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8-Hydroxy-2-methylquinolinium dichlorido(2-methylquinolin-8-olato-κ^2N,O)zincate(II) methanol solvate

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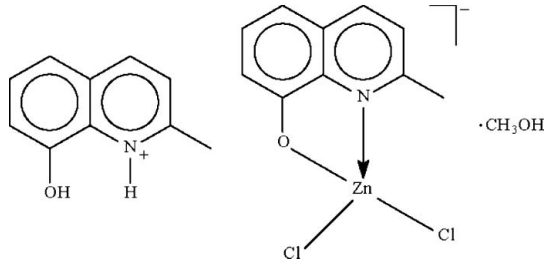
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 17.2.

The reaction of zinc chloride and 2-methyl-8-hydroxyquinoline in methanol yielded the title monosolvated salt, $(C_{10}H_{10}NO)[ZnCl_2(C_{10}H_8NO)]\cdot CH_3OH$, which has the Zn atom within a distorted Cl_2NO tetrahedral coordination geometry. Supramolecular chains feature in the crystal structure, comprising all components of the structure stabilized by a combination of O—H···O, N—H···O and O—H···Cl hydrogen bonding.

Related literature

Unlike 8-hydroxyquinoline, which yields a large number of metal derivatives, 2-methyl-8-hydroxyquinoline forms only a small number of metal chelates. Besides a related acetate salt (Sattarzadeh *et al.*, 2009), there is only one crystal structure report of another zinc derivative; for aquabis(2-methylquinolin-8-ato)zinc, see: da Silva *et al.* (2007).



Experimental

Crystal data

$(C_{10}H_{10}NO)[ZnCl_2(C_{10}H_8NO)]\cdot CH_4O$
M_r = 486.68
Monoclinic, $P2_1/n$
a = 10.0717 (2) Å
b = 13.7886 (3) Å
c = 15.4828 (3) Å
β = 105.48 (1)°
V = 2072.15 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.47 mm^{-1}
T = 100 K
0.32 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.651, T_{max} = 0.892
18982 measured reflections
4753 independent reflections
3600 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.02
4753 reflections
277 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2O···O1	0.84 (1)	1.70 (1)	2.534 (3)	177 (4)
O3—H3O···Cl1^{i}	0.84 (1)	2.47 (3)	3.239 (4)	153 (5)
N2—H2N···O3	0.88 (1)	1.87 (2)	2.727 (4)	163 (3)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2423).

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supporting information

Acta Cryst. (2009). E**65**, m553 [doi:10.1107/S1600536809014202]

8-Hydroxy-2-methylquinolinium dichlorido(2-methylquinolin-8-olato-κ^2N,O)zincate(II) methanol solvate

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S1. Experimental

Zinc chloride (0.10 g, 0.75 mmol) and 2-methyl-8-hydroxyquinoline (0.24 g, 1.5 mmol) were loaded into a convection tube; the tube was filled with dry methanol and kept at 333 K. Crystals were collected from the side arm after several days.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C). The O–H and N–H hydrogen atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.84±0.01 Å and N–H 0.88±01 Å; their temperature factors were freely refined.

The final difference Fourier map had a large peak/deep hole in the vicinity of the O3 atom.

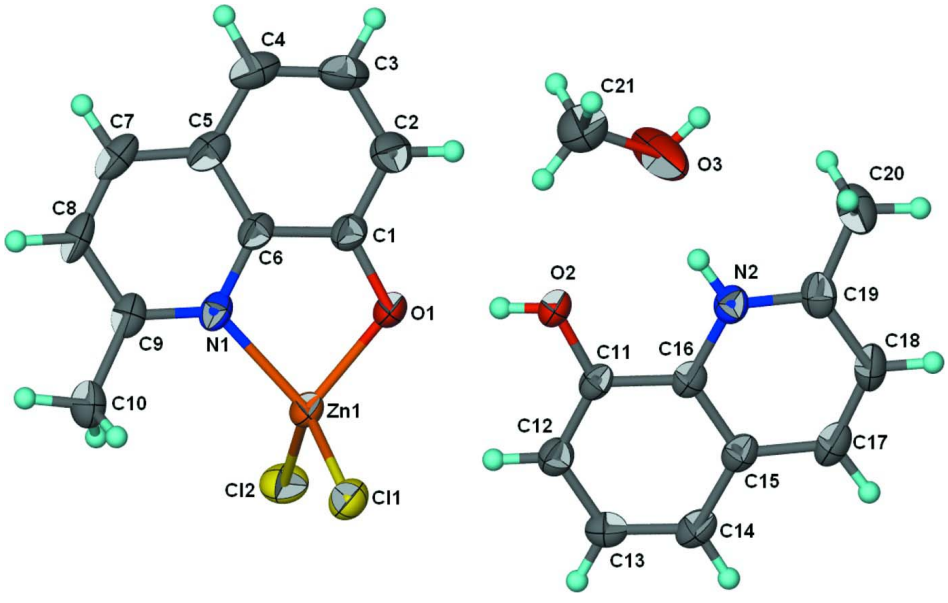

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $[C_{10}H_{10}NO][Zn(C_{10}H_8NO)Cl_2]\cdot CH_3OH$; ellipsoids are drawn at the 70% probability level and H atoms of arbitrary radius.

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Crystal data

$(C_{10}H_{10}NO)[ZnCl_2(C_{10}H_8NO)]\cdot CH_4O$
$M_r = 486.68$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.0717$ (2) Å
$b = 13.7886$ (3) Å
$c = 15.4828$ (3) Å
$\beta = 105.48$ (1)°
$V = 2072.15$ (7) Å^3
$Z = 4$
$F(000) = 1000$
$D_x = 1.560$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4908 reflections
$\theta = 2.6$–27.1°
$\mu = 1.47$ mm^{-1}
$T = 100$ K
Block, yellow
0.32 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.651$, $T_{max} = 0.892$
18982 measured reflections
4753 independent reflections
3600 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.5$°, $\theta_{min} = 2.0$°
$h = -13\rightarrow13$
$k = -17\rightarrow17$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.108$
$S = 1.02$
4753 reflections
277 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 2.8684P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.08$ e Å^{-3}
$\Delta\rho_{min} = -1.00$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.50382 (3)	0.63261 (3)	0.23689 (2)	0.02655 (11)
Cl1	0.48941 (8)	0.76378 (6)	0.31836 (5)	0.03149 (18)
Cl2	0.39683 (8)	0.50528 (6)	0.27699 (5)	0.03503 (19)
O1	0.6980 (2)	0.60686 (17)	0.23887 (13)	0.0318 (5)
O2	0.9135 (2)	0.63848 (15)	0.36428 (13)	0.0258 (4)
H2O	0.843 (3)	0.626 (3)	0.3225 (19)	0.054 (13)*
O3	1.1916 (3)	0.6985 (4)	0.3410 (2)	0.1114 (18)
H3O	1.2770 (14)	0.706 (5)	0.353 (4)	0.11 (2)*
N1	0.4760 (2)	0.63643 (17)	0.10133 (15)	0.0232 (5)
N2	1.1439 (2)	0.64419 (17)	0.49938 (16)	0.0239 (5)
H2N	1.143 (4)	0.657 (3)	0.4435 (10)	0.040 (10)*
C1	0.7143 (3)	0.6004 (2)	0.15652 (19)	0.0257 (6)

C2	0.8383 (3)	0.5781 (2)	0.1389 (2)	0.0345 (7)
H2	0.9178	0.5676	0.1872	0.041*
C3	0.8481 (3)	0.5708 (2)	0.0502 (2)	0.0363 (8)
H3	0.9347	0.5557	0.0401	0.044*
C4	0.7372 (4)	0.5847 (2)	−0.0217 (2)	0.0344 (7)
H4	0.7466	0.5793	−0.0810	0.041*
C5	0.6079 (3)	0.6075 (2)	−0.00683 (19)	0.0280 (6)
C6	0.5975 (3)	0.6156 (2)	0.08206 (18)	0.0238 (6)
C7	0.4857 (4)	0.6220 (2)	−0.0757 (2)	0.0324 (7)
H7	0.4873	0.6172	−0.1366	0.039*
C8	0.3656 (3)	0.6428 (2)	−0.05527 (19)	0.0303 (7)
H8	0.2839	0.6530	−0.1020	0.036*
C9	0.3619 (3)	0.6491 (2)	0.03512 (19)	0.0259 (6)
C10	0.2318 (3)	0.6695 (2)	0.0599 (2)	0.0322 (7)
H10A	0.2445	0.7264	0.0992	0.048*
H10B	0.2074	0.6134	0.0914	0.048*
H10C	0.1577	0.6823	0.0056	0.048*
C11	0.8990 (3)	0.61926 (19)	0.44627 (18)	0.0211 (5)
C12	0.7783 (3)	0.5956 (2)	0.46570 (19)	0.0254 (6)
H12	0.6953	0.5926	0.4189	0.031*
C13	0.7759 (3)	0.5758 (2)	0.5544 (2)	0.0267 (6)
H13	0.6909	0.5594	0.5664	0.032*
C14	0.8927 (3)	0.5795 (2)	0.62372 (19)	0.0279 (6)
H14	0.8887	0.5657	0.6831	0.033*
C15	1.0188 (3)	0.6040 (2)	0.60665 (18)	0.0241 (6)
C16	1.0214 (3)	0.62310 (19)	0.51737 (18)	0.0218 (6)
C17	1.1463 (3)	0.6076 (2)	0.6733 (2)	0.0300 (7)
H17	1.1488	0.5961	0.7342	0.036*
C18	1.2650 (3)	0.6276 (2)	0.6509 (2)	0.0309 (7)
H18	1.3496	0.6293	0.6964	0.037*
C19	1.2646 (3)	0.6457 (2)	0.5617 (2)	0.0284 (6)
C20	1.3919 (3)	0.6644 (3)	0.5335 (2)	0.0381 (8)
H20A	1.3932	0.6227	0.4825	0.057*
H20B	1.4726	0.6504	0.5834	0.057*
H20C	1.3940	0.7326	0.5158	0.057*
C21	1.1182 (4)	0.7302 (3)	0.2615 (2)	0.0478 (9)
H21C	1.1577	0.7911	0.2471	0.072*
H21B	1.0228	0.7413	0.2632	0.072*
H21A	1.1200	0.6817	0.2156	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02484 (18)	0.0370 (2)	0.01749 (17)	−0.00010 (14)	0.00511 (13)	0.00387 (14)
Cl1	0.0333 (4)	0.0367 (4)	0.0238 (3)	−0.0047 (3)	0.0066 (3)	−0.0003 (3)
Cl2	0.0401 (4)	0.0349 (4)	0.0342 (4)	−0.0009 (3)	0.0170 (3)	0.0076 (3)
O1	0.0251 (11)	0.0528 (14)	0.0170 (10)	−0.0012 (10)	0.0047 (8)	0.0001 (9)
O2	0.0260 (10)	0.0327 (11)	0.0173 (10)	−0.0003 (9)	0.0032 (8)	0.0002 (8)

O3	0.0368 (18)	0.240 (5)	0.063 (2)	0.040 (2)	0.0233 (16)	0.091 (3)
N1	0.0269 (12)	0.0231 (12)	0.0180 (11)	−0.0054 (10)	0.0029 (9)	0.0023 (9)
N2	0.0252 (12)	0.0233 (12)	0.0219 (12)	0.0037 (10)	0.0037 (10)	0.0026 (10)
C1	0.0268 (15)	0.0291 (15)	0.0212 (14)	−0.0070 (12)	0.0063 (11)	−0.0022 (11)
C2	0.0294 (16)	0.0411 (19)	0.0340 (17)	−0.0086 (14)	0.0100 (13)	−0.0070 (14)
C3	0.0348 (18)	0.0404 (19)	0.0404 (19)	−0.0108 (14)	0.0216 (15)	−0.0121 (15)
C4	0.048 (2)	0.0317 (17)	0.0290 (16)	−0.0104 (15)	0.0197 (15)	−0.0057 (13)
C5	0.0413 (17)	0.0217 (14)	0.0222 (14)	−0.0087 (12)	0.0108 (13)	0.0003 (11)
C6	0.0286 (15)	0.0237 (14)	0.0189 (13)	−0.0073 (11)	0.0062 (11)	−0.0001 (10)
C7	0.053 (2)	0.0247 (15)	0.0175 (14)	−0.0061 (14)	0.0055 (13)	−0.0002 (11)
C8	0.0424 (18)	0.0250 (15)	0.0162 (13)	−0.0023 (13)	−0.0050 (12)	0.0019 (11)
C9	0.0306 (15)	0.0206 (14)	0.0230 (14)	−0.0036 (11)	0.0009 (12)	0.0017 (11)
C10	0.0299 (16)	0.0333 (16)	0.0288 (16)	0.0019 (13)	−0.0001 (13)	0.0029 (13)
C11	0.0276 (14)	0.0176 (13)	0.0170 (12)	0.0024 (11)	0.0041 (11)	0.0006 (10)
C12	0.0271 (15)	0.0254 (14)	0.0227 (14)	0.0006 (11)	0.0048 (12)	−0.0022 (11)
C13	0.0295 (15)	0.0253 (15)	0.0281 (15)	0.0009 (12)	0.0123 (12)	0.0011 (12)
C14	0.0379 (17)	0.0252 (15)	0.0210 (14)	0.0042 (13)	0.0086 (12)	0.0017 (11)
C15	0.0306 (15)	0.0196 (13)	0.0209 (14)	0.0044 (11)	0.0049 (11)	−0.0026 (11)
C16	0.0266 (14)	0.0181 (13)	0.0199 (13)	0.0033 (11)	0.0047 (11)	−0.0005 (10)
C17	0.0380 (17)	0.0286 (16)	0.0198 (14)	0.0054 (13)	0.0016 (12)	−0.0013 (12)
C18	0.0282 (15)	0.0321 (16)	0.0260 (15)	0.0031 (13)	−0.0040 (12)	−0.0026 (12)
C19	0.0274 (15)	0.0230 (15)	0.0307 (16)	0.0033 (12)	0.0005 (12)	0.0000 (12)
C20	0.0264 (16)	0.0411 (19)	0.043 (2)	−0.0007 (14)	0.0029 (14)	0.0084 (15)
C21	0.048 (2)	0.057 (2)	0.040 (2)	−0.0010 (18)	0.0137 (17)	0.0023 (18)

Geometric parameters (Å, º)

Zn1—N1	2.043 (2)	C8—H8	0.9500
Zn1—O1	1.980 (2)	C9—C10	1.488 (4)
Zn1—Cl1	2.2318 (8)	C10—H10A	0.9800
Zn1—Cl2	2.2331 (8)	C10—H10B	0.9800
O1—C1	1.331 (3)	C10—H10C	0.9800
O2—C11	1.342 (3)	C11—C12	1.368 (4)
O2—H2O	0.841 (10)	C11—C16	1.418 (4)
O3—C21	1.329 (5)	C12—C13	1.407 (4)
O3—H3O	0.836 (10)	C12—H12	0.9500
N1—C9	1.332 (4)	C13—C14	1.365 (4)
N1—C6	1.365 (4)	C13—H13	0.9500
N2—C19	1.335 (4)	C14—C15	1.406 (4)
N2—C16	1.367 (4)	C14—H14	0.9500
N2—H2N	0.881 (10)	C15—C16	1.414 (4)
C1—C2	1.382 (4)	C15—C17	1.417 (4)
C1—C6	1.426 (4)	C17—C18	1.359 (5)
C2—C3	1.406 (4)	C17—H17	0.9500
C2—H2	0.9500	C18—C19	1.402 (4)
C3—C4	1.364 (5)	C18—H18	0.9500
C3—H3	0.9500	C19—C20	1.484 (4)
C4—C5	1.417 (5)	C20—H20A	0.9800

C4—H4	0.9500	C20—H20B	0.9800
C5—C7	1.411 (4)	C20—H20C	0.9800
C5—C6	1.412 (4)	C21—H21C	0.9800
C7—C8	1.360 (5)	C21—H21B	0.9800
C7—H7	0.9500	C21—H21A	0.9800
C8—C9	1.413 (4)		

O1—Zn1—N1	83.36 (9)	H10A—C10—H10B	109.5
O1—Zn1—Cl1	110.46 (7)	C9—C10—H10C	109.5
N1—Zn1—Cl1	123.24 (7)	H10A—C10—H10C	109.5
O1—Zn1—Cl2	113.75 (7)	H10B—C10—H10C	109.5
N1—Zn1—Cl2	111.22 (7)	O2—C11—C12	125.6 (3)
Cl1—Zn1—Cl2	111.78 (3)	O2—C11—C16	115.8 (2)
C1—O1—Zn1	111.79 (18)	C12—C11—C16	118.5 (3)
C11—O2—H2O	114 (3)	C11—C12—C13	120.6 (3)
C21—O3—H3O	117 (4)	C11—C12—H12	119.7
C9—N1—C6	119.9 (2)	C13—C12—H12	119.7
C9—N1—Zn1	130.4 (2)	C14—C13—C12	121.6 (3)
C6—N1—Zn1	109.52 (18)	C14—C13—H13	119.2
C19—N2—C16	123.6 (3)	C12—C13—H13	119.2
C19—N2—H2N	118 (2)	C13—C14—C15	119.6 (3)
C16—N2—H2N	118 (2)	C13—C14—H14	120.2
O1—C1—C2	123.6 (3)	C15—C14—H14	120.2
O1—C1—C6	118.6 (3)	C14—C15—C16	118.8 (3)
C2—C1—C6	117.8 (3)	C14—C15—C17	124.1 (3)
C1—C2—C3	120.7 (3)	C16—C15—C17	117.0 (3)
C1—C2—H2	119.6	N2—C16—C15	119.5 (3)
C3—C2—H2	119.6	N2—C16—C11	119.7 (2)
C4—C3—C2	122.2 (3)	C15—C16—C11	120.9 (3)
C4—C3—H3	118.9	C18—C17—C15	120.7 (3)
C2—C3—H3	118.9	C18—C17—H17	119.7
C3—C4—C5	119.0 (3)	C15—C17—H17	119.7
C3—C4—H4	120.5	C17—C18—C19	121.0 (3)
C5—C4—H4	120.5	C17—C18—H18	119.5
C7—C5—C6	116.7 (3)	C19—C18—H18	119.5
C7—C5—C4	124.2 (3)	N2—C19—C18	118.1 (3)
C6—C5—C4	119.1 (3)	N2—C19—C20	118.8 (3)
N1—C6—C5	122.2 (3)	C18—C19—C20	123.0 (3)
N1—C6—C1	116.6 (2)	C19—C20—H20A	109.5
C5—C6—C1	121.1 (3)	C19—C20—H20B	109.5
C8—C7—C5	120.3 (3)	H20A—C20—H20B	109.5
C8—C7—H7	119.8	C19—C20—H20C	109.5
C5—C7—H7	119.8	H20A—C20—H20C	109.5
C7—C8—C9	120.2 (3)	H20B—C20—H20C	109.5
C7—C8—H8	119.9	O3—C21—H21C	109.5
C9—C8—H8	119.9	O3—C21—H21B	109.5
N1—C9—C8	120.6 (3)	H21C—C21—H21B	109.5
N1—C9—C10	117.7 (3)	O3—C21—H21A	109.5

C8—C9—C10	121.7 (3)	H21C—C21—H21A	109.5
C9—C10—H10A	109.5	H21B—C21—H21A	109.5
C9—C10—H10B	109.5		

N1—Zn1—O1—C1	−2.8 (2)	C5—C7—C8—C9	−0.5 (4)
Cl1—Zn1—O1—C1	−125.81 (18)	C6—N1—C9—C8	−1.0 (4)
Cl2—Zn1—O1—C1	107.55 (19)	Zn1—N1—C9—C8	−175.8 (2)
O1—Zn1—N1—C9	178.1 (3)	C6—N1—C9—C10	178.7 (3)
Cl1—Zn1—N1—C9	−71.7 (3)	Zn1—N1—C9—C10	3.8 (4)
Cl2—Zn1—N1—C9	65.2 (3)	C7—C8—C9—N1	1.0 (4)
O1—Zn1—N1—C6	2.88 (18)	C7—C8—C9—C10	−178.6 (3)
Cl1—Zn1—N1—C6	113.03 (17)	O2—C11—C12—C13	179.2 (3)
Cl2—Zn1—N1—C6	−110.05 (17)	C16—C11—C12—C13	0.1 (4)
Zn1—O1—C1—C2	−176.7 (3)	C11—C12—C13—C14	0.1 (4)
Zn1—O1—C1—C6	2.2 (3)	C12—C13—C14—C15	0.1 (4)
O1—C1—C2—C3	178.9 (3)	C13—C14—C15—C16	−0.7 (4)
C6—C1—C2—C3	0.1 (5)	C13—C14—C15—C17	−178.4 (3)
C1—C2—C3—C4	−0.3 (5)	C19—N2—C16—C15	1.7 (4)
C2—C3—C4—C5	0.1 (5)	C19—N2—C16—C11	−177.4 (3)
C3—C4—C5—C7	−179.0 (3)	C14—C15—C16—N2	−178.1 (3)
C3—C4—C5—C6	0.3 (4)	C17—C15—C16—N2	−0.2 (4)
C9—N1—C6—C5	0.5 (4)	C14—C15—C16—C11	0.9 (4)
Zn1—N1—C6—C5	176.3 (2)	C17—C15—C16—C11	178.9 (2)
C9—N1—C6—C1	−178.4 (3)	O2—C11—C16—N2	−0.8 (4)
Zn1—N1—C6—C1	−2.6 (3)	C12—C11—C16—N2	178.4 (2)
C7—C5—C6—N1	−0.1 (4)	O2—C11—C16—C15	−179.9 (2)
C4—C5—C6—N1	−179.4 (3)	C12—C11—C16—C15	−0.7 (4)
C7—C5—C6—C1	178.8 (3)	C14—C15—C17—C18	177.0 (3)
C4—C5—C6—C1	−0.6 (4)	C16—C15—C17—C18	−0.8 (4)
O1—C1—C6—N1	0.4 (4)	C15—C17—C18—C19	0.5 (5)
C2—C1—C6—N1	179.3 (3)	C16—N2—C19—C18	−2.0 (4)
O1—C1—C6—C5	−178.6 (3)	C16—N2—C19—C20	176.8 (3)
C2—C1—C6—C5	0.4 (4)	C17—C18—C19—N2	0.9 (4)
C6—C5—C7—C8	0.1 (4)	C17—C18—C19—C20	−177.8 (3)
C4—C5—C7—C8	179.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*O*···O1	0.84 (1)	1.70 (1)	2.534 (3)	177 (4)
O3—H3*O*···Cl1^{i}	0.84 (1)	2.47 (3)	3.239 (4)	153 (5)
N2—H2*N*···O3	0.88 (1)	1.87 (2)	2.727 (4)	163 (3)

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