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3,5-Dichloro-*N*-(2,4-dichlorophenyl)benzenesulfonamide

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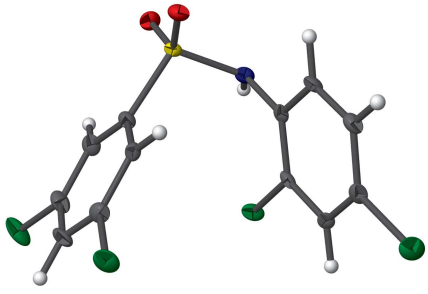
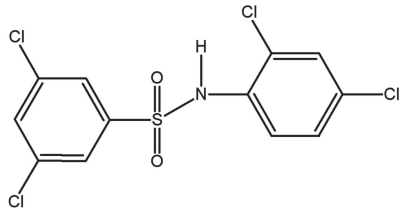
Structural data: full structural data are available from iucrdata.iucr.org

The molecule of the title compound, $C_{12}H_7Cl_4NO_2S$, is U-shaped, with the central C—S—N—C segment having a torsion angle of −58.7 (3)°. The dihedral angle between the benzene rings is 40.23 (2)°. Further, the *ortho* Cl atom on the aniline ring is *syn* to the N—H bond in the central –C—S(O_2)—NH—C– segment. In the crystal, molecules are linked by pairs of N—H···O hydrogen bonds, forming inversion dimers that enclose $R_2^2(8)$ loops. These dimers are linked by C—H···O hydrogen bonds that form a double $C(7)$ chain propagating along the *b*-axis direction. These chains are further consolidated by Cl···Cl halogen bonds [3.4331 (2) Å]. π–π contacts [centroid–centroid distance = 3.6574 (19) Å] between the aniline rings link adjacent chains into a three-dimensional supramolecular network with molecules stacked along the *b*-axis direction.

3D view



Chemical scheme



Structure description

In recent years, extensive research has been carried out on the synthesis and evaluation of the pharmacological activities of molecules containing the sulfonamide moiety (Mohan *et al.*, 2013). As part of our ongoing studies of sulfonamides (Shakuntala *et al.*, 2017), we report herein the crystal structure of the title sulfonamide derivative.

The molecule of the title compound (Fig. 1) is U shaped with the central C1—S1—N1—C7 segment displaying a torsion angle of −58.7 (3)°. The dihedral angle between the benzene rings is 40.23 (2)°. Further, the *ortho* chlorine atom on the aniline ring is *syn* to the N—H bond in the central –C—S(O_2)-NH—C– segment of the molecule.

In the crystal, pairs of molecules are linked by N1—H1···O2^{i} hydrogen bonds, forming inversion dimers that enclose $R_2^2(8)$ loops (Table 1 and Fig. 2). These dimers are joined

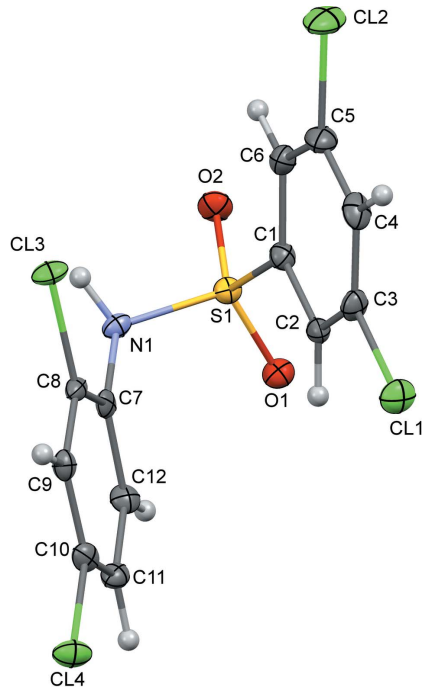


Figure 1
A view of the molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

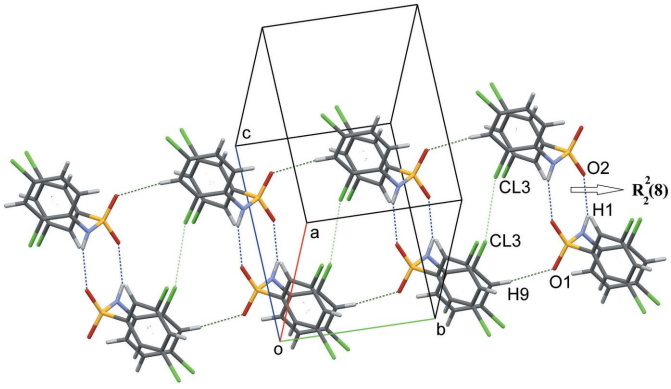


Figure 2
Double-chain architecture displayed in the crystal structure of the title compound, propagating along the *b* axis and formed by N—H···O and C—H···O hydrogen bonds (see Table 1). Cl···Cl contacts are also shown.

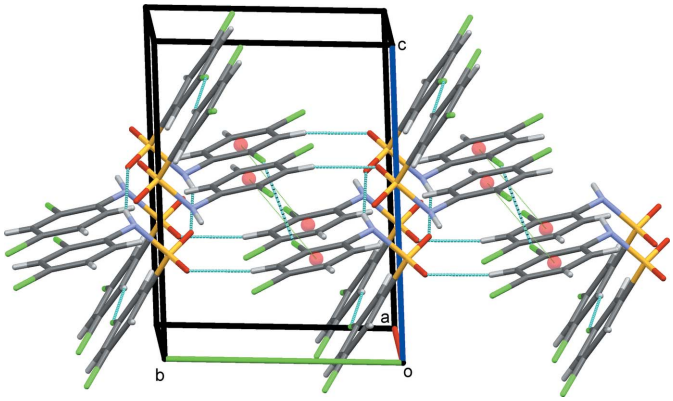


Figure 3
π_{aryl}–π_{aryl} contacts in the title compound viewed along *a*.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.20	3.0026	155
C9—H9···O1^{ii}	0.95	2.39	3.324 (4)	170

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_7Cl_4NO_2S$
M_r	371.05
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	8.1107 (4), 8.2615 (4), 11.2048 (5)
α, β, γ (°)	86.791 (2), 70.625 (2), 85.783 (2)
V (Å^3)	705.96 (6)
Z	2
Radiation type	Cu *Kα*
μ (mm^{-1})	9.01
Crystal size (mm)	0.26 × 0.23 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.144, 0.165
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6182, 2295, 2152
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.584
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.063, 0.190, 1.08
No. of reflections	2295
No. of parameters	185
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.15, −1.04

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

through C9—H9···O1^{ii} hydrogen bonds that form a double *C*(7) chain propagating along the *b*-axis direction. These chains are further consolidated by Cl3···Cl3^{iii} halogen bonds [3.4331 (2) Å; symmetry code: (iii) $-x, -y+1, -z+1$]. π–π contacts [centroid–centroid distance = 3.6574 (19) Å; symmetry code: $1-x, 1-y, 1-z$] between the C7–C12 rings, Fig. 3, link adjacent chains into a three-dimensional supramolecular network with molecules stacked along the *b*-axis direction.

Synthesis and crystallization

The title compound was prepared according to a literature method (Rodrigues *et al.*, 2015). The purity of the compound was checked by determining its melting point. Prismatic single crystals suitable for X-ray diffraction study were obtained by

slow evaporation of an ethanol solution of the compound at room temperature.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170372 [https://doi.org/10.1107/S2414314617003728]

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Crystal data

$C_{12}H_7Cl_4NO_2S$
M_r = 371.05
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.1107 (4) Å
b = 8.2615 (4) Å
c = 11.2048 (5) Å
α = 86.791 (2)°
β = 70.625 (2)°
γ = 85.783 (2)°
V = 705.96 (6) Å^3
Z = 2
$F(000)$ = 372
prism
D_x = 1.746 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 154 reflections
θ = 5.4–64.2°
μ = 9.01 mm^{-1}
T = 100 K
Prism, colourless
0.26 × 0.23 × 0.20 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.144, T_{max} = 0.165
6182 measured reflections
2295 independent reflections
2152 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 64.2°, θ_{min} = 5.4°
h = −9→9
k = −9→9
l = −12→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.190
S = 1.08
2295 reflections
185 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.153P)^2 + 0.3492P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 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}
C1	−0.0147 (4)	0.9271 (4)	0.7955 (3)	0.0146 (7)
C2	0.0650 (4)	0.8534 (4)	0.8789 (3)	0.0137 (7)
H2	0.185287	0.865134	0.866524	0.016*
C3	−0.0373 (5)	0.7626 (4)	0.9805 (3)	0.0169 (8)
C4	−0.2119 (5)	0.7464 (4)	1.0011 (3)	0.0202 (8)
H4	−0.279938	0.684198	1.071779	0.024*
C5	−0.2867 (5)	0.8225 (5)	0.9167 (4)	0.0208 (8)
C6	−0.1911 (5)	0.9131 (4)	0.8122 (3)	0.0183 (8)
H6	−0.243662	0.963513	0.754287	0.022*
C7	0.3233 (4)	0.7602 (4)	0.5954 (3)	0.0132 (7)
C8	0.2658 (4)	0.6040 (4)	0.6286 (3)	0.0123 (7)
C9	0.3685 (4)	0.4808 (4)	0.6637 (3)	0.0140 (7)
H9	0.329198	0.373986	0.683842	0.017*
C10	0.5287 (5)	0.5179 (4)	0.6686 (3)	0.0157 (8)
C11	0.5914 (5)	0.6721 (4)	0.6362 (3)	0.0160 (8)
H11	0.703132	0.694572	0.639253	0.019*
C12	0.4883 (4)	0.7922 (4)	0.5996 (3)	0.0154 (8)
H12	0.530101	0.897891	0.576927	0.018*
N1	0.2191 (4)	0.8860 (3)	0.5578 (3)	0.0142 (6)
O1	0.2543 (3)	1.0985 (3)	0.6941 (2)	0.0167 (6)
O2	0.0145 (3)	1.1270 (3)	0.6002 (2)	0.0198 (6)
S1	0.12158 (10)	1.02925 (9)	0.65887 (8)	0.0129 (3)
CL1	0.05978 (11)	0.66634 (11)	1.08447 (8)	0.0222 (3)
CL2	−0.50807 (12)	0.80140 (14)	0.94357 (9)	0.0313 (4)
CL3	0.06355 (10)	0.55785 (10)	0.62220 (8)	0.0180 (3)
CL4	0.65852 (11)	0.36568 (10)	0.71396 (8)	0.0215 (3)
H1	0.149 (4)	0.853 (5)	0.523 (4)	0.012 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0141 (17)	0.0164 (17)	0.0120 (17)	−0.0025 (13)	−0.0024 (13)	0.0005 (13)
C2	0.0123 (15)	0.0140 (17)	0.0142 (18)	−0.0004 (13)	−0.0032 (13)	−0.0038 (14)
C3	0.0211 (19)	0.0191 (19)	0.0114 (19)	−0.0003 (15)	−0.0068 (15)	0.0008 (15)
C4	0.0206 (19)	0.0231 (19)	0.0123 (18)	−0.0086 (15)	0.0022 (15)	0.0005 (15)
C5	0.0125 (17)	0.029 (2)	0.0195 (19)	−0.0047 (15)	−0.0029 (14)	−0.0018 (16)
C6	0.0179 (18)	0.023 (2)	0.0143 (18)	−0.0005 (14)	−0.0062 (15)	−0.0023 (14)
C7	0.0149 (17)	0.0174 (18)	0.0055 (16)	0.0002 (13)	−0.0014 (13)	−0.0006 (13)
C8	0.0094 (15)	0.0191 (18)	0.0077 (15)	−0.0042 (13)	−0.0012 (13)	−0.0008 (13)
C9	0.0176 (17)	0.0131 (17)	0.0098 (17)	−0.0018 (13)	−0.0025 (13)	0.0006 (13)
C10	0.0170 (17)	0.0192 (18)	0.0095 (17)	0.0017 (14)	−0.0036 (14)	0.0030 (14)
C11	0.0123 (16)	0.0219 (19)	0.0133 (18)	−0.0043 (14)	−0.0030 (13)	0.0005 (14)
C12	0.0135 (17)	0.0173 (18)	0.0128 (17)	−0.0046 (13)	−0.0008 (13)	0.0036 (13)
N1	0.0150 (14)	0.0159 (15)	0.0133 (15)	−0.0034 (11)	−0.0068 (12)	0.0024 (12)
O1	0.0172 (12)	0.0158 (12)	0.0172 (13)	−0.0052 (10)	−0.0052 (10)	0.0027 (10)

O2	0.0215 (13)	0.0180 (13)	0.0201 (14)	0.0022 (10)	−0.0084 (11)	0.0032 (10)
S1	0.0132 (5)	0.0127 (5)	0.0124 (5)	−0.0028 (4)	−0.0038 (4)	0.0030 (4)
CL1	0.0241 (5)	0.0271 (6)	0.0155 (5)	−0.0033 (4)	−0.0076 (4)	0.0072 (4)
CL2	0.0129 (5)	0.0571 (8)	0.0232 (6)	−0.0112 (4)	−0.0037 (4)	0.0027 (5)
CL3	0.0142 (5)	0.0201 (5)	0.0225 (6)	−0.0070 (4)	−0.0094 (4)	0.0045 (4)
CL4	0.0189 (5)	0.0227 (6)	0.0247 (6)	0.0014 (4)	−0.0110 (4)	0.0057 (4)

Geometric parameters (Å, º)

C1—C6	1.393 (5)	C7—N1	1.424 (4)
C1—C2	1.393 (5)	C8—C9	1.391 (5)
C1—S1	1.774 (4)	C8—CL3	1.736 (3)
C2—C3	1.385 (5)	C9—C10	1.376 (5)
C2—H2	0.9500	C9—H9	0.9500
C3—C4	1.372 (5)	C10—C11	1.391 (5)
C3—CL1	1.738 (3)	C10—CL4	1.742 (3)
C4—C5	1.384 (6)	C11—C12	1.383 (5)
C4—H4	0.9500	C11—H11	0.9500
C5—C6	1.385 (5)	C12—H12	0.9500
C5—CL2	1.740 (4)	N1—S1	1.651 (3)
C6—H6	0.9500	N1—H1	0.858 (19)
C7—C8	1.393 (5)	O1—S1	1.428 (3)
C7—C12	1.400 (5)	O2—S1	1.433 (3)
C6—C1—C2	122.3 (3)	C7—C8—CL3	119.9 (3)
C6—C1—S1	120.4 (3)	C10—C9—C8	118.1 (3)
C2—C1—S1	117.2 (3)	C10—C9—H9	120.9
C3—C2—C1	117.6 (3)	C8—C9—H9	120.9
C3—C2—H2	121.2	C9—C10—C11	122.0 (3)
C1—C2—H2	121.2	C9—C10—CL4	118.9 (3)
C4—C3—C2	122.0 (3)	C11—C10—CL4	119.1 (3)
C4—C3—CL1	119.4 (3)	C12—C11—C10	118.9 (3)
C2—C3—CL1	118.6 (3)	C12—C11—H11	120.6
C3—C4—C5	118.7 (3)	C10—C11—H11	120.6
C3—C4—H4	120.7	C11—C12—C7	120.9 (3)
C5—C4—H4	120.7	C11—C12—H12	119.6
C4—C5—C6	122.2 (3)	C7—C12—H12	119.6
C4—C5—CL2	118.3 (3)	C7—N1—S1	118.4 (2)
C6—C5—CL2	119.4 (3)	C7—N1—H1	115 (3)
C5—C6—C1	117.1 (3)	S1—N1—H1	111 (3)
C5—C6—H6	121.4	O1—S1—O2	121.08 (15)
C1—C6—H6	121.4	O1—S1—N1	107.18 (15)
C8—C7—C12	118.3 (3)	O2—S1—N1	105.43 (15)
C8—C7—N1	121.8 (3)	O1—S1—C1	107.19 (15)
C12—C7—N1	119.9 (3)	O2—S1—C1	109.28 (16)
C9—C8—C7	121.8 (3)	N1—S1—C1	105.69 (15)
C9—C8—CL3	118.3 (3)		

C6—C1—C2—C3	0.6 (5)	C8—C9—C10—C11	−1.8 (5)
S1—C1—C2—C3	−175.0 (3)	C8—C9—C10—CL4	179.4 (3)
C1—C2—C3—C4	−1.0 (5)	C9—C10—C11—C12	0.8 (5)
C1—C2—C3—CL1	178.8 (3)	CL4—C10—C11—C12	179.6 (3)
C2—C3—C4—C5	0.5 (6)	C10—C11—C12—C7	0.3 (5)
CL1—C3—C4—C5	−179.4 (3)	C8—C7—C12—C11	−0.3 (5)
C3—C4—C5—C6	0.5 (6)	N1—C7—C12—C11	179.7 (3)
C3—C4—C5—CL2	−180.0 (3)	C8—C7—N1—S1	105.4 (3)
C4—C5—C6—C1	−0.9 (6)	C12—C7—N1—S1	−74.6 (4)
CL2—C5—C6—C1	179.6 (3)	C7—N1—S1—O1	55.4 (3)
C2—C1—C6—C5	0.3 (6)	C7—N1—S1—O2	−174.4 (2)
S1—C1—C6—C5	175.8 (3)	C7—N1—S1—C1	−58.7 (3)
C12—C7—C8—C9	−0.8 (5)	C6—C1—S1—O1	150.1 (3)
N1—C7—C8—C9	179.2 (3)	C2—C1—S1—O1	−34.1 (3)
C12—C7—C8—CL3	−178.9 (3)	C6—C1—S1—O2	17.2 (4)
N1—C7—C8—CL3	1.1 (5)	C2—C1—S1—O2	−167.0 (3)
C7—C8—C9—C10	1.8 (5)	C6—C1—S1—N1	−95.8 (3)
CL3—C8—C9—C10	180.0 (3)	C2—C1—S1—N1	79.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.20	3.0026	155
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Symmetry codes: (i) −*x*, −*y*+2, −*z*+1; (ii) *x*, *y*−1, *z*.