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2-(4-Chloro-3-nitrophenyl)-4-(4-chlorophenyl)-1,3-thiazole

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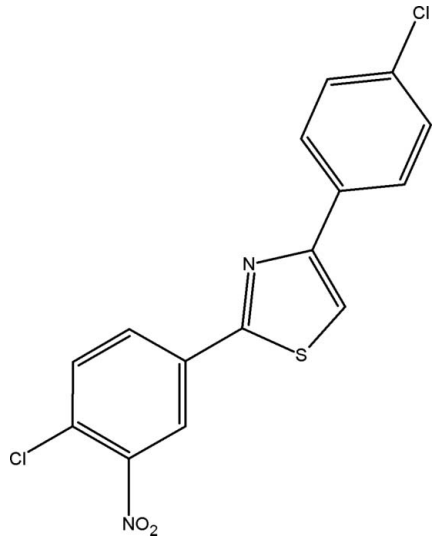
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.006 Å; R factor = 0.058; wR factor = 0.130; data-to-parameter ratio = 13.2.

The title compound, $C_{15}H_8Cl_2N_2O_2S$, crystallizes with two molecules in the asymmetric unit. The dihedral angles between the 4-chloro-3-nitrophenyl ring and the thiazole ring are 0.5 (1) and 7.1 (1)° and those between the 4-chlorophenyl ring and the thiazole ring are 7.1 (1) and 7.4 (1)° in the two molecules. The crystal structure is stabilized by intermolecular C—H···Cl and C—H···O hydrogen bonds.

Related literature

The aminothiazole ring system is a useful structural element in medicinal chemistry and has found broad applications in drug development, see: Fortuna *et al.* (1988); Frank *et al.* (1995); Karl *et al.* (1983); Tsuji & Ishikawa (1994).



Experimental

Crystal data

$C_{15}H_8Cl_2N_2O_2S$
M_r = 351.20
Triclinic, $P\overline{1}$
a = 7.4379 (19) Å
b = 12.305 (3) Å
c = 16.808 (4) Å
α = 88.596 (5)°
β = 84.131 (4)°
γ = 76.721 (5)°
V = 1489.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 292 K
0.28 × 0.24 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.854, T_{max} = 0.918
14507 measured reflections
5235 independent reflections
2855 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.130
S = 0.97
5235 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O1^{i}	0.93	2.48	3.285 (5)	145
C15′—H15′···Cl2^{ii}	0.93	2.73	3.610 (4)	158

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXL97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2009).

We thank the DST–IRHPA for the CCD X-ray facility at IISc and SKN thanks the CSIR (SRF), India, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2246).

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2-(4-Chloro-3-nitrophenyl)-4-(4-chlorophenyl)-1,3-thiazole

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S1. Comment

The aminothiazole ring system is a useful structural element in medicinal chemistry and has found broad applications in drug development as antiallergies (Karl *et al.*, 1983), anti-inflammatory (Fortuna *et al.*, 1988), antibacterial (Tsuji *et al.*, 1994) and anti-HIV agents (Frank *et al.*, 1995]. In view of different applications of this class of compounds, we have undertaken a single-crystal structure determination of the title compound. The compound is completely planar with the nitro group not planar with the 4-chloro-4-nitrophenyl ring to avoid electrostatic repulsion with the chlorine atom in an *ortho* position, the dihedral twist being 35.4 (3)° and 48.1 (3)° respectively in the two molecules. Relevant torsion angles are given in Table 1. Figure 1 gives an *ORTEP* view depicting two molecules (A) and (B) in the asymmetric unit. The C—N bond lengths of the five-membered thiazoyl ring is different indicating that the electrnoic environment around each nitrogen atom is different. The torsion angles N2—C7—C1—C6/N2′-C7′-C1′-C6′ and N2—C9—C10—C11/N2′-C9′-C10′-C11'are nearly equal to 180° indicating delocalization of the π electron density between all the three aromatic moieties, namely the thiazoyl ring and the adjacent aryl rings. The crystal structure is stabilized by C—H···O intermolecular hydrogen bonds (between molecules of the ′A′ type), each of which are held by C—H···Cl intermolecular interactions (with molecules of ′B′ type) between them (Figure 2).

S2. Experimental

A mixture of 4-chloro-3-nitrobenzonitrile, (0.1 mol), thioacetic acid (0.1 mol), boron trifluoride diethyletherate (0.1 mol) and 1,2 dichloro ethane was refluxed for 1 h at 80 C. The reaction medium was quenched with 1 N hydrochloric acid (congo red) and the obtained product i.e 4-chloro-3-nitrobenzothioamide was isolated with dichloromethane. The solvent was evaporated at reduced pressure and the crude product (Yield = 89%) left behind was recrystallized from ethyl acetate. This was taken with 2-bromo-1-(4-chlorophenyl)ethanone (0.1 mol) in absolute ethanol medium was refluxed under nitrogen atmosphere for 2 h at 80 C. Reaction medium was cooled to room temperature and poured into 50 ml of water containing sodium acetate. The precipitate obtained was filtered and recrystallized from ethanol. (Yield: 92%) and the melting point was 128–129 C.

S3. Refinement

All the aromatic H atoms were positioned geometrically, C—H = 0.93 Å, and refined using a riding model with U_{iso}(H)= 1.2 U_{eq}(C).

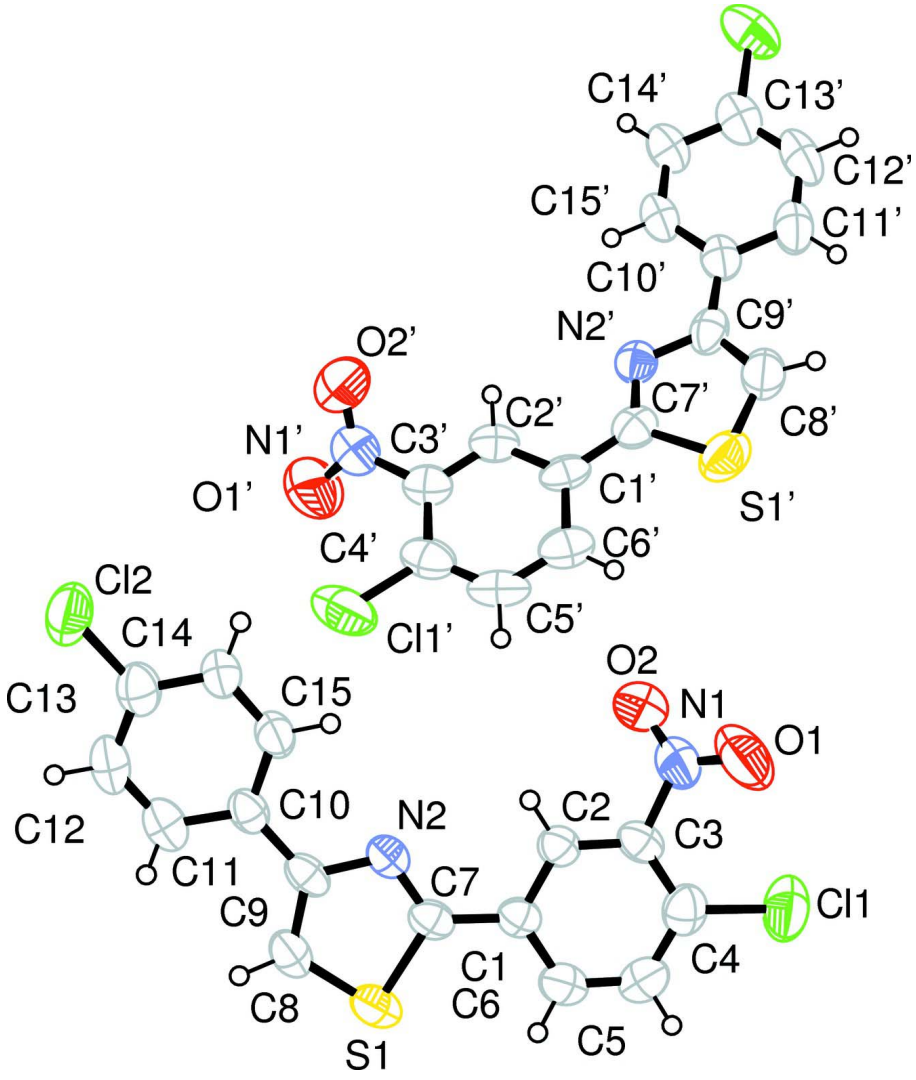

Figure 1

Molecular structure shows the atom labelling Scheme with displacement ellipsoids for non-H atoms at 50% probability level, hydrogen atoms are arbitary circle.

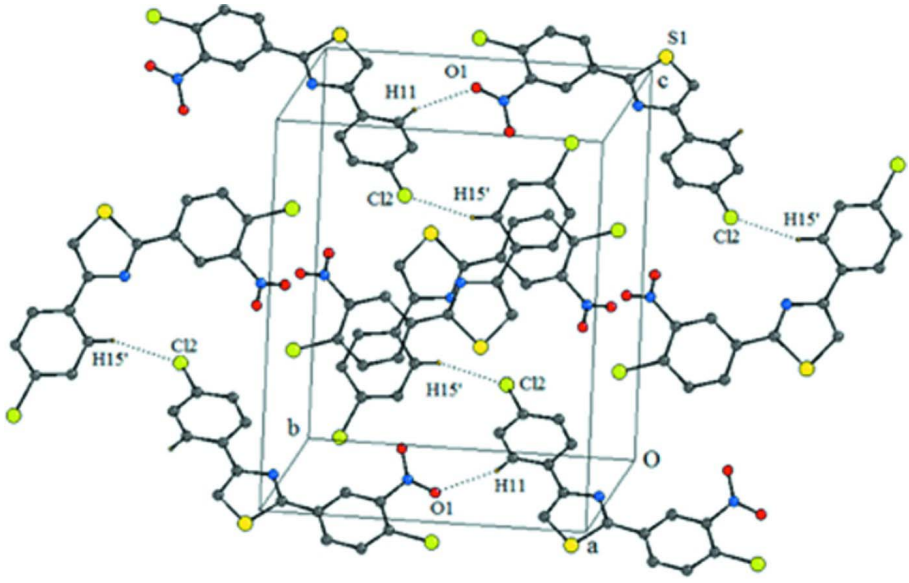

Figure 2

The molecular packing depicting C—H···O and C—H···Cl intermolecular interactions in the solid state.

2-(4-Chloro-3-nitrophenyl)-4-(4-chlorophenyl)-1,3-thiazole

Crystal data

$C_{15}H_8Cl_2N_2O_2S$
$M_r = 351.20$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.4379$ (19) Å
$b = 12.305$ (3) Å
$c = 16.808$ (4) Å
$\alpha = 88.596$ (5)°
$\beta = 84.131$ (4)°
$\gamma = 76.721$ (5)°
$V = 1489.3$ (6) Å^3
$Z = 4$
$F(000) = 712$
$D_x = 1.566$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 320 reflections
$\theta = 1.0$–$28.0°$
$\mu = 0.58$ mm^{-1}
$T = 292$ K
Plate, colorless
0.28 × 0.24 × 0.15 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*; Sheldrick, 1996)
$T_{min} = 0.854$, $T_{max} = 0.918$
14507 measured reflections
5235 independent reflections
2855 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.130$
$S = 0.97$
5235 reflections
397 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

$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.28130 (14)	−0.08178 (8)	1.08929 (6)	0.0671 (3)
S1′	0.55762 (17)	0.57562 (10)	0.65181 (7)	0.0872 (4)
Cl2′	1.01634 (16)	0.76240 (10)	0.20368 (8)	0.1005 (4)
Cl2	0.02483 (18)	−0.26482 (9)	0.64160 (7)	0.0962 (4)
Cl1′	0.55818 (19)	0.00327 (11)	0.69174 (8)	0.1110 (5)
Cl1	0.3241 (2)	0.48445 (10)	1.11376 (8)	0.1125 (5)
N2	0.2343 (4)	0.0036 (2)	0.95110 (18)	0.0511 (7)
N2′	0.7301 (4)	0.4815 (2)	0.52398 (18)	0.0561 (8)
C1	0.2750 (4)	0.1409 (3)	1.0459 (2)	0.0477 (8)
C9	0.2261 (4)	−0.1062 (3)	0.9456 (2)	0.0501 (9)
C10′	0.8033 (5)	0.6361 (3)	0.4402 (2)	0.0572 (10)
C1′	0.6345 (5)	0.3473 (3)	0.6178 (2)	0.0558 (10)
C2	0.2580 (4)	0.2243 (3)	0.9895 (2)	0.0514 (9)
H2	0.2385	0.2088	0.9376	0.062*
C10	0.1895 (4)	−0.1486 (3)	0.8695 (2)	0.0506 (9)
C7	0.2621 (4)	0.0289 (3)	1.0228 (2)	0.0497 (9)
C9′	0.7236 (5)	0.5945 (3)	0.5149 (2)	0.0582 (10)
C3	0.2695 (5)	0.3300 (3)	1.0087 (2)	0.0551 (9)
N1	0.2537 (5)	0.4131 (3)	0.9443 (3)	0.0807 (11)
C3′	0.6725 (5)	0.1531 (4)	0.5877 (2)	0.0627 (10)
C2′	0.6890 (5)	0.2590 (3)	0.5648 (2)	0.0575 (10)
H2′	0.7373	0.2712	0.5129	0.069*
C4	0.3003 (5)	0.3551 (3)	1.0859 (3)	0.0650 (10)
C12	0.1416 (5)	−0.2967 (3)	0.7884 (3)	0.0694 (11)
H12	0.1406	−0.3715	0.7822	0.083*
C15′	0.8695 (5)	0.5650 (3)	0.3768 (2)	0.0627 (10)
H15′	0.8679	0.4899	0.3830	0.075*
C13	0.0966 (5)	−0.2213 (3)	0.7275 (2)	0.0657 (11)
C6′	0.5613 (5)	0.3250 (4)	0.6947 (2)	0.0728 (12)
H6′	0.5253	0.3824	0.7320	0.087*

C5′	0.5417 (5)	0.2198 (4)	0.7162 (2)	0.0770 (13)
H5′	0.4892	0.2076	0.7673	0.092*
C15	0.1492 (5)	−0.0769 (3)	0.8060 (2)	0.0617 (10)
H15	0.1539	−0.0025	0.8110	0.074*
C14	0.1024 (5)	−0.1121 (3)	0.7358 (2)	0.0692 (11)
H14	0.0748	−0.0619	0.6940	0.083*
C11	0.1880 (5)	−0.2598 (3)	0.8587 (3)	0.0663 (11)
H11	0.2191	−0.3106	0.8998	0.080*
C4′	0.5983 (5)	0.1320 (4)	0.6634 (3)	0.0704 (11)
C6	0.3070 (5)	0.1658 (3)	1.1221 (2)	0.0633 (10)
H6	0.3202	0.1102	1.1610	0.076*
C7′	0.6514 (5)	0.4589 (3)	0.5922 (2)	0.0577 (10)
C14′	0.9381 (5)	0.6015 (3)	0.3042 (3)	0.0681 (11)
H14′	0.9827	0.5518	0.2621	0.082*
N1′	0.7310 (6)	0.0637 (3)	0.5286 (3)	0.0868 (11)
C13′	0.9395 (5)	0.7127 (4)	0.2952 (3)	0.0708 (11)
C5	0.3194 (5)	0.2702 (4)	1.1411 (2)	0.0697 (11)
H5	0.3415	0.2846	1.1929	0.084*
C8	0.2493 (5)	−0.1640 (3)	1.0153 (2)	0.0597 (10)
H8	0.2477	−0.2391	1.0214	0.072*
C12′	0.8791 (6)	0.7851 (3)	0.3577 (3)	0.0791 (13)
H12′	0.8836	0.8598	0.3512	0.095*
O2′	0.6821 (5)	0.0812 (3)	0.4624 (2)	0.1199 (13)
C11′	0.8114 (5)	0.7484 (3)	0.4306 (3)	0.0734 (12)
H11′	0.7713	0.7980	0.4731	0.088*
O1′	0.8319 (6)	−0.0236 (3)	0.5481 (2)	0.1366 (15)
O2	0.3185 (6)	0.3817 (3)	0.8786 (2)	0.1309 (15)
C8′	0.6340 (6)	0.6561 (3)	0.5786 (3)	0.0785 (12)
H8′	0.6164	0.7332	0.5819	0.094*
O1	0.1819 (6)	0.5084 (3)	0.9591 (2)	0.1363 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0729 (7)	0.0615 (7)	0.0633 (7)	−0.0124 (5)	−0.0007 (5)	0.0185 (5)
S1′	0.0982 (9)	0.0881 (9)	0.0658 (7)	−0.0012 (7)	−0.0043 (6)	−0.0207 (6)
Cl2′	0.0947 (9)	0.0892 (8)	0.1212 (10)	−0.0332 (7)	−0.0096 (7)	0.0432 (8)
Cl2	0.1247 (10)	0.0670 (7)	0.0990 (9)	−0.0185 (7)	−0.0239 (8)	−0.0217 (6)
Cl1′	0.1280 (11)	0.1157 (10)	0.1013 (10)	−0.0510 (9)	−0.0264 (8)	0.0499 (8)
Cl1	0.1490 (12)	0.0793 (8)	0.1167 (11)	−0.0433 (8)	−0.0024 (9)	−0.0282 (7)
N2	0.0489 (18)	0.0452 (18)	0.057 (2)	−0.0088 (14)	−0.0001 (15)	0.0068 (15)
N2′	0.0536 (19)	0.056 (2)	0.058 (2)	−0.0087 (15)	−0.0144 (16)	−0.0017 (16)
C1	0.041 (2)	0.052 (2)	0.048 (2)	−0.0085 (17)	0.0027 (16)	0.0034 (18)
C9	0.038 (2)	0.045 (2)	0.063 (3)	−0.0075 (17)	0.0035 (17)	0.0139 (19)
C10′	0.050 (2)	0.050 (2)	0.073 (3)	−0.0085 (18)	−0.022 (2)	0.001 (2)
C1′	0.046 (2)	0.082 (3)	0.038 (2)	−0.008 (2)	−0.0140 (17)	0.002 (2)
C2	0.054 (2)	0.053 (2)	0.049 (2)	−0.0172 (18)	−0.0032 (17)	0.0029 (19)
C10	0.047 (2)	0.043 (2)	0.060 (2)	−0.0117 (17)	0.0071 (18)	0.0029 (19)

C7	0.041 (2)	0.054 (2)	0.051 (2)	−0.0083 (17)	0.0048 (17)	0.0083 (18)
C9′	0.054 (2)	0.053 (3)	0.067 (3)	−0.0032 (19)	−0.021 (2)	−0.013 (2)
C3	0.051 (2)	0.055 (2)	0.057 (3)	−0.0135 (18)	0.0016 (18)	0.011 (2)
N1	0.105 (3)	0.057 (3)	0.082 (3)	−0.028 (2)	0.002 (2)	0.004 (2)
C3′	0.060 (3)	0.074 (3)	0.055 (3)	−0.015 (2)	−0.010 (2)	0.009 (2)
C2′	0.050 (2)	0.073 (3)	0.047 (2)	−0.010 (2)	−0.0025 (18)	0.009 (2)
C4	0.058 (2)	0.063 (3)	0.072 (3)	−0.014 (2)	0.008 (2)	−0.012 (2)
C12	0.068 (3)	0.044 (2)	0.097 (3)	−0.016 (2)	0.000 (2)	−0.008 (2)
C15′	0.062 (3)	0.044 (2)	0.083 (3)	−0.0150 (19)	−0.011 (2)	0.005 (2)
C13	0.063 (3)	0.052 (3)	0.079 (3)	−0.010 (2)	0.002 (2)	−0.007 (2)
C6′	0.067 (3)	0.095 (3)	0.054 (3)	−0.011 (2)	−0.014 (2)	0.004 (2)
C5′	0.070 (3)	0.116 (4)	0.046 (3)	−0.022 (3)	−0.009 (2)	0.023 (3)
C15	0.078 (3)	0.044 (2)	0.064 (3)	−0.021 (2)	0.005 (2)	0.000 (2)
C14	0.098 (3)	0.046 (2)	0.065 (3)	−0.021 (2)	−0.001 (2)	−0.003 (2)
C11	0.062 (3)	0.048 (2)	0.087 (3)	−0.0114 (19)	−0.004 (2)	0.008 (2)
C4′	0.064 (3)	0.086 (3)	0.066 (3)	−0.022 (2)	−0.021 (2)	0.025 (3)
C6	0.068 (3)	0.065 (3)	0.056 (3)	−0.016 (2)	−0.003 (2)	0.010 (2)
C7′	0.049 (2)	0.066 (3)	0.056 (3)	−0.0033 (19)	−0.0160 (19)	−0.003 (2)
C14′	0.065 (3)	0.054 (3)	0.085 (3)	−0.018 (2)	−0.004 (2)	0.010 (2)
N1′	0.108 (3)	0.070 (3)	0.082 (3)	−0.021 (2)	−0.009 (3)	0.006 (3)
C13′	0.053 (3)	0.062 (3)	0.099 (3)	−0.013 (2)	−0.015 (2)	0.007 (3)
C5	0.074 (3)	0.082 (3)	0.053 (3)	−0.019 (2)	−0.003 (2)	−0.008 (2)
C8	0.060 (2)	0.045 (2)	0.072 (3)	−0.0136 (18)	0.004 (2)	0.007 (2)
C12′	0.069 (3)	0.049 (3)	0.127 (4)	−0.022 (2)	−0.030 (3)	0.020 (3)
O2′	0.169 (4)	0.100 (3)	0.089 (3)	−0.018 (2)	−0.032 (2)	−0.013 (2)
C11′	0.074 (3)	0.051 (3)	0.099 (4)	−0.012 (2)	−0.029 (3)	−0.008 (2)
O1′	0.181 (4)	0.076 (2)	0.131 (3)	0.013 (2)	−0.015 (3)	0.011 (2)
O2	0.237 (5)	0.094 (3)	0.074 (2)	−0.070 (3)	−0.002 (3)	0.011 (2)
C8′	0.093 (3)	0.061 (3)	0.082 (3)	−0.012 (2)	−0.023 (3)	−0.007 (2)
O1	0.185 (4)	0.066 (2)	0.143 (3)	−0.014 (2)	0.011 (3)	0.028 (2)

Geometric parameters (Å, º)

S1—C8	1.692 (4)	C3′—C4′	1.377 (5)
S1—C7	1.730 (3)	C3′—C2′	1.378 (5)
S1′—C8′	1.695 (4)	C3′—N1′	1.459 (5)
S1′—C7′	1.737 (4)	C2′—H2′	0.9300
Cl2′—C13′	1.733 (4)	C4—C5	1.373 (5)
Cl2—C13	1.727 (4)	C12—C13	1.379 (5)
Cl1′—C4′	1.726 (4)	C12—C11	1.380 (5)
Cl1—C4	1.723 (4)	C12—H12	0.9300
N2—C7	1.300 (4)	C15′—C14′	1.380 (5)
N2—C9	1.372 (4)	C15′—H15′	0.9300
N2′—C7′	1.288 (4)	C13—C14	1.366 (5)
N2′—C9′	1.385 (4)	C6′—C5′	1.370 (5)
C1—C2	1.372 (4)	C6′—H6′	0.9300
C1—C6	1.380 (5)	C5′—C4′	1.376 (5)
C1—C7	1.468 (5)	C5′—H5′	0.9300

C9—C8	1.361 (5)	C15—C14	1.371 (5)
C9—C10	1.467 (5)	C15—H15	0.9300
C10′—C15′	1.372 (5)	C14—H14	0.9300
C10′—C11′	1.402 (5)	C11—H11	0.9300
C10′—C9′	1.465 (5)	C6—C5	1.357 (5)
C1′—C2′	1.383 (5)	C6—H6	0.9300
C1′—C6′	1.396 (5)	C14′—C13′	1.374 (5)
C1′—C7′	1.458 (5)	C14′—H14′	0.9300
C2—C3	1.372 (4)	N1′—O2′	1.205 (4)
C2—H2	0.9300	N1′—O1′	1.219 (4)
C10—C15	1.380 (5)	C13′—C12′	1.366 (5)
C10—C11	1.388 (5)	C5—H5	0.9300
C9′—C8′	1.352 (5)	C8—H8	0.9300
C3—C4	1.395 (5)	C12′—C11′	1.382 (5)
C3—N1	1.464 (5)	C12′—H12′	0.9300
N1—O1	1.193 (4)	C11′—H11′	0.9300
N1—O2	1.195 (4)	C8′—H8′	0.9300

C8—S1—C7	89.27 (18)	C14—C13—Cl2	119.9 (3)
C8′—S1′—C7′	89.0 (2)	C12—C13—Cl2	119.5 (3)
C7—N2—C9	111.8 (3)	C5′—C6′—C1′	121.2 (4)
C7′—N2′—C9′	112.2 (3)	C5′—C6′—H6′	119.4
C2—C1—C6	118.2 (3)	C1′—C6′—H6′	119.4
C2—C1—C7	119.1 (3)	C6′—C5′—C4′	121.1 (4)
C6—C1—C7	122.7 (3)	C6′—C5′—H5′	119.4
C8—C9—N2	113.8 (3)	C4′—C5′—H5′	119.4
C8—C9—C10	126.9 (3)	C14—C15—C10	122.0 (4)
N2—C9—C10	119.3 (3)	C14—C15—H15	119.0
C15′—C10′—C11′	118.2 (4)	C10—C15—H15	119.0
C15′—C10′—C9′	120.1 (3)	C13—C14—C15	119.5 (4)
C11′—C10′—C9′	121.7 (4)	C13—C14—H14	120.2
C2′—C1′—C6′	117.4 (4)	C15—C14—H14	120.2
C2′—C1′—C7′	120.0 (3)	C12—C11—C10	121.5 (4)
C6′—C1′—C7′	122.5 (4)	C12—C11—H11	119.3
C3—C2—C1	120.9 (3)	C10—C11—H11	119.3
C3—C2—H2	119.5	C5′—C4′—C3′	118.1 (4)
C1—C2—H2	119.5	C5′—C4′—Cl1′	119.0 (4)
C15—C10—C11	117.3 (4)	C3′—C4′—Cl1′	122.7 (4)
C15—C10—C9	120.3 (3)	C5—C6—C1	121.0 (4)
C11—C10—C9	122.3 (3)	C5—C6—H6	119.5
N2—C7—C1	123.5 (3)	C1—C6—H6	119.5
N2—C7—S1	113.8 (3)	N2′—C7′—C1′	124.4 (3)
C1—C7—S1	122.7 (3)	N2′—C7′—S1′	113.7 (3)
C8′—C9′—N2′	113.3 (4)	C1′—C7′—S1′	121.9 (3)
C8′—C9′—C10′	126.8 (4)	C13′—C14′—C15′	118.8 (4)
N2′—C9′—C10′	119.9 (3)	C13′—C14′—H14′	120.6
C2—C3—C4	120.6 (3)	C15′—C14′—H14′	120.6
C2—C3—N1	117.2 (3)	O2′—N1′—O1′	123.4 (4)

C4—C3—N1	122.2 (4)	O2′—N1′—C3′	118.3 (4)
O1—N1—O2	122.6 (4)	O1′—N1′—C3′	118.3 (4)
O1—N1—C3	119.8 (4)	C12′—C13′—C14′	120.7 (4)
O2—N1—C3	117.6 (4)	C12′—C13′—Cl2′	119.3 (3)
C4′—C3′—C2′	121.3 (4)	C14′—C13′—Cl2′	120.0 (4)
C4′—C3′—N1′	120.5 (4)	C6—C5—C4	121.7 (4)
C2′—C3′—N1′	118.2 (4)	C6—C5—H5	119.2
C3′—C2′—C1′	120.9 (4)	C4—C5—H5	119.2
C3′—C2′—H2′	119.6	C9—C8—S1	111.3 (3)
C1′—C2′—H2′	119.6	C9—C8—H8	124.4
C5—C4—C3	117.5 (4)	S1—C8—H8	124.4
C5—C4—Cl1	119.0 (3)	C13′—C12′—C11′	120.5 (4)
C3—C4—Cl1	123.4 (3)	C13′—C12′—H12′	119.8
C13—C12—C11	119.1 (4)	C11′—C12′—H12′	119.8
C13—C12—H12	120.4	C12′—C11′—C10′	119.7 (4)
C11—C12—H12	120.4	C12′—C11′—H11′	120.1
C10′—C15′—C14′	122.1 (4)	C10′—C11′—H11′	120.1
C10′—C15′—H15′	119.0	C9′—C8′—S1′	111.7 (3)
C14′—C15′—H15′	119.0	C9′—C8′—H8′	124.1
C14—C13—C12	120.5 (4)	S1′—C8′—H8′	124.1

C7—N2—C9—C8	−0.2 (4)	C9—C10—C15—C14	−175.7 (3)
C7—N2—C9—C10	178.1 (3)	C12—C13—C14—C15	−1.5 (6)
C6—C1—C2—C3	−1.1 (5)	Cl2—C13—C14—C15	176.2 (3)
C7—C1—C2—C3	−179.9 (3)	C10—C15—C14—C13	−0.5 (6)
C8—C9—C10—C15	173.0 (3)	C13—C12—C11—C10	0.3 (6)
N2—C9—C10—C15	−5.1 (5)	C15—C10—C11—C12	−2.3 (5)
C8—C9—C10—C11	−5.0 (5)	C9—C10—C11—C12	175.8 (3)
N2—C9—C10—C11	176.9 (3)	C6′—C5′—C4′—C3′	−1.1 (6)
C9—N2—C7—C1	−179.4 (3)	C6′—C5′—C4′—Cl1′	−176.4 (3)
C9—N2—C7—S1	0.2 (4)	C2′—C3′—C4′—C5′	−0.4 (5)
C2—C1—C7—N2	−0.3 (5)	N1′—C3′—C4′—C5′	−178.6 (4)
C6—C1—C7—N2	−179.2 (3)	C2′—C3′—C4′—Cl1′	174.7 (3)
C2—C1—C7—S1	−179.9 (2)	N1′—C3′—C4′—Cl1′	−3.6 (5)
C6—C1—C7—S1	1.3 (4)	C2—C1—C6—C5	0.7 (5)
C8—S1—C7—N2	−0.1 (3)	C7—C1—C6—C5	179.5 (3)
C8—S1—C7—C1	179.5 (3)	C9′—N2′—C7′—C1′	178.9 (3)
C7′—N2′—C9′—C8′	−1.1 (4)	C9′—N2′—C7′—S1′	1.0 (4)
C7′—N2′—C9′—C10′	−178.9 (3)	C2′—C1′—C7′—N2′	−6.4 (5)
C15′—C10′—C9′—C8′	−171.7 (4)	C6′—C1′—C7′—N2′	174.8 (3)
C11′—C10′—C9′—C8′	7.1 (6)	C2′—C1′—C7′—S1′	171.4 (3)
C15′—C10′—C9′—N2′	5.8 (5)	C6′—C1′—C7′—S1′	−7.5 (5)
C11′—C10′—C9′—N2′	−175.5 (3)	C8′—S1′—C7′—N2′	−0.6 (3)
C1—C2—C3—C4	0.6 (5)	C8′—S1′—C7′—C1′	−178.5 (3)
C1—C2—C3—N1	178.8 (3)	C10′—C15′—C14′—C13′	−0.2 (5)
C2—C3—N1—O1	146.7 (4)	C4′—C3′—N1′—O2′	132.4 (4)
C4—C3—N1—O1	−35.2 (6)	C2′—C3′—N1′—O2′	−45.9 (6)
C2—C3—N1—O2	−35.0 (5)	C4′—C3′—N1′—O1′	−50.1 (6)

C4—C3—N1—O2	143.1 (4)	C2′—C3′—N1′—O1′	131.7 (4)
C4′—C3′—C2′—C1′	1.2 (5)	C15′—C14′—C13′—C12′	1.9 (6)
N1′—C3′—C2′—C1′	179.5 (3)	C15′—C14′—C13′—Cl2′	−177.5 (3)
C6′—C1′—C2′—C3′	−0.5 (5)	C1—C6—C5—C4	0.2 (6)
C7′—C1′—C2′—C3′	−179.4 (3)	C3—C4—C5—C6	−0.7 (6)
C2—C3—C4—C5	0.3 (5)	Cl1—C4—C5—C6	−178.3 (3)
N1—C3—C4—C5	−177.8 (3)	N2—C9—C8—S1	0.2 (4)
C2—C3—C4—Cl1	177.7 (3)	C10—C9—C8—S1	−178.0 (3)
N1—C3—C4—Cl1	−0.3 (5)	C7—S1—C8—C9	0.0 (3)
C11′—C10′—C15′—C14′	−1.7 (5)	C14′—C13′—C12′—C11′	−1.6 (6)
C9′—C10′—C15′—C14′	177.1 (3)	Cl2′—C13′—C12′—C11′	177.8 (3)
C11—C12—C13—C14	1.6 (6)	C13′—C12′—C11′—C10′	−0.5 (6)
C11—C12—C13—Cl2	−176.1 (3)	C15′—C10′—C11′—C12′	2.1 (5)
C2′—C1′—C6′—C5′	−1.0 (5)	C9′—C10′—C11′—C12′	−176.7 (3)
C7′—C1′—C6′—C5′	177.9 (3)	N2′—C9′—C8′—S1′	0.7 (4)
C1′—C6′—C5′—C4′	1.9 (6)	C10′—C9′—C8′—S1′	178.2 (3)
C11—C10—C15—C14	2.4 (5)	C7′—S1′—C8′—C9′	−0.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.93	2.48	3.285 (5)	145
C15′—H15′···Cl2^{ii}	0.93	2.73	3.610 (4)	158

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