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4-(3-Methyl-4,5-dihydro-1*H*-benzo[*g*]-indazol-1-yl)benzenesulfonamide

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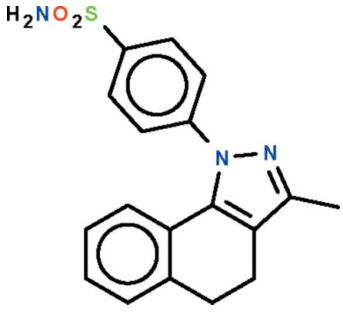
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.068; wR factor = 0.184; data-to-parameter ratio = 14.4.

In the title compound, $C_{18}H_{17}N_3O_2S$, the aromatic ring bearing the sulfamide unit is aligned at 61.65 (1)° with respect to the pyrrole ring; its amino group forms N—H···N and N—H···O hydrogen bonds to neighboring molecules, generating sheets in the *ac* plane.

Related literature

For the crystal structure of a pyrrole synthesized using 2-acetyltetralone as a reactant, see: Portilla *et al.* (2007).



Experimental

Crystal data

$C_{18}H_{17}N_3O_2S$
M_r = 339.41
Monoclinic, $P2_1/n$
a = 4.8838 (1) Å
b = 27.3894 (4) Å
c = 12.2399 (2) Å
β = 94.738 (1)°
V = 1631.67 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.600, T_{max} = 0.703
11808 measured reflections
3255 independent reflections
3166 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.184
S = 1.11
3255 reflections
226 parameters
14 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3^{i}	0.88 (1)	2.05 (1)	2.925 (4)	173 (5)
N1—H2···O2^{ii}	0.88 (1)	1.95 (2)	2.806 (4)	165 (4)

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5614).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Portilla, J., Quiroga, J., Cobo, J., Low, J. N. & Glidewell, C. (2007). *Acta Cryst.* C**63**, o458–o461.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, o2441 [doi:10.1107/S1600536811033186]

4-(3-Methyl-4,5-dihydro-1*H*-benzo[*g*]indazol-1-yl)benzenesulfonamide

Abdullah M. Asiri, Hassan M. Faidallah, Abdulrahman O. Al-Youbi, Mohamad S. I. T. Makki and Seik Weng Ng

S1. Comment

Among the wide range of compounds tested for medicinal properties, the compounds having the benzenesulfonamide unit that is grafted to pyrazoles, a class of chemotherapeutically active heterocycles, are expected to exhibit enhanced activity. The ketone, 2-acetyl-tetralone, condenses with a variety of primary amines such as 5-amino-3-methyl-1*H*-pyrazole and 5-amino-3-*tert*-butyl-1*H*-pyrazole (Portilla *et al.*, 2007). However, with 4-hydrazinobenzenesulfamide, the ketone yields a conventional Schiff base that cyclizes to form a pyrazole in a one-pot synthesis. In $C_{18}H_{17}N_3O_2S$ (Scheme I), the benzene and pyrrole rings that are fused to a central cyclohexadiene ring are somewhat twisted owing to the –CH_2CH_2– fragment of the cyclohexadiene ring (dihedral angle between benzene and pyrrole rings is 17.3 (2) °. The benzene ring bearing the sulfamide unit is aligned at 61.6 (1) ° with respect to the pyrrole ring; its amino group is hydrogen-bond donor to the acceptor sites of neighboring molecules to generating sheets in the *ac*-plane (Table 1).

S2. Experimental

2-Acetyl-1-tetralone (1.88 g, 10 mmol) in ethanol (50 ml) condensed with 4-hydrazinobenzenesulfonamide hydrochloride (2.2 g,10 mmol) by heating the reactants for 2 h. The mixture was allowed to cool, and the solid material was collected and recrystallized from ethanol.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.95 to 0.99 Å, U_{iso}(H) 1.2–1.5U_{eq}(C)] and were included in the refinement in the riding model approximation. The amino H atoms were located in a difference Fourier, and were refined isotropically with a distance restraint of N–H 0.88±0.01 Å.

As the two oxygen atoms showed somewhat elongated ellipsoids, their anisotropic temperature factors were restrained to be nearly isotropic.

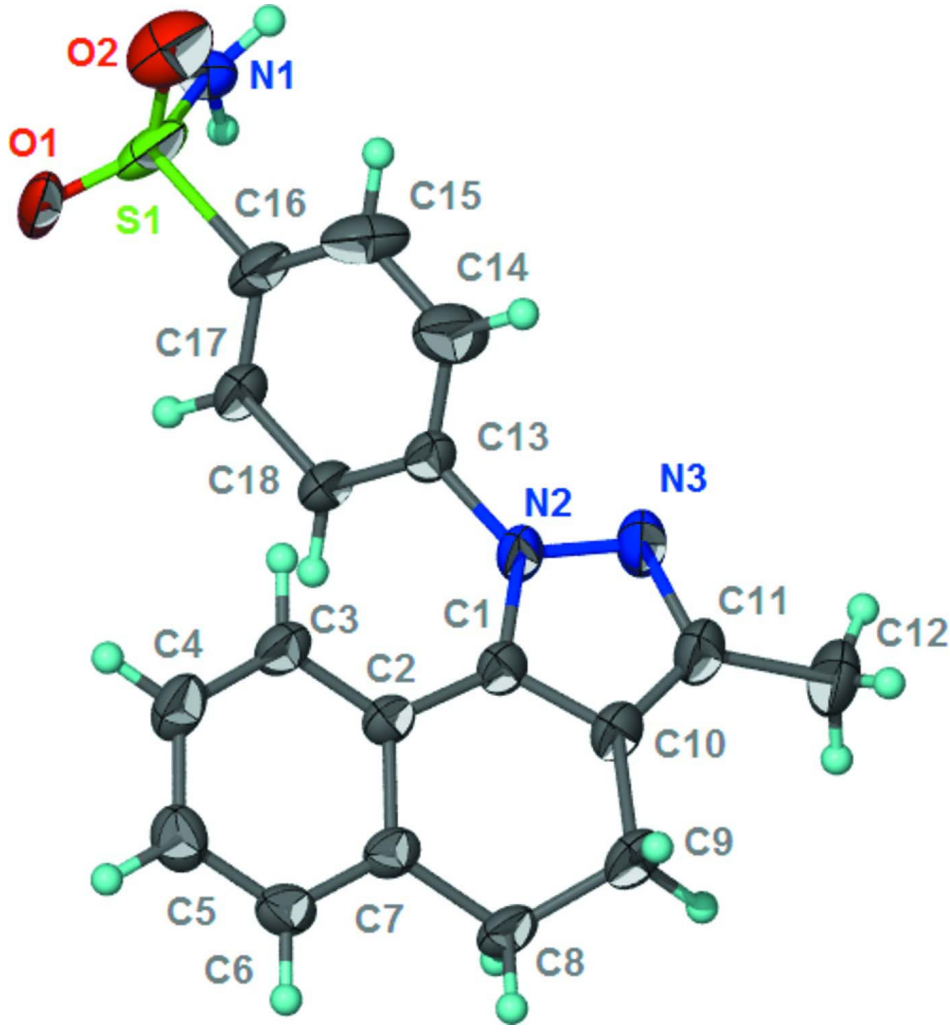


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{18}H_{17}N_3O_2S$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-(3-Methyl-4,5-dihydro-1*H*-benzo[*g*]indazol-1-yl)benzenesulfonamide

Crystal data

$C_{18}H_{17}N_3O_2S$
$M_r = 339.41$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 4.8838\ (1)$ Å
$b = 27.3894\ (4)$ Å
$c = 12.2399\ (2)$ Å
$\beta = 94.738\ (1)°$
$V = 1631.67\ (5)$ Å^3
$Z = 4$
$F(000) = 712$
$D_x = 1.382$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 7385 reflections
$\theta = 3.2–74.2°$
$\mu = 1.89$ mm^{-1}
$T = 100$ K
Prism, orange brown
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.600, T_{max} = 0.703
11808 measured reflections
3255 independent reflections
3166 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 74.4°, θ_{min} = 3.2°
h = −3→6
k = −34→33
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.184
S = 1.11
3255 reflections
226 parameters
14 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
$w = 1/[\sigma^2(F_o^2) + (0.0755P)^2 + 3.2939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.89421 (18)	0.67458 (3)	0.78209 (7)	0.0424 (3)
O1	0.8478 (8)	0.63001 (10)	0.8387 (2)	0.0718 (11)
O2	1.1649 (6)	0.69481 (19)	0.7792 (3)	0.0936 (15)
N1	0.7213 (6)	0.71611 (10)	0.8343 (2)	0.0316 (6)
N2	0.4538 (6)	0.64587 (9)	0.3184 (2)	0.0325 (6)
N3	0.2861 (7)	0.68173 (10)	0.2717 (2)	0.0430 (8)
C1	0.4586 (7)	0.60588 (11)	0.2510 (2)	0.0286 (6)
C2	0.6045 (6)	0.55949 (10)	0.2675 (2)	0.0260 (6)
C3	0.8268 (6)	0.55121 (11)	0.3446 (2)	0.0287 (6)
H3	0.8945	0.5771	0.3909	0.034*
C4	0.9494 (7)	0.50567 (12)	0.3544 (2)	0.0338 (7)
H4	1.1012	0.5004	0.4068	0.041*
C5	0.8501 (7)	0.46774 (12)	0.2875 (3)	0.0348 (7)
H5	0.9295	0.4361	0.2957	0.042*
C6	0.6338 (7)	0.47599 (11)	0.2082 (2)	0.0305 (7)
H6	0.5698	0.4500	0.1616	0.037*
C7	0.5095 (6)	0.52151 (11)	0.1959 (2)	0.0260 (6)
C8	0.2724 (7)	0.53032 (12)	0.1096 (2)	0.0312 (7)
H8A	0.0975	0.5235	0.1423	0.037*
H8B	0.2875	0.5070	0.0486	0.037*
C9	0.2622 (8)	0.58217 (12)	0.0634 (2)	0.0373 (8)
H9A	0.4125	0.5870	0.0149	0.045*
H9B	0.0850	0.5878	0.0199	0.045*
C10	0.2932 (7)	0.61727 (12)	0.1578 (2)	0.0340 (7)

C11	0.1879 (8)	0.66404 (13)	0.1747 (3)	0.0407 (8)
C12	−0.0164 (11)	0.69262 (15)	0.1018 (4)	0.0586 (12)
H12A	−0.0683	0.7222	0.1399	0.088*
H12B	−0.1802	0.6726	0.0836	0.088*
H12C	0.0660	0.7016	0.0343	0.088*
C13	0.5657 (7)	0.65231 (11)	0.4290 (2)	0.0293 (7)
C14	0.7437 (8)	0.69042 (14)	0.4540 (3)	0.0435 (9)
H14	0.7941	0.7118	0.3979	0.052*
C15	0.8491 (8)	0.69741 (14)	0.5616 (3)	0.0462 (9)
H15	0.9728	0.7235	0.5798	0.055*
C16	0.7714 (7)	0.66571 (12)	0.6426 (3)	0.0316 (7)
C17	0.5945 (7)	0.62796 (12)	0.6171 (3)	0.0344 (7)
H17	0.5436	0.6065	0.6729	0.041*
C18	0.4900 (7)	0.62110 (12)	0.5098 (3)	0.0333 (7)
H18	0.3664	0.5950	0.4917	0.040*
H1	0.756 (10)	0.7464 (7)	0.815 (4)	0.061 (14)*
H2	0.547 (3)	0.7076 (14)	0.829 (3)	0.041 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0376 (5)	0.0539 (6)	0.0321 (5)	0.0161 (4)	−0.0181 (3)	−0.0213 (4)
O1	0.134 (3)	0.0376 (14)	0.0361 (14)	0.0337 (17)	−0.0418 (17)	−0.0086 (11)
O2	0.0354 (16)	0.172 (4)	0.072 (2)	0.001 (2)	−0.0045 (15)	−0.070 (3)
N1	0.0401 (16)	0.0257 (13)	0.0280 (13)	−0.0022 (11)	−0.0041 (11)	−0.0051 (10)
N2	0.0532 (17)	0.0240 (12)	0.0185 (12)	0.0055 (11)	−0.0070 (11)	0.0000 (9)
N3	0.069 (2)	0.0290 (14)	0.0290 (15)	0.0111 (14)	−0.0105 (14)	0.0018 (11)
C1	0.0418 (17)	0.0252 (14)	0.0182 (13)	−0.0001 (12)	−0.0021 (12)	0.0003 (11)
C2	0.0346 (16)	0.0257 (14)	0.0173 (13)	−0.0009 (12)	−0.0006 (11)	−0.0018 (11)
C3	0.0326 (16)	0.0316 (15)	0.0210 (14)	0.0013 (12)	−0.0039 (11)	−0.0035 (11)
C4	0.0394 (18)	0.0405 (17)	0.0208 (14)	0.0080 (14)	−0.0018 (12)	−0.0006 (12)
C5	0.0451 (19)	0.0299 (15)	0.0296 (16)	0.0081 (14)	0.0041 (14)	0.0006 (12)
C6	0.0451 (18)	0.0264 (14)	0.0203 (14)	−0.0047 (13)	0.0041 (12)	−0.0035 (11)
C7	0.0313 (15)	0.0293 (14)	0.0175 (13)	−0.0038 (12)	0.0024 (11)	−0.0023 (11)
C8	0.0371 (17)	0.0366 (16)	0.0189 (14)	−0.0040 (13)	−0.0039 (12)	−0.0048 (12)
C9	0.051 (2)	0.0397 (18)	0.0191 (14)	0.0002 (15)	−0.0066 (13)	−0.0019 (13)
C10	0.0474 (19)	0.0321 (16)	0.0211 (14)	−0.0003 (14)	−0.0058 (13)	0.0024 (12)
C11	0.059 (2)	0.0350 (17)	0.0256 (16)	0.0056 (16)	−0.0105 (15)	0.0034 (13)
C12	0.083 (3)	0.043 (2)	0.044 (2)	0.016 (2)	−0.026 (2)	0.0050 (17)
C13	0.0408 (17)	0.0245 (14)	0.0211 (14)	0.0039 (12)	−0.0056 (12)	−0.0041 (11)
C14	0.057 (2)	0.0407 (19)	0.0329 (18)	−0.0142 (17)	0.0063 (16)	−0.0043 (15)
C15	0.046 (2)	0.049 (2)	0.044 (2)	−0.0169 (17)	0.0021 (16)	−0.0193 (17)
C16	0.0301 (16)	0.0381 (16)	0.0248 (15)	0.0071 (13)	−0.0074 (12)	−0.0104 (12)
C17	0.0456 (19)	0.0330 (16)	0.0227 (15)	0.0008 (14)	−0.0085 (13)	−0.0001 (12)
C18	0.0418 (18)	0.0312 (15)	0.0247 (15)	−0.0050 (13)	−0.0098 (13)	−0.0008 (12)

Geometric parameters (Å, º)

S1—O1	1.431 (3)	C7—C8	1.521 (4)
S1—O2	1.437 (4)	C8—C9	1.528 (5)
S1—N1	1.582 (3)	C8—H8A	0.9900
S1—C16	1.778 (3)	C8—H8B	0.9900
N1—H1	0.882 (11)	C9—C10	1.502 (4)
N1—H2	0.880 (11)	C9—H9A	0.9900
N2—N3	1.373 (4)	C9—H9B	0.9900
N2—C1	1.372 (4)	C10—C11	1.402 (5)
N2—C13	1.428 (4)	C11—C12	1.503 (5)
N3—C11	1.334 (5)	C12—H12A	0.9800
C1—C10	1.377 (4)	C12—H12B	0.9800
C1—C2	1.463 (4)	C12—H12C	0.9800
C2—C7	1.413 (4)	C13—C14	1.377 (5)
C2—C3	1.398 (4)	C13—C18	1.381 (4)
C3—C4	1.385 (4)	C14—C15	1.387 (5)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.385 (5)	C15—C16	1.395 (5)
C4—H4	0.9500	C15—H15	0.9500
C5—C6	1.392 (5)	C16—C17	1.367 (5)
C5—H5	0.9500	C17—C18	1.382 (4)
C6—C7	1.390 (4)	C17—H17	0.9500
C6—H6	0.9500	C18—H18	0.9500
O1—S1—O2	121.6 (3)	C9—C8—H8B	108.8
O1—S1—N1	107.85 (18)	H8A—C8—H8B	107.7
O2—S1—N1	104.8 (2)	C10—C9—C8	108.2 (2)
O1—S1—C16	107.07 (16)	C10—C9—H9A	110.1
O2—S1—C16	105.50 (19)	C8—C9—H9A	110.1
N1—S1—C16	109.67 (15)	C10—C9—H9B	110.1
S1—N1—H1	116 (3)	C8—C9—H9B	110.1
S1—N1—H2	109 (3)	H9A—C9—H9B	108.4
H1—N1—H2	116 (4)	C1—C10—C11	106.4 (3)
N3—N2—C1	111.1 (2)	C1—C10—C9	120.5 (3)
N3—N2—C13	118.3 (2)	C11—C10—C9	133.1 (3)
C1—N2—C13	130.1 (3)	N3—C11—C10	110.7 (3)
C11—N3—N2	105.6 (3)	N3—C11—C12	120.8 (3)
N2—C1—C10	106.2 (3)	C10—C11—C12	128.5 (3)
N2—C1—C2	130.0 (3)	C11—C12—H12A	109.5
C10—C1—C2	123.8 (3)	C11—C12—H12B	109.5
C7—C2—C3	119.8 (3)	H12A—C12—H12B	109.5
C7—C2—C1	115.0 (3)	C11—C12—H12C	109.5
C3—C2—C1	125.2 (3)	H12A—C12—H12C	109.5
C4—C3—C2	120.7 (3)	H12B—C12—H12C	109.5
C4—C3—H3	119.6	C14—C13—C18	120.8 (3)
C2—C3—H3	119.6	C14—C13—N2	119.3 (3)
C5—C4—C3	119.8 (3)	C18—C13—N2	119.9 (3)

C5—C4—H4	120.1	C13—C14—C15	119.6 (3)
C3—C4—H4	120.1	C13—C14—H14	120.2
C4—C5—C6	119.9 (3)	C15—C14—H14	120.2
C4—C5—H5	120.1	C14—C15—C16	119.2 (3)
C6—C5—H5	120.1	C14—C15—H15	120.4
C7—C6—C5	121.4 (3)	C16—C15—H15	120.4
C7—C6—H6	119.3	C17—C16—C15	120.8 (3)
C5—C6—H6	119.3	C17—C16—S1	118.7 (3)
C6—C7—C2	118.4 (3)	C15—C16—S1	120.5 (3)
C6—C7—C8	121.2 (3)	C16—C17—C18	119.8 (3)
C2—C7—C8	120.4 (3)	C16—C17—H17	120.1
C7—C8—C9	113.8 (3)	C18—C17—H17	120.1
C7—C8—H8A	108.8	C17—C18—C13	119.8 (3)
C9—C8—H8A	108.8	C17—C18—H18	120.1
C7—C8—H8B	108.8	C13—C18—H18	120.1

C1—N2—N3—C11	−0.4 (4)	C8—C9—C10—C1	34.6 (4)
C13—N2—N3—C11	−173.2 (3)	C8—C9—C10—C11	−147.1 (4)
N3—N2—C1—C10	1.3 (4)	N2—N3—C11—C10	−0.7 (4)
C13—N2—C1—C10	173.0 (3)	N2—N3—C11—C12	177.0 (4)
N3—N2—C1—C2	−179.2 (3)	C1—C10—C11—N3	1.5 (4)
C13—N2—C1—C2	−7.5 (6)	C9—C10—C11—N3	−177.0 (4)
N2—C1—C2—C7	163.9 (3)	C1—C10—C11—C12	−176.0 (4)
C10—C1—C2—C7	−16.6 (5)	C9—C10—C11—C12	5.5 (7)
N2—C1—C2—C3	−17.6 (5)	N3—N2—C13—C14	−63.9 (5)
C10—C1—C2—C3	161.8 (3)	C1—N2—C13—C14	124.9 (4)
C7—C2—C3—C4	−2.2 (5)	N3—N2—C13—C18	114.7 (4)
C1—C2—C3—C4	179.4 (3)	C1—N2—C13—C18	−56.5 (5)
C2—C3—C4—C5	−0.4 (5)	C18—C13—C14—C15	0.2 (6)
C3—C4—C5—C6	2.2 (5)	N2—C13—C14—C15	178.8 (3)
C4—C5—C6—C7	−1.5 (5)	C13—C14—C15—C16	−0.3 (6)
C5—C6—C7—C2	−1.1 (5)	C14—C15—C16—C17	0.3 (6)
C5—C6—C7—C8	−179.7 (3)	C14—C15—C16—S1	−178.1 (3)
C3—C2—C7—C6	2.9 (4)	O1—S1—C16—C17	18.0 (3)
C1—C2—C7—C6	−178.5 (3)	O2—S1—C16—C17	148.8 (3)
C3—C2—C7—C8	−178.5 (3)	N1—S1—C16—C17	−98.8 (3)
C1—C2—C7—C8	0.1 (4)	O1—S1—C16—C15	−163.6 (3)
C6—C7—C8—C9	−148.2 (3)	O2—S1—C16—C15	−32.7 (4)
C2—C7—C8—C9	33.2 (4)	N1—S1—C16—C15	79.7 (3)
C7—C8—C9—C10	−48.0 (4)	C15—C16—C17—C18	−0.3 (5)
N2—C1—C10—C11	−1.6 (4)	S1—C16—C17—C18	178.2 (3)
C2—C1—C10—C11	178.8 (3)	C16—C17—C18—C13	0.2 (5)
N2—C1—C10—C9	177.1 (3)	C14—C13—C18—C17	−0.2 (5)
C2—C1—C10—C9	−2.5 (5)	N2—C13—C18—C17	−178.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.88 (1)	2.05 (1)	2.925 (4)	173 (5)
N1—H2···O2^{ii}	0.88 (1)	1.95 (2)	2.806 (4)	165 (4)

Symmetry codes: (i) $x+1/2, -y+3/2, z+1/2$; (ii) $x-1, y, z$.