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Structural and physicochemical characterization of sulfonylhydrazone derivatives designed as hypoglycemic agents

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Supporting information

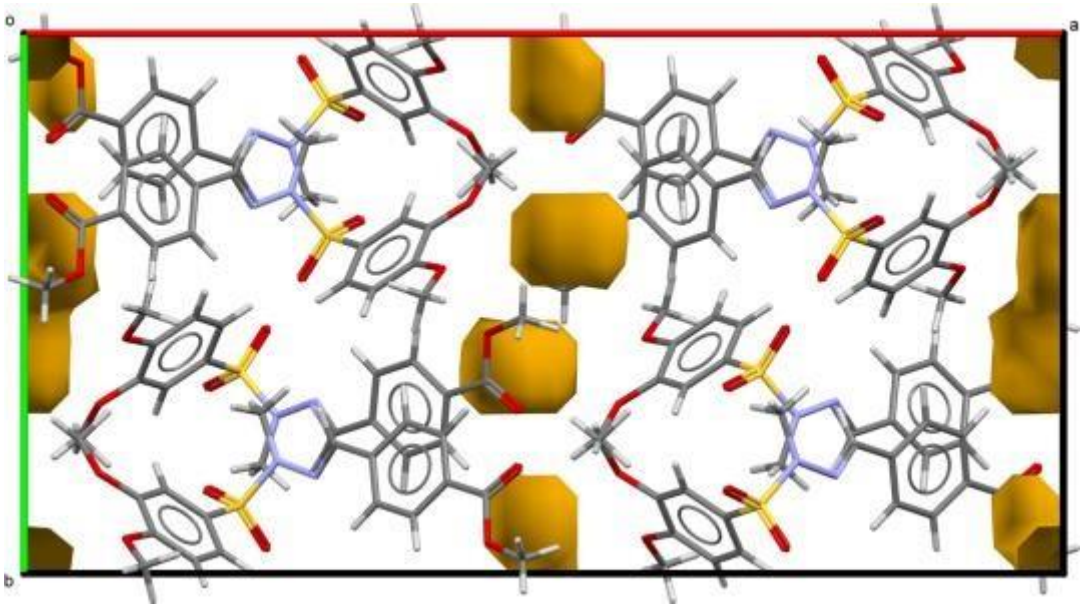

Figure S1. Crystal structure arrangement of (2) evidencing some voids (yellow channels) in the unit cell. Atoms are indicated as follows: carbon (gray), hydrogen (light gray), oxygen (red), nitrogen (blue), sulfur (yellow) and voids (yellow channels).

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Table S1. Compact nomenclature for the centre of gravity (Cg) for the aromatic rings in (**1**) and (**2**).

	(**1**)	(**2**)
Cg(A)	C_4-C_8-C_{11}-C_{15}-C_{12}-C_9	C_8-C_{12}-C_{15}-C_{19}-C_{16}-C_{13}
Cg(B)	C_{10}-C_{13}-C_{17}-C_{21}-C_{18}-C_{14}	C_{14}-C_{17}-C_{21}-C_{25}-C_{22}-C_{18}

Table S2. Selected π-π-stacking and T-shaped non-covalent interactions between aromatic rings in **1**. Distances are measured in Å and angles in (°) between adjacent centroids (Cg).

Centroid (I)…Centroid (J)	**Distance (Å)**	**Angle (°)**	**Symmetry codes**
π-π			
Cg (A) … Cg (B)	5.167(12)	9	*1/2+x,1/2-y,2-z*
T-shaped			
Cg (A) … Cg (A)	5.890(12)	61	1/2-x,-y,1/2+z

Table S3. Selected π-π-stacking and T-shaped non-covalent interactions between aromatic rings in (**2**). Distances are measured in Å and angles in (°) between adjacent centroids (Cg).

Centroid (I)…Centroid (J)	**Distance (Å)**	**Angle (°)**	**Symmetry codes**
π-π			
Cg (A) … Cg (B)	4.88(2)	29	*x,1/2-y,-1/2+z*
T-shaped			
Cg (A) … Cg (A)	5.44(2)	58	1/2-x,1-y,1/2+z

Table S4. Fractional coordinates of the structure (**1**).

Atom	***x***	***y***	***z***
N(1)	0.13953(63)	0.2350(13)	0.5044(19)
S(2)	0.19937(28)	0.31987(59)	0.50170(86)
N(3)	0.10618(79)	0.2384(15)	0.6682(21)
C(4)	0.24837(91)	0.2539(24)	0.6590(32)
O(5)	0.22403(51)	0.3080(14)	0.3193(17)
O(6)	0.18396(49)	0.4434(11)	0.5658(16)

C(7)	0.06430(81)	0.1571(20)	0.6837(26)
C(8)	0.26482(98)	0.3213(22)	0.8131(27)
C(9)	0.27081(82)	0.1355(19)	0.6283(29)
C(10)	0.02586(97)	0.1544(24)	0.8490(31)
C(11)	0.30367(81)	0.2702(19)	0.9397(28)
C(12)	0.3102(11)	0.0833(21)	0.7536(33)
C(13)	-0.01227(98)	0.0550(20)	0.8763(29)
C(14)	0.03106(68)	0.2457(19)	0.9836(31)
C(15)	0.32646(94)	0.1510(22)	0.9106(30)
O(16)	0.33562(57)	-0.0324(14)	0.7342(17)
C(17)	-0.04431(77)	0.0458(17)	1.0373(27)
C(18)	-0.00125(86)	0.2366(21)	1.1450(28)
O(19)	0.36443(48)	0.09274(99)	1.0276(18)
C(20)	0.32870(60)	-0.0956(12)	0.5617(23)
C(21)	-0.03939(97)	0.1375(22)	1.1711(32)
C(22)	0.37917(64)	0.1580(15)	1.1926(23)
C(23)	-0.07361(94)	0.1292(20)	1.3435(27)
O(24)	-0.07551(50)	0.2155(11)	1.4513(15)
O(25)	-0.10742(52)	0.0252(12)	1.3586(18)
C(26)	-0.14090(67)	0.0074(14)	1.5225(22)
H(27)	0.12906(63)	0.1891(13)	0.4111(19)
H(28)	0.05193(81)	0.1116(20)	0.5742(26)
H(29)	0.24870(98)	0.4035(22)	0.8354(27)
H(30)	0.25954(82)	0.0905(19)	0.5195(29)
H(31)	0.31506(81)	0.3171(19)	1.0481(28)
H(32)	-0.01425(98)	-0.0097(20)	0.7807(29)
H(33)	0.05756(68)	0.3154(19)	0.9660(31)
H(34)	-0.07072(77)	-0.0246(17)	1.0496(27)
H(35)	0.00111(86)	0.3010(21)	1.2368(28)
H(36)	0.34409(60)	-0.0449(12)	0.4591(23)

H(37)	0.34619(60)	-0.1757(12)	0.5576(23)
H(38)	0.28579(60)	-0.1068(12)	0.5306(23)
H(39)	0.34400(64)	0.1729(15)	1.2627(23)
H(40)	0.40600(64)	0.1085(15)	1.2645(23)
H(41)	0.39730(64)	0.2366(15)	1.1623(23)
H(42)	-0.17156(67)	0.0752(14)	1.5271(22)
H(43)	-0.16236(67)	-0.0703(14)	1.5240(22)
H(44)	-0.11856(67)	0.0153(14)	1.6340(22)

Table S5. Some selected bond distances for the structure (**1**).

Bonds	Lengths (Å)
N(1)-S(2)	1.63(2)
N(1)-N(3)	1.41(2)
N(1)-H(27)	0.87(2)
S(2)-C(4)	1.74(2)
S(2)-O(5)	1.44(1)
S(2)-O(6)	1.44(1)
N(3)-C(7)	1.29(3)
C(4)-C(8)	1.38(3)
C(4)-C(9)	1.38(3)
C(7)-C(10)	1.48(3)
C(7)-H(28)	0.97(3)
C(8)-C(11)	1.38(3)
C(8)-H(29)	0.96(3)
C(9)-C(12)	1.39(3)
C(9)-H(30)	0.96(3)
C(10)-C(13)	1.38(3)
C(10)-C(14)	1.38(3)
C(11)-C(15)	1.39(3)
C(11)-H(31)	0.97(3)

C(12)-C(15)	1.40(3)
C(12)-O(16)	1.37(3)
C(13)-C(17)	1.38(3)
C(13)-H(32)	0.98(3)
C(14)-C(18)	1.38(3)
C(14)-H(33)	0.97(3)
C(15)-O(19)	1.36(2)
O(16)-C(20)	1.43(2)
C(17)-C(21)	1.38(3)
C(17)-H(34)	0.97(3)
C(18)-C(21)	1.38(3)
C(18)-H(35)	0.96(3)
O(19)-C(22)	1.42(2)
C(20)-H(36)	0.98(2)
C(20)-H(37)	0.94(2)
C(20)-H(38)	1.01(2)
C(21)-C(23)	1.47(3)
C(22)-H(39)	0.96(2)
C(22)-H(40)	0.96(2)
C(22)-H(41)	0.96(2)
C(23)-O(24)	1.21(2)
C(23)-O(25)	1.35(2)
O(25)-C(26)	1.42(2)
C(26)-H(42)	1.01(2)
C(26)-H(43)	0.96(2)
C(26)-H(44)	0.96(2)

Table S6. Some selected bond angles for the structure (**1**).

Bonds	Angles (°)
S(2)-N(1)-N(3)	116(1)
S(2)-N(1)-H(27)	122(2)
N(3)-N(1)-H(27)	122(2)
N(1)-S(2)-C(4)	107(1)
N(1)-S(2)-O(5)	106.6(8)
N(1)-S(2)-O(6)	107.6(8)
C(4)-S(2)-O(5)	108(1)
C(4)-S(2)-O(6)	108(1)
O(5)-S(2)-O(6)	118.1(8)
N(1)-N(3)-C(7)	117(2)
S(2)-C(4)-C(8)	119(2)
S(2)-C(4)-C(9)	120(2)
C(8)-C(4)-C(9)	121(2)
N(3)-C(7)-C(10)	121(2)
N(3)-C(7)-H(28)	119(2)
C(10)-C(7)-H(28)	119(2)
C(4)-C(8)-C(11)	120(2)
C(4)-C(8)-H(29)	120(3)
C(11)-C(8)-H(29)	119(2)
C(4)-C(9)-C(12)	120(2)
C(4)-C(9)-H(30)	120(2)
C(12)-C(9)-H(30)	120(2)
C(7)-C(10)-C(13)	120(2)
C(7)-C(10)-C(14)	120(2)
C(13)-C(10)-C(14)	120(2)
C(8)-C(11)-C(15)	120(2)
C(8)-C(11)-H(31)	120(2)
C(15)-C(11)-H(31)	120(2)

C(9)-C(12)-C(12)	120(2)
C(9)-C(12)-O(16)	124(2)
C(15)-C(12)-O(16)	116(2)
C(10)-C(13)-C(17)	120(2)
C(10)-C(13)-H(32)	118(2)
C(17)-C(13)-H(32)	122(2)
C(10)-C(14)-C(18)	120(2)
C(10)-C(14)-H(33)	120(2)
C(18)-C(14)-H(33)	120(2)
C(11)-C(15)-C(12)	120(2)
C(11)-C(15)-O(19)	124(2)
C(12)-C(15)-O(19)	116(2)
C(12)-O(16)-C(20)	118(1)
C(13)-C(17)-C(21)	120(2)
C(13)-C(17)-H(34)	117(2)
C(21)-C(17)-H(34)	122(2)
C(14)-C(18)-C(21)	120(2)
C(14)-C(18)-H(35)	120(2)
C(21)-C(18)-H(35)	119(2)
C(15)-O(19)-C(22)	117(1)
O(16)-C(20)-H(36)	111(2)
O(16)-C(20)-H(37)	114(2)
O(16)-C(20)-H(38)	111(2)
H(36)-C(20)-H(37)	109(2)
H(36)-C(20)-H(38)	104(2)
H(37)-C(20)-H(38)	107(2)
C(17)-C(21)-C(18)	120(2)
C(17)-C(21)-C(23)	121(2)
C(18)-C(21)-C(23)	120(2)
O(19)-C(22)-H(39)	109(2)
O(19)-C(22)-H(40)	110(2)

O(19)-C(22)-H(41)	110(2)
H(39)-C(22)-H(40)	109(2)
H(39)-C(22)-H(41)	109(2)
H(40)-C(22)-H(41)	109(2)
C(21)-C(23)-O(24)	121(2)
C(21)-C(23)-O(25)	115(2)
O(24)-C(23)-O(25)	124(2)
C(23)-O(25)-C(26)	119(1)
O(25)-C(26)-H(42)	108(2)
O(25)-C(26)-H(43)	113(2)
O(25)-C(26)-H(44)	114(2)
H(42)-C(26)-H(43)	106(2)
H(42)-C(26)-H(43)	106(2)
H(43)-C(26)-H(44)	110(2)

Table S7. Some selected torsion angles for the structure (**1**).

Bonds	Angles (°)
N(3)-N(1)-S(2)-C(4)	67(1)
N(3)-N(1)-S(2)-O(5)	-177(1)
N(3)-N(1)-S(2)-O(6)	-49(1)
H(27)-N(1)-S(2)-C(4)	-112(2)
H(27)-N(1)-S(2)-O(5)	4(2)
H(27)-N(1)-S(2)-O(6)	132(2)
S(2)-N(1)-N(3)-C(7)	-169(1)
H(27)-N(1)-N(3)-C(7)	10(3)
N(1)-S(2)-C(4)-C(8)	-116(2)
N(1)-S(2)-C(4)-C(9)	65(2)

O(5)-S(2)-C(4)-C(8)	130(2)
O(5)-S(2)-C(4)-C(9)	-50(2)
O(6)-S(2)-C(4)-C(8)	0(2)
O(5)-S(2)-C(4)-C(9)	-179(2)
N(1)-N(3)-C(7)-C(10)	-179(2)
N(1)-N(3)-C(7)-H(28)	-14(3)
S(2)-C(4)-C(8)-C(11)	180(2)
S(2)-C(4)-C(8)-H(29)	1(4)
C(9)-C(4)-C(8)-C(11)	-1(3)
C(9)-C(4)-C(8)-H(29)	-179(3)
S(2)-C(4)-C(9)-C(12)	180(2)
S(2)-C(4)-C(9)-H(30)	1(3)
C(8)-C(4)-C(9)-C(12)	0(3)
C(8)-C(4)-C(9)-H(30)	-179(2)
N(3)-C(7)-C(10)-C(13)	-170(2)
N(3)-C(7)-C(10)-C(14)	5(3)
H(28)-C(7)-C(10)-C(13)	25(3)
H(28)-C(7)-C(10)-C(14)	-160(2)
C(4)-C(8)-C(11)-C(15)	0(3)
C(4)-C(8)-C(11)-H(31)	-180(2)
H(29)-C(8)-C(11)-C(15)	179(3)
H(29)-C(8)-C(11)-H(31)	-1(4)
C(4)-C(9)-C(12)-C(15)	0(3)
C(4)-C(9)-C(12)-O(16)	-179(2)
H(30)-C(9)-C(12)-C(15)	179(2)
H(30)-C(9)-C(12)-O(16)	0(4)
C(7)-C(10)-C(13)-C(17)	174(2)
C(7)-C(10)-C(13)-H(32)	-3(4)
C(14)-C(10)-C(13)-C(17)	-1(3)
C(14)-C(10)-C(13)-H(32)	-178(2)
C(14)-C(10)-C(14)-C(18)	-174(2)

C(7)-C(10)-C(14)-H(33)	5(4)
C(13)-C(10)-C(14)-C(18)	1(3)
C(13)-C(10)-C(14)-H(33)	180(2)
C(8)-C(11)-C(15)-C(12)	0(3)
C(8)-C(11)-C(15)-O(19)	-179(2)
H(31)-C(11)-C(15)-C(12)	-180(2)
H(31)-C(11)-C(15)-O(19)	1(4)
C(9)-C(12)-C(15)-C(11)	-1(3)
C(9)-C(12)-C(15)-O(19)	179(2)
O(16)-C(12)-C(15)-C(11)	179(2)
O(16)-C(12)-C(15)-O(19)	-2(3)
C(9)-C(12)-O(16)-C(20)	10(3)
C(15)-C(12)-O(16)-C(20)	-169(2)
C(10)-C(13)-C(17)-C(21)	1(3)
C(10)-C(13)-C(17)-H(34)	179(2)
H(32)-C(13)-C(17)-C(21)	179(3)
H(32)-C(13)-C(17)-H(34)	-4(4)
C(10)-C(14)-C(18)-C(21)	-1(3)
C(10)-C(14)-C(18)-H(35)	-178(3)
H(33)-C(14)-C(18)-C(21)	180(2)
H(33)-C(14)-C(18)-H(35)	3(4)
C(11)-C(15)-O(19)-C(22)	3(3)
C(12)-C(15)-O(19)-C(22)	-177(2)
C(12)-O(16)-C(20)-H(36)	58(2)
C(12)-O(16)-C(20)-H(37)	-178(2)
C(12)-O(16)-C(20)-H(38)	-57(2)
C(13)-C(16)-C(21)-C(18)	-2(3)
C(12)-C(17)-C(21)-C(23)	180(2)
H(34)-C(17)-C(21)-C(18)	-179(2)
H(34)-C(17)-C(21)-C(23)	2(4)
C(14)-C(17)-C(21)-C(18)	1(3)

C(14)-C(18)-C(21)-C(23)	-180(2)
H(35)-C(18)-C(21)-C(17)	178(2)
H(35)-C(18)-C(21)-C(23)	-3(4)
C(15)-O(19)-C(22)-H(39)	60(2)
C(15)-O(19)-C(22)-H(40)	180(2)
C(15)-O(19)-C(22)-H(41)	-60(2)
C(17)-C(21)-C(23)-O(24)	-171(2)
C(17)-C(21)-C(23)-O(25)	2(3)
C(18)-C(21)-C(23)-O(24)	11(3)
C(18)-C(21)-C(23)-O(25)	-177(2)
C(21)-C(21)-O(25)-C(26)	178(2)
O(24)-C(23)-O(25)-C(26)	-9(3)
C(23)-O(25)-C(26)-H(42)	66(2)
C(23)-O(25)-C(26)-H(43)	-178(2)
C(23)-O(25)-C(26)-H(44)	-51(2)

Table S8. Fractional coordinates of the structure (**2**).

Atom	*x*	*y*	*z*
O(1)	0.0153(9)	0.3992(19)	0.453(3)
H(2)	0.013(11)	0.335(14)	0.45(2)
H(3)	-0.014(9)	0.425(17)	0.44(3)
N(4)	0.2607(13)	0.293(2)	0.533(4)
S(5)	0.2944(5)	0.3769(8)	0.5793(14)
N(6)	0.2233(12)	0.318(2)	0.444(3)
C(7)	0.2657(8)	0.2051(19)	0.599(3)
C(8)	0.3277(18)	0.400(3)	0.422(5)
O(9)	0.3237(8)	0.3429(14)	0.693(3)
O(10)	0.2643(10)	0.4500(17)	0.6090(19)
C(11)	0.2025(13)	0.259(2)	0.368(3)
C(12)	0.3660(14)	0.347(2)	0.390(4)

C(13)	0.3123(13)	0.462(2)	0.322(4)
C(14)	0.1657(15)	0.283(3)	0.265(4)
C(15)	0.3902(16)	0.360(3)	0.262(5)
C(16)	0.3366(16)	0.476(2)	0.191(4)
C(17)	0.1608(14)	0.370(3)	0.214(4)
C(18)	0.1335(15)	0.220(2)	0.214(4)
C(19)	0.3757(15)	0.424(3)	0.162(4)
O(20)	0.4289(10)	0.3142(15)	0.221(2)
C(21)	0.1258(14)	0.392(3)	0.117(4)
C(22)	0.0988(13)	0.243(2)	0.117(3)
O(23)	0.4025(10)	0.4300(14)	0.042(2)
C(24)	0.4474(10)	0.2476(18)	0.317(3)
C(25)	0.0943(15)	0.330(3)	0.067(4)
C(26)	0.3928(10)	0.4958(18)	-0.067(3)
C(27)	0.0572(15)	0.355(3)	-0.038(4)
O(28)	0.0225(10)	0.3084(17)	-0.061(2)
O(29)	0.0610(8)	0.4399(17)	-0.085(3)
C(30)	0.0199(11)	0.4746(17)	-0.153(2)
H(31)	0.2555(8)	0.2121(19)	0.698(3)
H(32)	0.2970(8)	0.1831(19)	0.599(3)
H(33)	0.2461(8)	0.1631(19)	0.550(3)
H(34)	0.1985(13)	0.191(2)	0.407(3)
H(35)	0.3779(14)	0.301(2)	0.474(4)
H(36)	0.2803(13)	0.500(2)	0.336(4)
H(37)	0.3243(16)	0.522(2)	0.108(4)
H(38)	0.1897(14)	0.414(3)	0.242(4)
H(39)	0.1314(15)	0.154(2)	0.262(4)
H(40)	0.1283(14)	0.458(3)	0.066(4)
H(41)	0.0700(13)	0.199(2)	0.088(3)
H(42)	0.4225(10)	0.1929(18)	0.323(3)
H(43)	0.4801(10)	0.2249(18)	0.268(3)

H(44)	0.4536(10)	0.2767(18)	0.425(3)
H(45)	0.3914(10)	0.5542(18)	-0.025(3)
H(46)	0.4177(10)	0.4953(18)	-0.136(3)
H(47)	0.3641(10)	0.4823(18)	-0.115(3)
H(48)	-0.0042(11)	0.4540(17)	-0.096(2)
H(49)	0.0217(11)	0.5396(17)	-0.158(2)
H(50)	0.0186(11)	0.4525(17)	-0.252(2)

Table S9. Some selected bond distances for the structure (**2**).

Bonds	Lengths (Å)
O(1)-H(2)	1.0(2)
O(1)-H(3)	0.9(3)
N(4)-S(5)	1.65(4)
N(4)-N(6)	1.40(5)
N(4)-C(7)	1.46(4)
S(5)-C(8)	1.77(5)
S(5)-O(9)	1.44(3)
S(5)-O(10)	1.43(3)
N(6)-C(11)	1.28(4)
C(7)-H(31)	0.96(4)
C(7)-H(32)	0.96(3)
C(7)-H(33)	0.96(4)
C(8)-C(12)	1.39(6)
C(8)-C(13)	1.38(6)
C(11)-C(14)	1.47(5)
C(11)-H(34)	1.09(4)
C(12)-C(15)	1.38(6)
C(12)-H(35)	1.09(5)

C(13)-C(16)	1.40(5)
C(13)-H(36)	1.09(5)
C(14)-C(17)	1.40(6)
C(14)-C(18)	1.41(6)
C(15)-C(19)	1.39(6)
C(15)-O(20)	1.37(5)
C(16)-C(19)	1.40(6)
C(16)-H(37)	1.09(5)
C(17)-C(21)	1.39(6)
C(17)-H(38)	1.10(6)
C(18)-C(22)	1.38(5)
C(18)-H(39)	1.09(4)
C(19)-O(23)	1.35(4)
O(20)-C(24)	1.44(4)
C(21)-C(25)	1.38(6)
C(21)-H(40)	1.10(6)
C(22)-C(25)	1.39(5)
C(22)-H(41)	1.10(5)
O(23)-C(26)	1.43(3)
C(24)-H(42)	1.09(4)
C(24)-H(43)	1.10(4)
C(24)-H(44)	1.10(4)
C(25)-C(27)	1.49(6)
C(26)-H(45)	0.96(4)
C(26)-H(46)	0.96(4)
C(26)-H(47)	0.96(4)
C(27)-O(28)	1.24(5)
C(27)-O(29)	1.35(5)
O(29)-C(30)	1.44(4)
C(30)-H(48)	0.92(4)
C(30)-H(49)	0.98(4)

C(30)-H(50)	0.97(3)

Table S10. Some selected bond angles for the structure (**2**).

Bonds	Angles (°)
H(2)-O(1)-H(3)	110(22)
S(5)-N(4)-N(6)	113(3)
S(5)-N(4)-C(7)	122(3)
N(6)-N(4)-C(7)	124(3)
N(4)-S(5)-C(8)	105(2)
N(4)-S(5)-O(9)	105(2)
N(4)-S(5)-O(10)	106(2)
C(8)-S(5)-O(9)	110(2)
C(8)-S(5)-O(10)	110(2)
O(9)-S(5)-O(10)	120(2)
N(4)-N(6)-C(11)	119(3)
N(4)-C(7)-H(31)	105(3)
N(4)-C(7)-H(32)	114(3)
N(4)-C(7)-H(33)	110(3)
H(31)-C(7)-H(32)	109(3)
H(31)-C(7)-H(33)	109(3)
H(32)-C(7)-H(33)	109(3)
S(5)-C(8)-C(12)	119(3)
S(5)-C(8)-C(13)	120(3)
C(12)-C(8)-C(13)	120(4)
N(6)-C(11)-C(14)	121(3)
N(6)-C(11)-H(34)	122(3)
C(14)-C(11)-H(34)	111(3)
C(8)-C(12)-C(15)	120(4)
C(8)-C(12)-H(35)	118(4)
C(15)-C(12)-H(35)	122(4)

C(8)-C(13)-C(16)	120(4)
C(8)-C(13)-H(36)	123(4)
C(16)-C(13)-H(36)	116(4)
C(11)-C(14)-C(17)	121(4)
C(11)-C(14)-C(18)	122(3)
C(17)-C(14)-C(18)	117(4)
C(12)-C(15)-C(19)	120(4)
C(12)-C(15)-O(20)	125(4)
C(19)-C(15)-O(20)	114(4)
C(13)-C(15)-C(19)	119(3)
C(13)-C(16)-H(37)	122(4)
C(19)-C(16)-H(37)	119(4)
C(14)-C(17)-C(21)	121(4)
C(14)-C(17)-H(38)	114(4)
C(21)-C(17)-H(38)	124(4)
C(14)-C(18)-C(22)	122(3)
C(14)-C(18)-H(39)	121(4)
C(22)-C(18)-H(39)	117(4)
C(15)-C(19)-C(16)	120(4)
C(15)-C(19)-O(23)	114(4)
C(16)-C(19)-O(23)	126(4)
C(15)-O(20)-C(24)	119(3)
C(17)-C(21)-C(25)	122(4)
C(17)-C(21)-H(40)	116(4)
C(25)-C(21)-H(40)	121(4)
C(18)-C(22)-C(25)	121(3)
C(18)-C(22)-H(41)	124(3)
C(25)-C(22)-H(41)	115(3)
C(19)-O(23)-C(26)	120(3)
O(20)-C(24)-H(42)	108(3)
O(20)-C(24)-H(43)	107(3)

O(20)-C(24)-H(44)	110(3)
H(42)-C(24)-H(43)	111(3)
H(42)-C(24)-H(44)	111(3)
H(43)-C(24)-H(44)	111(3)
C(21)-C(25)-C(22)	118(4)
C(21)-C(25)-C(27)	121(4)
C(22)-C(25)-C(27)	121(4)
O(23)-C(26)-H(45)	111(3)
O(23)-C(26)-H(46)	108(3)
O(23)-C(26)-H(47)	110(3)
H(45)-C(26)-H(46)	108(4)
H(45)-C(26)-H(47)	110(4)
H(46)-C(26)-H(47)	110(4)
C(25)-C(27)-O(28)	123(4)
C(25)-C(27)-O(29)	113(3)
O(28)-C(27)-O(29)	123(4)
C(27)-O(29)-C(30)	114(3)
O(29)-C(30)-H(48)	105(3)
O(29)-C(30)-H(49)	110(3)
O(29)-C(30)-H(50)	108(3)
H(48)-C(30)-H(49)	114(3)
H(48)-C(30)-H(50)	113(3)
H(49)-C(30)-H(50)	108(3)

Table S11. Some selected torsion angles for the structure (**2**).

Bonds	Angles (°)
N(6)-N(4)-S(8)-C(8)	-76(3)
N(6)-N(4)-S(5)-O(9)	168(2)
N(6)-N(4)-S(5)-O(10)	40(3)

C(7)-N(4)-S(5)-C(8)	113(3)
C(7)-N(4)-S(5)-O(9)	-3(3)
C(7)-N(4)-S(5)-O(10)	-131(3)
S(5)-N(4)-N(6)-C(11)	161(3)
C(7)-N(4)-N(6)-C(11)	-29(5)
S(5)-N(4)-C(7)-H(31)	70(4)
S(5)-N(4)-C(7)-H(32)	-49(4)
S(5)-N(4)-C(7)-H(33)	-172(3)
N(6)-N(4)-C(7)-H(31)	-100(4)
N(6)-N(4)-C(7)-H(32)	141(4)
N(6)-N(4)-C(7)-H(33)	18(5)
N(4)-S(5)-C(8)-C(12)	-80(4)
N(4)-S(5)-C(8)-C(13)	92(4)
O(9)-S(5)-C(8)-C(12)	33(4)
O(9)-S(5)-C(8)-C(13)	-156(3)
O(10)-S(5)-C(8)-C(12)	167(3)
O(10)-S(5)-C(8)-C(13)	-22(4)
N(4)-N(6)-C(11)-C(14)	-175(3)
N(4)-N(6)-C(11)-H(34)	34(5)
S(5)-C(8)-C(12)-C(15)	175(3)
S(5)-C(8)-C(12)-H(35)	-11(6)
C(13)-C(8)-C(12)-C(15)	4(6)
C(13)-C(8)-C(12)-H(35)	177(4)
S(5)-C(8)-C(13)-C(16)	-175(3)
S(5)-C(8)-C(13)-H(36)	2(6)
C(12)-C(8)-C(13)-C(16)	-4(6)
C(12)-C(8)-C(13)-H(36)	173(4)
N(6)-C(11)-C(14)-C(17)	19(6)
N(6)-C(11)-C(14)-C(18)	-161(4)
H(34)-C(11)-C(14)-C(17)	173(4)
H(34)-C(11)-C(14)-C(18)	-7(5)

C(8)-C(12)-C(15)-C(19)	-2(6)
C(8)-C(12)-C(15)-O(20)	178(4)
H(35)-C(12)-C(15)-C(19)	-175(4)
H(35)-C(12)-C(15)-O(20)	5(7)
C(8)-C(13)-C(16)-C(19)	2(6)
C(8)-C(13)-C(16)-H(37)	177(4)
H(36)-C(13)-C(16)-C(19)	-175(4)
H(36)-C(13)-C(16)-H(37)	-0(6)
C(11)-C(14)-C(17)-C(21)	-180(4)
C(11)-C(14)-C(17)-H(38)	10(6)
C(18)-C(14)-C(17)-C(21)	-0(6)
C(18)-C(14)-C(17)-H(38)	-170(4)
C(11)-C(14)-C(18)-C(22)	180(3)
C(11)-C(14)-C(18)-H(39)	10(6)
C(17)-C(14)-C(18)-C(22)	0(6)
C(17)-C(14)-C(18)-H(39)	-170(4)
C(12)-C(15)-C(19)-C(16)	0(6)
C(12)-C(15)-C(19)-O(23)	180(4)
O(20)-C(15)-C(19)-C(16)	-180(4)
O(20)-C(15)-C(19)-O(23)	-0(5)
C(12)-C(15)-O(20)-C(24)	-1(6)
C(19)-C(15)-O(20)-C(24)	179(3)
C(13)-C(16)-C(19)-C(15)	-0(6)
C(13)-C(16)-C(19)-O(23)	-180(4)
H(37)-C(16)-C(19)-C(15)	-175(4)
H(37)-C(16)-C(19)-O(23)	5(7)
C(14)-C(17)-C(21)-C(15)	0(6)
C(14)-C(17)-C(21)-H(40)	-169(4)
H(38)-C(17)-C(21)-C(25)	169(5)
H(38)-C(17)-C(21)-H(40)	1(7)
C(14)-C(18)-C(22)-C(25)	-0(6)

C(14)-C(18)-C(22)-H(41)	-170(4)
H(39)-C(18)-C(22)-C(25)	170(4)
H(39)-C(18)-C(22)-H(41)	0(6)
C(15)-C(19)-O(23)-C(26)	-177(3)
C(16)-C(19)-O(23)-C(26)	2(5)
C(15)-O(20)-C(24)-H(42)	67(4)
C(15)-O(20)-C(24)-H(43)	-174(3)
C(15)-O(20)-C(24)-H(44)	-54(4)
C(17)-C(21)-C(25)-C(22)	-0(6)
C(17)-C(21)-C(25)-C(27)	-180(4)
H(40)-C(21)-C(25)-C(22)	168(4)
H(40)-C(21)-C(25)-C(27)	-11(7)
C(18)-C(22)-C(25)-C(21)	0(6)
C(18)-C(22)-C(25)-C(27)	180(4)
H(41)-C(22)-C(25)-C(21)	171(4)
H(41)-C(22)-C(25)-C(27)	-10(6)
C(19)-O(23)-C(26)-H(45)	54(4)
C(19)-O(23)-C(26)-H(46)	172(3)
C(19)-O(23)-C(26)-H(47)	-68(4)
C(21)-C(25)-C(27)-O(28)	-163(4)
C(21)-C(25)-C(27)-O(29)	5(6)
C(22)-C(25)-C(27)-O(28)	17(6)
C(22)-C(25)-C(27)-O(29)	-174(3)
C(25)-C(27)-O(29)-C(30)	-164(3)
O(28)-C(27)-O(29)-C(30)	5(5)
C(27)-O(29)-C(30)-H(48)	41(4)
C(27)-O(29)-C(30)-H(49)	163(3)
C(27)-O(29)-C(30)-H(50)	-79(4)