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Crystal structures of isomeric 4-bromo-*N*-[(2-nitrophenyl)sulfonyl]benzamide and 4-bromo-*N*-[(4-nitrophenyl)sulfonyl]benzamide

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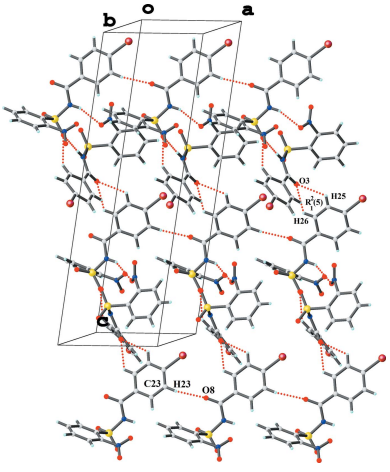
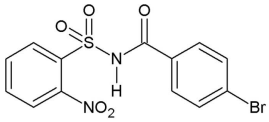
The syntheses and crystal structures of the isomeric 4-bromo-*N*-[(2-nitrophenyl)sulfonyl]benzamide, (I), and 4-bromo-*N*-[(4-nitrophenyl)sulfonyl]benzamide, (II), are described (molecular formula = $C_{13}H_9BrN_2O_5S$ in each case). The asymmetric unit of (I) contains two independent molecules [(I*A*) and (I*B*)], while that of (II) contains one molecule. The benzoic acid aromatic ring of molecule (I*A*) is disordered due to rotation about the C_{ar}—C(=O) bond over two orientations in a 0.525 (9):0.475 (9) ratio. The dihedral angle between the benzene rings is 85.9 (3)° in (I*A*) and 65.22 (19)° in (I*B*), while in (II), the corresponding value is 56.7 (7)°. In the crystals of (I) and (II), N—H···O, C—H···O and C—H···π interactions generate three-dimensional networks.

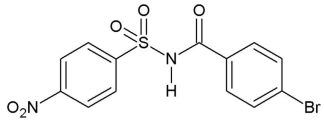
1. Chemical context

In recent years, *N*-(arylsulfonyl)arylamides have received much attention as they constitute an important class of drugs for treating Alzheimer's disease (Hasegawa & Yamamoto, 2000) and acting as anti-bacterial inhibitors of tRNA synthetases (Banwell *et al.*, 2000), antagonists for angiotensin II (Chang *et al.*, 1994) and as leukotriene D4-receptors (Musser *et al.*, 1990). Further, *N*-(arylsulfonyl)-arylamides are known to be potent anti-tumour agents against a broad spectrum of human tumour xenografts (colon, lung, breast, ovary and prostate) in mice (Mader *et al.*, 2005). In a continuation of our work on the synthesis and crystal structures of *N*-(2-nitrophenylsulfonyl)arylamides (Suchetan *et al.*, 2012*a*) and *N*-(4-nitrophenylsulfonyl)arylamides (Suchetan *et al.*, 2012*b*), compounds (I) and (II) were synthesized and their crystal structures determined.





(I)



(II)

2. Structural commentary

The asymmetric unit of (I) (Fig. 1) contains two independent molecules, (I*A*) and (I*B*), while that of (II) contains one

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

*Cg*1 and *Cg*2 are the centroids of the bromobenzene ring of molecule *A* and nitrobenzene ring of molecule *B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O6	0.81 (4)	2.03 (4)	2.837 (4)	172 (5)
N3—H*N*3···O4	0.82 (6)	2.29 (5)	3.021 (4)	148 (4)
C13*A*—H13*A*···O6	0.95	2.41	3.210 (8)	141
C23—H23···O8^{i}	0.95	2.50	3.425 (4)	165
C25—H25···O3^{ii}	0.95	2.51	3.117 (4)	122
C26—H26···O3^{ii}	0.95	2.51	3.123 (4)	122
C12*A*—H12*A*···*Cg*1^{iii}	0.95	2.99	3.635 (9)	126
C10*B*—H10*B*···*Cg*2^{iii}	0.95	2.76	3.532 (8)	139

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

molecule (Fig. 2). In both molecules (I*A*) and (I*B*), the *ortho*-nitro substitution on the benzenesulfonyl ring is *syn* to the N—H bond in the central –C—SO_2—*N*—C(O)– segment (Fig. 1). The benzoic acid ring of molecule (I*A*) is disordered due to rotation about the C_{ar}—C(═O) bond over two orientations in a 0.525 (9):0.475 (9) ratio, which are inclined to each other by 45.5 (4)°. The nitro groups in both the *A* and *B* molecules of (I) and the molecule of (II) are twisted relative to the attached benzenesulfonyl rings: the torsion angle C1—C2—N2—O4 in (I*A*) is 56.3 (4)°, while in (I*B*), the torsion angle C14—C15—N4—O9 is 35.6 (5)°, whereas in (II), the C5—C4—N2—O4 torsion angle has a value of 19.4 (5)°. The dihedral angle between the benzene rings is 85.9 (3)° in (I*A*), 65.22 (19)° in (I*B*) and 56.7 (7)° in (II). The conformation of (II) is supported by an intramolecular C2—H2···O3 interaction (Table 2), forming an *S*(7) motif.

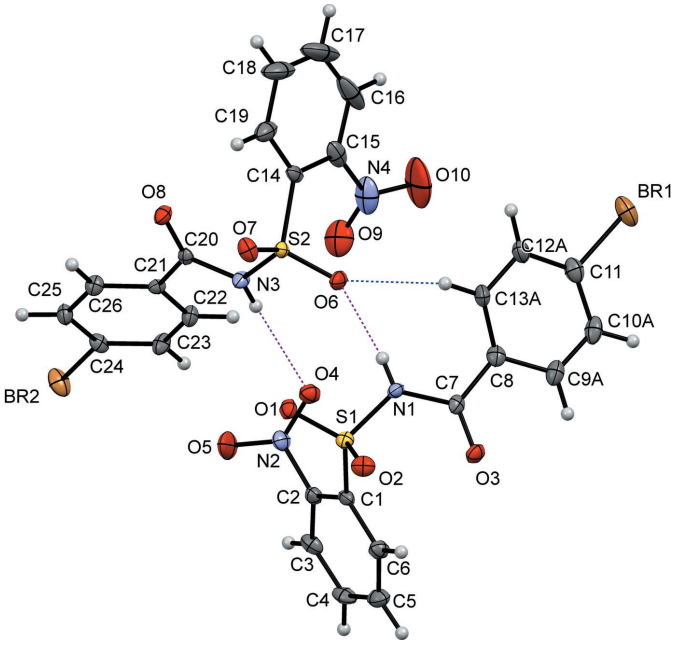


Figure 1
A view of (I*A*), showing displacement ellipsoids drawn at the 50% probability level.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O3^{i}	0.90	1.97	2.8530	168
C2—H2···O3	0.95	2.36	3.1280	138
C3—H3···O4^{ii}	0.95	2.45	3.3199	152
C9—H9···O2^{iii}	0.95	2.55	3.2599	132
C10—H10···O1^{iv}	0.95	2.48	3.1081	124
C12—H12···O4^{v}	0.95	2.56	3.4445	155
C13—H13···O3^{i}	0.95	2.53	3.3182	141

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

3. Supramolecular features

The crystal structure of (I) features two N—H···O hydrogen bonds, namely N1—H*N*1···O6 and N3—H*N*3···O4 (Table 1) between the *A* and *B* molecules, resulting in a hetero dimer with graph-set motif $R_2^2(11)$, which is consolidated by a C13—H13*A*···O6 interaction between the *A* and *B* molecules (Fig. 3). The *A* + *B* dimers assemble along the *a*-axis direction *via* C23—H23···O8 interactions, forming *C*6 chains (Table 1, Fig. 3). A dimeric $R_1^2(5)$ network generated by the C25—H25···O3 and C26—H26···O3 interactions (Table 1, Fig. 3) and the $R_2^2(11)$ network, which alternate along the *c*-axis direction, build a network of $C_2^2(14)$ and $C_2^2(15)$ chains as part of a zigzag sheet propagating in the *ac* plane, which features a short Br2···O3 contact [3.212 (2) Å]. Further, C10—H10*B*···π_1 [where π_1 is the nitrobenzene ring of molecule (I*B*)] and C12—H12*A*···π_2 [π_2 is the bromobenzene ring of molecule (I*A*)] extend the zigzag sheets into a three-dimensional architecture, which is consolidated by several aromatic π–π stacking interactions [centroid–centroid separations = 3.873 (4), 3.785 (5) and 3.698 (5) Å].

The crystal structure of (II) features N1—H*N*1···O3 hydrogen bonds forming *C*(4) chains along [100] (Table 2, Fig. 4): these chains are further strengthened by C13—H13···O3 interactions (Table 2) forming *C*(5) chains. The molecules of neighbouring chains are interlinked *via* C3—H3···O4 and C12—H12···O4 interactions (*i.e.* O4 acts as a double acceptor) and thus, a zigzag sheet propagates in the *ac* plane (Table 2). The C12—H12···O4 and C3—H3···O4 interactions run as *C*(13) and *C*(5) chains, respectively, along [001]. Molecules in adjacent layers are linked *via* C9—

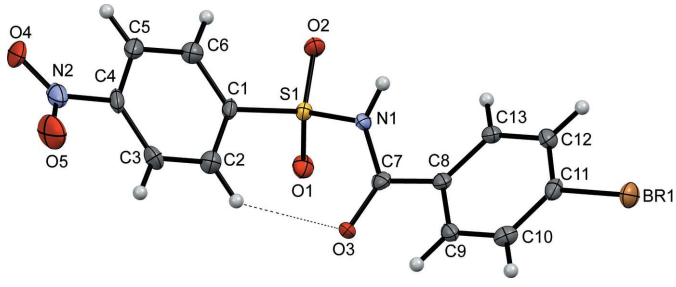


Figure 2
A view of (II), showing displacement ellipsoids drawn at the 50% probability level.

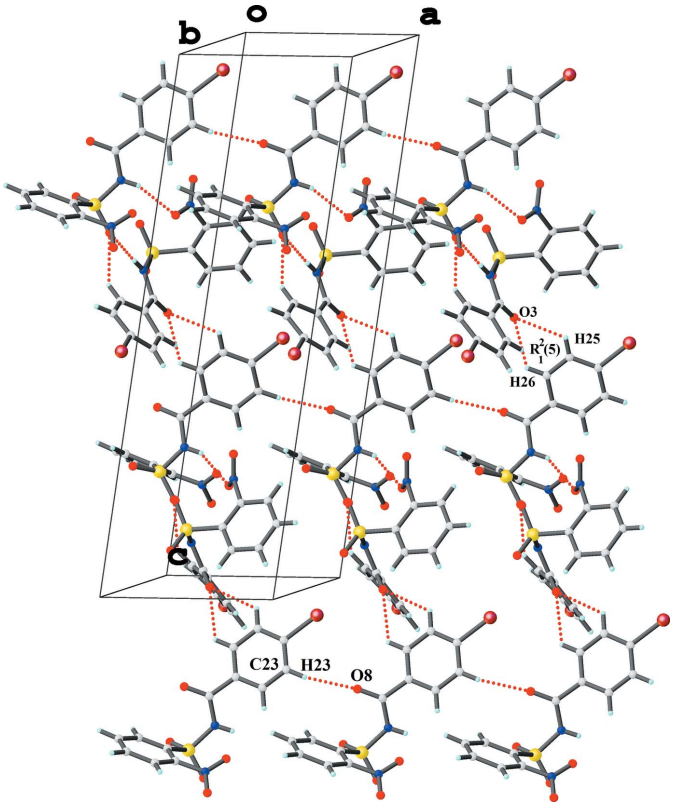


Figure 3
The crystal packing of (I), displaying the hetero $R_2^2(11)$ dimeric supramolecular synthon. Molecules assemble along the *a* axis forming *C*(6) chains *via* C—H···O interactions while two further C—H···O interactions involving the same acceptor atom lead to the formation of an $R_1^2(5)$ network.

H9···O2 and C10—H10···O1 interactions that form *C*(7) and *C*(8) chains propagating along the *b*-axis direction, and thus a three-dimensional network is obtained. A short O5···Br1 [3.173 (4) Å] contact is observed.

4. Database survey

A survey of the Cambridge Structural Database (Groom *et al.*, 2016) revealed 82 phenylsulfonyl-arylamide structures with different substituents attached to the benzene rings including the parent compound *N*-benzoylbenzenesulfonamide (Gowda *et al.*, 2009).

5. Synthesis and crystallization

Compounds (I) and (II) were prepared by refluxing a mixture of 4-bromobenzoic acid, the corresponding substituted benzenesulfonamide and phosphorus oxychloride for 3 h on a water bath. The resultant mixtures were cooled and poured into ice-cold water. The solids obtained were filtered, washed thoroughly with water and then dissolved in sodium bicarbonate solutions. The compounds were later reprecipitated by acidifying the filtered solutions with dilute HCl. They were filtered, dried and recrystallized. [m.p. = 486 for (I) and 498 K for (II)]. Colourless prisms of (I) and (II) were obtained by slow evaporation of the respective solutions of the compounds in methanol (with a few added drops of water).

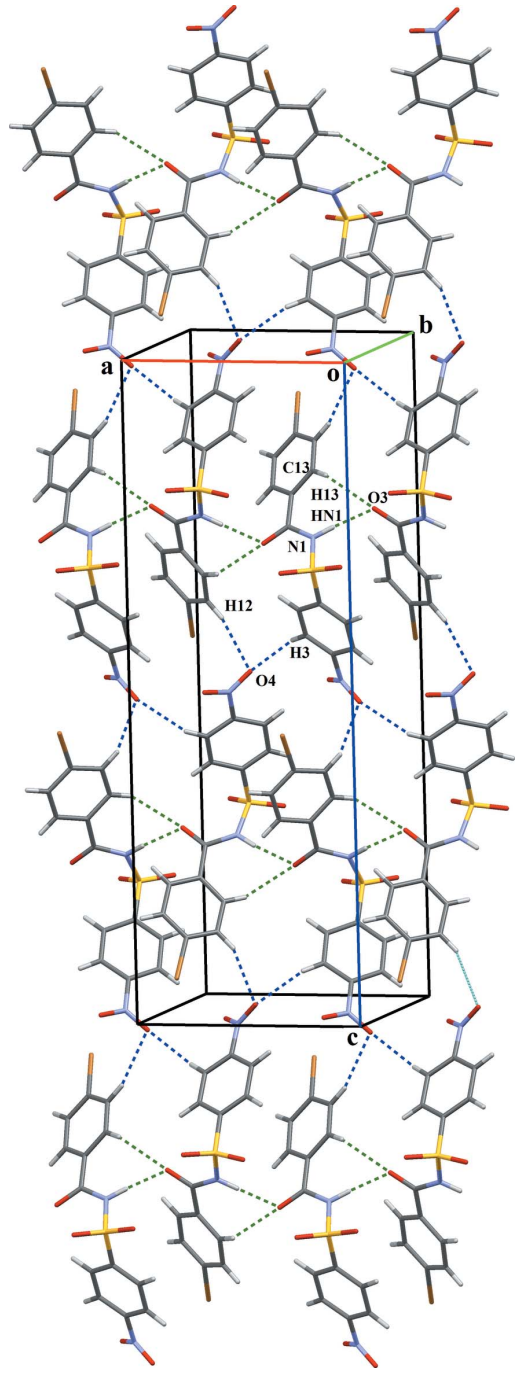


Figure 4
Structure-directing C—H···O interactions in the crystal structure of (II) propagating along the *b* axis as chains.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms of the NH groups in (I) and (II) were located in a difference map and later refined

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{13}H_9BrN_2O_5S$	$C_{13}H_9BrN_2O_5S$
M_r	385.19	385.19
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, *Pbca*
Temperature (K)	173	173
a, b, c (Å)	8.0209 (3), 14.5364 (5), 25.0008 (8)	9.6085 (4), 10.3246 (5), 27.7296 (13)
α, β, γ (°)	90, 98.499 (1), 90	90, 90, 90
V (Å^3)	2882.96 (17)	2750.9 (2)
Z	8	8
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	5.50	5.76
Crystal size (mm)	0.25 × 0.12 × 0.09	0.22 × 0.11 × 0.08
Data collection		
Diffractometer	Bruker APEXII	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.476, 0.610	0.491, 0.631
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17578, 4732, 4576	12896, 2256, 2221
R_{int}	0.051	0.055
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.585	0.585
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.139, 1.11	0.050, 0.138, 1.12
No. of reflections	4732	2256
No. of parameters	442	203
No. of restraints	1	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.71, −1.11	1.10, −1.69

Computer programs: *APEX2*, *SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2008).

freely. The carbon-bound H atoms were positioned with idealized geometry and refined using a riding model with C—H = 0.95 Å, and with $U_{iso} = 1.2U_{eq}$(parent atom).

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References

Banwell, M. G., Crasto, C. F., Easton, C. J., Forrest, A. K., Karoli, T., March, D. R., Mensah, L., Nairn, M. R., O'Hanlon, P. J., Oldham, M. D. & Yue, W. (2000). *Bioorg. Med. Chem. Lett.* **10**, 2263–2266.
Bruker (2009). *APEX2*, *SADABS*, *SAINT-Plus* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chang, L. L., Ashton, W. T., Flanagan, K. L., Chen, T. B., O'Malley, S. S., Zingaro, G. J., Siegl, P. K. S., Kivlighn, S. D., Lotti, V. J., Chang, R. S. L. & Greenlee, W. J. (1994). *J. Med. Chem.* **37**, 4464–4478.
Gowda, B. T., Foro, S., Suchetan, P. A. & Fuess, H. (2009). *Acta Cryst.* E**65**, o2516.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hasegawa, T. & Yamamoto, H. (2000). *Bull. Chem. Soc. Jpn*, **73**, 423–428.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Mader, M., Shih, C., Considine, E., De Dios, A., Grossman, C., Hipskind, P., Lin, H., Lobb, K., Lopez, B., Lopez, J., Cabrejas, L., Richett, M., White, W., Cheung, Y., Huang, Z., Reilly, J. & Dinn, S. (2005). *Bioorg. Med. Chem. Lett.* **15**, 617–620.
Musser, J. H., Kreft, A. F., Bender, R. H. W., Kubrak, D. M., Grimes, D., Carlson, R. P., Hand, J. M. & Chang, J. (1990). *J. Med. Chem.* **33**, 240–245.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Suchetan, P. A., Foro, S. & Gowda, B. T. (2012*a*). *Acta Cryst.* E**68**, o572.
Suchetan, P. A., Foro, S. & Gowda, B. T. (2012*b*). *Acta Cryst.* E**68**, o888.

supporting information

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Crystal structures of isomeric 4-bromo-*N*-[(2-nitrophenyl)sulfonyl]benzamide and 4-bromo-*N*-[(4-nitrophenyl)sulfonyl]benzamide

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Computing details

For both compounds, data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2016* (Sheldrick, 2015b).

(I) 4-Bromo-*N*-[(2-nitrophenyl)sulfonyl]benzamide

Crystal data

$C_{13}H_9BrN_2O_5S$
M_r = 385.19
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.0209 (3) Å
b = 14.5364 (5) Å
c = 25.0008 (8) Å
β = 98.499 (1)°
V = 2882.96 (17) Å^3
Z = 8
F(000) = 1536

Prism
D_x = 1.775 Mg m^{-3}
Melting point: 486 K
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 173 reflections
θ = 4.7–64.4°
μ = 5.50 mm^{-1}
T = 173 K
Prism, colourless
0.25 × 0.12 × 0.09 mm

Data collection

Bruker APEXII diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.476, T_{max} = 0.610
17578 measured reflections

4732 independent reflections
4576 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 64.4°, θ_{min} = 4.7°
h = −7→9
k = −16→16
l = −28→29
1 standard reflections every 1 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.139
S = 1.11
4732 reflections
442 parameters

1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2 + 3.8108P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -1.11$ 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)
BR2	1.02710 (5)	0.34737 (3)	0.05488 (2)	0.02901 (17)	
BR1	0.79778 (5)	0.67350 (3)	0.56143 (2)	0.03300 (18)	
S1	0.70457 (10)	0.15258 (5)	0.40128 (3)	0.0150 (2)	
S2	0.41557 (9)	0.38557 (5)	0.30456 (3)	0.0131 (2)	
O3	0.8626 (3)	0.21365 (18)	0.50821 (9)	0.0203 (5)	
O1	0.6105 (3)	0.16337 (17)	0.34822 (9)	0.0191 (5)	
O4	0.8579 (3)	0.29764 (17)	0.32525 (9)	0.0215 (5)	
O6	0.5231 (3)	0.38082 (18)	0.35563 (9)	0.0210 (5)	
O8	0.3425 (3)	0.40157 (18)	0.18734 (9)	0.0193 (5)	
O2	0.6549 (3)	0.08544 (17)	0.43717 (10)	0.0211 (5)	
O7	0.2785 (3)	0.32341 (17)	0.29277 (10)	0.0213 (5)	
N1	0.7047 (3)	0.2553 (2)	0.42926 (11)	0.0156 (6)	
N2	0.9067 (4)	0.2238 (2)	0.31015 (11)	0.0203 (6)	
O5	0.8932 (4)	0.2001 (2)	0.26277 (11)	0.0439 (8)	
N3	0.5424 (4)	0.3737 (2)	0.25907 (11)	0.0163 (6)	
O9	0.6914 (4)	0.5303 (3)	0.31353 (14)	0.0466 (8)	
C7	0.7894 (4)	0.2739 (2)	0.48080 (12)	0.0151 (7)	
C8	0.7857 (4)	0.3714 (3)	0.49883 (14)	0.0196 (7)	
C6	1.0096 (4)	0.0750 (2)	0.43391 (14)	0.0198 (7)	
H6	0.959542	0.053680	0.463750	0.024*	
C14	0.3326 (4)	0.4980 (2)	0.29766 (12)	0.0169 (7)	
C4	1.2453 (4)	0.0791 (3)	0.38479 (15)	0.0228 (8)	
H4	1.356869	0.060691	0.381307	0.027*	
C2	0.9934 (4)	0.1604 (2)	0.35111 (14)	0.0166 (7)	
C20	0.4900 (4)	0.3876 (2)	0.20422 (12)	0.0128 (6)	
C21	0.6240 (4)	0.3802 (2)	0.16921 (12)	0.0130 (6)	
N4	0.6001 (5)	0.5792 (3)	0.33590 (15)	0.0423 (10)	
C23	0.9132 (4)	0.3909 (3)	0.15395 (13)	0.0192 (7)	
H23	1.028007	0.404991	0.166430	0.023*	
C3	1.1560 (4)	0.1341 (2)	0.34542 (15)	0.0200 (7)	
H3	1.205261	0.153578	0.315019	0.024*	
C1	0.9180 (4)	0.1309 (2)	0.39488 (13)	0.0152 (7)	
C26	0.5760 (4)	0.3523 (2)	0.11605 (14)	0.0175 (7)	
H26	0.460520	0.340667	0.103073	0.021*	
C5	1.1745 (4)	0.0505 (3)	0.42912 (15)	0.0250 (8)	
H5	1.238345	0.014104	0.456339	0.030*	

C25	0.6958 (4)	0.3415 (2)	0.08176 (14)	0.0192 (7)	
H25	0.663981	0.320850	0.045635	0.023*	
C11	0.7929 (5)	0.5504 (3)	0.53672 (15)	0.0244 (8)	
O10	0.6496 (7)	0.6324 (3)	0.37231 (18)	0.0834 (15)	
C24	0.8631 (4)	0.3613 (2)	0.10135 (13)	0.0167 (7)	
C22	0.7935 (4)	0.3995 (3)	0.18771 (13)	0.0184 (7)	
H22	0.826368	0.418684	0.224058	0.022*	
C19	0.1607 (5)	0.5033 (3)	0.27804 (14)	0.0306 (9)	
H19	0.100878	0.449361	0.265210	0.037*	
C15	0.4186 (5)	0.5781 (3)	0.31678 (14)	0.0276 (8)	
C18	0.0767 (6)	0.5865 (4)	0.27715 (19)	0.0471 (13)	
H18	−0.039147	0.590113	0.262314	0.057*	
C16	0.3325 (9)	0.6615 (3)	0.31749 (19)	0.0496 (14)	
H16	0.389190	0.715932	0.331171	0.059*	
C17	0.1592 (8)	0.6624 (4)	0.2973 (2)	0.0573 (16)	
H17	0.098513	0.718418	0.297889	0.069*	
C13A	0.6630 (9)	0.4334 (5)	0.4788 (3)	0.024 (2)	0.525 (9)
H13A	0.575449	0.414218	0.451220	0.029*	0.525 (9)
C12A	0.6632 (10)	0.5234 (5)	0.4975 (3)	0.027 (2)	0.525 (9)
H12A	0.576235	0.565144	0.483732	0.032*	0.525 (9)
C13B	0.7728 (9)	0.4457 (5)	0.4604 (3)	0.0176 (19)	0.475 (9)
H13B	0.761456	0.433511	0.422743	0.021*	0.475 (9)
C12B	0.7772 (10)	0.5349 (6)	0.4794 (3)	0.024 (2)	0.475 (9)
H12B	0.770006	0.585306	0.454956	0.028*	0.475 (9)
C9A	0.9060 (13)	0.3985 (6)	0.5443 (3)	0.0228 (18)	0.525 (9)
H9A	0.983879	0.354712	0.561645	0.027*	0.525 (9)
C10A	0.9092 (13)	0.4875 (6)	0.5630 (3)	0.0252 (18)	0.525 (9)
H10A	0.988688	0.505882	0.593063	0.030*	0.525 (9)
C9B	0.8136 (15)	0.3881 (6)	0.5514 (3)	0.021 (2)	0.475 (9)
H9B	0.829992	0.338396	0.576281	0.025*	0.475 (9)
C10B	0.8190 (15)	0.4782 (6)	0.5704 (3)	0.023 (2)	0.475 (9)
H10B	0.841876	0.488856	0.608251	0.028*	0.475 (9)
HN1	0.657 (5)	0.295 (3)	0.4102 (17)	0.015 (10)*	
HN3	0.644 (7)	0.368 (3)	0.269 (2)	0.033 (12)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
BR2	0.0266 (3)	0.0357 (3)	0.0287 (3)	−0.00689 (15)	0.01712 (18)	−0.00913 (16)
BR1	0.0396 (3)	0.0287 (3)	0.0335 (3)	−0.01070 (17)	0.0147 (2)	−0.01360 (17)
S1	0.0117 (4)	0.0179 (5)	0.0157 (4)	0.0002 (3)	0.0030 (3)	0.0000 (3)
S2	0.0154 (4)	0.0140 (4)	0.0103 (4)	0.0014 (3)	0.0038 (3)	0.0012 (3)
O3	0.0218 (12)	0.0248 (14)	0.0140 (11)	0.0039 (10)	0.0020 (9)	0.0044 (10)
O1	0.0147 (11)	0.0253 (14)	0.0167 (12)	−0.0002 (9)	−0.0004 (9)	−0.0034 (9)
O4	0.0236 (12)	0.0209 (13)	0.0208 (12)	0.0031 (10)	0.0056 (9)	0.0024 (10)
O6	0.0236 (12)	0.0283 (14)	0.0114 (11)	0.0079 (10)	0.0035 (9)	0.0024 (10)
O8	0.0143 (12)	0.0288 (14)	0.0145 (11)	0.0032 (10)	0.0016 (9)	0.0018 (10)
O2	0.0173 (11)	0.0202 (13)	0.0271 (12)	−0.0020 (10)	0.0071 (9)	0.0032 (10)

O7	0.0247 (13)	0.0206 (13)	0.0205 (12)	−0.0071 (10)	0.0102 (10)	−0.0026 (10)
N1	0.0153 (13)	0.0183 (16)	0.0127 (12)	0.0049 (11)	0.0006 (10)	0.0028 (12)
N2	0.0232 (14)	0.0242 (17)	0.0150 (14)	0.0038 (12)	0.0075 (11)	−0.0001 (12)
O5	0.068 (2)	0.052 (2)	0.0121 (13)	0.0184 (17)	0.0063 (13)	−0.0014 (13)
N3	0.0121 (14)	0.0244 (16)	0.0131 (13)	0.0035 (11)	0.0040 (11)	0.0011 (11)
O9	0.0339 (16)	0.057 (2)	0.0490 (18)	−0.0216 (15)	0.0066 (14)	−0.0042 (17)
C7	0.0127 (14)	0.0231 (19)	0.0107 (14)	0.0001 (13)	0.0059 (12)	0.0010 (13)
C8	0.0151 (16)	0.026 (2)	0.0182 (17)	−0.0020 (14)	0.0048 (13)	−0.0019 (14)
C6	0.0222 (17)	0.0181 (18)	0.0196 (16)	0.0022 (14)	0.0044 (13)	0.0023 (13)
C14	0.0260 (17)	0.0148 (17)	0.0114 (14)	0.0053 (14)	0.0076 (12)	0.0016 (12)
C4	0.0116 (15)	0.0192 (18)	0.038 (2)	0.0015 (13)	0.0051 (14)	−0.0056 (15)
C2	0.0201 (17)	0.0133 (17)	0.0165 (16)	0.0004 (12)	0.0031 (13)	−0.0016 (12)
C20	0.0161 (16)	0.0102 (16)	0.0121 (14)	−0.0022 (12)	0.0020 (12)	−0.0001 (12)
C21	0.0123 (15)	0.0134 (16)	0.0134 (15)	0.0012 (12)	0.0023 (12)	0.0023 (12)
N4	0.057 (2)	0.037 (2)	0.0328 (19)	−0.029 (2)	0.0070 (17)	−0.0033 (17)
C23	0.0127 (15)	0.027 (2)	0.0179 (16)	−0.0034 (13)	0.0009 (12)	0.0004 (14)
C3	0.0186 (17)	0.0149 (17)	0.0284 (18)	−0.0035 (13)	0.0095 (14)	−0.0037 (14)
C1	0.0138 (15)	0.0138 (16)	0.0177 (16)	0.0016 (12)	0.0019 (12)	−0.0041 (13)
C26	0.0150 (16)	0.0211 (18)	0.0167 (16)	−0.0027 (13)	0.0031 (13)	0.0005 (13)
C5	0.0194 (17)	0.023 (2)	0.0307 (19)	0.0047 (14)	−0.0025 (14)	−0.0016 (15)
C25	0.0204 (17)	0.0231 (19)	0.0141 (16)	−0.0011 (13)	0.0026 (13)	−0.0043 (13)
C11	0.0251 (18)	0.026 (2)	0.0238 (18)	−0.0066 (15)	0.0079 (14)	−0.0058 (15)
O10	0.109 (4)	0.070 (3)	0.066 (3)	−0.047 (3)	−0.003 (3)	−0.036 (2)
C24	0.0186 (16)	0.0166 (17)	0.0171 (16)	−0.0005 (13)	0.0104 (13)	0.0008 (13)
C22	0.0168 (16)	0.0242 (19)	0.0137 (15)	−0.0028 (13)	0.0010 (12)	−0.0014 (13)
C19	0.0278 (19)	0.045 (3)	0.0198 (17)	0.0165 (18)	0.0051 (14)	0.0047 (17)
C15	0.051 (2)	0.0180 (19)	0.0166 (16)	−0.0036 (17)	0.0132 (16)	0.0021 (14)
C18	0.050 (3)	0.051 (3)	0.043 (2)	0.035 (3)	0.016 (2)	0.015 (2)
C16	0.108 (4)	0.014 (2)	0.034 (2)	−0.004 (2)	0.034 (3)	−0.0019 (17)
C17	0.085 (4)	0.041 (3)	0.054 (3)	0.042 (3)	0.035 (3)	0.023 (2)
C13A	0.027 (4)	0.025 (4)	0.018 (3)	0.002 (3)	−0.003 (3)	−0.009 (3)
C12A	0.038 (5)	0.025 (4)	0.016 (3)	0.005 (3)	0.004 (3)	−0.004 (3)
C13B	0.020 (4)	0.021 (4)	0.013 (3)	0.000 (3)	0.005 (3)	0.001 (3)
C12B	0.023 (4)	0.023 (4)	0.024 (4)	−0.005 (3)	0.001 (3)	−0.001 (3)
C9A	0.018 (4)	0.035 (5)	0.016 (3)	−0.005 (3)	0.002 (3)	−0.001 (3)
C10A	0.018 (4)	0.040 (5)	0.018 (4)	−0.009 (4)	0.003 (3)	−0.004 (3)
C9B	0.032 (6)	0.021 (4)	0.011 (4)	−0.001 (4)	0.007 (4)	−0.005 (3)
C10B	0.033 (6)	0.025 (5)	0.013 (4)	−0.004 (4)	0.009 (4)	−0.008 (3)

Geometric parameters (Å, º)

BR2—C24	1.890 (3)	C4—C3	1.383 (5)
BR1—C11	1.892 (4)	C4—H4	0.9500
S1—O2	1.422 (3)	C2—C3	1.386 (5)
S1—O1	1.434 (2)	C2—C1	1.394 (5)
S1—N1	1.649 (3)	C20—C21	1.487 (4)
S1—C1	1.771 (3)	C21—C26	1.388 (5)
S2—O7	1.420 (3)	C21—C22	1.398 (5)

S2—O6	1.433 (2)	N4—O10	1.215 (5)
S2—N3	1.643 (3)	N4—C15	1.464 (6)
S2—C14	1.764 (3)	C23—C22	1.374 (5)
O3—C7	1.210 (4)	C23—C24	1.386 (5)
O4—N2	1.221 (4)	C23—H23	0.9500
O8—C20	1.213 (4)	C3—H3	0.9500
N1—C7	1.392 (4)	C26—C25	1.388 (5)
N1—HN1	0.81 (5)	C26—H26	0.9500
N2—O5	1.223 (4)	C5—H5	0.9500
N2—C2	1.473 (4)	C25—C24	1.389 (5)
N3—C20	1.389 (4)	C25—H25	0.9500
N3—HN3	0.82 (5)	C11—C10B	1.343 (10)
O9—N4	1.214 (6)	C11—C12A	1.376 (8)
C7—C8	1.489 (5)	C11—C10A	1.398 (9)
C8—C9B	1.322 (8)	C11—C12B	1.438 (8)
C8—C13A	1.373 (8)	C22—H22	0.9500
C8—C9A	1.433 (8)	C19—C18	1.383 (6)
C8—C13B	1.438 (8)	C19—H19	0.9500
C6—C5	1.392 (5)	C15—C16	1.397 (6)
C6—C1	1.393 (5)	C18—C17	1.345 (9)
C6—H6	0.9500	C18—H18	0.9500
C14—C19	1.396 (5)	C16—C17	1.407 (9)
C14—C15	1.400 (5)	C16—H16	0.9500
C4—C5	1.382 (6)	C17—H17	0.9500

O2—S1—O1	120.04 (15)	O9—N4—O10	124.4 (5)
O2—S1—N1	109.66 (15)	O9—N4—C15	118.8 (3)
O1—S1—N1	105.10 (14)	O10—N4—C15	116.7 (5)
O2—S1—C1	107.44 (15)	C22—C23—C24	118.7 (3)
O1—S1—C1	108.61 (15)	C22—C23—H23	120.7
N1—S1—C1	105.04 (15)	C24—C23—H23	120.7
O7—S2—O6	119.98 (15)	C4—C3—C2	118.9 (3)
O7—S2—N3	109.22 (15)	C4—C3—H3	120.6
O6—S2—N3	105.01 (14)	C2—C3—H3	120.6
O7—S2—C14	107.45 (16)	C6—C1—C2	119.0 (3)
O6—S2—C14	107.49 (15)	C6—C1—S1	117.2 (3)
N3—S2—C14	107.05 (15)	C2—C1—S1	123.6 (3)
C7—N1—S1	122.6 (2)	C21—C26—C25	120.3 (3)
C7—N1—HN1	122 (3)	C21—C26—H26	119.8
S1—N1—HN1	115 (3)	C25—C26—H26	119.8
O4—N2—O5	124.1 (3)	C4—C5—C6	120.0 (3)
O4—N2—C2	118.3 (3)	C4—C5—H5	120.0
O5—N2—C2	117.5 (3)	C6—C5—H5	120.0
C20—N3—S2	122.7 (2)	C26—C25—C24	118.7 (3)
C20—N3—HN3	117 (3)	C26—C25—H25	120.7
S2—N3—HN3	119 (3)	C24—C25—H25	120.7
O3—C7—N1	120.9 (3)	C23—C24—C25	121.9 (3)
O3—C7—C8	123.2 (3)	C23—C24—BR2	119.1 (3)

N1—C7—C8	115.9 (3)	C25—C24—BR2	119.0 (3)
C5—C6—C1	119.9 (3)	C23—C22—C21	120.8 (3)
C5—C6—H6	120.0	C23—C22—H22	119.6
C1—C6—H6	120.0	C21—C22—H22	119.6
C19—C14—C15	119.1 (4)	C18—C19—C14	120.5 (5)
C19—C14—S2	115.1 (3)	C18—C19—H19	119.8
C15—C14—S2	125.2 (3)	C14—C19—H19	119.8
C5—C4—C3	120.9 (3)	C16—C15—C14	120.4 (4)
C5—C4—H4	119.6	C16—C15—N4	117.1 (4)
C3—C4—H4	119.6	C14—C15—N4	122.4 (4)
C3—C2—C1	121.3 (3)	C17—C18—C19	120.0 (5)
C3—C2—N2	117.1 (3)	C17—C18—H18	120.0
C1—C2—N2	121.5 (3)	C19—C18—H18	120.0
O8—C20—N3	120.4 (3)	C15—C16—C17	117.8 (5)
O8—C20—C21	124.0 (3)	C15—C16—H16	121.1
N3—C20—C21	115.5 (3)	C17—C16—H16	121.1
C26—C21—C22	119.6 (3)	C18—C17—C16	122.2 (4)
C26—C21—C20	117.5 (3)	C18—C17—H17	118.9
C22—C21—C20	122.9 (3)	C16—C17—H17	118.9

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the bromobenzene ring of molecule *A* and nitrobenzene ring of molecule *B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O6	0.81 (4)	2.03 (4)	2.837 (4)	172 (5)
N3—H*N*3···O4	0.82 (6)	2.29 (5)	3.021 (4)	148 (4)
C13*A*—H13*A*···O6	0.95	2.41	3.210 (8)	141
C23—H23···O8^{i}	0.95	2.50	3.425 (4)	165
C25—H25···O3^{ii}	0.95	2.51	3.117 (4)	122
C26—H26···O3^{ii}	0.95	2.51	3.123 (4)	122
C12*A*—H12*A*···*Cg*1^{iii}	0.95	2.99	3.635 (9)	126
C10*B*—H10*B*···*Cg*2^{iii}	0.95	2.76	3.532 (8)	139

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

(II) 4-Bromo-*N*-[(4-nitrophenyl)sulfonyl]benzamide

Crystal data

$C_{13}H_9BrN_2O_5S$
M_r = 385.19
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 9.6085 (4) Å
b = 10.3246 (5) Å
c = 27.7296 (13) Å
V = 2750.9 (2) Å^3
Z = 8
F(000) = 1536

Prism
D_x = 1.860 Mg m^{-3}
Melting point: 498 K
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 195 reflections
θ = 3.2–64.4°
μ = 5.76 mm^{-1}
T = 173 K
Prism, colourless
0.22 × 0.11 × 0.08 mm

Data collection

Bruker APEXII diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
phi and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.491, T_{max} = 0.631
12896 measured reflections
2256 independent reflections
2221 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 64.4°, θ_{min} = 3.2°
h = −10→11
k = −9→11
l = −30→32
1 standard reflections every 1 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.138
S = 1.12
2256 reflections
203 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 3.3998P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.10 e Å^{-3}
$\Delta\rho_{min}$ = −1.69 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}
BR1	0.84255 (4)	0.07764 (3)	0.93310 (2)	0.0173 (2)
S1	0.64837 (8)	0.55824 (8)	0.68971 (3)	0.0106 (3)
O3	0.9065 (2)	0.41915 (19)	0.72287 (8)	0.0121 (5)
O1	0.7620 (2)	0.6467 (2)	0.68874 (7)	0.0150 (5)
O2	0.5095 (2)	0.6044 (2)	0.69698 (8)	0.0142 (5)
O4	0.5406 (3)	0.2713 (3)	0.47917 (8)	0.0329 (7)
O5	0.7105 (3)	0.1538 (3)	0.50614 (9)	0.0336 (7)
N1	0.6740 (3)	0.4527 (3)	0.73423 (10)	0.0109 (6)
N2	0.6290 (3)	0.2439 (3)	0.50936 (10)	0.0226 (7)
C8	0.8049 (3)	0.3267 (3)	0.79323 (11)	0.0118 (6)
C9	0.9167 (3)	0.2414 (3)	0.79975 (11)	0.0123 (6)
H9	0.985687	0.233663	0.775389	0.015*
C13	0.7045 (3)	0.3383 (3)	0.82959 (11)	0.0120 (6)
H13	0.628340	0.395897	0.825434	0.014*
C10	0.9273 (3)	0.1686 (3)	0.84136 (11)	0.0145 (6)
H10	1.002921	0.110502	0.845651	0.017*
C12	0.7156 (3)	0.2662 (3)	0.87166 (11)	0.0138 (7)
H12	0.648375	0.274796	0.896577	0.017*
C5	0.5224 (4)	0.4010 (4)	0.56487 (11)	0.0175 (8)
H5	0.442958	0.404706	0.544537	0.021*
C4	0.6369 (3)	0.3257 (3)	0.55290 (12)	0.0161 (7)

C7	0.8014 (3)	0.4021 (3)	0.74789 (12)	0.0123 (7)
C6	0.5281 (3)	0.4704 (3)	0.60744 (11)	0.0156 (7)
H6	0.450494	0.520542	0.617544	0.019*
C11	0.8268 (3)	0.1812 (3)	0.87667 (11)	0.0133 (7)
C3	0.7578 (3)	0.3213 (3)	0.58033 (13)	0.0190 (7)
H3	0.834325	0.269078	0.570736	0.023*
C2	0.7638 (4)	0.3946 (3)	0.62190 (11)	0.0172 (7)
H2	0.845796	0.395971	0.641024	0.021*
C1	0.6477 (3)	0.4665 (3)	0.63527 (11)	0.0117 (7)
HN1	0.593 (4)	0.430 (3)	0.7485 (14)	0.015 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
BR1	0.0194 (3)	0.0203 (3)	0.0123 (3)	0.00086 (11)	−0.00126 (11)	0.00536 (11)
S1	0.0107 (5)	0.0135 (5)	0.0076 (5)	0.0010 (3)	−0.0005 (2)	0.0001 (3)
O3	0.0074 (12)	0.0210 (12)	0.0079 (11)	0.0002 (8)	0.0015 (9)	−0.0005 (7)
O1	0.0172 (12)	0.0143 (11)	0.0135 (11)	−0.0032 (9)	0.0000 (8)	0.0010 (8)
O2	0.0115 (12)	0.0186 (11)	0.0125 (10)	0.0044 (9)	−0.0009 (9)	0.0006 (9)
O4	0.0218 (13)	0.0647 (19)	0.0121 (12)	−0.0082 (13)	−0.0032 (10)	−0.0123 (12)
O5	0.0352 (16)	0.0397 (16)	0.0258 (14)	0.0004 (13)	0.0069 (12)	−0.0200 (12)
N1	0.0080 (13)	0.0162 (13)	0.0085 (13)	−0.0009 (10)	0.0008 (10)	0.0037 (11)
N2	0.0187 (14)	0.0352 (17)	0.0139 (15)	−0.0089 (14)	0.0035 (12)	−0.0089 (13)
C8	0.0087 (15)	0.0155 (16)	0.0112 (15)	−0.0021 (12)	−0.0004 (12)	−0.0020 (12)
C9	0.0103 (14)	0.0161 (15)	0.0105 (14)	−0.0016 (12)	0.0014 (12)	−0.0030 (11)
C13	0.0086 (15)	0.0159 (16)	0.0115 (15)	−0.0004 (12)	−0.0005 (12)	−0.0010 (12)
C10	0.0120 (15)	0.0148 (15)	0.0168 (15)	0.0001 (12)	−0.0025 (12)	0.0002 (12)
C12	0.0126 (16)	0.0181 (16)	0.0107 (15)	−0.0023 (12)	0.0012 (12)	0.0019 (12)
C5	0.0145 (18)	0.0268 (19)	0.0112 (17)	−0.0059 (14)	−0.0010 (12)	0.0017 (12)
C4	0.0188 (16)	0.0234 (17)	0.0062 (14)	−0.0050 (13)	0.0020 (12)	−0.0016 (14)
C7	0.0097 (15)	0.0151 (16)	0.0121 (15)	−0.0019 (12)	−0.0016 (13)	−0.0043 (12)
C6	0.0134 (15)	0.0188 (16)	0.0146 (15)	−0.0002 (12)	0.0002 (12)	0.0007 (13)
C11	0.0153 (15)	0.0144 (16)	0.0102 (16)	−0.0033 (12)	−0.0029 (11)	0.0010 (12)
C3	0.0162 (17)	0.029 (2)	0.0118 (16)	0.0021 (15)	0.0044 (12)	−0.0038 (13)
C2	0.0152 (16)	0.0235 (17)	0.0130 (15)	0.0003 (13)	−0.0006 (13)	−0.0012 (13)
C1	0.0141 (16)	0.0147 (16)	0.0065 (15)	−0.0022 (11)	−0.0010 (11)	−0.0010 (13)

Geometric parameters (Å, º)

BR1—C11	1.901 (3)	C13—C12	1.388 (4)
S1—O1	1.424 (2)	C13—H13	0.9500
S1—O2	1.431 (2)	C10—C11	1.381 (4)
S1—N1	1.665 (3)	C10—H10	0.9500
S1—C1	1.782 (3)	C12—C11	1.390 (4)
O3—C7	1.238 (4)	C12—H12	0.9500
O4—N2	1.226 (4)	C5—C6	1.382 (5)
O5—N2	1.219 (4)	C5—C4	1.387 (5)
N1—C7	1.384 (4)	C5—H5	0.9500

N1—HN1	0.90 (4)	C4—C3	1.389 (5)
N2—C4	1.475 (4)	C6—C1	1.384 (4)
C8—C13	1.400 (4)	C6—H6	0.9500
C8—C9	1.400 (5)	C3—C2	1.380 (5)
C8—C7	1.479 (4)	C3—H3	0.9500
C9—C10	1.381 (4)	C2—C1	1.390 (5)
C9—H9	0.9500	C2—H2	0.9500

O1—S1—O2	120.29 (14)	C11—C12—H12	120.6
O1—S1—N1	108.68 (14)	C6—C5—C4	117.6 (3)
O2—S1—N1	104.55 (14)	C6—C5—H5	121.2
O1—S1—C1	109.13 (14)	C4—C5—H5	121.2
O2—S1—C1	107.02 (14)	C5—C4—C3	123.4 (3)
N1—S1—C1	106.33 (16)	C5—C4—N2	118.4 (3)
C7—N1—S1	125.5 (2)	C3—C4—N2	118.2 (3)
C7—N1—HN1	123 (2)	O3—C7—N1	121.0 (3)
S1—N1—HN1	112 (2)	O3—C7—C8	122.2 (3)
O5—N2—O4	124.8 (3)	N1—C7—C8	116.8 (3)
O5—N2—C4	117.6 (3)	C5—C6—C1	119.6 (3)
O4—N2—C4	117.5 (3)	C5—C6—H6	120.2
C13—C8—C9	119.3 (3)	C1—C6—H6	120.2
C13—C8—C7	123.4 (3)	C10—C11—C12	121.7 (3)
C9—C8—C7	117.3 (3)	C10—C11—BR1	118.4 (2)
C10—C9—C8	120.4 (3)	C12—C11—BR1	119.9 (2)
C10—C9—H9	119.8	C2—C3—C4	118.3 (3)
C8—C9—H9	119.8	C2—C3—H3	120.8
C12—C13—C8	120.4 (3)	C4—C3—H3	120.8
C12—C13—H13	119.8	C3—C2—C1	118.8 (3)
C8—C13—H13	119.8	C3—C2—H2	120.6
C11—C10—C9	119.3 (3)	C1—C2—H2	120.6
C11—C10—H10	120.3	C6—C1—C2	122.2 (3)
C9—C10—H10	120.3	C6—C1—S1	117.4 (2)
C13—C12—C11	118.8 (3)	C2—C1—S1	120.4 (2)
C13—C12—H12	120.6		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O3^{i}	0.90	1.97	2.8530	168
C2—H2···O3	0.95	2.36	3.1280	138
C3—H3···O4^{ii}	0.95	2.45	3.3199	152
C9—H9···O2^{iii}	0.95	2.55	3.2599	132
C10—H10···O1^{iv}	0.95	2.48	3.1081	124
C12—H12···O4^{v}	0.95	2.56	3.4445	155
C13—H13···O3^{i}	0.95	2.53	3.3182	141

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