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Ethyl 2-{3-[(2-chloro-1,3-thiazol-5-yl)-methyl]-4-nitroimino-1,3,5-triazinan-1-yl}acetate

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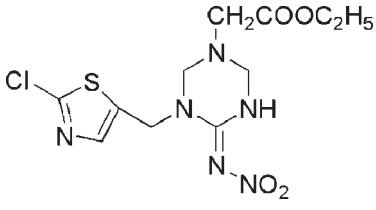
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.128; data-to-parameter ratio = 15.4.

In the title compound, $C_{11}H_{15}ClN_6O_4S$, which belongs to the neonicotinoid class of insecticidally active heterocyclic compounds, the six-membered triazine ring adopts an opened envelope conformation. The planar nitro imine group [dihedral angle between nitro and imine groups = 1.07 (7)°] and the thiazole ring are oriented at a dihedral angle of 69.62 (8)°. A classical intramolecular N—H···O hydrogen bond is found in the molecular structure. Moreover, one classical intermolecular N—H···N and four non-classical C—H···O and C—H···N hydrogen bonds are also present in the crystal structure. Besides intermolecular hydrogen bonds, the Cl atom forms an intermolecular short contact [3.020 (2) Å] with one of the nitro O atoms.

Related literature

For general background to neonicotinoid compounds and their application as insecticides, see: Kagabu (1996); Kagabu *et al.* (2005); Tian *et al.* (2007); Tomizawa *et al.* (2000); Tomizawa & Yamamoto (1993); Zhang *et al.* (2004). For halogen bonding, see: Riley & Merz (2007). For the synthesis of the title compound, see: Maienfisch *et al.* (2001).



Experimental

Crystal data

$C_{11}H_{15}ClN_6O_4S$
M_r = 362.81
Triclinic, $P\overline{1}$
a = 8.5066 (6) Å
b = 9.1114 (7) Å
c = 10.9071 (8) Å
α = 100.488 (2)°
β = 98.416 (3)°
γ = 101.281 (3)°
V = 800.55 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 298 K
0.40 × 0.23 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.857, T_{max} = 0.925
5350 measured reflections
3259 independent reflections
2670 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.128
S = 1.05
3259 reflections
212 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N6^{i}	0.79 (2)	2.55 (2)	3.133 (2)	132 (2)
N3—H3A···O3	0.79 (2)	1.98 (2)	2.570 (2)	131 (2)
C3—H3C···O3^{ii}	0.97	2.57	3.191 (3)	122
C5—H5A···N1^{iii}	0.97	2.61	3.449 (3)	144
C6—H6B···O4^{iv}	0.97	2.56	3.478 (3)	159
C10—H10···O1^{v}	0.93	2.45	3.278 (3)	149

Symmetry codes: (i) $x, y+1, z$; (ii) $x-1, y-1, z$; (iii) $-x, -y+2, -z+1$; (iv) $-x+1, -y+2, -z+1$; (v) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2201).

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supporting information

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Ethyl 2-{3-[(2-chloro-1,3-thiazol-5-yl)methyl]-4-nitroimino-1,3,5-triazinan-1-yl}acetate

Chuan-wen Sun, Jun Zhu, Jia Jin and Ding-rong Yang

S1. Comment

Neonicotinoid compounds (Tomizawa & Yamamoto, 1993; Kagabu, 1996; Tomizawa *et al.*, 2000) have received much attention on their applications as insecticide (Zhang *et al.*, 2004; Kagabu *et al.*, 2005; Tian *et al.*, 2007). We report here the molecular and crystal structures of the title compound.

The molecular structure of title compound, $C_{11}H_{15}ClN_6O_4S$, is depicted on Fig.1. The triazine moiety exhibits an opened envolope conformation with N1 out of the envolope plan defined by C5, N3, C7, N2 and C6. The dihedral angle between the thiazole ring and triazine envolope plan is 75.63 (7)°. The planar nitroimine–group and the thiazole ring are oriented the dihedral angle of 69.62 (8)°. The large discrepancy between (O4—N5···N4 115.65 (17)°) and (O3—N5···N4 123.84 (16)°) bond angles attributes to the hydrogen bond effect on O4 and O3 - look the Table 1. Another interesting structure feature that should be mentioned is that the bond lengths (C7—N2 1.340 (2)Å) and (C7—N3 1.329 (2)Å) are between the standard (C—N 1.47Å) single bond and (C═N 1.26Å) double bond, clearly showing the conjugated effect of the nirtoimine. The C7—N4 bond length is as long as to 1.357 (2)Å, due to being linked with a strong electron–attracting nitro–group. Moreover, except intermolecular hydrogen bonding, the crystal structure is further stabilized by the so–called halogen bonding (Riley & Merz, 2007), due to short intermolecular contact of Cl1—$O4^{i}$ with a distance of 3.020 (2)Å and an angle close to 180° (C11—Cl1···$O4^{i}$ 178.1 (1)°). Symmetry code: (i) 1-*x*,1-*y*,-*z*).

S2. Experimental

The title compound was prepared by the literature method (Maienfisch *et al.*, (2001). It was purified by silica gel chromatography using ethyl acetate and petroleum ether in the ratio of 1:1, as the flush to afford. This compound was obtained as white crystals, yield 46.7%, ^{1}H NMR($CDCl_3$, 400 Hz): 9.51 (1*H*, s, NH), 7.44 (1*H*, s, thiazole—H), 4.61 (2*H*,s,CH_2—thiazole), 4.48–4.49(4*H*, d, *J* = 5.2 Hz, triazine—4H), 4.21–4.15 (2*H*, m, OCH_2), 3.32 (2*H*, s, CHC═O) 1.29–1.26 (3*H*, t, *J* = 7.2 Hz, CH_3); IR(potassium bromide, cm^{-1}) 3288(N—H), 3000 (thiazole), 1730 (C═O) 1587 (C═N), 1398 (NO_2), 1224 (C—O—C), 1105 (C—N), Anal. calcd for $C_{11}H_{15}ClN_6O_4S$: C 36.42, H 4.17, N 23.16; found C 36.40, H 4.23, N 23.19. ESI–MS m/z: 363.8.

S3. Refinement

H atoms bonded to C atoms were positioned geometrically [C—H = 0.93Å (aromatic), 0.97Å (methylene) and 0.96Å (methyl)] and refined in riding modes with U_{iso}(H) = 1.2U_{eq}(C) for aromatic and methylene; U_{iso}(H) = 1.5U~eq~(C) for methyl. H atom bonded to N atom was found from Fourier difference maps and refined with the constraint U_{iso}(H) = 1.2U_{eq}(N), but coordinates refined freely.

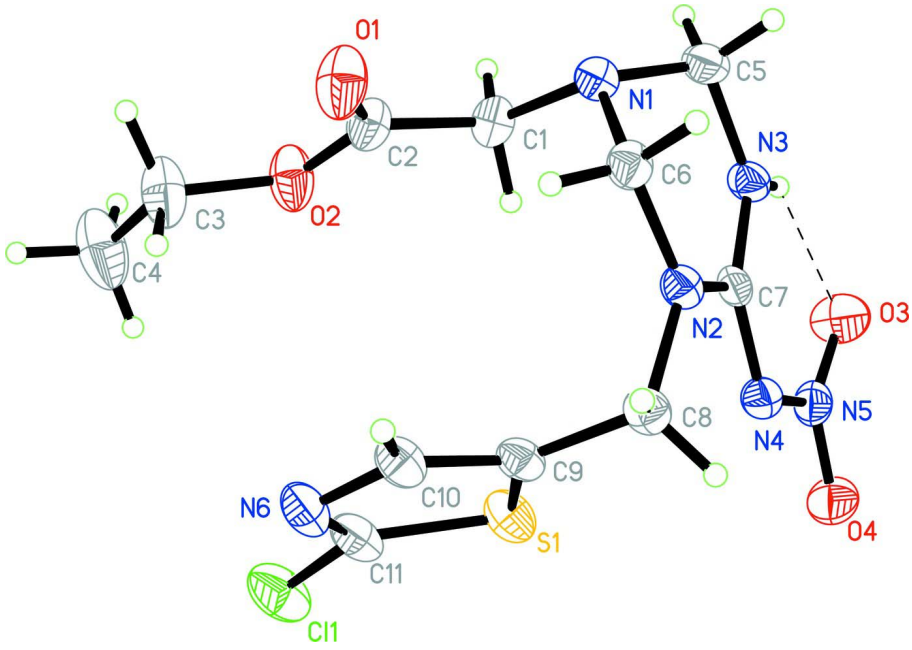

Figure 1

The molecular structure of title compound with the atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a small spheres of arbitrary radius. The intramolecular H–bond is marked by dashed line.

Ethyl 2-{3-[(2-chloro-1,3-thiazol-5-yl)methyl]- 4-nitroimino-1,3,5-triazinan-1-yl}acetate

Crystal data

$C_{11}H_{15}ClN_6O_4S$
$M_r = 362.81$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.5066$ (6) Å
$b = 9.1114$ (7) Å
$c = 10.9071$ (8) Å
$\alpha = 100.488$ (2)°
$\beta = 98.416$ (3)°
$\gamma = 101.281$ (3)°
$V = 800.55$ (10) Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.505$ Mg m^{-3}
Melting point: 449 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2512 reflections
$\theta = 2.3$–$28.2°$
$\mu = 0.40$ mm^{-1}
$T = 298$ K
Block, colourless
0.40 × 0.23 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine focus sealed Siemens Mo tube
Graphite monochromator
Detector resolution: 1.57 × 0.49 mm pixels mm^{-1}
0.3° wide ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.857$, $T_{max} = 0.925$
5350 measured reflections
3259 independent reflections
2670 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.9°$
$h = -10 \rightarrow 9$
$k = -10 \rightarrow 11$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.128$
$S = 1.05$
3259 reflections
212 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.0779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0095 (3)	0.7149 (2)	0.26414 (19)	0.0444 (5)
H1A	0.0880	0.7030	0.2309	0.053*
H1B	−0.0751	0.7574	0.2054	0.053*
C2	−0.1049 (2)	0.5590 (2)	0.2702 (2)	0.0454 (5)
C3	−0.2096 (4)	0.3054 (3)	0.1509 (3)	0.0701 (7)
H3C	−0.3189	0.3031	0.1674	0.084*
H3B	−0.1526	0.2605	0.2128	0.084*
C4	−0.2173 (5)	0.2185 (3)	0.0216 (3)	0.0943 (11)
H4A	−0.2647	0.2692	−0.0391	0.141*
H4B	−0.2831	0.1169	0.0105	0.141*
H4C	−0.1091	0.2126	0.0092	0.141*
C5	0.1108 (3)	0.9754 (2)	0.3748 (2)	0.0485 (5)
H5A	0.1225	1.0469	0.4549	0.058*
H5B	0.0397	1.0059	0.3108	0.058*
C6	0.1510 (2)	0.7783 (2)	0.47718 (18)	0.0405 (4)
H6A	0.1079	0.6734	0.4825	0.049*
H6B	0.1619	0.8435	0.5603	0.049*
C7	0.3648 (2)	0.88803 (19)	0.36999 (17)	0.0337 (4)
C8	0.4008 (2)	0.6726 (2)	0.46817 (19)	0.0408 (4)
H8A	0.3775	0.6440	0.5462	0.049*
H8B	0.5174	0.7146	0.4805	0.049*
C9	0.3537 (2)	0.5325 (2)	0.36264 (18)	0.0399 (4)
C10	0.2576 (3)	0.3953 (2)	0.3607 (2)	0.0468 (5)
H10	0.2113	0.3768	0.4302	0.056*
C11	0.3072 (3)	0.3403 (2)	0.1709 (2)	0.0527 (6)
Cl1	0.30601 (10)	0.23735 (8)	0.02224 (6)	0.0779 (3)
N1	0.03775 (19)	0.82249 (18)	0.38653 (16)	0.0408 (4)
N2	0.31341 (19)	0.79068 (17)	0.44198 (15)	0.0367 (4)

N3	0.2716 (2)	0.98200 (18)	0.33909 (17)	0.0393 (4)
H3A	0.306 (3)	1.039 (3)	0.297 (2)	0.047*
N4	0.50886 (19)	0.87424 (18)	0.33519 (16)	0.0402 (4)
N5	0.5757 (2)	0.97002 (19)	0.26754 (16)	0.0430 (4)
N6	0.2308 (2)	0.28347 (19)	0.25118 (19)	0.0544 (5)
O1	−0.1559 (2)	0.52487 (19)	0.36034 (15)	0.0659 (5)
O2	−0.1227 (2)	0.46316 (17)	0.16030 (15)	0.0614 (4)
O3	0.5158 (2)	1.0752 (2)	0.23700 (19)	0.0671 (5)
O4	0.70673 (19)	0.95104 (19)	0.23875 (17)	0.0607 (4)
S1	0.41711 (8)	0.52681 (6)	0.21876 (5)	0.0532 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0449 (11)	0.0457 (11)	0.0389 (10)	0.0019 (9)	0.0037 (9)	0.0122 (9)
C2	0.0434 (11)	0.0495 (12)	0.0386 (11)	0.0005 (9)	0.0066 (9)	0.0095 (9)
C3	0.0903 (19)	0.0483 (12)	0.0592 (14)	−0.0107 (12)	0.0183 (13)	0.0055 (11)
C4	0.144 (3)	0.0561 (15)	0.0660 (17)	−0.0045 (17)	0.0236 (19)	−0.0031 (12)
C5	0.0451 (11)	0.0377 (10)	0.0671 (14)	0.0144 (8)	0.0191 (10)	0.0106 (10)
C6	0.0430 (10)	0.0429 (10)	0.0331 (10)	0.0067 (8)	0.0087 (8)	0.0037 (8)
C7	0.0379 (9)	0.0256 (8)	0.0336 (9)	0.0057 (7)	0.0040 (7)	−0.0001 (7)
C8	0.0473 (11)	0.0370 (10)	0.0389 (10)	0.0130 (8)	0.0030 (8)	0.0106 (8)
C9	0.0479 (11)	0.0363 (10)	0.0398 (10)	0.0176 (8)	0.0065 (8)	0.0118 (8)
C10	0.0590 (13)	0.0391 (11)	0.0460 (12)	0.0163 (9)	0.0105 (10)	0.0122 (9)
C11	0.0731 (15)	0.0436 (11)	0.0427 (11)	0.0274 (10)	0.0013 (11)	0.0048 (10)
Cl1	0.1162 (6)	0.0694 (4)	0.0455 (3)	0.0420 (4)	0.0031 (3)	−0.0065 (3)
N1	0.0398 (9)	0.0382 (8)	0.0447 (9)	0.0101 (7)	0.0090 (7)	0.0074 (7)
N2	0.0405 (8)	0.0318 (8)	0.0385 (8)	0.0098 (6)	0.0071 (7)	0.0080 (7)
N3	0.0416 (9)	0.0306 (8)	0.0499 (10)	0.0112 (6)	0.0133 (7)	0.0124 (7)
N4	0.0375 (8)	0.0364 (8)	0.0468 (9)	0.0082 (6)	0.0106 (7)	0.0075 (7)
N5	0.0401 (9)	0.0421 (9)	0.0407 (9)	0.0023 (7)	0.0079 (7)	0.0009 (7)
N6	0.0704 (12)	0.0356 (9)	0.0545 (11)	0.0156 (8)	0.0039 (10)	0.0053 (8)
O1	0.0766 (11)	0.0650 (10)	0.0453 (9)	−0.0146 (8)	0.0207 (8)	0.0100 (8)
O2	0.0806 (11)	0.0484 (9)	0.0455 (9)	−0.0096 (8)	0.0202 (8)	0.0055 (7)
O3	0.0612 (10)	0.0647 (11)	0.0929 (14)	0.0183 (8)	0.0302 (9)	0.0448 (10)
O4	0.0468 (9)	0.0706 (11)	0.0654 (10)	0.0116 (7)	0.0249 (8)	0.0070 (8)
S1	0.0731 (4)	0.0452 (3)	0.0456 (3)	0.0181 (3)	0.0187 (3)	0.0098 (2)

Geometric parameters (Å, º)

C1—N1	1.455 (3)	C6—H6B	0.9700
C1—C2	1.510 (3)	C7—N3	1.329 (2)
C1—H1A	0.9700	C7—N2	1.340 (2)
C1—H1B	0.9700	C7—N4	1.357 (2)
C2—O1	1.198 (2)	C8—N2	1.468 (2)
C2—O2	1.318 (3)	C8—C9	1.498 (3)
C3—O2	1.460 (3)	C8—H8A	0.9700
C3—C4	1.472 (4)	C8—H8B	0.9700

C3—H3C	0.9700	C9—C10	1.348 (3)
C3—H3B	0.9700	C9—S1	1.728 (2)
C4—H4A	0.9600	C10—N6	1.380 (3)
C4—H4B	0.9600	C10—H10	0.9300
C4—H4C	0.9600	C11—N6	1.287 (3)
C5—N1	1.447 (2)	C11—S1	1.717 (2)
C5—N3	1.469 (3)	C11—Cl1	1.717 (2)
C5—H5A	0.9700	N3—H3A	0.79 (2)
C5—H5B	0.9700	N4—N5	1.339 (2)
C6—N1	1.444 (3)	N5—O4	1.237 (2)
C6—N2	1.476 (2)	N5—O3	1.243 (2)
C6—H6A	0.9700		

N1—C1—C2	113.48 (16)	N3—C7—N4	127.89 (17)
N1—C1—H1A	108.9	N2—C7—N4	113.62 (16)
C2—C1—H1A	108.9	N2—C8—C9	112.19 (16)
N1—C1—H1B	108.9	N2—C8—H8A	109.2
C2—C1—H1B	108.9	C9—C8—H8A	109.2
H1A—C1—H1B	107.7	N2—C8—H8B	109.2
O1—C2—O2	124.32 (19)	C9—C8—H8B	109.2
O1—C2—C1	126.2 (2)	H8A—C8—H8B	107.9
O2—C2—C1	109.47 (17)	C10—C9—C8	127.86 (19)
O2—C3—C4	108.0 (2)	C10—C9—S1	109.13 (15)
O2—C3—H3C	110.1	C8—C9—S1	123.00 (14)
C4—C3—H3C	110.1	C9—C10—N6	117.05 (19)
O2—C3—H3B	110.1	C9—C10—H10	121.5
C4—C3—H3B	110.1	N6—C10—H10	121.5
H3C—C3—H3B	108.4	N6—C11—S1	117.24 (17)
C3—C4—H4A	109.5	N6—C11—Cl1	123.01 (18)
C3—C4—H4B	109.5	S1—C11—Cl1	119.74 (15)
H4A—C4—H4B	109.5	C6—N1—C5	107.68 (16)
C3—C4—H4C	109.5	C6—N1—C1	113.41 (16)
H4A—C4—H4C	109.5	C5—N1—C1	111.93 (16)
H4B—C4—H4C	109.5	C7—N2—C8	121.33 (16)
N1—C5—N3	111.07 (15)	C7—N2—C6	120.93 (15)
N1—C5—H5A	109.4	C8—N2—C6	116.72 (15)
N3—C5—H5A	109.4	C7—N3—C5	122.00 (17)
N1—C5—H5B	109.4	C7—N3—H3A	115.8 (16)
N3—C5—H5B	109.4	C5—N3—H3A	122.2 (16)
H5A—C5—H5B	108.0	N5—N4—C7	118.95 (16)
N1—C6—N2	112.02 (15)	O4—N5—O3	120.48 (17)
N1—C6—H6A	109.2	O4—N5—N4	115.65 (17)
N2—C6—H6A	109.2	O3—N5—N4	123.84 (16)
N1—C6—H6B	109.2	C11—N6—C10	108.32 (18)
N2—C6—H6B	109.2	C2—O2—C3	116.56 (17)
H6A—C6—H6B	107.9	C11—S1—C9	88.24 (10)
N3—C7—N2	118.48 (17)		

N1—C1—C2—O1	7.9 (3)	N1—C6—N2—C8	−143.03 (17)
N1—C1—C2—O2	−171.21 (18)	N2—C7—N3—C5	−3.8 (3)
N2—C8—C9—C10	−105.2 (2)	N4—C7—N3—C5	174.62 (18)
N2—C8—C9—S1	73.8 (2)	N1—C5—N3—C7	−28.0 (3)
C8—C9—C10—N6	179.47 (18)	N3—C7—N4—N5	4.3 (3)
S1—C9—C10—N6	0.3 (2)	N2—C7—N4—N5	−177.22 (16)
N2—C6—N1—C5	−55.1 (2)	C7—N4—N5—O4	−179.85 (17)
N2—C6—N1—C1	69.28 (19)	C7—N4—N5—O3	2.1 (3)
N3—C5—N1—C6	56.0 (2)	S1—C11—N6—C10	0.8 (2)
N3—C5—N1—C1	−69.3 (2)	Cl1—C11—N6—C10	179.62 (16)
C2—C1—N1—C6	65.1 (2)	C9—C10—N6—C11	−0.7 (3)
C2—C1—N1—C5	−172.82 (16)	O1—C2—O2—C3	−0.5 (4)
N3—C7—N2—C8	173.29 (16)	C1—C2—O2—C3	178.7 (2)
N4—C7—N2—C8	−5.4 (2)	C4—C3—O2—C2	179.5 (2)
N3—C7—N2—C6	5.2 (3)	N6—C11—S1—C9	−0.57 (19)
N4—C7—N2—C6	−173.49 (16)	Cl1—C11—S1—C9	−179.41 (14)
C9—C8—N2—C7	−82.8 (2)	C10—C9—S1—C11	0.11 (16)
C9—C8—N2—C6	85.8 (2)	C8—C9—S1—C11	−179.09 (17)
N1—C6—N2—C7	25.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N6^{i}	0.79 (2)	2.55 (2)	3.133 (2)	132 (2)
N3—H3*A*···O3	0.79 (2)	1.98 (2)	2.570 (2)	131 (2)
C3—H3*C*···O3^{ii}	0.97	2.57	3.191 (3)	122
C5—H5*A*···N1^{iii}	0.97	2.61	3.449 (3)	144
C6—H6*B*···O4^{iv}	0.97	2.56	3.478 (3)	159
C10—H10···O1^{v}	0.93	2.45	3.278 (3)	149

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*−1, *y*−1, *z*; (iii) −*x*, −*y*+2, −*z*+1; (iv) −*x*+1, −*y*+2, −*z*+1; (v) −*x*, −*y*+1, −*z*+1.