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N,*N*′-Propylenedioxybis(2,4,6-trimethylbenzenesulfonamide): molecules of unexpected conformation form a molecular ladder built from two independent N—H···O=S hydrogen bonds

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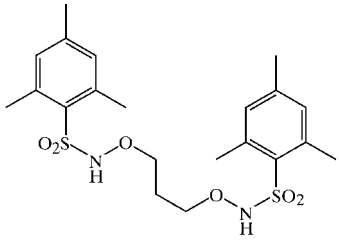
Molecules of the title compound, $C_{21}H_{30}N_2O_6S_2$, adopt a skeletal conformation which does not possess even approximate internal symmetry. The molecules are linked by two N—H···O=S hydrogen bonds [H···O = 1.97 Å (×2), N···O = 2.865 (2) and 2.864 (2) Å, and N—H···O = 160 and 159°] into molecular ladders, alternatively described as chains of edge-fused $R_2^2(20)$ rings.

Comment

Terminally disubstituted bis[(2,4,6-trimethylbenzenesulfonyl)aminooxy]alkanes are useful intermediates for the synthesis of oxaaza-macrocycles (Kuksa *et al.*, 1999), and we report here



(I)

the molecular and supramolecular structure of the title compound, (I), as a typical example of this class of intermediate.

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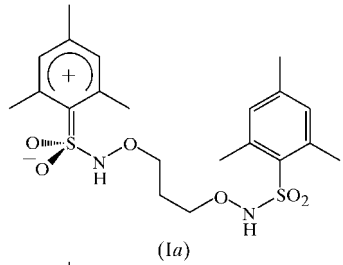
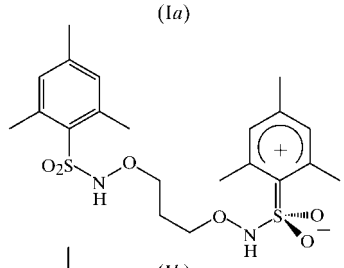
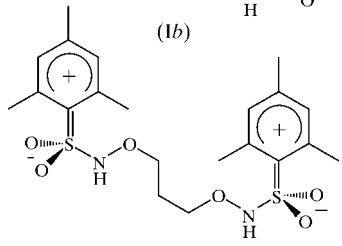
Molecules of (I) (Fig. 1) could, in principle, adopt a conformation having symmetry as high as C_{2v} (*mm*2); in the event, the molecules lie in general positions in space group $P\overline{1}$ ($Z' = 1$) and the molecular conformation precludes even approximate internal symmetry. Several of the corresponding pairs of torsion angles (Table 1) for the two halves of the molecule, from atom C2 to ring C11–C16 and from atom C2 to ring C21–C26, have similar values, but the conformations of



(I*a*)



(I*b*)



(I*c*)

the non-H atoms about the O1—C1 and O2—C3 bonds are antiperiplanar and synclinal, respectively, while those around the C1—C2 and C3—C2 bonds are synclinal and antiperiplanar, respectively, so that the molecule as a whole has only C_1 symmetry (Fig. 1). Both of the S—N—O—C torsion angles appear to be determined by the mutual repulsion of the lone pairs of electrons on the N and O atoms, while each of the

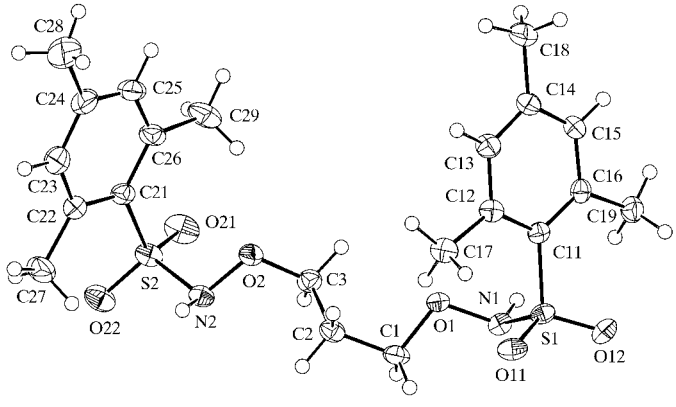


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

 DOI: 10.1107/S0108270104006109

two aryl rings is approximately orthogonal to the adjacent CSN fragment. The conformational behaviour of the central fragment of the molecule between atoms S1 and S2 is unexpected and, at present, unexplained; given the orthogonality of the lone-pair orbitals on the adjacent N and O atoms, conformations having either C_s (*m*) or C_2 (2) symmetry might have been expected.

The bond lengths within the SO_2NOC fragments are typical of those observed in sulfonylhydroxylamines, such as $PhSO_2NHOH$ and $PhSO_2NHOSO_2Ph$ (Scholz *et al.*, 1989). In the aryl rings, the C*n*1—C*n*2 and C*n*1—C*n*6 bonds (n = 1 or 2), adjacent to the sulfonyl substituents, have distances in the range 1.410 (2)–1.414 (2) Å, significantly longer than the other bonds in these rings, for which the distances lie in the range 1.382 (3)–1.399 (2) Å (mean 1.389 Å; Table 1). These values indicate some contribution to the overall molecular–electronic structure of charge-separated forms, such as (I*a*)–(I*c*).

Molecules of (I) are linked by pairs of inequivalent N—H···O=S hydrogen bonds (Table 2). Amine atoms N1 and N2 in the molecule at (x, y, z) act as hydrogen-bond donors, respectively, to atom O11 in the molecule at ($-1+x$, y, z) and to atom O21 in the molecule at ($1+x$, y, z), so generating by translation a pair of independent and antiparallel $C(4)$ (Bernstein *et al.*, 1995) chains. This $C(4)$ motif is characteristic of the supramolecular aggregation in sulfonamides, sulfonylhydrazines and sulfonylhydroxylamines (Vorontsova, 1966; Cotton & Stokeley, 1970; Klug, 1970; Brink & Mattes, 1986; Scholz *et al.*, 1989; Lightfoot *et al.*, 1993; Tremayne *et al.*, 1999, 2002).

The combination of the two $C(4)$ motifs generates a chain of edge-fused $R_2^2(20)$ (Bernstein *et al.*, 1995) rings running parallel to the [100] direction (Fig. 2). This chain may alternatively be regarded as a molecular ladder in which the two $C(4)$ chains provide the uprights and the sequence of atoms in the molecule running from N1 to N2 forms a rung of the ladder. This chain, or ladder, lies in the domain $-0.06 < z < 0.64$, and a second such ladder, related to the first by inversion, lies in the domain $0.36 < z < 1.06$. However, there are no direction-specific interactions between adjacent ladders. In particular, there are neither C—H···O nor C—H···π(arene) hydrogen bonds and no aromatic π–π stacking interactions; it seems probable that participation by the ring components in any of these interactions is precluded by the presence of the methyl substituents. The two shortest intermolecular H···O contacts both involve one the CH_2 groups in the central bridge, where the acidity of the C—H bonds is expected to be low. Since both have H···O distances above 2.55 Å, *i.e.* not significantly less than the sum of the van der Waals radii, these contacts are not regarded as structurally significant.

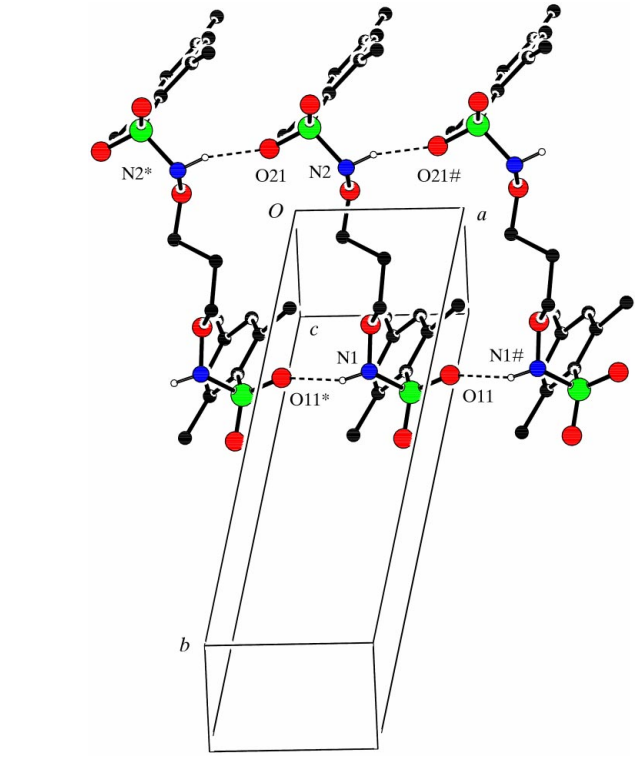


Figure 2
Part of the crystal structure of (I), showing the formation of a chain of edge-fused $R_2^2(20)$ rings along [100]. For clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions ($-1+x$, y, z) and ($1+x$, y, z), respectively.

Experimental

The title compound was prepared from 1,3-dibromopropane by means of successive reactions with (i) *N*-hydroxyphthalimide/dimethylformamide, (ii) HCl/acetic acid and (iii) 2,4,6-trimethylbenzenesulfonyl chloride/pyridine (Kuksa *et al.*, 1999). After recrystallization from toluene, the compound had a melting point of 433–435 K. Crystals suitable for single-crystal X-ray diffraction were selected directly from the recrystallized sample.

Crystal data

$C_{21}H_{30}N_2O_6S_2$
M_r = 470.59
Triclinic, $P\overline{1}$
a = 5.1689 (1) Å
b = 14.3184 (3) Å
c = 16.1506 (4) Å
α = 98.121 (1)°
β = 97.963 (1)°
γ = 99.033 (1)°
V = 1152.75 (4) Å^3
Z = 2
D_x = 1.356 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5176 reflections
θ = 3.4–27.5°
μ = 0.27 mm^{-1}
T = 120 (2) K
Plate, colourless
0.20 × 0.10 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*DENZO–SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.954, T_{max} = 0.989
17 653 measured reflections
5176 independent reflections
4173 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.5°
$h = -6 \rightarrow 6$
$k = -18 \rightarrow 18$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.108
S = 1.02
5176 reflections
286 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.3916P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O11	1.4312 (12)	S2—O21	1.4307 (13)
S1—O12	1.4263 (13)	S2—O22	1.4266 (13)
S1—N1	1.6608 (14)	S2—N2	1.6653 (14)
S1—C11	1.7799 (16)	S2—C21	1.7747 (17)
O1—N1	1.4270 (17)	O2—N2	1.4284 (17)
O1—C1	1.4448 (19)	O2—C3	1.442 (2)
C11—C12	1.414 (2)	C21—C22	1.410 (2)
C11—C16	1.413 (2)	C21—C26	1.413 (2)
C12—C13	1.399 (2)	C22—C23	1.389 (3)
C13—C14	1.386 (2)	C23—C24	1.385 (3)
C14—C15	1.384 (3)	C24—C25	1.382 (3)
C15—C16	1.391 (2)	C25—C26	1.396 (3)
C12—C11—S1—N1	90.86 (13)	C22—C21—S2—N2	−83.82 (14)
C11—S1—N1—O1	−56.25 (11)	C21—S2—N2—O2	−59.15 (11)
S1—N1—O1—C1	−114.34 (11)	S2—N2—O2—C3	−126.22 (11)
N1—O1—C1—C2	176.00 (12)	N2—O2—C3—C2	−80.35 (16)
O1—C1—C2—C3	59.76 (18)	O2—C3—C2—C1	−174.31 (13)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O11^{i}	0.94	1.97	2.865 (2)	160
N2—H2···O21^{ii}	0.93	1.97	2.864 (2)	159

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

Crystals of (I) are triclinic, and space group $P\overline{1}$ was selected and confirmed by the subsequent structure analysis. All H atoms were located from difference maps. H atoms bonded to C atoms were treated as riding atoms, with C—H distances of 0.95 (aromatic), 0.98 (CH_3) and 0.99 Å (CH_2). H atoms bonded to N atoms were allowed to ride at the positions identified from difference maps, giving N—H distances of 0.93 and 0.94 Å.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England; the authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants that have provided computing facilities for this work. SMSVW, MVDRS and PFP thank CNPq for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GG1212). Services for accessing these data are described at the back of the journal.

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supporting information

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Computing details

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO*–SMN (Otwinowski & Minor, 1997); data reduction: *DENZO*–SMN; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

1,3-Bis[(2,4,6-trimethylbenzenesulfonyl)aminooxy]propane

Crystal data

$C_{21}H_{30}N_2O_6S_2$
$M_r = 470.59$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.1689\ (1)$ Å
$b = 14.3184\ (3)$ Å
$c = 16.1506\ (4)$ Å
$\alpha = 98.121\ (1)°$
$\beta = 97.963\ (1)°$
$\gamma = 99.033\ (1)°$
$V = 1152.75\ (4)$ Å^3
$Z = 2$
$F(000) = 500$
$D_x = 1.356$ Mg m^{-3}
Melting point: 434 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5176 reflections
$\theta = 3.4–27.5°$
$\mu = 0.27$ mm^{-1}
$T = 120$ K
Plate, colourless
0.20 × 0.10 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: frotating anode
Graphite monochromator
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*DENZO*–SMN; Otwinowski & Minor, 1997)
$T_{min} = 0.954$, $T_{max} = 0.989$
17653 measured reflections
5176 independent reflections
4173 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -6\rightarrow6$
$k = -18\rightarrow18$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.108$
$S = 1.02$
5176 reflections
286 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
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.3916P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.85265 (7)	0.33140 (3)	0.37549 (3)	0.02281 (12)
S2	−0.02530 (8)	−0.19875 (3)	0.03182 (3)	0.02635 (12)
O1	0.5459 (2)	0.19945 (8)	0.27042 (7)	0.0224 (2)
O2	0.2761 (2)	−0.08003 (8)	0.14769 (7)	0.0269 (3)
O11	1.0708 (2)	0.30210 (9)	0.33938 (8)	0.0292 (3)
O12	0.8622 (2)	0.43108 (8)	0.40360 (8)	0.0324 (3)
O21	−0.2415 (2)	−0.15825 (11)	0.05907 (9)	0.0392 (3)
O22	−0.0360 (2)	−0.22995 (10)	−0.05667 (7)	0.0360 (3)
N1	0.5919 (3)	0.30065 (9)	0.29826 (8)	0.0225 (3)
N2	0.2397 (3)	−0.11135 (10)	0.05820 (8)	0.0247 (3)
C1	0.5935 (3)	0.18220 (13)	0.18398 (10)	0.0282 (4)
C2	0.5625 (3)	0.07488 (12)	0.15877 (11)	0.0270 (4)
C3	0.2883 (3)	0.02237 (12)	0.16410 (11)	0.0270 (4)
C11	0.7853 (3)	0.26306 (11)	0.45642 (10)	0.0212 (3)
C12	0.8647 (3)	0.17290 (12)	0.45564 (10)	0.0240 (3)
C13	0.7896 (3)	0.11977 (13)	0.51748 (11)	0.0287 (4)
C14	0.6440 (4)	0.15177 (13)	0.57808 (10)	0.0296 (4)
C15	0.5731 (4)	0.24092 (12)	0.57715 (10)	0.0286 (4)
C16	0.6368 (3)	0.29795 (11)	0.51732 (10)	0.0238 (3)
C17	1.0236 (4)	0.12821 (13)	0.39445 (11)	0.0299 (4)
C18	0.5638 (5)	0.09204 (15)	0.64319 (12)	0.0419 (5)
C19	0.5406 (4)	0.39231 (12)	0.52293 (11)	0.0310 (4)
C21	0.0403 (3)	−0.29131 (12)	0.08973 (10)	0.0249 (3)
C22	0.1885 (4)	−0.35811 (12)	0.05656 (11)	0.0321 (4)
C23	0.2503 (5)	−0.42710 (14)	0.10469 (13)	0.0443 (5)
C24	0.1755 (5)	−0.43231 (14)	0.18327 (12)	0.0419 (5)
C25	0.0322 (4)	−0.36523 (14)	0.21412 (11)	0.0373 (4)
C26	−0.0385 (3)	−0.29359 (13)	0.16987 (11)	0.0300 (4)
C27	0.2894 (5)	−0.36079 (15)	−0.02729 (13)	0.0464 (5)
C28	0.2533 (7)	−0.50753 (18)	0.23351 (16)	0.0668 (8)
C29	−0.1947 (4)	−0.22545 (17)	0.21237 (13)	0.0433 (5)
H1	0.4406	0.3153	0.3193	0.027*
H2	0.3877	−0.1375	0.0464	0.030*
H1A	0.7748	0.2139	0.1800	0.034*

H1B	0.4640	0.2077	0.1462	0.034*
H2A	0.6967	0.0511	0.1963	0.032*
H2B	0.5970	0.0603	0.1000	0.032*
H3A	0.2456	0.0414	0.2213	0.032*
H3B	0.1547	0.0406	0.1222	0.032*
H13	0.8408	0.0589	0.5180	0.034*
H15	0.4767	0.2642	0.6192	0.034*
H17A	1.2078	0.1625	0.4071	0.045*
H17B	0.9468	0.1322	0.3364	0.045*
H17C	1.0196	0.0608	0.4001	0.045*
H18A	0.6564	0.1237	0.6997	0.063*
H18B	0.6113	0.0286	0.6303	0.063*
H18C	0.3716	0.0851	0.6419	0.063*
H19A	0.4166	0.3948	0.5636	0.047*
H19B	0.4502	0.3986	0.4670	0.047*
H19C	0.6924	0.4450	0.5418	0.047*
H23	0.3486	−0.4729	0.0827	0.053*
H25	−0.0207	−0.3680	0.2679	0.045*
H27A	0.4079	−0.4077	−0.0318	0.070*
H27B	0.3868	−0.2972	−0.0303	0.070*
H27C	0.1387	−0.3792	−0.0739	0.070*
H28A	0.4399	−0.4884	0.2603	0.100*
H28B	0.2293	−0.5691	0.1955	0.100*
H28C	0.1414	−0.5139	0.2774	0.100*
H29A	−0.3794	−0.2396	0.1833	0.065*
H29B	−0.1164	−0.1593	0.2095	0.065*
H29C	−0.1898	−0.2333	0.2718	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0165 (2)	0.0245 (2)	0.0277 (2)	0.00084 (15)	0.00399 (16)	0.00824 (16)
S2	0.0164 (2)	0.0394 (3)	0.0247 (2)	0.00694 (16)	0.00293 (16)	0.00866 (17)
O1	0.0223 (6)	0.0233 (6)	0.0225 (5)	0.0024 (4)	0.0057 (4)	0.0071 (4)
O2	0.0317 (6)	0.0275 (6)	0.0232 (6)	0.0057 (5)	0.0061 (5)	0.0071 (5)
O11	0.0163 (6)	0.0384 (7)	0.0363 (7)	0.0043 (5)	0.0084 (5)	0.0140 (5)
O12	0.0338 (7)	0.0221 (6)	0.0398 (7)	−0.0018 (5)	0.0064 (6)	0.0069 (5)
O21	0.0194 (6)	0.0598 (9)	0.0445 (8)	0.0175 (6)	0.0086 (6)	0.0140 (7)
O22	0.0296 (7)	0.0542 (8)	0.0236 (6)	0.0075 (6)	0.0001 (5)	0.0083 (6)
N1	0.0175 (6)	0.0231 (7)	0.0282 (7)	0.0048 (5)	0.0032 (5)	0.0079 (5)
N2	0.0226 (7)	0.0312 (8)	0.0232 (7)	0.0082 (6)	0.0062 (6)	0.0080 (6)
C1	0.0280 (9)	0.0358 (10)	0.0204 (8)	−0.0007 (7)	0.0061 (7)	0.0082 (7)
C2	0.0217 (8)	0.0345 (9)	0.0256 (8)	0.0043 (7)	0.0074 (7)	0.0056 (7)
C3	0.0254 (9)	0.0267 (9)	0.0309 (9)	0.0058 (7)	0.0089 (7)	0.0066 (7)
C11	0.0169 (7)	0.0231 (8)	0.0220 (7)	0.0006 (6)	−0.0001 (6)	0.0047 (6)
C12	0.0201 (8)	0.0289 (9)	0.0234 (8)	0.0055 (6)	0.0010 (6)	0.0069 (7)
C13	0.0336 (9)	0.0286 (9)	0.0264 (8)	0.0107 (7)	0.0038 (7)	0.0086 (7)
C14	0.0360 (10)	0.0311 (9)	0.0213 (8)	0.0041 (7)	0.0043 (7)	0.0058 (7)

C15	0.0339 (9)	0.0293 (9)	0.0222 (8)	0.0036 (7)	0.0086 (7)	0.0011 (7)
C16	0.0210 (8)	0.0231 (8)	0.0245 (8)	0.0017 (6)	0.0005 (6)	0.0002 (6)
C17	0.0284 (9)	0.0339 (10)	0.0324 (9)	0.0134 (7)	0.0079 (7)	0.0110 (7)
C18	0.0621 (14)	0.0389 (11)	0.0285 (9)	0.0089 (9)	0.0148 (9)	0.0117 (8)
C19	0.0336 (10)	0.0263 (9)	0.0329 (9)	0.0064 (7)	0.0080 (8)	0.0008 (7)
C21	0.0201 (8)	0.0289 (9)	0.0237 (8)	−0.0014 (6)	0.0029 (6)	0.0051 (7)
C22	0.0427 (11)	0.0248 (9)	0.0295 (9)	0.0035 (7)	0.0112 (8)	0.0044 (7)
C23	0.0697 (15)	0.0264 (10)	0.0416 (11)	0.0142 (9)	0.0174 (10)	0.0080 (8)
C24	0.0606 (13)	0.0281 (10)	0.0342 (10)	−0.0016 (9)	0.0044 (9)	0.0104 (8)
C25	0.0429 (11)	0.0418 (11)	0.0233 (8)	−0.0081 (8)	0.0068 (8)	0.0083 (8)
C26	0.0236 (9)	0.0385 (10)	0.0259 (8)	−0.0033 (7)	0.0074 (7)	0.0048 (7)
C27	0.0748 (15)	0.0362 (11)	0.0399 (11)	0.0238 (10)	0.0303 (11)	0.0100 (9)
C28	0.112 (2)	0.0425 (14)	0.0492 (14)	0.0148 (14)	0.0094 (14)	0.0236 (11)
C29	0.0369 (11)	0.0634 (14)	0.0341 (10)	0.0101 (9)	0.0190 (9)	0.0096 (9)

Geometric parameters (Å, º)

S1—O11	1.4312 (12)	C2—H2B	0.99
S1—O12	1.4263 (13)	C3—H3A	0.99
S1—N1	1.6608 (14)	C3—H3B	0.99
S1—C11	1.7799 (16)	C12—C17	1.507 (2)
O1—N1	1.4270 (17)	C13—H13	0.95
O1—C1	1.4448 (19)	C14—C18	1.508 (2)
C11—C12	1.414 (2)	C15—H15	0.95
C11—C16	1.413 (2)	C16—C19	1.506 (2)
C12—C13	1.399 (2)	C17—H17A	0.98
C13—C14	1.386 (2)	C17—H17B	0.98
C14—C15	1.384 (3)	C17—H17C	0.98
C15—C16	1.391 (2)	C18—H18A	0.98
S2—O21	1.4307 (13)	C18—H18B	0.98
S2—O22	1.4266 (13)	C18—H18C	0.98
S2—N2	1.6653 (14)	C19—H19A	0.98
S2—C21	1.7747 (17)	C19—H19B	0.98
O2—N2	1.4284 (17)	C19—H19C	0.98
O2—C3	1.442 (2)	C22—C27	1.515 (3)
C21—C22	1.410 (2)	C23—H23	0.95
C21—C26	1.413 (2)	C24—C28	1.508 (3)
C22—C23	1.389 (3)	C25—H25	0.95
C23—C24	1.385 (3)	C26—C29	1.512 (3)
C24—C25	1.382 (3)	C27—H27A	0.98
C25—C26	1.396 (3)	C27—H27B	0.98
N1—H1	0.9362	C27—H27C	0.98
N2—H2	0.9337	C28—H28A	0.98
C1—C2	1.510 (2)	C28—H28B	0.98
C1—H1A	0.99	C28—H28C	0.98
C1—H1B	0.99	C29—H29A	0.98
C2—C3	1.516 (2)	C29—H29B	0.98
C2—H2A	0.99	C29—H29C	0.98

O12—S1—O11	118.68 (7)	C11—C16—C19	125.32 (15)
O12—S1—N1	104.25 (7)	C12—C17—H17A	109.5
O11—S1—N1	105.68 (7)	C12—C17—H17B	109.5
O12—S1—C11	111.31 (8)	H17A—C17—H17B	109.5
O11—S1—C11	109.01 (7)	C12—C17—H17C	109.5
N1—S1—C11	107.09 (7)	H17A—C17—H17C	109.5
O22—S2—O21	118.47 (8)	H17B—C17—H17C	109.5
O22—S2—N2	104.20 (7)	C14—C18—H18A	109.5
O21—S2—N2	105.91 (8)	C14—C18—H18B	109.5
O22—S2—C21	110.46 (8)	H18A—C18—H18B	109.5
O21—S2—C21	110.03 (8)	C14—C18—H18C	109.5
N2—S2—C21	106.92 (7)	H18A—C18—H18C	109.5
N1—O1—C1	108.14 (11)	H18B—C18—H18C	109.5
N2—O2—C3	108.95 (11)	C16—C19—H19A	109.5
O1—N1—S1	109.42 (9)	C16—C19—H19B	109.5
O1—N1—H1	107.3	H19A—C19—H19B	109.5
S1—N1—H1	109.3	C16—C19—H19C	109.5
O2—N2—S2	107.96 (9)	H19A—C19—H19C	109.5
O2—N2—H2	107.5	H19B—C19—H19C	109.5
S2—N2—H2	107.8	C22—C21—C26	121.03 (16)
O1—C1—C2	106.71 (13)	C22—C21—S2	118.36 (12)
O1—C1—H1A	110.4	C26—C21—S2	120.46 (14)
C2—C1—H1A	110.4	C23—C22—C21	117.73 (16)
O1—C1—H1B	110.4	C23—C22—C27	116.74 (17)
C2—C1—H1B	110.4	C21—C22—C27	125.53 (16)
H1A—C1—H1B	108.6	C24—C23—C22	123.11 (19)
C1—C2—C3	112.71 (14)	C24—C23—H23	118.4
C1—C2—H2A	109.0	C22—C23—H23	118.4
C3—C2—H2A	109.0	C25—C24—C23	117.59 (18)
C1—C2—H2B	109.0	C25—C24—C28	121.6 (2)
C3—C2—H2B	109.0	C23—C24—C28	120.8 (2)
H2A—C2—H2B	107.8	C24—C25—C26	123.00 (17)
O2—C3—C2	110.72 (13)	C24—C25—H25	118.5
O2—C3—H3A	109.5	C26—C25—H25	118.5
C2—C3—H3A	109.5	C25—C26—C21	117.53 (17)
O2—C3—H3B	109.5	C25—C26—C29	116.59 (16)
C2—C3—H3B	109.5	C21—C26—C29	125.88 (17)
H3A—C3—H3B	108.1	C22—C27—H27A	109.5
C16—C11—C12	121.29 (14)	C22—C27—H27B	109.5
C16—C11—S1	118.59 (12)	H27A—C27—H27B	109.5
C12—C11—S1	119.99 (12)	C22—C27—H27C	109.5
C13—C12—C11	117.20 (15)	H27A—C27—H27C	109.5
C13—C12—C17	116.56 (15)	H27B—C27—H27C	109.5
C11—C12—C17	126.25 (15)	C24—C28—H28A	109.5
C14—C13—C12	123.03 (16)	C24—C28—H28B	109.5
C14—C13—H13	118.5	H28A—C28—H28B	109.5
C12—C13—H13	118.5	C24—C28—H28C	109.5

C15—C14—C13	117.85 (16)	H28A—C28—H28C	109.5
C15—C14—C18	120.55 (16)	H28B—C28—H28C	109.5
C13—C14—C18	121.59 (17)	C26—C29—H29A	109.5
C14—C15—C16	122.87 (16)	C26—C29—H29B	109.5
C14—C15—H15	118.6	H29A—C29—H29B	109.5
C16—C15—H15	118.6	C26—C29—H29C	109.5
C15—C16—C11	117.74 (15)	H29A—C29—H29C	109.5
C15—C16—C19	116.94 (15)	H29B—C29—H29C	109.5
C12—C11—S1—N1	90.86 (13)	C18—C14—C15—C16	−178.50 (17)
C11—S1—N1—O1	−56.25 (11)	C14—C15—C16—C11	−1.4 (3)
S1—N1—O1—C1	−114.34 (11)	C14—C15—C16—C19	178.56 (16)
N1—O1—C1—C2	176.00 (12)	C12—C11—C16—C15	0.6 (2)
O1—C1—C2—C3	59.76 (18)	S1—C11—C16—C15	176.39 (12)
C22—C21—S2—N2	−83.82 (14)	C12—C11—C16—C19	−179.36 (15)
C21—S2—N2—O2	−59.15 (11)	S1—C11—C16—C19	−3.5 (2)
S2—N2—O2—C3	−126.22 (11)	O22—S2—C21—C22	28.96 (16)
N2—O2—C3—C2	−80.35 (16)	O21—S2—C21—C22	161.60 (13)
O2—C3—C2—C1	−174.31 (13)	O22—S2—C21—C26	−155.40 (13)
O12—S1—N1—O1	−174.30 (9)	O21—S2—C21—C26	−22.75 (16)
O11—S1—N1—O1	59.86 (10)	N2—S2—C21—C26	91.82 (14)
O22—S2—N2—O2	−176.15 (9)	C26—C21—C22—C23	1.1 (3)
O21—S2—N2—O2	58.17 (11)	S2—C21—C22—C23	176.68 (15)
O12—S1—C11—C16	28.30 (15)	C26—C21—C22—C27	−178.34 (18)
O11—S1—C11—C16	161.08 (12)	S2—C21—C22—C27	−2.7 (3)
N1—S1—C11—C16	−85.04 (13)	C21—C22—C23—C24	−0.6 (3)
O12—S1—C11—C12	−155.80 (12)	C27—C22—C23—C24	178.8 (2)
O11—S1—C11—C12	−23.03 (15)	C22—C23—C24—C25	0.1 (3)
C16—C11—C12—C13	0.2 (2)	C22—C23—C24—C28	−178.7 (2)
S1—C11—C12—C13	−175.63 (12)	C23—C24—C25—C26	−0.1 (3)
C16—C11—C12—C17	−179.76 (15)	C28—C24—C25—C26	178.7 (2)
S1—C11—C12—C17	4.5 (2)	C24—C25—C26—C21	0.5 (3)
C11—C12—C13—C14	−0.1 (2)	C24—C25—C26—C29	−179.80 (18)
C17—C12—C13—C14	179.80 (16)	C22—C21—C26—C25	−1.0 (2)
C12—C13—C14—C15	−0.6 (3)	S2—C21—C26—C25	−176.53 (13)
C12—C13—C14—C18	179.27 (17)	C22—C21—C26—C29	179.33 (17)
C13—C14—C15—C16	1.4 (3)	S2—C21—C26—C29	3.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O11^{i}	0.94	1.97	2.865 (2)	160
N2—H2···O21^{ii}	0.93	1.97	2.864 (2)	159
C1—H1*A*···O22^{iii}	0.99	2.57	3.337 (2)	134
C1—H1*B*···O22^{iv}	0.99	2.56	3.518 (2)	163

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