Electronic Supplementary Material (ESI) for CrystEngComm.
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Electronic Supplementary Information

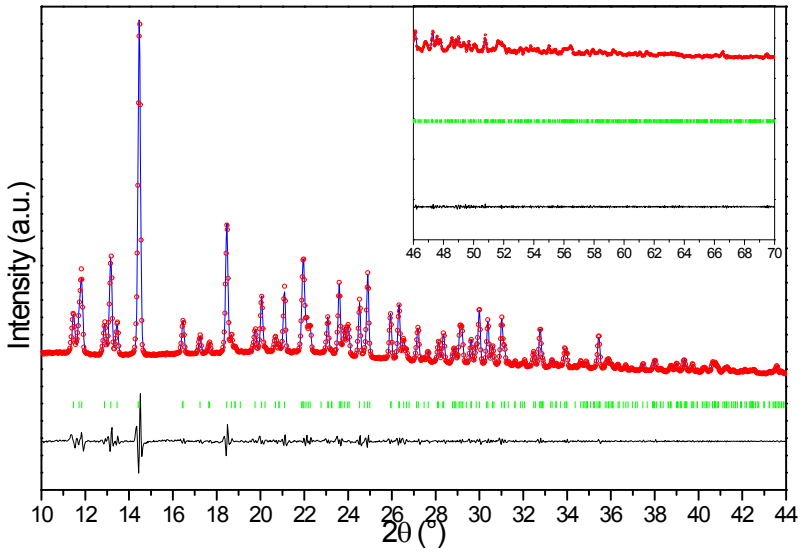

Fig. S1: Pawley Refinement of the XRPD data for Sibutramine Hydrochloride Monohydrate (rac.Sibut.HCl.H_2O) obtained at 294 K. Blue line: experimental pattern, empty red circles: calculated pattern, green vertical bars: peak positions, black line: residual XRPD patterns. The insert corresponds to the scale for the data between 46° and 70° magnified 15 times.

Table S1. Unit cell parameters for Sibutramine Hydrochloride Monohydrate (rac.Sibut.HCl.H_2O) obtained from XRPD (this work) and single crystal. Crystal system: orthorhombic. Space group: Pbcn (Z=8 and Z'=1)

	Ref [16]	This work
	Single crystal	powder
temperature	294 K	294 K
unit cell dimensions (Å)	a = 13.442(3)	a = 13.4088(12)
	b = 9.374(2)	b = 9.3919(8)
	c = 30.110(7)	c = 30.100(3)
volume ($Å^3$)	3794.0	3790.6(10)

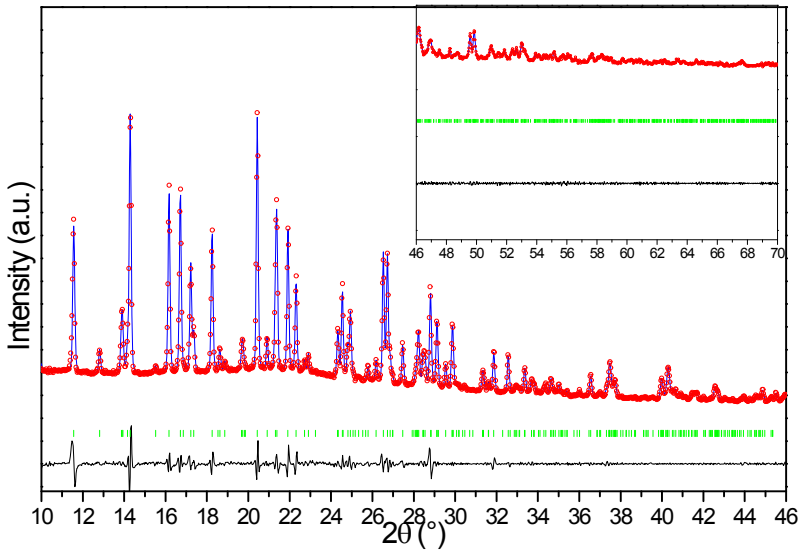

Fig. S2: Pawley Refinement of the XRPD data for Sibutramine Hydrochloride anhydrous A obtained at 294 K. Blue line: experimental pattern, empty red circles: calculated pattern, green vertical bars: peak positions, black line: residual XRPD patterns. The insert corresponds to the scale for the data between 46° and 70° magnified 15 times.

Table S2. Unit cell parameters for sibutramine anhydrous A obtained from XRPD (this work) and single crystal. . Crystal system: monoclinic. Space group: $P2_1/n$ (Z=4)

	Ref [10]	This work
	Single crystal	powder
temperature	293 K	294 K
unit cell dimensions (Å)	a = 7.321(2)	a = 7.3206(8)
	b = 25.456(2)	b = 25.475(3)
	c = 9.750(3)	c = 9.765(1)
	β = 101.60(2)°	β = 101.559(6)°
volume ($Å^3$)	1779.9(8)	1784.2(6)

Table S3. Rietveld refinement data of sibutramine anhydrous B.

Formula		$C_{17}H_{27}NCl_2$
FW (g mol^{-1})		316.3
temperature		295(1) K
wavelength		1.540562 Å
cryst. syst.		Monoclinic
space group		P 2_1
unit cell dimensions	length (Å)	a = 12.0282(19)
		b = 9.0364(15)
		c = 8.1578(11)
	angle (deg.)	β = 90.601(9)
volume (Å^3)		886.6(2)
Z(Z')		2(1)
Dx (g cm^{-3})		1.185
Rp		0.0315
Rwp		0.0436

Table S4. Inter-molecular H-bond distances and angles for anhydrous A (deduced from crystal structure reported in ref [10]).

D	H	A	D - H (Å)	H…A (Å)	D…A (Å)	D-H…A (deg.)	symmetry
N1	H1	Cl2	0.910	2.24	3.056	149.0	i
C12	H12B	Cl2	0.960	2.80	3.725	163	ii
C10	H10	Cl2	0.931	3.04	3.911	156.4	i
C11	H11	Cl2	0.981	2.99	3.936	162.3	iii
C14	H14A	Cl2	0.969	3.04	3.984	165.1	ii
C17	H17C	Cl1	0.960	3.17	4.087	161.6	iv

(i) x-1/2, -y-1/2, z+1/2; (ii) x, y, z; (iii) x-1, y, z; (iv) -x, -y, -z.

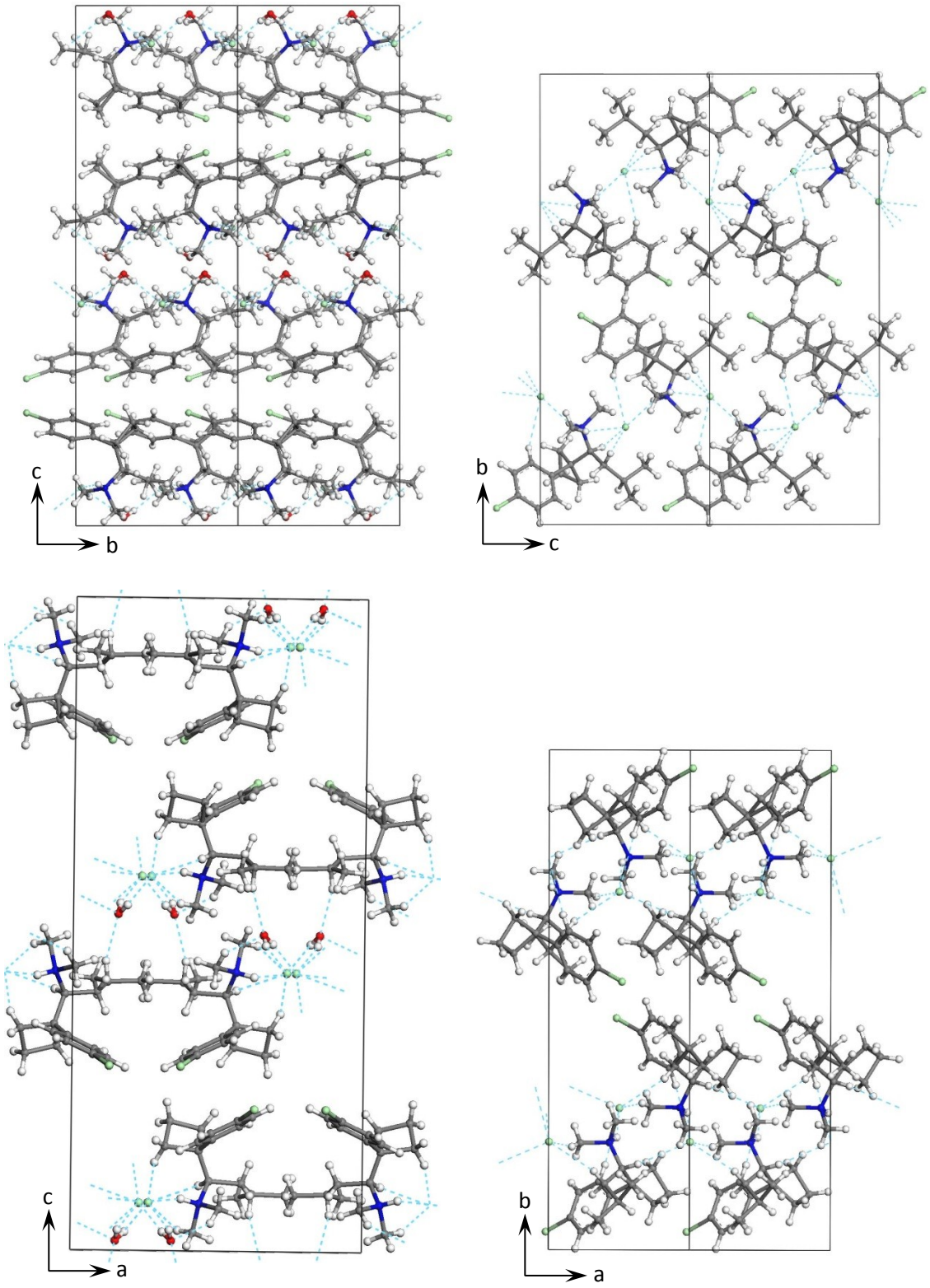

Fig. S3: Crystal packing of racemic sibutramine. Hydrated form viewed along a (top left) and along b (bottom left), Anhydrous A viewed along a (top right) and along c (bottom right).