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Molecular packings and specific-bond patterns in sulfonamides

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Electronic Supplementary Information

Table 1. Crystal data and structure refinement for compound I

Empirical formula	$C_{15}H_{16}N_2O_3S$
Formula weight	304.36
Temperature/K	293.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.0437(3)
b/Å	9.7182(2)
c/Å	19.7716(6)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	1545.55(8)
Z	4
ρ_{calc}mg/mm^3	1.308
m/mm^{-1}	1.964
F(000)	640.0
Crystal size/mm^3	? × ? × ?
2Θ range for data collection	8.94 to 152.66°
Index ranges	$-9 \leq h \leq 10$, $-11 \leq k \leq 12$, $-24 \leq l \leq 24$
Reflections collected	15858
Independent reflections	3224[R(int) = 0.0353]
Data/restraints/parameters	3224/0/215
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0297, wR_2 = 0.0743
Final R indexes [all data]	R_1 = 0.0321, wR_2 = 0.0763
Largest diff. peak/hole / e Å^{-3}	0.13/-0.23
Flack parameter	0.129(15)

Table 2. Bond lengths for compound I

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4244(12)	C2	C3	1.384(3)
S1	O2	1.4341(12)	C3	C4	1.378(3)
S1	N1	1.6452(14)	C4	C5	1.382(3)
S1	C1	1.7568(17)	C5	C6	1.376(3)
O3	C10	1.386(13)	C7	C8	1.488(2)
O3	C15A	1.34(2)	C7	C14	1.502(3)
O31	C10	1.357(13)	C8	C9	1.402(3)
O31	C15B	1.49(2)	C8	C13	1.382(3)
N1	N2	1.3982(18)	C9	C10	1.376(3)
N2	C7	1.278(2)	C10	C11	1.398(3)
C1	C2	1.385(2)	C11	C12	1.367(4)
C1	C6	1.384(2)	C12	C13	1.389(3)

Table 3. Bond angles for compound I

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	O2	119.75(8)	C5	C6	C1	118.99(18)
O1	S1	N1	104.91(8)	N2	C7	C8	115.21(15)
O1	S1	C1	109.64(9)	N2	C7	C14	123.99(17)
O2	S1	N1	106.85(7)	C8	C7	C14	120.80(16)
O2	S1	C1	107.82(7)	C9	C8	C7	119.60(15)
N1	S1	C1	107.21(8)	C13	C8	C7	121.43(18)
C15A	O3	C10	120.2(12)	C13	C8	C9	118.97(19)
C10	O31	C15B	114.1(12)	C10	C9	C8	120.44(18)
N2	N1	S1	112.27(10)	O3	C10	C11	116.5(6)
C7	N2	N1	117.38(14)	O31	C10	O3	12.9(14)
C2	C1	S1	119.53(12)	O31	C10	C9	125.9(6)
C6	C1	S1	119.03(13)	O31	C10	C11	113.3(6)
C6	C1	C2	121.42(16)	C9	C10	O3	123.0(6)
C3	C2	C1	118.53(17)	C9	C10	C11	120.2(2)
C4	C3	C2	120.61(19)	C12	C11	C10	119.1(2)
C3	C4	C5	120.0(2)	C11	C12	C13	121.3(2)
C6	C5	C4	120.47(19)	C8	C13	C12	120.0(2)

Table 4. Hydrogen bonds for compound I

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O2[1]	0.83(2)	2.13(2)	2.9481(18)	169.3(18)
[1]2-X,-1/2+Y,1/2-Z						

Table 5. Crystal data and structure refinement for compound II

Empirical formula	$C_{23}H_{21}N_2O_4SBr$
Formula weight	501.39
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.3535(2)
b/Å	15.3411(3)
c/Å	17.7711(5)
α/°	90.00
β/°	98.086(2)
γ/°	90.00
Volume/Å^3	2254.76(9)
Z	4
ρ_{calc}mg/mm^3	1.477
m/mm^{-1}	3.621
F(000)	1024.0
Crystal size/mm^3	0.43 × 0.30 × 0.21
2Θ range for data collection	7.64 to 153.1°
Index ranges	$-10 \leq h \leq 10$, $-14 \leq k \leq 19$, $-21 \leq l \leq 22$
Reflections collected	22055
Independent reflections	4720[R(int) = 0.0256]
Data/restraints/parameters	4720/0/286
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0420, wR_2 = 0.1086
Final R indexes [all data]	R_1 = 0.0462, wR_2 = 0.1119
Largest diff. peak/hole / e Å^{-3}	0.48/-0.54

Table 6. Bond lengths for compound II

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C4	1.897(3)	C5	C6	1.370(4)
S1	O1	1.4247(19)	C7	C14	1.464(3)
S1	O2	1.4267(19)	C8	C9	1.383(4)
S1	N1	1.653(2)	C8	C13	1.380(3)
S1	C8	1.760(2)	C9	C10	1.391(4)
O3	C20	1.366(3)	C10	C11	1.359(5)
O3	C23	1.416(3)	C11	C12	1.376(5)
O4	C19	1.363(3)	C12	C13	1.391(4)
O4	C22	1.434(3)	C14	C15	1.325(3)
N1	N2	1.412(3)	C15	C16	1.469(3)
N2	C7	1.295(3)	C16	C17	1.390(3)
C1	C2	1.387(3)	C16	C21	1.399(3)
C1	C6	1.400(3)	C17	C18	1.385(3)
C1	C7	1.482(3)	C18	C19	1.376(3)
C2	C3	1.381(4)	C19	C20	1.401(3)
C3	C4	1.377(4)	C20	C21	1.379(3)
C4	C5	1.382(4)			

Table 7. Bond angles for compound II

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	O2	120.54(12)	C9	C8	S1	118.79(19)
O1	S1	N1	107.27(12)	C13	C8	S1	119.96(19)
O1	S1	C8	108.09(11)	C13	C8	C9	121.2(2)
O2	S1	N1	104.76(11)	C8	C9	C10	119.0(3)
O2	S1	C8	108.70(11)	C11	C10	C9	120.2(3)
N1	S1	C8	106.68(10)	C10	C11	C12	120.8(3)
C20	O3	C23	117.9(2)	C11	C12	C13	120.2(3)
C19	O4	C22	117.33(19)	C8	C13	C12	118.6(3)
N2	N1	S1	111.60(15)	C15	C14	C7	125.4(2)
C7	N2	N1	115.74(19)	C14	C15	C16	125.8(2)
C2	C1	C6	118.0(2)	C17	C16	C15	123.7(2)
C2	C1	C7	122.5(2)	C17	C16	C21	118.2(2)
C6	C1	C7	119.6(2)	C21	C16	C15	118.1(2)
C3	C2	C1	121.2(2)	C18	C17	C16	120.9(2)
C4	C3	C2	119.2(2)	C19	C18	C17	120.7(2)
C3	C4	Br1	119.9(2)	O4	C19	C18	126.0(2)
C3	C4	C5	121.2(3)	O4	C19	C20	114.78(19)
C5	C4	Br1	118.9(2)	C18	C19	C20	119.3(2)
C6	C5	C4	119.0(2)	O3	C20	C19	114.96(19)
C5	C6	C1	121.4(2)	O3	C20	C21	125.1(2)
N2	C7	C1	114.8(2)	C21	C20	C19	119.9(2)
N2	C7	C14	124.1(2)	C20	C21	C16	121.0(2)
C14	C7	C1	121.09(19)				

Table 8. Hydrogen bonds for compound II

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O3[1]	0.85(3)	2.31(3)	3.114(3)	159(3)
N1	H1	O4[1]	0.85(3)	2.50(3)	3.175(3)	137(3)
[1]1-X,1-Y,2-Z						

Table 9. Crystal data and structure refinement for compound III

Empirical formula	$C_{15}H_{24}N_2O_6S$
Formula weight	360.42
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1$
a/Å	10.1962(11)
b/Å	5.9840(4)
c/Å	15.6595(16)
α/°	90.00
β/°	96.232(10)
γ/°	90.00
Volume/Å^3	949.80(15)
Z	2
ρ_{calc}mg/mm^3	1.260
m/mm^{-1}	1.791
F(000)	384.0
Crystal size/mm^3	0.28 × 0.07 × 0.05
2Θ range for data collection	8.72 to 153°
Index ranges	$-12 \leq h \leq 12$, $-4 \leq k \leq 7$, $-19 \leq l \leq 19$
Reflections collected	8328
Independent reflections	2865[R(int) = 0.0547]
Data/restraints/parameters	2865/3/241
Goodness-of-fit on F^2	1.104
Final R indexes [I>=2σ (I)]	R_1 = 0.0436, wR_2 = 0.0983
Final R indexes [all data]	R_1 = 0.0661, wR_2 = 0.1185
Largest diff. peak/hole / e Å^{-3}	0.21/-0.22
Flack parameter	-0.05(3)

Table 10. Bond lengths for compound III

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	N1	1.621(3)	C8	C7	1.516(4)
S1	O1	1.422(3)	C11	C12	1.532(5)
S1	O2	1.439(3)	C12	C14	1.513(7)
S1	C1	1.764(4)	C12	C13	1.506(7)
O3	C8	1.237(4)	C5	C4	1.393(6)
O5	C10	1.314(4)	C5	C6	1.375(6)
N2	C9	1.452(4)	C1	C2	1.381(5)
N2	C8	1.321(5)	C1	C6	1.375(5)
N1	C7	1.456(4)	C2	C3	1.383(6)
O4	C10	1.210(4)	C4	C3	1.373(7)
C9	C11	1.521(5)	C4	C15	1.517(6)
C9	C10	1.513(4)			

Table 11. Bond angles for compound III

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	S1	C1	106.95(16)	O4	C10	O5	123.0(3)
O1	S1	N1	105.8(2)	O4	C10	C9	124.1(3)
O1	S1	O2	120.8(2)	C14	C12	C11	111.7(4)
O1	S1	C1	108.89(19)	C13	C12	C11	110.1(4)
O2	S1	N1	106.51(17)	C13	C12	C14	111.8(5)
O2	S1	C1	107.22(19)	C6	C5	C4	121.6(4)
C8	N2	C9	123.5(3)	C2	C1	S1	120.2(3)
C7	N1	S1	117.7(2)	C6	C1	S1	119.4(3)
N2	C9	C11	109.8(3)	C6	C1	C2	120.4(4)
N2	C9	C10	110.7(3)	N1	C7	C8	112.5(3)
C10	C9	C11	110.2(3)	C1	C2	C3	119.3(4)
O3	C8	N2	123.4(3)	C5	C4	C15	120.7(5)
O3	C8	C7	119.7(3)	C3	C4	C5	117.7(4)
N2	C8	C7	116.9(3)	C3	C4	C15	121.6(5)
C9	C11	C12	114.7(3)	C5	C6	C1	119.3(4)
O5	C10	C9	112.8(3)	C4	C3	C2	121.7(4)

Table 12. Hydrogen bonds for compound III

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1N	O3[1]	0.75(5)	2.11(5)	2.856(4)	176(4)
O5	H5O	O6W[2]	1.07(5)	1.55(5)	2.579(4)	161(4)
O6W	H1W	O3[3]	0.881(10)	1.925(13)	2.802(4)	174(6)
O6W	H2W	O4[2]	0.881(10)	1.960(19)	2.819(4)	165(5)
[1]+X,-1+Y,+Z; [2]1-X,1/2+Y,1-Z; [3]1+X,+Y,+Z						