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3-(4-Amino-3-ethyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-yl)-1,3-diphenylpropan-1-one

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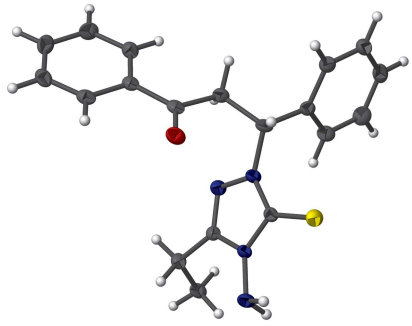
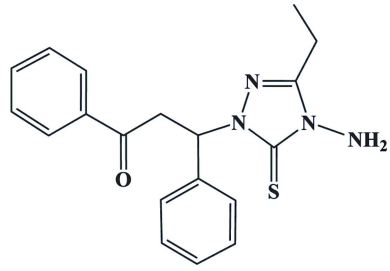
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{19}H_{20}N_4OS$, the 1,2,4-triazole ring forms dihedral angles of 58.64 (9) and 87.68 (9)° with the phenyl rings, which are inclined to one another by 43.30 (6)°. In the crystal, molecules are linked by N—H···O, N—H···S and C—H···S hydrogen bonds, forming chains propagating along the *c*-axis direction. Neighbouring chains are linked by three C—H···π interactions, forming layers parallel to the *bc* plane. Finally, the layers are linked by a fourth C—H···π interaction, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

The synthesis and crystal structures of some Mannich base derivatives have been reported (Wang, *et al.*, 2011; Shams, *et al.*, 2011). Now, we present here the crystal structure of the title 1,2,4-triazole derivative.

In the title compound, Fig. 1, the 1,2,4-triazole ring is almost planar, with an r.m.s. deviation of 0.0055 Å and a maximum deviation of 0.0087 (2) Å for atom C17. Atom C16 of the 1,2,4-triazole ring shows a distorted Csp^2 hybridization state with bond angles of 103.06 (13)° for N1—C16—N3, 129.69 (12)° for N1—C16—S1, and 127.19 (12)° for N3—C16—S1. These values are similar to those reported for other triazole derivatives (Zhao *et al.*, 2010; Gao *et al.*, 2011). The other bond lengths and angles are comparable with those reported for related 1,2,4-triazole-5(4*H*)-thione derivatives (Al-Tamimi *et al.*, 2010; Fun *et al.*, 2009; Tan *et al.*, 2010). The C10–C15 phenyl ring is normal to the triazole ring, making a dihedral angle of 87.68 (9)°, while the second phenyl ring (C1–C6) is inclined to the triazole ring by 58.64 (9)°. The phenyl rings are inclined to one another by 43.30 (6)°.

In the crystal, molecules are linked by N—H···O, N—H···S and C—H···S hydrogen bonds, forming chains propagating along the *c*-axis direction (Table 1 and Fig. 2). Neighbouring chains are linked by three C—H···π interactions, forming layers parallel

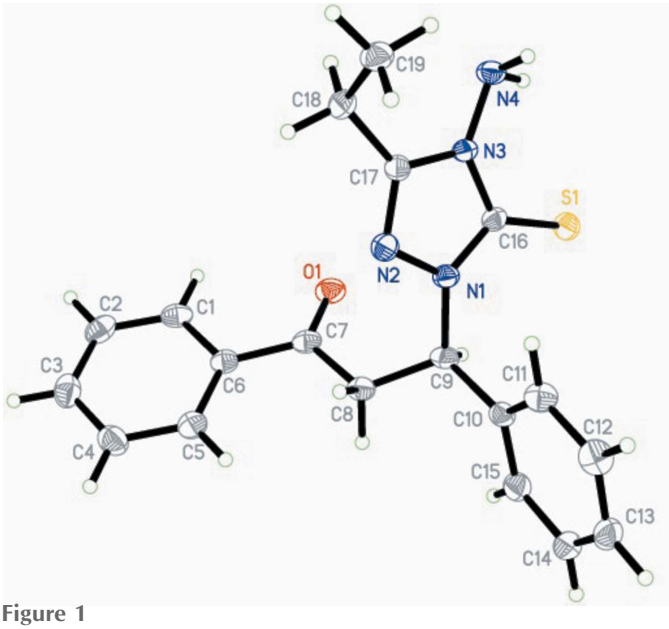


Figure 1
A view of the molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

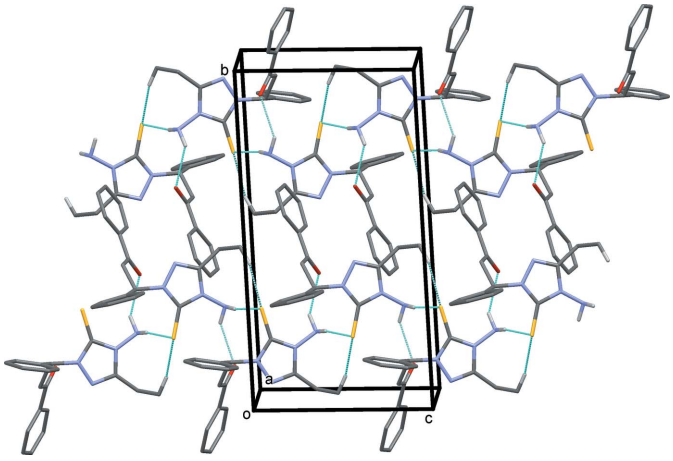


Figure 2
A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only the H atoms involved in the hydrogen bonds have been included.

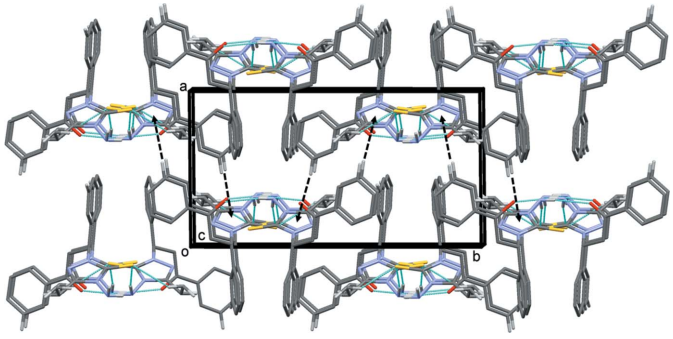


Figure 3
A view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines and the C—H···π interactions linking the layers are shown as black dashed arrows (see Table 1). For clarity, only the H atoms involved in the various intermolecular interactions have been included.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the N1/N2/N3/C17/C18, C1–C6 and C10–C15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O1^{i}	0.92 (2)	2.39 (2)	3.138 (2)	139 (2)
N4—H4*B*···S1^{i}	0.91 (2)	2.55 (2)	3.458 (2)	172 (2)
C19—H19*C*···S1^{i}	0.98	2.87	3.743 (2)	149
C12—H12···*Cg*2^{ii}	0.95	2.97	3.711 (2)	136
C18—H18*A*···*Cg*3^{ii}	0.99	2.75	3.7275 (18)	170
C19—H19*B*···*Cg*2^{iii}	0.98	2.75	3.5032 (19)	134
C2—H2···*Cg*1^{iv}	0.95	2.99	3.924 (2)	168

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{20}N_4OS$
M_r	352.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	113
a, *b*, *c* (Å)	10.4024 (15), 17.797 (2), 10.2829 (14)
β (°)	112.908 (7)
V (Å^3)	1753.5 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.20 × 0.18 × 0.14
Data collection	
Diffractometer	Rigaku Saturn CCD area detector
Absorption correction	Multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min}, T_{max}	0.961, 0.973
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18273, 4199, 2965
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.659
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.099, 0.97
No. of reflections	4199
No. of parameters	233
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.33

Computer programs: *CrystalClear* and *CrystalStructure* (Rigaku/MSC, 2005), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

to the *bc* plane, which are in turn linked by a fourth C—H···π interaction (C2—H2···*Cg*1^{iv}) forming a three-dimensional network (Table 1 and Fig. 3).

Synthesis and crystallization

Benzaldehyde (2.0 mmol) and 3-(4-amino-5-thioxo-3-ethyl-4,5-dihydro-1*H*-1,2,4-triazol-1-yl)-3-(4-methoxyphenyl)-1-phenylpropan-1-one (2.0 mmol) were refluxed in ethanol. The reaction progress was monitored by TLC. The resulting precipitate was filtered off, washed with cold ethanol, dried and purified to give the target product as a colourless solid in

85% yield. Crystals of the title compound suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform-ethanol (1:1).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2017). **2**, x162001 [https://doi.org/10.1107/S2414314616020010]

3-(4-Amino-3-ethyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-yl)-1,3-diphenylpropan-1-one

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3-(4-Amino-3-ethyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-yl)-1,3-diphenylpropan-1-one

Crystal data

$C_{19}H_{20}N_4OS$
M_r = 352.45
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.4024 (15) Å
b = 17.797 (2) Å
c = 10.2829 (14) Å
β = 112.908 (7)°
V = 1753.5 (4) Å^3
Z = 4
$F(000)$ = 744
D_x = 1.335 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6033 reflections
θ = 2.1–28.0°
μ = 0.20 mm^{-1}
T = 113 K
Prism, colorless
0.20 × 0.18 × 0.14 mm

Data collection

Rigaku Saturn CCD area detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.22 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)
T_{min} = 0.961, T_{max} = 0.973
18273 measured reflections
4199 independent reflections
2965 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 27.9°, θ_{min} = 2.1°
h = −13→13
k = −23→23
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.099
S = 0.97
4199 reflections
233 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.12424 (4)	0.20783 (2)	0.57027 (4)	0.02353 (13)
O1	0.29173 (11)	0.38597 (6)	0.39457 (12)	0.0258 (3)
N1	0.09813 (13)	0.35970 (7)	0.53152 (13)	0.0191 (3)
N2	0.14589 (13)	0.42626 (7)	0.60247 (14)	0.0215 (3)
N3	0.22893 (13)	0.32917 (7)	0.74060 (13)	0.0178 (3)
N4	0.31459 (14)	0.28805 (8)	0.85958 (15)	0.0225 (3)
H4A	0.3163 (17)	0.2402 (11)	0.8276 (19)	0.034*
H4B	0.2634 (19)	0.2836 (10)	0.914 (2)	0.034*
C1	0.39700 (16)	0.51862 (10)	0.33197 (17)	0.0236 (4)
H1	0.4613	0.4798	0.3783	0.028*
C2	0.44514 (17)	0.58554 (10)	0.30018 (18)	0.0274 (4)
H2	0.5426	0.5931	0.3277	0.033*
C3	0.35281 (18)	0.64159 (10)	0.22870 (19)	0.0300 (4)
H3	0.3865	0.6873	0.2058	0.036*
C4	0.21096 (18)	0.63089 (10)	0.19061 (19)	0.0293 (4)
H4	0.1470	0.6690	0.1404	0.035*
C5	0.16246 (17)	0.56481 (9)	0.22558 (18)	0.0243 (4)
H5	0.0652	0.5583	0.2010	0.029*
C6	0.25453 (15)	0.50757 (9)	0.29653 (16)	0.0203 (4)
C7	0.20880 (16)	0.43628 (9)	0.33978 (16)	0.0207 (4)
C8	0.05603 (16)	0.42832 (9)	0.31349 (17)	0.0212 (4)
H8A	0.0012	0.4275	0.2103	0.025*
H8B	0.0267	0.4731	0.3522	0.025*
C9	0.02112 (16)	0.35844 (9)	0.37787 (16)	0.0206 (4)
H9	0.0539	0.3139	0.3401	0.025*
C10	−0.13554 (16)	0.35072 (9)	0.33486 (17)	0.0196 (4)
C11	−0.19972 (17)	0.36120 (9)	0.42884 (18)	0.0248 (4)
H11	−0.1447	0.3715	0.5253	0.030*
C12	−0.34399 (17)	0.35674 (10)	0.3831 (2)	0.0289 (4)
H12	−0.3871	0.3634	0.4485	0.035*
C13	−0.42453 (17)	0.34270 (10)	0.2433 (2)	0.0290 (4)
H13	−0.5233	0.3411	0.2116	0.035*
C14	−0.36106 (17)	0.33084 (10)	0.14891 (19)	0.0275 (4)
H14	−0.4162	0.3202	0.0527	0.033*
C15	−0.21747 (16)	0.33454 (9)	0.19507 (18)	0.0247 (4)

H15	−0.1743	0.3259	0.1302	0.030*
C16	0.14737 (15)	0.29898 (9)	0.61269 (17)	0.0182 (4)
C17	0.22746 (16)	0.40574 (9)	0.72990 (16)	0.0188 (4)
C18	0.31117 (17)	0.45732 (9)	0.84495 (17)	0.0237 (4)
H18A	0.3114	0.5075	0.8036	0.028*
H18B	0.4088	0.4391	0.8846	0.028*
C19	0.26191 (17)	0.46595 (10)	0.96465 (17)	0.0251 (4)
H19A	0.1654	0.4841	0.9272	0.038*
H19B	0.3218	0.5021	1.0336	0.038*
H19C	0.2666	0.4172	1.0107	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0290 (2)	0.0178 (2)	0.0220 (2)	−0.00271 (18)	0.00791 (19)	−0.00223 (17)
O1	0.0233 (6)	0.0228 (7)	0.0258 (7)	0.0049 (5)	0.0036 (5)	−0.0002 (5)
N1	0.0200 (7)	0.0175 (7)	0.0163 (7)	0.0003 (6)	0.0033 (6)	−0.0006 (6)
N2	0.0261 (8)	0.0174 (8)	0.0194 (7)	−0.0013 (6)	0.0071 (6)	−0.0029 (6)
N3	0.0174 (7)	0.0180 (7)	0.0151 (7)	−0.0009 (6)	0.0033 (6)	−0.0003 (6)
N4	0.0225 (8)	0.0219 (8)	0.0180 (8)	0.0026 (6)	0.0024 (6)	0.0023 (6)
C1	0.0221 (8)	0.0313 (10)	0.0166 (8)	0.0037 (7)	0.0067 (7)	−0.0026 (7)
C2	0.0227 (9)	0.0377 (11)	0.0225 (9)	−0.0058 (8)	0.0095 (8)	−0.0080 (8)
C3	0.0379 (11)	0.0257 (10)	0.0296 (10)	−0.0080 (8)	0.0164 (9)	−0.0049 (8)
C4	0.0342 (10)	0.0232 (10)	0.0287 (10)	0.0038 (8)	0.0102 (9)	0.0026 (8)
C5	0.0214 (9)	0.0264 (10)	0.0245 (9)	0.0004 (7)	0.0082 (8)	−0.0015 (7)
C6	0.0212 (8)	0.0227 (9)	0.0160 (8)	0.0009 (7)	0.0060 (7)	−0.0031 (7)
C7	0.0229 (9)	0.0235 (10)	0.0138 (8)	0.0007 (7)	0.0050 (7)	−0.0050 (7)
C8	0.0205 (8)	0.0215 (9)	0.0190 (8)	0.0025 (7)	0.0050 (7)	0.0010 (7)
C9	0.0224 (8)	0.0225 (9)	0.0138 (8)	0.0023 (7)	0.0034 (7)	−0.0008 (7)
C10	0.0215 (8)	0.0167 (9)	0.0190 (8)	0.0011 (7)	0.0059 (7)	0.0015 (7)
C11	0.0273 (9)	0.0249 (10)	0.0213 (9)	0.0024 (7)	0.0086 (8)	−0.0029 (7)
C12	0.0299 (10)	0.0260 (10)	0.0342 (11)	0.0054 (8)	0.0163 (9)	0.0004 (8)
C13	0.0208 (9)	0.0238 (10)	0.0389 (11)	0.0002 (7)	0.0080 (9)	0.0048 (8)
C14	0.0263 (9)	0.0250 (10)	0.0258 (10)	−0.0048 (8)	0.0043 (8)	0.0012 (8)
C15	0.0270 (9)	0.0241 (10)	0.0224 (9)	−0.0021 (7)	0.0090 (8)	0.0002 (7)
C16	0.0152 (8)	0.0207 (9)	0.0179 (8)	−0.0002 (6)	0.0055 (7)	−0.0005 (7)
C17	0.0200 (8)	0.0192 (9)	0.0175 (8)	−0.0012 (7)	0.0076 (7)	−0.0008 (7)
C18	0.0269 (9)	0.0208 (9)	0.0218 (9)	−0.0046 (7)	0.0076 (8)	−0.0039 (7)
C19	0.0274 (9)	0.0254 (10)	0.0196 (9)	−0.0017 (7)	0.0059 (8)	−0.0042 (7)

Geometric parameters (Å, º)

S1—C16	1.6727 (16)	C8—C9	1.518 (2)
O1—C7	1.2185 (18)	C8—H8A	0.9900
N1—C16	1.3394 (19)	C8—H8B	0.9900
N1—N2	1.3784 (17)	C9—C10	1.520 (2)
N1—C9	1.4674 (19)	C9—H9	1.0000
N2—C17	1.3057 (19)	C10—C11	1.385 (2)

N3—C17	1.367 (2)	C10—C15	1.386 (2)
N3—C16	1.3674 (19)	C11—C12	1.389 (2)
N3—N4	1.4063 (18)	C11—H11	0.9500
N4—H4A	0.916 (19)	C12—C13	1.376 (2)
N4—H4B	0.91 (2)	C12—H12	0.9500
C1—C2	1.380 (2)	C13—C14	1.386 (2)
C1—C6	1.396 (2)	C13—H13	0.9500
C1—H1	0.9500	C14—C15	1.382 (2)
C2—C3	1.381 (2)	C14—H14	0.9500
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.385 (2)	C17—C18	1.483 (2)
C3—H3	0.9500	C18—C19	1.514 (2)
C4—C5	1.381 (2)	C18—H18A	0.9900
C4—H4	0.9500	C18—H18B	0.9900
C5—C6	1.394 (2)	C19—H19A	0.9800
C5—H5	0.9500	C19—H19B	0.9800
C6—C7	1.483 (2)	C19—H19C	0.9800
C7—C8	1.511 (2)		

C16—N1—N2	113.07 (12)	N1—C9—H9	107.7
C16—N1—C9	125.08 (13)	C8—C9—H9	107.7
N2—N1—C9	121.09 (12)	C10—C9—H9	107.7
C17—N2—N1	104.50 (13)	C11—C10—C15	118.87 (15)
C17—N3—C16	109.34 (13)	C11—C10—C9	122.59 (14)
C17—N3—N4	124.91 (13)	C15—C10—C9	118.52 (14)
C16—N3—N4	125.31 (13)	C10—C11—C12	120.46 (16)
N3—N4—H4A	105.5 (11)	C10—C11—H11	119.8
N3—N4—H4B	104.8 (11)	C12—C11—H11	119.8
H4A—N4—H4B	103.7 (15)	C13—C12—C11	120.14 (17)
C2—C1—C6	120.42 (15)	C13—C12—H12	119.9
C2—C1—H1	119.8	C11—C12—H12	119.9
C6—C1—H1	119.8	C12—C13—C14	119.80 (15)
C1—C2—C3	120.54 (16)	C12—C13—H13	120.1
C1—C2—H2	119.7	C14—C13—H13	120.1
C3—C2—H2	119.7	C15—C14—C13	119.88 (16)
C2—C3—C4	119.66 (17)	C15—C14—H14	120.1
C2—C3—H3	120.2	C13—C14—H14	120.1
C4—C3—H3	120.2	C14—C15—C10	120.81 (16)
C5—C4—C3	120.03 (16)	C14—C15—H15	119.6
C5—C4—H4	120.0	C10—C15—H15	119.6
C3—C4—H4	120.0	N1—C16—N3	103.06 (13)
C4—C5—C6	120.82 (16)	N1—C16—S1	129.69 (12)
C4—C5—H5	119.6	N3—C16—S1	127.19 (12)
C6—C5—H5	119.6	N2—C17—N3	110.01 (13)
C5—C6—C1	118.49 (15)	N2—C17—C18	125.30 (15)
C5—C6—C7	123.16 (14)	N3—C17—C18	124.64 (14)
C1—C6—C7	118.33 (14)	C17—C18—C19	115.59 (14)
O1—C7—C6	121.02 (15)	C17—C18—H18A	108.4

O1—C7—C8	121.32 (15)	C19—C18—H18A	108.4
C6—C7—C8	117.67 (13)	C17—C18—H18B	108.4
C7—C8—C9	114.34 (13)	C19—C18—H18B	108.4
C7—C8—H8A	108.7	H18A—C18—H18B	107.4
C9—C8—H8A	108.7	C18—C19—H19A	109.5
C7—C8—H8B	108.7	C18—C19—H19B	109.5
C9—C8—H8B	108.7	H19A—C19—H19B	109.5
H8A—C8—H8B	107.6	C18—C19—H19C	109.5
N1—C9—C8	109.51 (13)	H19A—C19—H19C	109.5
N1—C9—C10	112.89 (13)	H19B—C19—H19C	109.5
C8—C9—C10	111.02 (12)		

C16—N1—N2—C17	0.60 (18)	C8—C9—C10—C15	68.66 (19)
C9—N1—N2—C17	−169.86 (13)	C15—C10—C11—C12	−1.0 (2)
C6—C1—C2—C3	−2.2 (3)	C9—C10—C11—C12	177.20 (16)
C1—C2—C3—C4	1.0 (3)	C10—C11—C12—C13	−0.8 (3)
C2—C3—C4—C5	0.8 (3)	C11—C12—C13—C14	1.9 (3)
C3—C4—C5—C6	−1.4 (3)	C12—C13—C14—C15	−1.2 (3)
C4—C5—C6—C1	0.2 (2)	C13—C14—C15—C10	−0.6 (3)
C4—C5—C6—C7	178.47 (16)	C11—C10—C15—C14	1.7 (2)
C2—C1—C6—C5	1.5 (2)	C9—C10—C15—C14	−176.58 (15)
C2—C1—C6—C7	−176.78 (15)	N2—N1—C16—N3	0.44 (17)
C5—C6—C7—O1	175.84 (15)	C9—N1—C16—N3	170.45 (13)
C1—C6—C7—O1	−5.9 (2)	N2—N1—C16—S1	−176.68 (12)
C5—C6—C7—C8	−4.1 (2)	C9—N1—C16—S1	−6.7 (2)
C1—C6—C7—C8	174.09 (14)	C17—N3—C16—N1	−1.28 (17)
O1—C7—C8—C9	7.7 (2)	N4—N3—C16—N1	−173.98 (14)
C6—C7—C8—C9	−172.31 (14)	C17—N3—C16—S1	175.93 (12)
C16—N1—C9—C8	−146.40 (15)	N4—N3—C16—S1	3.2 (2)
N2—N1—C9—C8	22.87 (19)	N1—N2—C17—N3	−1.40 (17)
C16—N1—C9—C10	89.36 (18)	N1—N2—C17—C18	176.23 (15)
N2—N1—C9—C10	−101.38 (16)	C16—N3—C17—N2	1.76 (18)
C7—C8—C9—N1	60.17 (17)	N4—N3—C17—N2	174.50 (14)
C7—C8—C9—C10	−174.50 (13)	C16—N3—C17—C18	−175.88 (15)
N1—C9—C10—C11	13.9 (2)	N4—N3—C17—C18	−3.1 (2)
C8—C9—C10—C11	−109.55 (17)	N2—C17—C18—C19	109.40 (19)
N1—C9—C10—C15	−167.92 (14)	N3—C17—C18—C19	−73.3 (2)

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg3 are the centroids of the N1/N2/N3/C17/C18, C1–C6 and C10–C15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O1^{i}	0.92 (2)	2.39 (2)	3.138 (2)	139 (2)
N4—H4*B*···S1^{i}	0.91 (2)	2.55 (2)	3.458 (2)	172 (2)
C19—H19*C*···S1^{i}	0.98	2.87	3.743 (2)	149
C12—H12···*Cg*2^{ii}	0.95	2.97	3.711 (2)	136
C18—H18*A*···*Cg*3^{ii}	0.99	2.75	3.7275 (18)	170

C19—H19*B*···*Cg*2^{iii}	0.98	2.75	3.5032 (19)	134
C2—H2···*Cg*1^{iv}	0.95	2.99	3.924 (2)	168

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