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Sulfamethizole–2-amino-4,6-dimethoxypyrimidine (1/1)

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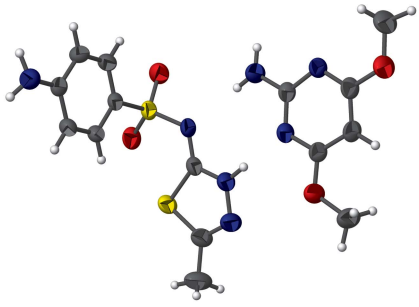
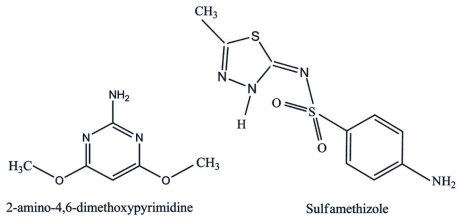
In the title 1:1 co-crystal, $C_9H_{10}N_4O_2S_2\cdot C_6H_9N_3O_2$ [systematic name: 4-amino-*N*-(5-methyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide–2-amino-4,6-dimethoxypyrimidine (1/1)], the sulfamethazole molecule is found in the form of the imidine tautomer. In the crystal, the components are linked by a pair of N—H···N hydrogen bonds, which generate an $R_2^2(8)$ loop. Further N—H···N and N—H···O hydrogen bonds link the dimers into [100] chains.

3D view



Chemical scheme



Structure description

Sulfamethizole [4-amino-*N*-(5-methyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide; SMT] is a bacteriostatic antibiotic drug that contains the sulfonamide group and acts through the competitive inhibition of folic acid synthesis in bacteria (Kerrn *et al.*, 2003). The crystal structure of SMT shows that the molecule exists as the imidine tautomer (Fuglp & Kalman, 1987). SMT displays good solubility in water, but it has a short biological half–life due to fast elimination and therefore bioavailability is limited (Suresh *et al.*, 2015). The drug dose should be increased to overcome this problem. Nevertheless, increasing the drug dosage leads to the occurrence of unwanted side effects and systemic toxicity. It has been reported that the biopharmaceutical properties of drugs can be improved by cocrystalization (Duggirala *et al.*, 2016). Pharmaceutical cocrystal formation can result in a lower dissolution rate and thus, the bioavailability of the drug is increased. The hydrogen-bonding groups in the drug molecule make it capable of forming cocrystals.

Sulfamethizole is a conformationally flexible drug and has rich hydrogen-bond groups (donors: amine NH_2 and imine NH; acceptors: sulfonyl O atoms, thiazolidine N and S, and imidine N). Therefore, sulfamethizole can easily form a cocrystal and this is reported extensively in the literature (Suresh *et al.*, 2015; Thomas *et al.*, 2015).

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N5	0.86 (3)	1.99 (3)	2.842 (2)	179 (2)
N4—H4A···N6^{i}	0.87 (2)	2.29 (3)	3.151 (2)	172 (2)
N4—H4B···O1^{ii}	0.84 (2)	2.25 (2)	3.026 (2)	153.4 (19)
N7—H7A···N1	0.83 (3)	2.33 (3)	3.160 (2)	179 (2)
N7—H7B···N4^{iii}	0.86 (3)	2.62 (2)	3.176 (3)	123.7 (18)

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

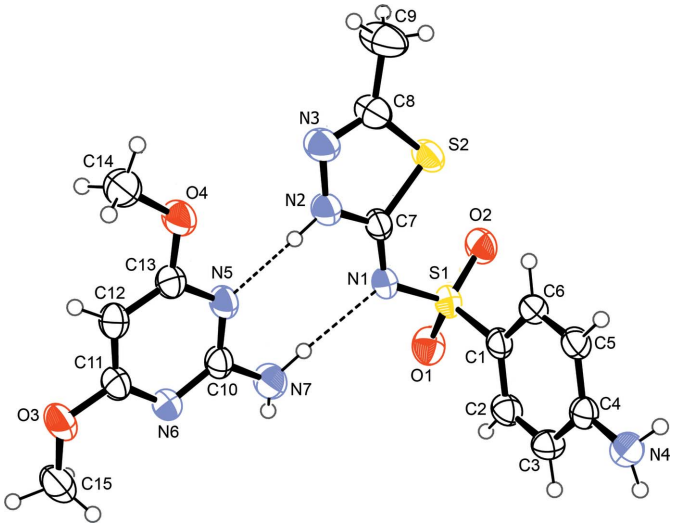


Figure 1
The molecular structure of the title co-crystal, with displacement elipsoids drawn at the 40% probability level.

We now report the structure of the 1:1 co-crystal between sulfamethizole and 2-amino-4,6-dimethoxypyrimidine (Fig. 1), which may provide insight into drug–protein recognition processes in biological systems.

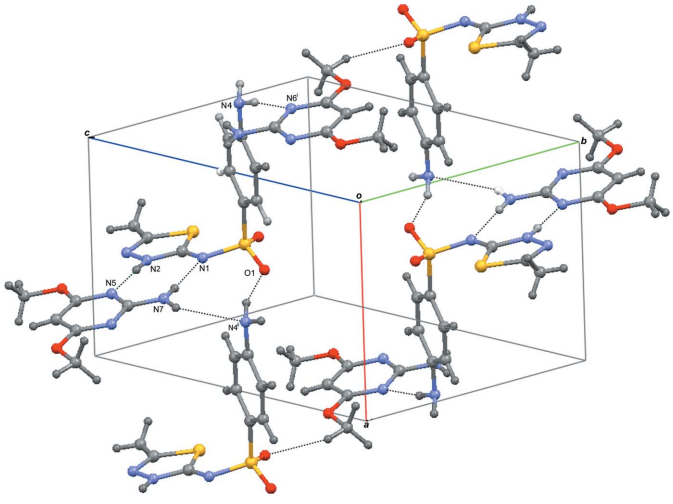


Figure 2
The hydrogen-bonding interactions in the title compound forming the crystal packing. The N—H···N hydrogen bonds form an $R_2^2(8)$ ring motif.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_9H_{10}N_4O_2S_2{\cdot}C_6H_9N_3O_2$
M_r	425.49
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	7.9645 (5), 10.3576 (6), 12.7222 (7)
α, β, γ (°)	101.576 (5), 101.640 (5), 100.566 (5)
V (Å^3)	979.21 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.31
Crystal size (mm)	0.55 × 0.50 × 0.43
Data collection	
Diffractometer	Stoe IPDS II
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.843, 0.875
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19762, 4515, 3910
R_{int}	0.118
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.652
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.111, 1.08
No. of reflections	4515
No. of parameters	273
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.28

Computer programs: *X-AREA* and, *X-RED32* (Stoe & Cie, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

The sulfamethizole molecule is found in the form of the imidine tautomer (see Scheme). Two intermolecular N—H···N hydrogen bonds appear in the asymmetric unit of the structure (Table 1). The first (N7—H7A···N1) is between the pyrimidine NH group and the sulfaimidine N atom. The other (N2—H2···N5) is between the H atom on the thiazole N atom and a pyrimidine ring N atom. These homonuclear hydrogen bonds generate an $R_2^2(8)$ loop motif (Fig. 2).

The dihedral angle between the planes of the thiazole and benzene rings is 82.97 (5)°. The S2—C7—N1—S1 torsion angle is 5.0 (2)°, which is comparable with the sulfa (2.8°) and selanate (5.7°) salts of sulfamethizole, but lower than in sulfamethizole–4-aminopyridine (7.16°) and much lower than in cocrystals of sulfamethizole–4-amino benzoic acid (30.8°) (Thomas *et al.*, 2015). These variations in the dihedral angle were attributed to the strength of the hydrogen bonding involved, since this affects the orientation, conformation and tautomeric form of sulfamethizole due to flexible rotation of the sulfonamide group (Suresh *et al.*, 2015).

Synthesis and crystallization

The title compound was prepared by mixing of 0.5 mmol quantities of 2-amino-4,6-dimethoxypyrimidine with 0.5 mmol sulfamethizole obtained commercially. The mixture was then refluxed for 30 min at 323 K and left for slow evaporation for

two weeks. Well-defined colourless crystals were collected for X-ray analysis.

Refinement

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

Acknowledgements

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full crystallographic data

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Sulfamethizole–2-amino-4,6-dimethoxypyrimidine (1/1)

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4-Amino-*N*-(5-methyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide; 2-amino-4,6-dimethoxypyrimidine

Crystal data

$C_9H_{10}N_4O_2S_2·C_6H_9N_3O_2$
M_r = 425.49
Triclinic, $P\overline{1}$
a = 7.9645 (5) Å
b = 10.3576 (6) Å
c = 12.7222 (7) Å
α = 101.576 (5)°
β = 101.640 (5)°
γ = 100.566 (5)°
V = 979.21 (10) Å^3
Z = 2
$F(000)$ = 444
D_x = 1.443 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 19970 reflections
θ = 2.7–26°
μ = 0.31 mm^{-1}
T = 293 K
Prism, colorless
0.55 × 0.50 × 0.43 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
T_{min} = 0.843, T_{max} = 0.875
19762 measured reflections
4515 independent reflections
3910 reflections with $I > 2\sigma(I)$
R_{int} = 0.118
θ_{max} = 27.6°, θ_{min} = 2.7°
h = −10→10
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.111
S = 1.08
4515 reflections
273 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.2223P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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	0.2941 (2)	0.31995 (17)	0.69271 (13)	0.0383 (3)
C2	0.3406 (2)	0.45325 (18)	0.75414 (15)	0.0445 (4)
H2C	0.4536	0.5053	0.7641	0.053*
C3	0.2202 (2)	0.50910 (18)	0.80052 (15)	0.0460 (4)
H3	0.2525	0.5989	0.8413	0.055*
C4	0.0504 (2)	0.43251 (17)	0.78698 (13)	0.0399 (3)
C5	0.0044 (2)	0.29768 (17)	0.72458 (14)	0.0421 (4)
H5	−0.1083	0.2452	0.7146	0.051*
C6	0.1245 (2)	0.24235 (17)	0.67801 (14)	0.0417 (4)
H6	0.0926	0.1529	0.6366	0.050*
C7	0.4293 (2)	0.01659 (18)	0.67771 (13)	0.0399 (3)
C8	0.2797 (3)	−0.2225 (2)	0.60952 (16)	0.0525 (4)
C9	0.1694 (4)	−0.3590 (2)	0.5459 (2)	0.0760 (7)
H9A	0.1019	−0.3523	0.4764	0.114*
H9B	0.2443	−0.4201	0.5326	0.114*
H9C	0.0910	−0.3925	0.5877	0.114*
C10	0.8114 (2)	0.15307 (18)	0.99761 (13)	0.0404 (4)
C11	0.9544 (3)	0.0998 (2)	1.14895 (14)	0.0456 (4)
C12	0.8567 (3)	−0.03299 (19)	1.11218 (14)	0.0478 (4)
H12	0.8727	−0.0975	1.1523	0.057*
C13	0.7345 (2)	−0.06289 (18)	1.01245 (14)	0.0421 (4)
C14	0.6485 (3)	−0.2931 (2)	1.0150 (2)	0.0664 (6)
H14A	0.5665	−0.3754	0.9712	0.100*
H14B	0.7666	−0.3054	1.0225	0.100*
H14C	0.6259	−0.2707	1.0870	0.100*
C15	1.1865 (4)	0.2621 (3)	1.28728 (18)	0.0719 (7)
H15A	1.2645	0.2678	1.3571	0.108*
H15B	1.2545	0.2803	1.2354	0.108*
H15C	1.1162	0.3276	1.2969	0.108*
N1	0.5048 (2)	0.14709 (15)	0.70960 (12)	0.0445 (3)
N2	0.4668 (2)	−0.06597 (16)	0.74267 (13)	0.0484 (4)
N3	0.3839 (2)	−0.20093 (17)	0.70591 (14)	0.0546 (4)
N4	−0.0696 (2)	0.48684 (19)	0.83644 (15)	0.0493 (4)
N5	0.7090 (2)	0.02878 (15)	0.95416 (11)	0.0428 (3)
N6	0.9366 (2)	0.19515 (15)	1.09468 (12)	0.0431 (3)
N7	0.7878 (3)	0.2465 (2)	0.93969 (16)	0.0560 (4)
O1	0.60116 (18)	0.35499 (15)	0.65218 (13)	0.0567 (3)
O2	0.36048 (19)	0.17430 (15)	0.52230 (10)	0.0543 (3)
O3	1.0740 (2)	0.12920 (16)	1.24624 (11)	0.0650 (4)
O4	0.62877 (19)	−0.18590 (14)	0.96184 (11)	0.0556 (3)
S1	0.44759 (6)	0.24784 (5)	0.63460 (3)	0.04182 (13)
S2	0.27661 (7)	−0.08031 (5)	0.55645 (4)	0.04938 (14)
H2	0.541 (3)	−0.037 (3)	0.806 (2)	0.066 (7)*
H4A	−0.043 (3)	0.575 (3)	0.8510 (18)	0.057 (6)*
H4B	−0.176 (3)	0.455 (2)	0.8035 (18)	0.049 (6)*

H7A	0.713 (3)	0.220 (2)	0.880 (2)	0.060 (7)*
H7B	0.860 (3)	0.324 (3)	0.9634 (19)	0.055 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0365 (8)	0.0400 (8)	0.0366 (7)	0.0094 (7)	0.0011 (6)	0.0131 (6)
C2	0.0389 (9)	0.0398 (9)	0.0495 (9)	0.0015 (7)	0.0043 (7)	0.0128 (7)
C3	0.0489 (10)	0.0340 (8)	0.0492 (9)	0.0052 (7)	0.0055 (8)	0.0075 (7)
C4	0.0429 (9)	0.0397 (8)	0.0372 (8)	0.0110 (7)	0.0038 (6)	0.0147 (6)
C5	0.0346 (8)	0.0399 (9)	0.0466 (9)	0.0044 (7)	0.0020 (7)	0.0107 (7)
C6	0.0388 (8)	0.0358 (8)	0.0434 (8)	0.0063 (7)	−0.0010 (7)	0.0072 (6)
C7	0.0359 (8)	0.0462 (9)	0.0355 (8)	0.0116 (7)	0.0033 (6)	0.0094 (7)
C8	0.0562 (11)	0.0498 (11)	0.0441 (9)	0.0000 (9)	0.0060 (8)	0.0126 (8)
C9	0.0939 (18)	0.0550 (13)	0.0570 (13)	−0.0162 (12)	−0.0001 (12)	0.0134 (10)
C10	0.0429 (9)	0.0455 (9)	0.0351 (8)	0.0137 (7)	0.0079 (7)	0.0140 (7)
C11	0.0513 (10)	0.0515 (10)	0.0329 (8)	0.0166 (8)	0.0036 (7)	0.0109 (7)
C12	0.0589 (11)	0.0471 (10)	0.0383 (8)	0.0151 (8)	0.0031 (8)	0.0189 (7)
C13	0.0461 (9)	0.0438 (9)	0.0376 (8)	0.0121 (7)	0.0081 (7)	0.0136 (7)
C14	0.0813 (15)	0.0459 (11)	0.0617 (12)	0.0022 (11)	−0.0037 (11)	0.0231 (10)
C15	0.0807 (16)	0.0658 (14)	0.0484 (11)	0.0068 (12)	−0.0171 (11)	0.0101 (10)
N1	0.0451 (8)	0.0440 (8)	0.0396 (7)	0.0137 (6)	−0.0037 (6)	0.0109 (6)
N2	0.0511 (9)	0.0451 (8)	0.0412 (8)	0.0075 (7)	−0.0040 (7)	0.0119 (6)
N3	0.0618 (10)	0.0451 (9)	0.0486 (9)	0.0025 (8)	0.0020 (7)	0.0141 (7)
N4	0.0477 (9)	0.0446 (9)	0.0549 (9)	0.0124 (7)	0.0109 (7)	0.0110 (7)
N5	0.0454 (8)	0.0464 (8)	0.0357 (7)	0.0109 (6)	0.0028 (6)	0.0153 (6)
N6	0.0462 (8)	0.0445 (8)	0.0362 (7)	0.0128 (6)	0.0043 (6)	0.0088 (6)
N7	0.0631 (11)	0.0478 (10)	0.0496 (9)	0.0045 (9)	−0.0049 (8)	0.0219 (8)
O1	0.0430 (7)	0.0598 (8)	0.0706 (9)	0.0088 (6)	0.0151 (6)	0.0252 (7)
O2	0.0626 (8)	0.0652 (9)	0.0357 (6)	0.0214 (7)	0.0056 (6)	0.0144 (6)
O3	0.0777 (10)	0.0597 (9)	0.0430 (7)	0.0112 (8)	−0.0150 (7)	0.0142 (6)
O4	0.0634 (9)	0.0467 (7)	0.0476 (7)	0.0032 (6)	−0.0043 (6)	0.0183 (6)
S1	0.0390 (2)	0.0474 (2)	0.0397 (2)	0.01207 (18)	0.00461 (16)	0.01532 (17)
S2	0.0511 (3)	0.0509 (3)	0.0368 (2)	0.0043 (2)	−0.00223 (18)	0.00978 (18)

Geometric parameters (Å, º)

C1—C2	1.385 (2)	C11—N6	1.325 (2)
C1—C6	1.395 (2)	C11—O3	1.341 (2)
C1—S1	1.7544 (17)	C11—C12	1.385 (3)
C2—C3	1.377 (3)	C12—C13	1.373 (2)
C2—H2C	0.9300	C12—H12	0.9300
C3—C4	1.395 (3)	C13—N5	1.336 (2)
C3—H3	0.9300	C13—O4	1.344 (2)
C4—N4	1.387 (2)	C14—O4	1.427 (2)
C4—C5	1.402 (2)	C14—H14A	0.9600
C5—C6	1.374 (2)	C14—H14B	0.9600
C5—H5	0.9300	C14—H14C	0.9600

C6—H6	0.9300	C15—O3	1.429 (3)
C7—N1	1.318 (2)	C15—H15A	0.9600
C7—N2	1.334 (2)	C15—H15B	0.9600
C7—S2	1.7437 (17)	C15—H15C	0.9600
C8—N3	1.286 (2)	N1—S1	1.6142 (14)
C8—C9	1.492 (3)	N2—N3	1.372 (2)
C8—S2	1.741 (2)	N2—H2	0.86 (3)
C9—H9A	0.9600	N4—H4A	0.87 (2)
C9—H9B	0.9600	N4—H4B	0.84 (2)
C9—H9C	0.9600	N7—H7A	0.83 (3)
C10—N5	1.332 (2)	N7—H7B	0.86 (3)
C10—N7	1.346 (2)	O1—S1	1.4387 (15)
C10—N6	1.356 (2)	O2—S1	1.4396 (14)
C2—C1—C6	119.65 (16)	C11—C12—H12	122.3
C2—C1—S1	120.42 (13)	N5—C13—O4	112.31 (15)
C6—C1—S1	119.92 (13)	N5—C13—C12	123.03 (17)
C3—C2—C1	120.25 (17)	O4—C13—C12	124.66 (16)
C3—C2—H2C	119.9	O4—C14—H14A	109.5
C1—C2—H2C	119.9	O4—C14—H14B	109.5
C2—C3—C4	120.73 (17)	H14A—C14—H14B	109.5
C2—C3—H3	119.6	O4—C14—H14C	109.5
C4—C3—H3	119.6	H14A—C14—H14C	109.5
N4—C4—C3	121.00 (17)	H14B—C14—H14C	109.5
N4—C4—C5	120.36 (17)	O3—C15—H15A	109.5
C3—C4—C5	118.62 (16)	O3—C15—H15B	109.5
C6—C5—C4	120.56 (16)	H15A—C15—H15B	109.5
C6—C5—H5	119.7	O3—C15—H15C	109.5
C4—C5—H5	119.7	H15A—C15—H15C	109.5
C5—C6—C1	120.20 (16)	H15B—C15—H15C	109.5
C5—C6—H6	119.9	C7—N1—S1	120.34 (12)
C1—C6—H6	119.9	C7—N2—N3	118.54 (15)
N1—C7—N2	120.79 (15)	C7—N2—H2	122.1 (17)
N1—C7—S2	131.24 (13)	N3—N2—H2	119.4 (17)
N2—C7—S2	107.97 (13)	C8—N3—N2	109.41 (16)
N3—C8—C9	123.13 (19)	C4—N4—H4A	111.3 (15)
N3—C8—S2	115.29 (16)	C4—N4—H4B	116.1 (15)
C9—C8—S2	121.58 (16)	H4A—N4—H4B	111 (2)
C8—C9—H9A	109.5	C10—N5—C13	116.13 (14)
C8—C9—H9B	109.5	C11—N6—C10	114.42 (16)
H9A—C9—H9B	109.5	C10—N7—H7A	116.6 (17)
C8—C9—H9C	109.5	C10—N7—H7B	117.5 (15)
H9A—C9—H9C	109.5	H7A—N7—H7B	125 (2)
H9B—C9—H9C	109.5	C11—O3—C15	119.04 (16)
N5—C10—N7	116.88 (16)	C13—O4—C14	117.21 (15)
N5—C10—N6	126.51 (15)	O1—S1—O2	117.78 (9)
N7—C10—N6	116.61 (17)	O1—S1—N1	106.72 (8)
N6—C11—O3	119.99 (18)	O2—S1—N1	111.25 (8)

N6—C11—C12	124.48 (16)	O1—S1—C1	107.18 (9)
O3—C11—C12	115.53 (16)	O2—S1—C1	107.85 (8)
C13—C12—C11	115.43 (16)	N1—S1—C1	105.32 (8)
C13—C12—H12	122.3	C8—S2—C7	88.79 (9)
C6—C1—C2—C3	0.0 (2)	O4—C13—N5—C10	−178.71 (15)
S1—C1—C2—C3	−179.37 (13)	C12—C13—N5—C10	0.7 (3)
C1—C2—C3—C4	0.3 (3)	O3—C11—N6—C10	−179.90 (16)
C2—C3—C4—N4	177.91 (16)	C12—C11—N6—C10	0.4 (3)
C2—C3—C4—C5	−0.4 (3)	N5—C10—N6—C11	0.0 (3)
N4—C4—C5—C6	−178.20 (15)	N7—C10—N6—C11	179.69 (17)
C3—C4—C5—C6	0.1 (2)	N6—C11—O3—C15	−2.9 (3)
C4—C5—C6—C1	0.2 (2)	C12—C11—O3—C15	176.8 (2)
C2—C1—C6—C5	−0.2 (2)	N5—C13—O4—C14	178.00 (17)
S1—C1—C6—C5	179.10 (12)	C12—C13—O4—C14	−1.4 (3)
N6—C11—C12—C13	−0.2 (3)	C7—N1—S1—O1	−149.25 (15)
O3—C11—C12—C13	−179.89 (16)	C7—N1—S1—O2	−19.54 (18)
C11—C12—C13—N5	−0.4 (3)	C7—N1—S1—C1	97.05 (15)
C11—C12—C13—O4	178.95 (17)	C2—C1—S1—O1	−7.28 (16)
N2—C7—N1—S1	−175.32 (13)	C6—C1—S1—O1	173.37 (13)
S2—C7—N1—S1	5.0 (2)	C2—C1—S1—O2	−135.02 (14)
N1—C7—N2—N3	179.62 (17)	C6—C1—S1—O2	45.64 (15)
S2—C7—N2—N3	−0.6 (2)	C2—C1—S1—N1	106.10 (14)
C9—C8—N3—N2	180.0 (2)	C6—C1—S1—N1	−73.24 (14)
S2—C8—N3—N2	0.5 (2)	N3—C8—S2—C7	−0.68 (18)
C7—N2—N3—C8	0.1 (3)	C9—C8—S2—C7	179.8 (2)
N7—C10—N5—C13	179.77 (16)	N1—C7—S2—C8	−179.59 (19)
N6—C10—N5—C13	−0.5 (3)	N2—C7—S2—C8	0.67 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N5	0.86 (3)	1.99 (3)	2.842 (2)	179 (2)
N4—H4*A*···N6^{i}	0.87 (2)	2.29 (3)	3.151 (2)	172 (2)
N4—H4*B*···O1^{ii}	0.84 (2)	2.25 (2)	3.026 (2)	153.4 (19)
N7—H7*A*···N1	0.83 (3)	2.33 (3)	3.160 (2)	179 (2)
N7—H7*B*···N4^{iii}	0.86 (3)	2.62 (2)	3.176 (3)	123.7 (18)

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