Supplementary Information

Structural studies and physicochemical properties of L-valine hydrochloride monohydrate

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Table S1. Crystal data and structure refinement parameters for (L.T.)and(R.T.) structures.

Structure	**L.T. (Present study)**	**R.T.**
Empirical formula	$C_5H_{12}NO_2^+Cl^-.H_2O$	$C_5H_{12}NO_2^+Cl^-.H_2O$
Formula Weight	171.62	171.62
Temperature (K)	120(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Orthorhombic	Orthorhombic
space group	$P2_12_12_1$	$P2_12_12_1$
a, b, c (Å)	6.115(2), 6.850(1), 20.781(2)	6.155(1), 6.828(1), 21.099(3)
α, β, γ (°)	90.0, 90.0, 90.0	90.0, 90.0, 90.0
Volume ($Å^3$)	870.5(3)	886.7(2)
Z / Density (calc.) (Mg/m^3)	4 / 1.310	4 / 1.286
Absorption coefficient (mm^{-1})	0.396	0.389
F(000)	368	368
Crystal size (mm^3)	0.28 × 0.19 × 0.09	0.48 × 0.36 × 0.32
θ range for data collection (°)	1.96 to 24.97	1.93 to 27.48
Limiting indices	-7<=h<=6,-8<=k<=8, -24<=l<=24	-7<=h<=7,-8<=k<=8, -27<=l<=27
Reflections collected / unique	8018/1522[R(int)=0.0372]	2442/2020[R(int)=0.0229]
Completeness to θ (%)	100.0	100.0
Absorption correction	Semi-empirical from equivalents	Psi-scan
Max. and min. transmission	0.96 and 0.91	0.88 and 0.84
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	1522 / 0 / 95	2020 / 0 / 148
Goodness-of - fit on F^2	1.171	0.973
Extinction coefficient	0.066(4)	0.065(5)
Final R indices [I > 2σ(I)]	R1=0.0178, *w*R2=0.0465	R1=0.355, *w*R2=0.0809
R indices (all data)	R1=0.0178, *w*R2=0.0465	R1=0.0433, *w*R2=0.0832
Largest diff. peak and hole ($e.Å^{-3}$)	0.166 and -0.141	0.295 and -0.159

$R_1 = \sum||F_o|-|F_c||/\sum|F_o|$, $wR_2 = [\sum\{(F_o^2-F_c^2)^2\}/\sum\{w(F_o^2)^2\}]^{1/2}$, $w = 1/\{\sigma^2(F_o^2) + (aP)^2 + bP\}$, where a = 0.0157and b = 0.1750 for (**L.T.**) and a = 0.0465 and b = 0.0 for (**R.T.**) structure. $P = (F_o^2 + 2F_c^2)/3$ for both the structures.

Table S2. Hydrogen bonding geometry of $C_5H_{14}N_1O_3Cl$ (L.T.) (Å, °).

D–H···A	d(D–H)	d(H···A)	d(D···A)	D–H···A	Symmetry
O2–H2···Cl1	0.82	2.20	3.010(2)	172	x, 1+y, z
O1W–H1W···Cl1	0.81	2.37	3.178(2)	172	1/2+x, 1/2-y, -z
O1W–H2W···Cl1	0.86	2.31	3.156(2)	168	---
N1–H1C···O1	0.89	2.36	2.873(2)	117	1/2+x, 3/2-y, -z
N1–H1A···O1W	0.89	1.98	2.848(2)	165	---
N1–H1C···O1W	0.89	2.02	2.861(2)	157	1/2+x, 3/2-y, -z
N1–H1B···Cl1	0.89	2.42	3.237(2)	153	1+x, y, z
C1–H1F···Cl1	0.96	2.83	3.750(2)	162	1+x, y, z
C3–H3···O2	0.98	2.54	2.914(2)	103	---