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2-Chloro-*N*-[4-(4-chlorophenyl)-1,3-thiazol-2-yl]-acetamide

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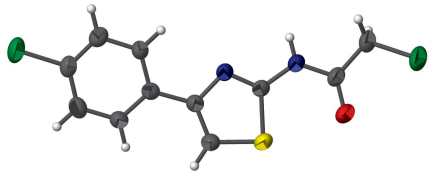
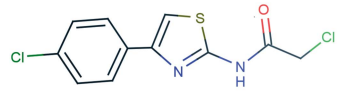
Structural data: full structural data are available from iucrdata.iucr.org

In the title acetamide, $C_{11}H_8Cl_2N_2OS$, the chlorophenyl ring is oriented at an angle of 7.1 (1)° with respect to the thiazole ring. In the crystal, molecules are linked *via* C—H···O intermolecular interactions, forming *C*(10) chains propagating in a zigzag manner along the *b* axis.

3D view



Chemical scheme



Structure description

In a continuation of our work on the crystal structure analysis of acetamide derivatives, we have undertaken a single-crystal X-ray diffraction study for the title compound, and the results are presented here. The molecular structure of the title compound is illustrated in Fig. 1. The geometry of the present structure, apart from atom Cl2. is comparable with that reported for a similar structure, namely 2-chloro-*N*-(4-phenyl-1,3-thiazol-2-yl)acetamide (II) (Saravanan *et al.*, 2016). The superposition of the structures (Fig. 2) using *Qmol* (Gans & Shalloway, 2001), gives r.m.s. deviations of 0.858 and 0.595 Å, respectively, for molecules *A* and *B* in (II). The thiazole ring is planar with a maximum deviation of 0.005 (3) Å for atom *C*7. Chlorine atom Cl2 is deviates by 0.033 (1) Å from the best plane through the chlorophenyl ring. The chlorophenyl ring is oriented at an angle of 7.1 (1)° to the thiazole ring. The molecular structure is influenced by an intramolecular C—H···N short contact (Table 1). In the crystal, C—H···O interactions link the molecules, forming *C*(10) chains propagating along the *b* axis in a zigzag manner (Fig. 3).

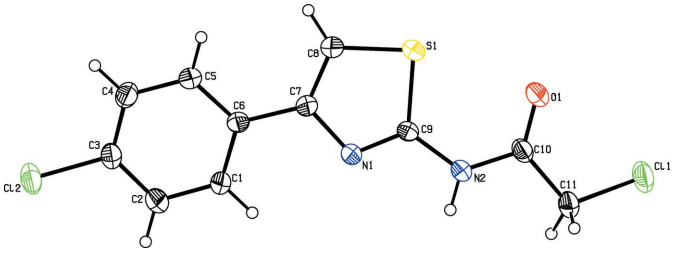


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

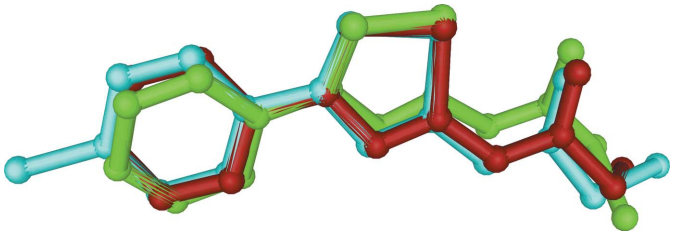


Figure 2
Superposition of the present structure except Cl2 (cyan) with the similar reported structure (molecule *A* *in* green and molecule *B* *in* brown; Saravanan *et al.*, 2016).

Synthesis and crystallization

To a solution of the 4-(4-chlorophenyl) thiazol-2-amine (1.5 g, 7.14 mmol) in dry toluene (25 ml), K_2CO_3 (1.97 g, 14.28 mmol) and chloroacetyl chloride (0.57 ml, 7.14 mmol) was added. The reaction mixture was heated to reflux for 3 h. After completion of the reaction (monitored by pre-coated TLC), the reaction mixture was cooled to RT and diluted with DCM (45 ml). The organic layer was washed with saturated $NaHCO_3$ solution, water (10 ml × 3) and dried over Na_2SO_4. The filtrate was concentrated and the crude product mass was purified by precipitation using petroleum ether and diethyl ether (3:1) to give a colorless solid. This solid was recrystallized in ethyl acetate to yield a colorless crystal of the title compound.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1	0.93	2.47	2.827 (4)	103
C5—H5···O1^{i}	0.93	2.58	3.498 (5)	169

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_8Cl_2N_2OS$
M_r	287.15
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	5.0940 (12), 14.738 (3), 15.703 (3)
β (°)	96.932 (9)
V (Å^3)	1170.3 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.72
Crystal size (mm)	0.24 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6510, 2688, 1679
R_{int}	0.100
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.652
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.178, 0.98
No. of reflections	2688
No. of parameters	160
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})	0.47, −0.41

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Refinement

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

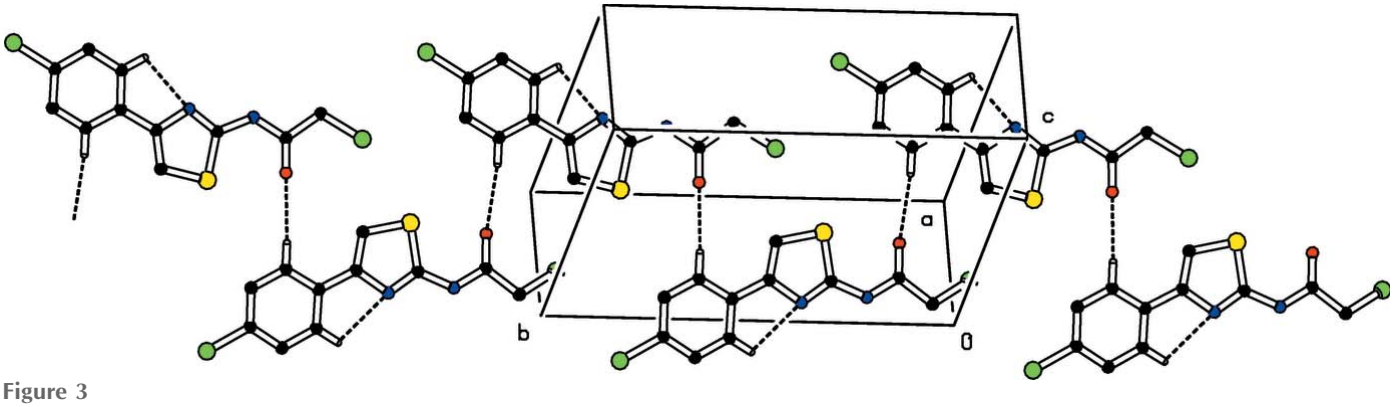


Figure 3
Crystal packing of the title compound, viewed down the *c* axis. The C—H···N and C—H···O hydrogen bonds are shown as dashed lines (see Table 1). For clarity, H atoms not involved in these hydrogen bonds have been omitted.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160903 [doi:10.1107/S2414314616009032]

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2-Chloro-*N*-[4-(4-chlorophenyl)-1,3-thiazol-2-yl]acetamide

Crystal data

$C_{11}H_8Cl_2N_2OS$
M_r = 287.15
Monoclinic, $P2_1/c$
a = 5.0940 (12) Å
b = 14.738 (3) Å
c = 15.703 (3) Å
β = 96.932 (9)°
V = 1170.3 (4) Å^3
Z = 4
$F(000)$ = 584
D_x = 1.630 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4320 reflections
θ = 3.2–26.9°
μ = 0.72 mm^{-1}
T = 296 K
Block, colourless
0.24 × 0.22 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scans
6510 measured reflections
2688 independent reflections
1679 reflections with $I > 2\sigma(I)$
R_{int} = 0.100
θ_{max} = 27.6°, θ_{min} = 3.1°
h = −6→6
k = −18→19
l = −20→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.178
S = 0.98
2688 reflections
160 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0772P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 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}
S1	0.40270 (17)	0.34381 (7)	0.21301 (7)	0.0471 (3)
O1	0.3657 (5)	0.15655 (18)	0.18809 (18)	0.0564 (7)

N1	−0.0350 (5)	0.39261 (18)	0.12588 (19)	0.0394 (7)
N2	0.0005 (6)	0.2354 (2)	0.1381 (2)	0.0438 (7)
Cl1	0.1848 (3)	−0.02066 (7)	0.11890 (9)	0.0789 (5)
Cl2	−0.4015 (2)	0.82462 (7)	0.03508 (7)	0.0614 (4)
C1	−0.2452 (7)	0.5616 (2)	0.0659 (2)	0.0453 (8)
H1	−0.3220	0.5072	0.0460	0.054*
C2	−0.3652 (8)	0.6429 (3)	0.0384 (2)	0.0476 (9)
H2A	−0.5208	0.6435	0.0008	0.057*
C3	−0.2477 (7)	0.7222 (2)	0.0683 (2)	0.0418 (8)
C4	−0.0174 (8)	0.7233 (2)	0.1237 (2)	0.0476 (9)
H4	0.0591	0.7780	0.1429	0.057*
C5	0.0987 (7)	0.6419 (2)	0.1506 (2)	0.0428 (8)
H5	0.2545	0.6419	0.1882	0.051*
C6	−0.0146 (6)	0.5598 (2)	0.1221 (2)	0.0358 (7)
C7	0.1045 (6)	0.4713 (2)	0.1506 (2)	0.0371 (7)
C8	0.3431 (7)	0.4571 (2)	0.1969 (2)	0.0450 (8)
H8	0.4594	0.5030	0.2173	0.054*
C9	0.0985 (6)	0.3231 (2)	0.1550 (2)	0.0376 (8)
C10	0.1383 (7)	0.1575 (2)	0.1540 (2)	0.0417 (8)
C11	−0.0185 (8)	0.0745 (2)	0.1235 (3)	0.0550 (10)
H11A	−0.1120	0.0860	0.0670	0.066*
H11B	−0.1490	0.0622	0.1622	0.066*
H2	−0.158 (4)	0.237 (3)	0.113 (3)	0.097 (18)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0321 (5)	0.0426 (5)	0.0636 (6)	0.0025 (4)	−0.0066 (4)	0.0069 (4)
O1	0.0468 (15)	0.0449 (15)	0.0721 (18)	0.0114 (12)	−0.0144 (13)	−0.0022 (12)
N1	0.0294 (13)	0.0330 (14)	0.0553 (18)	0.0026 (12)	0.0035 (12)	−0.0003 (12)
N2	0.0324 (15)	0.0346 (15)	0.063 (2)	0.0055 (12)	−0.0021 (14)	−0.0005 (13)
Cl1	0.0867 (9)	0.0387 (6)	0.1008 (10)	0.0226 (6)	−0.0312 (7)	−0.0140 (5)
Cl2	0.0659 (7)	0.0399 (5)	0.0780 (8)	0.0161 (5)	0.0067 (5)	0.0094 (4)
C1	0.0434 (19)	0.0308 (17)	0.059 (2)	0.0009 (15)	−0.0051 (16)	−0.0019 (15)
C2	0.046 (2)	0.045 (2)	0.050 (2)	0.0063 (17)	−0.0031 (16)	0.0050 (16)
C3	0.0453 (19)	0.0345 (18)	0.047 (2)	0.0061 (15)	0.0113 (16)	0.0048 (14)
C4	0.051 (2)	0.0354 (19)	0.057 (2)	−0.0032 (17)	0.0087 (17)	−0.0020 (16)
C5	0.0361 (17)	0.0380 (18)	0.053 (2)	−0.0023 (15)	−0.0014 (15)	−0.0026 (15)
C6	0.0310 (16)	0.0369 (17)	0.0398 (18)	−0.0022 (13)	0.0057 (13)	0.0013 (14)
C7	0.0323 (16)	0.0348 (17)	0.0439 (19)	−0.0018 (13)	0.0041 (14)	0.0007 (13)
C8	0.0373 (18)	0.040 (2)	0.055 (2)	−0.0026 (15)	−0.0048 (15)	0.0018 (15)
C9	0.0258 (15)	0.0360 (18)	0.051 (2)	0.0021 (13)	0.0047 (14)	0.0000 (14)
C10	0.0390 (18)	0.0384 (19)	0.047 (2)	0.0102 (15)	0.0011 (15)	0.0005 (14)
C11	0.054 (2)	0.0349 (19)	0.073 (3)	0.0117 (17)	−0.0055 (19)	−0.0040 (18)

Geometric parameters (Å, º)

S1—C8	1.710 (4)	C2—C3	1.369 (5)
S1—C9	1.727 (3)	C2—H2A	0.9300
O1—C10	1.216 (4)	C3—C4	1.374 (5)
N1—C9	1.283 (4)	C4—C5	1.381 (5)
N1—C7	1.390 (4)	C4—H4	0.9300
N2—C10	1.352 (4)	C5—C6	1.391 (5)
N2—C9	1.401 (4)	C5—H5	0.9300
N2—H2	0.856 (10)	C6—C7	1.485 (5)
Cl1—C11	1.750 (4)	C7—C8	1.355 (5)
Cl2—C3	1.751 (3)	C8—H8	0.9300
C1—C6	1.382 (5)	C10—C11	1.507 (5)
C1—C2	1.390 (5)	C11—H11A	0.9700
C1—H1	0.9300	C11—H11B	0.9700
C8—S1—C9	87.85 (16)	C1—C6—C7	119.7 (3)
C9—N1—C7	109.6 (3)	C5—C6—C7	121.9 (3)
C10—N2—C9	125.7 (3)	C8—C7—N1	114.6 (3)
C10—N2—H2	123 (3)	C8—C7—C6	127.2 (3)
C9—N2—H2	111 (3)	N1—C7—C6	118.1 (3)
C6—C1—C2	121.5 (3)	C7—C8—S1	111.2 (3)
C6—C1—H1	119.2	C7—C8—H8	124.4
C2—C1—H1	119.2	S1—C8—H8	124.4
C3—C2—C1	118.1 (3)	N1—C9—N2	120.5 (3)
C3—C2—H2A	120.9	N1—C9—S1	116.8 (3)
C1—C2—H2A	120.9	N2—C9—S1	122.7 (2)
C2—C3—C4	122.1 (3)	O1—C10—N2	122.5 (3)
C2—C3—Cl2	118.2 (3)	O1—C10—C11	124.8 (3)
C4—C3—Cl2	119.7 (3)	N2—C10—C11	112.8 (3)
C3—C4—C5	119.0 (3)	C10—C11—Cl1	111.7 (3)
C3—C4—H4	120.5	C10—C11—H11A	109.3
C5—C4—H4	120.5	Cl1—C11—H11A	109.3
C4—C5—C6	120.7 (3)	C10—C11—H11B	109.3
C4—C5—H5	119.6	Cl1—C11—H11B	109.3
C6—C5—H5	119.6	H11A—C11—H11B	107.9
C1—C6—C5	118.4 (3)		
C6—C1—C2—C3	0.3 (6)	C5—C6—C7—N1	173.7 (3)
C1—C2—C3—C4	0.2 (6)	N1—C7—C8—S1	−0.8 (4)
C1—C2—C3—Cl2	−179.0 (3)	C6—C7—C8—S1	−178.5 (3)
C2—C3—C4—C5	−0.4 (6)	C9—S1—C8—C7	0.3 (3)
Cl2—C3—C4—C5	178.8 (3)	C7—N1—C9—N2	−179.5 (3)
C3—C4—C5—C6	0.1 (5)	C7—N1—C9—S1	−0.9 (4)
C2—C1—C6—C5	−0.5 (5)	C10—N2—C9—N1	169.4 (3)
C2—C1—C6—C7	179.1 (3)	C10—N2—C9—S1	−9.1 (5)
C4—C5—C6—C1	0.3 (5)	C8—S1—C9—N1	0.4 (3)
C4—C5—C6—C7	−179.3 (3)	C8—S1—C9—N2	178.9 (3)

C9—N1—C7—C8	1.1 (4)	C9—N2—C10—O1	2.4 (6)
C9—N1—C7—C6	179.0 (3)	C9—N2—C10—C11	−176.6 (3)
C1—C6—C7—C8	171.7 (4)	O1—C10—C11—Cl1	−14.5 (5)
C5—C6—C7—C8	−8.6 (6)	N2—C10—C11—Cl1	164.5 (3)
C1—C6—C7—N1	−6.0 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1	0.93	2.47	2.827 (4)	103
C5—H5···O1^{i}	0.93	2.58	3.498 (5)	169

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+1/2.