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ISSN 2414-3146

4,4-Diphenyl-1-propyl-2-propylsulfanyl-4,5-dihydro-1*H*-imidazol-5-one

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Received 25 June 2018
Accepted 28 June 2018

Edited by J. Simpson, University of Otago, New Zealand

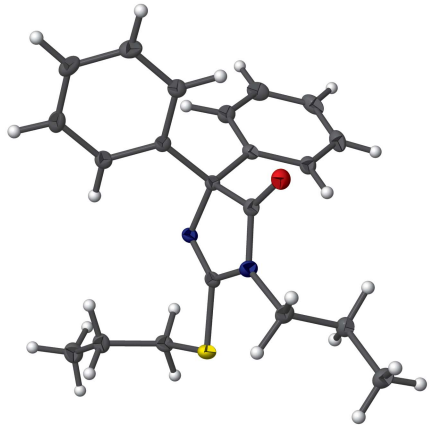
Keywords: crystal structure; dihydroimidazolone; hydrogen bond; C—H···π(ring) interaction.

CCDC reference: 1852189

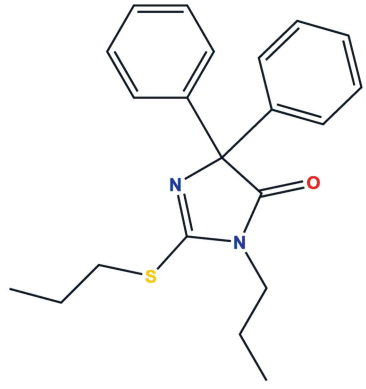
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{21}H_{24}N_2OS$, the five-membered ring is planar with an r.m.s. deviation of 0.0142 Å. The phenyl rings are inclined to the plane of the dihydroimidazolone ring by 60.81 (6) and 79.23 (6)°. In the crystal, inversion dimers are formed by a C—H···O hydrogen bond and a C—H···π(ring) interaction. Additional C—H···O hydrogen bonds and C—H···π(ring) interactions connect these dimers into chains along the *c*-axis direction.

3D view



Chemical scheme



Structure description

Over the past thirty years, imidazolone derivatives of hydantoin or thiohydantoin have been the focus of interest for the synthetic and pharmaceutical industries because of their biological properties. As part of our ongoing studies of 4,4- and 5,5-diphenylimidazolidine-2,4-dione and 5,5-diphenyl-2-thioxoimidazolidin-4-one derivatives (Ramli, Akrad *et al.*, 2017; Ramli, Guerrab *et al.*, 2017; Akrad *et al.*, 2017; Guerrab *et al.*, 2017*a*,*b*), the title compound was prepared and its crystal structure is reported here.

In the title molecule (Fig. 1), the C10–C15 and C16–C21 benzene rings are inclined to the plane of the central five-membered ring by 60.81 (6) and 79.23 (6)°, respectively. In the crystal, C8—H8*A*···O1 hydrogen bonds and C9—H9*A*···*Cg*3 interactions, Table 1, form inversion dimers, which are connected into chains extending along the *c*-axis direction by C19—H19···O1 hydrogen bonds and C20—H20···*Cg*2 interactions (Table 1 and Fig. 2).

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

*Cg*2 and *Cg*3 are the centroids of the C10–C15 and C16–C21 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···O1^{i}	1.005 (15)	2.607 (15)	3.5908 (14)	166.2 (11)
C9—H9*A*···*Cg*3^{i}	0.973 (16)	2.908 (15)	3.7370 (15)	143.8 (12)
C19—H19···O1^{ii}	0.955 (16)	2.596 (16)	3.4407 (15)	147.7 (12)
C20—H20···*Cg*2^{ii}	0.997 (16)	2.999 (17)	3.7390 (14)	131.9 (12)

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

Synthesis and crystallization

Thiohydantoin (0.7 g) was placed in a flask with K_2CO_3 (0.9 g, 0.0065 mmol) in absolute dimethylformamide (DMF), and two equivalents of propyl iodide were added. The solution was left stirring for 2 h at room temperature. The solvent was then removed after filtration of the base and the oil obtained was recrystallized from methanol solution to yield colourless block-shaped single crystals (Guerrab *et al.*, 2017*c*, 2018).

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{24}N_2OS$
M_r	352.48
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	14.898 (2), 14.878 (2), 8.4007 (13)
β (°)	96.780 (2)
V (Å^3)	1849.0 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.30 × 0.27 × 0.22
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.84, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35375, 5241, 4279
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.708
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.114, 1.07
No. of reflections	5241
No. of parameters	322
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.51, −0.19

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Funding information

JTM thanks Tulane University for support of the Tulane Crystallography Laboratory.

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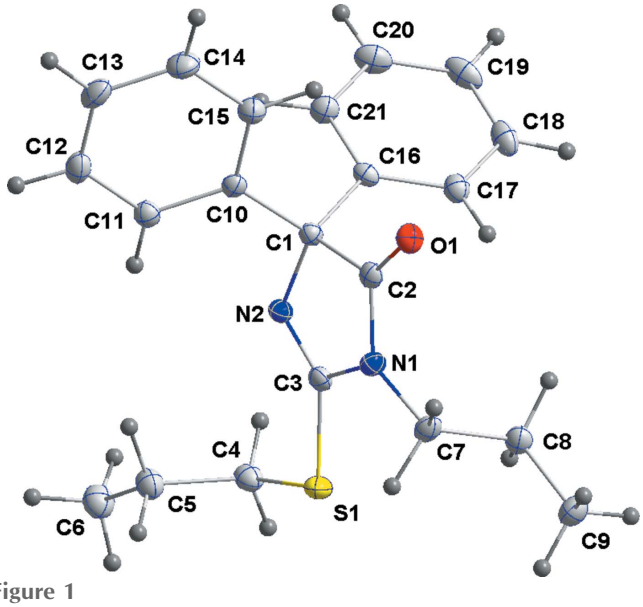

Figure 1
The title molecule with the atom-labelling scheme and 50% probability ellipsoids.

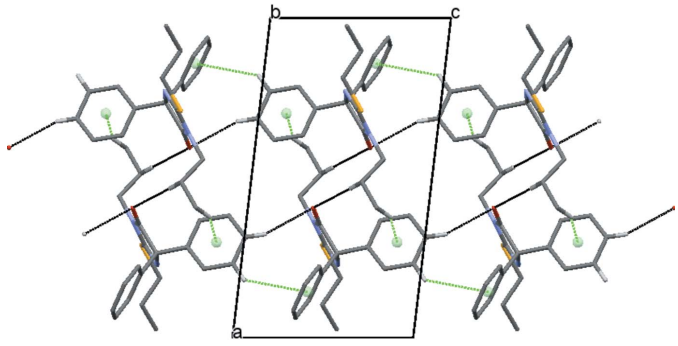

Figure 2
A portion of a chain of the title molecules viewed along the *b*-axis direction. C—H···O hydrogen bonds and C—H···π(ring) interactions are shown by black and green dashed lines, respectively.

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full crystallographic data

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Crystal data

$C_{21}H_{24}N_2OS$
M_r = 352.48
Monoclinic, $P2_1/c$
a = 14.898 (2) Å
b = 14.878 (2) Å
c = 8.4007 (13) Å
β = 96.780 (2)°
V = 1849.0 (5) Å^3
Z = 4
$F(000)$ = 752
D_x = 1.266 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9958 reflections
θ = 2.7–30.0°
μ = 0.19 mm^{-1}
T = 100 K
Block, colourless
0.30 × 0.27 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.84, T_{max} = 0.96
35375 measured reflections
5241 independent reflections
4279 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 30.2°, θ_{min} = 1.9°
h = −21→21
k = −20→20
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.07
5241 reflections
322 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0755P)^2 + 0.1235P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 20 sec/frame.

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	0.28969 (2)	0.21368 (2)	0.56491 (4)	0.02040 (10)
O1	0.40566 (5)	0.52459 (5)	0.63859 (9)	0.01851 (18)
N1	0.36245 (6)	0.37573 (6)	0.62527 (11)	0.01618 (19)
N2	0.22807 (6)	0.37922 (6)	0.46398 (11)	0.01469 (18)
C1	0.26378 (7)	0.47263 (7)	0.47678 (12)	0.0131 (2)
C2	0.35317 (7)	0.46531 (7)	0.59014 (12)	0.0146 (2)
C3	0.28811 (7)	0.33033 (7)	0.54480 (12)	0.0153 (2)
C4	0.18745 (8)	0.18173 (8)	0.44041 (14)	0.0203 (2)
H4A	0.1989 (11)	0.1189 (11)	0.404 (2)	0.037 (4)*
H4B	0.1770 (12)	0.2204 (10)	0.342 (2)	0.038 (5)*
C5	0.10239 (8)	0.18493 (8)	0.52482 (15)	0.0217 (2)
H5A	0.1147 (10)	0.1580 (10)	0.6326 (19)	0.027 (4)*
H5B	0.0847 (10)	0.2504 (11)	0.5396 (17)	0.025 (3)*
C6	0.02608 (9)	0.13272 (9)	0.42926 (17)	0.0264 (3)
H6A	0.0410 (11)	0.0673 (11)	0.4339 (19)	0.038 (4)*
H6B	0.0169 (10)	0.1538 (10)	0.3164 (19)	0.030 (4)*
H6C	−0.0330 (11)	0.1417 (10)	0.4759 (18)	0.032 (4)*
C7	0.44183 (7)	0.33597 (8)	0.71897 (13)	0.0181 (2)
H7A	0.4663 (10)	0.3808 (10)	0.7962 (18)	0.022 (3)*
H7B	0.4168 (11)	0.2821 (9)	0.7763 (18)	0.030 (4)*
C8	0.51335 (8)	0.30657 (8)	0.61454 (14)	0.0189 (2)
H8A	0.5325 (10)	0.3615 (10)	0.5576 (18)	0.025 (4)*
H8B	0.4848 (9)	0.2635 (9)	0.5348 (16)	0.018 (3)*
C9	0.59323 (8)	0.26092 (9)	0.71236 (16)	0.0232 (2)
H9A	0.6227 (10)	0.3009 (10)	0.7940 (19)	0.027 (4)*
H9B	0.6360 (11)	0.2419 (10)	0.6369 (19)	0.031 (4)*
H9C	0.5719 (12)	0.2071 (11)	0.765 (2)	0.038 (4)*
C10	0.19982 (7)	0.53663 (7)	0.54917 (12)	0.0139 (2)
C11	0.11947 (7)	0.50725 (7)	0.59961 (13)	0.0171 (2)
H11	0.1028 (9)	0.4450 (10)	0.5864 (17)	0.022 (3)*
C12	0.06233 (8)	0.56794 (8)	0.66487 (14)	0.0211 (2)
H12	0.0049 (10)	0.5497 (10)	0.7005 (17)	0.024 (4)*
C13	0.08580 (8)	0.65759 (8)	0.68128 (14)	0.0228 (2)
H13	0.0461 (10)	0.6994 (10)	0.7219 (18)	0.025 (4)*
C14	0.16667 (9)	0.68758 (8)	0.63317 (15)	0.0233 (2)
H14	0.1854 (10)	0.7476 (10)	0.6499 (17)	0.023 (3)*

C15	0.22333 (8)	0.62766 (7)	0.56654 (14)	0.0190 (2)
H15	0.2804 (10)	0.6485 (10)	0.5290 (17)	0.025 (4)*
C16	0.28335 (7)	0.50095 (7)	0.30928 (12)	0.0142 (2)
C17	0.36676 (8)	0.48304 (7)	0.25711 (14)	0.0181 (2)
H17	0.4160 (10)	0.4566 (10)	0.3323 (17)	0.027 (4)*
C18	0.38154 (9)	0.50281 (8)	0.10041 (14)	0.0228 (3)
H18	0.4394 (11)	0.4880 (11)	0.0687 (19)	0.038 (4)*
C19	0.31434 (9)	0.54172 (8)	−0.00507 (14)	0.0245 (3)
H19	0.3236 (10)	0.5579 (10)	−0.1119 (19)	0.033 (4)*
C20	0.23084 (9)	0.55984 (8)	0.04611 (14)	0.0236 (2)
H20	0.1804 (11)	0.5876 (11)	−0.026 (2)	0.035 (4)*
C21	0.21515 (8)	0.53930 (8)	0.20199 (13)	0.0189 (2)
H21	0.1559 (10)	0.5492 (9)	0.2374 (17)	0.026 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02010 (16)	0.01411 (15)	0.02723 (17)	0.00107 (9)	0.00377 (12)	0.00478 (10)
O1	0.0172 (4)	0.0200 (4)	0.0179 (4)	−0.0018 (3)	0.0004 (3)	−0.0023 (3)
N1	0.0156 (4)	0.0167 (4)	0.0156 (4)	0.0016 (3)	−0.0007 (3)	0.0024 (3)
N2	0.0165 (4)	0.0126 (4)	0.0154 (4)	−0.0007 (3)	0.0036 (3)	0.0000 (3)
C1	0.0130 (5)	0.0136 (5)	0.0125 (5)	−0.0004 (3)	0.0011 (4)	0.0006 (3)
C2	0.0155 (5)	0.0179 (5)	0.0108 (5)	0.0010 (4)	0.0030 (4)	0.0000 (4)
C3	0.0168 (5)	0.0155 (5)	0.0143 (5)	−0.0004 (4)	0.0048 (4)	0.0017 (4)
C4	0.0239 (6)	0.0158 (5)	0.0219 (6)	−0.0021 (4)	0.0061 (4)	−0.0009 (4)
C5	0.0214 (6)	0.0221 (6)	0.0225 (6)	−0.0015 (4)	0.0064 (5)	−0.0018 (5)
C6	0.0243 (6)	0.0254 (6)	0.0296 (7)	−0.0039 (5)	0.0038 (5)	−0.0027 (5)
C7	0.0171 (5)	0.0219 (5)	0.0149 (5)	0.0044 (4)	0.0002 (4)	0.0029 (4)
C8	0.0180 (5)	0.0226 (5)	0.0159 (5)	0.0016 (4)	0.0018 (4)	0.0016 (4)
C9	0.0205 (6)	0.0237 (6)	0.0248 (6)	0.0053 (5)	0.0007 (5)	0.0013 (5)
C10	0.0146 (5)	0.0158 (5)	0.0110 (5)	0.0015 (4)	0.0005 (4)	0.0011 (4)
C11	0.0175 (5)	0.0184 (5)	0.0155 (5)	−0.0003 (4)	0.0020 (4)	0.0007 (4)
C12	0.0173 (5)	0.0277 (6)	0.0187 (6)	0.0029 (4)	0.0044 (4)	0.0015 (4)
C13	0.0242 (6)	0.0250 (6)	0.0196 (6)	0.0103 (5)	0.0041 (5)	0.0003 (4)
C14	0.0281 (6)	0.0160 (5)	0.0258 (6)	0.0030 (4)	0.0036 (5)	−0.0014 (4)
C15	0.0193 (5)	0.0174 (5)	0.0206 (6)	−0.0001 (4)	0.0031 (4)	0.0001 (4)
C16	0.0175 (5)	0.0129 (5)	0.0122 (5)	−0.0025 (4)	0.0023 (4)	−0.0003 (4)
C17	0.0180 (5)	0.0182 (5)	0.0186 (5)	−0.0014 (4)	0.0040 (4)	−0.0021 (4)
C18	0.0252 (6)	0.0240 (6)	0.0209 (6)	−0.0065 (5)	0.0105 (5)	−0.0063 (4)
C19	0.0390 (7)	0.0230 (6)	0.0125 (5)	−0.0094 (5)	0.0068 (5)	−0.0025 (4)
C20	0.0311 (6)	0.0238 (6)	0.0146 (5)	−0.0026 (5)	−0.0024 (5)	0.0012 (4)
C21	0.0192 (5)	0.0211 (5)	0.0160 (5)	0.0006 (4)	0.0006 (4)	0.0001 (4)

Geometric parameters (Å, º)

S1—C3	1.7436 (11)	C9—H9A	0.973 (16)
S1—C4	1.8066 (13)	C9—H9B	0.991 (16)
O1—C2	1.2165 (13)	C9—H9C	0.987 (16)

N1—C2	1.3686 (14)	C10—C11	1.3867 (15)
N1—C3	1.4012 (14)	C10—C15	1.4022 (15)
N1—C7	1.4657 (14)	C11—C12	1.3967 (15)
N2—C3	1.2832 (14)	C11—H11	0.961 (15)
N2—C1	1.4874 (13)	C12—C13	1.3816 (18)
C1—C10	1.5236 (14)	C12—H12	0.977 (14)
C1—C16	1.5295 (14)	C13—C14	1.3889 (18)
C1—C2	1.5469 (15)	C13—H13	0.949 (15)
C4—C5	1.5242 (16)	C14—C15	1.3900 (16)
C4—H4A	1.003 (17)	C14—H14	0.941 (15)
C4—H4B	1.002 (17)	C15—H15	0.991 (14)
C5—C6	1.5248 (18)	C16—C17	1.3914 (15)
C5—H5A	0.987 (15)	C16—C21	1.3978 (15)
C5—H5B	1.020 (16)	C17—C18	1.3915 (16)
C6—H6A	0.997 (17)	C17—H17	0.992 (15)
C6—H6B	0.993 (16)	C18—C19	1.3832 (19)
C6—H6C	1.014 (16)	C18—H18	0.958 (16)
C7—C8	1.5222 (15)	C19—C20	1.3897 (18)
C7—H7A	0.971 (15)	C19—H19	0.955 (16)
C7—H7B	1.028 (15)	C20—C21	1.3911 (16)
C8—C9	1.5238 (16)	C20—H20	0.997 (16)
C8—H8A	1.005 (15)	C21—H21	0.976 (15)
C8—H8B	0.987 (14)		

C3—S1—C4	101.83 (5)	C9—C8—H8B	108.9 (8)
C2—N1—C3	108.15 (9)	H8A—C8—H8B	109.2 (11)
C2—N1—C7	124.29 (9)	C8—C9—H9A	111.5 (9)
C3—N1—C7	127.32 (9)	C8—C9—H9B	107.6 (9)
C3—N2—C1	105.69 (9)	H9A—C9—H9B	110.8 (13)
N2—C1—C10	112.18 (8)	C8—C9—H9C	109.4 (10)
N2—C1—C16	107.23 (8)	H9A—C9—H9C	108.7 (13)
C10—C1—C16	113.03 (8)	H9B—C9—H9C	108.8 (13)
N2—C1—C2	104.68 (8)	C11—C10—C15	119.12 (10)
C10—C1—C2	109.38 (8)	C11—C10—C1	121.87 (9)
C16—C1—C2	110.00 (8)	C15—C10—C1	119.00 (9)
O1—C2—N1	126.11 (10)	C10—C11—C12	120.28 (10)
O1—C2—C1	128.88 (10)	C10—C11—H11	119.3 (8)
N1—C2—C1	105.01 (8)	C12—C11—H11	120.4 (8)
N2—C3—N1	116.35 (10)	C13—C12—C11	120.30 (11)
N2—C3—S1	128.03 (8)	C13—C12—H12	117.3 (8)
N1—C3—S1	115.61 (8)	C11—C12—H12	122.4 (8)
C5—C4—S1	114.39 (8)	C12—C13—C14	119.94 (11)
C5—C4—H4A	110.5 (9)	C12—C13—H13	120.5 (9)
S1—C4—H4A	105.0 (9)	C14—C13—H13	119.6 (9)
C5—C4—H4B	107.9 (10)	C13—C14—C15	120.01 (11)
S1—C4—H4B	111.3 (10)	C13—C14—H14	120.9 (8)
H4A—C4—H4B	107.6 (13)	C15—C14—H14	119.0 (9)
C4—C5—C6	110.39 (10)	C14—C15—C10	120.34 (11)

C4—C5—H5A	109.8 (8)	C14—C15—H15	120.8 (8)
C6—C5—H5A	108.8 (9)	C10—C15—H15	118.8 (8)
C4—C5—H5B	109.1 (8)	C17—C16—C21	118.90 (10)
C6—C5—H5B	111.3 (8)	C17—C16—C1	120.76 (9)
H5A—C5—H5B	107.3 (12)	C21—C16—C1	120.18 (9)
C5—C6—H6A	109.1 (9)	C16—C17—C18	120.30 (11)
C5—C6—H6B	110.6 (9)	C16—C17—H17	119.8 (8)
H6A—C6—H6B	110.6 (13)	C18—C17—H17	119.9 (8)
C5—C6—H6C	110.9 (9)	C19—C18—C17	120.74 (11)
H6A—C6—H6C	108.2 (12)	C19—C18—H18	121.7 (10)
H6B—C6—H6C	107.4 (12)	C17—C18—H18	117.5 (10)
N1—C7—C8	112.44 (9)	C18—C19—C20	119.32 (11)
N1—C7—H7A	107.3 (9)	C18—C19—H19	122.3 (9)
C8—C7—H7A	110.4 (9)	C20—C19—H19	118.4 (9)
N1—C7—H7B	104.6 (9)	C19—C20—C21	120.30 (11)
C8—C7—H7B	111.3 (8)	C19—C20—H20	121.9 (9)
H7A—C7—H7B	110.6 (12)	C21—C20—H20	117.8 (9)
C7—C8—C9	111.87 (9)	C20—C21—C16	120.44 (11)
C7—C8—H8A	107.4 (8)	C20—C21—H21	120.8 (9)
C9—C8—H8A	111.8 (9)	C16—C21—H21	118.7 (9)
C7—C8—H8B	107.6 (8)		

C3—N2—C1—C10	−121.87 (9)	C16—C1—C10—C11	123.08 (10)
C3—N2—C1—C16	113.47 (9)	C2—C1—C10—C11	−114.01 (11)
C3—N2—C1—C2	−3.36 (10)	N2—C1—C10—C15	−178.90 (9)
C3—N1—C2—O1	−179.50 (10)	C16—C1—C10—C15	−57.51 (13)
C7—N1—C2—O1	−4.77 (17)	C2—C1—C10—C15	65.41 (12)
C3—N1—C2—C1	−0.08 (10)	C15—C10—C11—C12	0.83 (16)
C7—N1—C2—C1	174.66 (9)	C1—C10—C11—C12	−179.76 (10)
N2—C1—C2—O1	−178.56 (10)	C10—C11—C12—C13	−0.67 (17)
C10—C1—C2—O1	−58.17 (13)	C11—C12—C13—C14	−0.19 (18)
C16—C1—C2—O1	66.53 (13)	C12—C13—C14—C15	0.89 (18)
N2—C1—C2—N1	2.04 (10)	C13—C14—C15—C10	−0.73 (18)
C10—C1—C2—N1	122.43 (9)	C11—C10—C15—C14	−0.13 (17)
C16—C1—C2—N1	−112.87 (9)	C1—C10—C15—C14	−179.56 (10)
C1—N2—C3—N1	3.68 (12)	N2—C1—C16—C17	−88.04 (11)
C1—N2—C3—S1	−175.29 (8)	C10—C1—C16—C17	147.81 (10)
C2—N1—C3—N2	−2.40 (12)	C2—C1—C16—C17	25.24 (13)
C7—N1—C3—N2	−176.93 (10)	N2—C1—C16—C21	87.17 (11)
C2—N1—C3—S1	176.70 (7)	C10—C1—C16—C21	−36.98 (13)
C7—N1—C3—S1	2.17 (14)	C2—C1—C16—C21	−159.55 (9)
C4—S1—C3—N2	1.13 (11)	C21—C16—C17—C18	−0.24 (16)
C4—S1—C3—N1	−177.84 (8)	C1—C16—C17—C18	175.03 (10)
C3—S1—C4—C5	−85.29 (9)	C16—C17—C18—C19	1.00 (17)
S1—C4—C5—C6	−163.91 (9)	C17—C18—C19—C20	−0.98 (17)
C2—N1—C7—C8	−90.02 (12)	C18—C19—C20—C21	0.20 (18)
C3—N1—C7—C8	83.69 (13)	C19—C20—C21—C16	0.55 (18)
N1—C7—C8—C9	−177.00 (10)	C17—C16—C21—C20	−0.53 (16)

N2—C1—C10—C11	1.68 (14)	C1—C16—C21—C20	−175.83 (10)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the C10–C15 and C16–C21 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···O1^{i}	1.005 (15)	2.607 (15)	3.5908 (14)	166.2 (11)
C9—H9*A*···*Cg*3^{i}	0.973 (16)	2.908 (15)	3.7370 (15)	143.8 (12)
C19—H19···O1^{ii}	0.955 (16)	2.596 (16)	3.4407 (15)	147.7 (12)
C20—H20···*Cg*2^{ii}	0.997 (16)	2.999 (17)	3.7390 (14)	131.9 (12)

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