

Supporting Information

Impact of A2V Mutation and Histidine Tautomerism on A β 42 Monomer Structures from Atomistic Simulations

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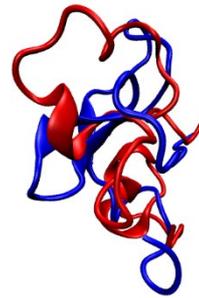
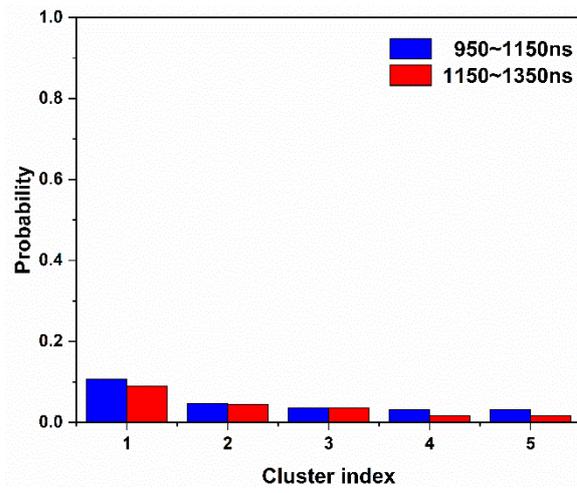
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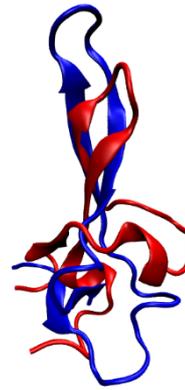
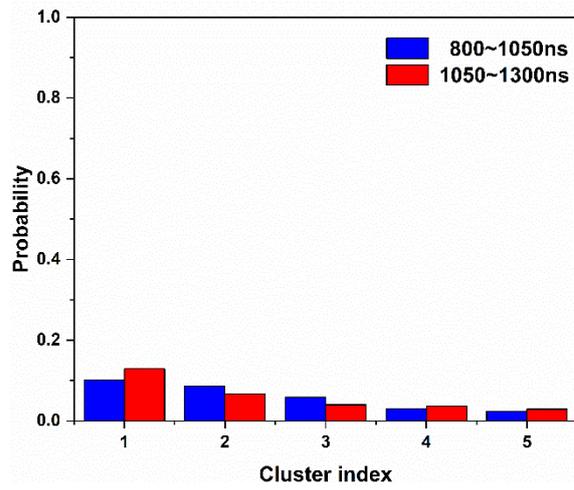
#These authors contributed equally to this work.

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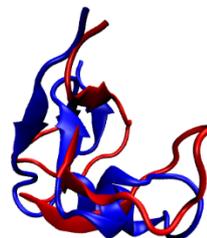
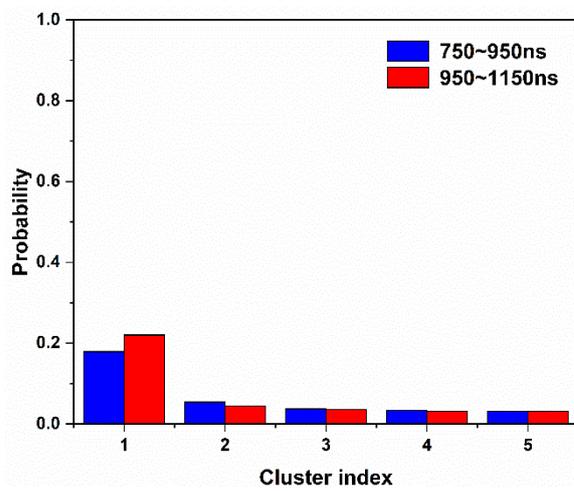
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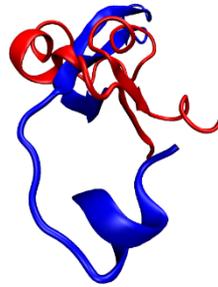
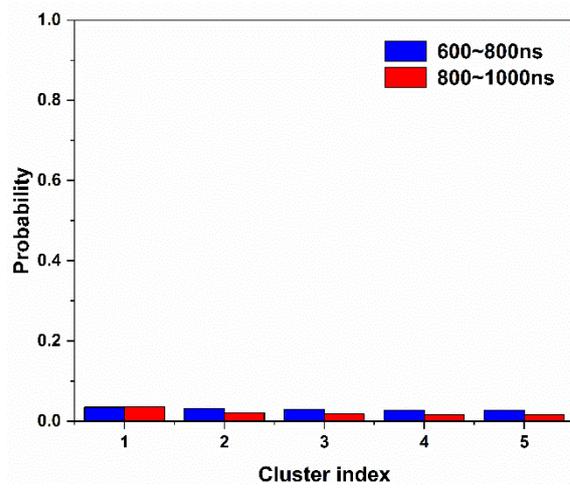
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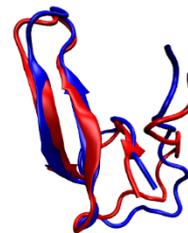
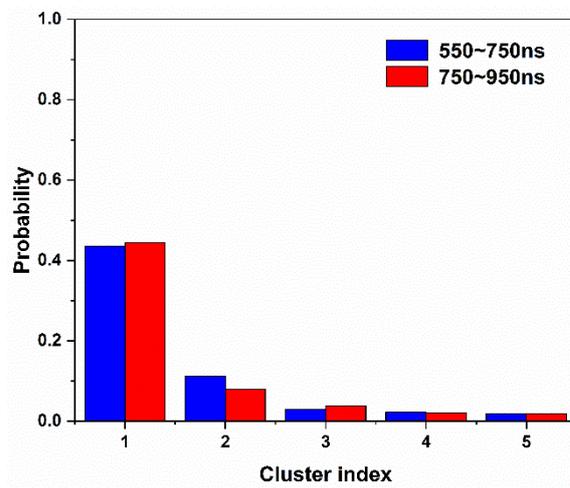
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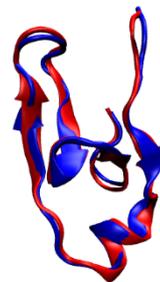
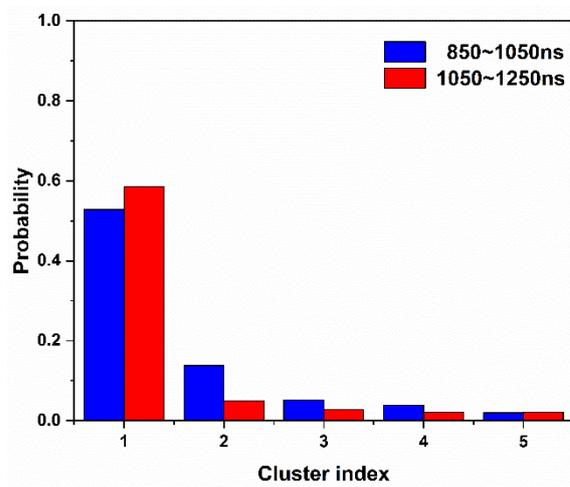
$\epsilon\delta\delta$



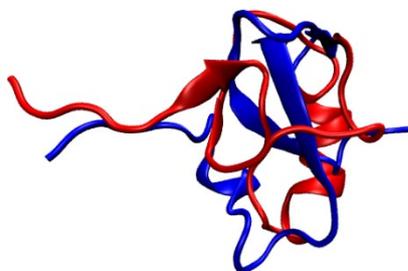
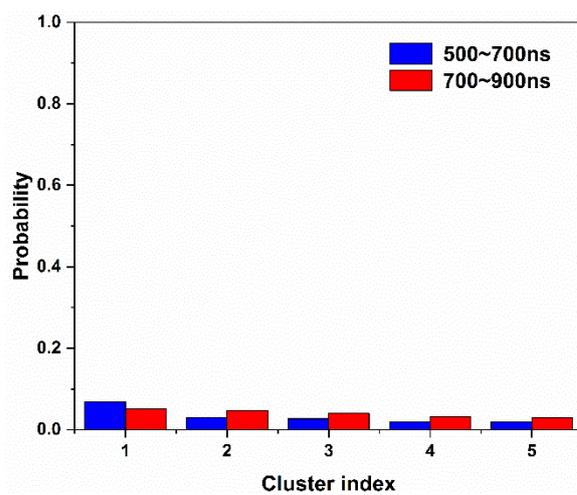
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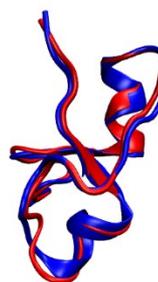
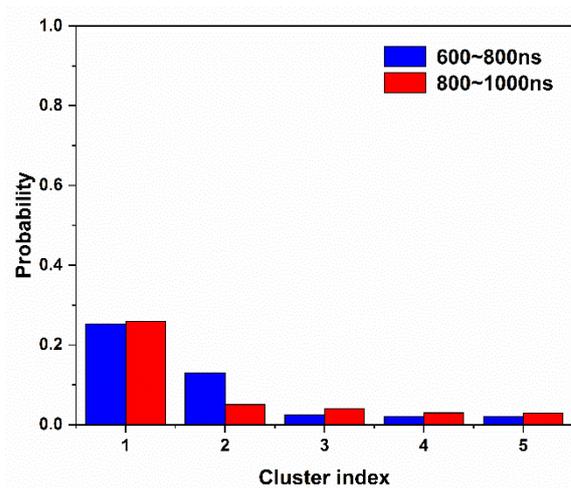


Figure S1. Cluster distributions (left) of each isomer, the most abundant structure (right).

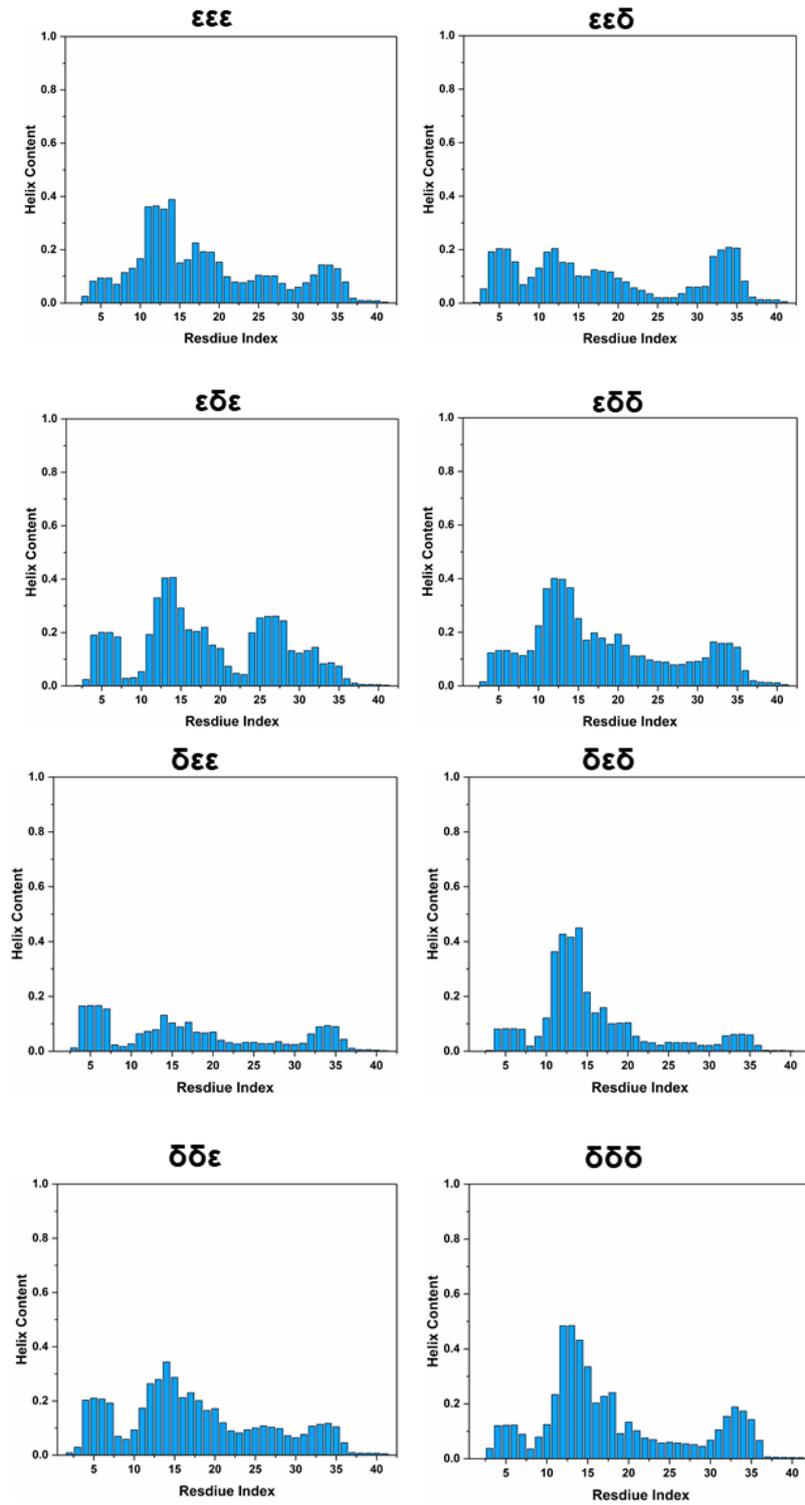


Figure S2. The α -helix contents of each amino acid of A2V A β 42 isomers.

Table S1. Hydrogen bond interactions of histidine residues of each isomer.

	$\epsilon\epsilon\epsilon$			$\epsilon\epsilon\delta$		
	P	Acceptor	Donor	P	Acceptor	Donor
Donor His6	6.22%	GLU_3@O	HIE_6@N	10.34%	GLU_3@O	HIE_6@N
Acceptor His6						
Donor His13	12.89%	TYR_10@O	HIE_13@N			
Acceptor His13	11.42%	HIE_13@O	LYS_16@N	7.61%	HIE_13@O	LYS_16@N
	7.32%	HIE_13@O	LEU_17@N			
Donor His14	13.35%	TYR_10@O	HIE_14@N	6.72%	GLU_11@O	HID_14@N
	5.65%	GLU_11@O	HIE_14@N	5.48%	TYR_10@O	HID_14@ND1
Acceptor His14						
	$\epsilon\delta\epsilon$			$\epsilon\delta\delta$		
	P	Acceptor	Donor	P	Acceptor	Donor
Donor His6	5.49%	GLU_3@O	HIE_6@N	6.66%	GLU_3@O	HIE_6@N
Acceptor His6						
Donor His13	24.19%	GLU_11@OE2	HID_13@ND1	13.66%	GLY_9@O	HID_13@ND1
	21.40%	GLU_11@OE1	HID_13@ND1	10.94%	TYR_10@O	HID_13@N
	7.29%	GLU_11@HG3	HID_13@N	10.86%	TYR_10@O	HID_13@ND1
	6.85%	GLU_11@OE2	HID_13@N	5.42%	GLU_11@OE2	HID_13@ND1
	5.27%	TYR_10@O	HID_13@ND1			
Acceptor His13	10.45%	HID_13@O	LEU_34@N	8.97%	HID_13@O	LYS_16@N
	6.46%	HID_13@O	LEU_17@N	7.78%	HID_13@O	LEU_17@N
	5.54%	HID_13@H	GLU_11@CG			
Donor His14	6.00%	GLU_11@O	HIE_14@N	13.01%	TYR_10@O	HID_14@N
				12.70%	GLU_11@O	HID_14@N
				11.06%	TYR_10@O	HID_14@ND1
				10.27%	GLU_11@O	HID_14@ND1
				5.00%	GLU_11@OE2	HID_14@ND1
Acceptor His14	10.06%	HIE_14@O	GLY_33@N	6.11%	HID_14@O	LEU_17@N
	5.32%	HIE_14@O	MET_35@N			
	$\delta\epsilon\epsilon$			$\delta\epsilon\delta$		
	P	Acceptor	Donor	P	Acceptor	Donor
Donor His6	13.66%	GLU_3@O	HID_6@N	31.41%	LEU_34@O	HID_6@N
	9.45%	ASP_7@O	HID_6@ND1	11.11%	ASP_7@O1	HID_6@ND1
Acceptor His6	6.82%	HID_6@O	ARG_5@NH2	43.54%	HID_6@O	VAL_36@N
Donor His13				10.37%	TYR_10@O	HIE_13@N
Acceptor His13	15.10%	HIE_13@O	LYS_16@N	10.32%	HIE_13@O	LYS_16@N
	8.03%	HIE_13@O	LEU_17@N	8.98%	HIE_13@O	LEU_17@N
Donor His14				13.59%	TYR_10@O	HID_14@ND1
				11.47%	GLU_11@O	HID_14@N
				9.69%	TYR_10@O	HID_14@N
				7.61%	GLU_11@O	HID_14@ND1

Acceptor His14

	$\delta\delta\epsilon$			$\delta\delta\delta$		
	P	Acceptor	Donor	P	Acceptor	Donor
Donor His6	16.30%	GLY_33@O	HID_6@N	25.40%	VAL_2@O	HID_6@N
	9.47%	GLU_3@O	HID_6@N	12.38%	GLU_3@O	HID_6@N
	7.33%	ASP_7@O	HID_6@ND1	5.33%	HID_6@O	HID_6@ND1
Acceptor His6	9.05%	HID_6@O	GLY_33@N	5.33%	HID_6@O	HID_6@ND1
Donor His13	13.13%	GLU_11@OE2	HID_13@ND1	17.27%	GLU_11@OE2	HID_13@ND1
	12.00%	GLU_11@OE1	HID_13@ND1	14.47%	GLU_11@OE1	HID_13@ND1
	7.47%	TYR_10@O	HID_13@N	9.66%	TYR_10@O	HID_13@ND1
	6.96%	TYR_10@O	HID_13@ND1	5.17%	TYR_10@O	HID_13@N
	5.05%	GLY_9@O	HID_13@ND1			
Acceptor His13	16.32%	HID_13@O	LYS_16@N			
	14.09%	HID_13@O	LEU_17@N			
Donor His14	11.96%	GLU_11@O	HIE_14@N	25.08%	GLU_11@O	HID_14@N
	9.33%	TYR_10@O	HIE_14@N	8.61%	TYR_10@O	HID_14@ND1
				8.03%	ARG_5@O	HID_14@ND1
			6.29%	GLU_11@O	HID_14@ND1	
			5.79%	TYR_10@O	HID_14@N	
Acceptor His14	5.80%	HIE_14@O	LEU_17@N	6.46%	HID_14@O	LEU_17@N