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catena-Poly[[[bis(quinoxaline-2-carboxylato-κ^2N^1,O)zinc(II)]-μ_2-1,2-bis(pyridin-4-yl)ethene-$\kappa^2N:N'$] hemihydrate]

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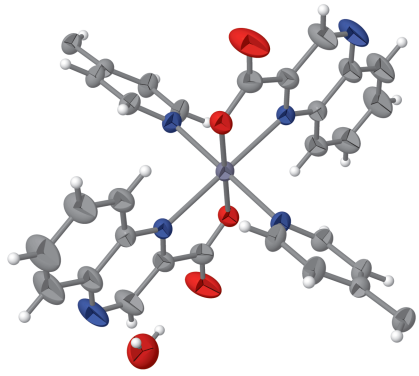
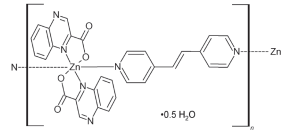
The title complex, $\{[Zn(C_9H_5N_2O_2)_2(C_{12}H_{10}N_2)]\cdot 0.5H_2O\}_n$, has six-coordinate Zn^{II} ions with two *trans*-bidentate quinoxaline-2-carboxylato ligands and a bridging 1,2-bis(pyridin-4-yl)ethylene ligand, resulting in polymeric chains along the $[10\bar{1}]$ direction. The offset packing of these one-dimensional chains gives rise to inter-chain H···O and H···ring interactions.

3D view



Chemical scheme



Structure description

The single repeating unit of the polymeric title complex has a six-coordinated zinc(II) ion lying on an inversion centre, with two *trans*-bidentate quinoxaline-2-carboxylate ligands and a 1,2-bis(pyridin-4-yl)ethylene ligand bridging each zinc centre (Fig. 1). The resulting polymeric chains propagate along the $[10\bar{1}]$ direction, with each one-dimensional chain offset from another by a half of the 1,2-bis(pyridin-4-yl)ethylene (Fig. 2). The Zn···Zn distances within each polymer is 13.7278 (5) Å and between offset polymers is 9.1330 (3) Å, which corresponds to the *c* dimension of the unit cell. This staggered packing gives rise to inter-chain close proximity of H15(x, y, $z-1$) and O2, 2.406 (3) Å. Additionally, the H5($1-x$, $1-y$, $1-z$) on the quinoxaline is positioned near the π system of the pyridyl ring with the H5···centroid[(N3/C10···C14)(x, $\frac{1}{2}-y$, $-\frac{1}{2}+z$)] distance of 2.795 Å (Fig. 2), which is similar to the range of H···centroid distances, 2.73–3.03 Å, observed in the sandwich packing of water between two C_6 rings (Dong *et al.*, 2016). The H atoms of the lattice water molecule are situated so as to hydrogen bond with O2 (Table 1, Fig. 2).

This *N*,*O*-bidentate quinoxaline-2-carboxylatate ligand, qlc, has also been employed with copper(II) to form molecular $[Cu(qlc)_2(H_2O)_2]$ (Feng *et al.*, 2007). Another derivative of the qlc ligand is 3-hydroxy-2-quinoxalinecarboxylate, hqxc. As an equatorial bidentate ligand with zinc(II), hqxc has been used to generate molecular complexes with

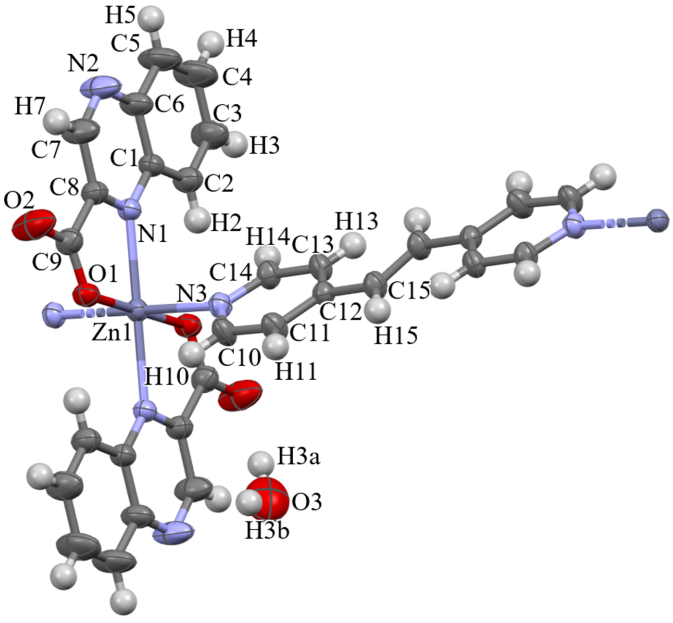


Figure 1
Displacement ellipsoid plot (50% probability) of a single repeating unit of the title compound with the distance between atom O2 and the H3*a* of the interstitial water molecule shown.

trans pyridine or DMSO ligands (Sakai *et al.*, 2010), or to form a polymeric complex using bridging *trans* 4,4-bipyridine (Xiao *et al.*, 2013), which forms similar offset polymer chains as the title compound.

Synthesis and crystallization

A DMF solution of 7 mg of $ZnCl_2$ and 17 mg of 2-quinoxalinecarboxylic acid was heated at 393 K for 1 d. After cooling, 7 mg of 1,10-methylenebis{4-[(*E*)-2-(pyridin-4-yl)vinyl]pyridinium} bis(hexafluorophosphate) (Blanco *et al.*, 2009) was added and the solution heated for a few days, then left to air cool in an oven for seven months. Dichroic brown/blue crystals of the title compound were harvested from the solution. Thermal decomposition of the pyridinium salt to *trans*-1,2-bis(pyridin-4-yl)ethylene likely occurred. Water of crystallization likely originated from prolonged air exposure.

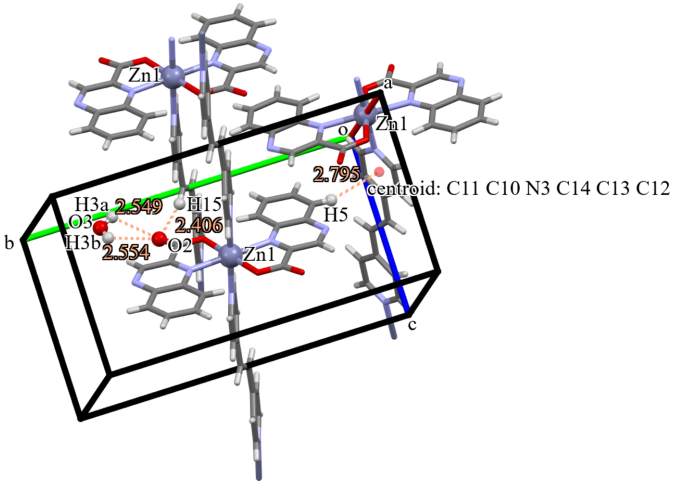


Figure 2
Partial packing of the title complex using capped or ball-and-stick models with the intermolecular H···O distances between O2 and atoms H3*a*, H3*b* and H15(x, y, $z-1$), as well as the H···centroid distance between H5($-x+1$, $-y+1$, $-z+1$) and the centroid of the pyridyl ring N3/C10···C14(x, $-y+\frac{1}{2}$, $z-\frac{1}{2}$).

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93 (1)	2.41 (1)	3.250 (3)	151 (1)
C15—H15···O2^{ii}	0.93 (1)	2.41 (1)	3.307 (3)	163 (1)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zn(C_9H_5N_2O_2)_2(C_{12}H_{10}N_2)]\cdot 0.5H_2O$
M_r	602.90
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	8.9506 (3), 17.1862 (6), 9.1330 (3)
β (°)	98.770 (3)
V (Å^3)	1388.47 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.93
Crystal size (mm)	0.51 × 0.28 × 0.26
Data collection	
Diffractometer	XtaLAB Mini II
Absorption correction	Analytical (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.626, 0.758
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20662, 4146, 2813
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.099, 1.00
No. of reflections	4146
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.44

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015), *OLEX2.refine* (Bourhis *et al.*, 2015), *Mercury* (Macrae *et al.*, 2020), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. The lattice water molecule was refined with a site occupancy factor fixed to 1/4, in such a way that the monomeric formula for the Zn^{II} complex is hemi-hydrated, since the Zn^{II} ion is placed on an inversion centre.

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full crystallographic data

IUCrData (2025). **10**, x250752 [https://doi.org/10.1107/S2414314625007527]

catena-Poly[[[bis(quinoxaline-2-carboxylato-κ^2N^1,O)zinc(II)]-μ_2-1,2-bis-(pyridin-4-yl)ethene-$\kappa^2N:N'$] hemihydrate]

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Crystal data

$[Zn(C_9H_5N_2O_2)_2(C_{12}H_{10}N_2)]\cdot 0.5H_2O$
M_r = 602.90
Monoclinic, $P2_1/c$
a = 8.9506 (3) Å
b = 17.1862 (6) Å
c = 9.1330 (3) Å
β = 98.770 (3)°
V = 1388.47 (8) Å^3
Z = 2
$F(000)$ = 619.085
D_x = 1.442 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5554 reflections
θ = 2.3–24.6°
μ = 0.93 mm^{-1}
T = 293 K
Prism, light yellow
0.51 × 0.28 × 0.26 mm

Data collection

XtaLAB Mini II diffractometer
Radiation source: fine-focus sealed X-ray tube, Rigaku (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: analytical (CrysAlis PRO; Rigaku OD, 2024)
T_{min} = 0.626, T_{max} = 0.758
20662 measured reflections
4146 independent reflections
2813 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 30.6°, θ_{min} = 2.4°
h = −12→12
k = −24→24
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.099
S = 1.00
4146 reflections
199 parameters
0 restraints
23 constraints
Primary atom site location: dual
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.5115P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.0004
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.5	0.5	0.5	0.02940 (10)	

O1	0.33184 (15)	0.54080 (8)	0.34057 (15)	0.0357 (3)	
N1	0.54028 (17)	0.62863 (9)	0.51597 (17)	0.0309 (4)	
N3	0.34623 (18)	0.51175 (9)	0.66291 (17)	0.0323 (4)	
C12	0.1566 (2)	0.51820 (11)	0.8812 (2)	0.0306 (4)	
C13	0.1040 (2)	0.49021 (11)	0.7382 (2)	0.0334 (4)	
H13	0.0049 (2)	0.47303 (11)	0.7134 (2)	0.0401 (5)*	
O2	0.2120 (2)	0.64790 (10)	0.2512 (2)	0.0799 (7)	
C11	0.3046 (2)	0.54536 (13)	0.9078 (2)	0.0401 (5)	
H11	0.3429 (2)	0.56663 (13)	0.9995 (2)	0.0481 (6)*	
C15	0.0653 (2)	0.51873 (12)	1.0016 (2)	0.0350 (5)	
H15	0.1013 (2)	0.54724 (12)	1.0862 (2)	0.0420 (5)*	
C1	0.6463 (2)	0.67477 (11)	0.6011 (2)	0.0353 (4)	
C14	0.2015 (2)	0.48856 (11)	0.6352 (2)	0.0341 (4)	
H14	0.1648 (2)	0.47029 (11)	0.5407 (2)	0.0410 (5)*	
C8	0.4346 (2)	0.66382 (12)	0.4235 (2)	0.0376 (5)	
C9	0.3153 (2)	0.61372 (13)	0.3298 (2)	0.0409 (5)	
C10	0.3948 (2)	0.54077 (13)	0.7980 (2)	0.0402 (5)	
H10	0.4939 (2)	0.55865 (13)	0.8188 (2)	0.0483 (6)*	
C2	0.7619 (3)	0.64133 (13)	0.7037 (3)	0.0444 (5)	
H2	0.7673 (3)	0.58763 (13)	0.7158 (3)	0.0533 (6)*	
N2	0.5273 (3)	0.79219 (12)	0.4877 (3)	0.0666 (7)	
C3	0.8666 (3)	0.68857 (15)	0.7855 (3)	0.0637 (8)	
H3	0.9435 (3)	0.66659 (15)	0.8527 (3)	0.0765 (9)*	
C6	0.6378 (3)	0.75669 (13)	0.5851 (3)	0.0492 (6)	
C7	0.4294 (3)	0.74598 (13)	0.4103 (3)	0.0586 (7)	
H7	0.3525 (3)	0.76813 (13)	0.3432 (3)	0.0703 (8)*	
C5	0.7479 (3)	0.80324 (15)	0.6718 (3)	0.0733 (9)	
H5	0.7441 (3)	0.85710 (15)	0.6621 (3)	0.0879 (10)*	
C4	0.8589 (3)	0.76983 (16)	0.7688 (4)	0.0799 (10)	
H4	0.9308 (3)	0.80101 (16)	0.8251 (4)	0.0959 (12)*	
O3	0.1505 (13)	0.7936 (6)	0.0902 (12)	0.102 (3)	0.250000
H3a	0.133 (19)	0.749 (4)	0.050 (16)	0.153 (5)*	0.250000
H3b	0.220 (15)	0.789 (8)	0.165 (13)	0.153 (5)*	0.250000

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03042 (16)	0.02834 (16)	0.03095 (16)	−0.00198 (14)	0.00956 (11)	−0.00164 (14)
O1	0.0373 (8)	0.0316 (7)	0.0370 (7)	−0.0035 (6)	0.0021 (6)	−0.0036 (6)
N1	0.0315 (8)	0.0273 (8)	0.0349 (9)	−0.0034 (6)	0.0083 (7)	−0.0033 (7)
N3	0.0323 (8)	0.0356 (10)	0.0309 (8)	−0.0017 (7)	0.0106 (6)	−0.0014 (7)
C12	0.0315 (10)	0.0310 (10)	0.0308 (9)	0.0002 (7)	0.0100 (7)	−0.0001 (7)
C13	0.0262 (9)	0.0429 (12)	0.0317 (9)	−0.0037 (8)	0.0063 (7)	−0.0007 (8)
O2	0.0717 (13)	0.0456 (11)	0.1053 (16)	0.0108 (9)	−0.0416 (12)	−0.0095 (10)
C11	0.0398 (11)	0.0504 (13)	0.0321 (10)	−0.0111 (10)	0.0116 (9)	−0.0111 (9)
C15	0.0346 (10)	0.0440 (12)	0.0281 (9)	−0.0023 (8)	0.0101 (8)	−0.0050 (8)
C1	0.0343 (11)	0.0293 (10)	0.0429 (11)	−0.0041 (8)	0.0077 (9)	−0.0041 (9)
C14	0.0327 (10)	0.0431 (12)	0.0274 (9)	−0.0005 (8)	0.0070 (7)	−0.0022 (8)

C8	0.0381 (11)	0.0295 (10)	0.0447 (12)	−0.0009 (9)	0.0047 (9)	−0.0034 (9)
C9	0.0379 (11)	0.0380 (12)	0.0453 (12)	0.0024 (9)	0.0011 (9)	−0.0045 (10)
C10	0.0329 (11)	0.0492 (13)	0.0409 (11)	−0.0120 (9)	0.0132 (9)	−0.0108 (10)
C2	0.0437 (12)	0.0336 (11)	0.0540 (13)	−0.0013 (9)	0.0012 (10)	−0.0045 (10)
N2	0.0731 (16)	0.0277 (10)	0.0897 (17)	−0.0030 (10)	−0.0167 (13)	0.0007 (10)
C3	0.0544 (16)	0.0477 (15)	0.0794 (19)	−0.0050 (12)	−0.0208 (14)	−0.0080 (13)
C6	0.0514 (14)	0.0305 (11)	0.0625 (16)	−0.0078 (10)	−0.0014 (12)	−0.0040 (11)
C7	0.0626 (17)	0.0319 (12)	0.0735 (18)	0.0016 (11)	−0.0144 (13)	0.0031 (12)
C5	0.0778 (19)	0.0340 (13)	0.099 (2)	−0.0169 (13)	−0.0166 (17)	−0.0072 (14)
C4	0.071 (2)	0.0485 (16)	0.107 (2)	−0.0198 (14)	−0.0284 (18)	−0.0109 (16)
O3	0.108 (9)	0.108 (8)	0.094 (8)	0.005 (6)	0.026 (6)	0.035 (6)

Geometric parameters (Å, º)

Zn1—O1	2.0515 (13)	C15—H15	0.9300
Zn1—O1^{i}	2.0515 (13)	C1—C2	1.408 (3)
Zn1—N1^{i}	2.2411 (16)	C1—C6	1.416 (3)
Zn1—N1	2.2411 (16)	C14—H14	0.9300
Zn1—N3	2.1848 (15)	C8—C9	1.528 (3)
Zn1—N3^{i}	2.1848 (15)	C8—C7	1.417 (3)
O1—C9	1.264 (2)	C10—H10	0.9300
N1—C1	1.382 (2)	C2—H2	0.9300
N1—C8	1.315 (3)	C2—C3	1.372 (3)
N3—C14	1.342 (2)	N2—C6	1.368 (3)
N3—C10	1.340 (2)	N2—C7	1.308 (3)
C12—C13	1.404 (3)	C3—H3	0.9300
C12—C11	1.390 (3)	C3—C4	1.405 (4)
C12—C15	1.467 (3)	C6—C5	1.414 (3)
C13—H13	0.9300	C7—H7	0.9300
C13—C14	1.378 (3)	C5—H5	0.9300
O2—C9	1.230 (3)	C5—C4	1.354 (4)
C11—H11	0.9300	C4—H4	0.9300
C11—C10	1.382 (3)	O3—H3a	0.8500
C15—C15^{ii}	1.331 (4)	O3—H3b	0.8501
O1^{i}—Zn1—O1	180.0	C6—C1—N1	119.38 (19)
N1—Zn1—O1	78.60 (6)	C6—C1—C2	119.80 (19)
N1—Zn1—O1^{i}	101.40 (6)	C13—C14—N3	123.96 (17)
N1^{i}—Zn1—O1	101.40 (6)	H14—C14—N3	118.02 (10)
N1^{i}—Zn1—O1^{i}	78.60 (6)	H14—C14—C13	118.02 (11)
N1^{i}—Zn1—N1	180.0	C9—C8—N1	118.25 (17)
N3^{i}—Zn1—O1	91.06 (6)	C7—C8—N1	121.59 (19)
N3^{i}—Zn1—O1^{i}	88.94 (6)	C7—C8—C9	120.16 (19)
N3—Zn1—O1	88.94 (6)	O2—C9—O1	126.0 (2)
N3—Zn1—O1^{i}	91.06 (6)	C8—C9—O1	116.82 (18)
N3—Zn1—N1	88.64 (5)	C8—C9—O2	117.2 (2)
N3—Zn1—N1^{i}	91.36 (5)	C11—C10—N3	123.03 (19)
N3^{i}—Zn1—N1	91.36 (5)	H10—C10—N3	118.48 (11)

N3^{i}—Zn1—N1^{i}	88.64 (5)	H10—C10—C11	118.48 (12)
N3^{i}—Zn1—N3	180.0	H2—C2—C1	120.25 (12)
C9—O1—Zn1	117.32 (13)	C3—C2—C1	119.5 (2)
C1—N1—Zn1	133.84 (13)	C3—C2—H2	120.25 (15)
C8—N1—Zn1	108.60 (12)	C7—N2—C6	116.0 (2)
C8—N1—C1	117.55 (17)	H3—C3—C2	119.63 (15)
C14—N3—Zn1	122.29 (12)	C4—C3—C2	120.7 (2)
C10—N3—Zn1	120.76 (13)	C4—C3—H3	119.63 (15)
C10—N3—C14	116.93 (16)	N2—C6—C1	122.2 (2)
C11—C12—C13	116.91 (17)	C5—C6—C1	118.8 (2)
C15—C12—C13	123.61 (17)	C5—C6—N2	119.0 (2)
C15—C12—C11	119.48 (17)	N2—C7—C8	123.2 (2)
H13—C13—C12	120.49 (11)	H7—C7—C8	118.38 (13)
C14—C13—C12	119.01 (17)	H7—C7—N2	118.38 (14)
C14—C13—H13	120.49 (11)	H5—C5—C6	119.81 (15)
H11—C11—C12	119.97 (11)	C4—C5—C6	120.4 (2)
C10—C11—C12	120.07 (18)	C4—C5—H5	119.81 (15)
C10—C11—H11	119.97 (12)	C5—C4—C3	120.8 (2)
C15^{ii}—C15—C12	124.6 (2)	H4—C4—C3	119.62 (15)
H15—C15—C12	117.69 (11)	H4—C4—C5	119.62 (15)
C2—C1—N1	120.82 (18)	H3b—O3—H3a	109.5

Zn1—O1—C9—O2	−172.45 (18)	C11—C12—C13—C14	2.2 (2)
Zn1—O1—C9—C8	7.37 (14)	C11—C12—C15—C15^{ii}	−166.6 (2)
Zn1—N1—C1—C2	0.96 (19)	C11—C10—N3—C14	1.9 (3)
Zn1—N1—C1—C6	−178.84 (19)	C15—C12—C13—C14	−176.65 (19)
Zn1—N1—C8—C9	−0.49 (14)	C15—C12—C11—C10	176.0 (2)
Zn1—N1—C8—C7	179.21 (16)	C1—N1—C8—C9	−179.27 (18)
Zn1—N3—C14—C13	175.49 (14)	C1—N1—C8—C7	0.4 (2)
Zn1—N3—C10—C11	−176.25 (16)	C1—C2—C3—C4	0.5 (3)
O1—C9—C8—N1	−4.4 (2)	C1—C6—N2—C7	0.1 (3)
O1—C9—C8—C7	175.9 (2)	C1—C6—C5—C4	−0.3 (3)
N1—C1—C2—C3	179.3 (2)	C8—N1—C1—C2	179.35 (19)
N1—C1—C6—N2	0.2 (2)	C8—N1—C1—C6	−0.5 (2)
N1—C1—C6—C5	−179.3 (2)	C8—C7—N2—C6	−0.1 (3)
N1—C8—C9—O2	175.4 (2)	C9—C8—C7—N2	179.6 (2)
N1—C8—C7—N2	−0.1 (3)	C2—C1—C6—N2	−179.6 (2)
N3—C14—C13—C12	0.5 (2)	C2—C1—C6—C5	0.8 (3)
N3—C10—C11—C12	0.9 (3)	C2—C3—C4—C5	0.1 (4)
C12—C15—C15^{ii}—C12^{ii}	180.0 (3)	N2—C6—C5—C4	−179.9 (3)
C13—C12—C11—C10	−2.9 (2)	C3—C2—C1—C6	−0.9 (3)
C13—C12—C15—C15^{ii}	12.3 (2)	C3—C4—C5—C6	−0.1 (4)
C13—C14—N3—C10	−2.6 (2)	C7—N2—C6—C5	179.6 (3)
O2—C9—C8—C7	−4.3 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93 (1)	2.40 (1)	3.250 (3)	151 (1)
C15—H15···O2^{iii}	0.93 (1)	2.41 (1)	3.307 (3)	163 (1)

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