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N,*N*-Bis(quinolin-8-yl)-2,2′-[(1,3,4-thiadiazole-2,5-diyl)bis(sulfanediyl)]-diacetamide monohydrate

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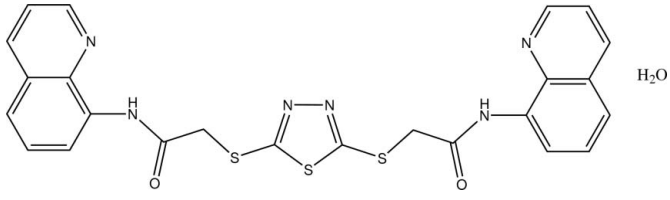
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.109; data-to-parameter ratio = 13.6.

In the title compound, $C_{24}H_{18}N_6O_2S_3\cdot H_2O$, the thiadiazole ring makes dihedral angles of 78.00 (13) and 77.27 (13)° with the quinoline ring systems. In the crystal, molecules are linked into a two-dimensional network by O—H···O and C—H···O hydrogen bonds.

Related literature

For background to the applications of 2,5-dimercapto-1,3,4-thiadiazole, see: Vullo *et al.* (2003); Gurn (2001). For related 2,5-dimercapto-1,3,4-thiadiazole structures, see: Wen *et al.* (2005); Zhang *et al.* (2005).



Experimental

Crystal data

$C_{24}H_{18}N_6O_2S_3\cdot H_2O$
M_r = 536.64
Monoclinic, $P2_1/n$
a = 10.8215 (8) Å
b = 10.2355 (8) Å
c = 21.5510 (16) Å
β = 90.068 (1)°
V = 2387.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 293 K
0.15 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.966
12711 measured reflections
4542 independent reflections
3469 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.02
4542 reflections
333 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1	0.95 (7)	2.07 (7)	2.990 (3)	162 (6)
O1W—H1WB···O2^{i}	0.94 (4)	1.91 (4)	2.841 (3)	175 (4)
C11—H11B···O1W^{ii}	0.97	2.49	3.332 (4)	145
C23—H23···O1^{iii}	0.93	2.55	3.411 (4)	155

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

Data collection: *APEX2* (Bruker 2001); cell refinement: *SAINT* (Bruker 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5124).

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supplementary materials

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N,*N*-Bis(quinolin-8-yl)-2,2'-[(1,3,4-thiadiazole-2,5-diyl)bis(sulfanediyl)]diacetamide monohydrate

X.-F. Li, Y. An, Q.-H. Huang and Y.-H. Wen

Comment

Thiodiazole and its derivatives have attracted much attention in the development of the new kind pesticide. 2,5-Dimercapto-1,3,4-thiadiazole (DMTD) is an effective stabilizer for emulsions, and its derivatives can be absorbed by plant cells, so they can be prepared as bactericides, herbicides and insecticides, *etc* (Vullo *et al.*, 2003; Gurn, 2001). In this paper, a new DMTD derivative of amide-based open-chain crown-ether, 2,5-di(quinolin-8-ylcarbamoylmethylthio)-1,3,4-thiodiazole, was synthesized and an X-ray crystal structure undertaken to elucidate its molecular conformation (Fig. 1).

The crystal structure of the title compound, consists of a $C_{24}H_{18}N_6O_2S_3$ molecule and a crystal water molecule. All bond lengths and angles in the title compound are within normal ranges, and are comparable with the structural related compounds (Wen *et al.*, 2005; Zhang *et al.*, 2005). The bond lengths in thiadiazole ring show a character intermediate between single and double bond because of the π-conjugation. The thiadiazole ring and two quinoline rings are each coplanar with their attached atoms, excluding the H atoms attached to them, while the whole molecule is not planar, with dihedral angles of 78.00 (13) and 77.27 (13)° between the thiadiazole ring and the two quinoline rings, respectively. The N1 atom adopts a planar configuration with the sum of the bond angles around atom N1 being 360.00°.

In the crystal packing, the molecules are linked into network structure by O1W—H1WA···O1, O1W—H1WB···O2, C11—H11B···O1W and C23—H23A···O1 hydrogen bond interactions (Table 1, Fig. 2).

Experimental

After stirring the 40 ml acetone solution of 2,5-dimercapto-1,3,4-thiodiazole (1.50 g, 10 mmole), K_2CO_3 (1.52 g, 11 mmole) and NaI (0.5 g) at room temperature for 30 minutes, a 20 ml solution of 2-chloro-*N*-quinolin-8-ylacetamide (4.41 g, 20 mmoles) in acetone was added drop by drop, and the mixture was refluxed at 329 K for 3 h. After cooling to room temperature, the mixture was washed three times with water (3 × 5 ml) and then filtered. The filter cake was washed three times with acetone (3 × 5 ml). 2,5-di(quinolin-8-ylcarbamoylmethylthio)-1,3,4-thiodiazole was obtained after dryness of the resulting coffee powders at room temperature for 48 h. Yield 3.91 g (80.1%), mp 166.5–167.5°C. Anal. Calcd. (%) for $C_{24}H_{18}N_6O_2S_3$: C, 55.58; H, 3.50; N, 16.20; S, 18.55. Found (%): C, 55.62; H, 3.55; N, 16.26; S, 18.53.

Brown single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation at room temperature from CH_3CH_2OH for 15 days.

Refinement

Water molecule bound H atoms were located in difference Fourier maps and their positional parameters refined with a distance restraint [O—H = 0.85 (10) Å] and a angle restraint. Other H atoms were positioned geometrically, with N—H = 0.86 Å and C—H = 0.95–0.99 Å, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C,*N*).

Figures

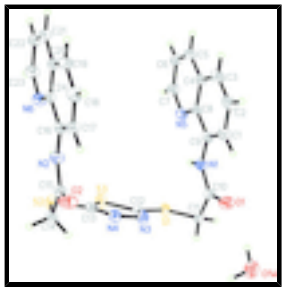

Fig. 1. The structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

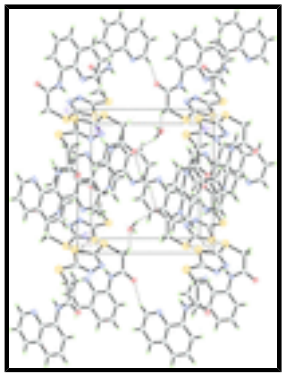

Fig. 2. The packing diagram of the title compound, viewed down the *c* axis.

N,*N*-Bis(quinolin-8-yl)-2,2'-[(1,3,4-thiadiazole- 2,5-diyl)bis(sulfanediyl)]diacetamide monohydrate

Crystal data

$C_{24}H_{18}N_6O_2S_3·H_2O$	$F(000) = 1112$
$M_r = 536.64$	$D_x = 1.493$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2913 reflections
$a = 10.8215$ (8) Å	$\theta = 2.2$–$24.6°$
$b = 10.2355$ (8) Å	$\mu = 0.35$ mm^{-1}
$c = 21.5510$ (16) Å	$T = 293$ K
$\beta = 90.068$ (1)°	Prism, brown
$V = 2387.1$ (3) Å^3	0.15 × 0.10 × 0.10 mm
$Z = 4$	

Data collection

Bruker APEXII CCD area-detector diffractometer	4542 independent reflections
Radiation source: fine-focus sealed tube	3469 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.031$
phi and ω scans	$\theta_{max} = 25.7°$, $\theta_{min} = 1.9°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -11 \rightarrow 13$
$T_{min} = 0.949$, $T_{max} = 0.966$	$k = -12 \rightarrow 11$

12711 measured reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.109$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2 + 0.3494P]$ where $P = (F_o^2 + 2F_c^2)/3$
4542 reflections	$(\Delta/\sigma)_{max} < 0.001$
333 parameters	$\Delta\rho_{max} = 0.28$ e Å^{-3}
3 restraints	$\Delta\rho_{min} = -0.19$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.48854 (6)	0.33999 (6)	0.03568 (3)	0.04181 (18)
S2	0.65584 (6)	0.67713 (6)	0.23342 (3)	0.04294 (18)
S3	0.52541 (6)	0.56902 (7)	0.12152 (3)	0.0484 (2)
N2	0.93916 (17)	0.68189 (19)	0.23701 (8)	0.0376 (5)
H2	0.8860	0.7272	0.2166	0.045*
N4	0.68075 (18)	0.4337 (2)	0.18382 (9)	0.0409 (5)
N5	0.78366 (18)	0.4925 (2)	−0.08496 (9)	0.0445 (5)
N6	0.98890 (17)	0.8914 (2)	0.16646 (9)	0.0422 (5)
O2	0.95579 (16)	0.5195 (2)	0.30789 (9)	0.0598 (5)
C24	1.0876 (2)	0.8188 (2)	0.18599 (10)	0.0342 (5)
C16	1.0642 (2)	0.7078 (2)	0.22398 (10)	0.0344 (5)
O1	0.76858 (17)	0.09593 (19)	0.04223 (9)	0.0592 (5)
C8	0.8872 (2)	0.4250 (2)	−0.06819 (10)	0.0375 (5)
C10	0.7060 (2)	0.1861 (2)	0.02251 (10)	0.0395 (6)
C20	1.2107 (2)	0.8493 (2)	0.16943 (11)	0.0374 (5)
C15	0.8927 (2)	0.5951 (2)	0.27744 (10)	0.0383 (5)

C9	0.8725 (2)	0.3130 (2)	−0.02972 (10)	0.0382 (5)
N3	0.63967 (18)	0.35305 (19)	0.13605 (8)	0.0413 (5)
N1	0.75026 (17)	0.2858 (2)	−0.01150 (9)	0.0416 (5)
H1	0.6958	0.3411	−0.0240	0.050*
C13	0.62927 (19)	0.5483 (2)	0.18185 (10)	0.0353 (5)
C4	1.0072 (2)	0.4606 (3)	−0.08780 (11)	0.0435 (6)
C12	0.5590 (2)	0.4104 (2)	0.10073 (10)	0.0361 (5)
C14	0.7546 (2)	0.5972 (2)	0.28903 (10)	0.0398 (6)
H14A	0.7410	0.6384	0.3290	0.080*
H14B	0.7271	0.5074	0.2927	0.080*
C11	0.5678 (2)	0.1851 (2)	0.03428 (11)	0.0416 (6)
H11A	0.5537	0.1423	0.0738	0.080*
H11B	0.5295	0.1314	0.0025	0.080*
C1	0.9732 (2)	0.2404 (3)	−0.01294 (12)	0.0499 (7)
H1A	0.9633	0.1663	0.0115	0.060*
C19	1.3081 (2)	0.7714 (3)	0.19269 (12)	0.0467 (6)
H19	1.3895	0.7920	0.1831	0.056*
C21	1.2295 (2)	0.9559 (3)	0.12920 (12)	0.0461 (6)
H21	1.3089	0.9783	0.1166	0.055*
C22	1.1310 (3)	1.0255 (3)	0.10913 (12)	0.0513 (7)
H22	1.1418	1.0958	0.0824	0.062*
C6	0.9135 (3)	0.6360 (3)	−0.14421 (12)	0.0560 (7)
H6	0.9186	0.7077	−0.1705	0.067*
C17	1.1607 (2)	0.6324 (2)	0.24427 (11)	0.0432 (6)
H17	1.1456	0.5584	0.2682	0.052*
C18	1.2827 (2)	0.6669 (3)	0.22894 (12)	0.0506 (7)
H18	1.3476	0.6166	0.2441	0.061*
C2	1.0919 (2)	0.2781 (3)	−0.03267 (13)	0.0585 (8)
H2A	1.1599	0.2284	−0.0208	0.070*
C23	1.0124 (3)	0.9901 (3)	0.12920 (12)	0.0517 (7)
H23	0.9459	1.0397	0.1153	0.062*
C7	0.7990 (3)	0.5934 (3)	−0.12173 (12)	0.0542 (7)
H7	0.7290	0.6398	−0.1337	0.065*
C3	1.1092 (2)	0.3847 (3)	−0.06834 (13)	0.0552 (7)
H3	1.1887	0.4084	−0.0802	0.066*
C5	1.0168 (3)	0.5704 (3)	−0.12682 (12)	0.0520 (7)
H5	1.0939	0.5980	−0.1407	0.062*
O1W	0.6164 (3)	−0.1290 (2)	0.08683 (12)	0.0789 (7)
H1WA	0.679 (6)	−0.071 (7)	0.073 (3)	0.27 (4)*
H1WB	0.593 (4)	−0.085 (4)	0.1230 (19)	0.130 (17)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0407 (4)	0.0475 (4)	0.0372 (3)	0.0041 (3)	−0.0073 (3)	−0.0041 (3)
S2	0.0381 (3)	0.0438 (4)	0.0470 (4)	0.0016 (3)	−0.0049 (3)	−0.0076 (3)
S3	0.0509 (4)	0.0457 (4)	0.0487 (4)	0.0147 (3)	−0.0176 (3)	−0.0088 (3)
N2	0.0308 (10)	0.0446 (12)	0.0373 (10)	0.0012 (8)	−0.0025 (8)	0.0077 (9)

N4	0.0423 (11)	0.0442 (13)	0.0363 (11)	0.0041 (9)	−0.0060 (9)	−0.0003 (9)
N5	0.0432 (12)	0.0470 (13)	0.0434 (12)	−0.0013 (10)	0.0001 (9)	0.0033 (10)
N6	0.0392 (11)	0.0471 (13)	0.0403 (11)	0.0049 (9)	0.0019 (9)	0.0064 (10)
O2	0.0464 (11)	0.0685 (13)	0.0645 (12)	0.0073 (9)	0.0055 (9)	0.0286 (10)
C24	0.0353 (13)	0.0353 (13)	0.0319 (11)	0.0013 (10)	−0.0001 (10)	−0.0070 (10)
C16	0.0321 (12)	0.0392 (14)	0.0321 (12)	0.0000 (10)	−0.0004 (9)	−0.0036 (10)
O1	0.0534 (11)	0.0576 (13)	0.0666 (12)	0.0114 (9)	0.0089 (9)	0.0233 (10)
C8	0.0389 (13)	0.0430 (14)	0.0307 (12)	−0.0013 (10)	0.0004 (10)	−0.0067 (11)
C10	0.0451 (14)	0.0397 (14)	0.0337 (12)	0.0017 (11)	−0.0002 (10)	0.0017 (11)
C20	0.0350 (13)	0.0375 (14)	0.0398 (13)	−0.0025 (10)	0.0018 (10)	−0.0083 (11)
C15	0.0380 (13)	0.0415 (14)	0.0355 (12)	−0.0014 (11)	−0.0010 (10)	−0.0017 (11)
C9	0.0379 (13)	0.0454 (15)	0.0313 (12)	0.0014 (11)	0.0027 (10)	−0.0061 (11)
N3	0.0487 (12)	0.0406 (12)	0.0345 (10)	0.0035 (9)	−0.0069 (9)	−0.0001 (9)
N1	0.0385 (11)	0.0450 (12)	0.0414 (11)	0.0037 (9)	0.0025 (9)	0.0054 (10)
C13	0.0276 (11)	0.0439 (14)	0.0346 (12)	−0.0019 (10)	0.0010 (9)	0.0009 (11)
C4	0.0447 (15)	0.0487 (16)	0.0373 (13)	−0.0034 (12)	0.0056 (11)	−0.0073 (12)
C12	0.0329 (12)	0.0422 (14)	0.0331 (12)	0.0008 (10)	0.0010 (10)	0.0006 (10)
C14	0.0366 (13)	0.0502 (16)	0.0326 (12)	−0.0058 (11)	0.0007 (10)	−0.0035 (11)
C11	0.0453 (14)	0.0381 (14)	0.0415 (13)	−0.0019 (11)	0.0010 (11)	−0.0014 (11)
C1	0.0477 (16)	0.0579 (18)	0.0440 (14)	0.0072 (13)	0.0041 (12)	0.0048 (13)
C19	0.0324 (13)	0.0504 (16)	0.0574 (16)	−0.0016 (11)	0.0048 (11)	−0.0051 (13)
C21	0.0440 (14)	0.0458 (16)	0.0484 (15)	−0.0084 (12)	0.0081 (12)	−0.0052 (12)
C22	0.0588 (17)	0.0461 (16)	0.0492 (15)	−0.0045 (13)	0.0042 (13)	0.0104 (13)
C6	0.067 (2)	0.0495 (17)	0.0520 (16)	−0.0082 (14)	0.0080 (14)	0.0066 (13)
C17	0.0412 (14)	0.0404 (15)	0.0479 (14)	0.0023 (11)	0.0007 (11)	0.0053 (12)
C18	0.0353 (14)	0.0530 (17)	0.0634 (17)	0.0087 (12)	−0.0035 (12)	0.0026 (14)
C2	0.0413 (15)	0.076 (2)	0.0586 (17)	0.0156 (14)	0.0047 (13)	0.0043 (16)
C23	0.0528 (17)	0.0515 (17)	0.0507 (16)	0.0107 (13)	0.0016 (12)	0.0124 (13)
C7	0.0529 (17)	0.0523 (18)	0.0575 (17)	0.0025 (13)	0.0021 (13)	0.0093 (14)
C3	0.0374 (15)	0.072 (2)	0.0567 (17)	0.0002 (13)	0.0064 (12)	−0.0029 (15)
C5	0.0480 (16)	0.0574 (18)	0.0505 (16)	−0.0131 (13)	0.0100 (12)	−0.0044 (14)
O1W	0.0971 (18)	0.0642 (15)	0.0753 (16)	−0.0058 (13)	−0.0050 (13)	−0.0143 (13)

Geometric parameters (Å, °)

S1—C12	1.750 (2)	N1—H1	0.8600
S1—C11	1.803 (3)	C4—C5	1.407 (4)
S2—C13	1.748 (2)	C4—C3	1.414 (4)
S2—C14	1.801 (2)	C14—H14A	0.9700
S3—C12	1.723 (2)	C14—H14B	0.9700
S3—C13	1.731 (2)	C11—H11A	0.9700
N2—C15	1.343 (3)	C11—H11B	0.9700
N2—C16	1.408 (3)	C1—C2	1.408 (4)
N2—H2	0.8600	C1—H1A	0.9300
N4—C13	1.299 (3)	C19—C18	1.353 (4)
N4—N3	1.392 (3)	C19—H19	0.9300
N5—C7	1.313 (3)	C21—C22	1.352 (4)
N5—C8	1.365 (3)	C21—H21	0.9300
N6—C23	1.316 (3)	C22—C23	1.403 (4)

N6—C24	1.367 (3)	C22—H22	0.9300
O2—C15	1.222 (3)	C6—C5	1.357 (4)
C24—C20	1.414 (3)	C6—C7	1.400 (4)
C24—C16	1.424 (3)	C6—H6	0.9300
C16—C17	1.370 (3)	C17—C18	1.406 (3)
O1—C10	1.221 (3)	C17—H17	0.9300
C8—C4	1.414 (3)	C18—H18	0.9300
C8—C9	1.424 (3)	C2—C3	1.347 (4)
C10—N1	1.345 (3)	C2—H2A	0.9300
C10—C11	1.517 (3)	C23—H23	0.9300
C20—C21	1.409 (3)	C7—H7	0.9300
C20—C19	1.413 (3)	C3—H3	0.9300
C15—C14	1.516 (3)	C5—H5	0.9300
C9—C1	1.367 (3)	O1W—H1WA	0.95 (6)
C9—N1	1.408 (3)	O1W—H1WB	0.93 (4)
N3—C12	1.298 (3)		
C12—S1—C11	99.71 (11)	C15—C14—H14B	107.6
C13—S2—C14	100.22 (11)	S2—C14—H14B	107.6
C12—S3—C13	86.72 (11)	H14A—C14—H14B	107.1
C15—N2—C16	127.9 (2)	C10—C11—S1	117.78 (17)
C15—N2—H2	116.0	C10—C11—H11A	107.9
C16—N2—H2	116.0	S1—C11—H11A	107.9
C13—N4—N3	112.00 (18)	C10—C11—H11B	107.9
C7—N5—C8	117.0 (2)	S1—C11—H11B	107.9
C23—N6—C24	117.0 (2)	H11A—C11—H11B	107.2
N6—C24—C20	122.5 (2)	C9—C1—C2	119.9 (3)
N6—C24—C16	118.1 (2)	C9—C1—H1A	120.0
C20—C24—C16	119.3 (2)	C2—C1—H1A	120.0
C17—C16—N2	124.3 (2)	C18—C19—C20	120.0 (2)
C17—C16—C24	119.8 (2)	C18—C19—H19	120.0
N2—C16—C24	115.88 (19)	C20—C19—H19	120.0
N5—C8—C4	123.0 (2)	C22—C21—C20	119.3 (2)
N5—C8—C9	118.0 (2)	C22—C21—H21	120.3
C4—C8—C9	119.1 (2)	C20—C21—H21	120.3
O1—C10—N1	124.5 (2)	C21—C22—C23	119.1 (2)
O1—C10—C11	118.9 (2)	C21—C22—H22	120.4
N1—C10—C11	116.6 (2)	C23—C22—H22	120.4
C21—C20—C19	123.2 (2)	C5—C6—C7	118.7 (3)
C21—C20—C24	117.6 (2)	C5—C6—H6	120.7
C19—C20—C24	119.2 (2)	C7—C6—H6	120.7
O2—C15—N2	123.9 (2)	C16—C17—C18	119.9 (2)
O2—C15—C14	118.1 (2)	C16—C17—H17	120.0
N2—C15—C14	117.8 (2)	C18—C17—H17	120.0
C1—C9—N1	124.6 (2)	C19—C18—C17	121.7 (2)
C1—C9—C8	120.1 (2)	C19—C18—H18	119.2
N1—C9—C8	115.3 (2)	C17—C18—H18	119.2
C12—N3—N4	112.3 (2)	C3—C2—C1	121.5 (3)
C10—N1—C9	129.6 (2)	C3—C2—H2A	119.3
C10—N1—H1	115.2	C1—C2—H2A	119.3

C9—N1—H1	115.2	N6—C23—C22	124.3 (2)
N4—C13—S3	114.42 (17)	N6—C23—H23	117.8
N4—C13—S2	126.16 (17)	C22—C23—H23	117.8
S3—C13—S2	119.42 (14)	N5—C7—C6	124.5 (3)
C5—C4—C3	123.9 (2)	N5—C7—H7	117.8
C5—C4—C8	117.0 (2)	C6—C7—H7	117.8
C3—C4—C8	119.1 (2)	C2—C3—C4	120.3 (2)
N3—C12—S3	114.56 (17)	C2—C3—H3	119.8
N3—C12—S1	125.12 (19)	C4—C3—H3	119.8
S3—C12—S1	120.31 (13)	C6—C5—C4	119.9 (2)
C15—C14—S2	118.78 (16)	C6—C5—H5	120.1
C15—C14—H14A	107.6	C4—C5—H5	120.1
S2—C14—H14A	107.6	H1WA—O1W—H1WB	99 (4)
C23—N6—C24—C20	2.3 (3)	N4—N3—C12—S3	0.5 (3)
C23—N6—C24—C16	−177.1 (2)	N4—N3—C12—S1	179.22 (15)
C15—N2—C16—C17	10.7 (4)	C13—S3—C12—N3	−0.37 (18)
C15—N2—C16—C24	−170.7 (2)	C13—S3—C12—S1	−179.18 (15)
N6—C24—C16—C17	179.8 (2)	C11—S1—C12—N3	−3.3 (2)
C20—C24—C16—C17	0.3 (3)	C11—S1—C12—S3	175.39 (14)
N6—C24—C16—N2	1.1 (3)	O2—C15—C14—S2	−165.45 (19)
C20—C24—C16—N2	−178.34 (19)	N2—C15—C14—S2	18.5 (3)
C7—N5—C8—C4	1.0 (3)	C13—S2—C14—C15	87.36 (19)
C7—N5—C8—C9	−178.3 (2)	O1—C10—C11—S1	154.2 (2)
N6—C24—C20—C21	−2.6 (3)	N1—C10—C11—S1	−28.2 (3)
C16—C24—C20—C21	176.8 (2)	C12—S1—C11—C10	−64.46 (19)
N6—C24—C20—C19	178.5 (2)	N1—C9—C1—C2	−178.6 (2)
C16—C24—C20—C19	−2.1 (3)	C8—C9—C1—C2	1.3 (4)
C16—N2—C15—O2	−3.4 (4)	C21—C20—C19—C18	−177.0 (2)
C16—N2—C15—C14	172.5 (2)	C24—C20—C19—C18	1.8 (4)
N5—C8—C9—C1	178.4 (2)	C19—C20—C21—C22	−180.0 (2)
C4—C8—C9—C1	−0.9 (3)	C24—C20—C21—C22	1.2 (3)
N5—C8—C9—N1	−1.7 (3)	C20—C21—C22—C23	0.4 (4)
C4—C8—C9—N1	179.0 (2)	N2—C16—C17—C18	−179.7 (2)
C13—N4—N3—C12	−0.3 (3)	C24—C16—C17—C18	1.8 (3)
O1—C10—N1—C9	−2.8 (4)	C20—C19—C18—C17	0.3 (4)
C11—C10—N1—C9	179.8 (2)	C16—C17—C18—C19	−2.1 (4)
C1—C9—N1—C10	−2.6 (4)	C9—C1—C2—C3	−0.3 (4)
C8—C9—N1—C10	177.5 (2)	C24—N6—C23—C22	−0.6 (4)
N3—N4—C13—S3	0.1 (2)	C21—C22—C23—N6	−0.7 (4)
N3—N4—C13—S2	179.95 (15)	C8—N5—C7—C6	−0.4 (4)
C12—S3—C13—N4	0.17 (18)	C5—C6—C7—N5	−0.7 (4)
C12—S3—C13—S2	−179.74 (14)	C1—C2—C3—C4	−1.1 (4)
C14—S2—C13—N4	−5.8 (2)	C5—C4—C3—C2	−177.7 (3)
C14—S2—C13—S3	174.10 (13)	C8—C4—C3—C2	1.4 (4)
N5—C8—C4—C5	−0.6 (3)	C7—C6—C5—C4	1.1 (4)
C9—C8—C4—C5	178.7 (2)	C3—C4—C5—C6	178.6 (3)
N5—C8—C4—C3	−179.8 (2)	C8—C4—C5—C6	−0.5 (4)
C9—C8—C4—C3	−0.4 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O1	0.95 (7)	2.07 (7)	2.990 (3)	162 (6)
O1W—H1WB···O2^{i}	0.94 (4)	1.91 (4)	2.841 (3)	175 (4)
C11—H11B···O1W^{ii}	0.97	2.49	3.332 (4)	145
C23—H23···O1^{iii}	0.93	2.55	3.411 (4)	155

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2; (ii) −*x*+1, −*y*, −*z*; (iii) *x*, *y*+1, *z*.

Fig. 1

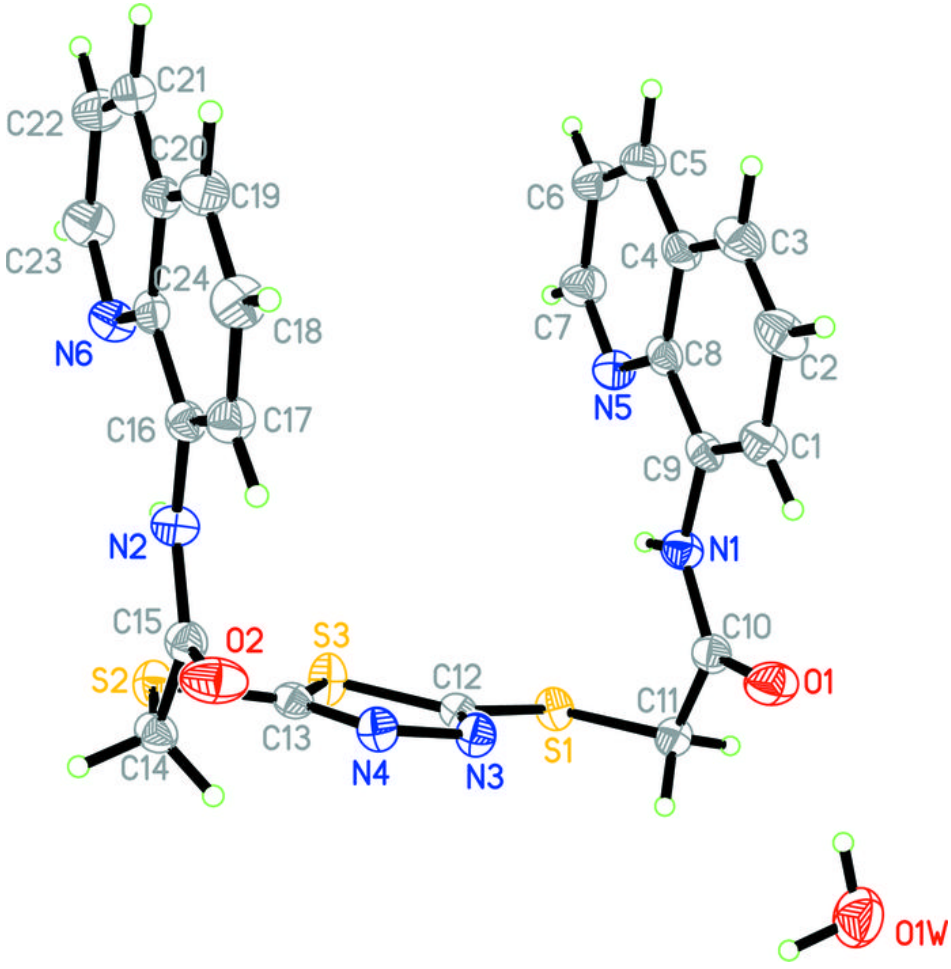
C21
C22
C20
C19
C23
C24
C18
N6
C16
C17
N2
C15
O2
S3
S2
C12
C13
C14
N4
N3
S1
C11
C10
O1
N1
C9
C1
C2
N5
C8
C7
C4
C3
C5
C6
O1W

Fig. 2