—C11A	0.7 (8)	S1B—C8B—C9B—C10B	−179.8 (4)
C9A—C10A—C11A—C12A	0.3 (8)	C8B—C9B—C10B—C11B	0.6 (8)
C9A—C10A—C11A—Cl1A	−179.6 (4)	C9B—C10B—C11B—C12B	−1.1 (9)
C10A—C11A—C12A—C13A	−0.6 (8)	C9B—C10B—C11B—Cl1B	178.0 (4)
Cl1A—C11A—C12A—C13A	179.3 (4)	C10B—C11B—C12B—C13B	0.8 (8)

C9A—C8A—C13A—C12A	0.9 (7)	Cl1B—C11B—C12B—C13B	−178.3 (4)
S1A—C8A—C13A—C12A	−178.2 (4)	C9B—C8B—C13B—C12B	−0.6 (7)
C11A—C12A—C13A—C8A	0.0 (8)	S1B—C8B—C13B—C12B	179.5 (3)
O2B—S1B—N1B—C2B	−25.1 (5)	C11B—C12B—C13B—C8B	0.0 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14*A*—H14*C*···O1*A*^{i}	0.96	2.59	3.271 (6)	128
C4*B*—H4*BA*···Cl1*B*^{ii}	0.93	2.95	3.800 (6)	153

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

2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-5-chloro-1*H*-benzimidazole; 2-*n*-butyl-1-(4-*tert*-butylphenylsulfonyl)-6-chloro-1*H*-benzimidazole (II)

Crystal data

$0.731C_{21}H_{25}ClN_2O_2S{\cdot}0.269C_{21}H_{25}ClN_2O_2S$
M_r = 404.94
Triclinic, $P\overline{1}$
a = 8.2990 (17) Å
b = 11.644 (2) Å
c = 12.279 (3) Å
α = 115.85 (3)°
β = 99.03 (3)°
γ = 94.96 (3)°
V = 1038.5 (4) Å^3
Z = 2
F(000) = 428
D_x = 1.295 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 2307 reflections
θ = 4.1–74.7°
μ = 2.71 mm^{-1}
T = 296 K
Prizmatic, colorless
0.36 × 0.20 × 0.20 mm

Data collection

Xcalibur, Ruby diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.2576 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.842, T_{max} = 1.000
7093 measured reflections
4179 independent reflections
3244 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 76.2°, θ_{min} = 4.1°
h = −9→10
k = −14→14
l = −15→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.152
S = 1.05
4179 reflections
258 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 0.1659P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.20524 (7)	0.60421 (6)	0.27060 (6)	0.0616 (2)	
O1	0.1971 (2)	0.73010 (19)	0.28074 (18)	0.0809 (6)	
O2	0.3383 (2)	0.5409 (2)	0.22959 (17)	0.0741 (5)	
Cl1	0.04322 (14)	0.99456 (11)	0.86571 (10)	0.0942 (4)	0.731 (2)
Cl1′	0.0497 (4)	1.0733 (2)	0.6922 (3)	0.0879 (11)	0.269 (2)
N1	0.2121 (2)	0.62283 (19)	0.41511 (18)	0.0572 (5)	
N3	0.2121 (2)	0.5667 (2)	0.56841 (18)	0.0601 (5)	
C2	0.2365 (3)	0.5296 (2)	0.4576 (2)	0.0557 (5)	
C3A	0.1665 (3)	0.6881 (2)	0.6048 (2)	0.0591 (6)	
C4	0.1301 (3)	0.7689 (3)	0.7172 (2)	0.0670 (6)	
H4A	0.130286	0.743758	0.779435	0.080*	
C5	0.0938 (3)	0.8879 (3)	0.7332 (3)	0.0752 (7)	
H5A	0.066479	0.943178	0.806841	0.090*	0.269 (2)
C6	0.0972 (3)	0.9266 (3)	0.6416 (3)	0.0790 (8)	
H6A	0.074455	1.008161	0.655985	0.095*	0.731 (2)
C7	0.1332 (3)	0.8475 (3)	0.5299 (3)	0.0718 (7)	
H7A	0.135532	0.874089	0.468797	0.086*	
C7A	0.1658 (3)	0.7272 (2)	0.5125 (2)	0.0576 (5)	
C8	0.0163 (3)	0.4999 (2)	0.1833 (2)	0.0552 (5)	
C9	−0.1303 (3)	0.5342 (2)	0.2174 (2)	0.0608 (6)	
H9A	−0.129886	0.612762	0.285345	0.073*	
C10	−0.2776 (3)	0.4498 (2)	0.1488 (2)	0.0604 (6)	
H10A	−0.375999	0.472137	0.172548	0.072*	
C11	−0.2830 (3)	0.3321 (2)	0.0452 (2)	0.0535 (5)	
C12	−0.1335 (3)	0.3031 (2)	0.0117 (2)	0.0618 (6)	
H12A	−0.133611	0.226523	−0.058291	0.074*	
C13	0.0161 (3)	0.3855 (3)	0.0801 (2)	0.0639 (6)	
H13A	0.114924	0.363844	0.056629	0.077*	
C14	0.2920 (3)	0.4038 (2)	0.3847 (2)	0.0606 (6)	
H14A	0.397881	0.421798	0.366095	0.073*	
H14B	0.212373	0.353996	0.306658	0.073*	
C15	0.3087 (3)	0.3245 (2)	0.4546 (2)	0.0621 (6)	
H15A	0.201796	0.304537	0.470730	0.074*	
H15B	0.385109	0.375959	0.533893	0.074*	
C16	0.3701 (3)	0.1993 (3)	0.3853 (3)	0.0718 (7)	
H16A	0.476404	0.218735	0.367995	0.086*	
H16B	0.292768	0.146655	0.306656	0.086*	
C17	0.3884 (4)	0.1230 (3)	0.4593 (3)	0.0899 (9)	
H17A	0.427770	0.044557	0.412930	0.135*	

H17B	0.282801	0.101922	0.475016	0.135*
H17C	0.466057	0.174357	0.536715	0.135*
C18	−0.4480 (3)	0.2395 (2)	−0.0235 (2)	0.0624 (6)
C19	−0.5259 (4)	0.2093 (3)	0.0686 (3)	0.0883 (9)
H19A	−0.629593	0.151107	0.025877	0.132*
H19B	−0.544544	0.288199	0.132867	0.132*
H19C	−0.452465	0.169645	0.104512	0.132*
C20	−0.4259 (4)	0.1129 (3)	−0.1283 (3)	0.0963 (10)
H20A	−0.532500	0.059832	−0.172766	0.145*
H20B	−0.359814	0.067746	−0.094261	0.145*
H20C	−0.371667	0.131430	−0.183790	0.145*
C21	−0.5653 (3)	0.3055 (3)	−0.0773 (3)	0.0812 (8)
H21A	−0.669470	0.248026	−0.120107	0.122*
H21B	−0.517354	0.326108	−0.134204	0.122*
H21C	−0.582711	0.383612	−0.011331	0.122*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0507 (3)	0.0742 (4)	0.0618 (4)	−0.0055 (3)	0.0076 (2)	0.0371 (3)
O1	0.0868 (13)	0.0788 (12)	0.0784 (12)	−0.0125 (10)	0.0024 (10)	0.0469 (10)
O2	0.0465 (9)	0.1040 (14)	0.0744 (11)	0.0001 (9)	0.0150 (8)	0.0448 (10)
Cl1	0.0803 (7)	0.0877 (7)	0.0813 (7)	0.0190 (5)	0.0135 (5)	0.0095 (5)
Cl1′	0.098 (2)	0.0607 (15)	0.0895 (19)	0.0184 (13)	−0.0046 (15)	0.0282 (13)
N1	0.0497 (10)	0.0615 (11)	0.0589 (11)	0.0008 (8)	0.0075 (8)	0.0290 (9)
N3	0.0553 (11)	0.0673 (12)	0.0596 (11)	0.0095 (9)	0.0113 (9)	0.0312 (9)
C2	0.0417 (11)	0.0633 (13)	0.0627 (13)	0.0009 (9)	0.0062 (9)	0.0323 (11)
C3A	0.0427 (11)	0.0686 (14)	0.0644 (14)	0.0046 (10)	0.0083 (10)	0.0308 (12)
C4	0.0541 (13)	0.0750 (16)	0.0634 (14)	0.0091 (12)	0.0089 (11)	0.0256 (12)
C5	0.0519 (13)	0.0718 (17)	0.0780 (17)	0.0038 (12)	0.0058 (12)	0.0170 (14)
C6	0.0609 (15)	0.0585 (15)	0.098 (2)	0.0067 (12)	0.0031 (14)	0.0237 (15)
C7	0.0638 (15)	0.0655 (15)	0.0821 (18)	0.0021 (12)	0.0048 (13)	0.0352 (14)
C7A	0.0398 (10)	0.0630 (13)	0.0653 (14)	−0.0009 (9)	0.0030 (9)	0.0295 (11)
C8	0.0464 (11)	0.0637 (13)	0.0569 (12)	0.0026 (10)	0.0067 (9)	0.0313 (11)
C9	0.0560 (13)	0.0583 (13)	0.0601 (13)	0.0090 (10)	0.0105 (10)	0.0207 (11)
C10	0.0451 (11)	0.0671 (14)	0.0662 (14)	0.0127 (10)	0.0126 (10)	0.0273 (12)
C11	0.0495 (11)	0.0557 (12)	0.0582 (12)	0.0063 (9)	0.0093 (9)	0.0300 (10)
C12	0.0569 (13)	0.0634 (14)	0.0583 (13)	0.0077 (11)	0.0146 (10)	0.0214 (11)
C13	0.0492 (12)	0.0779 (16)	0.0645 (14)	0.0112 (11)	0.0189 (11)	0.0304 (12)
C14	0.0509 (12)	0.0641 (14)	0.0638 (14)	0.0034 (10)	0.0112 (10)	0.0281 (11)
C15	0.0502 (12)	0.0635 (14)	0.0694 (15)	0.0031 (10)	0.0079 (11)	0.0306 (12)
C16	0.0567 (14)	0.0671 (15)	0.0841 (18)	0.0084 (12)	0.0067 (12)	0.0311 (13)
C17	0.086 (2)	0.0736 (18)	0.109 (2)	0.0114 (15)	0.0045 (18)	0.0464 (18)
C18	0.0547 (13)	0.0609 (14)	0.0672 (14)	−0.0009 (10)	0.0074 (11)	0.0293 (11)
C19	0.0721 (18)	0.101 (2)	0.095 (2)	−0.0168 (16)	0.0100 (15)	0.0567 (19)
C20	0.078 (2)	0.0700 (18)	0.103 (2)	−0.0111 (15)	0.0108 (17)	0.0137 (17)
C21	0.0565 (15)	0.094 (2)	0.089 (2)	−0.0063 (14)	−0.0062 (13)	0.0480 (17)

Geometric parameters (Å, º)

S1—O2	1.417 (2)	C11—C18	1.529 (3)
S1—O1	1.425 (2)	C12—C13	1.390 (3)
S1—N1	1.682 (2)	C12—H12A	0.9300
S1—C8	1.758 (2)	C13—H13A	0.9300
Cl1—C5	1.705 (3)	C14—C15	1.511 (3)
Cl1′—C6	1.652 (4)	C14—H14A	0.9700
N1—C2	1.410 (3)	C14—H14B	0.9700
N1—C7A	1.419 (3)	C15—C16	1.514 (4)
N3—C2	1.292 (3)	C15—H15A	0.9700
N3—C3A	1.391 (3)	C15—H15B	0.9700
C2—C14	1.504 (3)	C16—C17	1.525 (4)
C3A—C4	1.389 (3)	C16—H16A	0.9700
C3A—C7A	1.395 (3)	C16—H16B	0.9700
C4—C5	1.379 (4)	C17—H17A	0.9600
C4—H4A	0.9300	C17—H17B	0.9600
C5—C6	1.385 (4)	C17—H17C	0.9600
C5—H5A	0.9300	C18—C20	1.526 (4)
C6—C7	1.376 (4)	C18—C21	1.531 (4)
C6—H6A	0.9300	C18—C19	1.536 (4)
C7—C7A	1.380 (4)	C19—H19A	0.9600
C7—H7A	0.9300	C19—H19B	0.9600
C8—C13	1.381 (3)	C19—H19C	0.9600
C8—C9	1.384 (3)	C20—H20A	0.9600
C9—C10	1.385 (3)	C20—H20B	0.9600
C9—H9A	0.9300	C20—H20C	0.9600
C10—C11	1.396 (3)	C21—H21A	0.9600
C10—H10A	0.9300	C21—H21B	0.9600
C11—C12	1.391 (3)	C21—H21C	0.9600
O2—S1—O1	120.61 (12)	C8—C13—H13A	120.4
O2—S1—N1	106.88 (11)	C12—C13—H13A	120.4
O1—S1—N1	104.49 (12)	C2—C14—C15	111.9 (2)
O2—S1—C8	109.43 (12)	C2—C14—H14A	109.2
O1—S1—C8	109.75 (12)	C15—C14—H14A	109.2
N1—S1—C8	104.34 (10)	C2—C14—H14B	109.2
C2—N1—C7A	105.92 (19)	C15—C14—H14B	109.2
C2—N1—S1	127.14 (17)	H14A—C14—H14B	107.9
C7A—N1—S1	126.12 (17)	C14—C15—C16	113.1 (2)
C2—N3—C3A	106.4 (2)	C14—C15—H15A	109.0
N3—C2—N1	112.3 (2)	C16—C15—H15A	109.0
N3—C2—C14	123.6 (2)	C14—C15—H15B	109.0
N1—C2—C14	124.0 (2)	C16—C15—H15B	109.0
C4—C3A—N3	128.4 (2)	H15A—C15—H15B	107.8
C4—C3A—C7A	120.5 (2)	C15—C16—C17	111.7 (3)
N3—C3A—C7A	111.1 (2)	C15—C16—H16A	109.3
C5—C4—C3A	117.6 (3)	C17—C16—H16A	109.3

C5—C4—H4A	121.2	C15—C16—H16B	109.3
C3A—C4—H4A	121.2	C17—C16—H16B	109.3
C4—C5—C6	121.2 (3)	H16A—C16—H16B	107.9
C4—C5—Cl1	122.1 (3)	C16—C17—H17A	109.5
C6—C5—Cl1	116.7 (2)	C16—C17—H17B	109.5
C4—C5—H5A	119.4	H17A—C17—H17B	109.5
C6—C5—H5A	119.4	C16—C17—H17C	109.5
C7—C6—C5	121.8 (3)	H17A—C17—H17C	109.5
C7—C6—Cl1′	130.0 (3)	H17B—C17—H17C	109.5
C5—C6—Cl1′	108.2 (3)	C20—C18—C11	111.8 (2)
C7—C6—H6A	119.1	C20—C18—C21	109.2 (3)
C5—C6—H6A	119.1	C11—C18—C21	109.0 (2)
C6—C7—C7A	117.1 (3)	C20—C18—C19	109.0 (3)
C6—C7—H7A	121.4	C11—C18—C19	109.1 (2)
C7A—C7—H7A	121.4	C21—C18—C19	108.5 (2)
C7—C7A—C3A	121.7 (2)	C18—C19—H19A	109.5
C7—C7A—N1	133.9 (2)	C18—C19—H19B	109.5
C3A—C7A—N1	104.3 (2)	H19A—C19—H19B	109.5
C13—C8—C9	120.9 (2)	C18—C19—H19C	109.5
C13—C8—S1	119.42 (18)	H19A—C19—H19C	109.5
C9—C8—S1	119.72 (18)	H19B—C19—H19C	109.5
C8—C9—C10	118.9 (2)	C18—C20—H20A	109.5
C8—C9—H9A	120.6	C18—C20—H20B	109.5
C10—C9—H9A	120.6	H20A—C20—H20B	109.5
C9—C10—C11	122.1 (2)	C18—C20—H20C	109.5
C9—C10—H10A	119.0	H20A—C20—H20C	109.5
C11—C10—H10A	119.0	H20B—C20—H20C	109.5
C12—C11—C10	117.2 (2)	C18—C21—H21A	109.5
C12—C11—C18	122.9 (2)	C18—C21—H21B	109.5
C10—C11—C18	119.9 (2)	H21A—C21—H21B	109.5
C13—C12—C11	121.8 (2)	C18—C21—H21C	109.5
C13—C12—H12A	119.1	H21A—C21—H21C	109.5
C11—C12—H12A	119.1	H21B—C21—H21C	109.5
C8—C13—C12	119.2 (2)		

O2—S1—N1—C2	−44.7 (2)	S1—N1—C7A—C7	−13.3 (4)
O1—S1—N1—C2	−173.60 (18)	C2—N1—C7A—C3A	0.1 (2)
C8—S1—N1—C2	71.2 (2)	S1—N1—C7A—C3A	170.24 (15)
O2—S1—N1—C7A	147.17 (18)	O2—S1—C8—C13	−9.6 (2)
O1—S1—N1—C7A	18.3 (2)	O1—S1—C8—C13	124.9 (2)
C8—S1—N1—C7A	−96.96 (19)	N1—S1—C8—C13	−123.6 (2)
C3A—N3—C2—N1	1.0 (2)	O2—S1—C8—C9	171.52 (18)
C3A—N3—C2—C14	178.5 (2)	O1—S1—C8—C9	−54.0 (2)
C7A—N1—C2—N3	−0.7 (2)	N1—S1—C8—C9	57.5 (2)
S1—N1—C2—N3	−170.73 (16)	C13—C8—C9—C10	2.2 (4)
C7A—N1—C2—C14	−178.2 (2)	S1—C8—C9—C10	−178.88 (19)
S1—N1—C2—C14	11.8 (3)	C8—C9—C10—C11	−1.1 (4)
C2—N3—C3A—C4	−178.7 (2)	C9—C10—C11—C12	−0.9 (4)

C2—N3—C3A—C7A	−0.9 (3)	C9—C10—C11—C18	177.0 (2)
N3—C3A—C4—C5	177.6 (2)	C10—C11—C12—C13	1.8 (4)
C7A—C3A—C4—C5	0.0 (3)	C18—C11—C12—C13	−176.1 (2)
C3A—C4—C5—C6	−1.5 (4)	C9—C8—C13—C12	−1.4 (4)
C3A—C4—C5—Cl1	178.72 (19)	S1—C8—C13—C12	179.73 (19)
C4—C5—C6—C7	1.4 (4)	C11—C12—C13—C8	−0.7 (4)
Cl1—C5—C6—C7	−178.7 (2)	N3—C2—C14—C15	2.2 (3)
C4—C5—C6—Cl1′	−179.4 (2)	N1—C2—C14—C15	179.46 (19)
C5—C6—C7—C7A	0.1 (4)	C2—C14—C15—C16	−178.03 (19)
Cl1′—C6—C7—C7A	−178.9 (2)	C14—C15—C16—C17	179.0 (2)
C6—C7—C7A—C3A	−1.6 (4)	C12—C11—C18—C20	1.7 (4)
C6—C7—C7A—N1	−177.5 (2)	C10—C11—C18—C20	−176.1 (2)
C4—C3A—C7A—C7	1.5 (3)	C12—C11—C18—C21	−119.2 (3)
N3—C3A—C7A—C7	−176.4 (2)	C10—C11—C18—C21	63.0 (3)
C4—C3A—C7A—N1	178.5 (2)	C12—C11—C18—C19	122.4 (3)
N3—C3A—C7A—N1	0.5 (2)	C10—C11—C18—C19	−55.4 (3)
C2—N1—C7A—C7	176.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···O2^{i}	0.93	2.67	3.595 (3)	176

Symmetry code: (i) *x*−1, *y*, *z*.

2-*n*-Butyl-5-chloro-1-(4-methylphenylsulfonyl)-1*H*-benzimidazole (III)

Crystal data

$C_{18}H_{19}ClN_2O_2S$
M_r = 362.86
Triclinic, $P\overline{1}$
a = 8.1491 (16) Å
b = 10.039 (2) Å
c = 12.485 (3) Å
α = 112.23 (3)°
β = 105.49 (3)°
γ = 96.02 (3)°
V = 886.5 (4) Å^3
Z = 2
F(000) = 380
D_x = 1.359 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 4862 reflections
θ = 4.9–76.1°
μ = 3.11 mm^{-1}
T = 297 K
Prizmatic, colorless
0.40 × 0.34 × 0.28 mm

Data collection

Xcalibur, Ruby diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.2576 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.394, T_{max} = 1.000
8070 measured reflections
3662 independent reflections
3088 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 76.7°, θ_{min} = 4.9°
h = −10→7
k = −12→12
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.151$
$S = 1.06$
3662 reflections
219 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0949P)^2 + 0.1961P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ 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}
S1	0.14167 (6)	0.68003 (5)	0.49351 (5)	0.05023 (18)
Cl1	−0.14634 (10)	1.03713 (9)	0.10476 (6)	0.0805 (2)
O1	−0.0423 (2)	0.61981 (18)	0.44279 (18)	0.0639 (5)
O2	0.2329 (2)	0.71457 (18)	0.61788 (16)	0.0621 (4)
N1	0.1723 (2)	0.84081 (18)	0.47964 (17)	0.0484 (4)
N3	0.2844 (2)	1.07202 (19)	0.51200 (17)	0.0502 (4)
C2	0.2986 (2)	0.9753 (2)	0.5575 (2)	0.0463 (4)
C3A	0.1486 (3)	1.0042 (2)	0.40047 (19)	0.0467 (4)
C4	0.0822 (3)	1.0625 (2)	0.3172 (2)	0.0544 (5)
H4A	0.126985	1.159347	0.332202	0.065*
C5	−0.0529 (3)	0.9701 (3)	0.2118 (2)	0.0569 (5)
C6	−0.1219 (3)	0.8249 (3)	0.1868 (2)	0.0612 (6)
H6A	−0.211662	0.765974	0.113421	0.073*
C7	−0.0585 (3)	0.7670 (3)	0.2698 (2)	0.0592 (5)
H7A	−0.104578	0.670410	0.254779	0.071*
C7A	0.0771 (3)	0.8598 (2)	0.3767 (2)	0.0477 (4)
C8	0.2445 (3)	0.5723 (2)	0.3976 (2)	0.0484 (5)
C9	0.1471 (3)	0.4447 (3)	0.2933 (2)	0.0623 (6)
H9A	0.027067	0.414879	0.274444	0.075*
C10	0.2313 (4)	0.3638 (3)	0.2186 (2)	0.0684 (6)
H10A	0.167128	0.277938	0.149341	0.082*
C11	0.4103 (3)	0.4072 (3)	0.2443 (2)	0.0611 (6)
C12	0.5044 (3)	0.5332 (3)	0.3486 (2)	0.0614 (6)
H12A	0.624448	0.562930	0.367126	0.074*
C13	0.4237 (3)	0.6159 (2)	0.4260 (2)	0.0569 (5)
H13A	0.488914	0.700014	0.496580	0.068*
C14	0.4290 (3)	1.0024 (2)	0.6776 (2)	0.0523 (5)
H14A	0.506517	0.935467	0.663068	0.063*
H14B	0.367723	0.980399	0.727873	0.063*
C15	0.5380 (3)	1.1608 (3)	0.7474 (2)	0.0544 (5)

H15A	0.605879	1.180599	0.699777	0.065*
H15B	0.460274	1.228107	0.756961	0.065*
C16	0.6611 (4)	1.1901 (3)	0.8731 (2)	0.0674 (6)
H16A	0.593770	1.165935	0.919366	0.081*
H16B	0.742375	1.125984	0.863339	0.081*
C17	0.7634 (5)	1.3493 (4)	0.9447 (3)	0.0946 (10)
H17A	0.836419	1.363259	1.024234	0.142*
H17B	0.683530	1.413398	0.953948	0.142*
H17C	0.834961	1.372367	0.901381	0.142*
C18	0.5008 (5)	0.3202 (4)	0.1594 (3)	0.0903 (10)
H18D	0.621201	0.334121	0.205306	0.135*
H18A	0.494375	0.354141	0.096386	0.135*
H18B	0.444249	0.217126	0.122491	0.135*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0441 (3)	0.0451 (3)	0.0725 (4)	0.0097 (2)	0.0245 (2)	0.0332 (2)
Cl1	0.0847 (5)	0.0901 (5)	0.0704 (4)	0.0155 (4)	0.0130 (3)	0.0477 (4)
O1	0.0460 (8)	0.0580 (9)	0.1005 (13)	0.0095 (7)	0.0315 (8)	0.0428 (9)
O2	0.0709 (10)	0.0570 (9)	0.0736 (10)	0.0155 (8)	0.0317 (8)	0.0382 (8)
N1	0.0427 (8)	0.0424 (8)	0.0655 (10)	0.0093 (7)	0.0184 (7)	0.0285 (8)
N3	0.0503 (9)	0.0421 (8)	0.0611 (10)	0.0093 (7)	0.0198 (8)	0.0243 (8)
C2	0.0408 (9)	0.0434 (9)	0.0604 (11)	0.0107 (8)	0.0220 (9)	0.0241 (9)
C3A	0.0455 (10)	0.0422 (10)	0.0582 (11)	0.0122 (8)	0.0230 (9)	0.0229 (8)
C4	0.0597 (12)	0.0490 (11)	0.0634 (13)	0.0147 (9)	0.0250 (10)	0.0296 (10)
C5	0.0552 (12)	0.0670 (13)	0.0589 (12)	0.0204 (10)	0.0231 (10)	0.0331 (11)
C6	0.0533 (12)	0.0599 (13)	0.0629 (13)	0.0095 (10)	0.0143 (10)	0.0225 (11)
C7	0.0517 (12)	0.0490 (11)	0.0711 (14)	0.0043 (9)	0.0145 (10)	0.0255 (10)
C7A	0.0425 (9)	0.0455 (10)	0.0630 (12)	0.0131 (8)	0.0233 (9)	0.0267 (9)
C8	0.0450 (10)	0.0423 (10)	0.0648 (12)	0.0098 (8)	0.0188 (9)	0.0295 (9)
C9	0.0453 (11)	0.0576 (13)	0.0753 (15)	0.0025 (9)	0.0133 (10)	0.0262 (11)
C10	0.0627 (14)	0.0648 (14)	0.0627 (14)	0.0085 (11)	0.0129 (11)	0.0186 (11)
C11	0.0617 (13)	0.0694 (14)	0.0608 (13)	0.0233 (11)	0.0214 (11)	0.0337 (11)
C12	0.0434 (11)	0.0690 (14)	0.0779 (15)	0.0151 (10)	0.0232 (10)	0.0350 (12)
C13	0.0435 (10)	0.0492 (11)	0.0724 (14)	0.0061 (9)	0.0166 (10)	0.0229 (10)
C14	0.0499 (11)	0.0518 (11)	0.0603 (12)	0.0132 (9)	0.0203 (9)	0.0275 (10)
C15	0.0482 (11)	0.0567 (12)	0.0573 (12)	0.0088 (9)	0.0187 (9)	0.0233 (10)
C16	0.0634 (14)	0.0746 (16)	0.0594 (14)	0.0156 (12)	0.0189 (11)	0.0244 (12)
C17	0.085 (2)	0.092 (2)	0.0710 (18)	−0.0069 (17)	0.0106 (15)	0.0157 (16)
C18	0.088 (2)	0.118 (3)	0.0685 (17)	0.0433 (19)	0.0335 (16)	0.0324 (17)

Geometric parameters (Å, º)

S1—O2	1.4163 (19)	C10—C11	1.390 (4)
S1—O1	1.4235 (17)	C10—H10A	0.9300
S1—N1	1.6875 (17)	C11—C12	1.379 (4)
S1—C8	1.747 (2)	C11—C18	1.510 (4)

Cl1—C5	1.751 (2)	C12—C13	1.379 (3)
N1—C7A	1.405 (3)	C12—H12A	0.9300
N1—C2	1.417 (3)	C13—H13A	0.9300
N3—C2	1.298 (3)	C14—C15	1.523 (3)
N3—C3A	1.389 (3)	C14—H14A	0.9700
C2—C14	1.494 (3)	C14—H14B	0.9700
C3A—C7A	1.391 (3)	C15—C16	1.518 (3)
C3A—C4	1.394 (3)	C15—H15A	0.9700
C4—C5	1.376 (3)	C15—H15B	0.9700
C4—H4A	0.9300	C16—C17	1.513 (4)
C5—C6	1.388 (4)	C16—H16A	0.9700
C6—C7	1.383 (4)	C16—H16B	0.9700
C6—H6A	0.9300	C17—H17A	0.9600
C7—C7A	1.387 (3)	C17—H17B	0.9600
C7—H7A	0.9300	C17—H17C	0.9600
C8—C13	1.386 (3)	C18—H18D	0.9600
C8—C9	1.392 (3)	C18—H18A	0.9600
C9—C10	1.373 (4)	C18—H18B	0.9600
C9—H9A	0.9300		

O2—S1—O1	120.39 (11)	C12—C11—C10	118.6 (2)
O2—S1—N1	105.87 (10)	C12—C11—C18	120.3 (2)
O1—S1—N1	105.72 (10)	C10—C11—C18	121.2 (3)
O2—S1—C8	110.71 (10)	C11—C12—C13	121.2 (2)
O1—S1—C8	109.53 (11)	C11—C12—H12A	119.4
N1—S1—C8	103.00 (9)	C13—C12—H12A	119.4
C7A—N1—C2	106.35 (17)	C12—C13—C8	119.4 (2)
C7A—N1—S1	123.54 (15)	C12—C13—H13A	120.3
C2—N1—S1	129.95 (15)	C8—C13—H13A	120.3
C2—N3—C3A	106.66 (17)	C2—C14—C15	112.90 (19)
N3—C2—N1	111.37 (19)	C2—C14—H14A	109.0
N3—C2—C14	124.58 (19)	C15—C14—H14A	109.0
N1—C2—C14	124.04 (18)	C2—C14—H14B	109.0
N3—C3A—C7A	110.97 (19)	C15—C14—H14B	109.0
N3—C3A—C4	128.68 (19)	H14A—C14—H14B	107.8
C7A—C3A—C4	120.4 (2)	C16—C15—C14	112.5 (2)
C5—C4—C3A	116.9 (2)	C16—C15—H15A	109.1
C5—C4—H4A	121.6	C14—C15—H15A	109.1
C3A—C4—H4A	121.6	C16—C15—H15B	109.1
C4—C5—C6	122.8 (2)	C14—C15—H15B	109.1
C4—C5—Cl1	119.36 (19)	H15A—C15—H15B	107.8
C6—C5—Cl1	117.79 (19)	C17—C16—C15	112.5 (3)
C7—C6—C5	120.6 (2)	C17—C16—H16A	109.1
C7—C6—H6A	119.7	C15—C16—H16A	109.1
C5—C6—H6A	119.7	C17—C16—H16B	109.1
C6—C7—C7A	116.9 (2)	C15—C16—H16B	109.1
C6—C7—H7A	121.6	H16A—C16—H16B	107.8
C7A—C7—H7A	121.6	C16—C17—H17A	109.5

C7—C7A—C3A	122.4 (2)	C16—C17—H17B	109.5
C7—C7A—N1	133.0 (2)	H17A—C17—H17B	109.5
C3A—C7A—N1	104.63 (18)	C16—C17—H17C	109.5
C13—C8—C9	120.5 (2)	H17A—C17—H17C	109.5
C13—C8—S1	119.27 (17)	H17B—C17—H17C	109.5
C9—C8—S1	120.27 (17)	C11—C18—H18D	109.5
C10—C9—C8	118.9 (2)	C11—C18—H18A	109.5
C10—C9—H9A	120.6	H18D—C18—H18A	109.5
C8—C9—H9A	120.6	C11—C18—H18B	109.5
C9—C10—C11	121.5 (2)	H18D—C18—H18B	109.5
C9—C10—H10A	119.2	H18A—C18—H18B	109.5
C11—C10—H10A	119.2		

O2—S1—N1—C7A	−167.75 (16)	C4—C3A—C7A—N1	−178.69 (18)
O1—S1—N1—C7A	−38.97 (19)	C2—N1—C7A—C7	178.3 (2)
C8—S1—N1—C7A	75.96 (18)	S1—N1—C7A—C7	2.5 (3)
O2—S1—N1—C2	17.4 (2)	C2—N1—C7A—C3A	−1.5 (2)
O1—S1—N1—C2	146.22 (19)	S1—N1—C7A—C3A	−177.31 (14)
C8—S1—N1—C2	−98.86 (19)	O2—S1—C8—C13	−48.5 (2)
C3A—N3—C2—N1	−0.8 (2)	O1—S1—C8—C13	176.40 (18)
C3A—N3—C2—C14	−179.80 (18)	N1—S1—C8—C13	64.3 (2)
C7A—N1—C2—N3	1.5 (2)	O2—S1—C8—C9	131.96 (19)
S1—N1—C2—N3	176.97 (15)	O1—S1—C8—C9	−3.1 (2)
C7A—N1—C2—C14	−179.54 (18)	N1—S1—C8—C9	−115.25 (19)
S1—N1—C2—C14	−4.0 (3)	C13—C8—C9—C10	−0.6 (4)
C2—N3—C3A—C7A	−0.2 (2)	S1—C8—C9—C10	178.9 (2)
C2—N3—C3A—C4	179.5 (2)	C8—C9—C10—C11	−0.7 (4)
N3—C3A—C4—C5	179.2 (2)	C9—C10—C11—C12	1.3 (4)
C7A—C3A—C4—C5	−1.1 (3)	C9—C10—C11—C18	−177.9 (3)
C3A—C4—C5—C6	−0.3 (3)	C10—C11—C12—C13	−0.5 (4)
C3A—C4—C5—Cl1	178.52 (16)	C18—C11—C12—C13	178.7 (3)
C4—C5—C6—C7	1.3 (4)	C11—C12—C13—C8	−0.7 (4)
Cl1—C5—C6—C7	−177.49 (19)	C9—C8—C13—C12	1.3 (3)
C5—C6—C7—C7A	−0.9 (4)	S1—C8—C13—C12	−178.24 (18)
C6—C7—C7A—C3A	−0.5 (3)	N3—C2—C14—C15	4.0 (3)
C6—C7—C7A—N1	179.8 (2)	N1—C2—C14—C15	−174.85 (19)
N3—C3A—C7A—C7	−178.8 (2)	C2—C14—C15—C16	175.97 (18)
C4—C3A—C7A—C7	1.5 (3)	C14—C15—C16—C17	−177.4 (2)
N3—C3A—C7A—N1	1.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···O1^{i}	0.93	2.55	3.467 (3)	170
C18—H18*D*···O2^{ii}	0.96	2.46	3.199 (4)	133

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