

Structural data for L-leucine hydrochloride monohydrate:

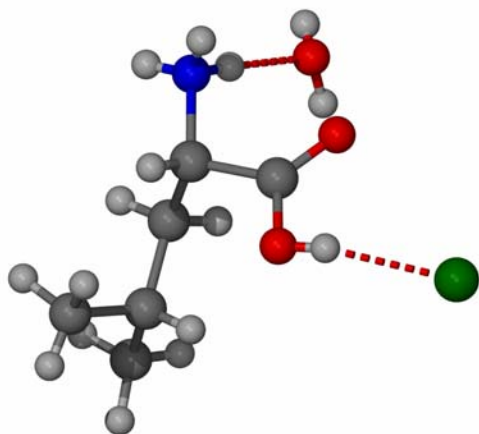


Figure 1. Ball and stick representation of the asymmetric unit found in the crystal structure of L-leucine hydrochloride monohydrate showing hydrogen bonding between the structural components.

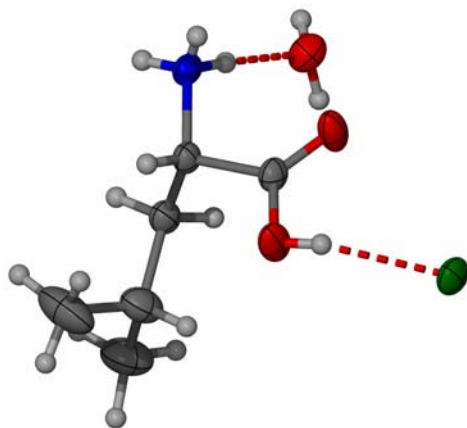


Figure 2. The asymmetric unit found in the crystal structure of L-leucine hydrochloride monohydrate, anisotropic displacement parameters shown at the 50% level. Hydrogen bonding between structural components is also shown.

Table 1. Crystal data and structure refinement for L-leucine hydrochloride monohydrate.

Identification code	L-Leucine hydrochloride monohydrate	
Formula	C ₆ H ₁₆ ClNO ₃	
Formula weight	185.65	
Size	0.46 x 0.18 x 0.08 mm	
Crystal morphology	Colourless plate	
Temperature	150(2) K	
Wavelength	0.71073 Å [Mo-K _α]	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	$a = 6.2563(13) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 6.3951(13) \text{ \AA}$	$\beta = 90^\circ$
	$c = 26.865(5) \text{ \AA}$	$\gamma = 90^\circ$
Volume	1074.9(4) Å ³	
Z	4	
Density (calculated)	1.147 Mg/m ³	
Absorption coefficient	0.325 mm ⁻¹	
F(000)	400	
Data collection range	3.34 ≤ θ ≤ 27.5°	
Index ranges	-8 ≤ h ≤ 4, -7 ≤ k ≤ 4, -11 ≤ l ≤ 33	
Reflections collected	1746	
Independent reflections	1473 [R(int) = 0.0678]	
Observed reflections	1299 [I > 2σ(I)]	
Absorption correction	multi-scan	
Max. and min. transmission	0.949 and 0.104	
Refinement method	Full	
Data / restraints / parameters	1473 / 0 / 164	
Goodness of fit	1.033	
Final R indices [I > 2σ(I)]	R ₁ = 0.0343, wR ₂ = 0.0777	
R indices (all data)	R ₁ = 0.0418, wR ₂ = 0.0818	

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Largest diff. peak and hole	0.159 and -0.167e.Å ⁻³
Absolute structure parameter	-0.01(9)