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4-[2-(Anthracen-9-ylmethylidene)-hydrazinylidene]-3-chloro-1-methyl-3,4-dihydro-1*H*-2λ^6,1-benzothiazine-2,2-dione

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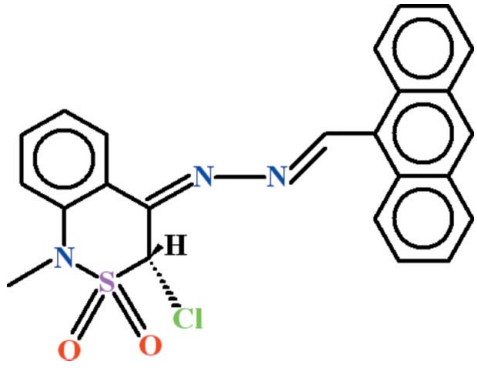
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.136; data-to-parameter ratio = 13.5.

In the title compound, $C_{24}H_{18}ClN_3O_2S$, the dihedral angle between the benzene ring and the anthracene ring system is 41.10 (8)°. The thiazine ring has a half-chair conformation and the Cl atom is in an axial orientation. In the crystal, molecules are linked by C—H···O interactions, generating $C(8)$ chains along [100]. A C—H···N short contact occurs in the molecule, generating an $S(6)$ ring.

Related literature

For a related structure and references to further synthetic details, see: Shafiq *et al.* (2012). For puckering parameters, see: Cremer & Pople (1975). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{24}H_{18}ClN_3O_2S$
M_r = 447.92
Monoclinic, $P2_1/c$
a = 8.5133 (4) Å
b = 19.8999 (8) Å
c = 12.7849 (6) Å
β = 105.026 (2)°
V = 2091.88 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 296 K
0.26 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.930, T_{max} = 0.960
16154 measured reflections
3788 independent reflections
2827 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 1.04
3788 reflections
281 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.93	2.59	3.370 (4)	142
C22—H22···N3	0.93	2.29	2.913 (4)	123

Symmetry code: (i) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. The authors also acknowledge the technical support provided by Syed Muhammad Hussain Rizvi of Bana International, Karachi, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6779).

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supplementary materials

Acta Cryst. (2012). E**68**, o1788 [doi:10.1107/S1600536812021642]

4-[2-(Anthracen-9-ylmethylidene)hydrazinylidene]-3-chloro-1-methyl-3,4-dihydro-1*H*-2λ^6,1-benzothiazine-2,2-dione

Muhammad Shafiq, M. Nawaz Tahir, Islam Ullah Khan, Tanveer Hussain Bokhari and Muhammad Nadeem Asghar

Comment

As part of our ongoing studies of thiazine derivatives (Shafiq *et al.*, 2012), we now describe the structure of the title compound, (I), (Fig. 1).

In (I), the benzene ring A (C1—C6) and anthracene group B (C10—C23) are almost planar with r. m. s. deviation of 0.0090 and 0.0144 Å, respectively. The dihedral angle between A/B is 41.10 (8)°. The central group C (N2/N3/C9) is of course planar. The dihedral angle between A/C and B/C is 13.63 (26) and 27.48 (26)°, respectively. The thiazine ring D (C1/C6/C7/C8/S1/N1) is in the half-chair form, with the maximum puckering amplitude (Cremer & Pople, 1975), Q = 0.578 (2) Å. There exist *S*(6) ring motif (Bernstein *et al.*, 1995) due to H-bonding of C—H···N type (Table 1, Fig. 1). The molecules form C(8) chains extending along the *a*-axis due to H-bonding of C—H···O type (Table 1, Fig. 2).

Experimental

Schiff base derivative of (4*Z*)-4-hydrazinylidene-1-methyl-3,4-dihydro -1*H*-2,1-benzothiazine 2,2-dioxide and anthracene-9-carbaldehyde was prepared using the method reported previously (Shafiq *et al.* 2012). The chlorination of the schiff base was undertaken using *N*-chloro succinimide and dibenzoylperoxide (Shafiq *et al.*, 2012). The crude product of (I) was re-crystallized in ethyl acetate to get orange prisms.

Refinement

The H-atoms were positioned geometrically (C–H = 0.93–0.98 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl and x = 1.2 for aryl H-atoms.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

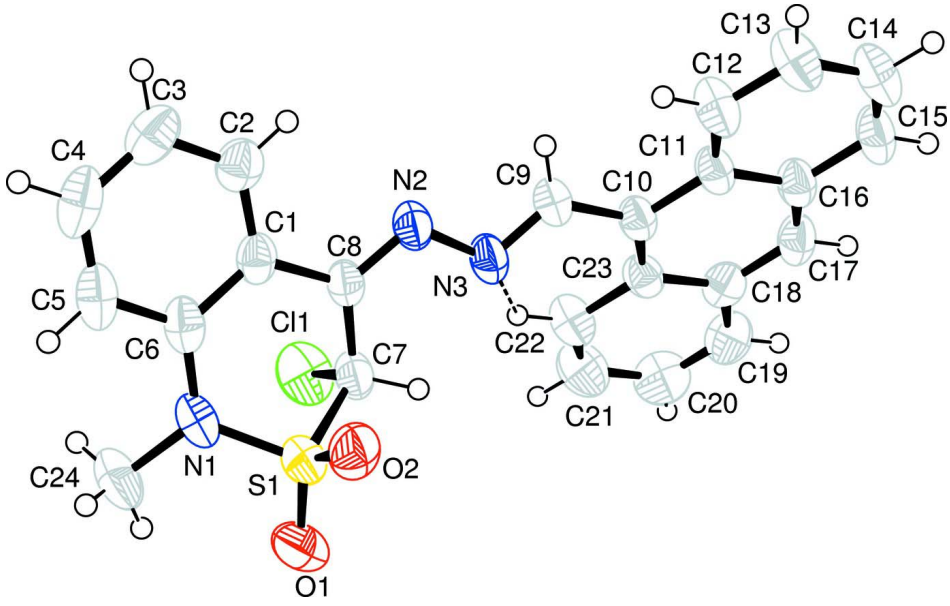

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level. The dotted line indicates the intra-molecular short contact.

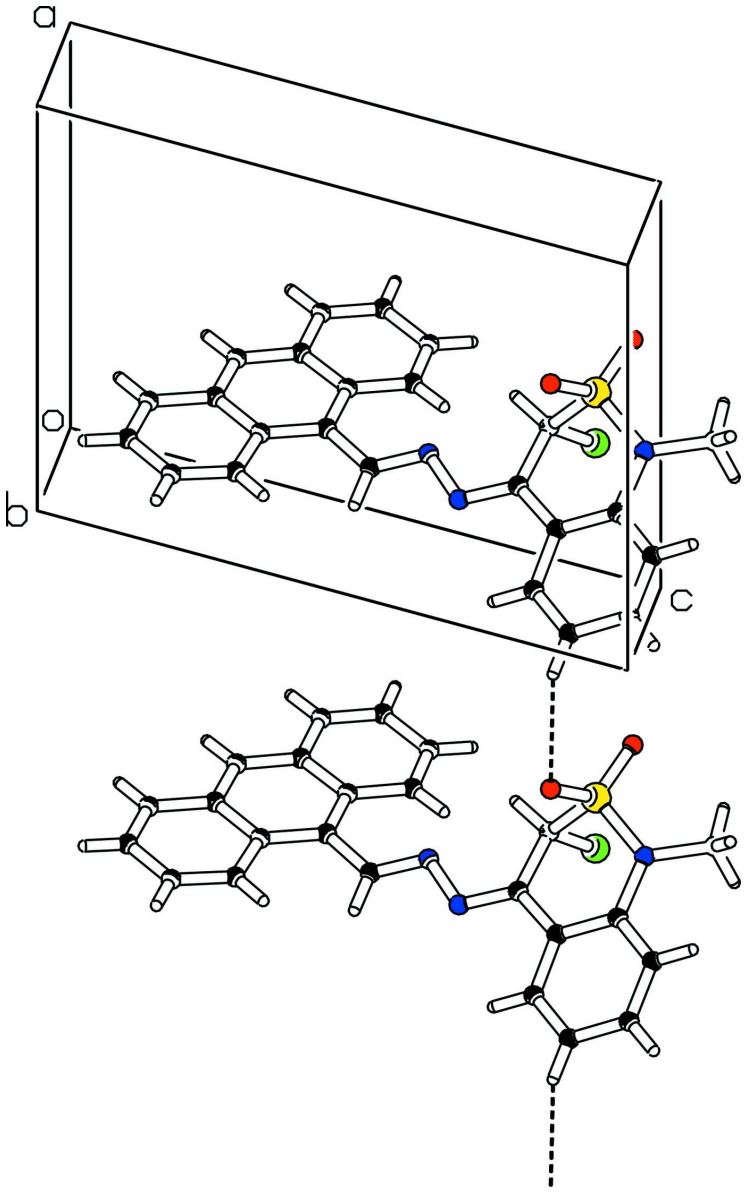

Figure 2

The partial packing, which shows that molecules form one-dimensional polymeric chains extending along the [100] direction.

4-[2-(Anthracen-9-ylmethylidene)hydrazinylidene]-3-chloro-1-methyl- 3,4-dihydro-1*H*-2λ^6,1-benzothiazine-2,2-dione

Crystal data

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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.5133$ (4) Å
$b = 19.8999$ (8) Å
$c = 12.7849$ (6) Å
$\beta = 105.026$ (2)°
$V = 2091.88$ (16) Å^3
$Z = 4$
$F(000) = 928$
$D_x = 1.422$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2827 reflections

θ = 2.1–25.3°
μ = 0.31 mm^{-1}
T = 296 K

Prism, orange
0.26 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.930, T_{max} = 0.960

16154 measured reflections
3788 independent reflections
2827 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.3°, θ_{min} = 2.1°
h = −10→9
k = −23→18
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 1.04
3788 reflections
281 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
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.8876P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.31773 (12)	0.02405 (4)	0.89027 (7)	0.0772 (3)
S1	0.47338 (9)	0.15552 (4)	0.89884 (6)	0.0561 (3)
O1	0.6215 (3)	0.12587 (13)	0.95945 (17)	0.0790 (8)
O2	0.4770 (2)	0.20988 (10)	0.82508 (16)	0.0625 (7)
N1	0.3657 (3)	0.17603 (12)	0.98246 (17)	0.0581 (8)
N2	0.1106 (3)	0.12240 (10)	0.66521 (16)	0.0470 (7)
N3	0.1929 (3)	0.07899 (11)	0.61082 (16)	0.0520 (8)
C1	0.1136 (3)	0.17431 (11)	0.8339 (2)	0.0436 (8)
C2	−0.0466 (3)	0.19551 (13)	0.7960 (2)	0.0533 (9)
C3	−0.1214 (4)	0.23414 (14)	0.8580 (3)	0.0632 (11)
C4	−0.0340 (4)	0.25376 (14)	0.9606 (3)	0.0665 (13)
C5	0.1253 (4)	0.23567 (14)	0.9993 (2)	0.0596 (10)
C6	0.2010 (4)	0.19540 (13)	0.9382 (2)	0.0498 (9)
C7	0.3445 (3)	0.09596 (13)	0.8164 (2)	0.0485 (8)

C8	0.1851 (3)	0.13033 (12)	0.76582 (18)	0.0414 (8)
C9	0.1181 (3)	0.07213 (12)	0.51179 (19)	0.0456 (8)
C10	0.1765 (3)	0.03012 (12)	0.43534 (19)	0.0430 (8)
C11	0.1245 (3)	0.04805 (12)	0.32402 (19)	0.0456 (8)
C12	0.0261 (4)	0.10529 (14)	0.2848 (2)	0.0619 (10)
C13	−0.0196 (4)	0.12103 (16)	0.1775 (2)	0.0676 (10)
C14	0.0306 (4)	0.08209 (16)	0.1014 (2)	0.0667 (10)
C15	0.1244 (4)	0.02818 (15)	0.1340 (2)	0.0603 (10)
C16	0.1755 (3)	0.00887 (13)	0.2453 (2)	0.0473 (8)
C17	0.2714 (3)	−0.04692 (13)	0.2787 (2)	0.0534 (10)
C18	0.3237 (3)	−0.06616 (12)	0.3865 (2)	0.0490 (9)
C19	0.4221 (4)	−0.12438 (15)	0.4175 (3)	0.0641 (11)
C20	0.4705 (4)	−0.14389 (16)	0.5208 (3)	0.0742 (13)
C21	0.4206 (4)	−0.10726 (15)	0.6017 (3)	0.0723 (11)
C22	0.3269 (4)	−0.05134 (14)	0.5762 (2)	0.0596 (10)
C23	0.2760 (3)	−0.02744 (12)	0.4675 (2)	0.0447 (8)
C24	0.4352 (5)	0.1704 (2)	1.0998 (2)	0.0851 (15)
H2	−0.10484	0.18318	0.72662	0.0639*
H3	−0.22948	0.24698	0.83144	0.0757*
H4	−0.08417	0.27945	1.00339	0.0798*
H5	0.18372	0.25048	1.06725	0.0716*
H7	0.39378	0.08215	0.75851	0.0582*
H9	0.02056	0.09509	0.48613	0.0547*
H12	−0.00791	0.13259	0.33383	0.0744*
H13	−0.08517	0.15836	0.15457	0.0813*
H14	−0.00106	0.09351	0.02836	0.0801*
H15	0.15741	0.00253	0.08271	0.0725*
H17	0.30231	−0.07276	0.22679	0.0640*
H19	0.45336	−0.14929	0.36469	0.0764*
H20	0.53679	−0.18145	0.53962	0.0887*
H21	0.45241	−0.12174	0.67323	0.0865*
H22	0.29546	−0.02823	0.63070	0.0713*
H24A	0.46719	0.21406	1.12959	0.1277*
H24B	0.52845	0.14138	1.11401	0.1277*
H24C	0.35525	0.15194	1.13268	0.1277*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1028 (7)	0.0585 (5)	0.0677 (5)	0.0011 (4)	0.0176 (5)	0.0132 (4)
S1	0.0554 (4)	0.0686 (5)	0.0428 (4)	−0.0061 (3)	0.0100 (3)	−0.0092 (3)
O1	0.0610 (13)	0.1054 (17)	0.0592 (13)	0.0087 (12)	−0.0049 (10)	−0.0130 (12)
O2	0.0646 (13)	0.0666 (12)	0.0617 (12)	−0.0183 (10)	0.0263 (10)	−0.0031 (10)
N1	0.0694 (16)	0.0683 (15)	0.0333 (12)	−0.0026 (12)	0.0076 (11)	−0.0079 (11)
N2	0.0551 (13)	0.0515 (12)	0.0352 (11)	0.0019 (10)	0.0131 (10)	−0.0046 (9)
N3	0.0600 (14)	0.0615 (13)	0.0347 (12)	0.0041 (11)	0.0127 (10)	−0.0103 (10)
C1	0.0547 (16)	0.0401 (13)	0.0410 (14)	−0.0090 (11)	0.0215 (12)	−0.0026 (11)
C2	0.0561 (17)	0.0506 (15)	0.0574 (17)	−0.0084 (13)	0.0225 (14)	−0.0053 (13)
C3	0.0625 (19)	0.0526 (16)	0.085 (2)	−0.0038 (14)	0.0378 (17)	−0.0041 (16)
C4	0.095 (3)	0.0477 (16)	0.075 (2)	−0.0053 (16)	0.055 (2)	−0.0096 (15)

C5	0.091 (2)	0.0487 (16)	0.0480 (16)	−0.0079 (15)	0.0339 (16)	−0.0090 (13)
C6	0.0706 (19)	0.0436 (14)	0.0406 (14)	−0.0100 (13)	0.0239 (13)	−0.0041 (11)
C7	0.0562 (16)	0.0547 (15)	0.0354 (13)	−0.0003 (12)	0.0132 (12)	−0.0057 (11)
C8	0.0504 (15)	0.0433 (13)	0.0330 (13)	−0.0080 (11)	0.0152 (11)	−0.0037 (10)
C9	0.0561 (16)	0.0464 (14)	0.0343 (13)	−0.0019 (12)	0.0120 (12)	−0.0022 (11)
C10	0.0514 (15)	0.0441 (13)	0.0337 (13)	−0.0074 (11)	0.0114 (11)	−0.0054 (10)
C11	0.0569 (16)	0.0455 (14)	0.0335 (13)	−0.0095 (12)	0.0103 (11)	−0.0059 (11)
C12	0.089 (2)	0.0559 (16)	0.0392 (15)	0.0073 (15)	0.0136 (14)	−0.0011 (13)
C13	0.094 (2)	0.0603 (17)	0.0434 (16)	0.0009 (16)	0.0084 (16)	0.0050 (14)
C14	0.096 (2)	0.0651 (19)	0.0341 (15)	−0.0196 (18)	0.0083 (15)	0.0018 (14)
C15	0.083 (2)	0.0653 (18)	0.0354 (14)	−0.0200 (16)	0.0202 (14)	−0.0123 (13)
C16	0.0590 (16)	0.0473 (14)	0.0371 (13)	−0.0133 (12)	0.0154 (12)	−0.0083 (11)
C17	0.0653 (18)	0.0554 (16)	0.0461 (16)	−0.0120 (14)	0.0265 (13)	−0.0138 (13)
C18	0.0510 (16)	0.0436 (14)	0.0555 (17)	−0.0076 (12)	0.0192 (13)	−0.0077 (12)
C19	0.072 (2)	0.0532 (16)	0.073 (2)	0.0051 (15)	0.0296 (17)	−0.0012 (15)
C20	0.078 (2)	0.0541 (18)	0.090 (3)	0.0105 (16)	0.0211 (19)	0.0066 (17)
C21	0.089 (2)	0.0621 (19)	0.0595 (19)	0.0060 (17)	0.0081 (17)	0.0120 (15)
C22	0.077 (2)	0.0533 (16)	0.0454 (16)	0.0013 (14)	0.0103 (14)	0.0003 (13)
C23	0.0504 (15)	0.0436 (13)	0.0386 (13)	−0.0086 (11)	0.0086 (11)	−0.0028 (11)
C24	0.092 (3)	0.124 (3)	0.0344 (16)	−0.008 (2)	0.0078 (16)	−0.0069 (18)

Geometric parameters (Å, º)

Cl1—C7	1.762 (3)	C16—C17	1.379 (4)
S1—O1	1.426 (3)	C17—C18	1.388 (3)
S1—O2	1.441 (2)	C18—C19	1.424 (4)
S1—N1	1.630 (3)	C18—C23	1.432 (4)
S1—C7	1.766 (3)	C19—C20	1.335 (5)
N1—C6	1.423 (4)	C20—C21	1.418 (5)
N1—C24	1.467 (3)	C21—C22	1.359 (4)
N2—N3	1.405 (3)	C22—C23	1.426 (4)
N2—C8	1.288 (3)	C2—H2	0.9300
N3—C9	1.269 (3)	C3—H3	0.9300
C1—C2	1.389 (4)	C4—H4	0.9300
C1—C6	1.412 (4)	C5—H5	0.9300
C1—C8	1.473 (3)	C7—H7	0.9800
C2—C3	1.374 (4)	C9—H9	0.9300
C3—C4	1.386 (5)	C12—H12	0.9300
C4—C5	1.366 (5)	C13—H13	0.9300
C5—C6	1.389 (4)	C14—H14	0.9300
C7—C8	1.508 (4)	C15—H15	0.9300
C9—C10	1.467 (3)	C17—H17	0.9300
C10—C11	1.422 (3)	C19—H19	0.9300
C10—C23	1.421 (3)	C20—H20	0.9300
C11—C12	1.426 (4)	C21—H21	0.9300
C11—C16	1.427 (4)	C22—H22	0.9300
C12—C13	1.362 (4)	C24—H24A	0.9600
C13—C14	1.395 (4)	C24—H24B	0.9600
C14—C15	1.338 (4)	C24—H24C	0.9600
C15—C16	1.429 (4)		

O1—S1—O2	120.04 (14)	C18—C19—C20	121.3 (3)
O1—S1—N1	108.40 (13)	C19—C20—C21	119.9 (3)
O1—S1—C7	111.82 (14)	C20—C21—C22	121.0 (3)
O2—S1—N1	110.63 (12)	C21—C22—C23	121.2 (3)
O2—S1—C7	103.22 (12)	C10—C23—C18	119.0 (2)
N1—S1—C7	101.03 (13)	C10—C23—C22	124.0 (2)
S1—N1—C6	118.09 (17)	C18—C23—C22	117.0 (2)
S1—N1—C24	120.3 (2)	C1—C2—H2	119.00
C6—N1—C24	121.5 (3)	C3—C2—H2	119.00
N3—N2—C8	113.0 (2)	C2—C3—H3	120.00
N2—N3—C9	112.0 (2)	C4—C3—H3	120.00
C2—C1—C6	117.9 (2)	C3—C4—H4	120.00
C2—C1—C8	119.6 (2)	C5—C4—H4	120.00
C6—C1—C8	122.5 (2)	C4—C5—H5	120.00
C1—C2—C3	121.9 (3)	C6—C5—H5	120.00
C2—C3—C4	119.2 (3)	Cl1—C7—H7	109.00
C3—C4—C5	120.5 (3)	S1—C7—H7	109.00
C4—C5—C6	120.7 (3)	C8—C7—H7	108.00
N1—C6—C1	121.3 (2)	N3—C9—H9	118.00
N1—C6—C5	119.1 (2)	C10—C9—H9	118.00
C1—C6—C5	119.7 (3)	C11—C12—H12	119.00
Cl1—C7—S1	111.83 (14)	C13—C12—H12	119.00
Cl1—C7—C8	111.80 (18)	C12—C13—H13	120.00
S1—C7—C8	107.60 (17)	C14—C13—H13	119.00
N2—C8—C1	119.4 (2)	C13—C14—H14	120.00
N2—C8—C7	121.9 (2)	C15—C14—H14	120.00
C1—C8—C7	118.7 (2)	C14—C15—H15	119.00
N3—C9—C10	123.9 (2)	C16—C15—H15	119.00
C9—C10—C11	116.9 (2)	C16—C17—H17	119.00
C9—C10—C23	123.1 (2)	C18—C17—H17	119.00
C11—C10—C23	120.0 (2)	C18—C19—H19	119.00
C10—C11—C12	123.7 (2)	C20—C19—H19	119.00
C10—C11—C16	119.7 (2)	C19—C20—H20	120.00
C12—C11—C16	116.6 (2)	C21—C20—H20	120.00
C11—C12—C13	121.8 (3)	C20—C21—H21	119.00
C12—C13—C14	121.1 (3)	C22—C21—H21	120.00
C13—C14—C15	119.6 (2)	C21—C22—H22	119.00
C14—C15—C16	121.9 (3)	C23—C22—H22	119.00
C11—C16—C15	119.1 (2)	N1—C24—H24A	110.00
C11—C16—C17	119.1 (2)	N1—C24—H24B	110.00
C15—C16—C17	121.9 (2)	N1—C24—H24C	109.00
C16—C17—C18	122.8 (2)	H24A—C24—H24B	110.00
C17—C18—C19	121.0 (3)	H24A—C24—H24C	109.00
C17—C18—C23	119.5 (2)	H24B—C24—H24C	109.00
C19—C18—C23	119.6 (2)		

O1—S1—N1—C6	−169.0 (2)	S1—C7—C8—C1	−43.3 (3)
O1—S1—N1—C24	7.3 (3)	N3—C9—C10—C11	−154.0 (3)

O2—S1—N1—C6	57.5 (2)	N3—C9—C10—C23	28.1 (4)
O2—S1—N1—C24	−126.2 (2)	C9—C10—C11—C12	2.7 (4)
C7—S1—N1—C6	−51.3 (2)	C9—C10—C11—C16	−179.4 (2)
C7—S1—N1—C24	125.0 (3)	C23—C10—C11—C12	−179.3 (3)
O1—S1—C7—Cl1	50.62 (19)	C23—C10—C11—C16	−1.3 (4)
O1—S1—C7—C8	173.77 (17)	C9—C10—C23—C18	178.5 (2)
O2—S1—C7—Cl1	−178.99 (14)	C9—C10—C23—C22	1.3 (4)
O2—S1—C7—C8	−55.85 (19)	C11—C10—C23—C18	0.7 (4)
N1—S1—C7—Cl1	−64.50 (17)	C11—C10—C23—C22	−176.6 (3)
N1—S1—C7—C8	58.64 (19)	C10—C11—C12—C13	179.3 (3)
S1—N1—C6—C1	23.8 (3)	C16—C11—C12—C13	1.3 (4)
S1—N1—C6—C5	−156.4 (2)	C10—C11—C16—C15	−179.0 (3)
C24—N1—C6—C1	−152.4 (3)	C10—C11—C16—C17	1.6 (4)
C24—N1—C6—C5	27.4 (4)	C12—C11—C16—C15	−0.9 (4)
C8—N2—N3—C9	−179.6 (2)	C12—C11—C16—C17	179.8 (3)
N3—N2—C8—C1	−179.8 (2)	C11—C12—C13—C14	−1.0 (5)
N3—N2—C8—C7	0.4 (3)	C12—C13—C14—C15	0.4 (5)
N2—N3—C9—C10	179.6 (2)	C13—C14—C15—C16	0.0 (5)
C6—C1—C2—C3	−1.9 (4)	C14—C15—C16—C11	0.3 (5)
C8—C1—C2—C3	177.1 (2)	C14—C15—C16—C17	179.6 (3)
C2—C1—C6—N1	−179.7 (2)	C11—C16—C17—C18	−1.3 (4)
C2—C1—C6—C5	0.5 (4)	C15—C16—C17—C18	179.3 (3)
C8—C1—C6—N1	1.3 (4)	C16—C17—C18—C19	179.7 (3)
C8—C1—C6—C5	−178.6 (2)	C16—C17—C18—C23	0.6 (4)
C2—C1—C8—N2	13.1 (4)	C17—C18—C19—C20	−178.8 (3)
C2—C1—C8—C7	−167.1 (2)	C23—C18—C19—C20	0.3 (5)
C6—C1—C8—N2	−167.9 (2)	C17—C18—C23—C10	−0.3 (4)
C6—C1—C8—C7	11.9 (4)	C17—C18—C23—C22	177.1 (3)
C1—C2—C3—C4	1.3 (4)	C19—C18—C23—C10	−179.4 (3)
C2—C3—C4—C5	0.8 (5)	C19—C18—C23—C22	−2.0 (4)
C3—C4—C5—C6	−2.2 (5)	C18—C19—C20—C21	1.5 (5)
C4—C5—C6—N1	−178.2 (3)	C19—C20—C21—C22	−1.6 (5)
C4—C5—C6—C1	1.6 (4)	C20—C21—C22—C23	−0.2 (5)
Cl1—C7—C8—N2	−100.3 (3)	C21—C22—C23—C10	179.2 (3)
Cl1—C7—C8—C1	79.9 (2)	C21—C22—C23—C18	1.9 (4)
S1—C7—C8—N2	136.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{i}	0.93	2.59	3.370 (4)	142
C22—H22···N3	0.93	2.29	2.913 (4)	123

Symmetry code: (i) *x*−1, *y*, *z*.