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N-Cyclohexyl-2-(2,3-dichlorophenylsulfanyl)acetamide

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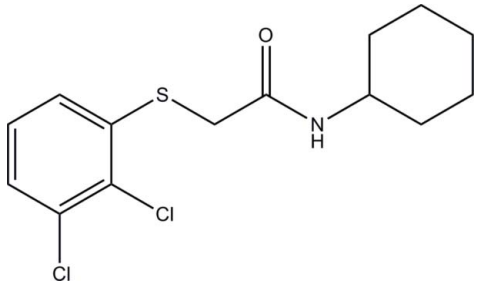
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.095; data-to-parameter ratio = 15.7.

In the crystal structure of title compound, $C_{14}H_{17}Cl_2NOS$, the cyclohexyl ring has a chair conformation and connects with an equatorial N atom. Molecules are connected *via* N—H···O hydrogen bonds into chains.

Related literature

For related literature, see: Li *et al.* (2008*a*,*b*).



Experimental

Crystal data

$C_{14}H_{17}Cl_2NOS$ M_r = 318.25
Monoclinic, $P2_1/c$
a = 13.427 (2) Å
b = 12.877 (2) Å
c = 9.1807 (16) Å
β = 104.849 (3)°
V = 1534.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 293 (2) K
0.10 × 0.06 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.947, T_{max} = 0.989
7968 measured reflections
2712 independent reflections
1972 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.095
S = 1.05
2712 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···O2^{i}	0.86	2.01	2.867 (2)	177

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2098).

References

Bruker (2005). *SMART*, *SAINT* and*SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Li, Z.-B., Zuo, H., Dong, W.-L., He, X.-Y. & Chen, Z.-B. (2008*b*). *Acta Cryst.* E**64**, o1609.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o32 [doi:10.1107/S1600536808040464]

N-Cyclohexyl-2-(2,3-dichlorophenylsulfanyl)acetamide

Zhu-Bo Li, Jing Li, Wen-Liang Dong, Hua Zuo and Xiao-Yan He

S1. Comment

The structure determination was performed as a part of a project on the interactions of small molecules with proteins. The structures of the similar compounds *N*-benzyl-2-(2-chloro-4-methylphenoxy)acetamide (Li *et al.*, 2008*a*) and *N*-benzyl-2-(2,6-dichlorophenoxy)acetamide (Li *et al.*, 2008*b*) were reported previously.

In the crystal structure the cyclohexyl ring is in a chair conformation. The molecules are connected *via* N—H···O hydrogen bonding between the N—H H atom and the carbonyl O atom into chains, that extend in the direction of the *c* axis.

S2. Experimental

The solution of 2,3-dichlorobenzenethiol (1.0 mmol), *N*-cyclohexyl-2-chloroacetamide (1.1 mmol), K_2CO_3 (1.1 mmol) and CH_3CN (20 ml) was refluxed for 4 h. After completion of the reaction (by TLC monitoring), the solution was cooled and solvent was evaporated under reduced pressure. The residue was poured into water and adjusted the pH 6–7 with dilute hydrochloric acid (10%) and extracted with ethyl acetate, washed with brine and dried over anhydrous $MgSO_4$ to obtain the corresponding crude product. The product was purified by column chromatography on silica gel using ethyl acetate as eluent (yield 80%). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid dissolved in ethyl acetate/hexane at room temperatures for 6 d.

S3. Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.97 Å (for CH_2 groups).

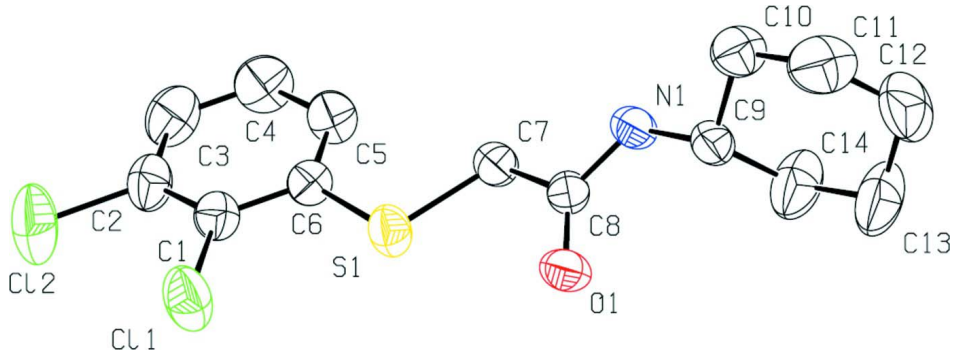

Figure 1

The molecular structure of the title compound showing displacement ellipsoids drawn at 50% probability level. H atoms are omitted for clarity.

N-Cyclohexyl-2-(2,3-dichlorophenylsulfanyl)acetamide

Crystal data

$C_{14}H_{17}Cl_2NOS$
$M_r = 318.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.427$ (2) Å
$b = 12.877$ (2) Å
$c = 9.1807$ (16) Å
$\beta = 104.849$ (3)°
$V = 1534.3$ (5) Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.378$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1963 reflections
$\theta = 2.8$–$23.3°$
$\mu = 0.55$ mm^{-1}
$T = 293$ K
Needle, colourless
0.10 × 0.06 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.947$, $T_{max} = 0.989$
7968 measured reflections
2712 independent reflections
1972 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.6°$
$h = -15 \rightarrow 15$
$k = -15 \rightarrow 15$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.095$
$S = 1.05$
2712 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.4415P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0083 (12)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.85908 (5)	0.72227 (5)	0.05020 (7)	0.0493 (2)
Cl1	1.06216 (5)	0.73736 (6)	−0.03167 (9)	0.0719 (3)
Cl2	1.24245 (6)	0.58238 (7)	0.09765 (11)	0.0941 (3)
O1	0.66239 (12)	0.81810 (13)	−0.02975 (18)	0.0506 (4)
C1	1.04846 (17)	0.64033 (18)	0.0911 (3)	0.0455 (6)
C2	1.12759 (19)	0.5724 (2)	0.1488 (3)	0.0549 (7)
C3	1.1172 (2)	0.4955 (2)	0.2479 (3)	0.0647 (8)
H3	1.1712	0.4502	0.2875	0.078*
C4	1.0261 (2)	0.4870 (2)	0.2872 (3)	0.0639 (7)
H4	1.0184	0.4352	0.3541	0.077*
C5	0.94551 (19)	0.55371 (19)	0.2295 (3)	0.0528 (6)
H5	0.8838	0.5460	0.2567	0.063*

C6	0.95562 (17)	0.63200 (17)	0.1317 (3)	0.0409 (5)
C7	0.75922 (16)	0.69227 (18)	0.1412 (3)	0.0436 (6)
H7A	0.7322	0.6232	0.1129	0.052*
H7B	0.7862	0.6945	0.2498	0.052*
C8	0.67521 (16)	0.77252 (17)	0.0911 (3)	0.0395 (5)
N1	0.61760 (14)	0.78834 (15)	0.1866 (2)	0.0483 (5)
H1	0.6331	0.7557	0.2711	0.058*
C9	0.52927 (17)	0.85822 (19)	0.1558 (3)	0.0461 (6)
H9	0.5418	0.9135	0.0893	0.055*
C10	0.5189 (2)	0.9077 (2)	0.2997 (3)	0.0596 (7)
H10A	0.5807	0.9472	0.3443	0.072*
H10B	0.5121	0.8539	0.3704	0.072*
C11	0.4258 (3)	0.9791 (3)	0.2719 (4)	0.0849 (10)
H11A	0.4185	1.0055	0.3676	0.102*
H11B	0.4368	1.0379	0.2118	0.102*
C12	0.3288 (3)	0.9245 (3)	0.1922 (4)	0.0917 (11)
H12A	0.2721	0.9736	0.1706	0.110*
H12B	0.3133	0.8707	0.2571	0.110*
C13	0.3393 (2)	0.8767 (3)	0.0481 (4)	0.0904 (11)
H13A	0.3477	0.9311	−0.0210	0.108*
H13B	0.2772	0.8383	0.0015	0.108*
C14	0.4319 (2)	0.8039 (3)	0.0773 (4)	0.0812 (10)
H14A	0.4203	0.7460	0.1386	0.097*
H14B	0.4389	0.7763	−0.0178	0.097*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0419 (3)	0.0507 (4)	0.0586 (4)	0.0076 (3)	0.0191 (3)	0.0136 (3)
Cl1	0.0579 (4)	0.0733 (5)	0.0933 (6)	0.0049 (3)	0.0355 (4)	0.0264 (4)
Cl2	0.0492 (5)	0.1011 (7)	0.1388 (8)	0.0170 (4)	0.0364 (5)	0.0111 (6)
O1	0.0577 (10)	0.0588 (10)	0.0387 (9)	0.0133 (8)	0.0183 (8)	0.0075 (8)
C1	0.0441 (13)	0.0426 (14)	0.0500 (15)	0.0009 (11)	0.0124 (11)	−0.0024 (12)
C2	0.0416 (14)	0.0547 (16)	0.0675 (18)	0.0065 (12)	0.0124 (12)	−0.0051 (14)
C3	0.0586 (17)	0.0533 (17)	0.076 (2)	0.0156 (14)	0.0058 (15)	0.0047 (15)
C4	0.0727 (19)	0.0484 (16)	0.0700 (19)	0.0114 (14)	0.0175 (15)	0.0152 (14)
C5	0.0537 (15)	0.0471 (14)	0.0599 (16)	0.0036 (12)	0.0189 (13)	0.0064 (13)
C6	0.0425 (13)	0.0366 (12)	0.0431 (13)	0.0022 (10)	0.0100 (10)	−0.0015 (11)
C7	0.0432 (13)	0.0476 (14)	0.0417 (13)	0.0029 (11)	0.0142 (10)	0.0024 (11)
C8	0.0374 (12)	0.0429 (13)	0.0383 (13)	−0.0024 (10)	0.0101 (10)	−0.0063 (11)
N1	0.0471 (11)	0.0620 (13)	0.0394 (11)	0.0143 (10)	0.0174 (9)	0.0104 (10)
C9	0.0431 (13)	0.0552 (15)	0.0429 (14)	0.0087 (11)	0.0165 (11)	0.0060 (12)
C10	0.0648 (17)	0.0590 (17)	0.0545 (16)	0.0130 (14)	0.0140 (14)	−0.0059 (14)
C11	0.100 (3)	0.084 (2)	0.070 (2)	0.044 (2)	0.0194 (19)	−0.0107 (18)
C12	0.068 (2)	0.113 (3)	0.105 (3)	0.034 (2)	0.042 (2)	0.009 (2)
C13	0.0447 (17)	0.106 (3)	0.111 (3)	0.0128 (17)	0.0022 (17)	−0.025 (2)
C14	0.0518 (17)	0.088 (2)	0.095 (2)	0.0106 (16)	0.0030 (16)	−0.0380 (19)

Geometric parameters (Å, º)

S1—C6	1.759 (2)	N1—H1	0.8600
S1—C7	1.794 (2)	C9—C14	1.495 (4)
Cl1—C1	1.724 (2)	C9—C10	1.505 (3)
Cl2—C2	1.728 (3)	C9—H9	0.9800
O1—C8	1.228 (2)	C10—C11	1.520 (4)
C1—C2	1.373 (3)	C10—H10A	0.9700
C1—C6	1.394 (3)	C10—H10B	0.9700
C2—C3	1.376 (4)	C11—C12	1.496 (4)
C3—C4	1.365 (4)	C11—H11A	0.9700
C3—H3	0.9300	C11—H11B	0.9700
C4—C5	1.377 (3)	C12—C13	1.499 (4)
C4—H4	0.9300	C12—H12A	0.9700
C5—C6	1.380 (3)	C12—H12B	0.9700
C5—H5	0.9300	C13—C14	1.524 (4)
C7—C8	1.512 (3)	C13—H13A	0.9700
C7—H7A	0.9700	C13—H13B	0.9700
C7—H7B	0.9700	C14—H14A	0.9700
C8—N1	1.325 (3)	C14—H14B	0.9700
N1—C9	1.457 (3)		
C6—S1—C7	102.52 (11)	N1—C9—H9	108.0
C2—C1—C6	120.3 (2)	C14—C9—H9	108.0
C2—C1—Cl1	120.80 (19)	C10—C9—H9	108.0
C6—C1—Cl1	118.90 (18)	C9—C10—C11	111.5 (2)
C1—C2—C3	120.9 (2)	C9—C10—H10A	109.3
C1—C2—Cl2	120.3 (2)	C11—C10—H10A	109.3
C3—C2—Cl2	118.8 (2)	C9—C10—H10B	109.3
C4—C3—C2	118.9 (2)	C11—C10—H10B	109.3
C4—C3—H3	120.6	H10A—C10—H10B	108.0
C2—C3—H3	120.6	C12—C11—C10	111.9 (3)
C3—C4—C5	121.1 (3)	C12—C11—H11A	109.2
C3—C4—H4	119.4	C10—C11—H11A	109.2
C5—C4—H4	119.4	C12—C11—H11B	109.2
C4—C5—C6	120.5 (2)	C10—C11—H11B	109.2
C4—C5—H5	119.7	H11A—C11—H11B	107.9
C6—C5—H5	119.7	C11—C12—C13	110.9 (3)
C5—C6—C1	118.3 (2)	C11—C12—H12A	109.4
C5—C6—S1	125.10 (18)	C13—C12—H12A	109.4
C1—C6—S1	116.58 (17)	C11—C12—H12B	109.4
C8—C7—S1	107.41 (15)	C13—C12—H12B	109.4
C8—C7—H7A	110.2	H12A—C12—H12B	108.0
S1—C7—H7A	110.2	C12—C13—C14	110.7 (3)
C8—C7—H7B	110.2	C12—C13—H13A	109.5
S1—C7—H7B	110.2	C14—C13—H13A	109.5
H7A—C7—H7B	108.5	C12—C13—H13B	109.5
O1—C8—N1	123.6 (2)	C14—C13—H13B	109.5

O1—C8—C7	121.53 (19)	H13A—C13—H13B	108.1
N1—C8—C7	114.8 (2)	C9—C14—C13	111.7 (2)
C8—N1—C9	123.41 (19)	C9—C14—H14A	109.3
C8—N1—H1	118.3	C13—C14—H14A	109.3
C9—N1—H1	118.3	C9—C14—H14B	109.3
N1—C9—C14	111.9 (2)	C13—C14—H14B	109.3
N1—C9—C10	110.20 (19)	H14A—C14—H14B	107.9
C14—C9—C10	110.7 (2)		

S1—C7—C8—O1	25.9 (3)	C14—C9—C10—C11	−54.3 (3)
S1—C7—C8—N1	−154.55 (17)	C9—C10—C11—C12	54.7 (4)
O1—C8—N1—C9	3.0 (4)	C10—C11—C12—C13	−55.3 (4)
C7—C8—N1—C9	−176.6 (2)	C11—C12—C13—C14	55.8 (4)
C8—N1—C9—C14	89.3 (3)	N1—C9—C14—C13	178.9 (3)
C8—N1—C9—C10	−147.0 (2)	C10—C9—C14—C13	55.5 (3)
N1—C9—C10—C11	−178.6 (2)	C12—C13—C14—C9	−56.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0A···O2^{i}	0.86	2.01	2.867 (2)	177

Symmetry code: (i) x, $-y+3/2$, $z+1/2$.