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4-Phenyl-2,5,5a,6,7,8,9,9a-hexahydro-1*H*-1,5-benzodiazepine-2-thione ethanol monosolvate

Wedad Al Garadi,[a]* Youssef Ramli,[b] Lhoussaine El Ghayati,[a] Mohamed El Hafi,[a] Ahmed Moussaif,[c] El Mokhtar Essassi[a] and Joel T. Mague[d]

[a]Laboratoire de Chimie Organique Heterocyclique URAC 21, Av. Ibn Battouta, BP 1014, Faculté des Sciences, Université Mohammed V, Rabat, Morocco, [b]Laboratory of Medicinal Chemistry, Drug Sciences Research Center, Faculty of Medicine and Pharmacy, Mohammed V University, Rabat, Morocco, [c]National Center of Energy Sciences and Nuclear Techniques, Rabat, Morocco, and [d]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: awedad17@yahoo.com

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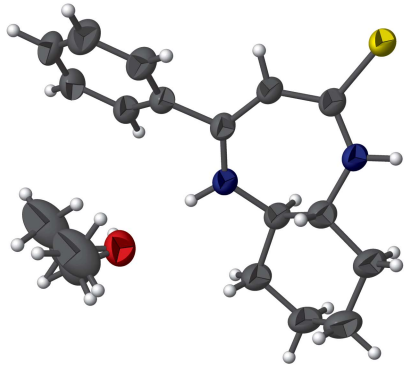
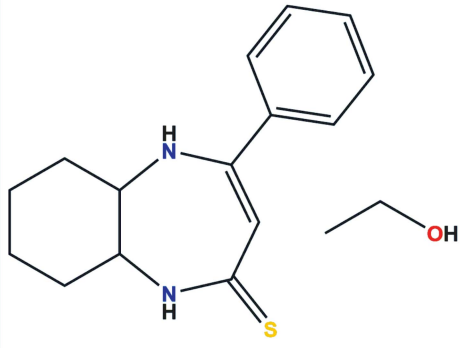
Structural data: full structural data are available from iucrdata.iucr.org

In the solvated title compound, $C_{15}H_{18}N_2S\cdot C_2H_5OH$, the seven-membered ring has a twisted envelope conformation and the cyclohexyl ring has a chair conformation. In the crystal, N—H$\cdots$O and O—H$\cdots$S hydrogen bonds as well as C—H$\cdots\pi$(ring) interactions form helical chains in which the thione and solvent ethanol molecules alternate. These chains are formed into layers parallel to (101) by inversion-related pairs of N—H$\cdots$S hydrogen bonds. The ethanol solvent molecule is disordered over two sets of sites [occupancy ratio 0.880 (8): 0.120 (8)] with the oxygen atom in common.

3D view



Chemical scheme



Structure description

Benzodiazepine derivatives have attracted significant attention because of their biological and therapeutic activities. They are used as sedatives, hypnotics, anxiolytics, anticonvulsants, analgesic, antidepressants, hypnotic, anti-inflammatory and muscle relaxant agents (Pasha & Jayashankara, 2006; Radatz *et al.* 2011; Naga Prashant & Ravi Kuma, 2015). As a continuation of our research into 1,5-benzodiazepine derivatives (Al Garadi *et al.*, 2018), we prepared the title compound (Fig. 1) and characterized it by X-ray diffraction.

From the C8—C7—C10—C11 torsion angle of 44.3 (3)°, the pendant phenyl ring is inclined to the approximately planar portion of the seven-membered ring. This ring adopts a twisted envelope conformation with C1 at the flap and a Cremer–Pople puckering analysis gave the parameters $Q(2)$ = 0.5165 (19) Å, $Q(3)$ = 0.3634 (19) Å, $\varphi(2)$ = 301.7 (2)° and $\varphi(3)$ = 217.2 (2)° with a total puckering amplitude of 0.632 (2) Å. The

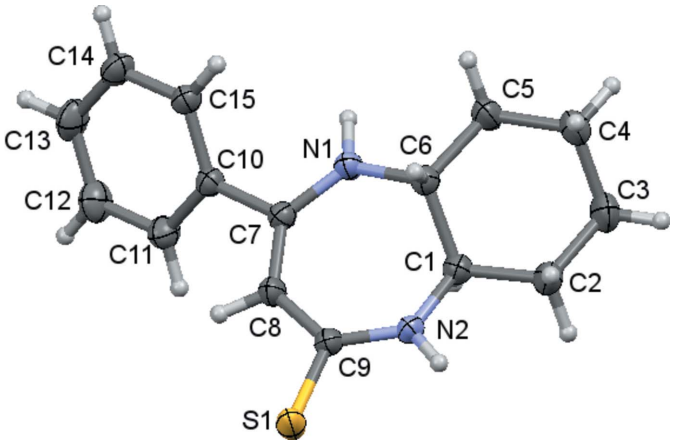


Figure 1
The title molecule with 30% probability ellipsoids. The disordered solvent molecule is omitted.

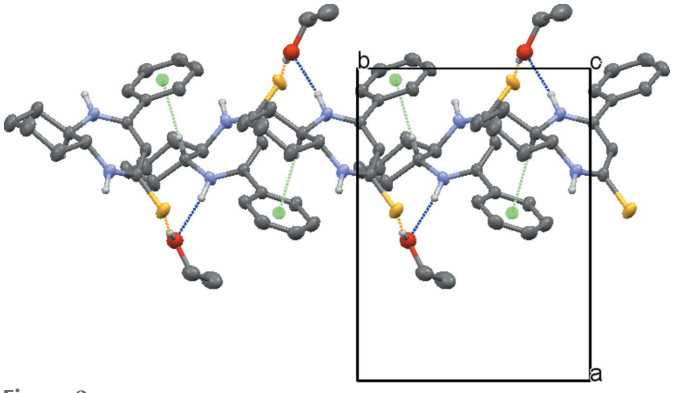


Figure 2
Portion of one chain viewed along the *c*-axis direction. N—H···O and O—H···S hydrogen bonds and the C—H···π(ring) interactions are shown, respectively, by blue, orange and green dashed lines.

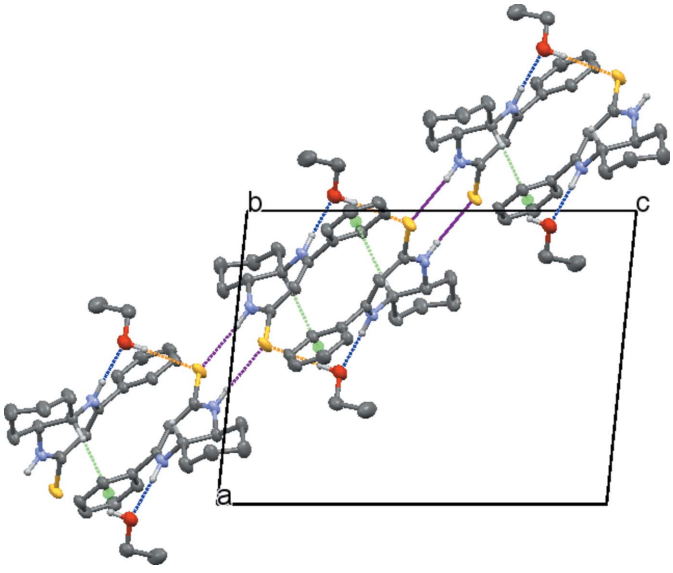


Figure 3
Packing viewed along the *b*-axis direction with the N—H···S hydrogen bonds linking chains shown by purple dashed lines. Other intermolecular interations are depicted as in Fig. 2.

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

*Cg*2 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1	0.91	2.13	3.030 (2)	173
N2—H2···S1^{i}	0.91	2.53	3.4312 (15)	171
O1—H1*B*···S1^{ii}	0.87	2.42	3.2886 (18)	173
C6—H6···*Cg*2^{ii}	0.98	2.54	3.516 (2)	177

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{18}N_2S{\cdot}C_2H_6O$
M_r	304.44
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, *b*, *c* (Å)	12.0255 (2), 8.9303 (2), 15.8822 (3)
β (°)	95.813 (1)
V (Å^3)	1696.84 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.69
Crystal size (mm)	0.22 × 0.13 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.71, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12459, 3209, 2613
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.125, 1.07
No. of reflections	3209
No. of parameters	199
No. of restraints	26
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.18

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008) and *SHELXTL* (Sheldrick, 2008).

cyclohexyl ring adopts a chair conformation with puckering parameters Q = 0.550 (3) Å, θ = 9.4 (2)° and φ = 142.2 (16)°.

In the crystal, each molecule is connected to an ethanol solvent molecule by an N1—H1*A*···O1 hydrogen bond and these units are formed into helical chains extending along the *b*-axis direction by O1—H1*B*···S1 hydrogen bonds and C6—H6···*Cg*2 interactions (Table 1 and Fig. 2). The chains are connected by inversion-related pairs of N2—H2···S1 hydrogen bonds, forming layers parallel to (101) (Table 1 and Fig. 3).

Synthesis and crystallization

Phosphorus pentasulfide (5.55 g, 0.025 mol) was added to a solution of 4-phenyl-5a,6,7,8,9,9a-hexahydro-1*H*-1,5-benzodiazepin-2(5*H*)-one (4.84 g, 0.02 mol) in 100 ml of pyridine. The mixture was refluxed for 3 h and the solvent was then

evaporated under reduced pressure. The precipitate formed was washed with hot water. The residue obtained was crystallized from ethanol solution to afford colourless plates of the title compound.

Refinement

Crystal and refinement details are presented in Table 2. Hydrogen atoms attached to carbon were placed in idealized positions while those attached to nitrogen and oxygen were located in difference maps and their coordinates adjusted to give N—H = 0.91 Å and O—H = 0.87 Å. All were included as riding contributions. The ethanol solvent molecule is disordered over two sets of sites [occupancy ratio 0.880 (8): 0.120 (8)] with the oxygen atom in common. The components of the disorder were refined with restraints that their geometries be comparable.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x181276 [https://doi.org/10.1107/S2414314618012762]

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Crystal data

$C_{15}H_{18}N_2S·C_2H_6O$
M_r = 304.44
Monoclinic, $P2_1/n$
a = 12.0255 (2) Å
b = 8.9303 (2) Å
c = 15.8822 (3) Å
β = 95.813 (1)°
V = 1696.84 (6) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.192 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8452 reflections
θ = 4.9–70.1°
μ = 1.69 mm^{-1}
T = 298 K
Plate, colourless
0.22 × 0.13 × 0.04 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.71, T_{max} = 0.93
12459 measured reflections
3209 independent reflections
2613 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 70.1°, θ_{min} = 4.9°
h = −14→14
k = −10→10
l = −19→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.07
3209 reflections
199 parameters
26 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.7241P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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.

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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.93 - 0.98 Å) while those attached to nitrogen and oxygen were placed in locations derived from a difference map and their coordinates adjusted to give N—H = 0.91 %A. and O—H = 0.87 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. The lattice ethanol is disordered over two sites with the oxygen atom in common. The components of the disorder were refined with restraints that their geometries be comparable.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.04411 (5)	0.33255 (6)	0.41909 (4)	0.0606 (2)	
N1	0.35246 (13)	0.63053 (17)	0.34690 (10)	0.0464 (4)	
H1A	0.415425	0.668287	0.327593	0.056*	
N2	0.16991 (13)	0.56183 (17)	0.46634 (9)	0.0470 (4)	
H2	0.109900	0.578865	0.495602	0.056*	
C1	0.26404 (17)	0.6658 (2)	0.47957 (12)	0.0484 (5)	
H1	0.329705	0.611765	0.505524	0.058*	
C2	0.2299 (2)	0.7841 (3)	0.54160 (14)	0.0638 (6)	
H2A	0.157157	0.823675	0.520850	0.077*	
H2B	0.223027	0.736859	0.595837	0.077*	
C3	0.3128 (2)	0.9130 (3)	0.55427 (15)	0.0740 (7)	
H3A	0.286707	0.985167	0.593474	0.089*	
H3B	0.384858	0.875486	0.578180	0.089*	
C4	0.3246 (2)	0.9874 (3)	0.47095 (15)	0.0664 (6)	
H4A	0.376771	1.070253	0.479142	0.080*	
H4B	0.252863	1.026899	0.447656	0.080*	
C5	0.3667 (2)	0.8748 (2)	0.40967 (16)	0.0630 (6)	
H5A	0.441443	0.843268	0.431149	0.076*	
H5B	0.371657	0.923603	0.355604	0.076*	
C6	0.29211 (16)	0.7361 (2)	0.39586 (12)	0.0453 (4)	
H6	0.222356	0.764715	0.362434	0.054*	
C7	0.32591 (15)	0.4872 (2)	0.33075 (11)	0.0402 (4)	
C8	0.23849 (16)	0.4073 (2)	0.35782 (12)	0.0461 (4)	
H8	0.229905	0.311777	0.334793	0.055*	
C9	0.15903 (16)	0.4448 (2)	0.41463 (11)	0.0440 (4)	
C10	0.39812 (14)	0.4097 (2)	0.27311 (11)	0.0417 (4)	
C11	0.43429 (17)	0.2639 (2)	0.28946 (13)	0.0521 (5)	
H11	0.415250	0.214890	0.337637	0.062*	
C12	0.49857 (19)	0.1908 (3)	0.23445 (16)	0.0640 (6)	
H12	0.522541	0.093252	0.245910	0.077*	
C13	0.52694 (18)	0.2624 (3)	0.16295 (15)	0.0636 (6)	

H13	0.569293	0.212846	0.125778	0.076*	
C14	0.49280 (18)	0.4067 (3)	0.14656 (14)	0.0586 (5)	
H14	0.512929	0.455074	0.098518	0.070*	
C15	0.42842 (16)	0.4814 (2)	0.20098 (12)	0.0478 (4)	
H15	0.405520	0.579352	0.189269	0.057*	
O1	0.55130 (14)	0.7823 (2)	0.28035 (11)	0.0695 (4)	
H1B	0.527520	0.804551	0.228297	0.083*	
C16	0.6566 (3)	0.7119 (5)	0.2791 (2)	0.0730 (10)	0.880 (8)
H16A	0.714534	0.786480	0.275471	0.088*	0.880 (8)
H16B	0.655933	0.645981	0.230550	0.088*	0.880 (8)
C17	0.6787 (3)	0.6240 (6)	0.3592 (4)	0.1058 (17)	0.880 (8)
H17A	0.620071	0.552021	0.362783	0.159*	0.880 (8)
H17B	0.681220	0.690618	0.406817	0.159*	0.880 (8)
H17C	0.748986	0.572968	0.359468	0.159*	0.880 (8)
C16A	0.6613 (11)	0.734 (3)	0.308 (2)	0.0730 (10)	0.120 (8)
H16C	0.678136	0.768901	0.365371	0.088*	0.120 (8)
H16D	0.711080	0.787784	0.273674	0.088*	0.120 (8)
C17A	0.694 (3)	0.573 (3)	0.306 (3)	0.1058 (17)	0.120 (8)
H17D	0.768610	0.560942	0.332235	0.159*	0.120 (8)
H17E	0.689151	0.538366	0.248687	0.159*	0.120 (8)
H17F	0.643514	0.515141	0.336788	0.159*	0.120 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0667 (3)	0.0529 (3)	0.0685 (4)	−0.0219 (2)	0.0373 (3)	−0.0206 (2)
N1	0.0516 (9)	0.0382 (8)	0.0527 (9)	−0.0079 (7)	0.0223 (7)	−0.0065 (7)
N2	0.0554 (9)	0.0428 (8)	0.0464 (8)	−0.0098 (7)	0.0230 (7)	−0.0088 (7)
C1	0.0574 (11)	0.0449 (10)	0.0446 (10)	−0.0076 (8)	0.0127 (8)	−0.0047 (8)
C2	0.0852 (16)	0.0587 (13)	0.0515 (11)	−0.0194 (12)	0.0257 (11)	−0.0165 (10)
C3	0.0958 (18)	0.0668 (15)	0.0605 (13)	−0.0214 (13)	0.0133 (12)	−0.0239 (12)
C4	0.0845 (16)	0.0473 (12)	0.0701 (14)	−0.0178 (11)	0.0210 (12)	−0.0161 (10)
C5	0.0766 (14)	0.0470 (11)	0.0702 (14)	−0.0181 (10)	0.0305 (11)	−0.0142 (10)
C6	0.0518 (10)	0.0390 (9)	0.0471 (10)	−0.0035 (8)	0.0145 (8)	−0.0050 (8)
C7	0.0450 (9)	0.0378 (9)	0.0394 (9)	0.0009 (7)	0.0121 (7)	0.0000 (7)
C8	0.0538 (10)	0.0369 (9)	0.0506 (10)	−0.0051 (8)	0.0203 (8)	−0.0074 (8)
C9	0.0543 (10)	0.0380 (9)	0.0422 (9)	−0.0044 (8)	0.0168 (8)	−0.0010 (7)
C10	0.0430 (9)	0.0409 (9)	0.0425 (9)	−0.0020 (7)	0.0109 (7)	−0.0039 (7)
C11	0.0605 (12)	0.0456 (11)	0.0515 (11)	0.0078 (9)	0.0129 (9)	0.0008 (9)
C12	0.0637 (13)	0.0555 (13)	0.0734 (15)	0.0176 (10)	0.0092 (11)	−0.0094 (11)
C13	0.0520 (11)	0.0755 (15)	0.0661 (14)	0.0061 (10)	0.0210 (10)	−0.0197 (12)
C14	0.0576 (12)	0.0697 (14)	0.0524 (11)	−0.0101 (10)	0.0243 (9)	−0.0083 (10)
C15	0.0517 (10)	0.0457 (10)	0.0483 (10)	−0.0049 (8)	0.0165 (8)	−0.0027 (8)
O1	0.0703 (10)	0.0719 (11)	0.0691 (10)	−0.0013 (8)	0.0199 (8)	0.0040 (8)
C16	0.0624 (14)	0.087 (2)	0.071 (2)	−0.0080 (13)	0.0133 (14)	0.0089 (17)
C17	0.083 (2)	0.120 (3)	0.110 (3)	−0.015 (2)	−0.007 (2)	0.048 (3)
C16A	0.0624 (14)	0.087 (2)	0.071 (2)	−0.0080 (13)	0.0133 (14)	0.0089 (17)
C17A	0.083 (2)	0.120 (3)	0.110 (3)	−0.015 (2)	−0.007 (2)	0.048 (3)

Geometric parameters (Å, º)

S1—C9	1.7143 (18)	C10—C11	1.389 (3)
N1—C7	1.338 (2)	C10—C15	1.393 (3)
N1—C6	1.461 (2)	C11—C12	1.387 (3)
N1—H1A	0.9100	C11—H11	0.9300
N2—C9	1.328 (2)	C12—C13	1.376 (3)
N2—C1	1.463 (2)	C12—H12	0.9300
N2—H2	0.9099	C13—C14	1.369 (3)
C1—C2	1.528 (3)	C13—H13	0.9300
C1—C6	1.538 (3)	C14—C15	1.388 (3)
C1—H1	0.9800	C14—H14	0.9300
C2—C3	1.523 (3)	C15—H15	0.9300
C2—H2A	0.9700	O1—C16	1.416 (3)
C2—H2B	0.9700	O1—C16A	1.416 (4)
C3—C4	1.501 (3)	O1—H1B	0.8700
C3—H3A	0.9700	C16—C17	1.495 (5)
C3—H3B	0.9700	C16—H16A	0.9700
C4—C5	1.521 (3)	C16—H16B	0.9700
C4—H4A	0.9700	C17—H17A	0.9600
C4—H4B	0.9700	C17—H17B	0.9600
C5—C6	1.532 (3)	C17—H17C	0.9600
C5—H5A	0.9700	C16A—C17A	1.495 (6)
C5—H5B	0.9700	C16A—H16C	0.9700
C6—H6	0.9800	C16A—H16D	0.9700
C7—C8	1.375 (2)	C17A—H17D	0.9600
C7—C10	1.494 (2)	C17A—H17E	0.9600
C8—C9	1.419 (2)	C17A—H17F	0.9600
C8—H8	0.9300		
C7—N1—C6	126.71 (15)	N2—C9—C8	123.24 (16)
C7—N1—H1A	118.7	N2—C9—S1	117.65 (13)
C6—N1—H1A	114.5	C8—C9—S1	119.09 (14)
C9—N2—C1	127.96 (15)	C11—C10—C15	118.79 (17)
C9—N2—H2	114.5	C11—C10—C7	120.66 (16)
C1—N2—H2	117.6	C15—C10—C7	120.53 (16)
N2—C1—C2	106.07 (16)	C12—C11—C10	120.5 (2)
N2—C1—C6	111.68 (15)	C12—C11—H11	119.8
C2—C1—C6	111.82 (16)	C10—C11—H11	119.8
N2—C1—H1	109.1	C13—C12—C11	120.1 (2)
C2—C1—H1	109.1	C13—C12—H12	119.9
C6—C1—H1	109.1	C11—C12—H12	119.9
C3—C2—C1	113.13 (19)	C14—C13—C12	119.97 (19)
C3—C2—H2A	109.0	C14—C13—H13	120.0
C1—C2—H2A	109.0	C12—C13—H13	120.0
C3—C2—H2B	109.0	C13—C14—C15	120.6 (2)
C1—C2—H2B	109.0	C13—C14—H14	119.7
H2A—C2—H2B	107.8	C15—C14—H14	119.7

C4—C3—C2	109.73 (19)	C14—C15—C10	120.0 (2)
C4—C3—H3A	109.7	C14—C15—H15	120.0
C2—C3—H3A	109.7	C10—C15—H15	120.0
C4—C3—H3B	109.7	C16—O1—H1B	107.3
C2—C3—H3B	109.7	C16A—O1—H1B	124.5
H3A—C3—H3B	108.2	O1—C16—C17	107.7 (3)
C3—C4—C5	109.8 (2)	O1—C16—H16A	110.2
C3—C4—H4A	109.7	C17—C16—H16A	110.2
C5—C4—H4A	109.7	O1—C16—H16B	110.2
C3—C4—H4B	109.7	C17—C16—H16B	110.2
C5—C4—H4B	109.7	H16A—C16—H16B	108.5
H4A—C4—H4B	108.2	C16—C17—H17A	109.5
C4—C5—C6	113.44 (17)	C16—C17—H17B	109.5
C4—C5—H5A	108.9	H17A—C17—H17B	109.5
C6—C5—H5A	108.9	C16—C17—H17C	109.5
C4—C5—H5B	108.9	H17A—C17—H17C	109.5
C6—C5—H5B	108.9	H17B—C17—H17C	109.5
H5A—C5—H5B	107.7	O1—C16A—C17A	122 (2)
N1—C6—C5	106.42 (15)	O1—C16A—H16C	107.0
N1—C6—C1	111.14 (16)	C17A—C16A—H16C	107.0
C5—C6—C1	112.51 (16)	O1—C16A—H16D	107.0
N1—C6—H6	108.9	C17A—C16A—H16D	107.0
C5—C6—H6	108.9	H16C—C16A—H16D	106.7
C1—C6—H6	108.9	C16A—C17A—H17D	109.5
N1—C7—C8	127.71 (16)	C16A—C17A—H17E	109.5
N1—C7—C10	114.72 (15)	H17D—C17A—H17E	109.5
C8—C7—C10	117.50 (16)	C16A—C17A—H17F	109.5
C7—C8—C9	131.47 (17)	H17D—C17A—H17F	109.5
C7—C8—H8	114.3	H17E—C17A—H17F	109.5
C9—C8—H8	114.3		

C9—N2—C1—C2	176.7 (2)	C10—C7—C8—C9	176.8 (2)
C9—N2—C1—C6	54.7 (3)	C1—N2—C9—C8	−4.3 (3)
N2—C1—C2—C3	−172.9 (2)	C1—N2—C9—S1	174.38 (15)
C6—C1—C2—C3	−50.9 (3)	C7—C8—C9—N2	−13.8 (4)
C1—C2—C3—C4	58.6 (3)	C7—C8—C9—S1	167.52 (18)
C2—C3—C4—C5	−60.0 (3)	N1—C7—C10—C11	138.34 (19)
C3—C4—C5—C6	56.8 (3)	C8—C7—C10—C11	−44.4 (3)
C7—N1—C6—C5	169.86 (19)	N1—C7—C10—C15	−43.0 (2)
C7—N1—C6—C1	47.0 (3)	C8—C7—C10—C15	134.25 (19)
C4—C5—C6—N1	−171.3 (2)	C15—C10—C11—C12	−0.6 (3)
C4—C5—C6—C1	−49.4 (3)	C7—C10—C11—C12	178.09 (19)
N2—C1—C6—N1	−76.6 (2)	C10—C11—C12—C13	−0.1 (3)
C2—C1—C6—N1	164.69 (17)	C11—C12—C13—C14	0.8 (4)
N2—C1—C6—C5	164.15 (17)	C12—C13—C14—C15	−0.8 (3)
C2—C1—C6—C5	45.5 (2)	C13—C14—C15—C10	0.1 (3)
C6—N1—C7—C8	−1.6 (3)	C11—C10—C15—C14	0.6 (3)
C6—N1—C7—C10	175.40 (17)	C7—C10—C15—C14	−178.09 (18)

N1—C7—C8—C9	−6.4 (4)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1	0.91	2.13	3.030 (2)	173
N2—H2···S1^{i}	0.91	2.53	3.4312 (15)	171
O1—H1*B*···S1^{ii}	0.87	2.42	3.2886 (18)	173
C6—H6···*Cg*2^{ii}	0.98	2.54	3.516 (2)	177

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