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3,7,11,19,23,27-Hexaazatricyclo-[27.3.1.1^{13,17}]tetratriaconta-1(32),-13,15,17(34),29(33),30-hexaene hexachloride tetrahydrate

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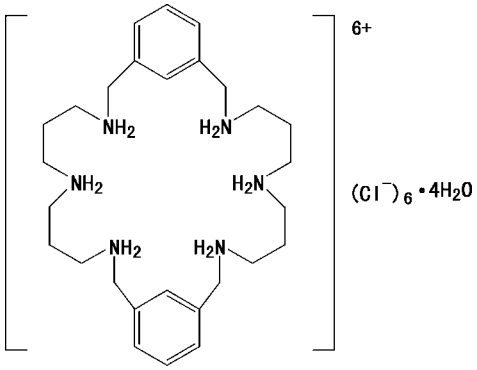
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.130; data-to-parameter ratio = 19.5.

The title compound, $C_{28}H_{52}N_6^{6+}\cdot 6Cl^-\cdot 4H_2O$, is a dinucleating 28-membered centrosymmetric hexaazamacrocyclic complex. The macrocyclic ligand adopts a chair-like conformation, with the crystallographic inversion center located in the macrocyclic cavity. The six chloride ions and four water molecules are situated symmetrically outside the macrocyclic cavity. The crystal structure is stabilized by N—H···Cl, N—H···O and O—H···Cl hydrogen bonds.

Related literature

For studies on hexaazamacrocyclic complexes, see: Llobet *et al.* (1994). For related literature, see: Anda *et al.* (2000); Costas *et al.* (2004); Lu *et al.* (1995).



Experimental

Crystal data

$C_{28}H_{52}N_6^{6+}\cdot 6Cl^-\cdot 4H_2O$
M_r = 757.52
Monoclinic, $P2_1/c$
a = 17.012 (7) Å
b = 7.469 (2) Å
c = 17.329 (7) Å
β = 113.841 (13)°
V = 2014.0 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 293 (2) K
0.19 × 0.18 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (Higashi, 1995)
T_{min} = 0.895, T_{max} = 0.932
18546 measured reflections
4594 independent reflections
2416 reflections with $I > 2\sigma(I)$
R_{int} = 0.102

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.130
S = 1.04
4594 reflections
235 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl2	0.86 (2)	2.24 (1)	3.082 (3)	168 (3)
N1—H1B···Cl1^{i}	0.89 (3)	2.24 (3)	3.115 (3)	169 (3)
O1W—H1O···Cl3	0.84 (4)	2.46 (5)	3.287 (4)	169 (4)
N2—H2A···Cl1	0.89 (3)	2.28 (3)	3.162 (3)	177 (3)
N2—H2B···Cl2^{i}	0.95 (3)	2.17 (3)	3.113 (3)	177 (3)
O1W—H2O···Cl1	0.84 (5)	2.40 (5)	3.222 (4)	166 (5)
N3—H3A···Cl3	0.85 (2)	2.25 (2)	3.104 (3)	173 (3)
N3—H3B···O2W	0.86 (2)	1.94 (2)	2.782 (4)	169 (2)
O2W—H3O···Cl3^{ii}	0.84 (2)	2.30 (2)	3.144 (3)	176 (6)
O2W—H4O···Cl3^{iii}	0.84 (3)	2.30 (3)	3.133 (4)	168 (4)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2525).

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supporting information

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3,7,11,19,23,27-Hexaazatricyclo-[27.3.1.1^{13,17}]tetratriaconta-1(32),13,15,17(34),29(33),30-hexaene hexachloride tetrahydrate

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S1. Comment

It has been shown that macrocyclic polyamines have numerous advantages as enzyme models. They can participate in molecular recongnition phenomena with different kinds of substrates, such as organic, inorganic, and biologically important anions (Lu *et al.*, 1995; Anda *et al.*, 2000). In addition, hexaaza macrocycles can form dinuclear metal complexes which in turn are capable of coordinating anions (Costas *et al.*, 2004). In this paper, the synthesis and the crystal structure of a hexaazamacrocyclic complex, L.6HCl.4H_2O [*L* is 3,7,11,19, 23,27-hexaazztricyclo-[27.3.1.1^{13,17}]tetratriaconta-1(32),13,15,17 (34),29 (33),30-hexaene] is presented.

The structure of the title compound is shown in Fig.1. It consists of a centrosymmetric hexaprotonated macrocycle, six chloride counterions, and four water molecules of crystallization. In the macrocycle, each of the aliphatic chains adopts a planar *trans* configuration, and each of the benzene rings is tilted from the mean plane of chains by 108.9 (1)°. All six N atoms are protonated with hydrogen atoms directed outside the ring. None of the chloride counterions are situated inside the macrocyclic cavity. The macrocycle adopts a chair conformation, similar to that observed in related compounds (Llobet *et al.*, 1994). The crystal structure is stabilized by N—H···Cl, N—H···O and O—H···Cl hydrogen bonds (Table 1).

S2. Experimental

A solution of 3,3′-iminobis(propylamine) (1.31 g, 10 mmol) in CH_3OH (400 ml) was added dropwise from a dropping funnel to a stirred solution of 97% *m*-phthalaldehyde (1.34 g, 10 mmol) in CH_3OH (400 ml) in a round-bottomed three-neck flask over 12 h at room temperature. Then the volume of the mixture was concentrated to 200 ml. $NaBH_4$ (2 g) was added to the solution and the suspension was magnetically stirred for about 5 h at room temperature. The solvent was removed under reduced pressure, and the product was extracted with CH_2Cl_2 from an aqueous solution (CH_2Cl_2/H_2O, 120 ml/50 ml). Evaporation of CH_2Cl_2 under reduced pressure yielded a colourless oil which was then dissolved in 50 ml of 8% HCl. The volume was reduced under low pressure until at approximately 5 ml, a white crystalline solid precipitated.

S3. Refinement

N-bound H atoms were located in a difference map and refined freely; N—H distances involving atoms N1 and N3 were restrained to 0.85 (1) Å. H atoms bonded to water molecules were located in a difference Fourier map and refined isotropically, with distance restraints of O—H = 0.85 (1) Å and H···H = 1.30 (1) Å, and with U_{iso}(H) = 1.5 U_{eq}(O). C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier).

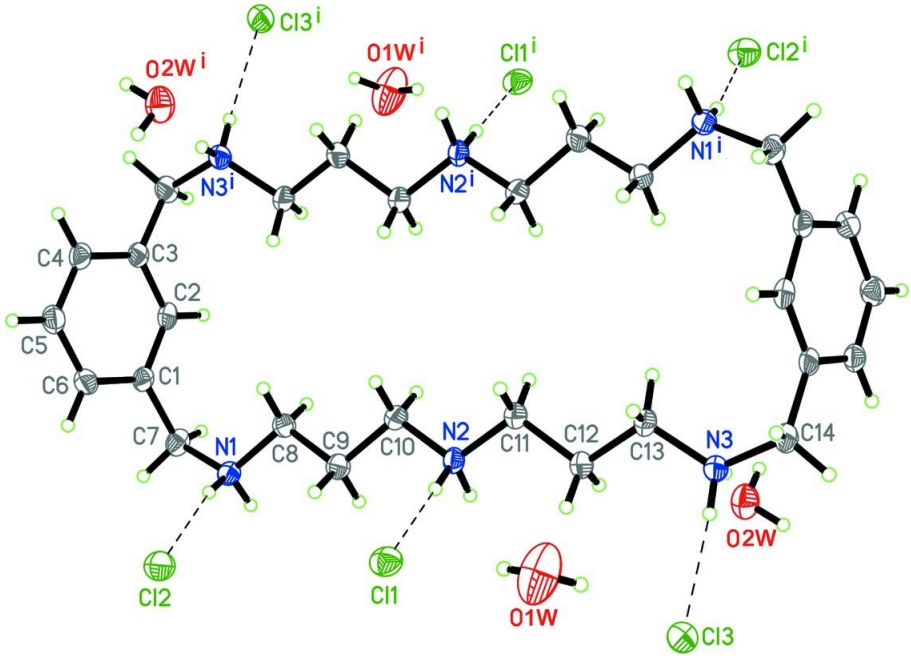

Figure 1

The structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) 1 - *x*, -*y*, 1 - *z*.

3,7,11,19,23,27-Hexaazatricyclo[27.3.1.1^{13,17}]tetratriaconta- 1(32),13,15,17 (34),29 (33),30-hexaene hexachloride tetrahydrate

Crystal data

$C_{28}H_{52}N_6^{6+}\cdot 6Cl^-\cdot 4H_2O$
$M_r = 757.52$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.012\ (7)$ Å
$b = 7.469\ (2)$ Å
$c = 17.329\ (7)$ Å
$\beta = 113.841\ (13)°$
$V = 2014.0\ (13)$ Å^3
$Z = 2$
$F(000) = 808$
$D_x = 1.249$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 4594 reflections
$\theta = 3.0–27.5°$
$\mu = 0.46$ mm^{-1}
$T = 293$ K
Block, colourless
0.19 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (Higashi, 1995)
$T_{min} = 0.895$, $T_{max} = 0.932$
18546 measured reflections
4594 independent reflections
2416 reflections with $I > 2\sigma(I)$
$R_{int} = 0.102$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -22\rightarrow22$
$k = -9\rightarrow8$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.130$
$S = 1.04$
4594 reflections
235 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.1273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.82877 (18)	0.1791 (4)	0.39938 (18)	0.0355 (7)
C2	0.84179 (18)	0.0147 (4)	0.44031 (19)	0.0368 (7)
H2	0.8105	−0.0843	0.4115	0.044*
C3	0.90031 (19)	−0.0047 (4)	0.52305 (19)	0.0350 (7)
C4	0.94848 (19)	0.1433 (4)	0.5644 (2)	0.0400 (8)
H4	0.9890	0.1320	0.6196	0.048*
C5	0.9369 (2)	0.3061 (4)	0.5244 (2)	0.0450 (8)
H5	0.9693	0.4044	0.5528	0.054*
C6	0.8769 (2)	0.3245 (4)	0.4419 (2)	0.0420 (8)
H6	0.8692	0.4351	0.4151	0.050*
C7	0.76289 (18)	0.1935 (5)	0.30992 (19)	0.0431 (8)
H7A	0.7856	0.2686	0.2781	0.052*
H7B	0.7527	0.0754	0.2845	0.052*
C8	0.63910 (18)	0.1810 (4)	0.35545 (18)	0.0367 (7)
H8A	0.6756	0.1954	0.4149	0.044*
H8B	0.6329	0.0539	0.3428	0.044*
C9	0.55173 (19)	0.2631 (4)	0.33619 (19)	0.0395 (8)
H9A	0.5580	0.3911	0.3465	0.047*
H9B	0.5149	0.2447	0.2771	0.047*
C10	0.51067 (18)	0.1803 (4)	0.39031 (19)	0.0385 (7)
H10A	0.5066	0.0517	0.3820	0.046*
H10B	0.5460	0.2037	0.4493	0.046*
C11	0.37784 (18)	0.1881 (4)	0.41939 (19)	0.0411 (8)
H11A	0.4035	0.2392	0.4756	0.049*

H11B	0.3838	0.0590	0.4245	0.049*
C12	0.28364 (19)	0.2373 (4)	0.3786 (2)	0.0435 (8)
H12A	0.2782	0.3645	0.3663	0.052*
H12B	0.2566	0.1734	0.3256	0.052*
C13	0.23772 (18)	0.1922 (4)	0.4348 (2)	0.0412 (8)
H13A	0.2536	0.0728	0.4577	0.049*
H13B	0.2544	0.2762	0.4814	0.049*
C14	0.08870 (19)	0.1827 (4)	0.4337 (2)	0.0434 (8)
H14A	0.0289	0.1977	0.3957	0.052*
H14B	0.1033	0.2769	0.4757	0.052*
N1	0.67900 (17)	0.2703 (4)	0.30374 (17)	0.0345 (6)
H1A	0.683 (2)	0.3817 (17)	0.3174 (19)	0.049 (10)*
H1B	0.6425 (19)	0.256 (4)	0.2505 (19)	0.037 (8)*
N2	0.42311 (16)	0.2566 (4)	0.36763 (17)	0.0341 (6)
H2A	0.4253 (18)	0.375 (4)	0.3706 (18)	0.038 (9)*
H2B	0.391 (2)	0.238 (4)	0.309 (2)	0.052 (10)*
N3	0.14354 (16)	0.2017 (4)	0.38479 (18)	0.0385 (6)
H3A	0.129 (2)	0.303 (2)	0.3601 (18)	0.053 (11)*
H3B	0.130 (2)	0.120 (3)	0.3470 (14)	0.046 (10)*
O1W	0.2694 (2)	0.7467 (6)	0.4322 (2)	0.1099 (12)
H1O	0.226 (2)	0.690 (7)	0.400 (3)	0.165*
H2O	0.307 (2)	0.711 (8)	0.416 (4)	0.165*
O2W	0.09052 (17)	−0.0279 (3)	0.24667 (18)	0.0595 (7)
H3O	0.090 (3)	−0.1386 (18)	0.256 (3)	0.089*
H4O	0.0390 (11)	0.005 (5)	0.232 (3)	0.089*
Cl1	0.43151 (6)	0.67844 (11)	0.38468 (5)	0.0500 (2)
Cl2	0.68078 (6)	0.68054 (11)	0.32358 (5)	0.0545 (3)
Cl3	0.10025 (6)	0.55940 (11)	0.28508 (6)	0.0543 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0243 (15)	0.0496 (19)	0.0374 (16)	0.0022 (15)	0.0175 (13)	0.0018 (15)
C2	0.0258 (15)	0.0446 (18)	0.0432 (17)	−0.0034 (13)	0.0172 (14)	−0.0063 (15)
C3	0.0252 (15)	0.0397 (17)	0.0454 (18)	0.0035 (13)	0.0197 (14)	0.0033 (15)
C4	0.0295 (16)	0.054 (2)	0.0393 (17)	−0.0024 (15)	0.0172 (14)	0.0001 (16)
C5	0.0406 (19)	0.0457 (19)	0.0478 (19)	−0.0110 (15)	0.0169 (16)	−0.0032 (16)
C6	0.0391 (18)	0.0430 (18)	0.0475 (19)	−0.0013 (15)	0.0213 (15)	0.0061 (16)
C7	0.0331 (17)	0.064 (2)	0.0373 (17)	0.0027 (16)	0.0192 (14)	−0.0028 (16)
C8	0.0329 (16)	0.0444 (17)	0.0362 (16)	0.0022 (14)	0.0174 (14)	0.0044 (14)
C9	0.0350 (17)	0.0436 (17)	0.0449 (18)	0.0044 (14)	0.0210 (15)	0.0038 (15)
C10	0.0293 (16)	0.0456 (18)	0.0400 (17)	0.0042 (14)	0.0133 (14)	0.0056 (15)
C11	0.0302 (16)	0.0512 (19)	0.0434 (18)	−0.0002 (15)	0.0165 (14)	0.0063 (16)
C12	0.0327 (17)	0.053 (2)	0.0496 (19)	0.0028 (15)	0.0213 (15)	0.0107 (16)
C13	0.0279 (16)	0.054 (2)	0.0423 (17)	−0.0007 (15)	0.0151 (14)	0.0043 (16)
C14	0.0343 (17)	0.0475 (19)	0.057 (2)	0.0081 (15)	0.0279 (16)	0.0075 (16)
N1	0.0321 (14)	0.0430 (17)	0.0290 (14)	−0.0003 (13)	0.0130 (12)	−0.0010 (13)
N2	0.0267 (14)	0.0355 (15)	0.0413 (16)	−0.0016 (12)	0.0152 (12)	−0.0004 (13)

N3	0.0328 (14)	0.0379 (16)	0.0460 (16)	0.0016 (13)	0.0170 (13)	0.0068 (15)
O1W	0.077 (2)	0.147 (3)	0.101 (3)	−0.015 (2)	0.031 (2)	−0.065 (2)
O2W	0.0507 (16)	0.0587 (15)	0.0750 (17)	−0.0019 (14)	0.0317 (15)	−0.0071 (15)
Cl1	0.0533 (5)	0.0491 (5)	0.0392 (4)	−0.0022 (4)	0.0098 (4)	−0.0021 (4)
Cl2	0.0599 (6)	0.0452 (5)	0.0469 (5)	−0.0075 (4)	0.0096 (4)	−0.0035 (4)
Cl3	0.0492 (5)	0.0495 (5)	0.0622 (6)	−0.0017 (4)	0.0206 (4)	0.0085 (4)

Geometric parameters (Å, º)

C1—C6	1.380 (4)	C11—N2	1.489 (4)
C1—C2	1.391 (4)	C11—C12	1.512 (4)
C1—C7	1.505 (4)	C11—H11A	0.97
C2—C3	1.383 (4)	C11—H11B	0.97
C2—H2	0.93	C12—C13	1.512 (4)
C3—C4	1.390 (4)	C12—H12A	0.97
C3—C14^{i}	1.500 (4)	C12—H12B	0.97
C4—C5	1.374 (4)	C13—N3	1.483 (4)
C4—H4	0.93	C13—H13A	0.97
C5—C6	1.387 (4)	C13—H13B	0.97
C5—H5	0.93	C14—N3	1.500 (4)
C6—H6	0.93	C14—C3^{i}	1.500 (4)
C7—N1	1.501 (4)	C14—H14A	0.97
C7—H7A	0.97	C14—H14B	0.97
C7—H7B	0.97	N1—H1A	0.861 (10)
C8—N1	1.483 (4)	N1—H1B	0.89 (3)
C8—C9	1.515 (4)	N2—H2A	0.89 (3)
C8—H8A	0.97	N2—H2B	0.95 (3)
C8—H8B	0.97	N3—H3A	0.857 (10)
C9—C10	1.510 (4)	N3—H3B	0.857 (10)
C9—H9A	0.97	O1W—H1O	0.84 (4)
C9—H9B	0.97	O1W—H2O	0.84 (5)
C10—N2	1.492 (4)	O2W—H3O	0.841 (10)
C10—H10A	0.97	O2W—H4O	0.84 (3)
C10—H10B	0.97		
C6—C1—C2	119.0 (3)	N2—C11—H11A	109.7
C6—C1—C7	121.9 (3)	C12—C11—H11A	109.7
C2—C1—C7	119.1 (3)	N2—C11—H11B	109.7
C3—C2—C1	121.4 (3)	C12—C11—H11B	109.7
C3—C2—H2	119.3	H11A—C11—H11B	108.2
C1—C2—H2	119.3	C13—C12—C11	111.7 (3)
C2—C3—C4	118.6 (3)	C13—C12—H12A	109.3
C2—C3—C14^{i}	120.1 (3)	C11—C12—H12A	109.3
C4—C3—C14^{i}	121.3 (3)	C13—C12—H12B	109.3
C5—C4—C3	120.7 (3)	C11—C12—H12B	109.3
C5—C4—H4	119.7	H12A—C12—H12B	107.9
C3—C4—H4	119.7	N3—C13—C12	109.3 (3)
C4—C5—C6	120.2 (3)	N3—C13—H13A	109.8

C4—C5—H5	119.9	C12—C13—H13A	109.8
C6—C5—H5	119.9	N3—C13—H13B	109.8
C1—C6—C5	120.2 (3)	C12—C13—H13B	109.8
C1—C6—H6	119.9	H13A—C13—H13B	108.3
C5—C6—H6	119.9	N3—C14—C3^{i}	112.7 (2)
N1—C7—C1	113.0 (2)	N3—C14—H14A	109.1
N1—C7—H7A	109.0	C3^{i}—C14—H14A	109.1
C1—C7—H7A	109.0	N3—C14—H14B	109.1
N1—C7—H7B	109.0	C3^{i}—C14—H14B	109.1
C1—C7—H7B	109.0	H14A—C14—H14B	107.8
H7A—C7—H7B	107.8	C8—N1—C7	116.1 (2)
N1—C8—C9	109.4 (2)	C8—N1—H1A	106 (2)
N1—C8—H8A	109.8	C7—N1—H1A	112 (2)
C9—C8—H8A	109.8	C8—N1—H1B	106 (2)
N1—C8—H8B	109.8	C7—N1—H1B	106 (2)
C9—C8—H8B	109.8	H1A—N1—H1B	110 (3)
H8A—C8—H8B	108.2	C11—N2—C10	114.5 (2)
C10—C9—C8	110.9 (2)	C11—N2—H2A	109 (2)
C10—C9—H9A	109.5	C10—N2—H2A	110.6 (19)
C8—C9—H9A	109.5	C11—N2—H2B	112 (2)
C10—C9—H9B	109.5	C10—N2—H2B	108 (2)
C8—C9—H9B	109.5	H2A—N2—H2B	102 (3)
H9A—C9—H9B	108.1	C13—N3—C14	115.9 (3)
N2—C10—C9	110.1 (2)	C13—N3—H3A	111 (2)
N2—C10—H10A	109.6	C14—N3—H3A	104 (2)
C9—C10—H10A	109.6	C13—N3—H3B	108 (2)
N2—C10—H10B	109.6	C14—N3—H3B	109 (2)
C9—C10—H10B	109.6	H3A—N3—H3B	108 (3)
H10A—C10—H10B	108.2	H1O—O1W—H2O	102 (5)
N2—C11—C12	110.0 (2)	H3O—O2W—H4O	105 (4)

C6—C1—C2—C3	1.6 (5)	C2—C1—C7—N1	99.6 (3)
C7—C1—C2—C3	−178.7 (3)	N1—C8—C9—C10	−177.8 (3)
C1—C2—C3—C4	−2.0 (5)	C8—C9—C10—N2	−177.3 (2)
C1—C2—C3—C14^{i}	178.4 (3)	N2—C11—C12—C13	−172.3 (3)
C2—C3—C4—C5	1.4 (5)	C11—C12—C13—N3	−166.5 (3)
C14^{i}—C3—C4—C5	−179.1 (3)	C9—C8—N1—C7	−174.9 (2)
C3—C4—C5—C6	−0.3 (5)	C1—C7—N1—C8	−53.3 (4)
C2—C1—C6—C5	−0.5 (5)	C12—C11—N2—C10	−166.3 (3)
C7—C1—C6—C5	179.8 (3)	C9—C10—N2—C11	−178.1 (3)
C4—C5—C6—C1	−0.2 (5)	C12—C13—N3—C14	−172.8 (3)
C6—C1—C7—N1	−80.7 (4)	C3^{i}—C14—N3—C13	−62.0 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl2	0.86 (2)	2.24 (1)	3.082 (3)	168 (3)

N1—H1*B*···Cl1^{ii}	0.89 (3)	2.24 (3)	3.115 (3)	169 (3)
O1*W*—H1*O*···Cl3	0.84 (4)	2.46 (5)	3.287 (4)	169 (4)
N2—H2*A*···Cl1	0.89 (3)	2.28 (3)	3.162 (3)	177 (3)
N2—H2*B*···Cl2^{ii}	0.95 (3)	2.17 (3)	3.113 (3)	177 (3)
O1*W*—H2*O*···Cl1	0.84 (5)	2.40 (5)	3.222 (4)	166 (5)
N3—H3*A*···Cl3	0.85 (2)	2.25 (2)	3.104 (3)	173 (3)
N3—H3*B*···O2*W*	0.86 (2)	1.94 (2)	2.782 (4)	169 (2)
O2*W*—H3*O*···Cl3^{iii}	0.84 (2)	2.30 (2)	3.144 (3)	176 (6)
O2*W*—H4*O*···Cl3^{iv}	0.84 (3)	2.30 (3)	3.133 (4)	168 (4)

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