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4-Iodo-N-(o-tolylsulfonyl)benzamide

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The title compound, $C_{14}H_{12}INO_3S$, crystallizes with two independent molecules (A and B) in the asymmetric unit. The dihedral angle between the two aryl rings is 83.1 (4)° in molecule A and 79.8 (4)° in molecule B. In the crystal, the two molecules are linked by a pair of N—H$\cdots$O hydrogen bonds, forming an A–B dimer with an $R_2^2(8)$ ring motif. The dimer is further strengthened by a pair of C—H$\cdots$O hydrogen bonds with an $R_2^2(14)$ motif. Another pair of C—H$\cdots$O interactions assembles these dimers along the diagonal of the bc plane, forming ribbons. Adjacent ribbons are connected by C—H$\cdots\pi_{aryl}$ interactions between the A molecules, and thus the overall supramolecular architecture is one-dimensional.

3D view

Chemical scheme

Structure description

Sulfonamide and amide moieties play a significant role as key constituents in a number of biologically active molecules (Mohan et al., 2013; Manojkumar et al., 2013; Hamad & Abed, 2014). In recent years, N-(arylsulfonyl)-arylamides have received much attention as they constitute an important class of drugs for Alzheimer's disease (Hasegawa & Yamamoto, 2000), 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 as potent anti-tumour agents against a broad spectrum of human tumour xenografts (colon, lung, breast, ovary and prostate) in nude mice (Mader et al., 2005). In view of the importance of N-(arylsulfonyl)-arylamides and in continuation of our work on the synthesis and crystal structures of N-(2-methylphenylsulfonyl)-arylamides (Suchetan et al., 2010a,b; Gowda et al., 2010; Suchetan et al., 2011), the title compound was synthesized and we report herein on its crystal structure.
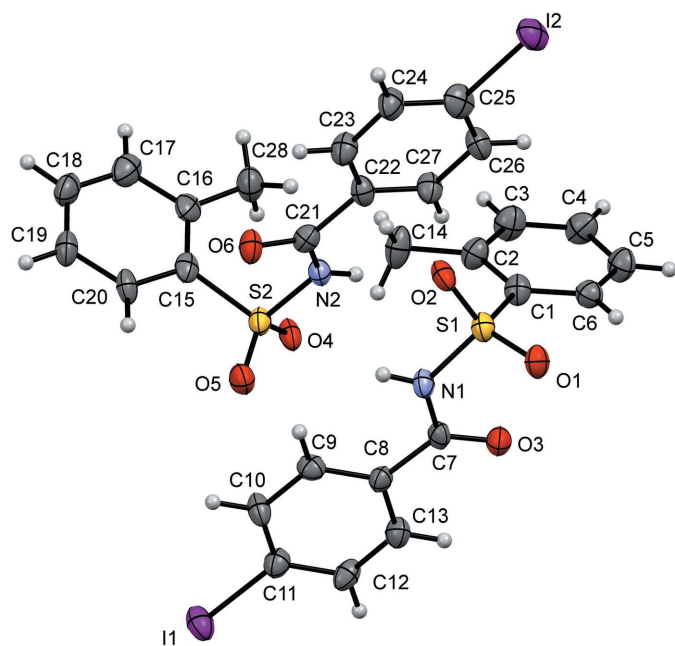
Figure 1
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

The asymmetric unit of the title compound, Fig. 1, contains two molecules [*A* (N1) and *B* N2)], similar to the situation observed for *N*-(4-chlorobenzoyl)-2-methylbenzene-sulfonamide (Suchetan *et al.*, 2010*b*) and *N*-(4-methylbenzo-yl)-2-methylbenzenesulfonamide (Gowda *et al.*, 2010). However, in the crystal structures of *N*-(benzoyl)-2-methyl-benzenesulfonamide (Suchetan *et al.*, 2010*a*) and *N*-(4-nitro-benzoyl)-2-methylbenzenesulfonamide (Suchetan *et al.*, 2011), there is only one molecule in the asymmetric unit. The dihe-dral angles between the two aryl rings are 83.1 (4) and 79.8 (4)° in molecules *A* and *B*, respectively, while the corre-
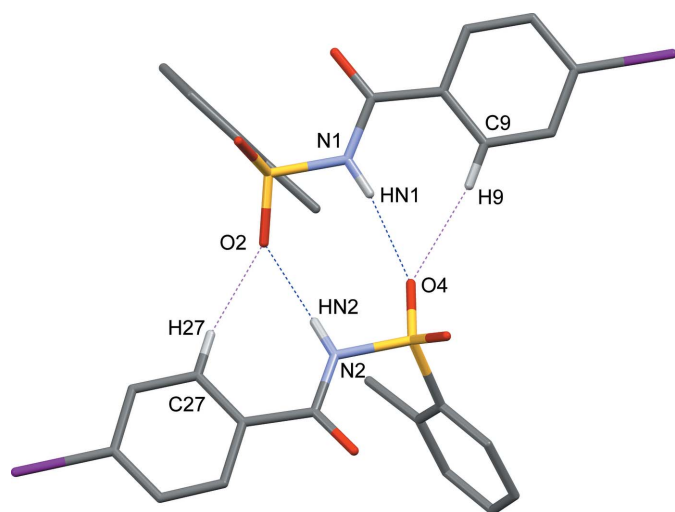
Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the iodobenzene ring (C8–C13) of molecule *A*

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1$\cdots$O4^{i}	0.88	2.06	2.900 (10)	158
N2—H2$\cdots$O2^{i}	0.88	2.12	2.970 (10)	161
C9—H9$\cdots$O4^{i}	0.95	2.36	3.301 (10)	170
C13—H13$\cdots$O6^{ii}	0.95	2.56	3.378 (11)	144
C23—H23$\cdots$O3^{ii}	0.95	2.40	3.201 (11)	142
C27—H27$\cdots$O2^{i}	0.95	2.51	3.428 (9)	163
C4—H4$\cdots$Cg^{iii}	0.93	2.81	3.656 (11)	151

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y, -z$; (iii) $-x+1, -y+2, -z+2$.

sponding angle is 73.9 (1)° in *N*-(benzoyl)-2-methylbenzene-sulfonamide, 89.4 (1) and 82.4 (1)° in the two molecules of *N*-(4-chlorobenzoyl)-2-methylbenzenesulfonamide, 88.1 (1) and 83.5 (1)° in the two molecules of *N*-(4-methylbenzoyl)-2-methylbenzenesulfonamide, and 83.8 (2)° in *N*-(4-nitrobenzo-yl)-2-methylbenzenesulfonamide. In both molecules of the title compound, the *ortho*-methyl substituent is *syn* to N—H bond in the central –C—SO₂—N(H)—C(O)– segment, similar to that observed in all the reported structures, the only exception being *N*-(4-methylbenzene)-2-methylbenzene-sulfonamide, where the conformation is *anti*.

The crystal structure, features two N—H$\cdots$O hydrogen bonds, namely, N1—H1$\cdots$O4^{i} and N2—H2$\cdots$O2^{i} (Table 1), linking the *A* and *B* molecules and resulting in an $R_2^2(8)$ dimer. This arrangement is further strengthened by C9—H9$\cdots$O4^{i} and C27—H27$\cdots$O2^{i} hydrogen bonds (Table 1), with an $R_2^2(14)$ ring motif (Fig. 2). Further, another pair of C—H$\cdots$O interactions, C13—H13$\cdots$O6^{ii} and C23—H23$\cdots$O3^{ii}, assemble these dimers along the diagonal of the *bc* plane forming ribbons (Fig. 3, Table 1). Adjacent ribbons are connected by C4—H4$\cdots\pi_{\text{aryl}}$ (the π-electron system of the iodobenzene ring of molecule *A*) interactions between the *A* molecules (Fig. 4, Table 1). Thus, the overall supramolecular architecture is one-dimensional. In the structures mentioned above, the assembly of molecules is only due to the N—H$\cdots$O

Figure 2
A view of the $R_2^2(8)$ and $R_2^2(14)$ dimeric patterns displayed in the crystal structure of the title compound, resulting from N—H$\cdots$O hydrogen bonds and C—H$\cdots$O interactions, respectively (dashed lines, see Table 1).
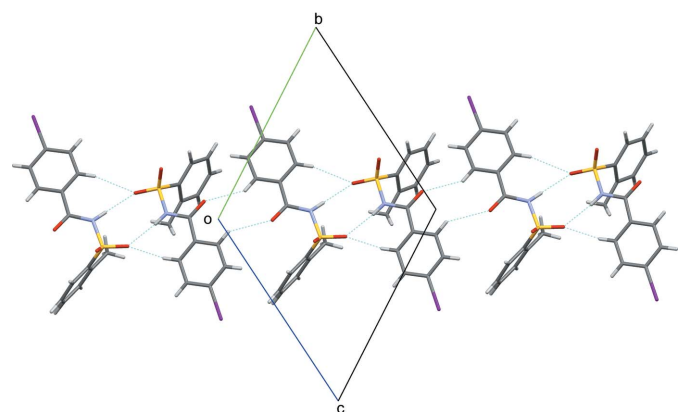

Figure 3
Generation of the ribbons *via* C—H$\cdots$O intermolecular interactions (dashed lines, see Table 1).
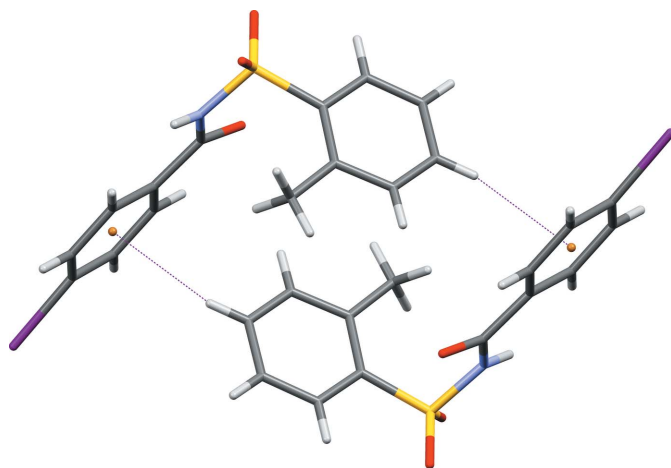
Figure 4
A view of the C—H···π_{aryl} interactions observed in the crystal structure of the title compound (dashed lines, see Table 1).

hydrogen-bonded $R_2^2(8)$ rings or $C(4)$ chains that result in either zero- or one-dimensional architectures.

Synthesis and crystallization

The title compound was prepared by refluxing a mixture of 4-iodobenzoic acid, 2-methylbenzenesulfonamide and phosphorousoxychloride for 3 h on a water bath. The resultant mixture was cooled and poured into ice-cold water. The solid obtained was filtered, washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. It was then filtered, dried and recrystallized from methanol (m.p. 450 K). Colourless prismatic crystals were obtained by slow evaporation of a solution of the title compound in methanol (with a few drops of water).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{12}INO_3S$
M_r	401.21
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	173
a, b, c (Å)	11.0543 (10), 12.1612 (10), 12.3464 (10)
α, β, γ (°)	119.140 (4), 94.668 (5), 93.182 (5)
V (Å^3)	1436.2 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	18.94
Crystal size (mm)	$0.25 \times 0.12 \times 0.07$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.124, 0.266
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17365, 4724, 3621
R_{int}	0.092
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.585
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.182, 1.05
No. of reflections	4724
No. of parameters	363
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	1.40, −1.39

Computer programs: *APEX2, SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXT2016* (Sheldrick, 2015a), *SHELXL2016* (Sheldrick, 2015b) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

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Crystal data

$C_{14}H_{12}INO_3S$
$M_r = 401.21$
Triclinic, $P\bar{1}$
$a = 11.0543\,(10)$ Å
$b = 12.1612\,(10)$ Å
$c = 12.3464\,(10)$ Å
$\alpha = 119.140\,(4)°$
$\beta = 94.668\,(5)°$
$\gamma = 93.182\,(5)°$
$V = 1436.2\,(2)$ Å^3
$Z = 4$

$F(000) = 784$
$D_x = 1.855$ Mg m^{-3}
Melting point: 450 K
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 133 reflections
$\theta = 4.0–64.4°$
$\mu = 18.94$ mm^{-1}
$T = 173$ K
Prism, colourless
$0.25 \times 0.12 \times 0.07$ mm

Data collection

Bruker APEXII CCD
    diffractometer
Radiation source: sealed X-ray tube
ω and φ scans
Absorption correction: multi-scan
    (SADABS; Bruker, 2009)
$T_{min} = 0.124$, $T_{max} = 0.266$
17365 measured reflections

4724 independent reflections
3621 reflections with $I > 2\sigma(I)$
$R_{int} = 0.092$
$\theta_{max} = 64.4°$, $\theta_{min} = 5.4°$
$h = -12 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.182$
$S = 1.05$
4724 reflections
363 parameters
0 restraints

Secondary atom site location: difference Fourier
    map
Hydrogen site location: inferred from
    neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.113P)^2]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.40$ e Å^{-3}
$\Delta\rho_{min} = -1.39$ 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	$U_{iso}*/U_{eq}$
I1	0.99795 (6)	0.28147 (5)	−0.25297 (5)	0.0394 (2)
S1	0.7516 (2)	0.17454 (18)	0.35284 (17)	0.0273 (5)
O1	0.8316 (6)	0.1073 (5)	0.3869 (5)	0.0318 (13)
O2	0.7190 (6)	0.2922 (5)	0.4501 (5)	0.0321 (14)
O3	0.8181 (6)	0.0118 (5)	0.1084 (5)	0.0330 (14)
N1	0.8113 (7)	0.2141 (6)	0.2560 (6)	0.0269 (15)
H1	0.827821	0.294813	0.279541	0.032*
C1	0.6178 (8)	0.0717 (7)	0.2660 (7)	0.0297 (19)
C2	0.5212 (9)	0.1108 (8)	0.2142 (8)	0.033 (2)
C3	0.4173 (10)	0.0220 (9)	0.1534 (9)	0.042 (2)
H3	0.350362	0.043818	0.117099	0.051*
C4	0.4096 (9)	−0.0963 (8)	0.1449 (9)	0.039 (2)
H4	0.337588	−0.153414	0.103983	0.047*
C5	0.5066 (9)	−0.1317 (8)	0.1958 (8)	0.038 (2)
H5	0.502342	−0.213616	0.187899	0.045*
C6	0.6086 (8)	−0.0465 (7)	0.2577 (7)	0.0304 (19)
H6	0.673931	−0.068811	0.295485	0.036*
C7	0.8359 (8)	0.1234 (7)	0.1386 (7)	0.0256 (18)
C8	0.8786 (8)	0.1684 (7)	0.0545 (7)	0.0258 (17)
C9	0.8854 (8)	0.2944 (8)	0.0827 (7)	0.0289 (19)
H9	0.865884	0.357746	0.161014	0.035*
C10	0.9214 (9)	0.3274 (8)	−0.0055 (7)	0.032 (2)
H10	0.926372	0.413321	0.013469	0.039*
C11	0.9497 (9)	0.2338 (8)	−0.1213 (7)	0.0316 (19)
C12	0.9445 (8)	0.1084 (8)	−0.1473 (7)	0.0310 (19)
H12	0.965631	0.044622	−0.224612	0.037*
C13	0.9083 (8)	0.0768 (8)	−0.0598 (7)	0.0314 (19)
H13	0.903828	−0.009000	−0.078578	0.038*
C14	0.5249 (10)	0.2348 (9)	0.2182 (9)	0.044 (2)
H14A	0.446169	0.241537	0.180359	0.066*
H14B	0.589802	0.241554	0.171524	0.066*
H14C	0.541018	0.303192	0.305187	0.066*
I2	0.35056 (6)	0.47630 (6)	−0.11241 (5)	0.0407 (2)
S2	0.1444 (2)	0.40351 (17)	0.52510 (17)	0.0275 (5)
O4	0.1960 (6)	0.5154 (5)	0.6401 (5)	0.0320 (14)
O5	0.0172 (6)	0.3659 (5)	0.5076 (5)	0.0355 (14)
O6	0.1204 (6)	0.2389 (5)	0.2576 (5)	0.0338 (14)
N2	0.1819 (6)	0.4363 (6)	0.4157 (6)	0.0268 (15)
H2	0.212606	0.513728	0.437907	0.032*
C15	0.2244 (9)	0.2757 (7)	0.5050 (6)	0.0288 (19)
C16	0.3543 (9)	0.2878 (8)	0.5247 (7)	0.034 (2)
C17	0.4071 (10)	0.1809 (9)	0.5084 (8)	0.041 (2)
H17	0.493510	0.185113	0.521427	0.049*
C18	0.3371 (10)	0.0675 (9)	0.4733 (8)	0.041 (2)
H18	0.376524	−0.004767	0.459878	0.049*

C19	0.2115 (9)	0.0583 (8)	0.4578 (7)	0.035 (2)
H19	0.164404	−0.018055	0.438802	0.042*
C20	0.1550 (9)	0.1618 (7)	0.4703 (7)	0.032 (2)
H20	0.068594	0.155170	0.455117	0.038*
C21	0.1661 (8)	0.3449 (8)	0.2899 (7)	0.0278 (18)
C22	0.2132 (8)	0.3842 (8)	0.2011 (7)	0.0288 (18)
C23	0.2159 (9)	0.2872 (8)	0.0803 (7)	0.034 (2)
H23	0.189032	0.202605	0.058519	0.041*
C24	0.2564 (9)	0.3118 (8)	−0.0073 (8)	0.035 (2)
H24	0.260178	0.244419	−0.089385	0.042*
C25	0.2927 (9)	0.4363 (9)	0.0234 (8)	0.038 (2)
C26	0.2897 (9)	0.5353 (8)	0.1443 (7)	0.033 (2)
H26	0.314058	0.620255	0.165411	0.040*
C27	0.2505 (9)	0.5079 (7)	0.2332 (7)	0.031 (2)
H27	0.249286	0.574251	0.316386	0.038*
C28	0.4340 (10)	0.4063 (8)	0.5610 (9)	0.041 (2)
H28A	0.431842	0.466625	0.649623	0.062*
H28B	0.404602	0.443550	0.510389	0.062*
H28C	0.518041	0.386688	0.546863	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0546 (5)	0.0361 (4)	0.0307 (3)	−0.0023 (3)	0.0084 (3)	0.0191 (2)
S1	0.0345 (12)	0.0241 (10)	0.0250 (9)	0.0008 (8)	0.0023 (8)	0.0140 (7)
O1	0.039 (4)	0.031 (3)	0.030 (3)	0.002 (3)	−0.002 (2)	0.020 (2)
O2	0.046 (4)	0.026 (3)	0.024 (3)	−0.004 (3)	0.008 (2)	0.013 (2)
O3	0.040 (4)	0.027 (3)	0.036 (3)	0.007 (3)	0.010 (3)	0.018 (2)
N1	0.036 (4)	0.025 (3)	0.024 (3)	0.002 (3)	0.004 (3)	0.016 (3)
C1	0.039 (6)	0.025 (4)	0.023 (4)	0.002 (4)	0.000 (3)	0.011 (3)
C2	0.035 (5)	0.030 (4)	0.034 (4)	0.005 (4)	0.000 (4)	0.015 (3)
C3	0.039 (6)	0.039 (5)	0.046 (5)	0.002 (4)	−0.004 (4)	0.021 (4)
C4	0.030 (5)	0.033 (5)	0.044 (5)	0.000 (4)	−0.002 (4)	0.012 (4)
C5	0.041 (6)	0.026 (4)	0.040 (5)	−0.001 (4)	−0.001 (4)	0.013 (4)
C6	0.031 (5)	0.031 (4)	0.030 (4)	0.003 (4)	0.005 (3)	0.015 (3)
C7	0.024 (5)	0.019 (4)	0.033 (4)	−0.003 (3)	0.000 (3)	0.014 (3)
C8	0.027 (5)	0.024 (4)	0.029 (4)	0.006 (3)	0.003 (3)	0.015 (3)
C9	0.031 (5)	0.029 (4)	0.024 (4)	0.002 (4)	0.005 (3)	0.011 (3)
C10	0.050 (6)	0.024 (4)	0.024 (4)	−0.004 (4)	0.004 (4)	0.013 (3)
C11	0.041 (6)	0.028 (4)	0.028 (4)	0.008 (4)	0.005 (4)	0.015 (3)
C12	0.041 (6)	0.028 (4)	0.023 (4)	0.012 (4)	0.001 (3)	0.011 (3)
C13	0.037 (5)	0.024 (4)	0.033 (4)	0.002 (4)	0.003 (4)	0.013 (3)
C14	0.054 (7)	0.033 (5)	0.047 (5)	0.001 (4)	−0.012 (5)	0.024 (4)
I2	0.0423 (4)	0.0562 (4)	0.0381 (3)	0.0068 (3)	0.0069 (3)	0.0340 (3)
S2	0.0382 (13)	0.0222 (9)	0.0259 (9)	0.0050 (8)	0.0072 (8)	0.0142 (7)
O4	0.053 (4)	0.019 (3)	0.025 (3)	−0.001 (3)	0.011 (3)	0.011 (2)
O5	0.041 (4)	0.029 (3)	0.041 (3)	0.001 (3)	0.009 (3)	0.020 (2)
O6	0.048 (4)	0.021 (3)	0.031 (3)	0.001 (3)	0.001 (3)	0.013 (2)

N2	0.031 (4)	0.024 (3)	0.032 (3)	0.002 (3)	0.006 (3)	0.019 (3)
C15	0.047 (6)	0.026 (4)	0.017 (3)	0.007 (4)	0.006 (3)	0.012 (3)
C16	0.046 (6)	0.038 (5)	0.030 (4)	0.011 (4)	0.014 (4)	0.024 (4)
C17	0.052 (7)	0.045 (5)	0.034 (4)	0.016 (5)	0.009 (4)	0.024 (4)
C18	0.054 (7)	0.037 (5)	0.044 (5)	0.019 (5)	0.012 (4)	0.028 (4)
C19	0.053 (7)	0.023 (4)	0.033 (4)	0.003 (4)	0.002 (4)	0.017 (3)
C20	0.047 (6)	0.026 (4)	0.027 (4)	−0.003 (4)	−0.001 (4)	0.018 (3)
C21	0.029 (5)	0.025 (4)	0.029 (4)	0.005 (4)	0.002 (3)	0.012 (3)
C22	0.032 (5)	0.029 (4)	0.029 (4)	0.000 (4)	−0.001 (3)	0.018 (3)
C23	0.047 (6)	0.029 (4)	0.028 (4)	0.006 (4)	0.003 (4)	0.014 (3)
C24	0.049 (6)	0.034 (5)	0.031 (4)	0.010 (4)	0.007 (4)	0.022 (4)
C25	0.041 (6)	0.052 (6)	0.033 (4)	0.007 (4)	−0.002 (4)	0.029 (4)
C26	0.039 (6)	0.032 (4)	0.032 (4)	−0.003 (4)	0.003 (4)	0.020 (4)
C27	0.046 (6)	0.026 (4)	0.023 (4)	0.005 (4)	0.005 (4)	0.012 (3)
C28	0.044 (6)	0.036 (5)	0.051 (5)	0.002 (4)	0.002 (4)	0.028 (4)

Geometric parameters (Å, °)

I1—C11	2.071 (8)	I2—C25	2.095 (9)
S1—O1	1.408 (6)	S2—O5	1.420 (7)
S1—O2	1.440 (6)	S2—O4	1.447 (6)
S1—N1	1.659 (7)	S2—N2	1.659 (6)
S1—C1	1.770 (9)	S2—C15	1.753 (8)
O3—C7	1.219 (9)	O6—C21	1.213 (10)
N1—C7	1.390 (10)	N2—C21	1.389 (10)
N1—H1	0.8800	N2—H2	0.8800
C1—C6	1.388 (11)	C15—C20	1.393 (12)
C1—C2	1.419 (12)	C15—C16	1.424 (13)
C2—C3	1.407 (13)	C16—C17	1.385 (13)
C2—C14	1.483 (12)	C16—C28	1.490 (13)
C3—C4	1.387 (13)	C17—C18	1.390 (14)
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.392 (13)	C18—C19	1.376 (14)
C4—H4	0.9500	C18—H18	0.9500
C5—C6	1.375 (13)	C19—C20	1.383 (12)
C5—H5	0.9500	C19—H19	0.9500
C6—H6	0.9500	C20—H20	0.9500
C7—C8	1.485 (11)	C21—C22	1.509 (11)
C8—C13	1.387 (11)	C22—C23	1.383 (12)
C8—C9	1.392 (12)	C22—C27	1.384 (12)
C9—C10	1.409 (11)	C23—C24	1.357 (12)
C9—H9	0.9500	C23—H23	0.9500
C10—C11	1.401 (12)	C24—C25	1.395 (13)
C10—H10	0.9500	C24—H24	0.9500
C11—C12	1.395 (12)	C25—C26	1.393 (13)
C12—C13	1.390 (12)	C26—C27	1.386 (12)
C12—H12	0.9500	C26—H26	0.9500
C13—H13	0.9500	C27—H27	0.9500

C14—H14A	0.9800	C28—H28A	0.9800
C14—H14B	0.9800	C28—H28B	0.9800
C14—H14C	0.9800	C28—H28C	0.9800
O1—S1—O2	118.2 (3)	O5—S2—O4	118.4 (4)
O1—S1—N1	110.5 (4)	O5—S2—N2	110.8 (4)
O2—S1—N1	103.9 (3)	O4—S2—N2	103.2 (3)
O1—S1—C1	108.4 (4)	O5—S2—C15	109.0 (4)
O2—S1—C1	109.7 (4)	O4—S2—C15	109.2 (4)
N1—S1—C1	105.3 (4)	N2—S2—C15	105.4 (4)
C7—N1—S1	121.8 (5)	C21—N2—S2	121.8 (6)
C7—N1—H1	119.1	C21—N2—H2	119.1
S1—N1—H1	119.1	S2—N2—H2	119.1
C6—C1—C2	121.5 (8)	C20—C15—C16	121.3 (8)
C6—C1—S1	116.5 (6)	C20—C15—S2	117.0 (7)
C2—C1—S1	121.8 (6)	C16—C15—S2	121.7 (6)
C3—C2—C1	115.9 (8)	C17—C16—C15	116.4 (8)
C3—C2—C14	119.5 (8)	C17—C16—C28	119.5 (9)
C1—C2—C14	124.6 (8)	C15—C16—C28	124.1 (8)
C4—C3—C2	122.1 (9)	C16—C17—C18	121.8 (10)
C4—C3—H3	119.0	C16—C17—H17	119.1
C2—C3—H3	119.0	C18—C17—H17	119.1
C3—C4—C5	120.4 (9)	C19—C18—C17	121.1 (8)
C3—C4—H4	119.8	C19—C18—H18	119.5
C5—C4—H4	119.8	C17—C18—H18	119.5
C6—C5—C4	119.0 (9)	C18—C19—C20	119.0 (8)
C6—C5—H5	120.5	C18—C19—H19	120.5
C4—C5—H5	120.5	C20—C19—H19	120.5
C5—C6—C1	121.1 (9)	C19—C20—C15	120.3 (9)
C5—C6—H6	119.5	C19—C20—H20	119.9
C1—C6—H6	119.5	C15—C20—H20	119.9
O3—C7—N1	118.9 (7)	O6—C21—N2	119.8 (7)
O3—C7—C8	123.4 (7)	O6—C21—C22	123.6 (7)
N1—C7—C8	117.6 (6)	N2—C21—C22	116.5 (7)
C13—C8—C9	119.6 (7)	C23—C22—C27	120.0 (8)
C13—C8—C7	116.7 (7)	C23—C22—C21	115.7 (7)
C9—C8—C7	123.6 (7)	C27—C22—C21	124.3 (7)
C8—C9—C10	119.7 (7)	C24—C23—C22	120.6 (8)
C8—C9—H9	120.2	C24—C23—H23	119.7
C10—C9—H9	120.2	C22—C23—H23	119.7
C11—C10—C9	120.2 (7)	C23—C24—C25	119.9 (8)
C11—C10—H10	119.9	C23—C24—H24	120.1
C9—C10—H10	119.9	C25—C24—H24	120.1
C12—C11—C10	119.5 (8)	C26—C25—C24	120.3 (8)
C12—C11—I1	120.3 (6)	C26—C25—I2	119.4 (7)
C10—C11—I1	120.2 (6)	C24—C25—I2	120.3 (6)
C13—C12—C11	119.8 (7)	C27—C26—C25	118.9 (8)
C13—C12—H12	120.1	C27—C26—H26	120.5

C11—C12—H12	120.1	C25—C26—H26	120.5
C8—C13—C12	121.2 (8)	C22—C27—C26	120.2 (7)
C8—C13—H13	119.4	C22—C27—H27	119.9
C12—C13—H13	119.4	C26—C27—H27	119.9
C2—C14—H14A	109.5	C16—C28—H28A	109.5
C2—C14—H14B	109.5	C16—C28—H28B	109.5
H14A—C14—H14B	109.5	H28A—C28—H28B	109.5
C2—C14—H14C	109.5	C16—C28—H28C	109.5
H14A—C14—H14C	109.5	H28A—C28—H28C	109.5
H14B—C14—H14C	109.5	H28B—C28—H28C	109.5
O1—S1—N1—C7	63.1 (7)	O5—S2—N2—C21	−62.5 (7)
O2—S1—N1—C7	−169.1 (6)	O4—S2—N2—C21	169.7 (7)
C1—S1—N1—C7	−53.8 (7)	C15—S2—N2—C21	55.2 (8)
O1—S1—C1—C6	6.3 (7)	O5—S2—C15—C20	3.3 (7)
O2—S1—C1—C6	−124.1 (6)	O4—S2—C15—C20	134.0 (6)
N1—S1—C1—C6	124.6 (6)	N2—S2—C15—C20	−115.7 (6)
O1—S1—C1—C2	−177.6 (6)	O5—S2—C15—C16	−176.0 (6)
O2—S1—C1—C2	52.0 (8)	O4—S2—C15—C16	−45.2 (7)
N1—S1—C1—C2	−59.3 (8)	N2—S2—C15—C16	65.0 (7)
C6—C1—C2—C3	−0.6 (12)	C20—C15—C16—C17	−0.5 (11)
S1—C1—C2—C3	−176.5 (7)	S2—C15—C16—C17	178.8 (6)
C6—C1—C2—C14	−179.3 (8)	C20—C15—C16—C28	179.5 (8)
S1—C1—C2—C14	4.8 (12)	S2—C15—C16—C28	−1.2 (11)
C1—C2—C3—C4	0.1 (14)	C15—C16—C17—C18	0.7 (12)
C14—C2—C3—C4	178.9 (9)	C28—C16—C17—C18	−179.3 (8)
C2—C3—C4—C5	−0.7 (15)	C16—C17—C18—C19	−2.4 (13)
C3—C4—C5—C6	1.8 (14)	C17—C18—C19—C20	3.8 (13)
C4—C5—C6—C1	−2.4 (13)	C18—C19—C20—C15	−3.6 (12)
C2—C1—C6—C5	1.8 (12)	C16—C15—C20—C19	2.0 (11)
S1—C1—C6—C5	177.9 (7)	S2—C15—C20—C19	−177.3 (6)
S1—N1—C7—O3	−3.3 (11)	S2—N2—C21—O6	2.3 (12)
S1—N1—C7—C8	174.6 (6)	S2—N2—C21—C22	−175.2 (6)
O3—C7—C8—C13	−5.3 (13)	O6—C21—C22—C23	−8.0 (13)
N1—C7—C8—C13	177.0 (8)	N2—C21—C22—C23	169.4 (8)
O3—C7—C8—C9	172.1 (8)	O6—C21—C22—C27	171.0 (9)
N1—C7—C8—C9	−5.6 (12)	N2—C21—C22—C27	−11.6 (13)
C13—C8—C9—C10	0.5 (13)	C27—C22—C23—C24	0.9 (14)
C7—C8—C9—C10	−176.8 (8)	C21—C22—C23—C24	180.0 (9)
C8—C9—C10—C11	0.2 (14)	C22—C23—C24—C25	−1.8 (15)
C9—C10—C11—C12	−1.3 (14)	C23—C24—C25—C26	1.3 (15)
C9—C10—C11—I1	178.3 (7)	C23—C24—C25—I2	−178.2 (7)
C10—C11—C12—C13	1.6 (14)	C24—C25—C26—C27	0.2 (14)
I1—C11—C12—C13	−178.0 (7)	I2—C25—C26—C27	179.6 (7)
C9—C8—C13—C12	−0.2 (13)	C23—C22—C27—C26	0.6 (14)
C7—C8—C13—C12	177.4 (8)	C21—C22—C27—C26	−178.4 (8)
C11—C12—C13—C8	−0.9 (14)	C25—C26—C27—C22	−1.1 (14)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the iodobenzene ring (C8–C13) of molecule *A*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4[i]	0.88	2.06	2.900 (10)	158
N2—H2···O2[i]	0.88	2.12	2.970 (10)	161
C9—H9···O4[i]	0.95	2.36	3.301 (10)	170
C13—H13···O6[ii]	0.95	2.56	3.378 (11)	144
C23—H23···O3[ii]	0.95	2.40	3.201 (11)	142
C27—H27···O2[i]	0.95	2.51	3.428 (9)	163
C4—H4···*Cg*[iii]	0.93	2.81	3.656 (11)	151

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