Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis[2,5-dichloro-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)benzenesulfonamidato-κ*N*]zinc(II)

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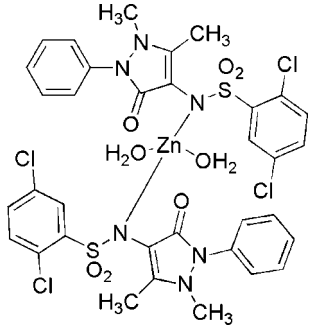
Received 19 November 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.118; data-to-parameter ratio = 15.6.

In the title compound, $[Zn(C_{17}H_{14}Cl_2N_3O_3S)_2(H_2O)_2]$, the Zn^{II} ion has a tetrahedral coordination formed by the two N atoms of the sulfonamide groups and the two water molecules. Two inter- and two intramolecular O—H···O hydrogen bonds are observed in the crystal structure.

Related literature

For related literature, see: Burdulene *et al.* (1999); Hernández-Delgadillo & Cruz (2006); Macías *et al.* (2003); Nardelli (1999); Prasad & Agarwal (2007); Raman *et al.* (2003); Xue *et al.* (2000).



Experimental

Crystal data

$[Zn(C_{17}H_{14}Cl_2N_3O_3S)_2(H_2O)_2]$
M_r = 923.95
Monoclinic, $P2_1/n$
a = 15.0683 (7) Å
b = 12.3009 (5) Å
c = 21.8256 (9) Å
β = 104.681 (4)°
V = 3913.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 299 (2) K
0.50 × 0.42 × 0.36 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.597, T_{max} = 0.698
29052 measured reflections
7987 independent reflections
5392 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.118
S = 1.09
7987 reflections
512 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Zn1	2.024 (2)	O1—Zn1	2.028 (3)
N4—Zn1	2.031 (3)	O2—Zn1	2.004 (3)
O2—Zn1—N1	108.83 (12)	O2—Zn1—N4	114.00 (13)
O2—Zn1—O1	114.56 (15)	N1—Zn1—N4	112.12 (10)
N1—Zn1—O1	105.49 (11)	O1—Zn1—N4	101.44 (11)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11*O*···O5^{i}	0.884 (18)	2.52 (3)	3.277 (4)	145 (4)
O1—H12*O*···O8	0.896 (18)	2.06 (2)	2.914 (4)	160 (4)
O2—H21*O*···O4	0.883 (19)	2.22 (3)	2.928 (4)	137 (4)
O2—H22*O*···O8^{i}	0.881 (19)	2.05 (3)	2.868 (4)	154 (5)

Symmetry code: (i) $-x+1, -y+1, -z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors thank Professor Dr. Hartmut Fuess, Technische Universität Darmstadt, for diffractometer time.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2502).

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supporting information

Acta Cryst. (2008). E**64**, m22–m23 [https://doi.org/10.1107/S1600536807061533]

Diaquabis[2,5-dichloro-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)benzenesulfonamidato-κN]zinc(II)

Luiz Everson da Silva, Paulo Teixeira de Sousa, Evandro Luiz Dall'Oglio and Sabine Foro

S1. Comment

The interest to develop the coordination chemistry of pyrazolone derivatives is because of their biological and medicinal properties. They present a variety of biological activities ranging from anti-tumour, fungicide, bactericide, antiinflamatory and anti-viral activities (Prasad and Agarwal, 2007; Hernández-Delgadillo *et al.*, 2006; Raman *et al.*, 2003; Burdulene *et al.*, 1999). As part of our efforts to investigate transition metal (II) complexes based on 4-amino-antypirine derivatives and sulfonamide pharmacophoric group, we describe the X-ray characterization of the title compound, (I).

The Zn^{II} ion has a tetrahedral coordination formed by the two sulfonamide N atoms and the two water molecules (Table 1). The bond angles around the central Zn atom are close to the 109° angle of an ideal tetrahedral value. Both hydrogen atoms of each water molecule are involved in an intermolecular O—H···O [O—H···O = 2.52 (3) Å, O—H···O = 2.05 (3) Å, respectively] and an intramolecular O—H···O [O—H···O = 2.06 (2) Å, O—H···O = 2.22 (3) Å, respectively] hydrogen bonds (Table 2).

S2. Experimental

The ligand was obtained according to the procedure previously described (Xue *et al.*, 2000). Compound (I) was prepared by a literature procedure (Macías *et al.*, 2003). Single crystals of (I) suitable for X-ray data collection appeared after a few days from a methanol solution.

S3. Refinement

The O-bound H atoms were located in difference map and were refined with restrained geometry (Nardelli, 1999), *viz*. O—H distances were restrained to 0.85 (2) Å and H···H distances were restrained to 1.365 (2) Å, thus leading to the angle of 107°.

The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93Å (aromatic), 0.96Å (methyl). All H atoms were refined with isotropic displacement parameters (set to 1.2 or 1.5 times of the U_{eq} of the parent atom).

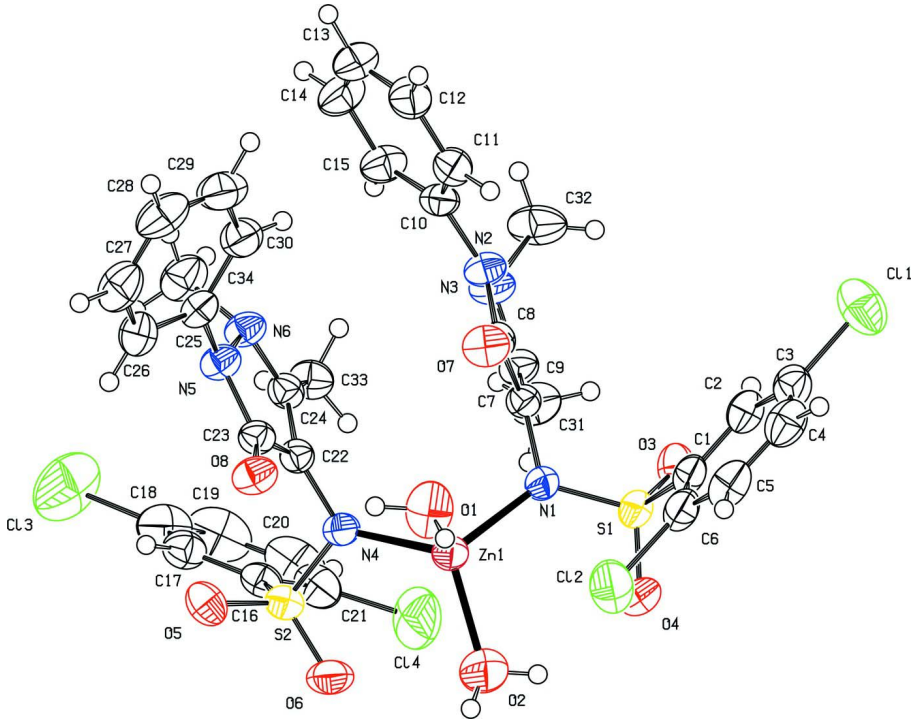

Figure 1

Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

Diaquabis[2,5-dichloro-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro- 1*H*-pyrazol-4-yl)benzenesulfonamidato-*κN*]zinc(II)

Crystal data

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$M_r = 923.95$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.0683\ (7)$ Å
$b = 12.3009\ (5)$ Å
$c = 21.8256\ (9)$ Å
$\beta = 104.681\ (4)°$
$V = 3913.4\ (3)$ Å^3
$Z = 4$
$F(000) = 1888$
$D_x = 1.568$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8931 reflections
$\theta = 1.9–25.0°$
$\mu = 1.07$ mm^{-1}
$T = 299$ K
Prism, colourless
0.50 × 0.42 × 0.36 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using ω and phi scans.
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.597$, $T_{max} = 0.698$
29052 measured reflections
7987 independent reflections
5392 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.2°$
$h = -18\rightarrow18$
$k = -11\rightarrow15$
$l = -27\rightarrow27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.118$
$S = 1.09$
7987 reflections
512 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 4.1837P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5603 (2)	0.6796 (3)	0.28912 (16)	0.0409 (7)
C2	0.5768 (2)	0.6727 (3)	0.35422 (16)	0.0440 (8)
H2	0.5301	0.6517	0.3725	0.053*
C3	0.6630 (2)	0.6972 (3)	0.39213 (17)	0.0494 (9)
C4	0.7332 (2)	0.7298 (3)	0.36661 (19)	0.0527 (9)
H4	0.7902	0.7481	0.3927	0.063*
C5	0.7176 (2)	0.7347 (3)	0.3020 (2)	0.0530 (9)
H5	0.7647	0.7554	0.2841	0.064*
C6	0.6323 (2)	0.7093 (3)	0.26338 (17)	0.0469 (8)
C7	0.4364 (2)	0.4486 (2)	0.24139 (14)	0.0333 (7)
C8	0.5111 (2)	0.3709 (3)	0.25951 (14)	0.0346 (7)
C9	0.3639 (2)	0.4081 (3)	0.25942 (15)	0.0383 (7)
C10	0.5135 (2)	0.1837 (3)	0.30486 (14)	0.0389 (7)
C11	0.6071 (2)	0.1694 (3)	0.32822 (15)	0.0439 (8)
H11	0.6464	0.2290	0.3344	0.053*
C12	0.6417 (3)	0.0660 (3)	0.34219 (17)	0.0528 (9)
H12	0.7046	0.0560	0.3576	0.063*
C13	0.5844 (3)	−0.0222 (3)	0.33367 (18)	0.0583 (10)
H13	0.6083	−0.0913	0.3442	0.070*
C14	0.4915 (3)	−0.0087 (3)	0.3095 (2)	0.0577 (10)
H14	0.4527	−0.0687	0.3029	0.069*
C15	0.4561 (2)	0.0943 (3)	0.29522 (17)	0.0477 (8)
H15	0.3932	0.1036	0.2790	0.057*
C16	0.2069 (2)	0.3622 (3)	0.00350 (14)	0.0396 (7)

C17	0.1821 (2)	0.2601 (3)	−0.02154 (16)	0.0466 (8)
H17	0.2209	0.2220	−0.0408	0.056*
C18	0.1005 (3)	0.2152 (4)	−0.0180 (2)	0.0654 (11)
C19	0.0418 (3)	0.2701 (5)	0.0092 (2)	0.0807 (15)
H19	−0.0139	0.2390	0.0106	0.097*
C20	0.0652 (3)	0.3710 (5)	0.0345 (2)	0.0777 (15)
H20	0.0253	0.4087	0.0531	0.093*
C21	0.1481 (2)	0.4170 (3)	0.03238 (17)	0.0557 (10)
C22	0.4052 (2)	0.2880 (2)	0.08708 (13)	0.0334 (7)
C23	0.4841 (2)	0.2373 (3)	0.07336 (14)	0.0350 (7)
C24	0.3656 (2)	0.2139 (3)	0.11794 (14)	0.0360 (7)
C25	0.5654 (2)	0.0663 (3)	0.11081 (16)	0.0399 (7)
C26	0.6037 (2)	0.0348 (3)	0.06249 (17)	0.0479 (8)
H26	0.5750	0.0518	0.0206	0.057*
C27	0.6851 (3)	−0.0223 (3)	0.0771 (2)	0.0608 (10)
H27	0.7117	−0.0434	0.0449	0.073*
C28	0.7271 (3)	−0.0482 (3)	0.1386 (2)	0.0641 (11)
H28	0.7824	−0.0860	0.1481	0.077*
C29	0.6876 (3)	−0.0182 (3)	0.1860 (2)	0.0616 (10)
H29	0.7156	−0.0371	0.2277	0.074*
C30	0.6065 (2)	0.0399 (3)	0.17273 (17)	0.0492 (8)
H30	0.5802	0.0609	0.2051	0.059*
C31	0.2695 (2)	0.4531 (3)	0.25029 (19)	0.0547 (9)
H31A	0.2563	0.5015	0.2146	0.066*
H31B	0.2656	0.4920	0.2876	0.066*
H31C	0.2258	0.3946	0.2427	0.066*
C32	0.3580 (3)	0.2902 (4)	0.34843 (19)	0.0653 (11)
H32A	0.3842	0.2232	0.3673	0.078*
H32B	0.2924	0.2865	0.3401	0.078*
H32C	0.3803	0.3492	0.3769	0.078*
C33	0.2803 (2)	0.2221 (3)	0.14020 (16)	0.0452 (8)
H33A	0.2929	0.1995	0.1837	0.054*
H33B	0.2340	0.1760	0.1147	0.054*
H33C	0.2592	0.2960	0.1366	0.054*
C34	0.3762 (3)	0.0120 (3)	0.1241 (2)	0.0578 (10)
H34A	0.4233	−0.0411	0.1395	0.069*
H34B	0.3460	−0.0036	0.0808	0.069*
H34C	0.3324	0.0096	0.1493	0.069*
N1	0.44014 (18)	0.5439 (2)	0.20587 (12)	0.0362 (6)
N2	0.47815 (17)	0.2898 (2)	0.29227 (12)	0.0380 (6)
N3	0.38412 (17)	0.3080 (2)	0.28874 (13)	0.0418 (6)
N4	0.37893 (17)	0.3976 (2)	0.07149 (11)	0.0359 (6)
N5	0.48516 (17)	0.1322 (2)	0.09505 (12)	0.0382 (6)
N6	0.41734 (17)	0.1203 (2)	0.12843 (12)	0.0391 (6)
O1	0.5833 (2)	0.4718 (3)	0.12585 (15)	0.0683 (8)
H11O	0.625 (2)	0.516 (3)	0.118 (2)	0.082*
H12O	0.582 (3)	0.418 (2)	0.0979 (17)	0.082*
O2	0.4242 (3)	0.6670 (3)	0.07039 (15)	0.0901 (11)

H21O	0.431 (4)	0.721 (3)	0.0980 (18)	0.108*
H22O	0.451 (3)	0.692 (4)	0.0415 (17)	0.108*
O3	0.39205 (16)	0.6519 (2)	0.28993 (11)	0.0501 (6)
O4	0.42301 (18)	0.74189 (19)	0.19750 (12)	0.0553 (6)
O5	0.34501 (15)	0.3405 (2)	−0.04321 (10)	0.0480 (6)
O6	0.30904 (17)	0.5236 (2)	−0.01506 (11)	0.0535 (6)
O7	0.58658 (14)	0.3693 (2)	0.24759 (11)	0.0461 (6)
O8	0.54446 (15)	0.27471 (18)	0.04963 (11)	0.0441 (5)
Cl1	0.68388 (7)	0.68768 (11)	0.47414 (5)	0.0732 (3)
Cl2	0.62100 (8)	0.71621 (9)	0.18265 (5)	0.0690 (3)
Cl3	0.07311 (10)	0.08467 (13)	−0.04885 (9)	0.1168 (6)
Cl4	0.17694 (9)	0.54153 (11)	0.06876 (6)	0.0899 (4)
S1	0.44404 (6)	0.65578 (7)	0.24313 (4)	0.03951 (19)
S2	0.31731 (5)	0.41072 (7)	0.00093 (4)	0.03802 (19)
Zn1	0.45325 (3)	0.52527 (3)	0.116433 (17)	0.03809 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0483 (19)	0.0283 (16)	0.0476 (19)	−0.0001 (14)	0.0150 (15)	−0.0068 (15)
C2	0.0430 (18)	0.0366 (18)	0.054 (2)	0.0020 (14)	0.0149 (16)	−0.0062 (16)
C3	0.052 (2)	0.044 (2)	0.051 (2)	0.0089 (16)	0.0104 (17)	−0.0064 (17)
C4	0.0405 (19)	0.043 (2)	0.072 (3)	0.0043 (16)	0.0109 (18)	−0.0070 (19)
C5	0.049 (2)	0.039 (2)	0.077 (3)	−0.0023 (16)	0.0265 (19)	−0.0066 (19)
C6	0.061 (2)	0.0317 (17)	0.054 (2)	−0.0056 (16)	0.0260 (18)	−0.0063 (16)
C7	0.0366 (16)	0.0326 (16)	0.0326 (15)	0.0011 (13)	0.0127 (13)	0.0015 (13)
C8	0.0351 (16)	0.0368 (17)	0.0328 (15)	−0.0030 (13)	0.0101 (13)	−0.0013 (14)
C9	0.0386 (17)	0.0355 (17)	0.0437 (17)	0.0072 (14)	0.0158 (14)	0.0043 (15)
C10	0.0437 (18)	0.0388 (18)	0.0346 (16)	0.0035 (14)	0.0108 (14)	0.0083 (14)
C11	0.0434 (18)	0.045 (2)	0.0407 (17)	0.0015 (15)	0.0048 (14)	0.0002 (16)
C12	0.048 (2)	0.055 (2)	0.048 (2)	0.0158 (18)	0.0000 (16)	−0.0009 (18)
C13	0.072 (3)	0.041 (2)	0.060 (2)	0.013 (2)	0.013 (2)	0.0081 (19)
C14	0.061 (2)	0.038 (2)	0.073 (3)	−0.0053 (17)	0.015 (2)	0.0061 (19)
C15	0.0412 (18)	0.042 (2)	0.058 (2)	−0.0020 (15)	0.0092 (16)	0.0106 (17)
C16	0.0343 (16)	0.050 (2)	0.0336 (16)	0.0065 (14)	0.0068 (13)	0.0073 (15)
C17	0.0419 (19)	0.052 (2)	0.0443 (19)	−0.0029 (16)	0.0073 (15)	0.0061 (17)
C18	0.048 (2)	0.072 (3)	0.070 (3)	−0.011 (2)	0.004 (2)	0.015 (2)
C19	0.040 (2)	0.122 (5)	0.080 (3)	−0.009 (3)	0.016 (2)	0.019 (3)
C20	0.043 (2)	0.129 (5)	0.065 (3)	0.027 (3)	0.022 (2)	0.010 (3)
C21	0.049 (2)	0.073 (3)	0.046 (2)	0.0192 (19)	0.0139 (16)	0.0030 (19)
C22	0.0346 (15)	0.0334 (16)	0.0321 (15)	−0.0023 (13)	0.0083 (12)	0.0006 (13)
C23	0.0352 (16)	0.0356 (17)	0.0349 (16)	−0.0033 (13)	0.0104 (13)	0.0035 (14)
C24	0.0367 (16)	0.0393 (18)	0.0327 (15)	−0.0031 (14)	0.0102 (13)	0.0008 (14)
C25	0.0431 (18)	0.0289 (16)	0.0489 (19)	−0.0004 (14)	0.0139 (15)	0.0008 (15)
C26	0.0486 (19)	0.045 (2)	0.052 (2)	0.0025 (16)	0.0163 (16)	−0.0065 (17)
C27	0.060 (2)	0.048 (2)	0.083 (3)	0.0109 (19)	0.032 (2)	−0.007 (2)
C28	0.052 (2)	0.043 (2)	0.097 (3)	0.0128 (18)	0.019 (2)	0.010 (2)
C29	0.067 (3)	0.049 (2)	0.065 (2)	0.005 (2)	0.009 (2)	0.016 (2)

C30	0.055 (2)	0.043 (2)	0.051 (2)	0.0042 (17)	0.0167 (17)	0.0036 (17)
C31	0.043 (2)	0.056 (2)	0.071 (2)	0.0095 (17)	0.0243 (18)	0.012 (2)
C32	0.067 (3)	0.073 (3)	0.069 (3)	0.014 (2)	0.041 (2)	0.029 (2)
C33	0.0418 (18)	0.052 (2)	0.0458 (18)	0.0006 (16)	0.0184 (15)	0.0066 (17)
C34	0.062 (2)	0.046 (2)	0.074 (3)	−0.0101 (18)	0.034 (2)	0.002 (2)
N1	0.0462 (15)	0.0300 (14)	0.0340 (13)	−0.0019 (11)	0.0133 (11)	0.0005 (11)
N2	0.0339 (13)	0.0354 (15)	0.0464 (15)	0.0016 (11)	0.0133 (12)	0.0086 (12)
N3	0.0370 (14)	0.0426 (16)	0.0515 (16)	0.0043 (12)	0.0215 (12)	0.0135 (13)
N4	0.0387 (14)	0.0328 (14)	0.0356 (13)	0.0014 (11)	0.0081 (11)	0.0045 (12)
N5	0.0389 (14)	0.0349 (15)	0.0462 (15)	0.0005 (11)	0.0206 (12)	0.0058 (12)
N6	0.0411 (14)	0.0342 (15)	0.0475 (15)	0.0002 (12)	0.0211 (12)	0.0076 (12)
O1	0.0611 (17)	0.072 (2)	0.080 (2)	−0.0129 (15)	0.0329 (15)	−0.0137 (16)
O2	0.156 (3)	0.055 (2)	0.062 (2)	−0.009 (2)	0.033 (2)	0.0071 (16)
O3	0.0474 (13)	0.0563 (15)	0.0507 (13)	0.0042 (11)	0.0197 (11)	−0.0130 (12)
O4	0.0726 (17)	0.0336 (13)	0.0566 (15)	0.0086 (12)	0.0109 (13)	0.0037 (12)
O5	0.0466 (13)	0.0632 (16)	0.0385 (12)	0.0005 (12)	0.0187 (10)	−0.0028 (12)
O6	0.0624 (15)	0.0448 (14)	0.0498 (14)	−0.0028 (12)	0.0074 (12)	0.0156 (12)
O7	0.0323 (12)	0.0529 (15)	0.0562 (14)	0.0009 (10)	0.0170 (10)	0.0070 (12)
O8	0.0415 (12)	0.0425 (13)	0.0549 (14)	−0.0006 (10)	0.0244 (11)	0.0090 (11)
Cl1	0.0562 (6)	0.1051 (9)	0.0530 (6)	0.0131 (6)	0.0042 (4)	−0.0111 (6)
Cl2	0.0884 (7)	0.0679 (7)	0.0600 (6)	−0.0338 (6)	0.0361 (5)	−0.0118 (5)
Cl3	0.0875 (9)	0.0850 (10)	0.1688 (15)	−0.0411 (8)	0.0159 (9)	−0.0023 (10)
Cl4	0.0998 (9)	0.0860 (9)	0.0894 (8)	0.0301 (7)	0.0343 (7)	−0.0232 (7)
S1	0.0458 (4)	0.0321 (4)	0.0415 (4)	0.0033 (3)	0.0126 (3)	−0.0032 (3)
S2	0.0391 (4)	0.0404 (5)	0.0346 (4)	−0.0002 (3)	0.0096 (3)	0.0048 (4)
Zn1	0.0460 (2)	0.0346 (2)	0.0361 (2)	−0.00316 (17)	0.01467 (16)	0.00228 (16)

Geometric parameters (Å, º)

C1—C2	1.382 (5)	C23—O8	1.243 (3)
C1—C6	1.391 (5)	C23—N5	1.375 (4)
C1—S1	1.809 (3)	C24—N6	1.377 (4)
C2—C3	1.385 (5)	C24—C33	1.487 (4)
C2—H2	0.9300	C25—C30	1.375 (5)
C3—C4	1.374 (5)	C25—C26	1.380 (5)
C3—Cl1	1.741 (4)	C25—N5	1.423 (4)
C4—C5	1.370 (5)	C26—C27	1.379 (5)
C4—H4	0.9300	C26—H26	0.9300
C5—C6	1.383 (5)	C27—C28	1.368 (6)
C5—H5	0.9300	C27—H27	0.9300
C6—Cl2	1.729 (4)	C28—C29	1.370 (6)
C7—C9	1.348 (4)	C28—H28	0.9300
C7—N1	1.414 (4)	C29—C30	1.381 (5)
C7—C8	1.452 (4)	C29—H29	0.9300
C8—O7	1.230 (3)	C30—H30	0.9300
C8—N2	1.390 (4)	C31—H31A	0.9600
C9—N3	1.386 (4)	C31—H31B	0.9600
C9—C31	1.492 (4)	C31—H31C	0.9600

C10—C15	1.383 (5)	C32—N3	1.470 (4)
C10—C11	1.384 (4)	C32—H32A	0.9600
C10—N2	1.410 (4)	C32—H32B	0.9600
C11—C12	1.379 (5)	C32—H32C	0.9600
C11—H11	0.9300	C33—H33A	0.9600
C12—C13	1.370 (5)	C33—H33B	0.9600
C12—H12	0.9300	C33—H33C	0.9600
C13—C14	1.375 (5)	C34—N6	1.462 (4)
C13—H13	0.9300	C34—H34A	0.9600
C14—C15	1.380 (5)	C34—H34B	0.9600
C14—H14	0.9300	C34—H34C	0.9600
C15—H15	0.9300	N1—S1	1.592 (3)
C16—C17	1.382 (5)	N1—Zn1	2.024 (2)
C16—C21	1.386 (5)	N2—N3	1.417 (3)
C16—S2	1.781 (3)	N4—S2	1.592 (3)
C17—C18	1.369 (5)	N4—Zn1	2.031 (3)
C17—H17	0.9300	N5—N6	1.405 (3)
C18—C19	1.362 (7)	O1—Zn1	2.028 (3)
C18—Cl3	1.750 (5)	O1—H11O	0.884 (18)
C19—C20	1.367 (7)	O1—H12O	0.896 (18)
C19—H19	0.9300	O2—Zn1	2.004 (3)
C20—C21	1.384 (6)	O2—H21O	0.883 (19)
C20—H20	0.9300	O2—H22O	0.881 (19)
C21—Cl4	1.729 (4)	O3—S1	1.437 (2)
C22—C24	1.358 (4)	O4—S1	1.433 (2)
C22—N4	1.422 (4)	O5—S2	1.433 (2)
C22—C23	1.440 (4)	O6—S2	1.430 (3)

C2—C1—C6	118.5 (3)	C28—C27—C26	120.6 (4)
C2—C1—S1	117.2 (2)	C28—C27—H27	119.7
C6—C1—S1	124.3 (3)	C26—C27—H27	119.7
C1—C2—C3	119.8 (3)	C27—C28—C29	119.8 (4)
C1—C2—H2	120.1	C27—C28—H28	120.1
C3—C2—H2	120.1	C29—C28—H28	120.1
C4—C3—C2	121.6 (3)	C28—C29—C30	120.8 (4)
C4—C3—Cl1	118.6 (3)	C28—C29—H29	119.6
C2—C3—Cl1	119.8 (3)	C30—C29—H29	119.6
C5—C4—C3	118.7 (3)	C25—C30—C29	118.9 (3)
C5—C4—H4	120.6	C25—C30—H30	120.6
C3—C4—H4	120.6	C29—C30—H30	120.6
C4—C5—C6	120.6 (3)	C9—C31—H31A	109.5
C4—C5—H5	119.7	C9—C31—H31B	109.5
C6—C5—H5	119.7	H31A—C31—H31B	109.5
C5—C6—C1	120.8 (3)	C9—C31—H31C	109.5
C5—C6—Cl2	116.6 (3)	H31A—C31—H31C	109.5
C1—C6—Cl2	122.6 (3)	H31B—C31—H31C	109.5
C9—C7—N1	127.9 (3)	N3—C32—H32A	109.5
C9—C7—C8	107.8 (3)	N3—C32—H32B	109.5

N1—C7—C8	124.0 (3)	H32A—C32—H32B	109.5
O7—C8—N2	124.6 (3)	N3—C32—H32C	109.5
O7—C8—C7	130.3 (3)	H32A—C32—H32C	109.5
N2—C8—C7	105.0 (2)	H32B—C32—H32C	109.5
C7—C9—N3	111.3 (3)	C24—C33—H33A	109.5
C7—C9—C31	129.8 (3)	C24—C33—H33B	109.5
N3—C9—C31	118.8 (3)	H33A—C33—H33B	109.5
C15—C10—C11	119.7 (3)	C24—C33—H33C	109.5
C15—C10—N2	121.0 (3)	H33A—C33—H33C	109.5
C11—C10—N2	119.3 (3)	H33B—C33—H33C	109.5
C12—C11—C10	119.5 (3)	N6—C34—H34A	109.5
C12—C11—H11	120.3	N6—C34—H34B	109.5
C10—C11—H11	120.3	H34A—C34—H34B	109.5
C13—C12—C11	120.7 (3)	N6—C34—H34C	109.5
C13—C12—H12	119.7	H34A—C34—H34C	109.5
C11—C12—H12	119.7	H34B—C34—H34C	109.5
C12—C13—C14	120.2 (4)	C7—N1—S1	116.0 (2)
C12—C13—H13	119.9	C7—N1—Zn1	117.49 (19)
C14—C13—H13	119.9	S1—N1—Zn1	126.19 (14)
C13—C14—C15	119.7 (4)	C8—N2—C10	126.7 (3)
C13—C14—H14	120.2	C8—N2—N3	110.0 (2)
C15—C14—H14	120.2	C10—N2—N3	118.7 (2)
C14—C15—C10	120.3 (3)	C9—N3—N2	105.4 (2)
C14—C15—H15	119.8	C9—N3—C32	117.7 (3)
C10—C15—H15	119.8	N2—N3—C32	114.7 (3)
C17—C16—C21	118.8 (3)	C22—N4—S2	112.7 (2)
C17—C16—S2	117.0 (2)	C22—N4—Zn1	122.10 (19)
C21—C16—S2	124.1 (3)	S2—N4—Zn1	120.23 (14)
C18—C17—C16	120.1 (4)	C23—N5—N6	109.3 (2)
C18—C17—H17	120.0	C23—N5—C25	123.6 (2)
C16—C17—H17	120.0	N6—N5—C25	120.0 (2)
C19—C18—C17	121.1 (4)	C24—N6—N5	106.4 (2)
C19—C18—Cl3	120.5 (4)	C24—N6—C34	122.6 (3)
C17—C18—Cl3	118.4 (4)	N5—N6—C34	114.4 (3)
C18—C19—C20	119.7 (4)	Zn1—O1—H11O	120 (3)
C18—C19—H19	120.1	Zn1—O1—H12O	108 (3)
C20—C19—H19	120.1	H11O—O1—H12O	102 (2)
C19—C20—C21	120.0 (4)	Zn1—O2—H21O	110 (3)
C19—C20—H20	120.0	Zn1—O2—H22O	126 (4)
C21—C20—H20	120.0	H21O—O2—H22O	103 (3)
C20—C21—C16	120.2 (4)	O4—S1—O3	117.03 (15)
C20—C21—Cl4	118.1 (3)	O4—S1—N1	108.11 (14)
C16—C21—Cl4	121.6 (3)	O3—S1—N1	112.20 (14)
C24—C22—N4	128.6 (3)	O4—S1—C1	106.15 (16)
C24—C22—C23	107.6 (3)	O3—S1—C1	103.70 (15)
N4—C22—C23	123.8 (3)	N1—S1—C1	109.20 (14)
O8—C23—N5	123.1 (3)	O6—S2—O5	116.33 (15)
O8—C23—C22	131.0 (3)	O6—S2—N4	109.16 (14)

N5—C23—C22	105.9 (2)	O5—S2—N4	113.04 (14)
C22—C24—N6	110.0 (3)	O6—S2—C16	107.99 (15)
C22—C24—C33	129.9 (3)	O5—S2—C16	104.64 (15)
N6—C24—C33	120.1 (3)	N4—S2—C16	104.83 (14)
C30—C25—C26	120.9 (3)	O2—Zn1—N1	108.83 (12)
C30—C25—N5	121.0 (3)	O2—Zn1—O1	114.56 (15)
C26—C25—N5	118.0 (3)	N1—Zn1—O1	105.49 (11)
C27—C26—C25	119.1 (4)	O2—Zn1—N4	114.00 (13)
C27—C26—H26	120.4	N1—Zn1—N4	112.12 (10)
C25—C26—H26	120.4	O1—Zn1—N4	101.44 (11)

C6—C1—C2—C3	1.3 (5)	C11—C10—N2—C8	47.2 (5)
S1—C1—C2—C3	−175.7 (3)	C15—C10—N2—N3	19.4 (4)
C1—C2—C3—C4	0.8 (5)	C11—C10—N2—N3	−159.5 (3)
C1—C2—C3—Cl1	−179.6 (3)	C7—C9—N3—N2	3.9 (4)
C2—C3—C4—C5	−2.0 (5)	C31—C9—N3—N2	−178.1 (3)
Cl1—C3—C4—C5	178.4 (3)	C7—C9—N3—C32	133.2 (3)
C3—C4—C5—C6	1.2 (5)	C31—C9—N3—C32	−48.8 (5)
C4—C5—C6—C1	0.9 (5)	C8—N2—N3—C9	−6.6 (3)
C4—C5—C6—Cl2	−179.0 (3)	C10—N2—N3—C9	−164.0 (3)
C2—C1—C6—C5	−2.1 (5)	C8—N2—N3—C32	−137.7 (3)
S1—C1—C6—C5	174.7 (3)	C10—N2—N3—C32	65.0 (4)
C2—C1—C6—Cl2	177.8 (3)	C24—C22—N4—S2	−96.7 (3)
S1—C1—C6—Cl2	−5.4 (4)	C23—C22—N4—S2	85.3 (3)
C9—C7—C8—O7	172.7 (3)	C24—C22—N4—Zn1	108.1 (3)
N1—C7—C8—O7	−2.0 (5)	C23—C22—N4—Zn1	−69.8 (3)
C9—C7—C8—N2	−4.2 (3)	O8—C23—N5—N6	170.1 (3)
N1—C7—C8—N2	−178.8 (3)	C22—C23—N5—N6	−7.3 (3)
N1—C7—C9—N3	174.5 (3)	O8—C23—N5—C25	19.9 (5)
C8—C7—C9—N3	0.1 (4)	C22—C23—N5—C25	−157.6 (3)
N1—C7—C9—C31	−3.2 (6)	C30—C25—N5—C23	109.5 (4)
C8—C7—C9—C31	−177.7 (3)	C26—C25—N5—C23	−67.0 (4)
C15—C10—C11—C12	−0.7 (5)	C30—C25—N5—N6	−37.8 (4)
N2—C10—C11—C12	178.3 (3)	C26—C25—N5—N6	145.8 (3)
C10—C11—C12—C13	−0.5 (5)	C22—C24—N6—N5	−8.0 (3)
C11—C12—C13—C14	1.6 (6)	C33—C24—N6—N5	172.4 (3)
C12—C13—C14—C15	−1.4 (6)	C22—C24—N6—C34	−142.5 (3)
C13—C14—C15—C10	0.2 (6)	C33—C24—N6—C34	38.0 (4)
C11—C10—C15—C14	0.9 (5)	C23—N5—N6—C24	9.5 (3)
N2—C10—C15—C14	−178.1 (3)	C25—N5—N6—C24	161.0 (3)
C21—C16—C17—C18	0.5 (5)	C23—N5—N6—C34	148.1 (3)
S2—C16—C17—C18	176.4 (3)	C25—N5—N6—C34	−60.4 (4)
C16—C17—C18—C19	0.9 (6)	C7—N1—S1—O4	−164.9 (2)
C16—C17—C18—Cl3	−178.7 (3)	Zn1—N1—S1—O4	21.9 (2)
C17—C18—C19—C20	−1.1 (7)	C7—N1—S1—O3	−34.3 (3)
Cl3—C18—C19—C20	178.4 (4)	Zn1—N1—S1—O3	152.46 (17)
C18—C19—C20—C21	−0.1 (7)	C7—N1—S1—C1	80.1 (2)
C19—C20—C21—C16	1.5 (6)	Zn1—N1—S1—C1	−93.1 (2)

C19—C20—C21—Cl4	−176.6 (4)	C2—C1—S1—O4	133.1 (3)
C17—C16—C21—C20	−1.6 (5)	C6—C1—S1—O4	−43.7 (3)
S2—C16—C21—C20	−177.2 (3)	C2—C1—S1—O3	9.2 (3)
C17—C16—C21—Cl4	176.3 (3)	C6—C1—S1—O3	−167.6 (3)
S2—C16—C21—Cl4	0.8 (4)	C2—C1—S1—N1	−110.6 (3)
C24—C22—C23—O8	−174.8 (3)	C6—C1—S1—N1	72.6 (3)
N4—C22—C23—O8	3.5 (5)	C22—N4—S2—O6	−168.7 (2)
C24—C22—C23—N5	2.3 (3)	Zn1—N4—S2—O6	−13.0 (2)
N4—C22—C23—N5	−179.4 (3)	C22—N4—S2—O5	−37.5 (2)
N4—C22—C24—N6	−174.6 (3)	Zn1—N4—S2—O5	118.13 (17)
C23—C22—C24—N6	3.6 (3)	C22—N4—S2—C16	75.8 (2)
N4—C22—C24—C33	5.0 (5)	Zn1—N4—S2—C16	−128.50 (17)
C23—C22—C24—C33	−176.9 (3)	C17—C16—S2—O6	139.8 (2)
C30—C25—C26—C27	−1.1 (5)	C21—C16—S2—O6	−44.6 (3)
N5—C25—C26—C27	175.3 (3)	C17—C16—S2—O5	15.3 (3)
C25—C26—C27—C28	0.5 (6)	C21—C16—S2—O5	−169.1 (3)
C26—C27—C28—C29	0.7 (6)	C17—C16—S2—N4	−103.9 (3)
C27—C28—C29—C30	−1.3 (6)	C21—C16—S2—N4	71.7 (3)
C26—C25—C30—C29	0.5 (5)	C7—N1—Zn1—O2	165.5 (2)
N5—C25—C30—C29	−175.8 (3)	S1—N1—Zn1—O2	−21.4 (2)
C28—C29—C30—C25	0.7 (6)	C7—N1—Zn1—O1	−71.1 (2)
C9—C7—N1—S1	76.1 (4)	S1—N1—Zn1—O1	101.98 (19)
C8—C7—N1—S1	−110.3 (3)	C7—N1—Zn1—N4	38.4 (2)
C9—C7—N1—Zn1	−110.1 (3)	S1—N1—Zn1—N4	−148.45 (17)
C8—C7—N1—Zn1	63.5 (3)	C22—N4—Zn1—O2	163.1 (2)
O7—C8—N2—C10	−15.3 (5)	S2—N4—Zn1—O2	9.8 (2)
C7—C8—N2—C10	161.8 (3)	C22—N4—Zn1—N1	−72.6 (2)
O7—C8—N2—N3	−170.4 (3)	S2—N4—Zn1—N1	134.01 (15)
C7—C8—N2—N3	6.6 (3)	C22—N4—Zn1—O1	39.5 (2)
C15—C10—N2—C8	−133.8 (3)	S2—N4—Zn1—O1	−113.89 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11*O*···O5^{i}	0.88 (2)	2.52 (3)	3.277 (4)	145 (4)
O1—H12*O*···O8	0.90 (2)	2.06 (2)	2.914 (4)	160 (4)
O2—H21*O*···O4	0.88 (2)	2.22 (3)	2.928 (4)	137 (4)
O2—H22*O*···O8^{i}	0.88 (2)	2.05 (3)	2.868 (4)	154 (5)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.