

Poly[(μ_6 -4-amino-3,5,6-trichloro-pyridine-2-carboxylato)aquacaesium]

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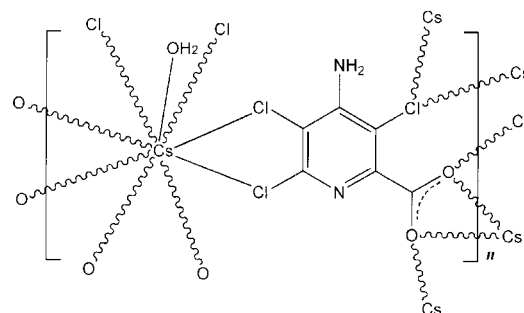
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Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.021; wR factor = 0.053; data-to-parameter ratio = 13.1.

In the structure of the title complex, $[\text{Cs}(\text{C}_6\text{H}_2\text{Cl}_3\text{N}_2\text{O}_2)(\text{H}_2\text{O})]_n$, the caesium salt of the commercial herbicide picloram, the Cs^+ cation lies on a crystallographic mirror plane, which also contains the coordinating water molecule and all non-H atoms of the 4-amino-3,5,6-trichloropicolinate anion except the carboxylate O-atom donors. The irregular CsCl_4O_5 coordination polyhedron comprises chlorine donors from the *ortho*-related ring substituents of the picloramate ligand in a bidentate chelate mode, with a third chlorine bridging $[\text{Cs}-\text{Cl}$ range 3.6052 (11)–3.7151 (11) Å] as well as a bidentate chelate carboxylate group giving sheets extending parallel to (010). A three-dimensional coordination polymer structure is generated through the carboxylate group, which also bridges the sheets down [010]. Within the structure, there are intra-unit water $\text{O}-\text{H}\cdots\text{O}_{\text{carboxylate}}$ and amine $\text{N}-\text{H}\cdots\text{N}_{\text{pyridine}}$ hydrogen-bonding interactions.

Related literature

For background information on picloram, see: Mullinson (1985); O'Neil (2001). For examples of structures of metal complexes with picloram, see: Smith *et al.* (1981*a,b*); O'Reilly *et al.* (1983). For another structure with caesium cations involving coordinating carbon-bound Cl, see: Levitskaia *et al.* (2000). For a caesium complex with dipicolinic acid, see: Santra *et al.* (2011).



Experimental

Crystal data

$[\text{Cs}(\text{C}_6\text{H}_2\text{Cl}_3\text{N}_2\text{O}_2)(\text{H}_2\text{O})]$	$V = 545.58$ (4) Å ³
$M_r = 391.37$	$Z = 2$
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation
$a = 7.0816$ (3) Å	$\mu = 4.11$ mm ⁻¹
$b = 6.6863$ (2) Å	$T = 200$ K
$c = 11.7382$ (5) Å	$0.25 \times 0.20 \times 0.08$ mm
$\beta = 101.005$ (4)°	

Data collection

Oxford Diffraction Gemini-S CCD detector diffractometer	3773 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2012)	1164 independent reflections
$T_{\min} = 0.67$, $T_{\max} = 0.98$	1118 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$	89 parameters
$wR(F^2) = 0.053$	H-atom parameters constrained
$S = 0.98$	$\Delta\rho_{\text{max}} = 0.55$ e Å ⁻³
1164 reflections	$\Delta\rho_{\text{min}} = -0.56$ e Å ⁻³

Table 1

Selected bond lengths (Å).

Cs1—Cl5	3.7151 (11)	Cs1—O21 ⁱⁱⁱ	3.150 (2)
Cs1—Cl6	3.6052 (11)	Cs1—O21 ^{iv}	3.150 (2)
Cs1—O1W	3.129 (3)	Cs1—Cl3 ^v	3.7127 (4)
Cs1—O21 ⁱ	3.116 (2)	Cs1—Cl3 ^{vi}	3.7127 (4)
Cs1—O21 ⁱⁱ	3.116 (2)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H11W \cdots O21 ^{vii}	0.92	2.00	2.905 (3)	168
N4—H42 \cdots N1 ^{viii}	0.79	2.44	2.985 (5)	127

Symmetry codes: (vii) $-x, -y, -z + 1$; (viii) $x - 1, y, z$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2705).

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supporting information

Acta Cryst. (2013). E69, m22–m23 [https://doi.org/10.1107/S1600536812049562]

Poly[(μ_6 -4-amino-3,5,6-trichloropyridine-2-carboxylato)caesium]**Graham Smith****S1. Comment**

4-Amino-3,5,6-trichloropyridine-2-carboxylic acid (picloram) is a commercial herbicide (Mullinson, 1985) introduced by Dow Chemicals as Tordon (O'Neil, 2001). Although it has potential as a metal chelating ligand similar to picolinic acid, there are only five metal complexes with picloramate ligands in the crystallographic literature. Examples include picloram as a bidentate chelate ligand [with Mn^{II} (Smith *et al.*, 1981*a*) and Cu^{II} (O'Reilly *et al.*, 1983)], while in the Mg complex (Smith *et al.*, 1981*b*), picloram acts as a counter-anion. A caesium complex derived from dipicolinic acid has also been reported (Santra *et al.*, 2011).

The reaction of picloram with caesium hydroxide in aqueous ethanol gave crystals of the title compound [Cs(C₆H₂Cl₃N₂O₂)(H₂O)]_n and the structure is reported herein. In this structure, the Cs⁺ cation lies on a crystallographic mirror plane which also contains the coordinating monodentate water molecule and all non-H atoms of the picloramate ligand except the carboxyl O-atom donors (Fig. 1). The irregular CsCl₄O₅ coordination sphere comprises chlorine donors from the *ortho*-related ring substituents (Cl5, Cl6) in a bidentate chelate mode [Cs—Cl, 3.6052 (11), 3.7151 (11) Å], with the third chlorine (Cl3) [Cs—Cl, 3.7127 (4) Å] bridging neighbouring Cs⁺ cations [Cs⁺⋯Cs^x, Cs⁺⋯Cs^{xi} = 4.9008 (3) Å] [for (x), -x + 1, y - 1/2, -z + 2; for (xi), -x + 1, y + 1/2, -z + 2], as well as a bidentate chelate and bridging carboxyl group. Although in most structures containing caesium and related ligands, the Cl atom is anionic rather than coordinating, an example of a coordinating carbon-bound Cl is known in which 1,2-dichloroethane acts as a bidentate chelate ligand (Levitskaia *et al.*, 2000). The Cs—Cl bond lengths in that structure are shorter than those in the title complex (3.46–3.56 Å).

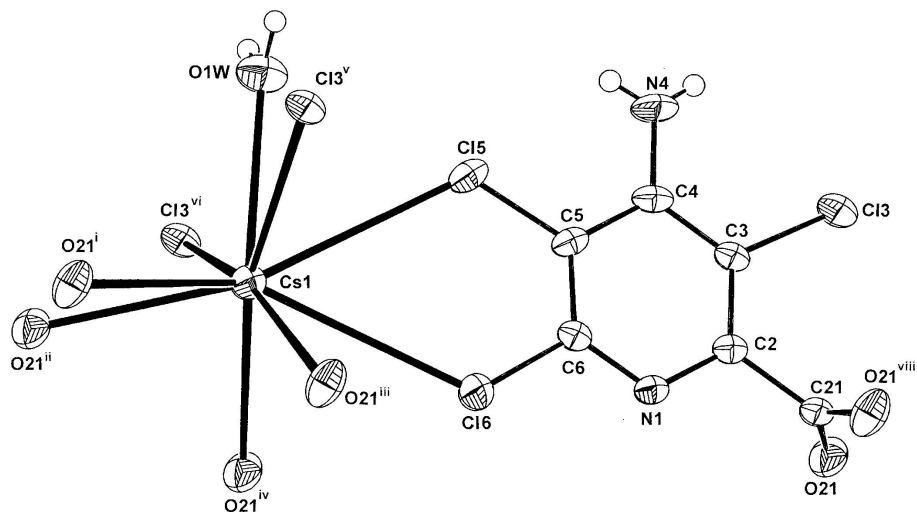
In the present complex, sheets are formed parallel to (010) (Fig. 2) and these are extended into a three-dimensional coordination polymer structure through the carboxyl group of the picloram ligand which bridges the sheets down [010] (Fig. 3). The amine group gives weak intramolecular N—H⋯Cl5 and ⋯Cl6 interactions and as well forms inter-complex N—H⋯N_{pyridine} hydrogen bonds which accompany water O—H⋯O_{carboxyl} hydrogen-bonding interactions in the structure (Table 2).

S2. Experimental

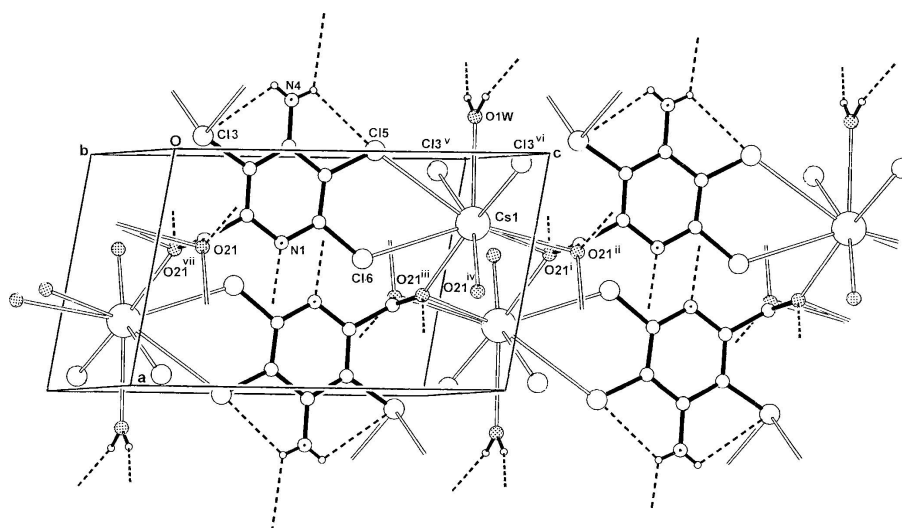
The title compound was synthesized by heating together under reflux for 10 minutes, 0.5 mmol of caesium hydroxide and 0.5 mmol of 4-amino-3,5,6-trichloropicolinic acid in 20 ml of 10% ethanol–water. Room temperature evaporation of the solution to incipient dryness gave colourless crystal plates of the title complex from which a specimen was cleaved for the X-ray analysis.

S3. Refinement

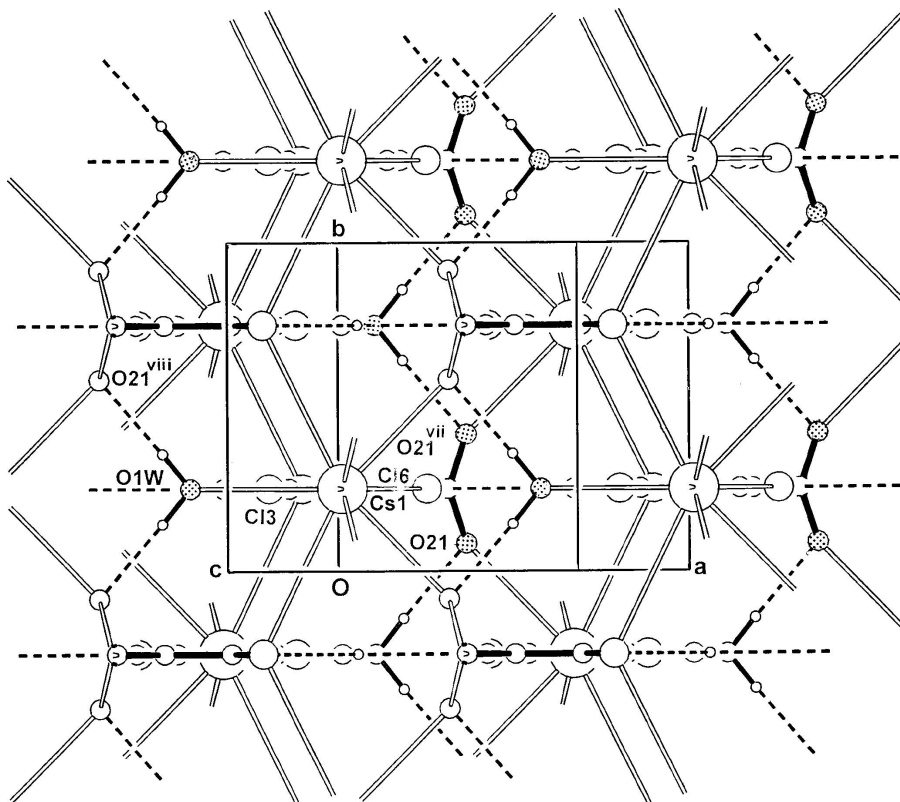
Hydrogen atoms of the coordinating water molecule and the amine group were located in a difference-Fourier synthesis but were allowed to ride in the refinement with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ or $1.5U_{\text{eq}}(\text{O})$.

**Figure 1**

The molecular configuration and atom-numbering scheme for the title compound, with non-H atoms drawn as 50% probability ellipsoids. For symmetry codes: see Table 1.

**Figure 2**

The sheet structure viewed perpendicular to the crystallographic mirror planes, with intermolecular hydrogen bonds and intramolecular N—H...Cl associations shown as dashed lines. For symmetry codes, see Fig. 1 and Table 1.


Figure 3

The packing in the unit cell viewed along the the mirror planes showing inter-plane carboxyl bridges and hydrogen-bonding associations (Table 2) as dashed lines.

Poly[(μ_6 -4-amino-3,5,6-trichloropyridine-2-carboxylato)aquacaesium]

Crystal data

[Cs(C₆H₂Cl₃N₂O₂)(H₂O)]

$M_r = 391.37$

Monoclinic, $P2_1/m$

Hall symbol: -P 2yb

$a = 7.0816$ (3) Å

$b = 6.6863$ (2) Å

$c = 11.7382$ (5) Å

$\beta = 101.005$ (4)°

$V = 545.58$ (4) Å³

$Z = 2$

$F(000) = 368$

$D_x = 2.382$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3047 reflections

$\theta = 3.5$ – 28.7°

$\mu = 4.11$ mm⁻¹

$T = 200$ K

Plate, colourless

$0.25 \times 0.20 \times 0.08$ mm

Data collection

Oxford Diffraction Gemini-S CCD detector
diffractometer

Radiation source: Enhance Mo X-ray source

Graphite monochromator

Detector resolution: 16.077 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2012)

$T_{\min} = 0.67$, $T_{\max} = 0.98$

3773 measured reflections

1164 independent reflections

1118 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 3.5^\circ$

$h = -8 \rightarrow 7$

$k = -8 \rightarrow 8$

$l = -11 \rightarrow 14$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.021$ $wR(F^2) = 0.053$ $S = 0.98$

1164 reflections

89 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 0.1378P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.55 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,
2008) within *WinGX* (Farrugia, 2012), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0132 (11)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cs1	0.29271 (3)	0.2500	0.885412 (19)	0.02831 (13)
Cl3	-0.06235 (13)	0.2500	0.12344 (9)	0.0326 (2)
Cl5	-0.01008 (14)	0.2500	0.58974 (9)	0.0291 (2)
Cl6	0.44747 (14)	0.2500	0.61009 (9)	0.0335 (2)
O1W	-0.1573 (4)	0.2500	0.8385 (3)	0.0433 (8)
H11W	-0.2387	0.1425	0.8335	0.065*
O21	0.4110 (3)	0.0836 (3)	0.14016 (17)	0.0369 (5)
N1	0.3823 (4)	0.2500	0.3865 (3)	0.0223 (6)
N4	-0.2153 (5)	0.2500	0.3441 (3)	0.0380 (8)
H41	-0.2870	0.2500	0.2908	0.046*
H42	-0.2700	0.2500	0.3968	0.046*
C2	0.2692 (5)	0.2500	0.2807 (3)	0.0211 (7)
C3	0.0719 (5)	0.2500	0.2649 (3)	0.0230 (7)
C4	-0.0239 (5)	0.2500	0.3586 (3)	0.0241 (8)
C5	0.0961 (5)	0.2500	0.4690 (3)	0.0224 (7)
C6	0.2937 (5)	0.2500	0.4763 (3)	0.0221 (7)
C21	0.3725 (5)	0.2500	0.1780 (3)	0.0253 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.02573 (17)	0.03285 (17)	0.02648 (18)	0.000	0.00536 (11)	0.000
Cl3	0.0204 (5)	0.0427 (5)	0.0316 (5)	0.000	-0.0029 (4)	0.000

Cl5	0.0277 (5)	0.0283 (5)	0.0359 (5)	0.000	0.0172 (4)	0.000
Cl6	0.0263 (5)	0.0492 (6)	0.0243 (5)	0.000	0.0034 (4)	0.000
O1W	0.0298 (16)	0.0423 (17)	0.056 (2)	0.000	0.0042 (15)	0.000
O21	0.0456 (12)	0.0340 (11)	0.0352 (12)	0.0137 (9)	0.0178 (10)	0.0035 (9)
N1	0.0173 (15)	0.0238 (15)	0.0266 (17)	0.000	0.0061 (12)	0.000
N4	0.0158 (16)	0.058 (2)	0.041 (2)	0.000	0.0076 (14)	0.000
C2	0.0187 (17)	0.0181 (16)	0.027 (2)	0.000	0.0048 (14)	0.000
C3	0.0169 (17)	0.0240 (17)	0.027 (2)	0.000	0.0008 (15)	0.000
C4	0.0164 (17)	0.0187 (16)	0.037 (2)	0.000	0.0052 (15)	0.000
C5	0.0198 (17)	0.0196 (16)	0.030 (2)	0.000	0.0116 (15)	0.000
C6	0.0194 (17)	0.0216 (16)	0.0243 (19)	0.000	0.0020 (14)	0.000
C21	0.0149 (16)	0.036 (2)	0.0238 (19)	0.000	0.0002 (14)	0.000

Geometric parameters (Å, °)

Cs1—Cl5	3.7151 (11)	O1W—H11W	0.9200
Cs1—Cl6	3.6052 (11)	O1W—H11W ^{vii}	0.9200
Cs1—O1W	3.129 (3)	N1—C2	1.343 (5)
Cs1—O21 ⁱ	3.116 (2)	N1—C6	1.326 (5)
Cs1—O21 ⁱⁱ	3.116 (2)	N4—C4	1.333 (5)
Cs1—O21 ⁱⁱⁱ	3.150 (2)	N4—H42	0.7900
Cs1—O21 ^{iv}	3.150 (2)	N4—H41	0.7300
Cs1—Cl3 ^v	3.7127 (4)	C2—C3	1.374 (5)
Cs1—Cl3 ^{vi}	3.7127 (4)	C2—C21	1.525 (5)
Cl5—C5	1.727 (4)	C3—C4	1.398 (5)
Cl6—C6	1.732 (4)	C3—Cl3	1.749 (4)
C21—O21	1.247 (3)	C4—C5	1.408 (5)
C21—O21 ^{vii}	1.247 (3)	C5—C6	1.386 (5)
Cl5—Cs1—Cl6	51.87 (2)	Cl3 ^{vi} —Cs1—O21 ⁱⁱⁱ	75.19 (4)
Cl5—Cs1—O1W	56.55 (7)	O21 ⁱ —Cs1—O21 ⁱⁱ	91.43 (5)
Cl5—Cs1—O21 ^{iv}	152.65 (4)	O21 ⁱ —Cs1—O21 ⁱⁱⁱ	77.10 (5)
Cl3 ^v —Cs1—Cl5	78.56 (2)	O21 ⁱⁱ —Cs1—O21 ⁱⁱⁱ	106.40 (5)
Cl3 ^{vi} —Cs1—Cl5	78.56 (2)	Cs1 ^v —Cl3—C3	100.54 (5)
Cl5—Cs1—O21 ⁱ	100.91 (4)	Cs1 ^{vi} —Cl3—C3	100.54 (5)
Cl5—Cs1—O21 ⁱⁱ	100.91 (4)	Cs1 ^v —Cl3—Cs1 ^{vi}	128.44 (3)
Cl5—Cs1—O21 ⁱⁱⁱ	152.65 (4)	Cs1—Cl5—C5	120.18 (13)
Cl6—Cs1—O1W	108.42 (7)	Cs1—Cl6—C6	124.53 (13)
Cl6—Cs1—O21 ^{iv}	141.22 (4)	Cs1 ^{viii} —O21—Cs1 ^{ix}	102.90 (6)
Cl3 ^v —Cs1—Cl6	100.49 (2)	Cs1—O1W—H11W	128.00
Cl3 ^{vi} —Cs1—Cl6	100.49 (2)	Cs1—O1W—H11W ^{vii}	128.00
Cl6—Cs1—O21 ⁱ	65.68 (4)	H11W—O1W—H11W ^{vii}	103.00
Cl6—Cs1—O21 ⁱⁱ	65.68 (4)	C2—N1—C6	116.5 (3)
Cl6—Cs1—O21 ⁱⁱⁱ	141.22 (4)	C4—N4—H41	130.00
O1W—Cs1—O21 ^{iv}	104.15 (7)	H41—N4—H42	108.00
Cl3 ^v —Cs1—O1W	64.39 (1)	C4—N4—H42	123.00
Cl3 ^{vi} —Cs1—O1W	64.39 (1)	N1—C2—C21	116.1 (3)
O1W—Cs1—O21 ⁱ	131.69 (4)	N1—C2—C3	122.4 (3)

O1W—Cs1—O21 ⁱⁱ	131.69 (4)	C3—C2—C21	121.5 (3)
O1W—Cs1—O21 ⁱⁱⁱ	104.15 (7)	C2—C3—C4	121.8 (3)
Cl3 ^v —Cs1—O21 ^{iv}	75.19 (4)	Cl3—C3—C2	118.9 (3)
Cl3 ^{vi} —Cs1—O21 ^{iv}	112.36 (4)	Cl3—C3—C4	119.3 (3)
O21 ^{iv} —Cs1—O21 ⁱ	106.40 (5)	N4—C4—C5	122.5 (3)
O21 ^{iv} —Cs1—O21 ⁱⁱ	77.10 (5)	C3—C4—C5	115.2 (3)
O21 ^{iv} —Cs1—O21 ⁱⁱⁱ	41.36 (5)	N4—C4—C3	122.3 (3)
Cl3 ^v —Cs1—Cl3 ^{vi}	128.44 (2)	C4—C5—C6	118.8 (3)
Cl3 ^v —Cs1—O21 ⁱ	160.44 (4)	Cl5—C5—C4	118.4 (3)
Cl3 ^v —Cs1—O21 ⁱⁱ	69.70 (4)	Cl5—C5—C6	122.8 (3)
Cl3 ^v —Cs1—O21 ⁱⁱⁱ	112.36 (4)	Cl6—C6—C5	120.6 (3)
Cl3 ^{vi} —Cs1—O21 ⁱ	69.70 (4)	Cl6—C6—N1	114.2 (3)
Cl3 ^{vi} —Cs1—O21 ⁱⁱ	160.44 (4)	N1—C6—C5	125.2 (3)
Cl6—Cs1—Cl5—C5	0.00 (1)	C21—C2—C3—C4	180.00 (1)
O1W—Cs1—Cl5—C5	180.00 (1)	N1—C2—C21—O21	89.9 (3)
Cl5—Cs1—Cl6—C6	0.00 (1)	C3—C2—C21—O21	-90.1 (3)
O1W—Cs1—Cl6—C6	0.00 (1)	Cl3—C3—C4—N4	0.00 (1)
Cs1—Cl5—C5—C4	180.00 (1)	Cl3—C3—C4—C5	180.00 (1)
Cs1—Cl5—C5—C6	0.00 (1)	C2—C3—C4—N4	180.00 (1)
Cs1—Cl6—C6—N1	180.00 (1)	C2—C3—C4—C5	0.00 (1)
Cs1—Cl6—C6—C5	0.00 (1)	N4—C4—C5—Cl5	0.00 (1)
C6—N1—C2—C3	0.00 (1)	N4—C4—C5—C6	180.00 (1)
C6—N1—C2—C21	180.00 (1)	C3—C4—C5—Cl5	180.00 (1)
C2—N1—C6—Cl6	180.00 (1)	C3—C4—C5—C6	0.00 (1)
C2—N1—C6—C5	0.00 (1)	Cl5—C5—C6—Cl6	0.00 (1)
N1—C2—C3—Cl3	180.00 (1)	Cl5—C5—C6—N1	180.00 (1)
N1—C2—C3—C4	0.00 (1)	C4—C5—C6—Cl6	180.00 (1)
C21—C2—C3—Cl3	0.00 (1)	C4—C5—C6—N1	0.00 (1)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—H11W \cdots O21 ^x	0.92	2.00	2.905 (3)	168
N4—H42 \cdots N1 ^{xi}	0.79	2.44	2.985 (5)	127
N4—H42 \cdots Cl5	0.79	2.63	2.971 (4)	108
N4—H41 \cdots Cl3	0.73	2.75	2.992 (4)	102

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