organic compounds

N-[Phenyl(piperidin-1-yl)methyl]-1,3,4-thiadiazol-2-amine

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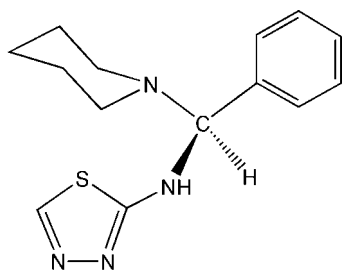Correspondence e-mail: dyh@mail.cnu.edu.cn

In the crystal structure of the title compound, $C_{14}H_{18}N_4S$, there is a chiral C atom with a tetrahedral configuration which connects two N atoms from piperidine and 2-amino-1,3,4-thiadiazole groups, one C atom from the benzene ring, and one H atom. A centrosymmetric dimer is constructed by a pair of chiral molecules of types S and R via intermolecular N—H⋯N hydrogen bonds, forming an $S_2^2(8)$ ring. In addition, C—H⋯N weak interactions link the dimers into an infinite supramolecular sheet.

Related literature

For related literature, see: Allen *et al.* (1987); Berkovitch-Yellin & Leiserowitz (1984); Bernstein *et al.* (1995); Dawood *et al.* (2005); Fleita *et al.* (2005); Glusker *et al.* (1995); Jurčík & Wilhelm (2004); Khrustalev *et al.* (1998); Marjo *et al.* (1994, 2001); Wu *et al.* (1998).

Experimental

Crystal data

$C_{14}H_{18}N_4S$	V = 2826.2 (10) Å³
M_r = 274.38	Z = 8
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 19.165 (4) Å	μ = 0.22 mm⁻¹
b = 6.4232 (13) Å	T = 293 (2) K
c = 23.093 (5) Å	0.37 × 0.32 × 0.26 mm
β = 96.19 (3)°	

Data collection

Brucker SMART APEX CCD diffractometer	12197 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3498 independent reflections
T_{min} = 0.923, T_{max} = 0.945	2435 reflections with $I > 2\sigma(I)$
	R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053	172 parameters
$wR(F^2)$ = 0.123	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.30 e Å⁻³
3498 reflections	$\Delta\rho_{min}$ = −0.31 e Å⁻³

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3—H3⋯N2ⁱ	0.86	2.27	2.999 (2)	143
C1—H1⋯N1ⁱⁱ	0.93	2.60	3.416 (3)	147

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXTL*.

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.
Berkovitch-Yellin, Z. & Leiserowitz, L. (1984). *Acta Cryst.* B**40**, 159–165.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Brandenburg, K. (2001). *DIAMOND*. Version 2.1. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SAINT* (Version 6.28a) and *SMART* (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
Dawood, K. M., Farag, A. M. & Abdel-Aziz, H. A. (2005). *Heteroatom. Chem.* **16**, 621–627.
Fleita, D., El-Banna, A. & Mohareb, R. (2005). *Phosphorus Sulfur Silicon Relat. Elem.* **180**, 2315–2333.
Glusker, J. P., Lewis, M. & Rossi, M. (1995). *Crystal Structure Analysis for Chemists and Biologists*, p. 406. New York: VCH Publisher Inc.
Jurčík, V. & Wilhelm, R. (2004). *Tetrahedron*, **60**, 3205–3210.
Khrustalev, V. N., Lindeman, S. V., Ukhin, L. Y., Orlova, Z. I., Gribanova, T. N. & Shishkin, O. V. (1998). *Z. Kristallogr.* **213**, 296–298.
Marjo, C. E., Bishop, R., Craig, D. C., O'Brien, A. & Scudder, M. L. (1994). *J. Chem. Soc. Chem. Commun.* pp. 2513–2514.
Marjo, C. E., Bishop, R., Craig, D. C. & Scudder, M. L. (2001). *Eur. J. Org. Chem.* pp. 863–873.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Wu, J., Liu, X.-F., Xu, H.-S., Huang, J.-W., Hu, S.-Z. & Seik, W. N. (1998). *Acta Cryst.* C**54**, IUC9800066.

supplementary materials

N-[Phenyl(piperidin-1-yl)methyl]-1,3,4-thiadiazol-2-amine

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Comment

Aminals, which are usually used as protecting groups for aldehydes (Jurčík & Wilhelm, 2004) in organic syntheses, can be either of open-chain or cyclic form. However, a few crystal structures of the open-chain aminals are reported yet (Wu *et al.*, 1998). In this work, we intended to prepare Schiff ligand using benzaldehyde and primary amine in the presence of piperidine as a catalyst (Dawood *et al.*, 2005; Fleita *et al.*, 2005). But the result product was characterized structurally to be an open-chain aminal *N*-(phenyl (piperidin-1-yl)methyl)-1,3,4-thiadiazol-2-amine (I) with a chiral carbon as shown in the scheme.

As shown in Fig.1, the title compound I contains a chiral carbon atom C3 showing a tetrahedral configuration that connects the N3 atom from 2-amino-1,3,4-thiadiazole, N4 atom from piperidine, C2 atom from benzene ring and H3A atom. The piperidine ring adopts a normal chair conformation. Atoms C1, C2, N1, N2 and S1 compose the thiadiazole ring which has an excellent coplanarity with tiny deviations (max. 0.0084 (14) to min. 0.0012 (12) Å) from its least-square plane. The dihedral angle between the benzene and thiadiazole planes is 56.23 (6) °. The torsion angles C2—N3—C3—N4 and C2—N3—C3—C4 are 50.70 (23) ° and 177.19 (17) °, respectively.

The bond angles around C3 are 108.45 (15) °, 109.49 (15) °, 115.22 (15) ° for N3—C3—N4, N3—C3—C4, N4—C3—C4, respectively, indicating the sp^3 hybridization of C3. The bond lengths of C3—N3 and C3—N4 with 1.459 (3) Å and 1.469 (2) Å fall in the normal range of C—N single bond (1.470 Å) (Allen *et al.*, 1987) and the C3—C4 bond length of 1.516 (3) Å comply exactly with the C—C single bond rule (about 1.51 Å) (Glusker *et al.*, 1995). The C2—N3 (1.354 (2) Å) bond has partial double-bond character, which could be attributed to conjugation of the five-membered thiadiazole ring. Few crystal structures that have similar tetrahedral configuration of the carbon atom were reported (Khrustalev *et al.*, 1998; Wu *et al.*, 1998).

In the crystal structure of I, a pair of molecules with S and *R* configuration are linked into a dimer *via* N—H···N intermolecular hydrogen bonds containing a $R^2_2(8)$ ring (Bernstein *et al.*, 1995) (Fig.2). Similarly, a dimer connected by a pair of molecules with S and *R* configuration *via* the C—H···O weak interaction can be seen in the compound N-[α-(*N*-Succimidyl)benzyl]selenamorpholine (Wu *et al.*, 1998). The racemic dimer of I has a symmetric center, leading to the crystal with the centrosymmetric space group, though the individual molecule has chirality. The dimers are further connected into an infinite sheet along the axis a by C—H···N (3.416 (3) Å) weak hydrogen bonds as shown in Fig.3. Though the H-bond length is slightly longer than that of the general C—H···N hydrogen bonds (Berkovitch-Ylellin & Leiserowitz, 1984), it plays a major role in construction of the infinite sheet in I. However, quite a few much longer C—H···N bonds in the centrosymmetric dimers have been discussed, which are considered as an important synthon for the crystal engineering (Marjo *et al.* 1994; 2001).

The packing diagram of I shown in Fig.4 indicates that the infinite sheets are aligned in the *ac* plane along the axis *a* and stacked along the axis *b*. There are no more significant weak interactions between the sheets.

supplementary materials

Experimental

2-Amino-1,3,4-thiadiazole (28 mmol, 2.5 g) and benzaldehyde (2.5 ml) were added in a 100 ml round-bottom flask, and 20 ml e thanol as solvent. The mixture was stirred at 80 ° for 1 hr. Then several drops of piperidine were added into the reaction mixture, which was continuously stirred for 3 hrs at 80 °. After reduced pressure distillation and recrystallization, the yellow product (0.088 g, yield 32.16%) was isolated from the solution. IR (KBr, cm^{-1}): 1618(C=N), 1021(C—N), 3306(N—H). Analysis calculated for $C_{14}H_{18}N_4S$: C 61.28%, H 6.61%, N 20.42%; Found C 60.75%, H 6.776%, N 20.64%.

Refinement

All the H atoms were treated as riding-model, with N—H=0.86 Å, C—H=0.93–0.98 Å, and their $U_{iso}=1.2U_{eq}$(carrier atom).
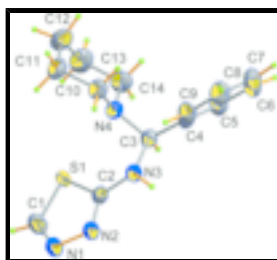
Figures

Fig. 1. *ORTEP* drawing of I with the atom-numbering scheme, showing 50% probability displacement ellipsoids.
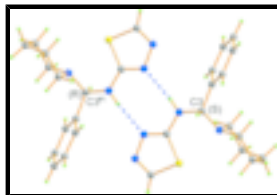
Fig. 2. The centrosymmetric dimer composed by S and *R* molecules *via* intermolecular N—H···N hydrogen bonds shown with blue dashed line.
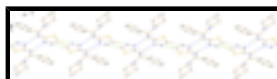
Fig. 3. Infinite sheets connected by weak intermolecular C—H···N interactions shown with green dashed line.

Fig. 4. Packing diagram of I viewed along the axis b (hydrogen bonds are shown as dashed lines).

N-[Phenyl(piperidin-1-yl)methyl]-1,3,4-thiadiazol-2-amine

Crystal data

$C_{14}H_{18}N_4S$	$F_{000} = 1168$
$M_r = 274.38$	$D_x = 1.290$ Mg m^{-3}

Monoclinic, *C*2/*c*

Mo *K*α radiation
λ = 0.71073 Å

Hall symbol: -C 2yc

Cell parameters from 13043 reflections
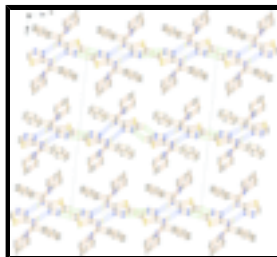
$a = 19.165$ (4) Å

θ = 1.8–28.3º

$b = 6.4232$ (13) Å

$μ = 0.22$ mm^{-1}

$c = 23.093$ (5) Å

$T = 293$ (2) K

β = 96.19 (3)º

Block, pale yellow

$V = 2826.2$ (10) Å^3

$0.37 × 0.32 × 0.26$ mm

$Z = 8$

Data collection

Brucker SMART Apex CCD
diffractometer

2435 reflections with $I > 2σ(I)$

Monochromator: graphite

$R_{int} = 0.042$

$T = 293(2)$ K

$θ_{max} = 28.3º$

phi and ω scans

$θ_{min} = 1.8º$

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$h = -25→25$

$T_{min} = 0.923$, $T_{max} = 0.945$

$k = -8→8$

12197 measured reflections

$l = -30→30$

3498 independent reflections

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2σ(F^2)] = 0.053$

H-atom parameters constrained

$wR(F^2) = 0.123$

$w = 1/[σ^2(F_o{}^2) + (0.0421P)^2 + 2.0932P]$
where $P = (F_o{}^2 + 2F_c{}^2)/3$

$S = 1.06$

$(Δ/σ)_{max} < 0.001$

3498 reflections

$Δρ_{max} = 0.30$ e Å^{-3}

172 parameters

$Δρ_{min} = -0.31$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 > 2sigma(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	$U_{iso}*/U_{eq}$
C1	0.04886 (11)	0.7153 (4)	0.02158 (10)	0.0546 (6)
H1	0.0013	0.6832	0.0172	0.066*
C2	0.16299 (9)	0.8538 (3)	0.04207 (8)	0.0355 (4)
C3	0.22536 (9)	1.1632 (3)	0.08492 (8)	0.0358 (4)
H3A	0.2056	1.2599	0.0547	0.043*
C4	0.30084 (10)	1.2265 (3)	0.10260 (8)	0.0357 (4)
C5	0.32101 (11)	1.4303 (4)	0.09465 (9)	0.0458 (5)
H5	0.2888	1.5248	0.0768	0.055*
C6	0.38900 (13)	1.4956 (4)	0.11311 (11)	0.0574 (6)
H6	0.4027	1.6313	0.1060	0.069*
C7	0.43584 (12)	1.3587 (4)	0.14187 (11)	0.0579 (7)
H7	0.4806	1.4035	0.1559	0.069*
C8	0.41645 (11)	1.1554 (4)	0.14985 (10)	0.0562 (6)
H8	0.4486	1.0618	0.1682	0.067*
C9	0.34917 (10)	1.0900 (4)	0.13062 (9)	0.0462 (5)
H9	0.3363	0.9527	0.1366	0.055*
C10	0.15910 (12)	1.3749 (4)	0.14777 (11)	0.0532 (6)
H10A	0.1445	1.4540	0.1128	0.064*
H10B	0.1989	1.4454	0.1687	0.064*
C11	0.09907 (14)	1.3638 (4)	0.18571 (12)	0.0663 (7)
H11A	0.0879	1.5030	0.1981	0.080*
H11B	0.0578	1.3074	0.1631	0.080*
C12	0.11794 (14)	1.2292 (5)	0.23849 (11)	0.0673 (7)
H12A	0.0770	1.2119	0.2594	0.081*
H12B	0.1541	1.2976	0.2643	0.081*
C13	0.14385 (12)	1.0186 (4)	0.22176 (10)	0.0557 (6)
H13A	0.1054	0.9408	0.2013	0.067*
H13B	0.1607	0.9417	0.2566	0.067*
C14	0.20278 (11)	1.0409 (4)	0.18299 (9)	0.0452 (5)
H14A	0.2430	1.1065	0.2047	0.054*
H14B	0.2170	0.9042	0.1708	0.054*
N1	0.09394 (9)	0.6053 (3)	−0.00162 (8)	0.0490 (5)
N2	0.16140 (8)	0.6861 (3)	0.00967 (7)	0.0416 (4)
N3	0.22363 (8)	0.9548 (3)	0.05965 (7)	0.0392 (4)
H3	0.2628	0.8935	0.0558	0.047*
N4	0.17963 (8)	1.1657 (3)	0.13202 (7)	0.0363 (4)
S1	0.08167 (3)	0.92670 (10)	0.06149 (3)	0.0541 (2)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0336 (11)	0.0644 (16)	0.0659 (15)	−0.0092 (11)	0.0054 (10)	−0.0167 (13)
C2	0.0304 (9)	0.0406 (12)	0.0364 (10)	0.0000 (8)	0.0075 (8)	−0.0015 (9)
C3	0.0324 (10)	0.0383 (11)	0.0370 (10)	0.0016 (8)	0.0052 (7)	0.0011 (8)

C4	0.0319 (10)	0.0396 (12)	0.0365 (10)	−0.0016 (8)	0.0076 (8)	−0.0011 (9)
C5	0.0453 (12)	0.0435 (13)	0.0494 (12)	−0.0042 (10)	0.0089 (9)	0.0028 (10)
C6	0.0537 (14)	0.0545 (15)	0.0662 (15)	−0.0178 (12)	0.0161 (12)	−0.0036 (12)
C7	0.0346 (12)	0.080 (2)	0.0605 (15)	−0.0159 (12)	0.0097 (10)	−0.0121 (13)
C8	0.0328 (11)	0.0731 (18)	0.0625 (14)	0.0059 (11)	0.0033 (10)	0.0005 (13)
C9	0.0375 (11)	0.0448 (13)	0.0566 (13)	0.0011 (10)	0.0059 (9)	0.0012 (11)
C10	0.0536 (13)	0.0432 (14)	0.0643 (15)	0.0062 (11)	0.0138 (11)	−0.0052 (11)
C11	0.0590 (15)	0.0577 (17)	0.0864 (19)	0.0124 (13)	0.0276 (14)	−0.0149 (15)
C12	0.0619 (16)	0.084 (2)	0.0593 (15)	−0.0026 (15)	0.0229 (12)	−0.0147 (15)
C13	0.0516 (13)	0.0710 (18)	0.0465 (13)	−0.0033 (12)	0.0135 (10)	0.0045 (12)
C14	0.0405 (11)	0.0532 (14)	0.0422 (11)	0.0046 (10)	0.0051 (9)	0.0040 (10)
N1	0.0367 (9)	0.0574 (13)	0.0535 (11)	−0.0115 (8)	0.0076 (8)	−0.0126 (9)
N2	0.0325 (9)	0.0469 (11)	0.0462 (9)	−0.0061 (8)	0.0079 (7)	−0.0079 (8)
N3	0.0282 (8)	0.0428 (10)	0.0474 (9)	−0.0012 (7)	0.0076 (7)	−0.0098 (8)
N4	0.0327 (8)	0.0370 (10)	0.0397 (9)	0.0038 (7)	0.0066 (7)	−0.0017 (7)
S1	0.0301 (3)	0.0621 (4)	0.0712 (4)	−0.0023 (3)	0.0102 (2)	−0.0233 (3)

Geometric parameters (Å, °)

C1—N1	1.278 (3)	C8—H8	0.9300
C1—S1	1.721 (2)	C9—H9	0.9300
C1—H1	0.9300	C10—N4	1.457 (3)
C2—N2	1.310 (3)	C10—C11	1.521 (3)
C2—N3	1.354 (2)	C10—H10A	0.9700
C2—S1	1.7321 (19)	C10—H10B	0.9700
C3—N3	1.459 (3)	C11—C12	1.506 (4)
C3—N4	1.469 (2)	C11—H11A	0.9700
C3—C4	1.516 (3)	C11—H11B	0.9700
N1—N2	1.392 (2)	C12—C13	1.506 (4)
C3—H3A	0.9800	C12—H12A	0.9700
C4—C5	1.383 (3)	C12—H12B	0.9700
C4—C9	1.384 (3)	C13—C14	1.522 (3)
C5—C6	1.391 (3)	C13—H13A	0.9700
C5—H5	0.9300	C13—H13B	0.9700
C6—C7	1.376 (4)	C14—N4	1.453 (3)
C6—H6	0.9300	C14—H14A	0.9700
C7—C8	1.375 (4)	C14—H14B	0.9700
C7—H7	0.9300	N3—H3	0.8600
C8—C9	1.383 (3)		
N1—C1—S1	115.87 (16)	C11—C10—H10A	109.7
C1—S1—C2	86.27 (10)	N4—C10—H10B	109.7
N1—C1—H1	122.1	C11—C10—H10B	109.7
S1—C1—H1	122.1	H10A—C10—H10B	108.2
C1—N1—N2	111.82 (18)	C12—C11—C10	111.3 (2)
C2—N2—N1	112.18 (16)	C12—C11—H11A	109.4
N2—C2—N3	122.09 (17)	C10—C11—H11A	109.4
N2—C2—S1	113.84 (14)	C12—C11—H11B	109.4
N3—C2—S1	124.04 (15)	C10—C11—H11B	109.4
N3—C3—N4	108.45 (15)	H11A—C11—H11B	108.0

N3—C3—C4	109.49 (16)	C11—C12—C13	111.4 (2)
N4—C3—C4	115.22 (15)	C11—C12—H12A	109.3
N3—C3—H3A	107.8	C13—C12—H12A	109.3
N4—C3—H3A	107.8	C11—C12—H12B	109.3
C4—C3—H3A	107.8	C13—C12—H12B	109.3
C5—C4—C9	118.63 (19)	H12A—C12—H12B	108.0
C5—C4—C3	119.38 (18)	C12—C13—C14	110.7 (2)
C9—C4—C3	121.81 (19)	C12—C13—H13A	109.5
C4—C5—C6	120.7 (2)	C14—C13—H13A	109.5
C4—C5—H5	119.6	C12—C13—H13B	109.5
C6—C5—H5	119.6	C14—C13—H13B	109.5
C7—C6—C5	119.7 (2)	H13A—C13—H13B	108.1
C7—C6—H6	120.1	N4—C14—C13	110.32 (17)
C5—C6—H6	120.1	N4—C14—H14A	109.6
C8—C7—C6	120.0 (2)	C13—C14—H14A	109.6
C8—C7—H7	120.0	N4—C14—H14B	109.6
C6—C7—H7	120.0	C13—C14—H14B	109.6
C7—C8—C9	120.1 (2)	H14A—C14—H14B	108.1
C7—C8—H8	120.0	C2—N3—C3	122.75 (16)
C9—C8—H8	120.0	C2—N3—H3	118.6
C8—C9—C4	120.7 (2)	C3—N3—H3	118.6
C8—C9—H9	119.6	C14—N4—C10	111.94 (17)
C4—C9—H9	119.6	C14—N4—C3	116.06 (15)
N4—C10—C11	110.0 (2)	C10—N4—C3	113.18 (17)
N4—C10—H10A	109.7		
N3—C3—C4—C5	141.88 (18)	S1—C2—N2—N1	0.0 (2)
N4—C3—C4—C5	−95.6 (2)	C1—N1—N2—C2	0.9 (3)
N3—C3—C4—C9	−43.1 (2)	N2—C2—N3—C3	166.71 (18)
N4—C3—C4—C9	79.4 (2)	S1—C2—N3—C3	−15.3 (3)
C9—C4—C5—C6	1.6 (3)	N4—C3—N3—C2	50.7 (2)
C3—C4—C5—C6	176.75 (19)	C4—C3—N3—C2	177.19 (17)
C4—C5—C6—C7	−2.9 (3)	C13—C14—N4—C10	60.6 (2)
C5—C6—C7—C8	3.1 (4)	C13—C14—N4—C3	−167.42 (18)
C6—C7—C8—C9	−2.0 (4)	C11—C10—N4—C14	−60.0 (2)
C7—C8—C9—C4	0.8 (4)	C11—C10—N4—C3	166.59 (18)
C5—C4—C9—C8	−0.6 (3)	N3—C3—N4—C14	67.3 (2)
C3—C4—C9—C8	−175.6 (2)	C4—C3—N4—C14	−55.8 (2)
N4—C10—C11—C12	55.3 (3)	N3—C3—N4—C10	−161.30 (16)
C10—C11—C12—C13	−52.4 (3)	C4—C3—N4—C10	75.6 (2)
C11—C12—C13—C14	52.5 (3)	N1—C1—S1—C2	1.3 (2)
C12—C13—C14—N4	−56.0 (3)	N2—C2—S1—C1	−0.68 (17)
S1—C1—N1—N2	−1.5 (3)	N3—C2—S1—C1	−178.81 (19)
N3—C2—N2—N1	178.19 (18)		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···N2[i]	0.86	2.27	2.999 (2)	143

| C1—H1···N1[ii] | 0.93 | 2.60 | 3.416 (3) | 147 |

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

Fig. 1

Fig. 2

Fig. 3

Fig. 4