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Salicylato[tris(*N*-methylbenzimidazol-2-ylmethyl)amine]zinc(II) perchlorate dimethylformamide sesquisolvate

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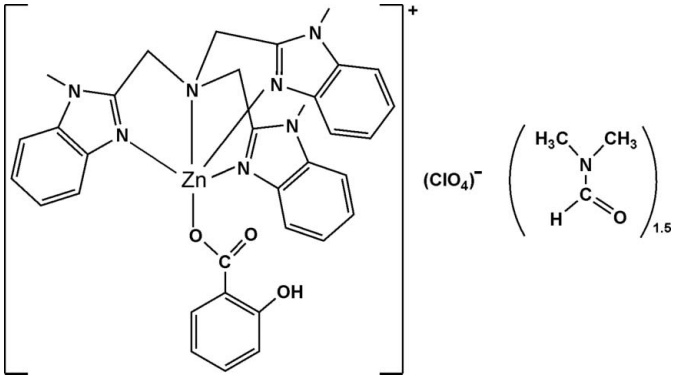
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.047; wR factor = 0.142; data-to-parameter ratio = 16.3.

In the title complex, $[Zn(C_7H_5O_3)(C_{27}H_{27}N_7)]ClO_4\cdot 1.5C_3H_7NO$, the Zn^{II} atom is five-coordinated by four N atoms from a tris(*N*-methylbenzimidazol-2-ylmethyl)amine ligand and one O atom from a salicylate ligand in a distorted trigonal-bipyramidal geometry (τ parameter = 0.84), with approximate molecular C_3 symmetry. One dimethylformamide molecule lies on a general position and is disordered over two coplanar orientations with equal occupancy. A second dimethylformamide molecule is disordered about a twofold rotation axis.

Related literature

For related literature, see: Addison *et al.* (1984); Youngme *et al.* (2007).



Experimental

Crystal data

$[Zn(C_7H_5O_3)(C_{27}H_{27}N_7)]ClO_4\cdot 1.5C_3H_7NO$
M_r = 861.13
Monoclinic, $C2/c$
a = 27.7110 (7) Å
b = 11.4499 (3) Å
c = 25.1395 (6) Å
β = 102.829 (1)°
V = 7777.3 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 153 (2) K
0.78 × 0.59 × 0.52 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.568, T_{max} = 0.670
37173 measured reflections
8884 independent reflections
7743 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.142
S = 1.06
8884 reflections
544 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.84	1.82	2.556 (3)	146

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2253).

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supporting information

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S1. Comment

The asymmetric unit of the title compound consists of a discrete $[Zn(Mentb)(salicylate)]^+$ cation (Mentb = tris(*N*-methylbenzimidazol-2-ylmethyl)amine) (Fig. 1), a perchlorate anion and 1.5 DMF molecules. The Zn^{II} atom is five-coordinated with a N_4O ligand set. The Mentb ligand acts as a tetradentate N-donor, and an O atom from the carboxylate group of the salicylate ligand completes the coordination. The geometry is best described as distorted trigonal bipyramidal (τ = 0.84, where β = O1—Zn—N7, α = N5—Zn—N1; Addison *et al.*, 1984). The equatorial plane is occupied by three N atoms of three benzimidazolyl groups, while the Zn^{II} atom is displaced towards O1 and is 0.560 (2) Å from the plane of atoms N1/N3/N5. The axial positions are occupyied by N7 and O1, with Zn—N7 = 2.434 (2) Å, Zn—O1 = 1.9974 (18) Å and O1—Zn—N7 = 165.76 (7) °. The three benzimidazole ring arms of the Mentb ligand form a cone-shaped cavity. The angles N3—Zn—N1, N5—Zn—N1 and N5—Zn—N3 are 113.00 (8), 115.30 (7) and 110.38 (8) °, respectively. The angles N7—Zn—N1 = 73.11 (7), N7—Zn—N3 = 74.69 (8) and N7—Zn—N5 = 74.93 (7) ° are all *ca* 16° less than the ideal value of 90°. This is imposed by the geometry of the Mentb ligand. The distance between Zn^{II} and O2 is 3.136 (2) °, so O2 is not coordinated.

S2. Experimental

To a stirred solution of tris(*N*-methylbenzimidazol-2-ylmethyl)amine (0.0899 g, 0.2 mmol) in hot MeOH (10 ml) was added $Zn(ClO_4)_2.6H_2O$ (0.0745 g, 0.2 mmol), followed by a solution of Na(salicylate) (0.0320 g, 0.2 mmol) in MeOH (5 ml). A colourless crystalline product formed rapidly. The precipitate was filtered off, washed with MeOH and absolute Et_2O, and dried *in vacuo*. The dried precipitate was dissolved in DMF to give a colourless solution that was allowed to evaporate at room temperature. Colourless crystals suitable for X-ray analysis were obtained after two weeks. Yield 0.085 g (49%). Elemental analysis found: C 53.74, H 5.01, N 13.66; calculated: C 53.70, H 4.97, N 13.83.

S3. Refinement

All H atoms associated with the cation were visible in difference Fourier maps but were placed geometrically with C—H distances in the range 0.95–0.98 Å and O—H = 0.82 Å. They were allowed to ride during subsequent refinement with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C/O). The DMF molecule on the general position is refined in two coplanar orientations, each with 50% site occupancy. The DMF molecule lying on the twofold rotation axis is modelled as one molecule with 50% site occupancy, with bond distances tightly restrained (C40—O9 = 1.200 (5), C40—N9 = 1.320 (5), N9—C37/C38 = 1.420 (5) Å) and the whole molecule restrained to be planar. The atoms of this molecule are refined with isotropic displacement parameters. The largest peak in the residual electron density (1.25 e $Å^{-3}$) is associated with the perchlorate anion.

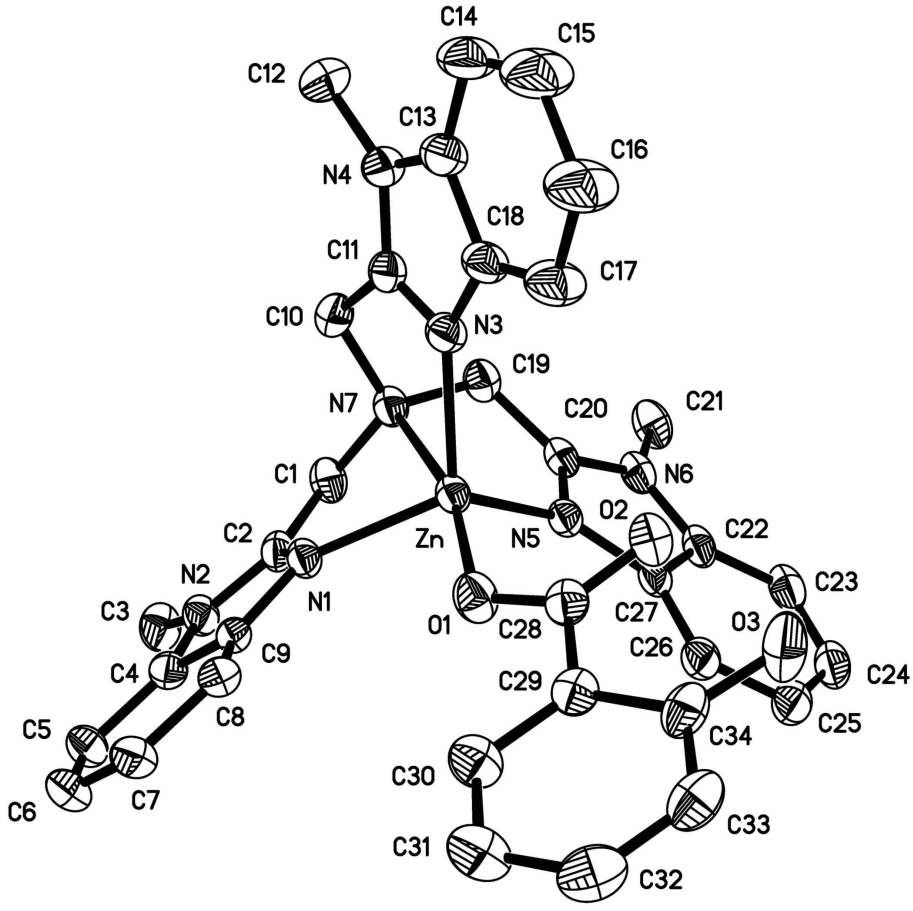

Figure 1

The $[C_{34}H_{32}N_7O_3Zn]^+$ cation with displacement ellipsoids drawn at the 50% probability level. H atoms are omitted.

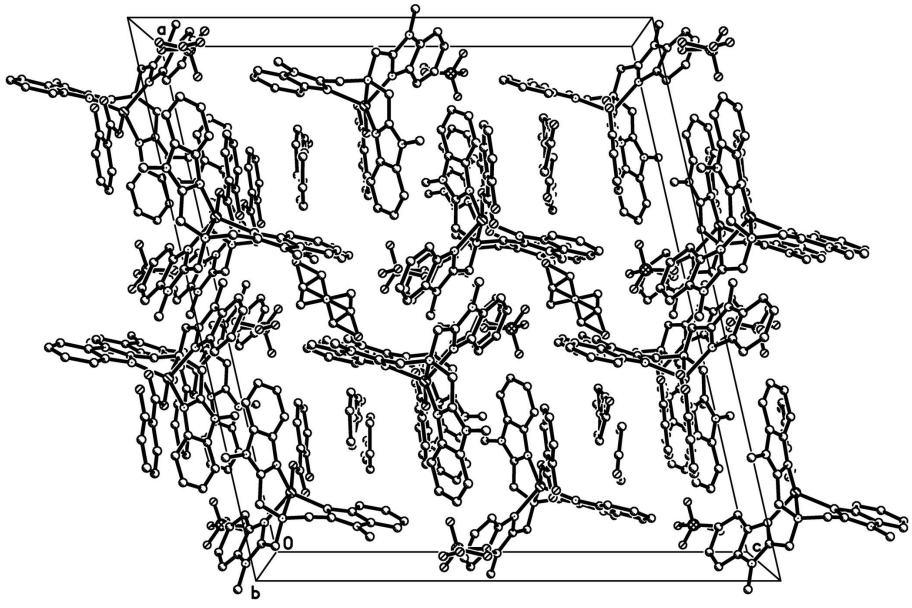

Figure 2

Packing diagram. H atoms are omitted for clarity.

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$M_r = 861.13$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 27.7110\ (7)$ Å
$b = 11.4499\ (3)$ Å
$c = 25.1395\ (6)$ Å
$\beta = 102.829\ (1)°$
$V = 7777.3\ (3)$ Å^3
$Z = 8$
$F(000) = 3584$
$D_x = 1.471$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 30068 reflections
$\theta = 3.0–27.5°$
$\mu = 0.77$ mm^{-1}
$T = 153$ K
Block, colourless
0.78 × 0.59 × 0.52 mm

Data collection

Rigaku R-AXIS Spider diffractometer
Radiation source: Rotating Anode
Graphite monochromator
ω scans
Absorption correction: empirical (using intensity measurements) (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.568$, $T_{max} = 0.670$
37173 measured reflections
8884 independent reflections
7743 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -35\rightarrow34$
$k = -14\rightarrow14$
$l = -32\rightarrow32$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.142$
$S = 1.06$
8884 reflections
544 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0822P)^2 + 15.4526P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.25$ e Å^{-3}
$\Delta\rho_{min} = -0.89$ 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}	Occ. (<1)
Zn	0.642944 (9)	0.84620 (2)	0.589173 (10)	0.02240 (10)	

O1	0.68899 (7)	0.98268 (15)	0.60013 (8)	0.0327 (4)
O2	0.63215 (7)	1.11523 (17)	0.60677 (8)	0.0335 (4)
O3	0.65424 (8)	1.33229 (17)	0.61367 (10)	0.0452 (5)
H3	0.6356	1.2737	0.6080	0.068*
N1	0.69813 (7)	0.73107 (17)	0.57875 (7)	0.0241 (4)
N2	0.72204 (8)	0.58518 (18)	0.53190 (8)	0.0277 (4)
N3	0.61492 (7)	0.80785 (19)	0.65594 (8)	0.0274 (4)
N4	0.58855 (8)	0.6825 (2)	0.71070 (9)	0.0326 (5)
N5	0.58658 (7)	0.87034 (17)	0.52174 (8)	0.0246 (4)
N6	0.51398 (7)	0.81871 (19)	0.46920 (8)	0.0283 (4)
N7	0.60436 (7)	0.65516 (17)	0.57040 (8)	0.0265 (4)
C1	0.63200 (9)	0.5940 (2)	0.53531 (10)	0.0296 (5)
H1A	0.6167	0.6093	0.4965	0.036*
H1B	0.6313	0.5088	0.5417	0.036*
C2	0.68426 (9)	0.6371 (2)	0.54853 (9)	0.0258 (5)
C3	0.71939 (11)	0.4822 (2)	0.49674 (11)	0.0370 (6)
H3A	0.6863	0.4772	0.4728	0.056*
H3B	0.7258	0.4118	0.5194	0.056*
H3C	0.7442	0.4889	0.4746	0.056*
C4	0.76425 (9)	0.6482 (2)	0.55369 (10)	0.0278 (5)
C5	0.81354 (10)	0.6319 (2)	0.55133 (11)	0.0358 (6)
H5A	0.8234	0.5697	0.5311	0.043*
C6	0.84742 (10)	0.7109 (3)	0.57999 (12)	0.0390 (6)
H6A	0.8814	0.7026	0.5795	0.047*
C7	0.83287 (9)	0.8028 (3)	0.60969 (11)	0.0343 (5)
H7A	0.8572	0.8554	0.6288	0.041*
C8	0.78364 (9)	0.8186 (2)	0.61178 (10)	0.0286 (5)
H8A	0.7738	0.8809	0.6320	0.034*
C9	0.74914 (8)	0.7397 (2)	0.58307 (9)	0.0246 (4)
C10	0.60888 (10)	0.6025 (2)	0.62449 (10)	0.0320 (5)
H10A	0.6415	0.5638	0.6362	0.038*
H10B	0.5827	0.5431	0.6233	0.038*
C11	0.60377 (9)	0.6977 (2)	0.66370 (10)	0.0286 (5)
C12	0.57507 (12)	0.5739 (3)	0.73413 (13)	0.0446 (7)
H12A	0.5709	0.5118	0.7066	0.067*
H12B	0.5439	0.5848	0.7459	0.067*
H12C	0.6013	0.5520	0.7656	0.067*
C13	0.59040 (9)	0.7902 (3)	0.73574 (10)	0.0337 (5)
C14	0.57910 (12)	0.8243 (3)	0.78500 (12)	0.0449 (7)
H14A	0.5673	0.7702	0.8078	0.054*
C15	0.58600 (15)	0.9400 (3)	0.79865 (13)	0.0559 (9)
H15A	0.5792	0.9666	0.8320	0.067*
C16	0.60278 (15)	1.0198 (3)	0.76492 (13)	0.0548 (9)
H16A	0.6073	1.0990	0.7761	0.066*
C17	0.61307 (12)	0.9863 (3)	0.71506 (11)	0.0412 (6)
H17A	0.6238	1.0412	0.6918	0.049*
C18	0.60686 (9)	0.8693 (2)	0.70125 (10)	0.0311 (5)
C19	0.55290 (9)	0.6784 (2)	0.54270 (10)	0.0292 (5)

H19A	0.5321	0.6865	0.5699	0.035*	
H19B	0.5398	0.6129	0.5180	0.035*	
C20	0.55155 (8)	0.7890 (2)	0.51075 (9)	0.0255 (4)	
C21	0.47023 (9)	0.7481 (3)	0.44612 (11)	0.0361 (6)	
H21A	0.4623	0.6980	0.4746	0.054*	
H21B	0.4770	0.6995	0.4165	0.054*	
H21C	0.4421	0.7997	0.4318	0.054*	
C22	0.52469 (9)	0.9281 (2)	0.45136 (10)	0.0287 (5)	
C23	0.49815 (10)	1.0003 (3)	0.41024 (10)	0.0357 (6)	
H23A	0.4668	0.9782	0.3887	0.043*	
C24	0.51999 (11)	1.1051 (3)	0.40270 (10)	0.0386 (6)	
H24A	0.5032	1.1569	0.3752	0.046*	
C25	0.56648 (11)	1.1380 (2)	0.43449 (11)	0.0361 (6)	
H25A	0.5806	1.2105	0.4275	0.043*	
C26	0.59215 (10)	1.0664 (2)	0.47582 (10)	0.0303 (5)	
H26A	0.6234	1.0889	0.4975	0.036*	
C27	0.57034 (9)	0.9600 (2)	0.48429 (9)	0.0266 (5)	
C28	0.67578 (9)	1.0869 (2)	0.60680 (9)	0.0274 (5)	
C29	0.71459 (9)	1.1799 (2)	0.61504 (9)	0.0270 (5)	
C30	0.76458 (10)	1.1524 (2)	0.62053 (11)	0.0344 (6)	
H30A	0.7739	1.0729	0.6186	0.041*	
C31	0.80082 (11)	1.2376 (3)	0.62864 (12)	0.0419 (6)	
H31A	0.8345	1.2173	0.6315	0.050*	
C32	0.78700 (12)	1.3540 (3)	0.63254 (12)	0.0423 (7)	
H32A	0.8116	1.4133	0.6385	0.051*	
C33	0.73832 (11)	1.3838 (2)	0.62789 (11)	0.0377 (6)	
H33A	0.7295	1.4633	0.6309	0.045*	
C34	0.70162 (10)	1.2980 (2)	0.61868 (10)	0.0318 (5)	
O8	0.69099 (12)	0.5249 (3)	0.73406 (12)	0.0713 (8)	0.50
N8	0.71843 (9)	0.3398 (2)	0.75385 (10)	0.0411 (6)	0.50
C35	0.6706 (3)	0.2884 (8)	0.7451 (3)	0.063 (2)	0.50
H35A	0.6453	0.3497	0.7367	0.095*	0.50
H35B	0.6671	0.2466	0.7781	0.095*	0.50
H35C	0.6662	0.2336	0.7145	0.095*	0.50
C36	0.7606 (4)	0.2671 (9)	0.7667 (3)	0.065 (2)	0.50
H36A	0.7906	0.3150	0.7714	0.098*	0.50
H36B	0.7598	0.2112	0.7370	0.098*	0.50
H36C	0.7607	0.2247	0.8006	0.098*	0.50
C37	0.7223 (3)	0.4587 (6)	0.7472 (3)	0.0459 (14)	0.50
H37A	0.7549	0.4894	0.7544	0.055*	0.50
O8A	0.69099 (12)	0.5249 (3)	0.73406 (12)	0.0713 (8)	0.50
N8A	0.71843 (9)	0.3398 (2)	0.75385 (10)	0.0411 (6)	0.50
C35A	0.7024 (3)	0.2147 (6)	0.7536 (3)	0.0605 (19)	0.50
H35D	0.6662	0.2105	0.7433	0.091*	0.50
H35E	0.7140	0.1812	0.7900	0.091*	0.50
H35F	0.7164	0.1706	0.7272	0.091*	0.50
C36A	0.7705 (3)	0.3607 (11)	0.7684 (3)	0.070 (3)	0.50
H36D	0.7768	0.4447	0.7673	0.106*	0.50

H36E	0.7866	0.3204	0.7426	0.106*	0.50
H36F	0.7839	0.3311	0.8053	0.106*	0.50
C37A	0.6847 (2)	0.4201 (6)	0.7380 (2)	0.0434 (13)	0.50
H37B	0.6514	0.3937	0.7284	0.052*	0.50
Cl	0.55496 (2)	0.47015 (6)	0.39812 (3)	0.04424 (18)	
O4	0.55287 (14)	0.5918 (3)	0.3936 (3)	0.138 (2)	
O5	0.54976 (15)	0.4453 (4)	0.45323 (14)	0.1082 (15)	
O6	0.51871 (11)	0.4007 (3)	0.36312 (11)	0.0824 (10)	
O7	0.60198 (10)	0.4316 (3)	0.39497 (16)	0.0792 (9)	
O9	0.5677 (4)	0.3054 (9)	0.7066 (4)	0.129 (3)*	0.50
N9	0.5000	0.2510 (5)	0.7500	0.1004 (19)*	
C38	0.4819 (6)	0.2026 (13)	0.6968 (3)	0.137 (5)*	0.50
H38A	0.5054	0.2186	0.6749	0.205*	0.50
H38B	0.4777	0.1197	0.6993	0.205*	0.50
H38C	0.4507	0.2379	0.6803	0.205*	0.50
C39	0.4779 (5)	0.2491 (11)	0.7952 (4)	0.130 (5)*	0.50
H39A	0.4990	0.2885	0.8253	0.195*	0.50
H39B	0.4464	0.2877	0.7862	0.195*	0.50
H39C	0.4734	0.1695	0.8052	0.195*	0.50
C40	0.5431 (2)	0.2957 (8)	0.7421 (5)	0.105 (4)*	0.50
H40A	0.5606	0.3324	0.7751	0.127*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.02145 (15)	0.02387 (15)	0.02202 (15)	0.00371 (9)	0.00515 (10)	−0.00118 (9)
O1	0.0295 (9)	0.0263 (8)	0.0419 (10)	0.0001 (7)	0.0071 (7)	−0.0061 (7)
O2	0.0291 (9)	0.0330 (9)	0.0372 (9)	0.0053 (7)	0.0047 (7)	−0.0021 (8)
O3	0.0413 (11)	0.0296 (10)	0.0596 (13)	0.0084 (8)	−0.0002 (10)	0.0013 (9)
N1	0.0234 (9)	0.0259 (9)	0.0233 (9)	0.0055 (7)	0.0059 (7)	−0.0002 (7)
N2	0.0313 (10)	0.0286 (10)	0.0245 (9)	0.0082 (8)	0.0092 (8)	−0.0014 (8)
N3	0.0259 (10)	0.0322 (10)	0.0249 (9)	0.0029 (8)	0.0071 (8)	0.0002 (8)
N4	0.0295 (11)	0.0393 (12)	0.0298 (10)	0.0036 (9)	0.0087 (9)	0.0072 (9)
N5	0.0241 (9)	0.0265 (9)	0.0238 (9)	0.0054 (7)	0.0069 (7)	0.0002 (7)
N6	0.0216 (9)	0.0347 (11)	0.0277 (10)	0.0056 (8)	0.0032 (8)	−0.0040 (8)
N7	0.0255 (10)	0.0257 (10)	0.0283 (10)	0.0046 (7)	0.0062 (8)	−0.0007 (7)
C1	0.0283 (12)	0.0286 (12)	0.0307 (12)	0.0046 (9)	0.0038 (9)	−0.0057 (9)
C2	0.0293 (12)	0.0257 (11)	0.0224 (10)	0.0088 (9)	0.0058 (9)	0.0014 (8)
C3	0.0478 (15)	0.0342 (13)	0.0303 (12)	0.0124 (11)	0.0112 (11)	−0.0058 (10)
C4	0.0315 (12)	0.0307 (12)	0.0235 (11)	0.0070 (9)	0.0114 (9)	0.0040 (9)
C5	0.0347 (13)	0.0404 (14)	0.0376 (14)	0.0125 (11)	0.0196 (11)	0.0055 (11)
C6	0.0271 (12)	0.0509 (16)	0.0432 (14)	0.0072 (11)	0.0167 (11)	0.0094 (12)
C7	0.0264 (12)	0.0414 (14)	0.0367 (13)	−0.0004 (10)	0.0101 (10)	0.0069 (11)
C8	0.0287 (12)	0.0316 (12)	0.0265 (11)	0.0024 (9)	0.0085 (9)	0.0055 (9)
C9	0.0247 (11)	0.0287 (11)	0.0220 (10)	0.0065 (9)	0.0085 (8)	0.0070 (8)
C10	0.0351 (13)	0.0272 (12)	0.0337 (12)	0.0050 (10)	0.0076 (10)	0.0048 (10)
C11	0.0233 (11)	0.0351 (13)	0.0263 (11)	0.0049 (9)	0.0035 (9)	0.0048 (9)
C12	0.0470 (16)	0.0453 (16)	0.0446 (15)	0.0019 (13)	0.0168 (13)	0.0162 (13)

C13	0.0287 (12)	0.0442 (15)	0.0292 (12)	0.0026 (10)	0.0088 (10)	0.0030 (11)
C14	0.0477 (17)	0.0611 (19)	0.0303 (13)	0.0009 (14)	0.0182 (12)	0.0038 (13)
C15	0.078 (2)	0.061 (2)	0.0372 (15)	−0.0008 (18)	0.0312 (16)	−0.0073 (14)
C16	0.080 (2)	0.0500 (18)	0.0432 (16)	−0.0056 (17)	0.0333 (17)	−0.0124 (14)
C17	0.0524 (17)	0.0439 (15)	0.0329 (13)	−0.0032 (13)	0.0213 (12)	−0.0076 (11)
C18	0.0295 (12)	0.0409 (14)	0.0242 (11)	0.0034 (10)	0.0089 (10)	−0.0004 (10)
C19	0.0245 (11)	0.0278 (11)	0.0344 (12)	0.0011 (9)	0.0043 (9)	−0.0017 (9)
C20	0.0213 (10)	0.0299 (11)	0.0252 (10)	0.0049 (9)	0.0051 (8)	−0.0041 (9)
C21	0.0233 (11)	0.0436 (15)	0.0374 (13)	0.0034 (10)	−0.0019 (10)	−0.0084 (11)
C22	0.0273 (11)	0.0330 (12)	0.0263 (11)	0.0114 (9)	0.0069 (9)	−0.0020 (9)
C23	0.0326 (13)	0.0488 (15)	0.0253 (11)	0.0171 (11)	0.0052 (10)	0.0004 (11)
C24	0.0450 (15)	0.0448 (15)	0.0281 (12)	0.0227 (12)	0.0126 (11)	0.0065 (11)
C25	0.0495 (16)	0.0327 (13)	0.0304 (12)	0.0126 (11)	0.0182 (12)	0.0036 (10)
C26	0.0347 (12)	0.0297 (12)	0.0288 (11)	0.0073 (10)	0.0119 (10)	−0.0005 (9)
C27	0.0291 (11)	0.0291 (11)	0.0236 (10)	0.0105 (9)	0.0101 (9)	−0.0005 (9)
C28	0.0301 (12)	0.0296 (12)	0.0213 (10)	0.0027 (9)	0.0035 (9)	−0.0012 (9)
C29	0.0325 (12)	0.0282 (11)	0.0194 (10)	0.0005 (9)	0.0041 (9)	−0.0031 (8)
C30	0.0364 (14)	0.0335 (13)	0.0347 (13)	−0.0007 (10)	0.0107 (11)	−0.0085 (10)
C31	0.0359 (14)	0.0460 (16)	0.0461 (15)	−0.0059 (12)	0.0142 (12)	−0.0104 (13)
C32	0.0512 (17)	0.0389 (15)	0.0367 (14)	−0.0137 (12)	0.0094 (13)	−0.0042 (11)
C33	0.0508 (16)	0.0274 (12)	0.0321 (13)	−0.0027 (11)	0.0032 (12)	0.0007 (10)
C34	0.0415 (14)	0.0282 (12)	0.0226 (11)	0.0032 (10)	0.0007 (10)	0.0022 (9)
O8	0.082 (2)	0.0578 (17)	0.0711 (18)	0.0077 (15)	0.0106 (15)	−0.0054 (14)
N8	0.0391 (13)	0.0522 (15)	0.0294 (11)	0.0040 (10)	0.0025 (10)	−0.0025 (10)
C35	0.072 (5)	0.068 (5)	0.049 (4)	−0.033 (4)	0.012 (3)	−0.014 (3)
C36	0.082 (6)	0.074 (5)	0.036 (3)	0.031 (5)	0.008 (3)	0.004 (4)
C37	0.051 (4)	0.041 (3)	0.040 (3)	−0.005 (3)	0.000 (3)	0.000 (2)
O8A	0.082 (2)	0.0578 (17)	0.0711 (18)	0.0077 (15)	0.0106 (15)	−0.0054 (14)
N8A	0.0391 (13)	0.0522 (15)	0.0294 (11)	0.0040 (10)	0.0025 (10)	−0.0025 (10)
C35A	0.097 (6)	0.048 (4)	0.037 (3)	0.012 (4)	0.016 (3)	−0.004 (3)
C36A	0.030 (3)	0.139 (9)	0.039 (4)	0.010 (4)	0.002 (3)	−0.009 (5)
C37A	0.033 (3)	0.054 (4)	0.040 (3)	0.002 (3)	0.003 (2)	−0.007 (3)
Cl	0.0316 (3)	0.0346 (3)	0.0695 (5)	−0.0046 (2)	0.0177 (3)	−0.0068 (3)
O4	0.079 (2)	0.0514 (19)	0.297 (7)	0.0192 (16)	0.071 (3)	0.042 (3)
O5	0.115 (3)	0.149 (3)	0.073 (2)	−0.080 (3)	0.0485 (19)	−0.056 (2)
O6	0.0594 (17)	0.125 (3)	0.0562 (16)	−0.0395 (18)	−0.0005 (13)	−0.0057 (17)
O7	0.0457 (14)	0.0543 (15)	0.146 (3)	0.0046 (11)	0.0397 (17)	−0.0089 (17)

Geometric parameters (Å, º)

Zn—O1	1.9974 (18)	C21—H21C	0.980
Zn—N3	2.047 (2)	C22—C27	1.398 (3)
Zn—N5	2.0528 (19)	C22—C23	1.398 (3)
Zn—N1	2.0791 (18)	C23—C24	1.376 (4)
Zn—N7	2.434 (2)	C23—H23A	0.950
O1—C28	1.270 (3)	C24—C25	1.408 (4)
O2—C28	1.252 (3)	C24—H24A	0.950
O3—C34	1.349 (3)	C25—C26	1.389 (4)

O3—H3	0.840	C25—H25A	0.950
N1—C2	1.323 (3)	C26—C27	1.397 (4)
N1—C9	1.397 (3)	C26—H26A	0.950
N2—C2	1.349 (3)	C28—C29	1.495 (3)
N2—C4	1.380 (3)	C29—C30	1.397 (4)
N2—C3	1.465 (3)	C29—C34	1.407 (3)
N3—C11	1.323 (3)	C30—C31	1.383 (4)
N3—C18	1.399 (3)	C30—H30A	0.950
N4—C11	1.351 (3)	C31—C32	1.397 (4)
N4—C13	1.381 (4)	C31—H31A	0.950
N4—C12	1.460 (4)	C32—C33	1.371 (4)
N5—C20	1.329 (3)	C32—H32A	0.950
N5—C27	1.398 (3)	C33—C34	1.396 (4)
N6—C20	1.344 (3)	C33—H33A	0.950
N6—C22	1.384 (3)	O8—C37	1.144 (7)
N6—C21	1.465 (3)	N8—C37	1.378 (7)
N7—C19	1.466 (3)	N8—C36	1.412 (8)
N7—C10	1.467 (3)	N8—C35	1.423 (7)
N7—C1	1.468 (3)	C35—H35A	0.980
C1—C2	1.496 (3)	C35—H35B	0.980
C1—H1A	0.990	C35—H35C	0.980
C1—H1B	0.990	C36—H36A	0.980
C3—H3A	0.980	C36—H36B	0.980
C3—H3B	0.980	C36—H36C	0.980
C3—H3C	0.980	C37—H37A	0.950
C4—C5	1.393 (4)	C35A—H35D	0.980
C4—C9	1.399 (3)	C35A—H35E	0.980
C5—C6	1.386 (4)	C35A—H35F	0.980
C5—H5A	0.950	C36A—H36D	0.980
C6—C7	1.400 (4)	C36A—H36E	0.980
C6—H6A	0.950	C36A—H36F	0.980
C7—C8	1.389 (3)	C37A—H37B	0.950
C7—H7A	0.950	Cl—O7	1.394 (3)
C8—C9	1.394 (3)	Cl—O4	1.398 (3)
C8—H8A	0.950	Cl—O6	1.423 (3)
C10—C11	1.498 (4)	Cl—O5	1.453 (3)
C10—H10A	0.990	O9—C40	1.242 (5)
C10—H10B	0.990	O9—C39^{i}	1.410 (14)
C12—H12A	0.980	N9—C40	1.355 (5)
C12—H12B	0.980	N9—C40^{i}	1.355 (5)
C12—H12C	0.980	N9—C39	1.407 (5)
C13—C18	1.398 (4)	N9—C39^{i}	1.407 (5)
C13—C14	1.399 (4)	N9—C38^{i}	1.431 (5)
C14—C15	1.371 (5)	N9—C38	1.431 (5)
C14—H14A	0.950	C38—C39^{i}	1.210 (17)
C15—C16	1.394 (5)	C38—H38A	0.960
C15—H15A	0.950	C38—H38B	0.960
C16—C17	1.399 (4)	C38—H38C	0.960

C16—H16A	0.950	C39—C40^{i}	1.123 (15)
C17—C18	1.385 (4)	C39—C38^{i}	1.210 (17)
C17—H17A	0.950	C39—O9^{i}	1.410 (14)
C19—C20	1.495 (3)	C39—H39A	0.960
C19—H19A	0.990	C39—H39B	0.960
C19—H19B	0.990	C39—H39C	0.960
C21—H21A	0.980	C40—C39^{i}	1.123 (15)
C21—H21B	0.980	C40—H40A	0.960

O1—Zn—N3	113.68 (8)	N5—C20—N6	112.8 (2)
O1—Zn—N5	110.75 (8)	N5—C20—C19	123.5 (2)
N3—Zn—N5	110.38 (8)	N6—C20—C19	123.7 (2)
O1—Zn—N1	92.77 (8)	N6—C21—H21A	109.5
N3—Zn—N1	113.00 (8)	N6—C21—H21B	109.5
N5—Zn—N1	115.30 (7)	H21A—C21—H21B	109.5
O1—Zn—N7	165.76 (7)	N6—C21—H21C	109.5
N3—Zn—N7	74.69 (8)	H21A—C21—H21C	109.5
N5—Zn—N7	74.93 (7)	H21B—C21—H21C	109.5
N1—Zn—N7	73.11 (7)	N6—C22—C27	106.0 (2)
C28—O1—Zn	123.99 (16)	N6—C22—C23	131.2 (2)
C34—O3—H3	109.5	C27—C22—C23	122.8 (3)
C2—N1—C9	105.19 (19)	C24—C23—C22	116.3 (3)
C2—N1—Zn	117.37 (15)	C24—C23—H23A	121.9
C9—N1—Zn	134.83 (16)	C22—C23—H23A	121.9
C2—N2—C4	107.1 (2)	C23—C24—C25	122.0 (2)
C2—N2—C3	127.1 (2)	C23—C24—H24A	119.0
C4—N2—C3	125.8 (2)	C25—C24—H24A	119.0
C11—N3—C18	106.0 (2)	C26—C25—C24	121.3 (3)
C11—N3—Zn	117.96 (17)	C26—C25—H25A	119.4
C18—N3—Zn	135.89 (18)	C24—C25—H25A	119.4
C11—N4—C13	107.3 (2)	C25—C26—C27	117.5 (3)
C11—N4—C12	128.3 (2)	C25—C26—H26A	121.3
C13—N4—C12	124.4 (2)	C27—C26—H26A	121.3
C20—N5—C27	105.27 (19)	C26—C27—N5	131.1 (2)
C20—N5—Zn	117.65 (16)	C26—C27—C22	120.2 (2)
C27—N5—Zn	136.64 (17)	N5—C27—C22	108.7 (2)
C20—N6—C22	107.2 (2)	O2—C28—O1	123.4 (2)
C20—N6—C21	126.7 (2)	O2—C28—C29	118.7 (2)
C22—N6—C21	126.1 (2)	O1—C28—C29	117.9 (2)
C19—N7—C10	112.9 (2)	C30—C29—C34	118.2 (2)
C19—N7—C1	112.55 (19)	C30—C29—C28	121.3 (2)
C10—N7—C1	114.34 (19)	C34—C29—C28	120.5 (2)
C19—N7—Zn	105.54 (14)	C31—C30—C29	121.8 (3)
C10—N7—Zn	104.26 (15)	C31—C30—H30A	119.1
C1—N7—Zn	106.25 (15)	C29—C30—H30A	119.1
N7—C1—C2	108.51 (19)	C30—C31—C32	118.9 (3)
N7—C1—H1A	110.0	C30—C31—H31A	120.6
C2—C1—H1A	110.0	C32—C31—H31A	120.6

N7—C1—H1B	110.0	C33—C32—C31	120.8 (3)
C2—C1—H1B	110.0	C33—C32—H32A	119.6
H1A—C1—H1B	108.4	C31—C32—H32A	119.6
N1—C2—N2	113.0 (2)	C32—C33—C34	120.4 (3)
N1—C2—C1	122.6 (2)	C32—C33—H33A	119.8
N2—C2—C1	124.4 (2)	C34—C33—H33A	119.8
N2—C3—H3A	109.5	O3—C34—C33	117.9 (2)
N2—C3—H3B	109.5	O3—C34—C29	122.1 (2)
H3A—C3—H3B	109.5	C33—C34—C29	120.0 (3)
N2—C3—H3C	109.5	C37—N8—C36	121.8 (6)
H3A—C3—H3C	109.5	C37—N8—C35	118.9 (5)
H3B—C3—H3C	109.5	C36—N8—C35	119.2 (7)
N2—C4—C5	131.8 (2)	N8—C35—H35A	109.5
N2—C4—C9	105.9 (2)	N8—C35—H35B	109.5
C5—C4—C9	122.3 (2)	H35A—C35—H35B	109.5
C6—C5—C4	116.6 (2)	N8—C35—H35C	109.5
C6—C5—H5A	121.7	H35A—C35—H35C	109.5
C4—C5—H5A	121.7	H35B—C35—H35C	109.5
C5—C6—C7	121.7 (2)	N8—C36—H36A	109.5
C5—C6—H6A	119.1	N8—C36—H36B	109.5
C7—C6—H6A	119.1	H36A—C36—H36B	109.5
C8—C7—C6	121.3 (3)	N8—C36—H36C	109.5
C8—C7—H7A	119.3	H36A—C36—H36C	109.5
C6—C7—H7A	119.3	H36B—C36—H36C	109.5
C7—C8—C9	117.5 (2)	O8—C37—N8	128.0 (6)
C7—C8—H8A	121.2	O8—C37—H37A	116.0
C9—C8—H8A	121.2	N8—C37—H37A	116.0
C8—C9—N1	130.7 (2)	H35D—C35A—H35E	109.5
C8—C9—C4	120.5 (2)	H35D—C35A—H35F	109.5
N1—C9—C4	108.8 (2)	H35E—C35A—H35F	109.5
N7—C10—C11	108.0 (2)	H36D—C36A—H36E	109.5
N7—C10—H10A	110.1	H36D—C36A—H36F	109.5
C11—C10—H10A	110.1	H36E—C36A—H36F	109.5
N7—C10—H10B	110.1	O7—Cl—O4	109.5 (2)
C11—C10—H10B	110.1	O7—Cl—O6	109.2 (2)
H10A—C10—H10B	108.4	O4—Cl—O6	119.8 (3)
N3—C11—N4	112.3 (2)	O7—Cl—O5	106.5 (3)
N3—C11—C10	122.5 (2)	O4—Cl—O5	105.2 (3)
N4—C11—C10	125.1 (2)	O6—Cl—O5	105.92 (18)
N4—C12—H12A	109.5	C40—N9—C40^{i}	135.6 (8)
N4—C12—H12B	109.5	C40—N9—C39	133.0 (8)
H12A—C12—H12B	109.5	C40^{i}—N9—C39^{i}	133.0 (8)
N4—C12—H12C	109.5	C39—N9—C39^{i}	178.3 (10)
H12A—C12—H12C	109.5	C40—N9—C38^{i}	98.4 (8)
H12B—C12—H12C	109.5	C40^{i}—N9—C38^{i}	98.4 (9)
N4—C13—C18	106.3 (2)	C39^{i}—N9—C38^{i}	128.7 (8)
N4—C13—C14	131.3 (3)	C40—N9—C38	98.4 (9)
C18—C13—C14	122.4 (3)	C40^{i}—N9—C38	98.4 (8)

C15—C14—C13	116.4 (3)	C39—N9—C38	128.7 (9)
C15—C14—H14A	121.8	N9—C38—H38A	108.7
C13—C14—H14A	121.8	C39^{i}—C38—H38B	123.0
C14—C15—C16	121.8 (3)	N9—C38—H38B	110.1
C14—C15—H15A	119.1	H38A—C38—H38B	109.5
C16—C15—H15A	119.1	N9—C38—H38C	109.6
C15—C16—C17	121.8 (3)	H38A—C38—H38C	109.5
C15—C16—H16A	119.1	H38B—C38—H38C	109.5
C17—C16—H16A	119.1	C40^{i}—C39—C38^{i}	129.4 (7)
C18—C17—C16	116.8 (3)	N9—C39—O9^{i}	121.0 (8)
C18—C17—H17A	121.6	C40^{i}—C39—H39A	123.2
C16—C17—H17A	121.6	N9—C39—H39A	109.3
C17—C18—C13	120.7 (2)	O9^{i}—C39—H39A	101.3
C17—C18—N3	131.1 (2)	N9—C39—H39B	109.8
C13—C18—N3	108.2 (2)	H39A—C39—H39B	109.5
N7—C19—C20	108.35 (19)	N9—C39—H39C	109.3
N7—C19—H19A	110.0	O9^{i}—C39—H39C	105.9
C20—C19—H19A	110.0	H39A—C39—H39C	109.5
N7—C19—H19B	110.0	H39B—C39—H39C	109.5
C20—C19—H19B	110.0	O9—C40—H40A	109.3
H19A—C19—H19B	108.4	N9—C40—H40A	109.3

N3—Zn—O1—C28	−66.4 (2)	C18—C13—C14—C15	−1.3 (5)
N5—Zn—O1—C28	58.6 (2)	C13—C14—C15—C16	0.8 (5)
N1—Zn—O1—C28	176.99 (19)	C14—C15—C16—C17	0.6 (6)
N7—Zn—O1—C28	169.8 (2)	C15—C16—C17—C18	−1.4 (5)
O1—Zn—N1—C2	−152.64 (17)	C16—C17—C18—C13	0.8 (4)
N3—Zn—N1—C2	90.15 (18)	C16—C17—C18—N3	−178.3 (3)
N5—Zn—N1—C2	−38.11 (19)	N4—C13—C18—C17	−179.6 (2)
N7—Zn—N1—C2	25.52 (16)	C14—C13—C18—C17	0.5 (4)
O1—Zn—N1—C9	5.9 (2)	N4—C13—C18—N3	−0.3 (3)
N3—Zn—N1—C9	−111.3 (2)	C14—C13—C18—N3	179.8 (2)
N5—Zn—N1—C9	120.4 (2)	C11—N3—C18—C17	179.1 (3)
N7—Zn—N1—C9	−176.0 (2)	Zn—N3—C18—C17	4.5 (4)
O1—Zn—N3—C11	−149.92 (17)	C11—N3—C18—C13	−0.1 (3)
N5—Zn—N3—C11	84.94 (19)	Zn—N3—C18—C13	−174.65 (18)
N1—Zn—N3—C11	−45.8 (2)	C10—N7—C19—C20	144.3 (2)
N7—Zn—N3—C11	17.85 (17)	C1—N7—C19—C20	−84.4 (2)
O1—Zn—N3—C18	24.1 (3)	Zn—N7—C19—C20	31.1 (2)
N5—Zn—N3—C18	−101.0 (2)	C27—N5—C20—N6	0.0 (3)
N1—Zn—N3—C18	128.2 (2)	Zn—N5—C20—N6	173.71 (15)
N7—Zn—N3—C18	−168.1 (2)	C27—N5—C20—C19	−177.7 (2)
O1—Zn—N5—C20	−176.78 (16)	Zn—N5—C20—C19	−4.0 (3)
N3—Zn—N5—C20	−49.99 (18)	C22—N6—C20—N5	−0.3 (3)
N1—Zn—N5—C20	79.56 (18)	C21—N6—C20—N5	178.6 (2)
N7—Zn—N5—C20	16.95 (16)	C22—N6—C20—C19	177.4 (2)
O1—Zn—N5—C27	−5.7 (2)	C21—N6—C20—C19	−3.7 (4)
N3—Zn—N5—C27	121.1 (2)	N7—C19—C20—N5	−22.1 (3)

N1—Zn—N5—C27	−109.3 (2)	N7—C19—C20—N6	160.4 (2)
N7—Zn—N5—C27	−172.0 (2)	C20—N6—C22—C27	0.4 (2)
O1—Zn—N7—C19	−142.5 (3)	C21—N6—C22—C27	−178.5 (2)
N3—Zn—N7—C19	89.58 (16)	C20—N6—C22—C23	−178.8 (3)
N5—Zn—N7—C19	−27.02 (15)	C21—N6—C22—C23	2.3 (4)
N1—Zn—N7—C19	−150.00 (16)	N6—C22—C23—C24	−179.5 (2)
O1—Zn—N7—C10	98.4 (3)	C27—C22—C23—C24	1.5 (4)
N3—Zn—N7—C10	−29.58 (14)	C22—C23—C24—C25	0.1 (4)
N5—Zn—N7—C10	−146.17 (16)	C23—C24—C25—C26	−1.1 (4)
N1—Zn—N7—C10	90.85 (15)	C24—C25—C26—C27	0.6 (4)
O1—Zn—N7—C1	−22.8 (4)	C25—C26—C27—N5	179.7 (2)
N3—Zn—N7—C1	−150.71 (16)	C25—C26—C27—C22	0.8 (3)
N5—Zn—N7—C1	92.70 (15)	C20—N5—C27—C26	−178.8 (2)
N1—Zn—N7—C1	−30.28 (14)	Zn—N5—C27—C26	9.4 (4)
C19—N7—C1—C2	144.8 (2)	C20—N5—C27—C22	0.2 (2)
C10—N7—C1—C2	−84.7 (2)	Zn—N5—C27—C22	−171.64 (17)
Zn—N7—C1—C2	29.7 (2)	N6—C22—C27—C26	178.8 (2)
C9—N1—C2—N2	−1.2 (3)	C23—C22—C27—C26	−2.0 (4)
Zn—N1—C2—N2	163.16 (15)	N6—C22—C27—N5	−0.3 (2)
C9—N1—C2—C1	178.1 (2)	C23—C22—C27—N5	178.9 (2)
Zn—N1—C2—C1	−17.5 (3)	Zn—O1—C28—O2	−0.6 (3)
C4—N2—C2—N1	1.3 (3)	Zn—O1—C28—C29	179.46 (15)
C3—N2—C2—N1	−178.0 (2)	O2—C28—C29—C30	174.0 (2)
C4—N2—C2—C1	−178.0 (2)	O1—C28—C29—C30	−6.1 (3)
C3—N2—C2—C1	2.7 (4)	O2—C28—C29—C34	−4.6 (3)
N7—C1—C2—N1	−12.4 (3)	O1—C28—C29—C34	175.4 (2)
N7—C1—C2—N2	166.8 (2)	C34—C29—C30—C31	−0.8 (4)
C2—N2—C4—C5	177.6 (3)	C28—C29—C30—C31	−179.4 (2)
C3—N2—C4—C5	−3.1 (4)	C29—C30—C31—C32	1.3 (4)
C2—N2—C4—C9	−0.8 (2)	C30—C31—C32—C33	−0.6 (5)
C3—N2—C4—C9	178.5 (2)	C31—C32—C33—C34	−0.5 (4)
N2—C4—C5—C6	−177.8 (3)	C32—C33—C34—O3	−179.1 (3)
C9—C4—C5—C6	0.4 (4)	C32—C33—C34—C29	1.1 (4)
C4—C5—C6—C7	−0.2 (4)	C30—C29—C34—O3	179.8 (2)
C5—C6—C7—C8	0.1 (4)	C28—C29—C34—O3	−1.6 (4)
C6—C7—C8—C9	−0.1 (4)	C30—C29—C34—C33	−0.4 (4)
C7—C8—C9—N1	177.9 (2)	C28—C29—C34—C33	178.2 (2)
C7—C8—C9—C4	0.3 (3)	C36—N8—C37—O8	175.5 (6)
C2—N1—C9—C8	−177.1 (2)	C35—N8—C37—O8	−1.6 (9)
Zn—N1—C9—C8	22.6 (4)	C40—N9—C38—C39^{i}	1.7 (11)
C2—N1—C9—C4	0.7 (2)	C40^{i}—N9—C38—C39^{i}	140.4 (12)
Zn—N1—C9—C4	−159.61 (17)	C39—N9—C38—C39^{i}	−178.1 (11)
N2—C4—C9—C8	178.1 (2)	C38^{i}—N9—C38—C39^{i}	−108.9 (11)
C5—C4—C9—C8	−0.5 (4)	C40—N9—C39—C40^{i}	118.3 (10)
N2—C4—C9—N1	0.0 (2)	C38^{i}—N9—C39—C40^{i}	177.7 (14)
C5—C4—C9—N1	−178.5 (2)	C38—N9—C39—C40^{i}	−62.0 (10)
C19—N7—C10—C11	−79.2 (2)	C40—N9—C39—C38^{i}	−59.4 (16)
C1—N7—C10—C11	150.4 (2)	C40^{i}—N9—C39—C38^{i}	−177.7 (14)

Zn—N7—C10—C11	34.8 (2)	C38—N9—C39—C38^{i}	120.2 (16)
C18—N3—C11—N4	0.5 (3)	C40—N9—C39—O9^{i}	117.0 (14)
Zn—N3—C11—N4	176.18 (15)	C40^{i}—N9—C39—O9^{i}	−1.3 (7)
C18—N3—C11—C10	−178.3 (2)	C38^{i}—N9—C39—O9^{i}	176 (2)
Zn—N3—C11—C10	−2.7 (3)	C38—N9—C39—O9^{i}	−63.4 (14)
C13—N4—C11—N3	−0.7 (3)	C39^{i}—O9—C40—N9	−2.0 (11)
C12—N4—C11—N3	−177.4 (2)	C40^{i}—N9—C40—C39^{i}	−113.0 (9)
C13—N4—C11—C10	178.1 (2)	C39—N9—C40—C39^{i}	178.0 (11)
C12—N4—C11—C10	1.4 (4)	C38^{i}—N9—C40—C39^{i}	135.8 (10)
N7—C10—C11—N3	−26.1 (3)	C38—N9—C40—C39^{i}	−1.8 (11)
N7—C10—C11—N4	155.3 (2)	C40^{i}—N9—C40—O9	−110.9 (7)
C11—N4—C13—C18	0.5 (3)	C39—N9—C40—O9	−179.9 (3)
C12—N4—C13—C18	177.4 (2)	C39^{i}—N9—C40—O9	2.1 (11)
C11—N4—C13—C14	−179.5 (3)	C38^{i}—N9—C40—O9	137.9 (11)
C12—N4—C13—C14	−2.7 (5)	C38—N9—C40—O9	0.3 (4)
N4—C13—C14—C15	178.8 (3)		

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.84	1.82	2.556 (3)	146