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2-(2,4-Dichlorophenyl)-3-[5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-yl]-thiazolidin-4-one

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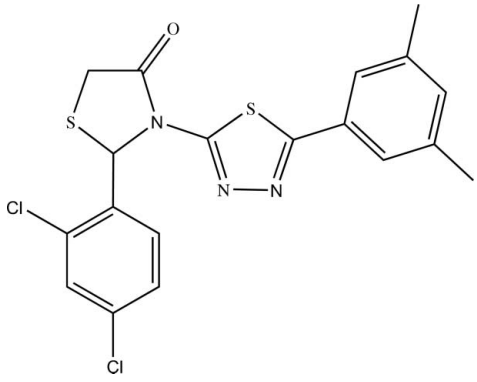
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.055; wR factor = 0.165; data-to-parameter ratio = 15.4.

The title compound, $C_{19}H_{15}Cl_2N_3OS_2$, was synthesized by the reaction of *N*-(2,4-dichlorophenyl)-5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-amine and mercaptoacetic acid. The thiazolidinone ring adopts a twist conformation. The 2,4-dichlorophenyl ring is almost perpendicular to the thiadiazole ring, the dihedral angle being 82.8 (2)°. The 3,5-dimethylphenyl ring is nearly coplanar with the thiadiazole ring, the dihedral angle being 2.7 (2)°. An intramolecular C—H···N hydrogen bond is present.

Related literature

For general background, see: Arun *et al.* (1999); Chen *et al.* (2000); Kidwai *et al.* (2000); Vicentini *et al.* (1998); Wasfy *et al.* (1996). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{19}H_{15}Cl_2N_3OS_2$
M_r = 436.36
Triclinic, $P\overline{1}$
a = 8.1760 (16) Å
b = 9.1650 (18) Å
c = 14.483 (3) Å
α = 80.60 (3)°
β = 80.82 (3)°
γ = 63.92 (3)°
V = 956.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 298 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.803, T_{max} = 0.894
4042 measured reflections
3761 independent reflections
2824 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.165
S = 1.03
3761 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···N3	0.93	2.49	2.842 (6)	102

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2029).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Arun, K. P., Nag, V. L. & Panda, C. S. (1999). *Indian J. Chem. Sect. B*, **38**, 998–1001.
Chen, H. S., Li, Z. M. & Han, Y. F. (2000). *J. Agric. Food Chem.* **48**, 5312–5315.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Kidwai, M., Negi, N. & Misra, P. (2000). *J. Indian Chem. Soc.* **77**, 46–48.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Vicentini, C. B., Manfrini, M., Veronese, A. C. & Guarneri, M. (1998). *J. Heterocycl. Chem.* **35**, 29–36.
Wasfy, A. A., Nassar, S. A. & Eissa, A. M. (1996). *Indian J. Chem. Sect. B*, **35**, 1218–1220.

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supplementary materials

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2-(2,4-Dichlorophenyl)-3-[5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2-yl]thiazolidin-4-one

R. Wan, L. Yin, F. Han, B. Wang and J. Wang

Comment

1,3,4-Thiadiazole derivatives containing the thiazolidinone unit are of great interest because of their chemical and pharmaceutical properties. Some derivatives have fungicidal activities and exhibit certain herbicidal activities (Chen *et al.*, 2000; Kidwai *et al.*, 2000; Vicentini *et al.*, 1998). Some show insecticidal activities (Arun *et al.*, 1999; Wasfy *et al.*, 1996). We report here the crystal structure of the titled compound, (I).

The molecular structure of (I) is shown in Fig.1. In this structure, the thiazolidinone adopts a twist conformation, the dihedral angle between the C11/S1/C12 and C11/N3/C12 is 24.4 (4)°. The thiadiazole ring (S2/C9/N1/N2/C10) is an aromatic heterocyclic ring, all atoms are in the same plane. The angle between the thiadiazole ring and the 3,5-dimethylphenyl ring is 2.7 (2)°. The other benzene ring (C14/C15/C16/C17/C18/C19) is nearly perpendicular to the thiadiazole ring, the dihedral angle is 82.8 (2)°. The molecule has a C—H···N intramolecular hydrogen bond.

Experimental

N-(2,4-dichlorobenzylidene)-5-(3,5-dimethylphenyl)-1,3,4-thiadiazol -2-amine (5 mmol) and mercapto-acetic acid (5 mmol) were added in toluene (50 ml). The water was removed by distillation for 5 h. The reaction mixture was left to cool to room temperature, filtered, and the filter cake was crystallized from acetone to give pure compound (I) (m.p. 476–477 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

Refinement

All H atoms bonded to the C atoms were placed geometrically at the distances of 0.93–0.97 Å and constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms. The methyl groups were allowed to rotate.

Figures

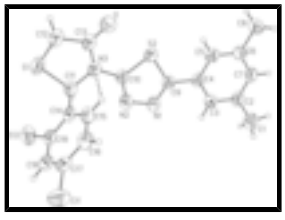


Fig. 1. The crystal structure of (I). Dashed lines indicate intramolecular C—H···N hydrogen bond.

2-(2,4-Dichlorophenyl)-3-[5-(3,5-dimethylphenyl)-1,3,4-thiadiazol-2- yl]thiazolidin-4-one

Crystal data

$C_{19}H_{15}Cl_2N_3OS_2$	$Z = 2$
$M_r = 436.36$	$F(000) = 448$
Triclinic, $P\overline{1}$	$D_x = 1.514$ Mg m^{-3}
Hall symbol: -P 1	Melting point = 476–477 K
$a = 8.1760$ (16) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.1650$ (18) Å	Cell parameters from 25 reflections
$c = 14.483$ (3) Å	$\theta = 10$–$14°$
$\alpha = 80.60$ (3)°	$\mu = 0.57$ mm^{-1}
$\beta = 80.82$ (3)°	$T = 298$ K
$\gamma = 63.92$ (3)°	Block, light yellow
$V = 956.9$ (4) Å^3	0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	2824 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.044$
graphite	$\theta_{max} = 26.0°$, $\theta_{min} = 1.4°$
ω/2θ scans	$h = -9 \rightarrow 10$
Absorption correction: ψ scan (North *et al.*, 1968)	$k = -11 \rightarrow 11$
$T_{min} = 0.803$, $T_{max} = 0.894$	$l = 0 \rightarrow 17$
4042 measured reflections	3 standard reflections every 200 reflections
3761 independent reflections	intensity decay: none

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.055$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.165$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 2.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
3761 reflections	$(\Delta/\sigma)_{max} < 0.001$
244 parameters	$\Delta\rho_{max} = 0.42$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.45$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.6127 (2)	0.7754 (2)	−0.14356 (11)	0.0843 (5)
Cl2	1.25961 (17)	0.62298 (16)	−0.02409 (9)	0.0667 (4)
S1	1.13265 (18)	0.90179 (17)	0.12924 (9)	0.0626 (4)
S2	0.80372 (16)	0.67126 (13)	0.42066 (7)	0.0469 (3)
O	0.7989 (6)	0.9660 (4)	0.3520 (3)	0.0818 (12)
N1	0.9137 (5)	0.4033 (4)	0.3485 (2)	0.0522 (9)
N2	0.9641 (5)	0.5066 (4)	0.2796 (2)	0.0523 (9)
N3	0.9527 (5)	0.7697 (4)	0.2528 (2)	0.0487 (8)
C1	0.7096 (8)	−0.0041 (6)	0.5859 (4)	0.0672 (13)
H1B	0.6622	−0.0377	0.6465	0.101*
H1C	0.8348	−0.0796	0.5727	0.101*
H1D	0.6386	−0.0023	0.5386	0.101*
C2	0.6989 (6)	0.1640 (6)	0.5861 (3)	0.0514 (11)
C3	0.7698 (6)	0.2378 (5)	0.5073 (3)	0.0469 (10)
H3A	0.8261	0.1815	0.4547	0.056*
C4	0.7565 (6)	0.3936 (5)	0.5074 (3)	0.0439 (9)
C5	0.6693 (6)	0.4783 (6)	0.5844 (3)	0.0496 (10)
H5A	0.6602	0.5831	0.5842	0.059*
C6	0.5944 (6)	0.4091 (6)	0.6629 (3)	0.0486 (10)
C7	0.6134 (6)	0.2527 (6)	0.6616 (3)	0.0527 (11)
H7A	0.5664	0.2048	0.7140	0.063*
C8	0.4899 (7)	0.5073 (7)	0.7442 (3)	0.0698 (14)
H8A	0.4485	0.4418	0.7920	0.105*
H8B	0.3863	0.6025	0.7226	0.105*
H8C	0.5683	0.5402	0.7698	0.105*
C9	0.8307 (5)	0.4717 (5)	0.4236 (3)	0.0409 (9)
C10	0.9149 (6)	0.6481 (5)	0.3094 (3)	0.0443 (9)
C11	1.0540 (6)	0.7385 (5)	0.1604 (3)	0.0480 (10)
H11A	1.1602	0.6323	0.1651	0.058*
C12	0.9563 (9)	1.0308 (7)	0.2078 (4)	0.0745 (16)
H12A	1.0026	1.0901	0.2380	0.089*
H12B	0.8546	1.1093	0.1738	0.089*
C13	0.8942 (7)	0.9217 (6)	0.2809 (3)	0.0576 (12)

C14	0.9401 (6)	0.7419 (5)	0.0871 (3)	0.0431 (9)
C15	0.7515 (6)	0.7987 (5)	0.1026 (3)	0.0500 (10)
H15A	0.6923	0.8314	0.1610	0.060*
C16	0.6505 (6)	0.8074 (6)	0.0324 (3)	0.0532 (11)
H16A	0.5239	0.8462	0.0431	0.064*
C17	0.7404 (7)	0.7576 (5)	−0.0542 (3)	0.0538 (11)
C18	0.9264 (6)	0.6968 (5)	−0.0713 (3)	0.0505 (10)
H18A	0.9855	0.6604	−0.1290	0.061*
C19	1.0239 (6)	0.6911 (5)	−0.0003 (3)	0.0461 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1062 (12)	0.1000 (11)	0.0749 (9)	−0.0627 (10)	−0.0278 (8)	−0.0105 (8)
Cl2	0.0586 (7)	0.0700 (8)	0.0645 (8)	−0.0285 (6)	0.0135 (6)	−0.0046 (6)
S1	0.0718 (8)	0.0738 (8)	0.0616 (7)	−0.0531 (7)	−0.0053 (6)	0.0051 (6)
S2	0.0603 (7)	0.0507 (6)	0.0407 (5)	−0.0345 (5)	−0.0035 (5)	−0.0034 (4)
O	0.130 (3)	0.067 (2)	0.062 (2)	−0.061 (2)	0.020 (2)	−0.0169 (18)
N1	0.071 (2)	0.051 (2)	0.0410 (19)	−0.0354 (19)	0.0016 (17)	0.0019 (16)
N2	0.064 (2)	0.050 (2)	0.046 (2)	−0.0316 (18)	0.0043 (17)	−0.0019 (16)
N3	0.060 (2)	0.049 (2)	0.0456 (19)	−0.0339 (18)	−0.0029 (16)	−0.0006 (16)
C1	0.079 (3)	0.058 (3)	0.066 (3)	−0.037 (3)	0.006 (3)	0.000 (2)
C2	0.063 (3)	0.065 (3)	0.041 (2)	−0.042 (2)	−0.007 (2)	0.003 (2)
C3	0.056 (2)	0.055 (2)	0.037 (2)	−0.032 (2)	0.0002 (18)	−0.0044 (18)
C4	0.048 (2)	0.053 (2)	0.041 (2)	−0.0301 (19)	−0.0090 (17)	0.0004 (18)
C5	0.057 (3)	0.059 (3)	0.047 (2)	−0.035 (2)	−0.0089 (19)	−0.006 (2)
C6	0.046 (2)	0.070 (3)	0.039 (2)	−0.032 (2)	−0.0046 (17)	−0.009 (2)
C7	0.061 (3)	0.078 (3)	0.038 (2)	−0.049 (2)	−0.0068 (19)	0.005 (2)
C8	0.075 (3)	0.095 (4)	0.056 (3)	−0.049 (3)	0.009 (2)	−0.028 (3)
C9	0.039 (2)	0.048 (2)	0.040 (2)	−0.0232 (18)	−0.0042 (16)	−0.0029 (17)
C10	0.058 (2)	0.052 (2)	0.034 (2)	−0.035 (2)	−0.0088 (17)	0.0044 (17)
C11	0.053 (2)	0.053 (2)	0.043 (2)	−0.031 (2)	0.0003 (18)	0.0011 (18)
C12	0.114 (5)	0.069 (3)	0.062 (3)	−0.064 (3)	−0.001 (3)	0.002 (3)
C13	0.080 (3)	0.052 (3)	0.053 (3)	−0.043 (2)	−0.001 (2)	0.000 (2)
C14	0.051 (2)	0.040 (2)	0.042 (2)	−0.0264 (18)	−0.0002 (18)	0.0020 (17)
C15	0.056 (3)	0.059 (3)	0.043 (2)	−0.035 (2)	−0.0004 (19)	−0.0006 (19)
C16	0.046 (2)	0.058 (3)	0.059 (3)	−0.027 (2)	−0.002 (2)	−0.004 (2)
C17	0.075 (3)	0.052 (3)	0.053 (3)	−0.043 (2)	−0.007 (2)	−0.004 (2)
C18	0.071 (3)	0.040 (2)	0.048 (2)	−0.033 (2)	0.005 (2)	−0.0052 (18)
C19	0.055 (2)	0.040 (2)	0.047 (2)	−0.0287 (19)	0.0016 (19)	0.0013 (17)

Geometric parameters (Å, °)

Cl1—C17	1.734 (5)	C5—C6	1.398 (6)
Cl2—C19	1.739 (4)	C5—H5A	0.9300
S1—C12	1.786 (6)	C6—C7	1.375 (6)
S1—C11	1.841 (4)	C6—C8	1.509 (6)
S2—C10	1.716 (4)	C7—H7A	0.9300
S2—C9	1.738 (4)	C8—H8A	0.9600

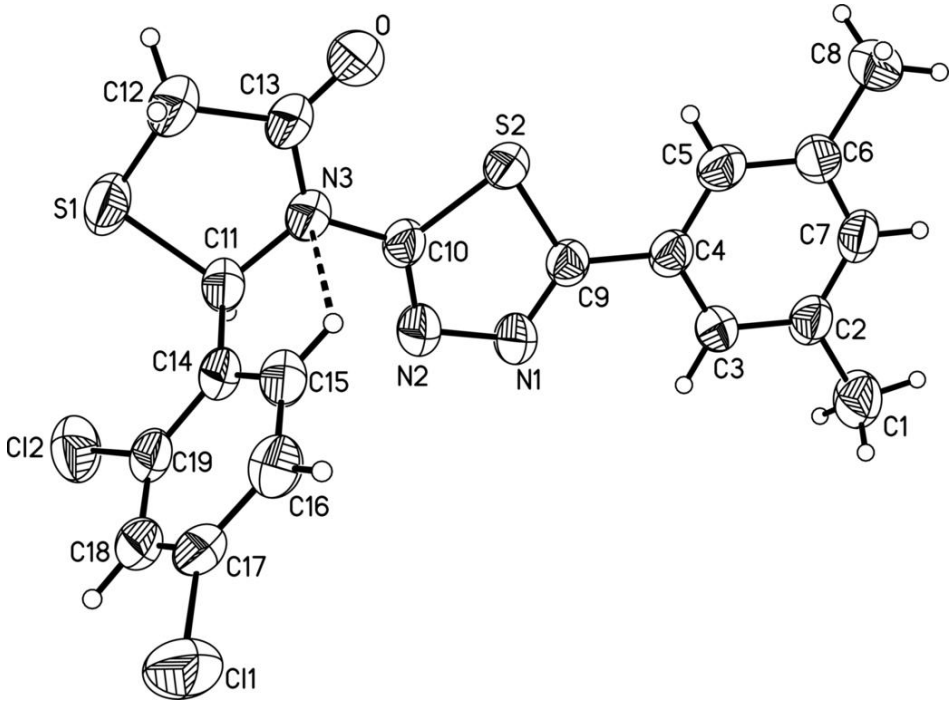
O—C13	1.198 (6)	C8—H8B	0.9600
N1—C9	1.285 (5)	C8—H8C	0.9600
N1—N2	1.401 (5)	C11—C14	1.507 (6)
N2—C10	1.303 (5)	C11—H11A	0.9800
N3—C13	1.368 (6)	C12—C13	1.518 (6)
N3—C10	1.391 (5)	C12—H12A	0.9700
N3—C11	1.458 (5)	C12—H12B	0.9700
C1—C2	1.504 (6)	C14—C15	1.386 (6)
C1—H1B	0.9600	C14—C19	1.388 (6)
C1—H1C	0.9600	C15—C16	1.380 (6)
C1—H1D	0.9600	C15—H15A	0.9300
C2—C7	1.376 (6)	C16—C17	1.385 (6)
C2—C3	1.406 (6)	C16—H16A	0.9300
C3—C4	1.383 (6)	C17—C18	1.365 (6)
C3—H3A	0.9300	C18—C19	1.378 (6)
C4—C5	1.378 (6)	C18—H18A	0.9300
C4—C9	1.488 (5)		
C12—S1—C11	92.2 (2)	N1—C9—S2	114.6 (3)
C10—S2—C9	86.20 (19)	C4—C9—S2	120.6 (3)
C9—N1—N2	112.7 (3)	N2—C10—N3	120.8 (4)
C10—N2—N1	110.8 (3)	N2—C10—S2	115.7 (3)
C13—N3—C10	121.6 (4)	N3—C10—S2	123.5 (3)
C13—N3—C11	118.1 (3)	N3—C11—C14	113.4 (3)
C10—N3—C11	120.2 (3)	N3—C11—S1	104.4 (3)
C2—C1—H1B	109.5	C14—C11—S1	110.7 (3)
C2—C1—H1C	109.5	N3—C11—H11A	109.4
H1B—C1—H1C	109.5	C14—C11—H11A	109.4
C2—C1—H1D	109.5	S1—C11—H11A	109.4
H1B—C1—H1D	109.5	C13—C12—S1	107.3 (4)
H1C—C1—H1D	109.5	C13—C12—H12A	110.3
C7—C2—C3	117.9 (4)	S1—C12—H12A	110.3
C7—C2—C1	121.2 (4)	C13—C12—H12B	110.3
C3—C2—C1	120.9 (4)	S1—C12—H12B	110.3
C4—C3—C2	120.5 (4)	H12A—C12—H12B	108.5
C4—C3—H3A	119.8	O—C13—N3	124.4 (4)
C2—C3—H3A	119.8	O—C13—C12	124.1 (4)
C5—C4—C3	119.7 (4)	N3—C13—C12	111.5 (4)
C5—C4—C9	120.0 (4)	C15—C14—C19	117.8 (4)
C3—C4—C9	120.3 (4)	C15—C14—C11	122.4 (4)
C4—C5—C6	121.0 (4)	C19—C14—C11	119.7 (4)
C4—C5—H5A	119.5	C16—C15—C14	120.9 (4)
C6—C5—H5A	119.5	C16—C15—H15A	119.6
C7—C6—C5	117.9 (4)	C14—C15—H15A	119.6
C7—C6—C8	121.8 (4)	C15—C16—C17	119.0 (4)
C5—C6—C8	120.2 (4)	C15—C16—H16A	120.5
C6—C7—C2	123.0 (4)	C17—C16—H16A	120.5
C6—C7—H7A	118.5	C18—C17—C16	121.8 (4)
C2—C7—H7A	118.5	C18—C17—Cl1	119.2 (4)
C6—C8—H8A	109.5	C16—C17—Cl1	119.0 (4)

C6—C8—H8B	109.5	C17—C18—C19	118.0 (4)
H8A—C8—H8B	109.5	C17—C18—H18A	121.0
C6—C8—H8C	109.5	C19—C18—H18A	121.0
H8A—C8—H8C	109.5	C18—C19—C14	122.4 (4)
H8B—C8—H8C	109.5	C18—C19—Cl2	117.9 (3)
N1—C9—C4	124.8 (4)	C14—C19—Cl2	119.6 (3)
C9—N1—N2—C10	0.5 (5)	C10—N3—C11—C14	76.7 (5)
C7—C2—C3—C4	1.3 (6)	C13—N3—C11—S1	18.4 (5)
C1—C2—C3—C4	178.9 (4)	C10—N3—C11—S1	−162.7 (3)
C2—C3—C4—C5	−1.5 (6)	C12—S1—C11—N3	−22.7 (3)
C2—C3—C4—C9	−179.6 (4)	C12—S1—C11—C14	99.6 (3)
C3—C4—C5—C6	0.2 (6)	C11—S1—C12—C13	22.1 (4)
C9—C4—C5—C6	178.4 (4)	C10—N3—C13—O	−4.5 (8)
C4—C5—C6—C7	1.2 (6)	C11—N3—C13—O	174.4 (5)
C4—C5—C6—C8	−176.4 (4)	C10—N3—C13—C12	178.8 (4)
C5—C6—C7—C2	−1.4 (7)	C11—N3—C13—C12	−2.4 (6)
C8—C6—C7—C2	176.2 (4)	S1—C12—C13—O	167.6 (5)
C3—C2—C7—C6	0.2 (7)	S1—C12—C13—N3	−15.6 (6)
C1—C2—C7—C6	−177.4 (4)	N3—C11—C14—C15	11.2 (6)
N2—N1—C9—C4	178.1 (4)	S1—C11—C14—C15	−105.7 (4)
N2—N1—C9—S2	−0.3 (5)	N3—C11—C14—C19	−170.7 (3)
C5—C4—C9—N1	−179.9 (4)	S1—C11—C14—C19	72.4 (4)
C3—C4—C9—N1	−1.8 (6)	C19—C14—C15—C16	−1.3 (6)
C5—C4—C9—S2	−1.6 (5)	C11—C14—C15—C16	176.9 (4)
C3—C4—C9—S2	176.5 (3)	C14—C15—C16—C17	0.3 (7)
C10—S2—C9—N1	0.0 (3)	C15—C16—C17—C18	1.4 (7)
C10—S2—C9—C4	−178.5 (3)	C15—C16—C17—Cl1	−177.7 (3)
N1—N2—C10—N3	179.3 (4)	C16—C17—C18—C19	−2.1 (6)
N1—N2—C10—S2	−0.5 (5)	Cl1—C17—C18—C19	177.1 (3)
C13—N3—C10—N2	176.7 (4)	C17—C18—C19—C14	1.1 (6)
C11—N3—C10—N2	−2.2 (6)	C17—C18—C19—Cl2	−176.9 (3)
C13—N3—C10—S2	−3.5 (6)	C15—C14—C19—C18	0.6 (6)
C11—N3—C10—S2	177.7 (3)	C11—C14—C19—C18	−177.6 (4)
C9—S2—C10—N2	0.3 (3)	C15—C14—C19—Cl2	178.6 (3)
C9—S2—C10—N3	−179.6 (4)	C11—C14—C19—Cl2	0.4 (5)
C13—N3—C11—C14	−102.2 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15A···N3	0.93	2.49	2.842 (6)	102

Fig. 1


O
C13
C12
S2
C8
C5
C6
N3
S1
C11
C10
C4
C7
C9
C2
C14
C15
N2
N1
C3
C1
Cl2
C19
C16
C18
C17
Cl1