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4-Hydroxyimino-2-phenylperhydroquinolinium chloride hemihydrate

A. Thiruvalluvar[a]* and D. Natarajan[b]

[a]Department of Physics, Rajah Serfoji Government College (Autonomous), Thanjavur 613 005, Tamilnadu, India, and [b]Department of Chemistry, Annamalai University, Annamalai Nagar 608 002, Tamilnadu, India
Correspondence e-mail: athiru@vsnl.net

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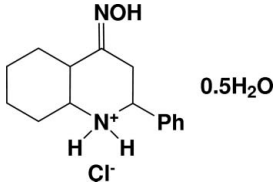
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 12.9.

The title compound, $C_{15}H_{21}N_2O^+\cdot Cl^-\cdot 0.5H_2O$, crystallizes with two cations, two anions and one water molecule in the asymmetric unit. Both the piperidine and cyclohexane rings adopt chair conformations and the oxime groups are basically planar. The cyclohexane ring is equatorially oriented with respect to the piperidine ring. The crystal structure is stabilized by N—H···Cl, C—H···Cl, C—H···O, N—H···N and O—H···Cl hydrogen bonds. A water molecule that bridges the two crystallographically independent chloride anions *via* hydrogen bonds is disordered over two chemically equivalent sites, with occupancy factors of *ca* 0.9:0.1.

Related literature

For a related crystal structure, see Thiruvalluvar *et al.*, 1995. For preparation of the title compound, see Baliah *et al.*, 1978.



Experimental

Crystal data

$C_{15}H_{21}N_2O^+\cdot Cl^-\cdot 0.5H_2O$
M_r = 289.81
Orthorhombic, $Pna2_1$
a = 13.1733 (4) Å
b = 18.2824 (5) Å
c = 12.6656 (4) Å
V = 3050.38 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 293 (2) K
0.28 × 0.18 × 0.18 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.743, T_{max} = 0.956
15501 measured reflections
4758 independent reflections
4335 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.04
4758 reflections
370 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), 1936 Friedel pairs
Flack parameter: −0.02 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1A1···N4A^{i}	0.90	2.08	2.9812 (16)	174
O1—H1A···Cl2^{ii}	0.857 (6)	2.587 (3)	3.410 (2)	161.3 (7)
O1—H1B···Cl1^{iii}	0.854 (4)	2.498 (4)	3.310 (2)	159.1 (6)
N1A—H1A2···Cl1	0.90	2.32	3.2011 (14)	168
O4A—H4A···Cl2^{iv}	0.82	2.23	3.0245 (14)	163
O4B—H4B···Cl2^{i}	0.82	2.23	3.0464 (13)	173
N1B—H1B1···Cl1	0.90	2.32	3.2013 (15)	168
N1B—H1B2···N4B^{v}	0.90	2.18	3.0774 (18)	173
C2B—H2B···Cl2	0.98	2.79	3.6194 (17)	143
C3A—H3A2···O4A	0.97	2.23	2.671 (2)	107
C3B—H3B1···O4B	0.97	2.23	2.669 (2)	106
C23B—H23B···O4A^{vi}	0.93	2.50	3.393 (3)	161
C25A—H25A···O4B^{vii}	0.93	2.47	3.355 (2)	160
C25B—H25B···O4A^{viii}	0.93	2.47	3.398 (2)	172
O2—H2C···Cl2^{ii}	0.842 (6)	2.587 (3)	3.261 (2)	137.9 (7)
O2—H2D···Cl1^{iii}	0.840 (4)	2.498 (4)	3.162 (2)	136.6 (6)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT-NT* (Bruker, 2004); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

The data collection was carried out by Dr A. Babu Vargheese and Mr K. Saminathan of the Sophisticated Analytical Instrument Facility (SAIF) of the Indian Institute of Technology (IIT), Chennai. This help is gratefully acknowledged by AT.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2073).

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supplementary materials

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4-Hydroxyimino-2-phenylperhydroquinolinium chloride hemihydrate

A. Thiruvalluvar and D. Natarajan

Comment

The title compound has been analysed as part of our crystallographic studies on substituted decahydroquinolines. Thiruvalluvar *et al.* (1995) have reported a crystal structure of *N*-benzoyl-2-phenyldecahydroquinolin-4-one, wherein the piperidine ring adopts a flexible twist conformation. The title compound, Fig. 1., crystallizes with two molecules per asymmetric unit. Both molecules are essentially identical, the r.m.s. deviation of an overlay of all non-hydrogen atoms is only 0.086 Å. The torsion angles (C8—C9—C10—C4 = −179.5 (1)° for molecule A and −178.1 (1)° for molecule B) confirm the *trans* fusion of the piperidine and cyclohexane rings in both independent molecules. It is evident from the ring torsion angles that the piperidine and cyclohexane rings are both in a chair conformation. The oxime moieties are essentially planar with r.m.s. deviations of only 0.024 (1) Å. The phenyl rings at C2 are equatorially oriented with respect to the piperidine rings. The crystal structure is stabilized by intramolecular N—H···Cl, C—H···Cl, and C—H···O and by intermolecular N—H···N, N—H···Cl, and O—H···Cl hydrogen bonds., see Fig. 2 and the hydrogen bonding table. A water molecule that bridges *via* hydrogen bonds the two crystallographically independent chlorine anions is disordered over two chemically equivalent sites. Its occupancy ratio refined to 0.905:0.095.

Experimental

The title compound was prepared following the procedure of Baliah et al. (1978). Crystals suitable for X-ray diffraction were grown by slow evaporation of an ethanolic solution.

Refinement

The solvate water molecule is disordered over two positions with an occupancy rate of 0.905 (3) to 0.095 (3). The ADPs of both oxygen atoms were set to be identical. The water hydrogen atoms were located in difference density Fourier maps and the O—H distances were restrained to be 0.84 (2) Å. To allow for a stable and meaningful refinement of the H atoms of the less occupied water molecule the hydrogen bonding distances to both chlorine atoms were restrained to be each the same in both moieties, as were the H···H distances in both water molecules. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms with N—H = 0.90 Å, C—H = 0.93–0.98 Å, O—H = 0.82 Å and U_{iso} = 1.2–1.5 U_{eq}(parent atom). Hydroxyl H atoms were allowed to rotate, but not to tip, to best fit the experimental electron density. A damping factor (damp 400 15 in the final refinement cycles) was applied to avoid large and erratic displacements of the hydrogen atoms of the less occupied water molecule.

Figures

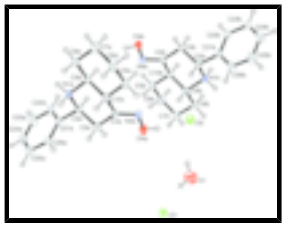

Fig. 1. View of the title molecule with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. H atoms are shown as small spheres of arbitray radii. The minor component water molecule is omitted for clarity.

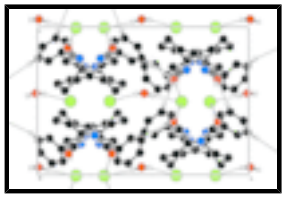

Fig. 2. The molecular packing of the title molecule, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. The minor component water molecule is omitted for clarity.

4-Hydroxyimino-2-phenylperhydroquinolinium chloride hemihydrate

Crystal data

$C_{15}H_{21}N_2O^+\cdot Cl^-\cdot 0.5H_2O$	$D_x = 1.262$ Mg m^{-3}
$M_r = 289.81$	Melting point: 521.5 K
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 7599 reflections
$a = 13.1733$ (4) Å	$\theta = 1.9$–25.0^o
$b = 18.2824$ (5) Å	$\mu = 0.25$ mm^{-1}
$c = 12.6656$ (4) Å	$T = 293$ (2) K
$V = 3050.38$ (16) Å^3	Block, colourless
$Z = 8$	0.28 × 0.18 × 0.18 mm
$F_{000} = 1240$	

Data collection

Bruker APEXII diffractometer	4758 independent reflections
Radiation source: fine-focus sealed tube	4335 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 298$(2) K	$\theta_{max} = 25.0^o$
φ and ω scans	$\theta_{min} = 1.9^o$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -11\rightarrow15$
$T_{min} = 0.743$, $T_{max} = 0.956$	$k = -21\rightarrow21$
15501 measured reflections	$l = -13\rightarrow15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.028$	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.4811P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.075$	$(\Delta/\sigma)_{max} = 0.021$
$S = 1.04$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
4758 reflections	$\Delta\rho_{min} = -0.14$ e Å^{-3}
370 parameters	Extinction correction: none
8 restraints	Absolute structure: Flack (1983), 1936 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.02 (5)
Secondary atom site location: difference Fourier map	

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2$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)
O4A	−0.08852 (9)	0.14775 (6)	0.14251 (11)	0.0470 (4)	
N1A	0.23310 (8)	0.22848 (7)	0.26652 (10)	0.0261 (4)	
N4A	−0.06632 (9)	0.20708 (7)	0.20969 (11)	0.0327 (4)	
C2A	0.19797 (11)	0.17058 (8)	0.19004 (13)	0.0287 (4)	
C3A	0.09632 (11)	0.14114 (8)	0.22857 (15)	0.0356 (5)	
C4A	0.02224 (11)	0.20168 (8)	0.24970 (13)	0.0299 (5)	
C5A	−0.01349 (12)	0.32273 (10)	0.34549 (15)	0.0415 (6)	
C6A	0.03391 (14)	0.38036 (11)	0.41681 (17)	0.0511 (6)	
C7A	0.12985 (14)	0.41068 (10)	0.36777 (17)	0.0525 (6)	
C8A	0.20610 (13)	0.35007 (9)	0.34488 (15)	0.0393 (5)	
C9A	0.15959 (11)	0.29081 (8)	0.27758 (13)	0.0293 (4)	
C10A	0.06029 (11)	0.26051 (9)	0.32326 (13)	0.0302 (5)	
C21A	0.27973 (11)	0.11392 (8)	0.17575 (13)	0.0309 (5)	
C22A	0.34608 (13)	0.12016 (11)	0.09173 (15)	0.0450 (6)	
C23A	0.42413 (15)	0.07005 (13)	0.07871 (17)	0.0614 (7)	
C24A	0.43615 (15)	0.01465 (11)	0.1498 (2)	0.0583 (7)	
C25A	0.37243 (15)	0.00811 (10)	0.23380 (18)	0.0521 (7)	
C26A	0.29358 (13)	0.05739 (9)	0.24692 (15)	0.0396 (5)	
O4B	0.55407 (9)	0.14436 (6)	0.85979 (11)	0.0467 (4)	
N1B	0.23888 (9)	0.22615 (7)	0.72882 (11)	0.0293 (4)	
N4B	0.53580 (10)	0.20112 (7)	0.78713 (12)	0.0348 (4)	

C2B	0.27362 (11)	0.16966 (9)	0.80739 (13)	0.0305 (5)	
C3B	0.37217 (11)	0.13598 (9)	0.76778 (15)	0.0367 (5)	
C4B	0.44839 (11)	0.19465 (8)	0.74485 (13)	0.0314 (5)	
C5B	0.48912 (13)	0.31285 (10)	0.64300 (16)	0.0457 (6)	
C6B	0.44378 (14)	0.36985 (12)	0.56901 (18)	0.0570 (7)	
C7B	0.34831 (14)	0.40309 (10)	0.61570 (18)	0.0533 (7)	
C8B	0.27053 (12)	0.34430 (10)	0.64105 (16)	0.0417 (6)	
C9B	0.31512 (11)	0.28649 (8)	0.71339 (13)	0.0305 (5)	
C10B	0.41304 (11)	0.25273 (9)	0.66891 (13)	0.0328 (5)	
C21B	0.18782 (12)	0.11607 (9)	0.82825 (14)	0.0342 (5)	
C22B	0.11709 (14)	0.13335 (11)	0.90508 (15)	0.0465 (6)	
C23B	0.03521 (16)	0.08800 (13)	0.92400 (18)	0.0630 (8)	
C24B	0.02430 (16)	0.02501 (12)	0.8665 (2)	0.0629 (8)	
C25B	0.09344 (15)	0.00736 (10)	0.7902 (2)	0.0619 (8)	
C26B	0.17489 (14)	0.05274 (10)	0.77065 (18)	0.0496 (6)	
O1	0.17392 (18)	0.49339 (11)	0.0517 (2)	0.1090 (9)	0.906 (3)
O2	0.3144 (15)	0.4868 (8)	−0.0019 (18)	0.1090 (9)	0.095 (3)
Cl1	0.23093 (3)	0.15663 (2)	0.49699 (4)	0.0410 (1)	
Cl2	0.23808 (3)	0.31712 (2)	0.99444 (5)	0.0463 (1)	
H1A1	0.29328	0.24616	0.24460	0.0314*	
H1A2	0.24260	0.20783	0.33025	0.0314*	
H2A	0.18667	0.19420	0.12159	0.0344*	
H3A1	0.10671	0.11322	0.29280	0.0427*	
H3A2	0.06834	0.10846	0.17572	0.0427*	
H4A	−0.14310	0.15490	0.11314	0.0705*	
H5A1	−0.07396	0.30328	0.37898	0.0498*	
H5A2	−0.03359	0.34522	0.27935	0.0498*	
H6A1	0.04972	0.35881	0.48483	0.0613*	
H6A2	−0.01417	0.41976	0.42815	0.0613*	
H7A1	0.11304	0.43574	0.30256	0.0631*	
H9A	0.14576	0.31090	0.20730	0.0352*	
H7A2	0.16012	0.44602	0.41542	0.0631*	
H10A	0.07643	0.23720	0.39088	0.0362*	
H8A1	0.22939	0.32910	0.41092	0.0472*	
H8A2	0.26445	0.37053	0.30870	0.0472*	
H22A	0.33836	0.15819	0.04363	0.0540*	
H23A	0.46817	0.07419	0.02163	0.0737*	
H24A	0.48844	−0.01896	0.14081	0.0699*	
H25A	0.38179	−0.02944	0.28237	0.0625*	
H26A	0.24965	0.05244	0.30395	0.0475*	
H2B	0.28847	0.19499	0.87381	0.0366*	
H4B	0.60021	0.15630	0.89968	0.0700*	
H9B	0.33005	0.30878	0.78202	0.0366*	
H10B	0.39548	0.22829	0.60251	0.0393*	
H1B1	0.22727	0.20419	0.66639	0.0351*	
H1B2	0.17993	0.24564	0.75114	0.0351*	
H3B1	0.39906	0.10292	0.82075	0.0440*	
H3B2	0.35908	0.10802	0.70413	0.0440*	
H5B1	0.54857	0.29132	0.61019	0.0548*	

H5B2	0.51057	0.33648	0.70785	0.0548*	
H6B1	0.49324	0.40815	0.55628	0.0684*	
H6B2	0.42772	0.34716	0.50183	0.0684*	
H7B1	0.31940	0.43761	0.56592	0.0640*	
H7B2	0.36541	0.42954	0.67966	0.0640*	
H22B	0.12475	0.17595	0.94440	0.0558*	
H8B1	0.21207	0.36650	0.67482	0.0500*	
H23B	−0.01222	0.10015	0.97548	0.0756*	
H8B2	0.24784	0.32150	0.57605	0.0500*	
H24B	−0.03042	−0.00586	0.87938	0.0755*	
H25B	0.08553	−0.03542	0.75134	0.0743*	
H26B	0.22140	0.04056	0.71828	0.0595*	
H1A	0.2045 (6)	0.45366 (7)	0.0351 (11)	0.1635*	0.906 (3)
H1B	0.2120 (4)	0.53110 (13)	0.0474 (8)	0.1635*	0.906 (3)
H2C	0.2816 (10)	0.4531 (3)	0.028 (2)	0.1635*	0.095 (3)
H2D	0.3179 (9)	0.52669 (19)	0.031 (2)	0.1635*	0.095 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4A	0.0355 (6)	0.0516 (7)	0.0538 (8)	0.0033 (5)	−0.0179 (6)	−0.0147 (6)
N1A	0.0186 (6)	0.0324 (6)	0.0274 (8)	0.0001 (5)	−0.0009 (5)	0.0013 (6)
N4A	0.0242 (6)	0.0399 (7)	0.0339 (8)	0.0007 (5)	−0.0042 (5)	−0.0050 (6)
C2A	0.0239 (7)	0.0359 (8)	0.0262 (8)	0.0033 (6)	−0.0043 (6)	0.0004 (7)
C3A	0.0255 (7)	0.0362 (8)	0.0450 (10)	0.0008 (6)	−0.0062 (7)	−0.0016 (8)
C4A	0.0203 (7)	0.0363 (8)	0.0332 (9)	−0.0004 (6)	0.0005 (6)	0.0031 (7)
C5A	0.0256 (8)	0.0575 (10)	0.0415 (11)	0.0081 (7)	−0.0021 (7)	−0.0120 (9)
C6A	0.0384 (9)	0.0608 (11)	0.0542 (12)	0.0112 (9)	−0.0038 (8)	−0.0261 (10)
C7A	0.0465 (10)	0.0474 (9)	0.0637 (14)	0.0037 (8)	−0.0067 (9)	−0.0226 (10)
C8A	0.0306 (8)	0.0416 (9)	0.0457 (11)	−0.0029 (7)	−0.0016 (8)	−0.0074 (8)
C9A	0.0256 (7)	0.0346 (7)	0.0278 (9)	0.0032 (6)	−0.0012 (6)	0.0007 (7)
C10A	0.0211 (7)	0.0417 (8)	0.0279 (9)	0.0035 (6)	−0.0025 (6)	0.0001 (7)
C21A	0.0241 (7)	0.0368 (8)	0.0318 (9)	0.0017 (6)	−0.0054 (6)	−0.0069 (7)
C22A	0.0390 (9)	0.0620 (11)	0.0341 (10)	0.0121 (8)	−0.0010 (8)	0.0035 (9)
C23A	0.0460 (11)	0.0932 (15)	0.0451 (12)	0.0246 (11)	0.0080 (9)	−0.0125 (12)
C24A	0.0480 (11)	0.0550 (11)	0.0718 (16)	0.0248 (9)	−0.0108 (10)	−0.0183 (11)
C25A	0.0503 (10)	0.0370 (9)	0.0689 (15)	0.0079 (8)	−0.0126 (10)	−0.0021 (9)
C26A	0.0365 (8)	0.0344 (8)	0.0479 (11)	0.0013 (7)	−0.0017 (8)	0.0042 (8)
O4B	0.0383 (6)	0.0441 (6)	0.0576 (9)	−0.0002 (5)	−0.0225 (6)	0.0093 (6)
N1B	0.0232 (6)	0.0370 (7)	0.0276 (8)	0.0031 (5)	0.0002 (5)	−0.0026 (6)
N4B	0.0253 (7)	0.0411 (7)	0.0379 (9)	0.0031 (5)	−0.0056 (6)	0.0014 (6)
C2B	0.0300 (8)	0.0367 (8)	0.0247 (9)	−0.0012 (6)	−0.0042 (6)	−0.0005 (7)
C3B	0.0273 (8)	0.0372 (8)	0.0455 (11)	0.0020 (7)	−0.0085 (7)	0.0012 (8)
C4B	0.0237 (7)	0.0404 (8)	0.0301 (9)	0.0033 (6)	−0.0016 (6)	−0.0041 (7)
C5B	0.0283 (8)	0.0634 (11)	0.0454 (12)	−0.0020 (8)	−0.0012 (8)	0.0157 (10)
C6B	0.0388 (10)	0.0727 (13)	0.0595 (14)	−0.0056 (9)	−0.0002 (9)	0.0284 (11)
C7B	0.0487 (11)	0.0512 (10)	0.0601 (13)	0.0000 (9)	−0.0026 (10)	0.0225 (10)
C8B	0.0320 (9)	0.0459 (10)	0.0471 (12)	0.0074 (7)	0.0007 (8)	0.0107 (9)

C9B	0.0274 (7)	0.0360 (8)	0.0281 (9)	−0.0001 (6)	−0.0008 (6)	0.0023 (7)
C10B	0.0217 (7)	0.0485 (9)	0.0281 (9)	0.0005 (7)	−0.0017 (6)	0.0007 (8)
C21B	0.0325 (8)	0.0363 (8)	0.0338 (10)	−0.0013 (7)	−0.0067 (7)	0.0014 (7)
C22B	0.0465 (10)	0.0593 (11)	0.0337 (10)	−0.0138 (9)	0.0015 (8)	−0.0067 (9)
C23B	0.0536 (12)	0.0916 (15)	0.0438 (13)	−0.0259 (11)	0.0113 (9)	−0.0024 (12)
C24B	0.0530 (12)	0.0615 (12)	0.0743 (17)	−0.0231 (10)	−0.0007 (11)	0.0099 (12)
C25B	0.0480 (11)	0.0406 (10)	0.0971 (19)	−0.0071 (9)	−0.0065 (12)	−0.0136 (12)
C26B	0.0357 (9)	0.0444 (10)	0.0687 (14)	−0.0009 (8)	0.0009 (9)	−0.0152 (10)
O1	0.1029 (16)	0.0790 (12)	0.145 (2)	−0.0179 (12)	0.0326 (15)	−0.0115 (13)
O2	0.1029 (16)	0.0790 (12)	0.145 (2)	−0.0179 (12)	0.0326 (15)	−0.0115 (13)
Cl1	0.0443 (2)	0.0488 (2)	0.0298 (2)	0.0058 (2)	−0.0018 (2)	−0.0005 (2)
Cl2	0.0433 (2)	0.0545 (2)	0.0410 (2)	0.0002 (2)	−0.0150 (2)	−0.0034 (3)

Geometric parameters (Å, °)

O4A—N4A	1.4093 (18)	C8A—H8A1	0.9700
O4A—H4A	0.8200	C8A—H8A2	0.9700
O4B—N4B	1.4077 (19)	C9A—H9A	0.9800
O4B—H4B	0.8200	C10A—H10A	0.9800
O1—H1A	0.857 (6)	C22A—H22A	0.9300
O1—H1B	0.854 (4)	C23A—H23A	0.9300
O2—H2C	0.84 (2)	C24A—H24A	0.9300
O2—H2D	0.84 (2)	C25A—H25A	0.9300
N1A—C9A	1.5020 (19)	C26A—H26A	0.9300
N1A—C2A	1.508 (2)	C2B—C3B	1.522 (2)
N4A—C4A	1.2758 (19)	C2B—C21B	1.519 (2)
N1A—H1A1	0.9000	C3B—C4B	1.498 (2)
N1A—H1A2	0.9000	C4B—C10B	1.507 (2)
N1B—C2B	1.505 (2)	C5B—C10B	1.523 (2)
N1B—C9B	1.5046 (19)	C5B—C6B	1.524 (3)
N4B—C4B	1.275 (2)	C6B—C7B	1.517 (3)
N1B—H1B2	0.9000	C7B—C8B	1.519 (3)
N1B—H1B1	0.9000	C8B—C9B	1.517 (2)
C2A—C21A	1.505 (2)	C9B—C10B	1.537 (2)
C2A—C3A	1.524 (2)	C21B—C22B	1.384 (3)
C3A—C4A	1.500 (2)	C21B—C26B	1.379 (3)
C4A—C10A	1.509 (2)	C22B—C23B	1.381 (3)
C5A—C6A	1.522 (3)	C23B—C24B	1.370 (3)
C5A—C10A	1.523 (2)	C24B—C25B	1.367 (3)
C6A—C7A	1.513 (3)	C25B—C26B	1.379 (3)
C7A—C8A	1.523 (3)	C2B—H2B	0.9800
C8A—C9A	1.509 (2)	C3B—H3B1	0.9700
C9A—C10A	1.534 (2)	C3B—H3B2	0.9700
C21A—C26A	1.384 (2)	C5B—H5B1	0.9700
C21A—C22A	1.382 (2)	C5B—H5B2	0.9700
C22A—C23A	1.387 (3)	C6B—H6B2	0.9700
C23A—C24A	1.364 (3)	C6B—H6B1	0.9700
C24A—C25A	1.360 (3)	C7B—H7B2	0.9700
C25A—C26A	1.385 (3)	C7B—H7B1	0.9700

C2A—H2A	0.9800	C8B—H8B1	0.9700
C3A—H3A2	0.9700	C8B—H8B2	0.9700
C3A—H3A1	0.9700	C9B—H9B	0.9800
C5A—H5A1	0.9700	C10B—H10B	0.9800
C5A—H5A2	0.9700	C22B—H22B	0.9300
C6A—H6A1	0.9700	C23B—H23B	0.9300
C6A—H6A2	0.9700	C24B—H24B	0.9300
C7A—H7A2	0.9700	C25B—H25B	0.9300
C7A—H7A1	0.9700	C26B—H26B	0.9300
Cl1···N1A	3.2011 (14)	H1A2···Cl1	2.3200
Cl1···N1B	3.2013 (15)	H2A···H22A	2.3200
Cl1···O2^{i}	3.162 (15)	H2A···H22B^{v}	2.4100
Cl1···O1^{i}	3.310 (2)	H2A···Cl2^{v}	2.8500
Cl2···O1^{ii}	3.410 (2)	H2A···H9A	2.4500
Cl2···O2^{ii}	3.261 (15)	H2A···C22B^{v}	3.1000
Cl2···O4B^{iii}	3.0464 (13)	H2B···H22A^{ii}	2.3500
Cl2···C2B	3.6194 (17)	H2B···H9B	2.4500
Cl1···H10A	2.8500	H2B···Cl2	2.7900
Cl1···H10B	2.8600	H2B···H22B	2.3600
Cl1···H1A2	2.3200	H2C···O4A^{iv}	2.904 (15)
Cl1···H2D^{i}	2.499 (6)	H2C···H4A^{iv}	2.4600
Cl1···H5B1^{iii}	2.9600	H2C···Cl2^{v}	2.587 (7)
Cl1···H26A	3.1100	H2D···H26B^{vi}	2.4400
Cl1···H5A1^{iv}	3.0600	H2D···Cl1^{vi}	2.499 (6)
Cl1···H1B^{i}	2.498 (4)	H2D···C26B^{vi}	3.07 (3)
Cl1···H1B1	2.3200	H3A1···H1A2	2.5300
Cl2···H2B	2.7900	H3A1···C26A	2.7300
Cl2···H9B	2.9500	H3A1···H26A	2.1900
Cl2···H22B	3.0500	H3A1···H24B^{viii}	2.4600
Cl2···H9A^{ii}	2.9600	H3A2···O4A	2.2300
Cl2···H2C^{ii}	2.587 (7)	H4A···H2C^{iii}	2.4600
Cl2···H2A^{ii}	2.8500	H4A···Cl2^{ix}	2.2300
Cl2···H4B^{iii}	2.2300	H4A···H1A1^{iii}	2.6000
Cl2···H1A^{ii}	2.587 (3)	H4B···Cl2^{iv}	2.2300
O1···Cl2^{v}	3.410 (2)	H5A1···Cl1^{iii}	3.0600
O1···C24A^{iii}	3.373 (3)	H5A1···N4A	2.7800
O1···Cl1^{vi}	3.310 (2)	H5A1···H1A2^{iii}	2.5000
O2···Cl1^{vi}	3.162 (15)	H5A2···H7A1	2.5600
O2···C24B^{vii}	3.24 (2)	H5A2···C21A^{iii}	2.8900
O2···C23B^{vii}	3.348 (19)	H5A2···C22A^{iii}	2.9300
O2···Cl2^{v}	3.261 (15)	H5A2···C23A^{iii}	3.0300
O4A···C25B^{viii}	3.398 (2)	H5A2···C24A^{iii}	3.0700
O4A···Cl2^{ix}	3.0245 (14)	H5A2···C25A^{iii}	3.0100

O4A···C23B^{v}	3.393 (3)	H5A2···C26A^{iii}	2.9200
O4B···C25A^{x}	3.355 (2)	H5A2···N4A	2.7100
O4B···Cl2^{iv}	3.0464 (13)	H6A1···H10A	2.5500
O1···H26B^{vi}	2.6600	H7A1···H5A2	2.5600
O1···H24A^{iii}	2.7300	H9A···H2A	2.4500
O1···H3B2^{vi}	2.8800	H9A···Cl2^{v}	2.9600
O2···H26A^{vi}	2.8600	H9B···H2B	2.4500
O2···H23B^{vii}	2.8000	H9B···Cl2	2.9500
O2···H24B^{vii}	2.5600	H10A···H1A2	2.3800
O4A···H1A1^{iii}	2.8000	H10A···H6A1	2.5500
O4A···H2C^{iii}	2.904 (15)	H10A···Cl1	2.8500
O4A···H8A2^{iii}	2.8800	H10B···H3B2	2.5900
O4A···H23B^{v}	2.5000	H10B···Cl1	2.8600
O4A···H25B^{viii}	2.4700	H10B···H1B1	2.4000
O4A···H3A2	2.2300	H10B···H6B2	2.5600
O4B···H23A^{ii}	2.6700	H8A1···C8B	2.9800
O4B···H3B1	2.2300	H8A1···H1A2	2.4500
O4B···H25A^{x}	2.4700	H8A1···H8B2	2.1100
N1A···Cl1	3.2011 (14)	H8A2···H1A1	2.4400
N1A···N4A^{iv}	2.9812 (16)	H8A2···O4A^{iv}	2.8800
N1B···N4B^{iii}	3.0774 (18)	H8A2···N4A^{iv}	2.9300
N1B···Cl1	3.2013 (15)	H1B1···C4B	3.0800
N4A···N1A^{iii}	2.9812 (16)	H1B1···H3B2	2.5200
N4B···N1B^{iv}	3.0774 (18)	H1B1···Cl1	2.3200
N1B···H5B1^{iii}	2.9400	H1B1···H5B1^{iii}	2.4600
N4A···H1A1^{iii}	2.0800	H1B1···H8B2	2.4500
N4A···H5A1	2.7800	H1B1···H10B	2.4000
N4A···H5A2	2.7100	H1B2···H8B1	2.4500
N4A···H8A2^{iii}	2.9300	H1B2···N4B^{iii}	2.1800
N4B···H5B1	2.7900	H1B2···C5B^{iii}	3.0600
N4B···H1B2^{iv}	2.1800	H1B2···C22B	2.9500
N4B···H5B2	2.6900	H1B2···H5B1^{iii}	2.5800
C2B···Cl2	3.6194 (17)	H3B1···O4B	2.2300
C5A···C26A^{iii}	3.581 (2)	H3B2···O1^{i}	2.8800
C23B···O2^{xi}	3.348 (19)	H3B2···H1B1	2.5200
C23B···O4A^{ii}	3.393 (3)	H3B2···C26B	2.7600
C24A···O1^{iv}	3.373 (3)	H3B2···H10B	2.5900
C24B···O2^{xi}	3.24 (2)	H3B2···H26B	2.2000
C25A···O4B^{xii}	3.355 (2)	H5B1···Cl1^{iv}	2.9600
C25B···O4A^{xiii}	3.398 (2)	H5B1···N1B^{iv}	2.9400
C26A···C5A^{iv}	3.581 (2)	H5B1···N4B	2.7900
C3A···H25B^{viii}	3.0900	H5B1···H1B1^{iv}	2.4600

C3A···H26A	2.7600	H5B1···H1B2^{iv}	2.5800
C3B···H26B	2.7200	H5B2···N4B	2.6900
C4A···H1A2	3.0800	H5B2···H7B2	2.5800
C4B···H1B1	3.0800	H5B2···C21B^{iv}	2.9200
C5B···H1B2^{iv}	3.0600	H5B2···C22B^{iv}	2.9200
C8A···H8B2	3.0200	H5B2···C23B^{iv}	3.0800
C8B···H8A1	2.9800	H5B2···C26B^{iv}	3.0700
C21A···H5A2^{iv}	2.8900	H6B2···H10B	2.5600
C21B···H5B2^{iii}	2.9200	H6B2···H8B2	2.5900
C22A···H5A2^{iv}	2.9300	H7B2···H5B2	2.5800
C22A···H1A1	3.0900	H22A···H2B^{v}	2.3500
C22B···H5B2^{iii}	2.9200	H22A···H2A	2.3200
C22B···H1B2	2.9500	H22B···Cl2	3.0500
C22B···H2A^{ii}	3.1000	H22B···H2A^{ii}	2.4100
C23A···H5A2^{iv}	3.0300	H22B···H2B	2.3600
C23B···H5B2^{iii}	3.0800	H8B1···H1B2	2.4500
C24A···H5A2^{iv}	3.0700	H8B1···C25A^{xv}	2.9200
C25A···H8B1^{xiv}	2.9200	H23A···O4B^{v}	2.6700
C25A···H5A2^{iv}	3.0100	H23B···O2^{xi}	2.8000
C26A···H1A2	3.0200	H23B···O4A^{ii}	2.5000
C26A···H5A2^{iv}	2.9200	H8B2···H8A1	2.1100
C26A···H3A1	2.7300	H8B2···H6B2	2.5900
C26B···H5B2^{iii}	3.0700	H8B2···H1B1	2.4500
C26B···H2D^{i}	3.07 (3)	H8B2···C8A	3.0200
C26B···H3B2	2.7600	H24A···O1^{iv}	2.7300
H1A1···C22A	3.0900	H24B···O2^{xi}	2.5600
H1A1···H4A^{iv}	2.6000	H24B···H3A1^{xiii}	2.4600
H1A1···N4A^{iv}	2.0800	H25A···O4B^{xii}	2.4700
H1A1···H8A2	2.4400	H25B···C3A^{xiii}	3.0900
H1A1···O4A^{iv}	2.8000	H25B···O4A^{xiii}	2.4700
H1A···Cl2^{v}	2.587 (3)	H26A···H3A1	2.1900
H1B···H26B^{vi}	2.3400	H26A···O2^{i}	2.8600
H1B···Cl1^{vi}	2.498 (4)	H26A···C3A	2.7600
H1A2···H8A1	2.4500	H26A···Cl1	3.1100
H1A2···H5A1^{iv}	2.5000	H26B···C3B	2.7200
H1A2···H3A1	2.5300	H26B···H3B2	2.2000
H1A2···H10A	2.3800	H26B···H1B^{i}	2.3400
H1A2···C4A	3.0800	H26B···H2D^{i}	2.4400
H1A2···C26A	3.0200	H26B···O1^{i}	2.6600
N4A—O4A—H4A	109.00	C23A—C22A—H22A	120.00
N4B—O4B—H4B	109.00	C22A—C23A—H23A	120.00
H1A—O1—H1B	113.1 (6)	C24A—C23A—H23A	120.00

H2C—O2—H2D	116 (3)	C25A—C24A—H24A	120.00
C2A—N1A—C9A	113.25 (11)	C23A—C24A—H24A	120.00
O4A—N4A—C4A	111.72 (12)	C26A—C25A—H25A	120.00
H1A1—N1A—H1A2	108.00	C24A—C25A—H25A	120.00
C2A—N1A—H1A1	109.00	C25A—C26A—H26A	120.00
C9A—N1A—H1A1	109.00	C21A—C26A—H26A	120.00
C9A—N1A—H1A2	109.00	C3B—C2B—C21B	115.54 (14)
C2A—N1A—H1A2	109.00	N1B—C2B—C21B	109.35 (12)
C2B—N1B—C9B	112.70 (11)	N1B—C2B—C3B	108.60 (13)
O4B—N4B—C4B	111.13 (12)	C2B—C3B—C4B	110.25 (13)
C2B—N1B—H1B1	109.00	N4B—C4B—C10B	118.80 (13)
H1B1—N1B—H1B2	108.00	N4B—C4B—C3B	126.18 (15)
C9B—N1B—H1B2	109.00	C3B—C4B—C10B	114.92 (13)
C2B—N1B—H1B2	109.00	C6B—C5B—C10B	111.60 (14)
C9B—N1B—H1B1	109.00	C5B—C6B—C7B	111.06 (17)
N1A—C2A—C21A	109.93 (12)	C6B—C7B—C8B	110.99 (16)
C3A—C2A—C21A	115.11 (12)	C7B—C8B—C9B	111.06 (14)
N1A—C2A—C3A	108.18 (12)	N1B—C9B—C10B	108.26 (12)
C2A—C3A—C4A	111.62 (12)	N1B—C9B—C8B	109.32 (12)
N4A—C4A—C3A	125.54 (14)	C8B—C9B—C10B	112.54 (14)
N4A—C4A—C10A	119.60 (13)	C4B—C10B—C5B	116.28 (13)
C3A—C4A—C10A	114.85 (13)	C5B—C10B—C9B	109.96 (13)
C6A—C5A—C10A	111.42 (14)	C4B—C10B—C9B	107.97 (13)
C5A—C6A—C7A	110.65 (16)	C2B—C21B—C26B	122.78 (16)
C6A—C7A—C8A	111.24 (15)	C22B—C21B—C26B	118.72 (16)
C7A—C8A—C9A	111.23 (14)	C2B—C21B—C22B	118.43 (15)
N1A—C9A—C8A	109.62 (12)	C21B—C22B—C23B	120.71 (18)
C8A—C9A—C10A	113.12 (14)	C22B—C23B—C24B	119.6 (2)
N1A—C9A—C10A	108.12 (12)	C23B—C24B—C25B	120.3 (2)
C4A—C10A—C5A	115.77 (13)	C24B—C25B—C26B	120.24 (19)
C4A—C10A—C9A	107.93 (13)	C21B—C26B—C25B	120.42 (19)
C5A—C10A—C9A	110.14 (13)	C3B—C2B—H2B	108.00
C2A—C21A—C26A	122.01 (14)	C21B—C2B—H2B	108.00
C22A—C21A—C26A	118.69 (15)	N1B—C2B—H2B	108.00
C2A—C21A—C22A	119.23 (15)	C4B—C3B—H3B1	110.00
C21A—C22A—C23A	120.39 (18)	C2B—C3B—H3B1	110.00
C22A—C23A—C24A	119.86 (19)	C2B—C3B—H3B2	110.00
C23A—C24A—C25A	120.65 (19)	H3B1—C3B—H3B2	108.00
C24A—C25A—C26A	119.96 (19)	C4B—C3B—H3B2	110.00
C21A—C26A—C25A	120.44 (17)	C6B—C5B—H5B2	109.00
C21A—C2A—H2A	108.00	C6B—C5B—H5B1	109.00
N1A—C2A—H2A	108.00	H5B1—C5B—H5B2	108.00
C3A—C2A—H2A	108.00	C10B—C5B—H5B1	109.00
C2A—C3A—H3A1	109.00	C10B—C5B—H5B2	109.00
C2A—C3A—H3A2	109.00	C7B—C6B—H6B1	109.00
C4A—C3A—H3A1	109.00	C7B—C6B—H6B2	109.00
C4A—C3A—H3A2	109.00	H6B1—C6B—H6B2	108.00
H3A1—C3A—H3A2	108.00	C5B—C6B—H6B1	109.00
C6A—C5A—H5A2	109.00	C5B—C6B—H6B2	109.00

H5A1—C5A—H5A2	108.00	C6B—C7B—H7B1	109.00
C10A—C5A—H5A2	109.00	C8B—C7B—H7B2	109.00
C6A—C5A—H5A1	109.00	C6B—C7B—H7B2	109.00
C10A—C5A—H5A1	109.00	C8B—C7B—H7B1	109.00
H6A1—C6A—H6A2	108.00	H7B1—C7B—H7B2	108.00
C5A—C6A—H6A1	110.00	C7B—C8B—H8B2	109.00
C7A—C6A—H6A2	110.00	C9B—C8B—H8B1	109.00
C7A—C6A—H6A1	110.00	H8B1—C8B—H8B2	108.00
C5A—C6A—H6A2	110.00	C9B—C8B—H8B2	109.00
C8A—C7A—H7A1	109.00	C7B—C8B—H8B1	109.00
C6A—C7A—H7A2	109.00	N1B—C9B—H9B	109.00
H7A1—C7A—H7A2	108.00	C10B—C9B—H9B	109.00
C6A—C7A—H7A1	109.00	C8B—C9B—H9B	109.00
C8A—C7A—H7A2	109.00	C5B—C10B—H10B	107.00
C7A—C8A—H8A1	109.00	C9B—C10B—H10B	107.00
C9A—C8A—H8A2	109.00	C4B—C10B—H10B	107.00
C7A—C8A—H8A2	109.00	C21B—C22B—H22B	120.00
C9A—C8A—H8A1	109.00	C23B—C22B—H22B	120.00
H8A1—C8A—H8A2	108.00	C22B—C23B—H23B	120.00
C10A—C9A—H9A	109.00	C24B—C23B—H23B	120.00
N1A—C9A—H9A	109.00	C25B—C24B—H24B	120.00
C8A—C9A—H9A	109.00	C23B—C24B—H24B	120.00
C9A—C10A—H10A	108.00	C24B—C25B—H25B	120.00
C5A—C10A—H10A	108.00	C26B—C25B—H25B	120.00
C4A—C10A—H10A	108.00	C25B—C26B—H26B	120.00
C21A—C22A—H22A	120.00	C21B—C26B—H26B	120.00
C9A—N1A—C2A—C3A	−58.84 (16)	C26A—C21A—C22A—C23A	0.8 (3)
C9A—N1A—C2A—C21A	174.71 (12)	C2A—C21A—C26A—C25A	−177.11 (16)
C2A—N1A—C9A—C8A	−173.23 (13)	C21A—C22A—C23A—C24A	−0.6 (3)
C2A—N1A—C9A—C10A	63.05 (16)	C22A—C23A—C24A—C25A	−0.2 (3)
O4A—N4A—C4A—C3A	0.9 (2)	C23A—C24A—C25A—C26A	0.9 (3)
O4A—N4A—C4A—C10A	179.48 (13)	C24A—C25A—C26A—C21A	−0.8 (3)
C9B—N1B—C2B—C3B	−59.89 (16)	N1B—C2B—C3B—C4B	53.73 (17)
C9B—N1B—C2B—C21B	173.23 (13)	C21B—C2B—C3B—C4B	176.97 (14)
C2B—N1B—C9B—C8B	−174.93 (13)	N1B—C2B—C21B—C22B	−86.26 (19)
C2B—N1B—C9B—C10B	62.15 (16)	N1B—C2B—C21B—C26B	90.68 (19)
O4B—N4B—C4B—C3B	0.7 (2)	C3B—C2B—C21B—C22B	150.90 (16)
O4B—N4B—C4B—C10B	176.86 (13)	C3B—C2B—C21B—C26B	−32.2 (2)
C3A—C2A—C21A—C26A	−40.8 (2)	C2B—C3B—C4B—N4B	120.99 (18)
C21A—C2A—C3A—C4A	175.02 (14)	C2B—C3B—C4B—C10B	−55.31 (19)
N1A—C2A—C21A—C22A	−95.33 (17)	N4B—C4B—C10B—C5B	4.0 (2)
N1A—C2A—C3A—C4A	51.65 (17)	N4B—C4B—C10B—C9B	−120.09 (16)
C3A—C2A—C21A—C22A	142.23 (16)	C3B—C4B—C10B—C5B	−179.41 (15)
N1A—C2A—C21A—C26A	81.69 (18)	C3B—C4B—C10B—C9B	56.50 (18)
C2A—C3A—C4A—N4A	125.11 (17)	C10B—C5B—C6B—C7B	57.0 (2)
C2A—C3A—C4A—C10A	−53.58 (19)	C6B—C5B—C10B—C4B	−177.83 (15)
N4A—C4A—C10A—C5A	1.0 (2)	C6B—C5B—C10B—C9B	−54.8 (2)
C3A—C4A—C10A—C9A	55.82 (18)	C5B—C6B—C7B—C8B	−56.7 (2)
N4A—C4A—C10A—C9A	−122.96 (15)	C6B—C7B—C8B—C9B	55.5 (2)

C3A—C4A—C10A—C5A	179.74 (14)	C7B—C8B—C9B—N1B	−175.11 (14)
C6A—C5A—C10A—C9A	−54.96 (19)	C7B—C8B—C9B—C10B	−54.77 (19)
C10A—C5A—C6A—C7A	57.8 (2)	N1B—C9B—C10B—C4B	−57.15 (16)
C6A—C5A—C10A—C4A	−177.73 (15)	N1B—C9B—C10B—C5B	175.05 (13)
C5A—C6A—C7A—C8A	−57.1 (2)	C8B—C9B—C10B—C4B	−178.09 (13)
C6A—C7A—C8A—C9A	54.7 (2)	C8B—C9B—C10B—C5B	54.11 (18)
C7A—C8A—C9A—N1A	−173.94 (14)	C2B—C21B—C22B—C23B	177.23 (17)
C7A—C8A—C9A—C10A	−53.20 (19)	C26B—C21B—C22B—C23B	0.2 (3)
C8A—C9A—C10A—C5A	53.22 (18)	C2B—C21B—C26B—C25B	−177.51 (18)
C8A—C9A—C10A—C4A	−179.52 (13)	C22B—C21B—C26B—C25B	−0.6 (3)
N1A—C9A—C10A—C4A	−57.94 (16)	C21B—C22B—C23B—C24B	0.4 (3)
N1A—C9A—C10A—C5A	174.81 (13)	C22B—C23B—C24B—C25B	−0.6 (3)
C2A—C21A—C22A—C23A	177.89 (17)	C23B—C24B—C25B—C26B	0.2 (3)
C22A—C21A—C26A—C25A	−0.1 (3)	C24B—C25B—C26B—C21B	0.4 (3)

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*+1/2; (ii) *x*, *y*, *z*+1; (iii) *x*−1/2, −*y*+1/2, *z*; (iv) *x*+1/2, −*y*+1/2, *z*; (v) *x*, *y*, *z*−1; (vi) −*x*+1/2, *y*+1/2, *z*−1/2; (vii) *x*+1/2, −*y*+1/2, *z*−1; (viii) −*x*, −*y*, *z*−1/2; (ix) *x*−1/2, −*y*+1/2, *z*−1; (x) −*x*+1, −*y*, *z*+1/2; (xi) *x*−1/2, −*y*+1/2, *z*+1; (xii) −*x*+1, −*y*, *z*−1/2; (xiii) −*x*, −*y*, *z*+1/2; (xiv) −*x*+1/2, *y*−1/2, *z*−1/2; (xv) −*x*+1/2, *y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1A—H1A1···N4A^{iv}	0.90	2.08	2.9812 (16)	174
O1—H1A···Cl2^{v}	0.857 (6)	2.587 (3)	3.410 (2)	161.3 (7)
O1—H1B···Cl1^{vi}	0.854 (4)	2.498 (4)	3.310 (2)	159.1 (6)
N1A—H1A2···Cl1	0.90	2.32	3.2011 (14)	168
O4A—H4A···Cl2^{ix}	0.82	2.23	3.0245 (14)	163
O4B—H4B···Cl2^{iv}	0.82	2.23	3.0464 (13)	173
N1B—H1B1···Cl1	0.90	2.32	3.2013 (15)	168
N1B—H1B2···N4B^{iii}	0.90	2.18	3.0774 (18)	173
C2B—H2B···Cl2	0.98	2.79	3.6194 (17)	143
C3A—H3A2···O4A	0.97	2.23	2.671 (2)	107
C3B—H3B1···O4B	0.97	2.23	2.669 (2)	106
C23B—H23B···O4A^{ii}	0.93	2.50	3.393 (3)	161
C25A—H25A···O4B^{xii}	0.93	2.47	3.355 (2)	160
C25B—H25B···O4A^{xiii}	0.93	2.47	3.398 (2)	172
O2—H2C···Cl2^{v}	0.842 (6)	2.587 (3)	3.261 (2)	137.9 (7)
O2—H2D···Cl1^{vi}	0.840 (4)	2.498 (4)	3.162 (2)	136.6 (6)

Symmetry codes: (iv) *x*+1/2, −*y*+1/2, *z*; (v) *x*, *y*, *z*−1; (vi) −*x*+1/2, *y*+1/2, *z*−1/2; (ix) *x*−1/2, −*y*+1/2, *z*−1; (iii) *x*−1/2, −*y*+1/2, *z*; (ii) *x*, *y*, *z*+1; (xii) −*x*+1, −*y*, *z*−1/2; (xiii) −*x*, −*y*, *z*+1/2.

Fig. 1

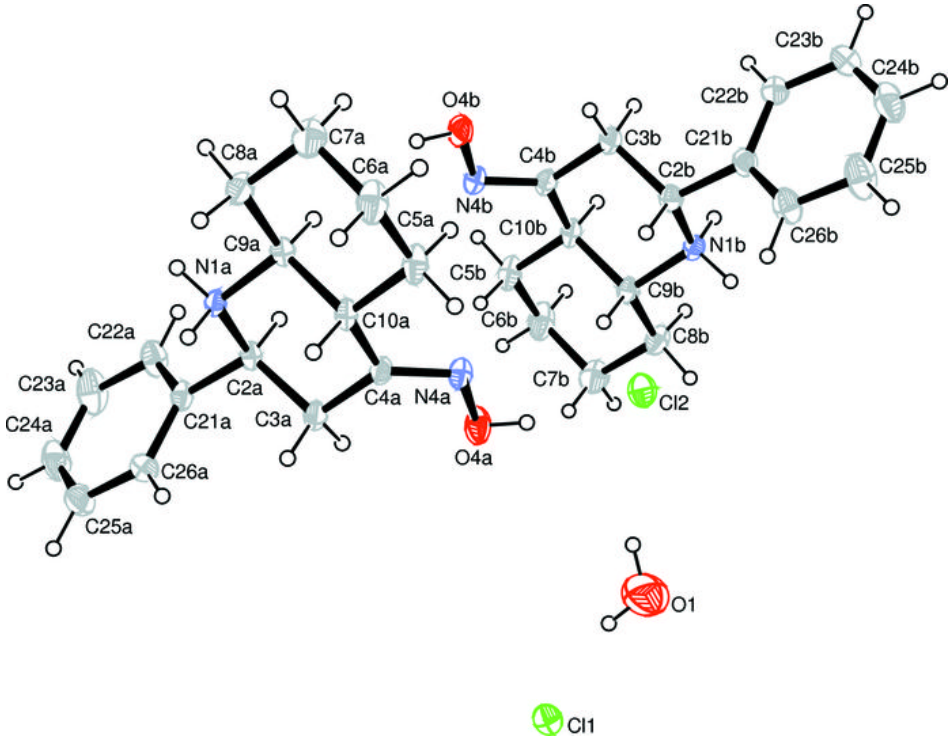
C23b
C24b
C22b
O4b
C7a
C8a
C6a
C3b
C21b
C4b
C2b
C25b
N4b
C5a
C10b
N1b
C26b
C9a
N1a
C5b
C9b
C10a
C6b
C8b
C22a
C23a
C2a
C4a
N4a
C7b
Cl2
C24a
C21a
C3a
O4a
C26a
C25a
O1
Cl1

Fig. 2