**X-ray Crystal Structure Analysis of (–)-Epidihydropinidine Hydrochloride (2·HCl)**

Single crystal of **2·HCl** suitable for X-ray analysis was obtained by slow evaporation of its ethanolic solution at room temperature. Data collection was performed at 100 K on a Oxford Diffraction GEMINI R diffractometer[1] equipped with a CCD detector with Cu Kα radiation (λ= 1.5418 Å) and graphite monochromator. The details of data collection and refinement are in Table S1. Crystal structure (Figure S1, S2) was solved and refined by SHELXS and SHELXL-97 suit of programs.[2]

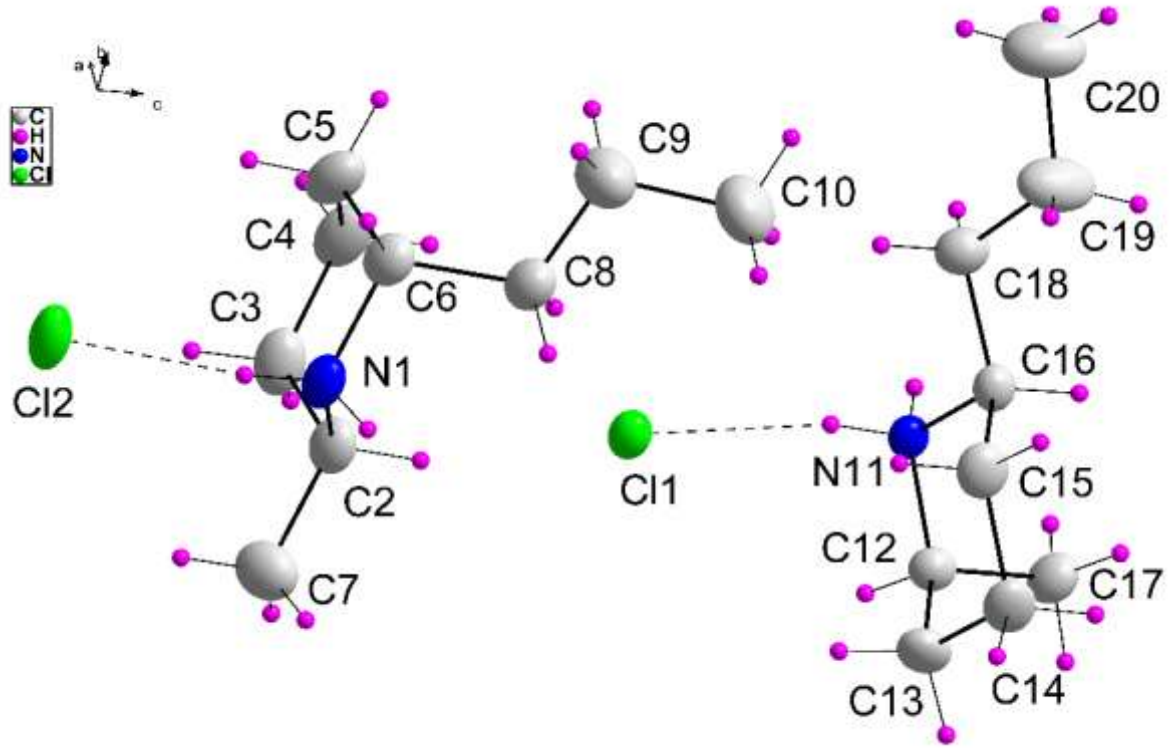


**Figure S1**. ORTEP[3] scheme of (–)-epidihydropinidine hydrochloride **2·HCl.** Thermal ellipsoids are drawn at the 20% probability level.

[1] Oxford Diffraction (2010). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
[2] Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
[3] Brandenburg, K. (1998). *DIAMOND*. Visual Information System for Crystal Structures, Bonn, Germany.

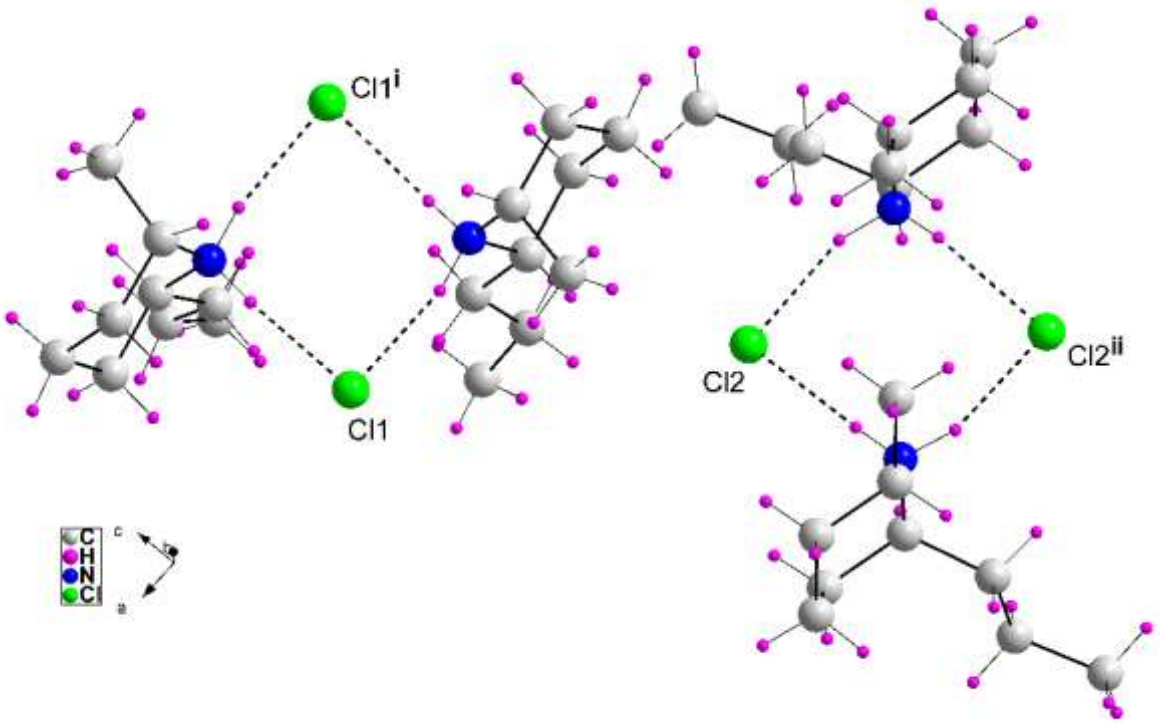


**Figure S2**. Schematic view of $Cl^-$ interactions with (–)-epidihydropinidine hydrochloride.

**Table S1.** Crystal data collection and refinement for (–)-epidihydropinidine hydrochloride **2**·**HCl**

*Crystal data*

| | |
|---|---|
| $C_9H_{20}Cl_1N_1$ | $F_{000}$ = 1568 |
| *Mr* = 177.71 | *D*x = 0.964 Mg m$^{-3}$ |
| Orthorhombic, *C 2 2 2* | Cu *K*α radiation |
| | λ = 1.5418 Å |
| Hall symbol: C 2 2 | Cell parameters from 28106 reflections |
| *a* = 9.90868(12) Å | θ = 3.07–74.87° |
| *b* = 34.4359(6) Å | μ = 2.363 mm$^{-1}$ |
| *c* = 14.35610(16) Å | *T* = 293 (1) K |
| *V* = 4898.51(11) Å$^3$ | Block, colourless |
| *Z* = 16 | 0.96 × 0.42 × 0.21 mm |

*Data collection*

| | |
|---|---|
| Goniometer Xcalibur, detector: Ruby (Gemini Cu) | |
| diffractometer | 4914 independent reflections |
| Radiation source: Enhance (Cu) X-ray Source | 4415 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.020 |
| Detector resolution: 10.4340 pixels mm$^{-1}$ | θmax = 74.87° |
| *T* = 293(1) K | θmin = 3.07° |
| Rotation method data acquisition using $\omega$ and $\phi$ scans | *h* = −10→12 |
| Absorption correction: analytical | *k* = −42→39 |
| CrysAlis RED, Oxford Diffraction Ltd. | *l* = −16→17 |

$T_{min}$ = 0.271, $T_{max}$ = 0.656
42033 measured reflections

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.066$ | $w = 1/[\sigma^2(Fo^2) + (0.0565P)^2 + 0.2803P]$ where $P = (Fo^2 + 2Fc^2)/3$ |
| $wR(F^2) = 0.068$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 1.13$ | $\Delta\rho_{max} = 0.93$ e A$^{-3}$ |
| 4914 reflections | $\Delta\rho_{min} = -0.26$ e A$^{-3}$ |
| 212 parameters | Extinction correction: 0.0011(2) |
| Primary atom site location: structure-invariant direct methods | Absolute structure: (Hooft, R. W. W., Straver, L. H. & Spek, A. L. (2008). J. Appl. Cryst. 41, 96-103) 'Rogers (1981), 12512 Friedel pairs' |
| Secondary atom site location: difference Fourier map | Flack parameter: 0.03(2) |

**Supplementary material:** Crystallographic data for the structural analysis have been deposited at the Cambridge Crystallographic Data Centre, CCDC no. 800711.