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4-Methoxy-*N*-(1-methyl-1*H*-indazol-7-yl)benzenesulfonamide hemihydrate

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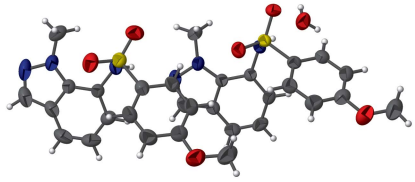
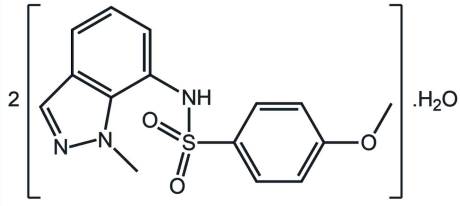
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $2C_{15}H_{15}N_3O_3S\cdot H_2O$, comprises two crystallographically independent organic molecules and one water molecule, all in general positions. Each organic molecule comprises an indazolyl system linked through a sulfonamide group to a methoxybenzene ring. The most important difference between the two organic molecules is the dihedral angle between the fused-ring system and the methoxybenzene ring, which is 56.32 (7)° in one molecule and 35.35 (8)° in the other. In the crystal, the organic and water molecules are connected into supramolecular chains along the *c* axis through O—H···N, O—H···O, N—H···O and N—-H···N hydrogen bonds; in addition, a π–π interaction between pyrazolyl rings [inter-centroid separation = 3.7547 (12) Å] is noted.

3D view



Chemical scheme



Structure description

Sulfonamides and their derivatives constitute an important class of therapeutic agents that exhibit a broad spectrum of pharmacological profiles, such as anti-bacterial, diuretic, hypoglycaemic, anti-thyroid, anti-viral, anti-inflammatory and anti-parasitic activities among others (Ranjith *et al.*, 2014; Shah *et al.*, 2013; Scozzafava *et al.*, 2013; Greig *et al.*, 2013). In our previous work, we have found that indazoles bearing arylsulfonamide groups showed anti-proliferative activity against human (colon and prostate) and murine (leukaemia) cell lines (Abbassi *et al.*, 2012, 2014; Bouissane, *et al.*, 2006).

The asymmetric unit of the title compound contains two independent organic molecules and one water molecule, as shown in Fig. 1. The fused five- and six-membered rings of each molecule are almost coplanar, with the maximum deviation from the mean plane being 0.020 (2) Å for the C12 atom and 0.022 (2) Å for the C27 atom in the first and

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···N6^{i}	0.83	2.03	2.828 (2)	160
O7—H7B···O2^{ii}	0.83	2.08	2.8831 (18)	162
N1—HN1···O7	0.86	1.92	2.7745 (18)	177
N4—HN4···N3	0.83	2.26	3.060 (2)	163

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

second molecules, respectively. The dihedral angles between the indazolyl system and the methoxybenzene ring are 56.32 (7) and 35.35 (8)° in the first and second molecules, respectively.

In the crystal, the organic molecules are connected through the water molecule by O7—H7A···N6, O7—H7B···O2, N1—HN1···O7 and N4—HN4···N3 hydrogen bonds (Table 1), in addition to π–π interactions between pyrazole rings as shown in Fig. 2.

Synthesis and crystallization

A mixture of 1-methyl-7-nitroindazole (1.22 mmol) and anhydrous $SnCl_2$ (1.1 g, 6.1 mmol) in ethanethiol (25 ml) was heated at 308 K for 4 h. After reduction, the starting material had been consumed and the solution was allowed to cool. The pH of the solution was made slightly basic (pH = 7–8) by addition of 5% aqueous potassium bicarbonate. Extraction with EtOAc followed. The organic phase was washed with brine and dried over magnesium sulfate. The solvent was removed to afford the amine, which was immediately dissolved in pyridine (5 ml) and then reacted with 4-methoxybenzenesulfonyl chloride (0.26 g, 1.25 mmol) at room temperature for 24 h. After the reaction mixture had been concentrated *in vacuo*, the resulting residue was purified by flash chromatography (elution was with EtOAc/hexane 1:9). The title compound was recrystallized from acetone solution, yield 62%; m.p. 439 K.

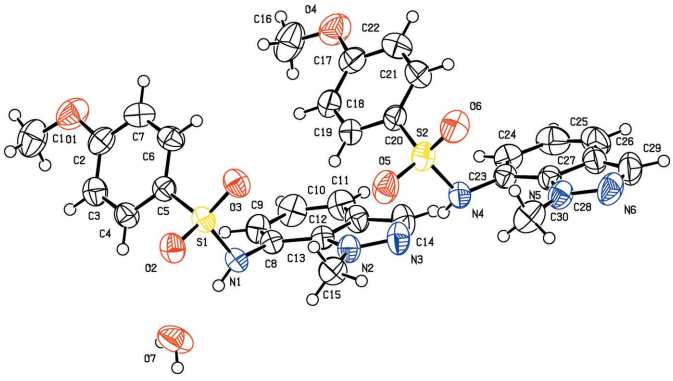


Figure 1
Plot of the molecules comprising the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_{15}H_{15}N_3O_3S\cdot H_2O$
M_r	652.73
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.3013 (5), 13.1934 (8), 15.3583 (9)
α, β, γ (°)	103.241 (3), 105.470 (3), 93.046 (3)
V (Å^3)	1566.30 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.33 × 0.26 × 0.22
Data collection	
Diffractometer	Bruker X8 APEX
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.663, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	52678, 8793, 6373
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.694
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.126, 1.01
No. of reflections	8793
No. of parameters	410
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.27

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXTL2014/7* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Three reflections, *i.e.* (010), (0$\overline{1}$1)

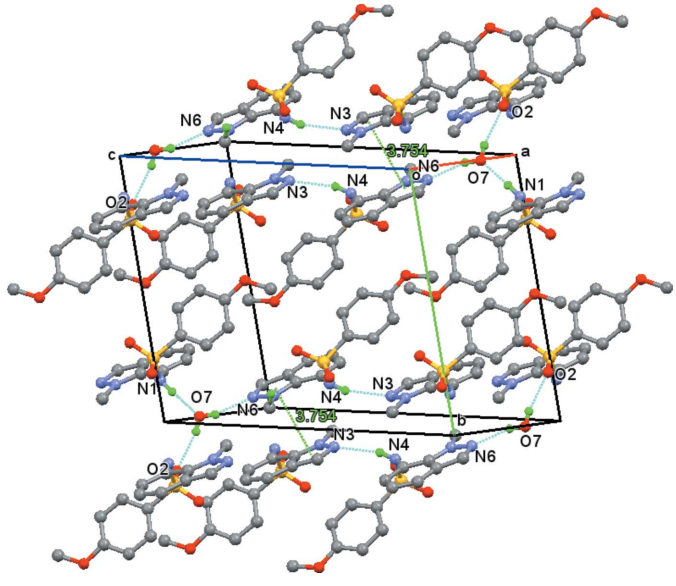


Figure 2
Crystal packing for the title compound showing hydrogen bonds as blue dashed lines and π–π interactions between pyrazole rings as green dashed lines.

and (001), were omitted from the final cycles of refinement owing to poor agreement.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170645 [https://doi.org/10.1107/S2414314617006459]

4-Methoxy-*N*-(1-methyl-1*H*-indazol-7-yl)benzenesulfonamide hemihydrate

Latifa Bouissane, Souad Mojahidi, El Mostapha Rakib, Hakima Chicha, Mohamed Saadi and Lahcen El Ammari

4-Methoxy-*N*-(1-methyl-1*H*-indazol-7-yl)benzenesulfonamide hemihydrate

Crystal data

$2C_{15}H_{15}N_3O_3S·H_2O$
M_r = 652.73
Triclinic, $P\overline{1}$
a = 8.3013 (5) Å
b = 13.1934 (8) Å
c = 15.3583 (9) Å
α = 103.241 (3)°
β = 105.470 (3)°
γ = 93.046 (3)°
V = 1566.30 (16) Å^3
Z = 2
$F(000)$ = 684
D_x = 1.384 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8793 reflections
θ = 2.4–29.6°
μ = 0.23 mm^{-1}
T = 296 K
Block, colourless
0.33 × 0.26 × 0.22 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.663, T_{max} = 0.746
52678 measured reflections
8793 independent reflections
6373 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 29.6°, θ_{min} = 2.4°
h = −11→11
k = −18→18
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.126
S = 1.01
8793 reflections
410 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.3677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7955 (3)	0.5081 (2)	1.36936 (15)	0.0819 (7)
H1A	0.7711	0.5670	1.4116	0.123*
H1B	0.9031	0.4886	1.3978	0.123*
H1C	0.7100	0.4500	1.3553	0.123*
C2	0.8330 (2)	0.46149 (14)	1.21830 (12)	0.0519 (4)
C3	0.8606 (2)	0.35988 (14)	1.22437 (12)	0.0523 (4)
H3	0.8550	0.3382	1.2771	0.063*
C4	0.8961 (2)	0.29174 (13)	1.15114 (11)	0.0475 (4)
H4	0.9146	0.2236	1.1545	0.057*
C5	0.90435 (18)	0.32425 (12)	1.07256 (11)	0.0413 (3)
C6	0.8740 (2)	0.42508 (13)	1.06623 (13)	0.0506 (4)
H6	0.8771	0.4465	1.0130	0.061*
C7	0.8392 (2)	0.49298 (14)	1.13927 (14)	0.0590 (4)
H7	0.8197	0.5608	1.1356	0.071*
C8	0.63751 (17)	0.16629 (12)	0.88692 (10)	0.0384 (3)
C9	0.5267 (2)	0.20653 (14)	0.93452 (12)	0.0490 (4)
H9	0.5570	0.2172	0.9991	0.059*
C10	0.3695 (2)	0.23200 (16)	0.88899 (13)	0.0581 (5)
H10	0.2985	0.2591	0.9239	0.070*
C11	0.3193 (2)	0.21774 (15)	0.79473 (13)	0.0555 (4)
H11	0.2160	0.2359	0.7649	0.067*
C12	0.42742 (19)	0.17504 (14)	0.74370 (11)	0.0471 (4)
C13	0.58508 (17)	0.14913 (11)	0.78936 (10)	0.0384 (3)
C14	0.4189 (2)	0.14518 (17)	0.64821 (12)	0.0588 (5)
H14	0.3280	0.1526	0.6003	0.071*
C15	0.8160 (2)	0.06416 (15)	0.72874 (13)	0.0546 (4)
H15A	0.8191	0.0273	0.6677	0.082*
H15B	0.8260	0.0165	0.7682	0.082*
H15C	0.9076	0.1198	0.7550	0.082*
C16	0.6073 (3)	0.5679 (2)	0.86652 (16)	0.0869 (7)
H16A	0.5583	0.6269	0.8937	0.130*
H16B	0.7230	0.5724	0.9018	0.130*
H16C	0.5469	0.5042	0.8674	0.130*
C17	0.6649 (2)	0.49176 (14)	0.72376 (13)	0.0549 (4)
C18	0.7408 (2)	0.41260 (14)	0.75749 (12)	0.0543 (4)
H18	0.7482	0.4088	0.8181	0.065*
C19	0.8056 (2)	0.33912 (14)	0.70115 (11)	0.0521 (4)
H19	0.8576	0.2861	0.7242	0.063*
C20	0.7939 (2)	0.34356 (13)	0.61088 (11)	0.0470 (4)
C21	0.7174 (2)	0.42338 (15)	0.57673 (13)	0.0586 (4)
H21	0.7093	0.4270	0.5160	0.070*
C22	0.6541 (3)	0.49656 (16)	0.63312 (15)	0.0650 (5)
H22	0.6033	0.5501	0.6104	0.078*
C23	0.57109 (19)	0.17150 (12)	0.41223 (11)	0.0419 (3)
C24	0.4319 (2)	0.21437 (14)	0.42935 (13)	0.0530 (4)

H24	0.4268	0.2339	0.4906	0.064*
C25	0.2974 (2)	0.22982 (16)	0.35798 (17)	0.0661 (5)
H25	0.2048	0.2580	0.3727	0.079*
C26	0.3001 (2)	0.20434 (16)	0.26802 (16)	0.0675 (5)
H26	0.2119	0.2163	0.2210	0.081*
C27	0.4389 (2)	0.15954 (14)	0.24732 (12)	0.0544 (4)
C28	0.57333 (19)	0.14280 (12)	0.31873 (11)	0.0425 (3)
C29	0.4819 (3)	0.11994 (18)	0.16507 (13)	0.0704 (6)
H29	0.4157	0.1199	0.1058	0.085*
C30	0.8443 (2)	0.06187 (16)	0.31512 (15)	0.0652 (5)
H30A	0.8662	0.0060	0.2690	0.098*
H30B	0.8409	0.0372	0.3688	0.098*
H30C	0.9321	0.1194	0.3331	0.098*
N1	0.79869 (15)	0.14195 (10)	0.93399 (9)	0.0409 (3)
HN1	0.8019	0.1000	0.9697	0.049*
N2	0.65791 (16)	0.10768 (11)	0.72168 (9)	0.0458 (3)
N3	0.55537 (19)	0.10556 (14)	0.63529 (10)	0.0578 (4)
N4	0.70516 (16)	0.15252 (11)	0.48502 (9)	0.0456 (3)
HN4	0.6730	0.1276	0.5232	0.055*
N5	0.68470 (18)	0.09626 (12)	0.27673 (10)	0.0515 (3)
N6	0.6269 (3)	0.08297 (14)	0.18201 (11)	0.0690 (5)
O1	0.7990 (2)	0.53534 (11)	1.28620 (10)	0.0743 (4)
O2	1.09600 (13)	0.18909 (10)	1.02068 (8)	0.0530 (3)
O3	0.96160 (15)	0.29187 (10)	0.91188 (8)	0.0534 (3)
O4	0.5979 (2)	0.56814 (12)	0.77337 (11)	0.0761 (4)
O5	0.98772 (16)	0.19783 (11)	0.59488 (9)	0.0679 (4)
O6	0.90416 (17)	0.28627 (11)	0.46690 (9)	0.0658 (4)
O7	0.8147 (2)	0.01367 (11)	1.05542 (10)	0.0801 (5)
H7A	0.7595	0.0187	1.0937	0.120*
H7B	0.8402	−0.0470	1.0451	0.120*
S1	0.95253 (4)	0.23680 (3)	0.98091 (3)	0.04128 (10)
S2	0.86491 (5)	0.24489 (4)	0.53781 (3)	0.05034 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0833 (15)	0.0967 (17)	0.0597 (13)	0.0026 (13)	0.0285 (11)	0.0002 (12)
C2	0.0429 (8)	0.0515 (9)	0.0548 (10)	−0.0010 (7)	0.0146 (7)	0.0015 (8)
C3	0.0503 (9)	0.0619 (10)	0.0455 (9)	0.0055 (8)	0.0141 (7)	0.0148 (8)
C4	0.0465 (8)	0.0496 (9)	0.0477 (9)	0.0107 (7)	0.0115 (7)	0.0161 (7)
C5	0.0319 (7)	0.0465 (8)	0.0444 (8)	0.0041 (6)	0.0086 (6)	0.0124 (6)
C6	0.0512 (9)	0.0494 (9)	0.0564 (10)	0.0037 (7)	0.0180 (8)	0.0212 (8)
C7	0.0639 (11)	0.0436 (9)	0.0728 (12)	0.0073 (8)	0.0240 (9)	0.0159 (8)
C8	0.0340 (7)	0.0427 (7)	0.0395 (7)	0.0028 (6)	0.0114 (6)	0.0120 (6)
C9	0.0442 (8)	0.0609 (10)	0.0425 (8)	0.0045 (7)	0.0171 (7)	0.0090 (7)
C10	0.0388 (8)	0.0741 (12)	0.0627 (11)	0.0111 (8)	0.0225 (8)	0.0095 (9)
C11	0.0333 (7)	0.0688 (11)	0.0637 (11)	0.0078 (7)	0.0118 (7)	0.0175 (9)
C12	0.0350 (7)	0.0586 (9)	0.0465 (8)	0.0006 (7)	0.0081 (6)	0.0167 (7)

C13	0.0346 (7)	0.0420 (7)	0.0394 (7)	0.0013 (6)	0.0119 (6)	0.0112 (6)
C14	0.0418 (9)	0.0862 (13)	0.0460 (9)	−0.0006 (9)	0.0045 (7)	0.0232 (9)
C15	0.0563 (10)	0.0571 (10)	0.0557 (10)	0.0161 (8)	0.0254 (8)	0.0119 (8)
C16	0.0716 (14)	0.1005 (18)	0.0711 (14)	0.0149 (13)	0.0200 (11)	−0.0130 (13)
C17	0.0530 (9)	0.0466 (9)	0.0579 (10)	0.0013 (7)	0.0119 (8)	0.0047 (8)
C18	0.0607 (10)	0.0539 (10)	0.0411 (8)	0.0004 (8)	0.0087 (7)	0.0061 (7)
C19	0.0582 (10)	0.0487 (9)	0.0421 (8)	0.0054 (8)	0.0037 (7)	0.0100 (7)
C20	0.0454 (8)	0.0475 (9)	0.0418 (8)	−0.0002 (7)	0.0062 (6)	0.0075 (7)
C21	0.0665 (11)	0.0605 (11)	0.0521 (10)	0.0080 (9)	0.0149 (8)	0.0231 (8)
C22	0.0736 (13)	0.0541 (10)	0.0705 (12)	0.0168 (9)	0.0172 (10)	0.0242 (9)
C23	0.0410 (7)	0.0429 (8)	0.0404 (8)	0.0030 (6)	0.0108 (6)	0.0092 (6)
C24	0.0499 (9)	0.0535 (10)	0.0587 (10)	0.0091 (7)	0.0222 (8)	0.0116 (8)
C25	0.0444 (9)	0.0633 (11)	0.0949 (16)	0.0151 (8)	0.0205 (10)	0.0261 (11)
C26	0.0470 (10)	0.0710 (12)	0.0803 (14)	0.0057 (9)	−0.0016 (9)	0.0346 (11)
C27	0.0530 (10)	0.0577 (10)	0.0474 (9)	−0.0054 (8)	0.0028 (7)	0.0199 (8)
C28	0.0409 (7)	0.0442 (8)	0.0404 (8)	−0.0002 (6)	0.0106 (6)	0.0091 (6)
C29	0.0777 (14)	0.0827 (14)	0.0419 (10)	−0.0124 (12)	0.0044 (9)	0.0180 (9)
C30	0.0521 (10)	0.0683 (12)	0.0724 (13)	0.0089 (9)	0.0279 (9)	0.0002 (10)
N1	0.0403 (6)	0.0462 (7)	0.0392 (6)	0.0078 (5)	0.0107 (5)	0.0173 (5)
N2	0.0427 (7)	0.0572 (8)	0.0379 (7)	0.0051 (6)	0.0134 (5)	0.0105 (6)
N3	0.0528 (8)	0.0804 (11)	0.0369 (7)	−0.0020 (7)	0.0103 (6)	0.0137 (7)
N4	0.0461 (7)	0.0519 (7)	0.0365 (6)	0.0035 (6)	0.0084 (5)	0.0110 (6)
N5	0.0542 (8)	0.0567 (8)	0.0421 (7)	0.0012 (6)	0.0191 (6)	0.0044 (6)
N6	0.0888 (13)	0.0728 (11)	0.0403 (8)	−0.0145 (10)	0.0256 (8)	0.0013 (7)
O1	0.0868 (10)	0.0645 (8)	0.0705 (9)	0.0059 (8)	0.0361 (8)	−0.0005 (7)
O2	0.0393 (6)	0.0674 (7)	0.0522 (7)	0.0187 (5)	0.0100 (5)	0.0160 (6)
O3	0.0507 (6)	0.0659 (7)	0.0529 (7)	0.0045 (6)	0.0208 (5)	0.0266 (6)
O4	0.0813 (10)	0.0655 (9)	0.0754 (10)	0.0197 (8)	0.0236 (8)	0.0019 (7)
O5	0.0500 (7)	0.0782 (9)	0.0602 (8)	0.0173 (6)	−0.0015 (6)	0.0052 (7)
O6	0.0613 (8)	0.0764 (9)	0.0588 (8)	−0.0076 (7)	0.0245 (6)	0.0107 (7)
O7	0.1307 (14)	0.0656 (9)	0.0751 (9)	0.0411 (9)	0.0604 (10)	0.0357 (7)
S1	0.03386 (17)	0.0517 (2)	0.0421 (2)	0.00845 (15)	0.01207 (14)	0.01725 (16)
S2	0.0423 (2)	0.0591 (3)	0.0438 (2)	0.00319 (18)	0.00828 (16)	0.00708 (18)

Geometric parameters (Å, º)

C1—O1	1.411 (3)	C17—C22	1.387 (3)
C1—H1A	0.9600	C18—C19	1.377 (2)
C1—H1B	0.9600	C18—H18	0.9300
C1—H1C	0.9600	C19—C20	1.379 (2)
C2—O1	1.356 (2)	C19—H19	0.9300
C2—C7	1.382 (3)	C20—C21	1.391 (2)
C2—C3	1.392 (3)	C20—S2	1.7512 (17)
C3—C4	1.379 (2)	C21—C22	1.368 (3)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.387 (2)	C22—H22	0.9300
C4—H4	0.9300	C23—C24	1.374 (2)
C5—C6	1.387 (2)	C23—C28	1.404 (2)

C5—S1	1.7544 (16)	C23—N4	1.4301 (19)
C6—C7	1.372 (3)	C24—C25	1.402 (3)
C6—H6	0.9300	C24—H24	0.9300
C7—H7	0.9300	C25—C26	1.352 (3)
C8—C9	1.376 (2)	C25—H25	0.9300
C8—C13	1.404 (2)	C26—C27	1.400 (3)
C8—N1	1.4324 (18)	C26—H26	0.9300
C9—C10	1.404 (2)	C27—C29	1.398 (3)
C9—H9	0.9300	C27—C28	1.408 (2)
C10—C11	1.360 (3)	C28—N5	1.358 (2)
C10—H10	0.9300	C29—N6	1.307 (3)
C11—C12	1.401 (2)	C29—H29	0.9300
C11—H11	0.9300	C30—N5	1.442 (2)
C12—C14	1.410 (2)	C30—H30A	0.9600
C12—C13	1.410 (2)	C30—H30B	0.9600
C13—N2	1.3619 (19)	C30—H30C	0.9600
C14—N3	1.316 (2)	N1—S1	1.6256 (13)
C14—H14	0.9300	N1—HN1	0.8600
C15—N2	1.448 (2)	N2—N3	1.3651 (19)
C15—H15A	0.9600	N4—S2	1.6441 (14)
C15—H15B	0.9600	N4—HN4	0.8284
C15—H15C	0.9600	N5—N6	1.371 (2)
C16—O4	1.413 (3)	O2—S1	1.4337 (11)
C16—H16A	0.9600	O3—S1	1.4307 (12)
C16—H16B	0.9600	O5—S2	1.4259 (13)
C16—H16C	0.9600	O6—S2	1.4259 (14)
C17—O4	1.356 (2)	O7—H7A	0.8299
C17—C18	1.378 (3)	O7—H7B	0.8299

O1—C1—H1A	109.5	C19—C20—C21	119.72 (16)
O1—C1—H1B	109.5	C19—C20—S2	119.93 (13)
H1A—C1—H1B	109.5	C21—C20—S2	120.25 (13)
O1—C1—H1C	109.5	C22—C21—C20	119.56 (17)
H1A—C1—H1C	109.5	C22—C21—H21	120.2
H1B—C1—H1C	109.5	C20—C21—H21	120.2
O1—C2—C7	115.49 (17)	C21—C22—C17	120.74 (18)
O1—C2—C3	124.28 (17)	C21—C22—H22	119.6
C7—C2—C3	120.23 (16)	C17—C22—H22	119.6
C4—C3—C2	119.14 (16)	C24—C23—C28	116.88 (15)
C4—C3—H3	120.4	C24—C23—N4	122.16 (15)
C2—C3—H3	120.4	C28—C23—N4	120.92 (14)
C3—C4—C5	120.33 (16)	C23—C24—C25	122.49 (18)
C3—C4—H4	119.8	C23—C24—H24	118.8
C5—C4—H4	119.8	C25—C24—H24	118.8
C4—C5—C6	120.26 (15)	C26—C25—C24	120.99 (18)
C4—C5—S1	119.56 (12)	C26—C25—H25	119.5
C6—C5—S1	120.19 (12)	C24—C25—H25	119.5
C7—C6—C5	119.37 (16)	C25—C26—C27	118.40 (17)

C7—C6—H6	120.3	C25—C26—H26	120.8
C5—C6—H6	120.3	C27—C26—H26	120.8
C6—C7—C2	120.64 (16)	C29—C27—C26	134.62 (19)
C6—C7—H7	119.7	C29—C27—C28	104.63 (17)
C2—C7—H7	119.7	C26—C27—C28	120.72 (17)
C9—C8—C13	116.97 (14)	N5—C28—C23	132.75 (15)
C9—C8—N1	121.96 (13)	N5—C28—C27	106.74 (14)
C13—C8—N1	121.07 (13)	C23—C28—C27	120.50 (15)
C8—C9—C10	122.28 (15)	N6—C29—C27	111.51 (17)
C8—C9—H9	118.9	N6—C29—H29	124.2
C10—C9—H9	118.9	C27—C29—H29	124.2
C11—C10—C9	121.10 (15)	N5—C30—H30A	109.5
C11—C10—H10	119.4	N5—C30—H30B	109.5
C9—C10—H10	119.4	H30A—C30—H30B	109.5
C10—C11—C12	118.25 (15)	N5—C30—H30C	109.5
C10—C11—H11	120.9	H30A—C30—H30C	109.5
C12—C11—H11	120.9	H30B—C30—H30C	109.5
C11—C12—C14	135.14 (16)	C8—N1—S1	118.27 (10)
C11—C12—C13	120.65 (15)	C8—N1—HN1	118.1
C14—C12—C13	104.18 (14)	S1—N1—HN1	110.3
N2—C13—C8	132.50 (14)	C13—N2—N3	110.83 (13)
N2—C13—C12	106.78 (13)	C13—N2—C15	130.26 (14)
C8—C13—C12	120.72 (13)	N3—N2—C15	118.85 (14)
N3—C14—C12	111.63 (15)	C14—N3—N2	106.58 (14)
N3—C14—H14	124.2	C23—N4—S2	118.47 (11)
C12—C14—H14	124.2	C23—N4—HN4	113.9
N2—C15—H15A	109.5	S2—N4—HN4	111.1
N2—C15—H15B	109.5	C28—N5—N6	110.14 (15)
H15A—C15—H15B	109.5	C28—N5—C30	131.09 (14)
N2—C15—H15C	109.5	N6—N5—C30	118.77 (15)
H15A—C15—H15C	109.5	C29—N6—N5	106.98 (16)
H15B—C15—H15C	109.5	C2—O1—C1	117.75 (17)
O4—C16—H16A	109.5	C17—O4—C16	118.23 (17)
O4—C16—H16B	109.5	H7A—O7—H7B	107.4
H16A—C16—H16B	109.5	O3—S1—O2	118.81 (7)
O4—C16—H16C	109.5	O3—S1—N1	107.97 (7)
H16A—C16—H16C	109.5	O2—S1—N1	105.66 (7)
H16B—C16—H16C	109.5	O3—S1—C5	107.83 (8)
O4—C17—C18	124.60 (18)	O2—S1—C5	107.82 (7)
O4—C17—C22	115.79 (17)	N1—S1—C5	108.38 (7)
C18—C17—C22	119.62 (17)	O6—S2—O5	120.27 (9)
C19—C18—C17	119.84 (17)	O6—S2—N4	106.67 (7)
C19—C18—H18	120.1	O5—S2—N4	105.43 (8)
C17—C18—H18	120.1	O6—S2—C20	108.53 (8)
C18—C19—C20	120.52 (16)	O5—S2—C20	108.31 (8)
C18—C19—H19	119.7	N4—S2—C20	106.89 (7)
C20—C19—H19	119.7		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···N6^{i}	0.83	2.03	2.828 (2)	160
O7—H7*B*···O2^{ii}	0.83	2.08	2.8831 (18)	162
N1—H*N*1···O7	0.86	1.92	2.7745 (18)	177
N4—H*N*4···N3	0.83	2.26	3.060 (2)	163

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