STRUCTURAL
CHEMISTRY

Volume 75 (2019)

Supporting information for article:

Structure and electrostatic properties of the pyrimethamine–3,5-di-hydroxybenzoic acid cocrystal in water solvent studied using transferred electron-density parameters

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Table S1: Geometry of all H bonds based on the ELMAM2 model

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O1^{i}	1.04(4)	2.08(4)	2.850(3)	129.(2)
N6—H6A···O2^{ii}	1.08(4)	1.67(4)	2.741(3)	169.5(9)
N6—H6A··· C25^{ii}	1.08(4)	2.55(4)	3.513(3)	148.(2)
N8—H8B··· O1^{ii}	1.07(4)	1.73(4)	2.793(3)	170.2(8)
N8—H8B··· O2^{ii}	1.07(4)	2.54(4)	3.336(3)	130.(2)
N8—H8B··· C25^{ii}	1.07(4)	2.33(4)	3.348(3)	158.(1)
C24—H24C··· O2^{ii}	1.1	2.6	3.502(4)	144
O7—H7··· O2^{ii}	0.94(4)	1.85(4)	2.792(3)	173.9(4)
O7—H7··· C25^{ii}	0.94(4)	2.63(4)	3.510(3)	157.(1)
O9—H9B··· O1^{ii}	1.02(4)	1.87(4)	2.885(3)	178.80(9)
C18—H18··· C30^{iii}	1.08	2.59	3.512(4)	143
C18—H18··· C31^{iii}	1.08	2.77	3.461(4)	122
N3—H3A··· O9^{iv}	0.99(4)	1.96(4)	2.924(3)	166.(1)
N4—H4A··· N5^{iv}	0.97(4)	2.11(4)	3.086(3)	175.3(3)
C38—H38··· N5^{iv}	1.1	2.5	3.390(3)	141
C2—H2··· N4^{v}	1.08	2.6	3.550(4)	146
O4—H4··· Cl1^{vi}	0.98(16)	2.86(15)	3.555(3)	129.(9)
N3—H3B··· C1	1.04(4)	2.48(4)	2.857(3)	100.(2)
N3—H3B··· C6	1.04(4)	2.57(4)	3.159(4)	115.(2)
C11—H11B··· C1	1.1	2.62	3.063(4)	103
C11—H11B··· C2	1.1	2.76	3.372(4)	115
N7—H7B··· C18	1.08(4)	2.59(4)	3.156(4)	112.(2)
C15—H15··· O3	1.08	2.61	3.362(5)	126
C23—H23A··· C13	1.1	2.58	3.066(4)	106
C36—H36··· O9	1.08	2.49	3.255(3)	127
O8—H8··· O9	0.99(4)	1.76(4)	2.744(3)	171.1(7)
N7—H7B··· O7^{vii}	1.08(4)	2.49(4)	3.497(4)	156.(1)
N7—H7B··· C35^{vii}	1.08(4)	2.53(4)	3.323(4)	129.(2)
O3—H3C··· O6^{vii}	0.98(4)	1.68(4)	2.652(3)	171.5(8)
N2—H2A··· O5^{viii}	1.03(4)	1.65(4)	2.684(3)	178.15(16)
N2—H2A··· C32^{viii}	1.03(4)	2.43(4)	3.380(3)	152.(1)
N4—H4B··· O6^{viii}	1.01(4)	1.84(4)	2.824(3)	164.(1)
N4—H4B··· C32^{viii}	1.01(4)	2.59(4)	3.511(3)	151.(1)
N7—H7A··· O8^{viii}	1.00(4)	2.09(4)	3.078(3)	171.0(7)
N8—H8A··· N1^{viii}	1.01(4)	2.07(4)	3.069(3)	168.6(8)
O9—H9A··· O5^{viii}	0.93(4)	1.94(4)	2.828(3)	161.(1)
O9—H9A··· C32^{viii}	0.93(4)	2.64(4)	3.352(3)	134.(2)

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

(vi). −*x*+3/2, −*y*+1/2, −*z* ***(vii)***. *x*+1/2, *y*+1/2, *z* ***(viii)***. −*x*+1/2, *y*+1/2, −*z*+1/2

Table S2. Topological properties of (3, -1) CPs on the intermolecular interactions: distances (Å), electron density (e/Å^3), Laplacian (e/Å^5), Hessian eigenvalues (e/Å^5), ellipticity, G_{cp} = Bond Kinetic energy V_{cp}= Bond Potential Energy (KJ /mol/Bohr^3)

Interacting atoms	d_{12} (Å)	d_{1cp} (Å)	d_{2cp} (Å)	$\rho_{(rb)}$ (e/Å3)	$\nabla 2\rho_{(cp)}$ (e/Å5)	λ_1 (e/Å5)	λ_2 (e/Å5)	λ_3 (e/Å5)	ε	G_{cp}	V_{cp}
N2—H2A•••O5^{viii}	1.03(4)	1.65(4)	2.684(3)	0.3365	2.37	-2.24	-2.18	6.79	0.03	93.89	-123.35
O3—H3C•••O6^{vii}	0.98(4)	1.68(4)	2.652(3)	0.3129	1.48	-2.15	-2.07	5.7	0.04	71.91	-103.61
N6—H6A•••O2^{ii}	1.08(4)	1.67(4)	2.741(3)	0.2815	2.18	-1.74	-1.71	5.62	0.02	77.37	-95.41
O7—H7•••O2^{ii}	0.94(4)	1.85(4)	2.792(3)	0.254	1.14	-1.58	-1.55	4.26	0.02	52.55	-74.07
N8—H8B•••O1ii	1.07(4)	1.73(4)	2.793(3)	0.2498	2.24	-1.5	-1.47	5.21	0.02	71.74	-82.35
O9—H9B•••O1^{ii}	1.02(4)	1.87(4)	2.885(3)	0.2423	1.18	-1.49	-1.48	4.15	0.01	50.94	-69.66
O9—H9A•••O5^{viii}	0.93(4)	1.94(4)	2.828(3)	0.2323	1.33	-1.37	-1.35	4.05	0.01	51.64	-67.01
N4—H4B•••O6^{viii}	1.01(4)	1.84(4)	2.824(3)	0.2319	2.02	-1.4	-1.39	4.82	0.01	64.13	-73.13
N3—H3A•••O9^{v}	0.99(4)	1.96(4)	2.924(3)	0.1754	1.66	-0.96	-0.95	3.57	0.02	47.24	-49.4
N8—H8A•••N1^{viii}	1.01(4)	2.07(4)	3.069(3)	0.1539	1.18	-0.84	-0.79	2.81	0.06	35.26	-38.37
N4—H4A•••N5^{v}	0.97(4)	2.11(4)	3.086(3)	0.1525	1.14	-0.81	-0.79	2.74	0.02	34.31	-37.57
N7—H7A•••O8^{viii}	1.00(4)	2.09(4)	3.078(3)	0.1298	1.15	-0.69	-0.67	2.51	0.03	31.38	-31.3
N3—H3B•••O1^{i}	1.04(4)	2.08(4)	2.850(3)	0.1296	1.79	-0.63	-0.48	2.89	0.32	42.8	-36.97
C38—H38•••N5^{v}	2.475	1.493	0.982	0.065	0.85	-0.25	-0.19	1.3	0.31	18.74	-14.24
C18—H18•••C30^{iii}	1.08	2.59	3.512(4)	0.0592	0.67	-0.18	-0.1	0.96	0.77	15.06	-11.75
N7—H7B•••O7^{vii}	1.08(4)	2.49(4)	3.497(4)	0.0576	0.59	-0.21	-0.11	0.9	0.88	13.35	-10.71
C27—H27•••O6^{vii}	2.452	1.014	1.44	0.056	0.94	-0.2	-0.14	1.28	0.49	19.53	-13.57
C2—H2•••N4^{ix}	1.08	2.6	3.550(4)	0.0478	0.61	-0.15	-0.15	0.91	0.05	13.07	-9.49
C24—H24C•••O2^{ii}	1.1	2.6	3.502(4)	0.0442	0.62	-0.15	-0.12	0.89	0.29	12.99	-9.08
C24—H24B•••Cl2^{xiii}	3.614	2.183	1.437	0.011	0.13	-0.03	-0.02	0.17	0.21	2.44	-1.46

(i). *x*−1/2, *y*−1/2, *z* ***(ii)***. *x*−1, *y*, *z* ***(iii)***. *x*−1/2, *y*+1/2, *z* ***(iv)***. −*x*+1/2, *y*−1/2, −*z*+1/2 ***(v)***. −*x*+1, *y*, −*z*+1/2

(vi). −*x*+3/2, −*y*+1/2, −*z* ***(vii)***. *x*+1/2, *y*+1/2, *z* ***(viii)***. −*x*+1/2, *y*+1/2, −*z*+1/2

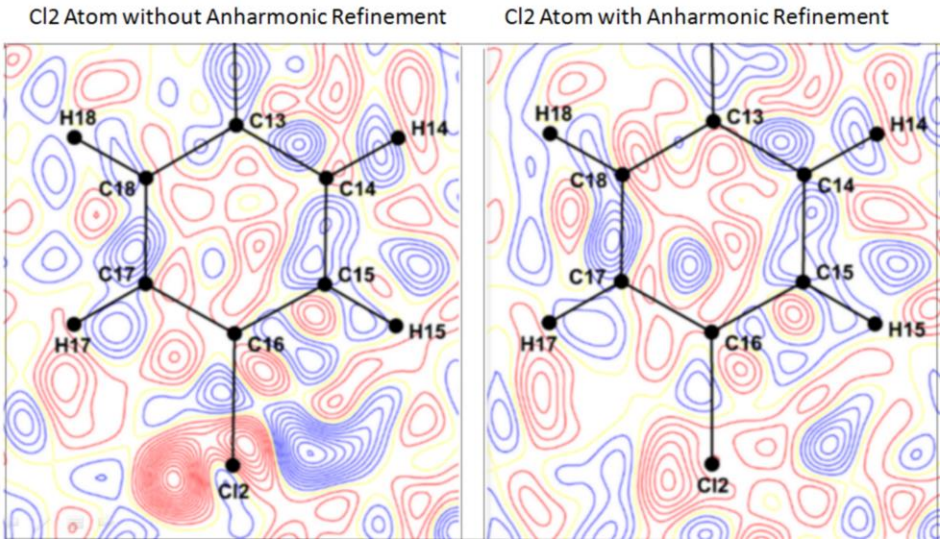

Fig. S1. Residual electron-density maps for the Cl atom.

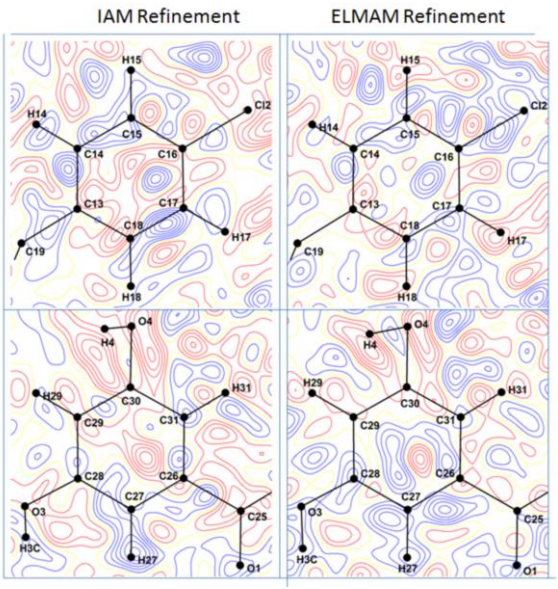

Fig. S2. Residual electron-density maps after IAM refinement.