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2-Chloro-*N*-(4-phenyl-1,3-thiazol-2-yl)acetamide

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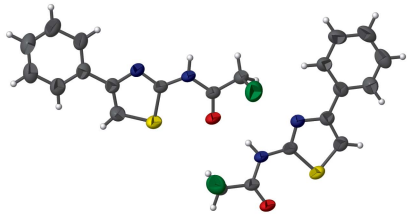
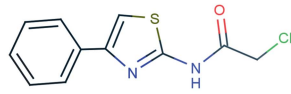
Structural data: full structural data are available from iucrdata.iucr.org

The title acetamide, $C_{11}H_9ClN_2OS$, crystallizes with two independent molecules in the asymmetric unit whose geometrical features are similar. The phenyl ring is oriented at angles of 2.5 (1) and 6.2 (1)° with respect to the thiazole ring in the two molecules. In the crystal, molecules are linked *via* C—H···N hydrogen bonds which form $C(10)$ chains along the [$\bar{1}$00] direction. The chains are linked by N—H···O and C—H···O hydrogen bonds, forming $C(8)$ chains along the [100] direction.

3D view



Chemical scheme



Structure description

Acetamide derivatives are new potential PET tracers for imaging nucleotide pyrophosphatase/phosphodiesterase (Gao *et al.*, 2016). These derivatives act as anticholinesterase agents for a possible role in the management of Alzheimer's disease (Sun *et al.*, 2016). Acetamide derivatives possess anticonvulsant, antidepressant (Zhen *et al.*, 2015) and anti-HIV (Huang *et al.*, 2016) activities. In view of the many interesting applications of acetamide derivatives we synthesized the title compound and report herein its crystal structure.

The X-ray study confirmed the molecular structure and atomic connectivity, as illustrated in Fig. 1. The asymmetric unit contains two molecules (Fig. 1); their corresponding bond lengths and bond angles are in good agreement. Fig. 2 shows a superposition of the thiazole ring of both the molecules using *Qmol* (Gans & Shalloway, 2001); the r.m.s. deviation is 0.734 Å. The phenyl ring and thiazole rings are coplanar with the maximum deviation of 0.007 (3) and 0.003 (3) Å for atom C9 in molecules *A* and *B*, respectively. The phenyl ring is oriented at angles of 2.5 (1) and 6.2 (1)°, respectively, to the thiazole ring in molecules *A* and *B*. The molecular structure is influenced by four intramolecular hydrogen bonds of N—H···O, C—H···N and C—H···O types (Table 1).

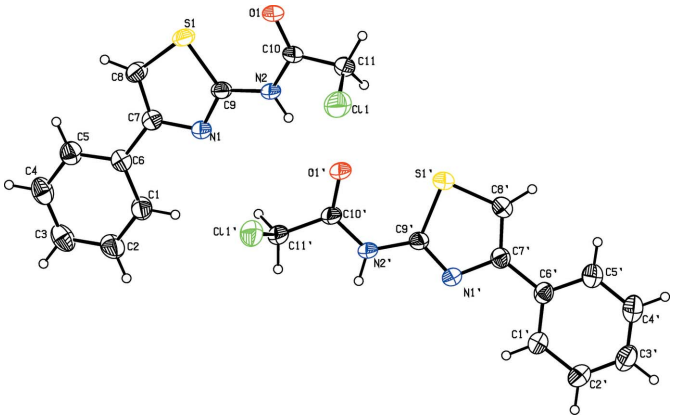


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

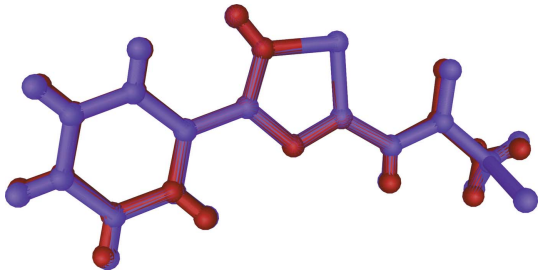


Figure 2
Superposition of molecule *A* (red) with the molecule *B* (purple).

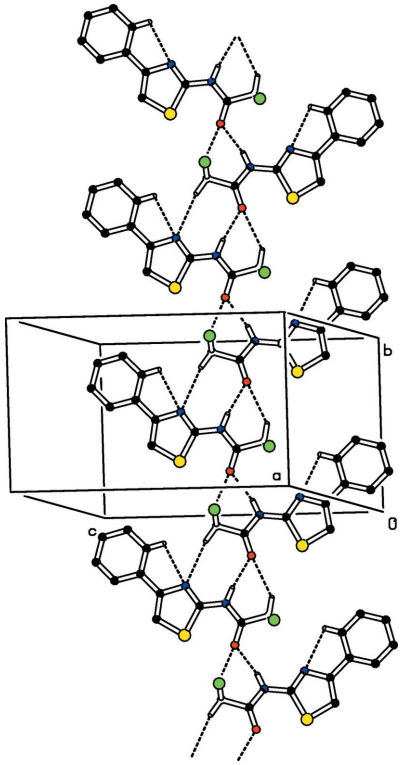


Figure 3
Crystal packing of the title compound, viewed along the *a* axis. The C—H···N, N—H···O and C—H···O hydrogen bonds are shown as dashed lines (see Table 1). For clarity, H atoms not involved in these hydrogen bonds have been omitted.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···N1′^{i}	0.97	2.62	3.565 (4)	165
N2′—H2′···O1^{ii}	0.86	1.98	2.835 (3)	172
C11′—H11*C*···O1^{ii}	0.97	2.48	3.329 (3)	146
N2—H2···O1′	0.86	1.98	2.825 (3)	168
C1—H1···N1	0.93	2.54	2.869 (4)	101
C1′—H1′···N1′	0.93	2.56	2.880 (4)	101
C11—H11*B*···O1′	0.97	2.55	3.204 (3)	125

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_9ClN_2OS$
M_r	252.71
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.0406 (9), 9.2313 (14), 15.9898 (17)
α, β, γ (°)	85.693 (19), 76.448 (19), 87.082 (19)
V (Å^3)	1149.9 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.49
Crystal size (mm)	0.22 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6721, 5129, 3519
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.174, 1.03
No. of reflections	5129
No. of parameters	289
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.52

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

In the crystal, C—H···N hydrogen bonds link the molecules, forming $C(10)$ chains propagating along [$\overline{1}$00]. In addition to this, N—H···O and C—H···O hydrogen bonds also link the molecules into $C(8)$ chains propagating along [100]; see Fig. 3.

Synthesis and crystallization

To a solution of 4-phenylthiazol-2-amine (1.5 g, 8.52 mmol) in dry toluene (25 ml), K_2CO_3 (2.32 g, 17.04 mmol) and chloroacetyl chloride (0.67 ml, 8.52 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 concen-

trated 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 colorless crystals of the title compound.

Refinement

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

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full crystallographic data

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Crystal data

$C_{11}H_9ClN_2OS$
$M_r = 252.71$
Triclinic, $P\overline{1}$
$a = 8.0406$ (9) Å
$b = 9.2313$ (14) Å
$c = 15.9898$ (17) Å
$\alpha = 85.693$ (19)°
$\beta = 76.448$ (19)°
$\gamma = 87.082$ (19)°
$V = 1149.9$ (3) Å^3
$Z = 4$
$F(000) = 520$
$D_x = 1.460$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4218 reflections
$\theta = 3.2$–$26.8°$
$\mu = 0.49$ mm^{-1}
$T = 296$ K
Block, colourless
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scans
6721 measured reflections
5129 independent reflections
3519 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -10\rightarrow10$
$k = -11\rightarrow7$
$l = -20\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.174$
$S = 1.03$
5129 reflections
289 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0971P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ 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	0.41465 (9)	0.74959 (7)	0.15473 (5)	0.0538 (2)

O1	0.6150 (3)	0.66650 (18)	0.27078 (12)	0.0597 (5)
N1	0.4150 (3)	1.0270 (2)	0.15895 (13)	0.0471 (5)
N2	0.5584 (3)	0.9072 (2)	0.25671 (14)	0.0519 (5)
H2	0.5680	0.9893	0.2769	0.062*
Cl1	0.94512 (12)	0.88155 (11)	0.28862 (7)	0.0922 (3)
C1	0.2855 (4)	1.2645 (3)	0.06344 (19)	0.0622 (7)
H1	0.3388	1.2834	0.1070	0.075*
C2	0.2265 (5)	1.3788 (4)	0.0159 (2)	0.0750 (9)
H2A	0.2410	1.4739	0.0277	0.090*
C3	0.1468 (4)	1.3534 (4)	−0.0483 (2)	0.0714 (9)
H3	0.1069	1.4307	−0.0799	0.086*
C4	0.1266 (4)	1.2125 (4)	−0.0654 (2)	0.0695 (8)
H4	0.0721	1.1944	−0.1087	0.083*
C5	0.1860 (3)	1.0988 (3)	−0.01938 (18)	0.0599 (7)
H5	0.1726	1.0043	−0.0325	0.072*
C6	0.2660 (3)	1.1213 (3)	0.04659 (16)	0.0493 (6)
C7	0.3300 (3)	0.9994 (3)	0.09627 (16)	0.0467 (5)
C8	0.3176 (3)	0.8557 (3)	0.08623 (18)	0.0554 (6)
H8	0.2633	0.8197	0.0472	0.066*
C9	0.4664 (3)	0.9065 (2)	0.19303 (16)	0.0460 (5)
C10	0.6333 (4)	0.7901 (3)	0.28888 (16)	0.0518 (6)
C11	0.7436 (5)	0.8203 (3)	0.3497 (2)	0.0696 (8)
H11A	0.7600	0.7325	0.3845	0.084*
H11B	0.6877	0.8940	0.3879	0.084*
S1′	0.69249 (11)	1.20434 (7)	0.49270 (4)	0.0608 (2)
O1′	0.6147 (3)	1.15393 (19)	0.33948 (13)	0.0642 (5)
N1′	0.7240 (3)	1.4819 (2)	0.47406 (13)	0.0466 (5)
N2′	0.6465 (3)	1.3901 (2)	0.35679 (13)	0.0468 (5)
H2′	0.6406	1.4773	0.3344	0.056*
Cl1′	0.76597 (12)	1.26828 (10)	0.14499 (5)	0.0814 (3)
C1′	0.8038 (4)	1.6899 (3)	0.58315 (19)	0.0668 (8)
H1′	0.7653	1.7229	0.5344	0.080*
C2′	0.8529 (5)	1.7902 (4)	0.6332 (2)	0.0803 (10)
H2′1	0.8495	1.8890	0.6168	0.096*
C3′	0.9056 (4)	1.7439 (4)	0.7057 (2)	0.0743 (9)
H3′	0.9367	1.8108	0.7395	0.089*
C4′	0.9128 (4)	1.6001 (4)	0.7287 (2)	0.0722 (9)
H4′	0.9494	1.5688	0.7783	0.087*
C5′	0.8667 (4)	1.4990 (4)	0.67955 (18)	0.0635 (7)
H5′	0.8725	1.4006	0.6964	0.076*
C6′	0.8115 (3)	1.5434 (3)	0.60490 (15)	0.0499 (6)
C8′	0.7508 (4)	1.2908 (3)	0.57165 (17)	0.0616 (7)
H8′	0.7719	1.2440	0.6219	0.074*
C7′	0.7626 (3)	1.4359 (3)	0.55226 (16)	0.0484 (6)
C9′	0.6865 (3)	1.3722 (2)	0.43644 (15)	0.0442 (5)
C10′	0.6162 (3)	1.2810 (3)	0.31178 (17)	0.0493 (6)
C11′	0.5852 (4)	1.3246 (3)	0.22428 (18)	0.0606 (7)
H11C	0.5675	1.4292	0.2180	0.073*

H11D	0.4836	1.2792	0.2172	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0635 (4)	0.0347 (3)	0.0662 (4)	−0.0070 (3)	−0.0186 (3)	−0.0062 (3)
O1	0.0932 (14)	0.0277 (9)	0.0627 (11)	−0.0032 (8)	−0.0277 (10)	−0.0004 (7)
N1	0.0563 (12)	0.0366 (11)	0.0501 (11)	0.0005 (8)	−0.0161 (10)	−0.0035 (8)
N2	0.0778 (14)	0.0266 (10)	0.0575 (12)	−0.0018 (9)	−0.0284 (11)	−0.0016 (8)
Cl1	0.0911 (6)	0.0810 (6)	0.1208 (8)	−0.0078 (5)	−0.0587 (6)	0.0006 (5)
C1	0.0819 (19)	0.0519 (16)	0.0561 (15)	0.0180 (14)	−0.0240 (15)	−0.0127 (12)
C2	0.100 (2)	0.0563 (18)	0.0677 (18)	0.0238 (16)	−0.0231 (18)	−0.0052 (14)
C3	0.0649 (18)	0.082 (2)	0.0639 (18)	0.0227 (16)	−0.0162 (15)	0.0076 (16)
C4	0.0519 (16)	0.096 (3)	0.0615 (17)	−0.0006 (15)	−0.0196 (14)	0.0078 (16)
C5	0.0510 (14)	0.0690 (18)	0.0610 (16)	−0.0056 (12)	−0.0153 (13)	−0.0022 (13)
C6	0.0421 (12)	0.0552 (15)	0.0483 (13)	0.0050 (10)	−0.0075 (11)	−0.0026 (11)
C7	0.0437 (12)	0.0469 (14)	0.0483 (13)	0.0017 (10)	−0.0079 (11)	−0.0059 (10)
C8	0.0569 (15)	0.0481 (15)	0.0657 (16)	−0.0042 (11)	−0.0208 (13)	−0.0100 (12)
C9	0.0536 (13)	0.0337 (12)	0.0492 (12)	−0.0032 (10)	−0.0092 (11)	−0.0015 (10)
C10	0.0728 (16)	0.0315 (12)	0.0519 (14)	−0.0019 (11)	−0.0179 (13)	0.0020 (10)
C11	0.111 (2)	0.0408 (15)	0.0692 (18)	−0.0006 (15)	−0.0469 (18)	0.0018 (13)
S1′	0.0902 (5)	0.0375 (4)	0.0573 (4)	−0.0053 (3)	−0.0232 (4)	0.0022 (3)
O1′	0.1028 (15)	0.0296 (9)	0.0690 (12)	−0.0025 (9)	−0.0376 (11)	−0.0031 (8)
N1′	0.0553 (12)	0.0376 (10)	0.0483 (11)	−0.0034 (8)	−0.0133 (9)	−0.0060 (8)
N2′	0.0636 (12)	0.0273 (9)	0.0530 (11)	−0.0020 (8)	−0.0204 (10)	−0.0024 (8)
Cl1′	0.0989 (6)	0.0854 (6)	0.0611 (5)	−0.0138 (5)	−0.0171 (4)	−0.0099 (4)
C1′	0.090 (2)	0.0596 (18)	0.0573 (16)	−0.0143 (15)	−0.0277 (16)	−0.0062 (13)
C2′	0.115 (3)	0.062 (2)	0.070 (2)	−0.0206 (18)	−0.028 (2)	−0.0120 (16)
C3′	0.078 (2)	0.086 (2)	0.0618 (18)	−0.0208 (17)	−0.0133 (16)	−0.0223 (17)
C4′	0.074 (2)	0.092 (3)	0.0545 (16)	−0.0065 (17)	−0.0194 (15)	−0.0140 (16)
C5′	0.0713 (18)	0.0669 (19)	0.0530 (15)	−0.0022 (14)	−0.0145 (14)	−0.0088 (13)
C6′	0.0498 (13)	0.0573 (15)	0.0399 (12)	−0.0065 (11)	−0.0022 (11)	−0.0089 (10)
C8′	0.0834 (19)	0.0532 (17)	0.0498 (14)	−0.0042 (13)	−0.0200 (14)	0.0033 (12)
C7′	0.0498 (13)	0.0512 (14)	0.0428 (12)	−0.0022 (10)	−0.0074 (11)	−0.0044 (10)
C9′	0.0510 (13)	0.0352 (12)	0.0458 (12)	0.0007 (9)	−0.0103 (11)	−0.0032 (9)
C10′	0.0606 (15)	0.0331 (13)	0.0576 (14)	0.0004 (10)	−0.0203 (12)	−0.0046 (10)
C11′	0.085 (2)	0.0399 (14)	0.0648 (16)	−0.0004 (12)	−0.0335 (15)	−0.0056 (12)

Geometric parameters (Å, º)

S1—C8	1.712 (3)	S1′—C8′	1.708 (3)
S1—C9	1.720 (2)	S1′—C9′	1.737 (2)
O1—C10	1.222 (3)	O1′—C10′	1.222 (3)
N1—C9	1.294 (3)	N1′—C9′	1.298 (3)
N1—C7	1.383 (3)	N1′—C7′	1.389 (3)
N2—C10	1.338 (3)	N2′—C10′	1.344 (3)
N2—C9	1.393 (3)	N2′—C9′	1.381 (3)
N2—H2	0.8600	N2′—H2′	0.8600

Cl1—C11	1.780 (4)	Cl1′—C11′	1.774 (3)
C1—C2	1.384 (4)	C1′—C6′	1.373 (4)
C1—C6	1.392 (4)	C1′—C2′	1.397 (4)
C1—H1	0.9300	C1′—H1′	0.9300
C2—C3	1.370 (5)	C2′—C3′	1.358 (5)
C2—H2A	0.9300	C2′—H2′1	0.9300
C3—C4	1.375 (5)	C3′—C4′	1.352 (5)
C3—H3	0.9300	C3′—H3′	0.9300
C4—C5	1.367 (4)	C4′—C5′	1.381 (4)
C4—H4	0.9300	C4′—H4′	0.9300
C5—C6	1.391 (4)	C5′—C6′	1.395 (4)
C5—H5	0.9300	C5′—H5′	0.9300
C6—C7	1.470 (3)	C6′—C7′	1.473 (4)
C7—C8	1.359 (4)	C8′—C7′	1.354 (4)
C8—H8	0.9300	C8′—H8′	0.9300
C10—C11	1.510 (4)	C10′—C11′	1.500 (4)
C11—H11A	0.9700	C11′—H11C	0.9700
C11—H11B	0.9700	C11′—H11D	0.9700
C8—S1—C9	88.17 (12)	C8′—S1′—C9′	88.18 (13)
C9—N1—C7	110.4 (2)	C9′—N1′—C7′	110.5 (2)
C10—N2—C9	125.1 (2)	C10′—N2′—C9′	124.7 (2)
C10—N2—H2	117.4	C10′—N2′—H2′	117.6
C9—N2—H2	117.4	C9′—N2′—H2′	117.6
C2—C1—C6	120.6 (3)	C6′—C1′—C2′	121.0 (3)
C2—C1—H1	119.7	C6′—C1′—H1′	119.5
C6—C1—H1	119.7	C2′—C1′—H1′	119.5
C3—C2—C1	120.7 (3)	C3′—C2′—C1′	120.1 (3)
C3—C2—H2A	119.7	C3′—C2′—H2′1	119.9
C1—C2—H2A	119.7	C1′—C2′—H2′1	119.9
C2—C3—C4	119.3 (3)	C4′—C3′—C2′	119.8 (3)
C2—C3—H3	120.4	C4′—C3′—H3′	120.1
C4—C3—H3	120.4	C2′—C3′—H3′	120.1
C5—C4—C3	120.5 (3)	C3′—C4′—C5′	120.9 (3)
C5—C4—H4	119.8	C3′—C4′—H4′	119.5
C3—C4—H4	119.8	C5′—C4′—H4′	119.5
C4—C5—C6	121.5 (3)	C4′—C5′—C6′	120.5 (3)
C4—C5—H5	119.2	C4′—C5′—H5′	119.7
C6—C5—H5	119.2	C6′—C5′—H5′	119.7
C5—C6—C1	117.5 (3)	C1′—C6′—C5′	117.6 (3)
C5—C6—C7	121.7 (3)	C1′—C6′—C7′	121.8 (2)
C1—C6—C7	120.8 (2)	C5′—C6′—C7′	120.6 (3)
C8—C7—N1	114.1 (2)	C7′—C8′—S1′	111.8 (2)
C8—C7—C6	126.2 (2)	C7′—C8′—H8′	124.1
N1—C7—C6	119.7 (2)	S1′—C8′—H8′	124.1
C7—C8—S1	111.3 (2)	C8′—C7′—N1′	114.1 (2)
C7—C8—H8	124.3	C8′—C7′—C6′	126.6 (2)
S1—C8—H8	124.3	N1′—C7′—C6′	119.3 (2)

N1—C9—N2	120.7 (2)	N1′—C9′—N2′	121.4 (2)
N1—C9—S1	116.1 (2)	N1′—C9′—S1′	115.38 (19)
N2—C9—S1	123.19 (18)	N2′—C9′—S1′	123.22 (18)
O1—C10—N2	123.0 (3)	O1′—C10′—N2′	122.7 (2)
O1—C10—C11	121.6 (2)	O1′—C10′—C11′	121.6 (2)
N2—C10—C11	115.4 (2)	N2′—C10′—C11′	115.7 (2)
C10—C11—Cl1	109.2 (2)	C10′—C11′—Cl1′	108.7 (2)
C10—C11—H11A	109.8	C10′—C11′—H11C	110.0
Cl1—C11—H11A	109.8	Cl1′—C11′—H11C	110.0
C10—C11—H11B	109.8	C10′—C11′—H11D	110.0
Cl1—C11—H11B	109.8	Cl1′—C11′—H11D	110.0
H11A—C11—H11B	108.3	H11C—C11′—H11D	108.3
C6—C1—C2—C3	0.4 (5)	C6′—C1′—C2′—C3′	−1.5 (5)
C1—C2—C3—C4	−0.3 (5)	C1′—C2′—C3′—C4′	1.0 (5)
C2—C3—C4—C5	−0.4 (5)	C2′—C3′—C4′—C5′	−0.2 (5)
C3—C4—C5—C6	0.9 (4)	C3′—C4′—C5′—C6′	0.0 (5)
C4—C5—C6—C1	−0.8 (4)	C2′—C1′—C6′—C5′	1.3 (5)
C4—C5—C6—C7	180.0 (2)	C2′—C1′—C6′—C7′	−179.1 (3)
C2—C1—C6—C5	0.2 (4)	C4′—C5′—C6′—C1′	−0.5 (4)
C2—C1—C6—C7	179.4 (3)	C4′—C5′—C6′—C7′	179.9 (3)
C9—N1—C7—C8	1.1 (3)	C9′—S1′—C8′—C7′	−0.1 (2)
C9—N1—C7—C6	−177.7 (2)	S1′—C8′—C7′—N1′	0.5 (3)
C5—C6—C7—C8	−1.3 (4)	S1′—C8′—C7′—C6′	−179.2 (2)
C1—C6—C7—C8	179.5 (3)	C9′—N1′—C7′—C8′	−0.7 (3)
C5—C6—C7—N1	177.4 (2)	C9′—N1′—C7′—C6′	179.0 (2)
C1—C6—C7—N1	−1.8 (4)	C1′—C6′—C7′—C8′	−173.7 (3)
N1—C7—C8—S1	−0.6 (3)	C5′—C6′—C7′—C8′	5.9 (4)
C6—C7—C8—S1	178.07 (19)	C1′—C6′—C7′—N1′	6.6 (4)
C9—S1—C8—C7	0.0 (2)	C5′—C6′—C7′—N1′	−173.8 (2)
C7—N1—C9—N2	178.7 (2)	C7′—N1′—C9′—N2′	−178.8 (2)
C7—N1—C9—S1	−1.1 (3)	C7′—N1′—C9′—S1′	0.7 (3)
C10—N2—C9—N1	−172.1 (2)	C10′—N2′—C9′—N1′	176.0 (2)
C10—N2—C9—S1	7.7 (4)	C10′—N2′—C9′—S1′	−3.5 (4)
C8—S1—C9—N1	0.7 (2)	C8′—S1′—C9′—N1′	−0.3 (2)
C8—S1—C9—N2	−179.2 (2)	C8′—S1′—C9′—N2′	179.1 (2)
C9—N2—C10—O1	−6.9 (4)	C9′—N2′—C10′—O1′	3.0 (4)
C9—N2—C10—C11	173.0 (2)	C9′—N2′—C10′—C11′	−176.5 (2)
O1—C10—C11—Cl1	100.9 (3)	O1′—C10′—C11′—Cl1′	−71.5 (3)
N2—C10—C11—Cl1	−79.0 (3)	N2′—C10′—C11′—Cl1′	108.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···N1′^{i}	0.97	2.62	3.565 (4)	165
N2′—H2′···O1^{ii}	0.86	1.98	2.835 (3)	172
C11′—H11*C*···O1^{ii}	0.97	2.48	3.329 (3)	146
N2—H2···O1′	0.86	1.98	2.825 (3)	168

C1—H1···N1	0.93	2.54	2.869 (4)	101
C1′—H1′···N1′	0.93	2.56	2.880 (4)	101
C11—H11*B*···O1′	0.97	2.55	3.204 (3)	125

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