

Supplementary Information

Cobalt(III) Complexes with Thiosemicarbazones as Potential anti-*Mycobacterium tuberculosis* Agents

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Crystallographic data (excluding structure factors) for the structures in this work were deposited in the Cambridge Crystallographic Data Centre as supplementary publication numbers CCDC 988971 (**1**·H₂O) and 988972 (**5**·MeOH). Copies of the data can be obtained, free of charge, via

www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033. E-mail: deposit@ccdc.cam.ac.uk.

IR spectra of compounds

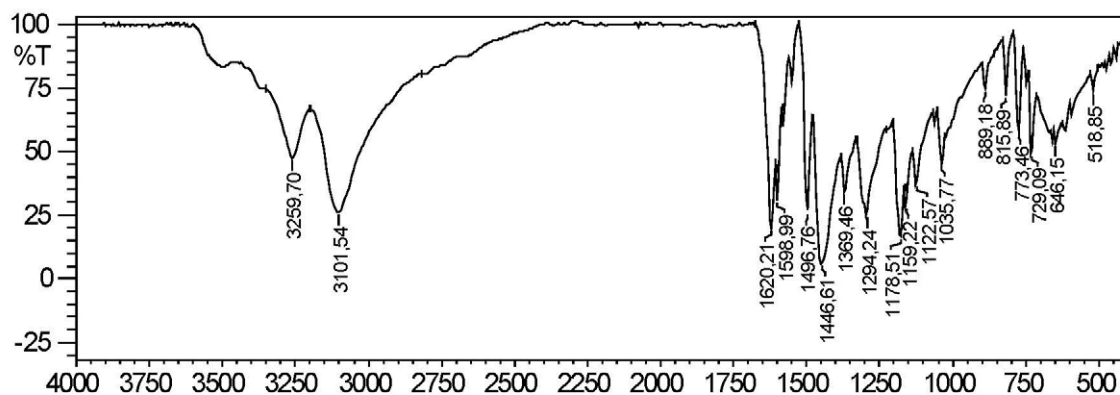


Figure S1. IR spectrum (KBr) of complex **1**.

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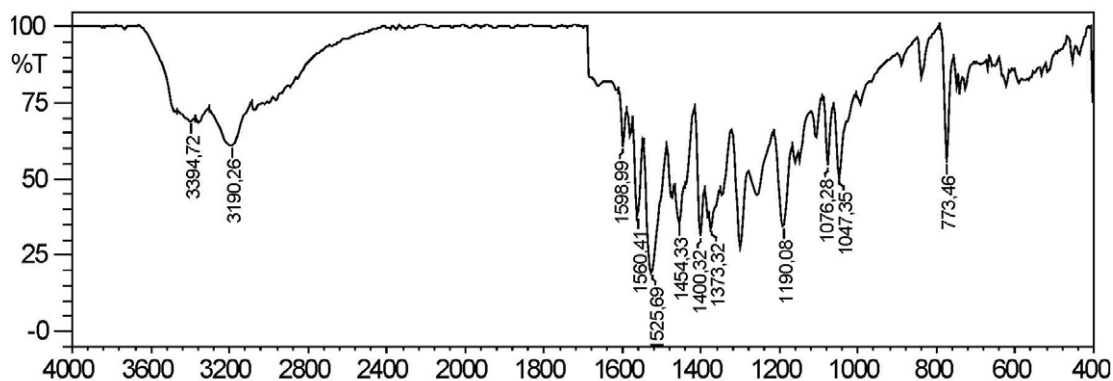


Figure S2. IR spectrum (KBr) of complex 2.

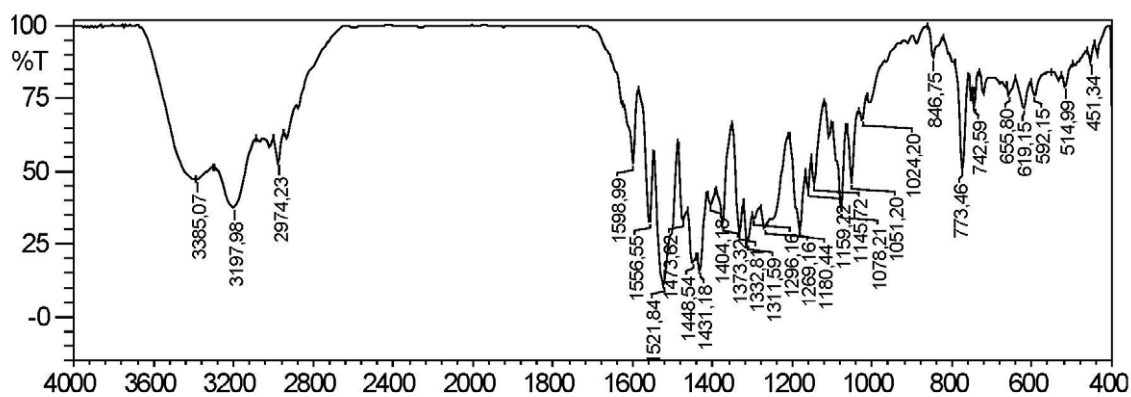


Figure S3. IR spectrum (KBr) of complex 3.

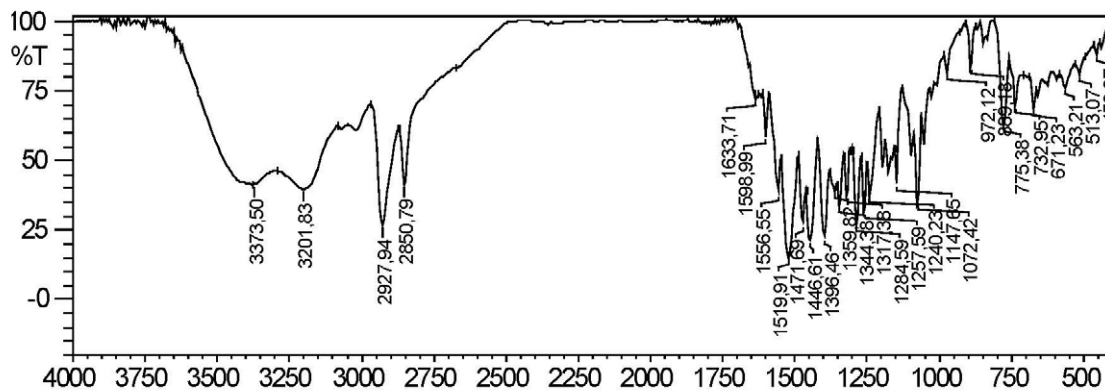


Figure S4. IR spectrum (KBr) of complex 4.

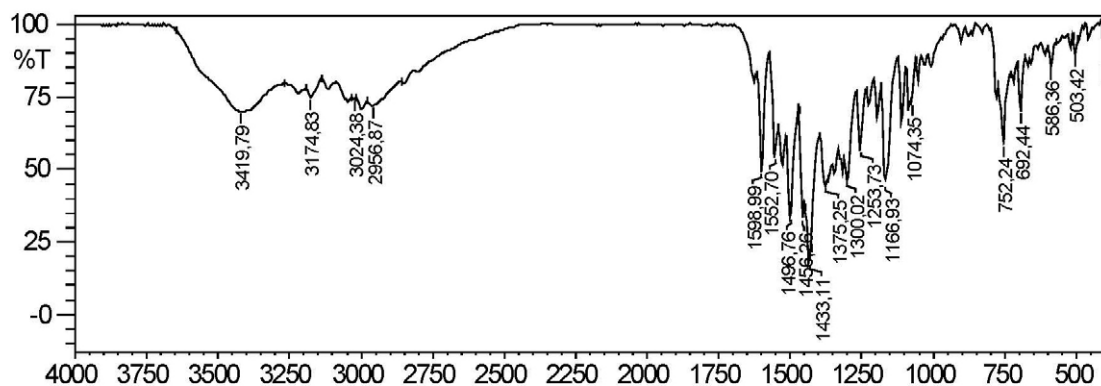


Figure S5. IR spectrum (KBr) of complex 5.

¹H NMR spectra of compounds

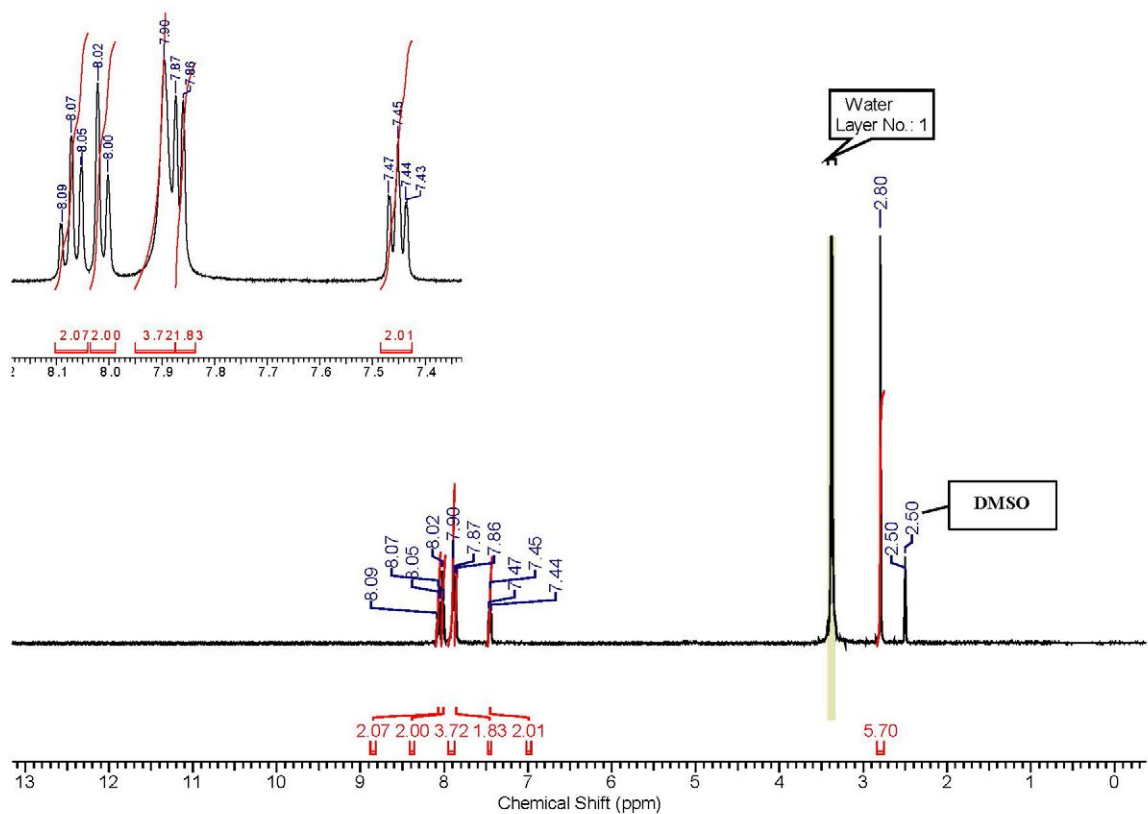


Figure S6. ¹H NMR spectrum (DMSO, 399.8 MHz) of complex 1.

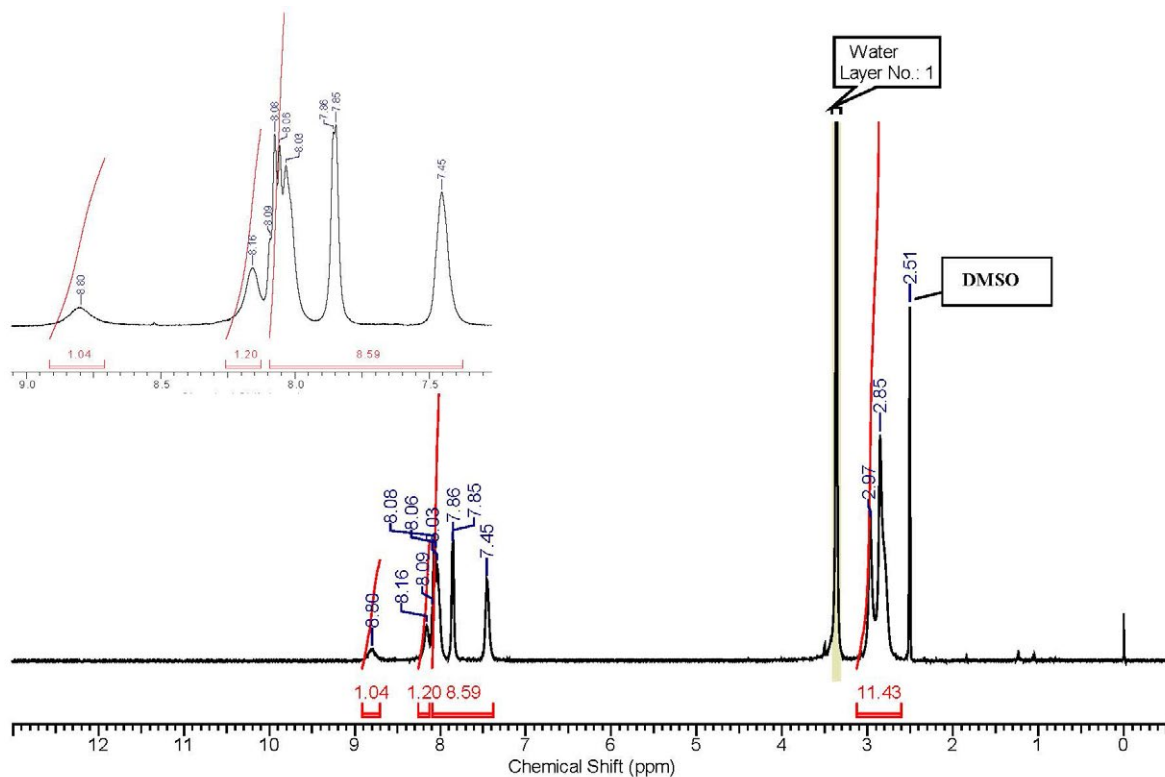


Figure S7. ^1H NMR spectrum (DMSO, 399.8 MHz) of complex 2.

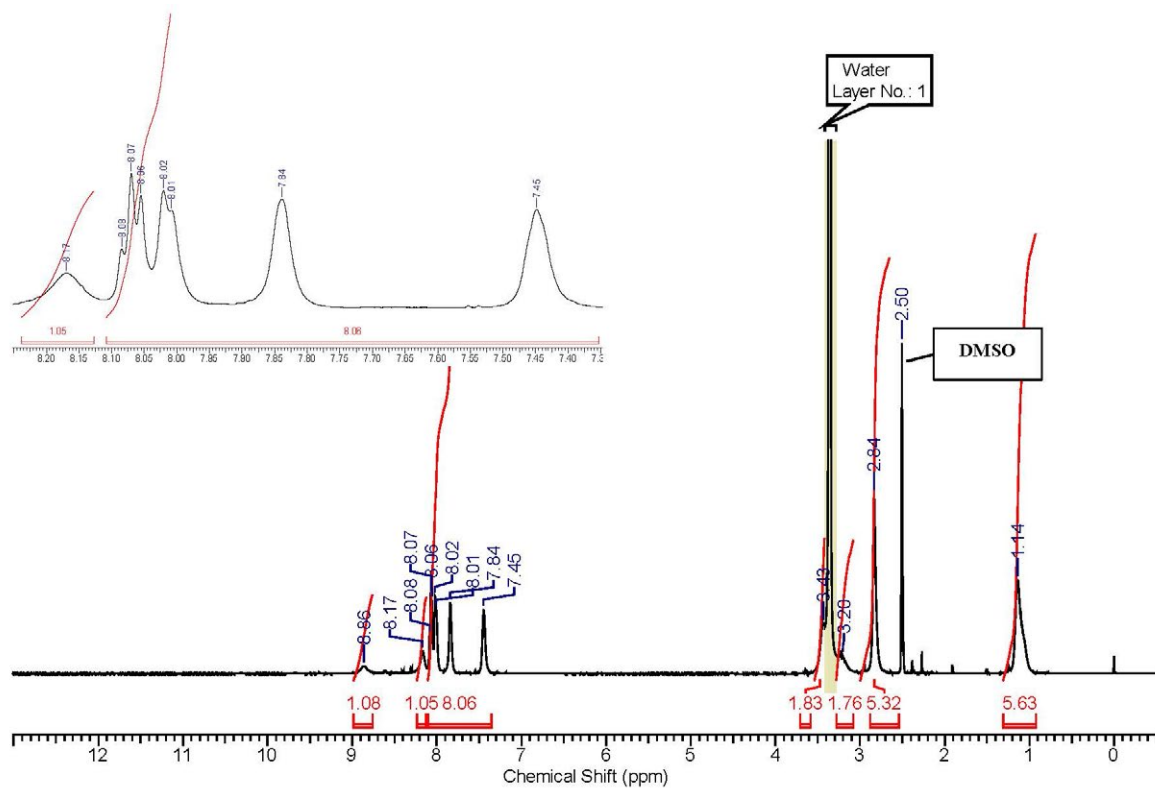


Figure S8. ^1H NMR spectrum (DMSO, 399.8 MHz) of complex 3.

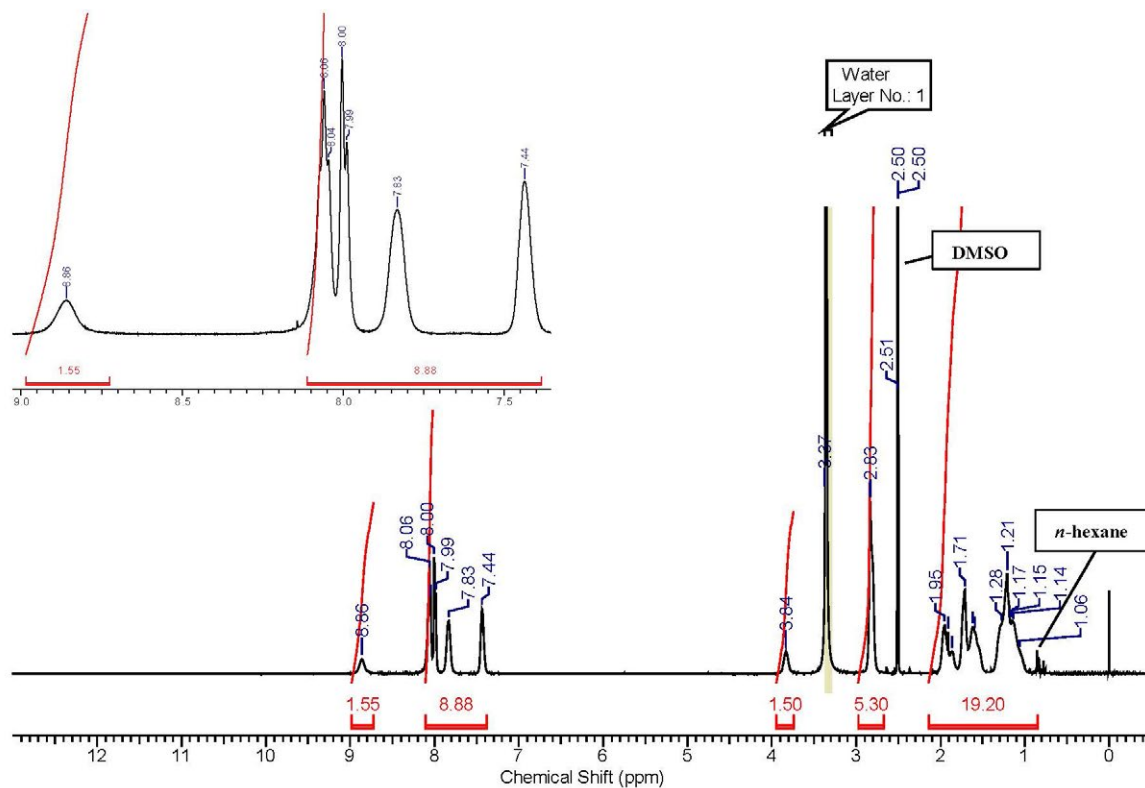


Figure S9. ^1H NMR spectrum (DMSO, 399.8 MHz) of complex 4.

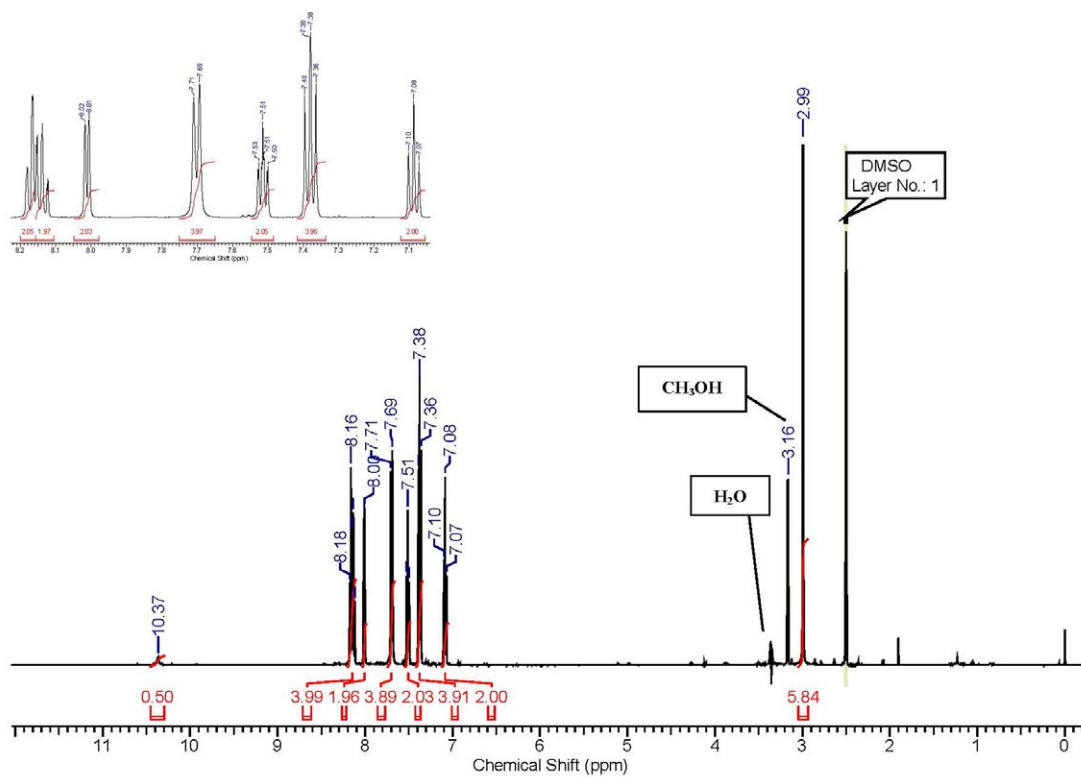


Figure S10. ^1H NMR spectrum (DMSO, 399.8 MHz) of complex 5.

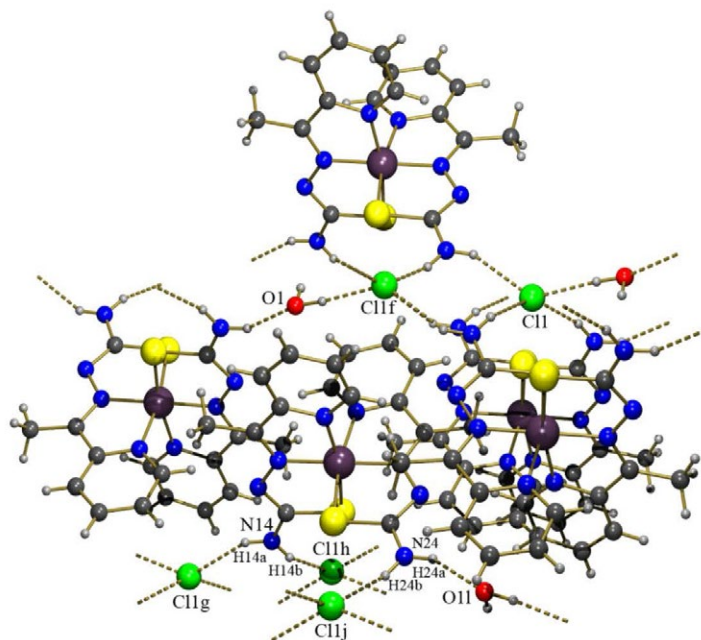


Figure S11. Crystalline and molecular structure of $[\text{Co}(\text{atc})_2]\text{Cl}\cdot\text{H}_2\text{O}$ [$\text{N}(24)\cdots\text{O}(1\text{L}) = 2.910(5) \text{ \AA}$, $\text{N}(24)\text{-H}(24\text{A})\cdots\text{O}(1\text{L}) = 146.5^\circ$], [$\text{N}(24)\cdots\text{Cl}(1\text{J}) = 3.258(3) \text{ \AA}$, $\text{N}(24)\text{-H}(24\text{B})\cdots\text{Cl}(1\text{J}) = 157.6^\circ$], [$\text{N}(14)\cdots\text{Cl}(1\text{G}) = 3.223(3) \text{ \AA}$, $\text{N}(14)\text{-H}(14\text{A})\cdots\text{Cl}(1\text{G}) = 147.5^\circ$], [$\text{N}(14)\cdots\text{Cl}(1\text{H}) = 3.222(3) \text{ \AA}$, $\text{N}(14)\text{-H}(14\text{B})\cdots\text{Cl}(1\text{H}) = 152.3^\circ$], [$\text{O}(1)\cdots\text{Cl}(1\text{F}) = 3.081(4) \text{ \AA}$, $\text{O}(1)\text{-H}(1\text{w})\cdots\text{Cl}(1\text{F}) = 174(4)^\circ$]. Symmetry operations used: ^F $1-x, -y, 1-z$; ^L $1/2+x, 1/2-y, 1/2+z$; ^J $1/2+x, 1/2-y, -1/2+z$; ^G $1/2-x, 1/2+y, 1/2-z$; ^H $-1/2+x, 1/2-y, -1/2+z$.