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N-Ethyl-*N*′-(3-methylbenzoyl)-*S*,*S*-diphenylsulfodiimide

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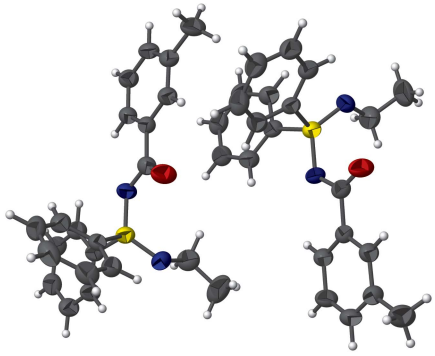
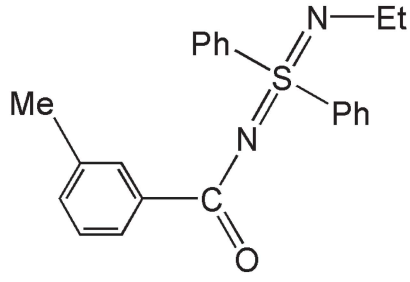
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title sulfodiimide, $C_{22}H_{22}N_2OS$, consists of two crystallographically independent molecules with similar conformations The environment around each sulfur atom is a slightly distorted tetrahedron with two S═N bonds and two S—C bonds. The S═ N(*m*-methylbenzoyl) and S═N(NEt) bond lengths are 1.584 (3) and 1.528 (2) Å, respectively, for one molecule, and 1.575 (2) and 1.529 (3) Å, respectively, for the other. The dihedral angles between the two phenyl rings in the molecules are 86.76 (8) and 82.49 (8)°. The N—S—N—C(*m*-methylbenzoyl) and N—S—N—C(ethyl) torsion angles are −60.5 (2) and −50.28 (19)°, respectively, for one molecule, and 62.9 (2) and 44.2 (3)°, respectively, for the other. In the crystal, each independent molecule is linked to its inversion-related molecule *via* a pair of C—H···O hydrogen bonds, forming a dimer.

3D view



Chemical scheme



Structure description

Sulfoximines and sulfonediimines are relatively unexplored organic compounds in the aza analogues of sulfones family. The latter display various biological activities (Sellinger *et al.*, 1969; Kennewell *et al.*, 1975; Haake, 1976; Park *et al.*, 2011; Sparks *et al.*, 2013; Chen *et al.*, 2012). In view of the biological activities of these sulfones, which are related to structural aspects, and as part of our studies on *N*-tosyl-sulfonediimine (Sheikh *et al.*, 2019), we report herein the synthesis and crystal structure of the title compound (Fig. 1). The S1—N1 (*m*-methylbenzoyl) and S1—N2 (NEt) bond lengths are 1.584 (3) and 1.528 (2) Å, respectively [1.575 (2) and 1.529 (3) Å in the other independent molecule], which are significantly longer than the S≡N triple bond of triphenylsulfanenitrile

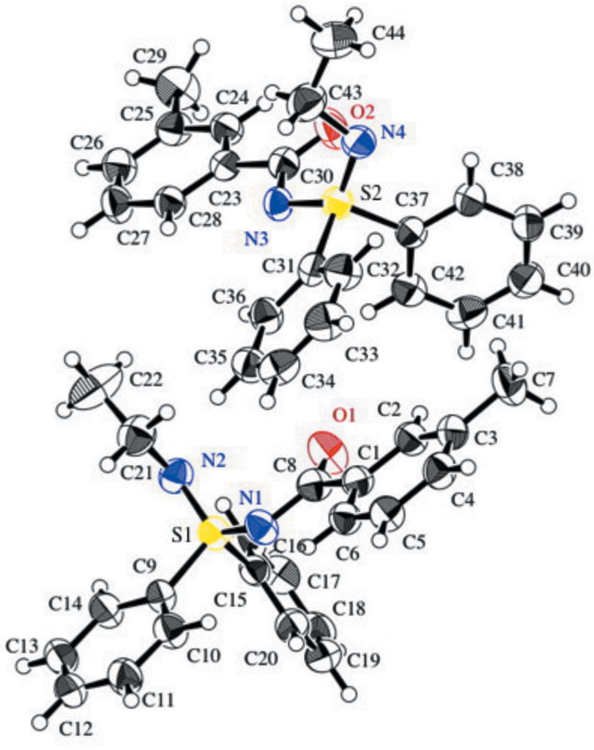


Figure 1
A view of the two independent molecules of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

(1.462 Å; Yoshimura *et al.*, 1997), and close to the S═N double bonds of *S,S*-dimethylsulfonediimine (1.533 Å, electron diffraction; Oberhammer *et al.*, 1970), *S,S*-diphenyl-*S*-pyrrolidinoiminosulfonium perchlorate [1.503 (2) Å for S—N (NH), X-ray; Sheikh *et al.*, 2017] and *S,S*-diphenylsulfodiimide-*N*-phenyl [1.526 Å for S—N (NH) and 1.546 (1) Å for S—N (Ph), X-ray; Yoshimura *et al.*, 2008], and shorter than the S—N bond of *S,S*-diphenyl-*N*-tosylsulfilimine (1.628 Å, X-ray; Kálmán *et al.*, 1971). The N—S—N bond angles are larger than

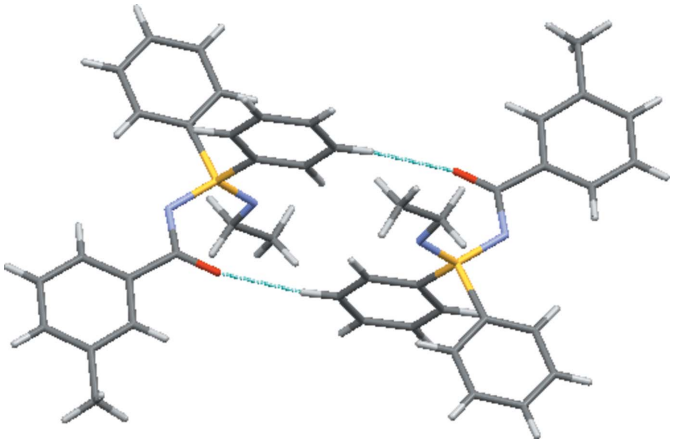


Figure 2
A view of the title compound, showing a pair of C—H···O hydrogen bonds (blue dashed lines) forming an $R_2^2(16)$ ring motif (S1-containing molecule is shown).

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H14···O1^{i}	0.95	2.37	3.307 (4)	170
C39—H36···O2^{ii}	0.95	2.35	3.296 (4)	173

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{22}N_2OS$
M_r	362.49
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	11.0780 (2), 13.2775 (3), 13.3258 (3)
α, β, γ (°)	91.717 (1), 100.9442 (10), 90.9017 (10)
V (Å^3)	1923.08 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.58
Crystal size (mm)	0.46 × 0.27 × 0.17
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.436, 0.770
No. of measured, independent and observed [$F^2 > 2\sigma(F^2)$] reflections	22182, 6901, 4159
R_{int}	0.099
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.151, 0.94
No. of reflections	6901
No. of parameters	473
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, −0.38

Computer programs: *RAPID-AUTO* (Rigaku, 2001), *SIR92* (Altomare *et al.*, 1993), *SHELXL97* (Sheldrick, 2008) and *CrystalStructure* (Rigaku, 2010).

109.5° expected for the sp^3 hybrid configuration, while the N—S—C and C—S—C bond angles are smaller.

In the crystal, the two independent molecules are each linked *via* a pair of C—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(16)$ ring motif (Fig. 2 and Table 1).

Synthesis and crystallization

The compound precursor, *N*-ethyl-*S,S*-diphenylsulfodiimide (100 mg, 0.40 mmol) was allowed to react with *m*-methylbenzoyl chloride (80.3 mg, 0.52 mmol) in dry pyridine (100 μmol) at room temperature for 25 min. The reaction mixture was washed, poured into water, acidified with 3% H_2SO_4, and extracted with $CHCl_3$ (3 × 10 ml). The combined organic layer washed with 10% aq. NaOH and with water, and then dried over anhydrous $MgSO_4$. The solution was concentrated under reduced pressure affording the title compound was collected as a colourless solid and crystallized

from a hot ethanol solution (yield: 84.0 mg, 90%; m.p. 140–141°C).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190946 [https://doi.org/10.1107/S2414314619009465]

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N-[(Ethylimino)diphenyl-λ^6-sulfanylidene]-3-methylbenzamide

Crystal data

$C_{22}H_{22}N_2OS$
M_r = 362.49
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 11.0780 (2) Å
b = 13.2775 (3) Å
c = 13.3258 (3) Å
α = 91.717 (1)°
β = 100.9442 (10)°
γ = 90.9017 (10)°
V = 1923.08 (6) Å^3
Z = 4
$F(000)$ = 768.00
D_x = 1.252 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 17291 reflections
θ = 3.3–68.4°
μ = 1.58 mm^{-1}
T = 173 K
Platelet, colorless
0.46 × 0.27 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.436, T_{max} = 0.770
22182 measured reflections
6901 independent reflections
4159 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.099
θ_{max} = 68.3°
h = −13→13
k = −15→15
l = −16→16

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.151
S = 0.94
6901 reflections
473 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.05317 (6)	0.61479 (5)	0.25436 (5)	0.0437 (2)
S2	0.33971 (6)	0.11964 (5)	0.24369 (5)	0.0437 (2)
O1	0.23346 (16)	0.48853 (14)	0.36079 (15)	0.0633 (6)
O2	0.20456 (16)	−0.01130 (14)	0.34751 (16)	0.0650 (6)
N1	0.19221 (19)	0.61318 (16)	0.24099 (16)	0.0475 (6)
N2	−0.03602 (18)	0.52441 (15)	0.23212 (16)	0.0493 (6)
N3	0.19529 (18)	0.11556 (15)	0.23012 (15)	0.0434 (6)
N4	0.41579 (19)	0.03189 (16)	0.21521 (16)	0.0509 (6)
C1	0.3969 (3)	0.54786 (19)	0.28407 (19)	0.0428 (7)
C2	0.4785 (3)	0.4807 (2)	0.3372 (2)	0.0473 (7)
C3	0.6002 (3)	0.4774 (2)	0.3254 (2)	0.0494 (7)
C4	0.6399 (3)	0.5449 (2)	0.2601 (2)	0.0511 (8)
C5	0.5604 (3)	0.6128 (2)	0.2073 (2)	0.0505 (8)
C6	0.4386 (3)	0.61333 (19)	0.21783 (19)	0.0447 (7)
C7	0.6861 (3)	0.4019 (3)	0.3822 (3)	0.0671 (9)
C8	0.2661 (3)	0.5456 (2)	0.2999 (2)	0.0481 (7)
C9	0.0020 (3)	0.71746 (19)	0.17606 (18)	0.0422 (7)
C10	0.0785 (3)	0.77799 (19)	0.1321 (2)	0.0516 (8)
C11	0.0294 (3)	0.8534 (3)	0.0691 (3)	0.0599 (9)
C12	−0.0948 (3)	0.8698 (2)	0.0508 (2)	0.0580 (8)
C13	−0.1718 (3)	0.8105 (2)	0.0952 (3)	0.0575 (8)
C14	−0.1240 (3)	0.7346 (2)	0.1581 (2)	0.0519 (8)
C15	0.0389 (3)	0.65915 (18)	0.37817 (19)	0.0414 (7)
C16	−0.0374 (3)	0.6097 (2)	0.4320 (2)	0.0491 (7)
C17	−0.0476 (3)	0.6478 (3)	0.5276 (2)	0.0583 (8)
C18	0.0186 (3)	0.7323 (3)	0.5676 (3)	0.0623 (9)
C19	0.0957 (3)	0.7809 (2)	0.5137 (3)	0.0603 (8)
C20	0.1065 (3)	0.7447 (2)	0.4187 (2)	0.0516 (8)
C21	−0.0438 (3)	0.4717 (3)	0.1319 (3)	0.0648 (9)
C22	−0.1434 (4)	0.3937 (3)	0.1150 (3)	0.0992 (13)
C23	0.0078 (3)	0.04398 (19)	0.26800 (19)	0.0415 (7)
C24	−0.0516 (3)	−0.02016 (19)	0.3237 (2)	0.0476 (7)
C25	−0.1792 (3)	−0.0255 (2)	0.3110 (3)	0.0520 (8)
C26	−0.2467 (3)	0.0374 (2)	0.2409 (3)	0.0551 (8)
C27	−0.1889 (3)	0.1027 (2)	0.1847 (2)	0.0554 (8)
C28	−0.0613 (3)	0.10573 (19)	0.19778 (19)	0.0466 (7)
C29	−0.2404 (3)	−0.0967 (3)	0.3727 (3)	0.0743 (10)
C30	0.1458 (3)	0.0460 (2)	0.2862 (2)	0.0464 (7)
C31	0.3579 (3)	0.22967 (19)	0.17269 (18)	0.0424 (7)
C32	0.4696 (3)	0.2423 (2)	0.1429 (2)	0.0575 (8)
C33	0.4901 (3)	0.3245 (3)	0.0867 (3)	0.0638 (9)
C34	0.3985 (3)	0.3937 (3)	0.0621 (2)	0.0575 (8)
C35	0.2879 (3)	0.3818 (2)	0.0925 (2)	0.0543 (8)
C36	0.2668 (3)	0.2995 (2)	0.14851 (19)	0.0495 (7)
C37	0.4115 (3)	0.15642 (19)	0.36964 (19)	0.0418 (7)

C38	0.5126 (3)	0.1052 (2)	0.4187 (2)	0.0504 (7)
C39	0.5688 (3)	0.1355 (3)	0.5173 (3)	0.0567 (8)
C40	0.5238 (3)	0.2155 (3)	0.5649 (3)	0.0590 (9)
C41	0.4221 (3)	0.2665 (2)	0.5160 (2)	0.0577 (8)
C42	0.3656 (3)	0.2374 (2)	0.4175 (2)	0.0501 (7)
C43	0.3710 (3)	−0.0217 (3)	0.1178 (3)	0.0690 (9)
C44	0.4426 (4)	−0.1135 (3)	0.1098 (3)	0.0883 (12)
H1	0.4503	0.4361	0.3826	0.0568*
H2	0.7231	0.5444	0.2517	0.0613*
H3	0.5895	0.6590	0.1638	0.0606*
H4	0.3833	0.6584	0.1798	0.0537*
H5	0.7504	0.3859	0.3433	0.0805*
H6	0.6396	0.3403	0.3905	0.0805*
H7	0.7239	0.4306	0.4497	0.0805*
H8	0.1647	0.7677	0.1452	0.0620*
H9	0.0820	0.8944	0.0379	0.0719*
H10	−0.1277	0.9222	0.0074	0.0697*
H11	−0.2577	0.8219	0.0825	0.0690*
H12	−0.1769	0.6938	0.1891	0.0622*
H13	−0.0821	0.5505	0.4039	0.0589*
H14	−0.1006	0.6153	0.5655	0.0700*
H15	0.0114	0.7580	0.6334	0.0748*
H16	0.1414	0.8394	0.5426	0.0723*
H17	0.1593	0.7776	0.3810	0.0619*
H18	0.0356	0.4397	0.1290	0.0777*
H19	−0.0598	0.5210	0.0769	0.0777*
H20	−0.1292	0.3463	0.1709	0.1190*
H21	−0.1440	0.3572	0.0499	0.1190*
H22	−0.2227	0.4260	0.1132	0.1190*
H23	−0.0039	−0.0618	0.3721	0.0571*
H24	−0.3339	0.0357	0.2312	0.0662*
H25	−0.2365	0.1453	0.1373	0.0665*
H26	−0.0216	0.1499	0.1588	0.0559*
H27	−0.1934	−0.1587	0.3825	0.0892*
H28	−0.3242	−0.1129	0.3363	0.0892*
H29	−0.2433	−0.0648	0.4395	0.0892*
H30	0.5323	0.1945	0.1609	0.0690*
H31	0.5665	0.3333	0.0652	0.0766*
H32	0.4123	0.4504	0.0236	0.0690*
H33	0.2256	0.4300	0.0750	0.0652*
H34	0.1905	0.2912	0.1702	0.0594*
H35	0.5431	0.0497	0.3852	0.0605*
H36	0.6382	0.1008	0.5516	0.0680*
H37	0.5628	0.2363	0.6323	0.0708*
H38	0.3913	0.3215	0.5501	0.0693*
H39	0.2964	0.2723	0.3832	0.0601*
H40	0.3784	0.0228	0.0609	0.0828*
H41	0.2831	−0.0404	0.1123	0.0828*

H42	0.5293	−0.0947	0.1135	0.1059*
H43	0.4109	−0.1492	0.0444	0.1059*
H44	0.4351	−0.1575	0.1661	0.1059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0368 (4)	0.0468 (5)	0.0487 (4)	0.0005 (4)	0.0104 (3)	0.0066 (3)
S2	0.0351 (4)	0.0450 (5)	0.0502 (4)	−0.0014 (4)	0.0059 (3)	0.0022 (3)
O1	0.0473 (12)	0.0719 (14)	0.0776 (14)	0.0055 (11)	0.0248 (11)	0.0311 (12)
O2	0.0406 (13)	0.0670 (14)	0.0849 (15)	−0.0002 (11)	0.0018 (11)	0.0298 (12)
N1	0.0337 (13)	0.0506 (15)	0.0601 (15)	0.0050 (11)	0.0124 (11)	0.0101 (12)
N2	0.0435 (14)	0.0503 (14)	0.0543 (14)	−0.0071 (12)	0.0104 (11)	0.0021 (12)
N3	0.0329 (12)	0.0484 (14)	0.0472 (13)	−0.0028 (11)	0.0029 (10)	0.0073 (11)
N4	0.0430 (14)	0.0478 (14)	0.0606 (15)	0.0072 (12)	0.0080 (11)	−0.0079 (12)
C1	0.0372 (16)	0.0416 (16)	0.0501 (16)	0.0009 (13)	0.0100 (13)	−0.0017 (13)
C2	0.0413 (17)	0.0468 (18)	0.0541 (17)	−0.0002 (14)	0.0088 (13)	0.0064 (14)
C3	0.0395 (17)	0.0508 (18)	0.0555 (18)	0.0010 (15)	0.0032 (14)	0.0020 (14)
C4	0.0345 (16)	0.060 (2)	0.0595 (19)	−0.0004 (15)	0.0108 (14)	−0.0010 (15)
C5	0.0459 (18)	0.0523 (19)	0.0552 (18)	−0.0005 (15)	0.0136 (14)	0.0083 (15)
C6	0.0395 (16)	0.0447 (17)	0.0503 (17)	0.0019 (14)	0.0089 (13)	0.0029 (13)
C7	0.0442 (19)	0.075 (3)	0.080 (3)	0.0084 (17)	0.0045 (16)	0.0207 (18)
C8	0.0434 (17)	0.0464 (18)	0.0567 (18)	0.0009 (15)	0.0150 (14)	−0.0009 (14)
C9	0.0386 (16)	0.0466 (17)	0.0407 (15)	0.0033 (14)	0.0046 (12)	0.0064 (12)
C10	0.0458 (17)	0.0529 (19)	0.0572 (18)	0.0003 (15)	0.0104 (14)	0.0137 (15)
C11	0.059 (2)	0.057 (2)	0.061 (2)	−0.0041 (17)	0.0020 (16)	0.0190 (16)
C12	0.071 (3)	0.0489 (19)	0.0479 (17)	0.0053 (17)	−0.0070 (16)	0.0093 (14)
C13	0.0493 (19)	0.055 (2)	0.066 (2)	0.0063 (16)	0.0028 (15)	0.0111 (16)
C14	0.0441 (18)	0.0521 (18)	0.0597 (18)	0.0032 (15)	0.0085 (14)	0.0141 (15)
C15	0.0362 (15)	0.0406 (16)	0.0469 (16)	0.0051 (13)	0.0061 (12)	0.0041 (12)
C16	0.0492 (18)	0.0465 (17)	0.0529 (17)	−0.0006 (14)	0.0118 (14)	0.0087 (14)
C17	0.063 (2)	0.063 (2)	0.0549 (19)	0.0086 (17)	0.0235 (16)	0.0096 (16)
C18	0.079 (3)	0.058 (2)	0.0496 (18)	0.0191 (19)	0.0106 (17)	0.0015 (16)
C19	0.071 (3)	0.0470 (18)	0.0581 (19)	−0.0004 (16)	0.0003 (16)	−0.0026 (15)
C20	0.0476 (18)	0.0503 (18)	0.0556 (18)	−0.0015 (15)	0.0063 (14)	0.0066 (14)
C21	0.060 (2)	0.073 (3)	0.061 (2)	0.0001 (18)	0.0128 (16)	−0.0069 (17)
C22	0.100 (3)	0.094 (3)	0.106 (3)	−0.034 (3)	0.035 (3)	−0.044 (3)
C23	0.0391 (16)	0.0403 (16)	0.0441 (15)	−0.0012 (13)	0.0060 (12)	0.0008 (12)
C24	0.0432 (17)	0.0441 (17)	0.0553 (17)	0.0013 (14)	0.0084 (14)	0.0062 (14)
C25	0.0433 (18)	0.0495 (18)	0.0651 (19)	−0.0038 (15)	0.0152 (15)	0.0020 (15)
C26	0.0357 (17)	0.060 (2)	0.070 (2)	0.0021 (15)	0.0112 (15)	0.0031 (16)
C27	0.0390 (17)	0.063 (2)	0.0614 (19)	0.0046 (16)	0.0019 (14)	0.0091 (15)
C28	0.0402 (17)	0.0474 (17)	0.0516 (17)	0.0003 (14)	0.0072 (13)	0.0041 (13)
C29	0.055 (2)	0.076 (3)	0.098 (3)	−0.0025 (18)	0.0288 (18)	0.020 (2)
C30	0.0430 (17)	0.0460 (18)	0.0481 (17)	−0.0022 (15)	0.0037 (13)	0.0019 (14)
C31	0.0392 (16)	0.0481 (17)	0.0384 (14)	−0.0050 (14)	0.0036 (12)	0.0024 (12)
C32	0.0473 (18)	0.056 (2)	0.072 (2)	−0.0020 (16)	0.0183 (15)	0.0036 (16)
C33	0.057 (2)	0.064 (3)	0.075 (3)	−0.0103 (18)	0.0264 (17)	0.0026 (17)

C34	0.070 (3)	0.054 (2)	0.0514 (18)	−0.0129 (18)	0.0221 (16)	0.0007 (15)
C35	0.058 (2)	0.0527 (19)	0.0525 (18)	0.0007 (16)	0.0100 (15)	0.0089 (14)
C36	0.0432 (17)	0.0552 (19)	0.0505 (17)	0.0015 (15)	0.0093 (13)	0.0071 (14)
C37	0.0342 (15)	0.0418 (16)	0.0496 (16)	−0.0034 (13)	0.0083 (12)	0.0053 (13)
C38	0.0414 (17)	0.0487 (18)	0.0579 (18)	−0.0032 (15)	0.0018 (14)	0.0014 (14)
C39	0.0503 (19)	0.055 (2)	0.0588 (19)	−0.0025 (16)	−0.0042 (15)	0.0085 (16)
C40	0.070 (3)	0.054 (2)	0.0495 (18)	−0.0111 (18)	0.0039 (16)	0.0067 (16)
C41	0.075 (3)	0.0490 (19)	0.0515 (18)	−0.0055 (17)	0.0188 (16)	−0.0025 (15)
C42	0.0478 (18)	0.0502 (18)	0.0538 (18)	0.0025 (15)	0.0128 (14)	0.0039 (14)
C43	0.069 (3)	0.067 (3)	0.069 (3)	−0.0003 (19)	0.0100 (17)	−0.0142 (17)
C44	0.101 (3)	0.064 (3)	0.094 (3)	0.017 (3)	0.006 (3)	−0.024 (2)

Geometric parameters (Å, º)

S1—N1	1.584 (3)	C37—C42	1.386 (4)
S1—N2	1.528 (2)	C38—C39	1.387 (4)
S1—C9	1.776 (3)	C39—C40	1.370 (5)
S1—C15	1.771 (3)	C40—C41	1.388 (5)
S2—N3	1.575 (2)	C41—C42	1.384 (4)
S2—N4	1.529 (3)	C43—C44	1.476 (5)
S2—C31	1.793 (3)	C2—H1	0.950
S2—C37	1.766 (3)	C4—H2	0.950
O1—C8	1.226 (4)	C5—H3	0.950
O2—C30	1.234 (4)	C6—H4	0.950
N1—C8	1.383 (4)	C7—H5	0.980
N2—C21	1.477 (4)	C7—H6	0.980
N3—C30	1.376 (4)	C7—H7	0.980
N4—C43	1.458 (4)	C10—H8	0.950
C1—C2	1.391 (4)	C11—H9	0.950
C1—C6	1.391 (4)	C12—H10	0.950
C1—C8	1.504 (4)	C13—H11	0.950
C2—C3	1.387 (4)	C14—H12	0.950
C3—C4	1.391 (4)	C16—H13	0.950
C3—C7	1.512 (4)	C17—H14	0.950
C4—C5	1.382 (4)	C18—H15	0.950
C5—C6	1.383 (4)	C19—H16	0.950
C9—C10	1.379 (4)	C20—H17	0.950
C9—C14	1.394 (4)	C21—H18	0.990
C10—C11	1.378 (4)	C21—H19	0.990
C11—C12	1.373 (5)	C22—H20	0.980
C12—C13	1.377 (5)	C22—H21	0.980
C13—C14	1.378 (4)	C22—H22	0.980
C15—C16	1.379 (4)	C24—H23	0.950
C15—C20	1.387 (4)	C26—H24	0.950
C16—C17	1.381 (4)	C27—H25	0.950
C17—C18	1.369 (4)	C28—H26	0.950
C18—C19	1.380 (5)	C29—H27	0.980
C19—C20	1.368 (5)	C29—H28	0.980

C21—C22	1.482 (5)	C29—H29	0.980
C23—C24	1.384 (4)	C32—H30	0.950
C23—C28	1.388 (4)	C33—H31	0.950
C23—C30	1.501 (4)	C34—H32	0.950
C24—C25	1.391 (4)	C35—H33	0.950
C25—C26	1.389 (4)	C36—H34	0.950
C25—C29	1.506 (5)	C38—H35	0.950
C26—C27	1.387 (5)	C39—H36	0.950
C27—C28	1.391 (4)	C40—H37	0.950
C31—C32	1.379 (5)	C41—H38	0.950
C31—C36	1.380 (4)	C42—H39	0.950
C32—C33	1.383 (5)	C43—H40	0.990
C33—C34	1.380 (5)	C43—H41	0.990
C34—C35	1.369 (5)	C44—H42	0.980
C35—C36	1.383 (4)	C44—H43	0.980
C37—C38	1.384 (4)	C44—H44	0.980

N1—S1—N2	124.42 (12)	C5—C6—H4	119.968
N1—S1—C9	99.34 (13)	C3—C7—H5	109.471
N1—S1—C15	111.93 (12)	C3—C7—H6	109.464
N2—S1—C9	111.85 (12)	C3—C7—H7	109.468
N2—S1—C15	104.30 (13)	H5—C7—H6	109.476
C9—S1—C15	103.29 (12)	H5—C7—H7	109.473
N3—S2—N4	123.76 (12)	H6—C7—H7	109.476
N3—S2—C31	99.52 (12)	C9—C10—H8	120.147
N3—S2—C37	112.11 (12)	C11—C10—H8	120.146
N4—S2—C31	112.28 (13)	C10—C11—H9	119.703
N4—S2—C37	104.46 (12)	C12—C11—H9	119.707
C31—S2—C37	103.05 (12)	C11—C12—H10	119.929
S1—N1—C8	115.9 (2)	C13—C12—H10	119.927
S1—N2—C21	116.3 (2)	C12—C13—H11	120.065
S2—N3—C30	116.68 (17)	C14—C13—H11	120.058
S2—N4—C43	117.30 (18)	C9—C14—H12	120.002
C2—C1—C6	119.1 (3)	C13—C14—H12	120.010
C2—C1—C8	118.2 (3)	C15—C16—H13	120.622
C6—C1—C8	122.7 (3)	C17—C16—H13	120.632
C1—C2—C3	121.5 (3)	C16—C17—H14	120.016
C2—C3—C4	118.2 (3)	C18—C17—H14	120.021
C2—C3—C7	120.4 (3)	C17—C18—H15	119.515
C4—C3—C7	121.5 (3)	C19—C18—H15	119.521
C3—C4—C5	121.2 (3)	C18—C19—H16	120.020
C4—C5—C6	120.0 (3)	C20—C19—H16	120.030
C1—C6—C5	120.1 (3)	C15—C20—H17	120.536
O1—C8—N1	125.9 (3)	C19—C20—H17	120.541
O1—C8—C1	120.8 (3)	N2—C21—H18	109.481
N1—C8—C1	113.3 (3)	N2—C21—H19	109.485
S1—C9—C10	124.0 (2)	C22—C21—H18	109.482
S1—C9—C14	116.3 (2)	C22—C21—H19	109.486

C10—C9—C14	119.7 (3)	H18—C21—H19	108.061
C9—C10—C11	119.7 (3)	C21—C22—H20	109.477
C10—C11—C12	120.6 (3)	C21—C22—H21	109.473
C11—C12—C13	120.1 (3)	C21—C22—H22	109.473
C12—C13—C14	119.9 (3)	H20—C22—H21	109.466
C9—C14—C13	120.0 (3)	H20—C22—H22	109.468
S1—C15—C16	120.58 (19)	H21—C22—H22	109.471
S1—C15—C20	118.0 (2)	C23—C24—H23	119.002
C16—C15—C20	121.4 (3)	C25—C24—H23	119.002
C15—C16—C17	118.7 (3)	C25—C26—H24	119.443
C16—C17—C18	120.0 (3)	C27—C26—H24	119.445
C17—C18—C19	121.0 (3)	C26—C27—H25	119.967
C18—C19—C20	120.0 (3)	C28—C27—H25	119.963
C15—C20—C19	118.9 (3)	C23—C28—H26	120.158
N2—C21—C22	110.8 (3)	C27—C28—H26	120.160
C24—C23—C28	119.3 (3)	C25—C29—H27	109.470
C24—C23—C30	119.0 (3)	C25—C29—H28	109.465
C28—C23—C30	121.6 (3)	C25—C29—H29	109.464
C23—C24—C25	122.0 (3)	H27—C29—H28	109.481
C24—C25—C26	117.8 (3)	H27—C29—H29	109.477
C24—C25—C29	120.3 (3)	H28—C29—H29	109.472
C26—C25—C29	121.8 (3)	C31—C32—H30	120.054
C25—C26—C27	121.1 (3)	C33—C32—H30	120.045
C26—C27—C28	120.1 (3)	C32—C33—H31	120.370
C23—C28—C27	119.7 (3)	C34—C33—H31	120.363
O2—C30—N3	125.7 (3)	C33—C34—H32	119.564
O2—C30—C23	120.1 (3)	C35—C34—H32	119.555
N3—C30—C23	114.2 (3)	C34—C35—H33	119.978
S2—C31—C32	116.4 (2)	C36—C35—H33	119.972
S2—C31—C36	123.0 (3)	C31—C36—H34	120.341
C32—C31—C36	120.6 (3)	C35—C36—H34	120.338
C31—C32—C33	119.9 (3)	C37—C38—H35	120.260
C32—C33—C34	119.3 (3)	C39—C38—H35	120.266
C33—C34—C35	120.9 (3)	C38—C39—H36	120.115
C34—C35—C36	120.0 (3)	C40—C39—H36	120.121
C31—C36—C35	119.3 (3)	C39—C40—H37	119.601
S2—C37—C38	120.1 (2)	C41—C40—H37	119.611
S2—C37—C42	118.89 (19)	C40—C41—H38	120.000
C38—C37—C42	121.0 (3)	C42—C41—H38	120.006
C37—C38—C39	119.5 (3)	C37—C42—H39	120.527
C38—C39—C40	119.8 (3)	C41—C42—H39	120.529
C39—C40—C41	120.8 (3)	N4—C43—H40	109.587
C40—C41—C42	120.0 (3)	N4—C43—H41	109.584
C37—C42—C41	118.9 (3)	C44—C43—H40	109.585
N4—C43—C44	110.3 (3)	C44—C43—H41	109.593
C1—C2—H1	119.237	H40—C43—H41	108.124
C3—C2—H1	119.239	C43—C44—H42	109.477
C3—C4—H2	119.421	C43—C44—H43	109.462

C5—C4—H2	119.429	C43—C44—H44	109.467
C4—C5—H3	120.008	H42—C44—H43	109.471
C6—C5—H3	120.017	H42—C44—H44	109.475
C1—C6—H4	119.971	H43—C44—H44	109.475

N1—S1—N2—C21	−50.28 (19)	C1—C2—C3—C7	−178.5 (2)
N2—S1—N1—C8	−60.5 (2)	C2—C3—C4—C5	−0.7 (4)
N1—S1—C9—C10	−6.6 (2)	C7—C3—C4—C5	179.1 (3)
N1—S1—C9—C14	172.15 (16)	C3—C4—C5—C6	−0.9 (4)
C9—S1—N1—C8	174.73 (15)	C4—C5—C6—C1	2.1 (4)
N1—S1—C15—C16	−134.65 (17)	S1—C9—C10—C11	177.38 (16)
N1—S1—C15—C20	45.4 (2)	S1—C9—C14—C13	−177.73 (16)
C15—S1—N1—C8	66.22 (18)	C10—C9—C14—C13	1.1 (4)
N2—S1—C9—C10	−139.73 (18)	C14—C9—C10—C11	−1.4 (4)
N2—S1—C9—C14	39.1 (2)	C9—C10—C11—C12	1.0 (4)
C9—S1—N2—C21	68.84 (17)	C10—C11—C12—C13	−0.3 (4)
N2—S1—C15—C16	2.3 (2)	C11—C12—C13—C14	0.0 (4)
N2—S1—C15—C20	−177.61 (16)	C12—C13—C14—C9	−0.4 (4)
C15—S1—N2—C21	179.80 (13)	S1—C15—C16—C17	−178.83 (15)
C9—S1—C15—C16	119.40 (18)	S1—C15—C20—C19	179.27 (16)
C9—S1—C15—C20	−60.56 (19)	C16—C15—C20—C19	−0.7 (4)
C15—S1—C9—C10	108.68 (19)	C20—C15—C16—C17	1.1 (4)
C15—S1—C9—C14	−72.53 (18)	C15—C16—C17—C18	−0.9 (4)
N3—S2—N4—C43	44.2 (3)	C16—C17—C18—C19	0.2 (5)
N4—S2—N3—C30	62.9 (2)	C17—C18—C19—C20	0.2 (5)
N3—S2—C31—C32	−162.49 (16)	C18—C19—C20—C15	0.0 (4)
N3—S2—C31—C36	17.8 (2)	C24—C23—C28—C27	0.3 (4)
C31—S2—N3—C30	−172.07 (14)	C28—C23—C24—C25	0.6 (4)
N3—S2—C37—C38	135.29 (18)	C24—C23—C30—O2	2.5 (4)
N3—S2—C37—C42	−45.2 (3)	C24—C23—C30—N3	−177.3 (2)
C37—S2—N3—C30	−63.70 (18)	C30—C23—C24—C25	179.7 (2)
N4—S2—C31—C32	−29.83 (19)	C28—C23—C30—O2	−178.4 (3)
N4—S2—C31—C36	150.48 (16)	C28—C23—C30—N3	1.8 (4)
C31—S2—N4—C43	−75.06 (18)	C30—C23—C28—C27	−178.8 (2)
N4—S2—C37—C38	−1.1 (3)	C23—C24—C25—C26	−1.0 (4)
N4—S2—C37—C42	178.40 (18)	C23—C24—C25—C29	179.7 (3)
C37—S2—N4—C43	173.98 (16)	C24—C25—C26—C27	0.6 (4)
C31—S2—C37—C38	−118.6 (2)	C29—C25—C26—C27	179.9 (3)
C31—S2—C37—C42	60.9 (2)	C25—C26—C27—C28	0.2 (4)
C37—S2—C31—C32	82.01 (18)	C26—C27—C28—C23	−0.7 (4)
C37—S2—C31—C36	−97.68 (19)	S2—C31—C32—C33	179.12 (16)
S1—N1—C8—O1	−0.5 (4)	S2—C31—C36—C35	−179.28 (15)
S1—N1—C8—C1	−179.82 (14)	C32—C31—C36—C35	1.0 (4)
S1—N2—C21—C22	−173.34 (15)	C36—C31—C32—C33	−1.2 (4)
S2—N3—C30—O2	1.8 (4)	C31—C32—C33—C34	0.7 (4)
S2—N3—C30—C23	−178.52 (14)	C32—C33—C34—C35	−0.1 (4)
S2—N4—C43—C44	−170.70 (17)	C33—C34—C35—C36	0.0 (4)
C2—C1—C6—C5	−1.5 (4)	C34—C35—C36—C31	−0.4 (4)

C6—C1—C2—C3	−0.2 (4)	S2—C37—C38—C39	179.39 (17)
C2—C1—C8—O1	2.5 (4)	S2—C37—C42—C41	−179.71 (17)
C2—C1—C8—N1	−178.1 (2)	C38—C37—C42—C41	−0.2 (4)
C8—C1—C2—C3	179.1 (2)	C42—C37—C38—C39	−0.1 (4)
C6—C1—C8—O1	−178.2 (3)	C37—C38—C39—C40	0.0 (5)
C6—C1—C8—N1	1.2 (4)	C38—C39—C40—C41	0.3 (5)
C8—C1—C6—C5	179.2 (2)	C39—C40—C41—C42	−0.7 (5)
C1—C2—C3—C4	1.3 (4)	C40—C41—C42—C37	0.6 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H14···O1^{i}	0.95	2.37	3.307 (4)	170
C39—H36···O2^{ii}	0.95	2.35	3.296 (4)	173

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