

Electronic Supplementary Information

Molecular Mechanism of Amyloidogenicity and Neurotoxicity of a Pro-aggregated Tau Mutant in the Presence of Histidine Tautomerism via Replica-Exchange Simulation

*Sompriya Chatterjee[§], Abbas Salimi[§], and Jin Yong Lee**

Department of Chemistry, Sungkyunkwan University, Suwon 440-746, Korea

[§] These authors contributed equally to this work

**Corresponding author: jinylee@skku.edu (J. Y. Lee), Orcid ID: 0000-0003-0360-5059*

Figure S1 [A]. The convergence evaluation of the REMD simulations at 310 K

Table S1 [A]. Hydrogen bond interactions of histidine for each mutant isomer

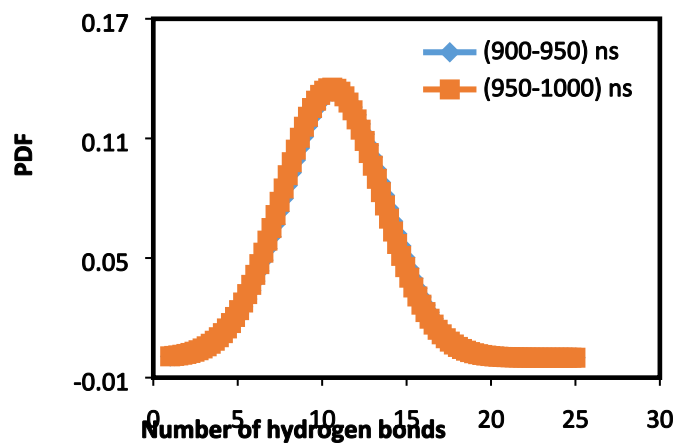
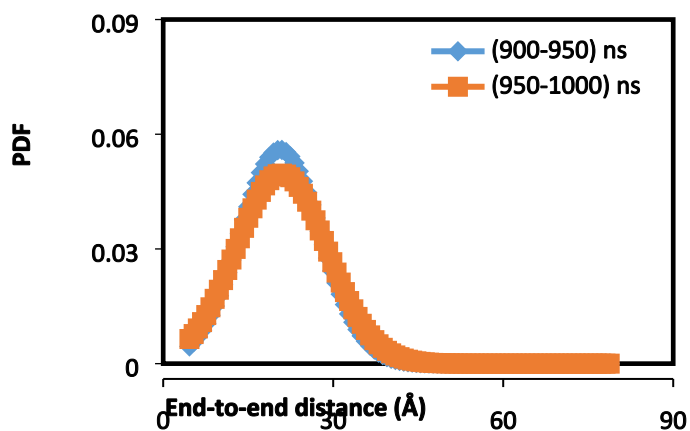
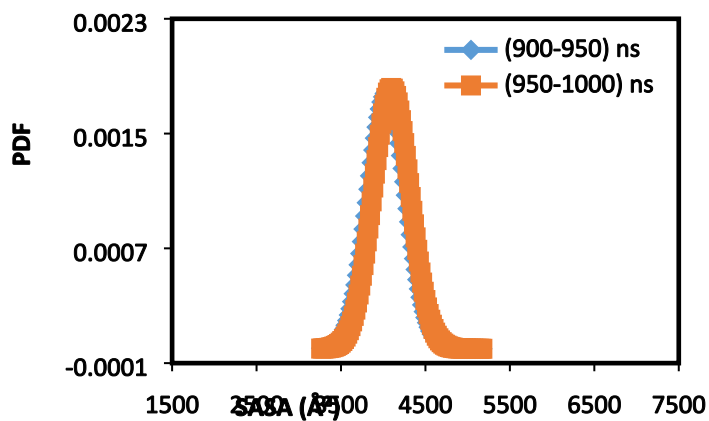
Figure S2 [A]. The convergence evaluation of P301L $\delta\epsilon$ and $\epsilon\epsilon$ isomers, at 310 K

Figure S3 [A]. a) Antiparallel sheet content, b) α -helical content, c) contact map, and d) clustering of P301L $\delta\epsilon$ isomer

Figure S4 [A]. a) Antiparallel sheet content, b) α -helical content, c) contact map, and d) clustering of P301L $\epsilon\epsilon$ isomer

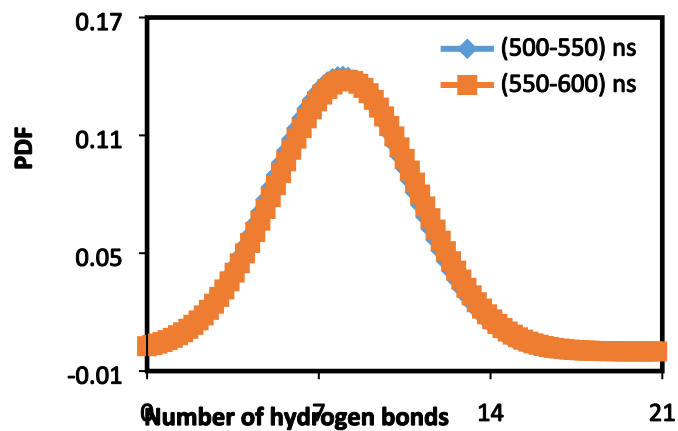
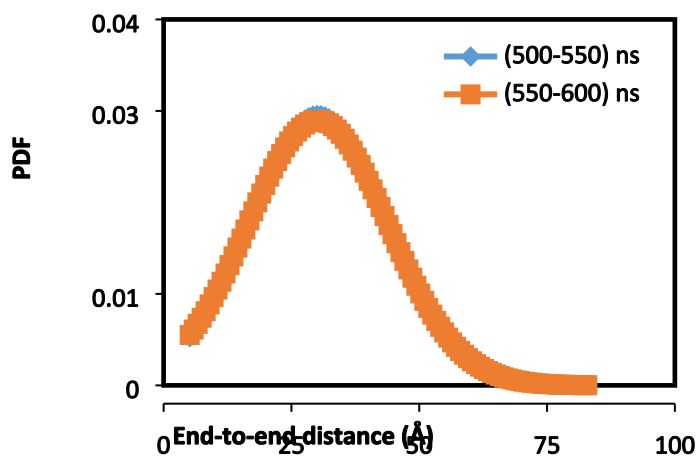
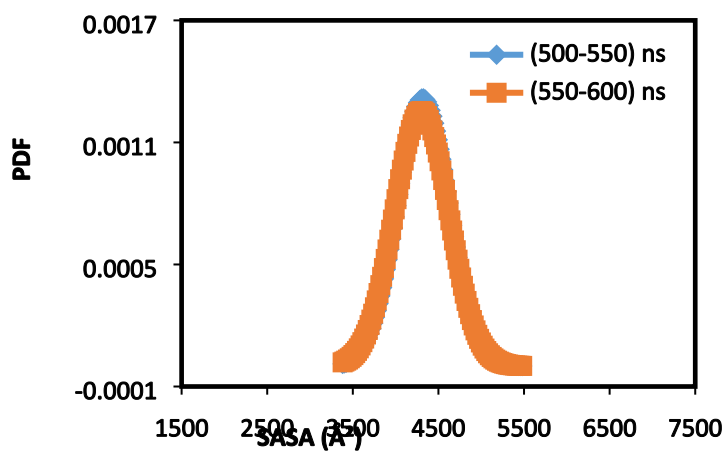
($\delta\delta$)

Isomer



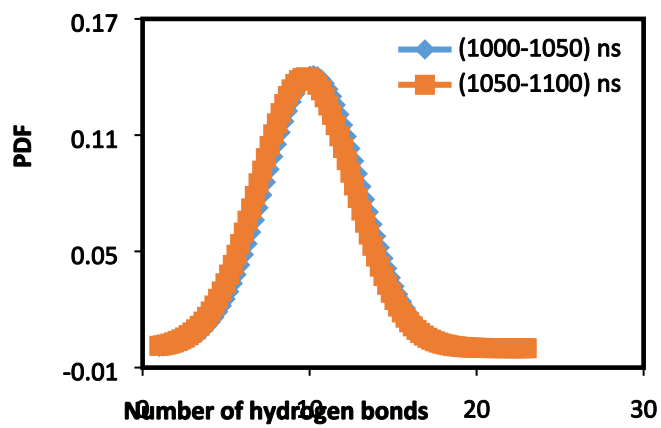
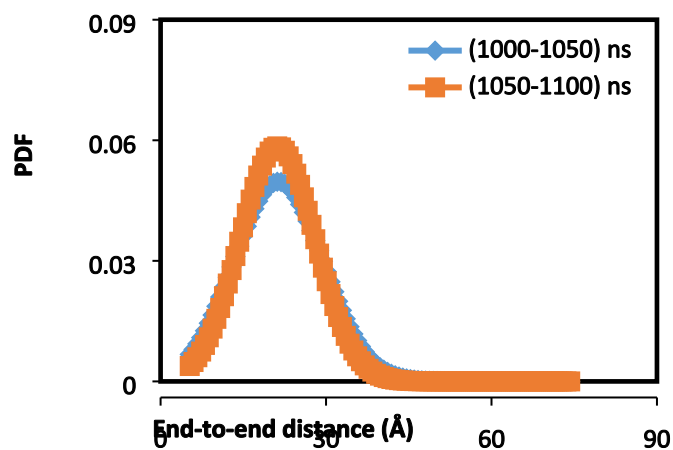
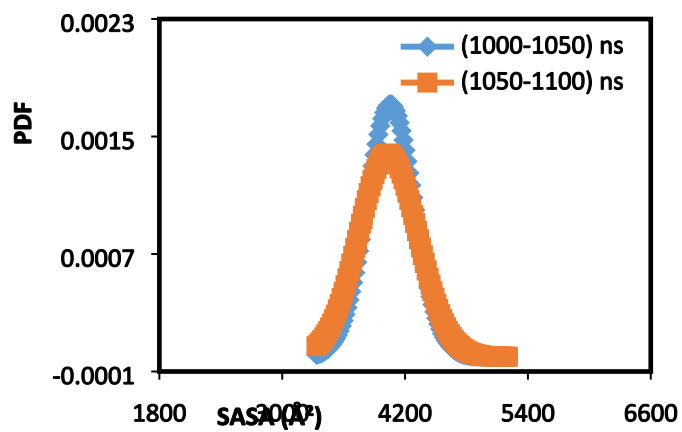
($\epsilon\epsilon$)

Isomer



($\delta\varepsilon$)

Isomer



($\epsilon\delta$)

Isomer

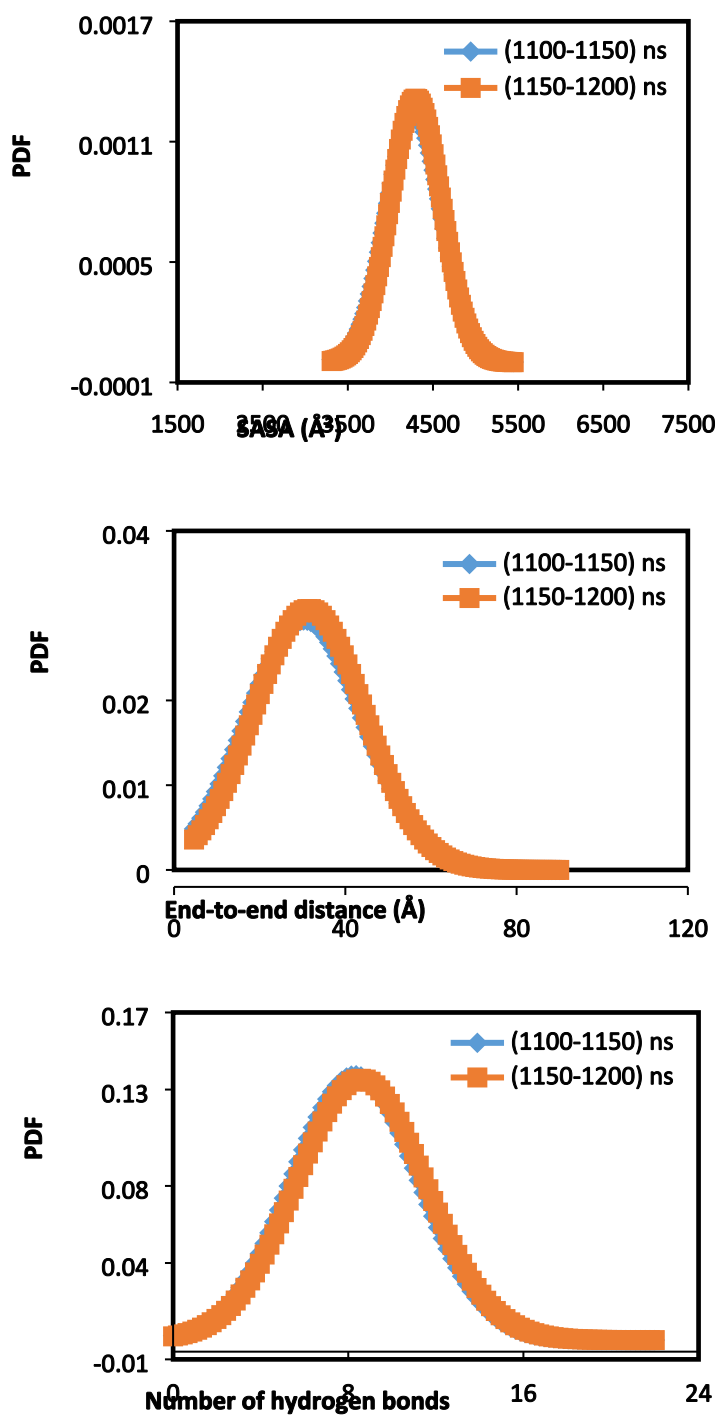


Figure S1 [A]. The convergence evaluation of the REMD simulations at 310 K

Table S1 [A]. Hydrogen bond interactions of histidine for each mutant isomer

($\delta\delta$) isomer

Donor HIS 268

P	Acceptor	Donor
14.22%	GLN_3@O	HID_2@ND1
1.38%	HID_2@O	HID_2@ND1
0.28%	LYS_1@O	HID_2@ND1
0.22%	PRO_45@O	HID_2@ND1
0.18%	GLN_3@OE1	HID_2@N
0.12%	GLN_3@OE1	HID_2@ND1
0.12%	VAL_33@O	HID_2@ND1
0.06%	PRO_34@O	HID_2@ND1
0.06%	PRO_45@OXT	HID_2@ND1
0.04%	GLY_6@O	HID_2@ND1
0.04%	GLY_35@O	HID_2@ND1
0.04%	TYR_43@O	HID_2@ND1
0.02%	ASP_16@OD1	HID_2@ND1
0.02%	TYR_43@OH	HID_2@ND1
0.02%	GLY_36@O	HID_2@ND1
0.02%	GLN_10@OE1	HID_2@ND1
0.02%	ILE_41@O	HID_2@ND1
0.02%	GLY_35@O	HID_2@N
0.02%	GLN_40@O	HID_2@ND1
0.02%	PRO_45@O	HID_2@N
0.02%	GLY_37@O	HID_2@N

Acceptor HIS 268

P	Acceptor	Donor
1.38%	HID_2@O	HID_2@ND1
0.94%	HID_2@O	GLN_3@NE2
0.12%	HID_2@O	TYR_43@OH
0.1%	HID_2@ND1	GLN_3@N
0.06%	HID_2@O	LYS_1@NZ
0.06%	HID_2@NE2	TYR_43@OH
0.04%	HID_2@O	LYS_1@NZ
0.02%	HID_2@NE2	GLN_3@NE2

Donor HIS 299

P	Acceptor	Donor
15%	VAL_33@O	HID_32@ND1
3.54%	ASN_29@O	HID_32@N
3.02%	ASN_29@O	HID_32@ND1
2.6%	HID_32@O	HID_32@ND1
2.1%	ASN_29@OD1	HID_32@N
1.84%	ASN_29@OD1	HID_32@ND1
1.7%	ILE_30@O	HID_32@ND1
1.62%	GLN_40@O	HID_32@N
1.34%	SER_26@O	HID_32@ND1
1.24%	GLN_40@OE1	HID_32@ND1
1.24%	ILE_30@O	HID_32@N
0.94%	LYS_31@O	HID_32@ND1
0.46%	ASP_28@OD1	HID_32@ND1
0.42%	ASP_28@OD2	HID_32@ND1
0.38%	SER_26@OG	HID_32@ND1
0.34%	GLY_25@O	HID_32@ND1
0.32%	CYS_24@O	HID_32@ND1
0.32%	GLY_37@O	HID_32@ND1
0.18%	ASP_28@O	HID_32@ND1
0.16%	SER_38@OG	HID_32@ND1
0.1%	TYR_43@O	HID_32@ND1
0.1%	GLY_36@O	HID_32@ND1
0.08%	LYS_23@O	HID_32@ND1
0.06%	VAL_39@O	HID_32@ND1
0.04%	ASP_16@OD2	HID_32@ND1
0.04%	LYS_27@O	HID_32@ND1
0.04%	VAL_20@O	HID_32@ND1
0.04%	SER_22@O	HID_32@ND1
0.02%	PRO_45@OXT	HID_32@ND1
0.02%	VAL_42@O	HID_32@ND1
0.02%	PRO_45@O	HID_32@ND1
0.02%	ILE_41@O	HID_32@ND1
0.02%	LYS_27@O	HID_32@N
0.02%	SER_22@OG	HID_32@ND1

Acceptor HIS 299

P	Acceptor	Donor
2.6%	HID_32@O	HID_32@ND1
1.8%	HID_32@O	ASP_28@N
1.2%	HID_32@O	SER_26@OG
0.96%	HID_32@O	GLN_40@N

0.38%	HID_32@O	GLY_25@N
0.24%	HID_32@O	LYS_27@NZ
0.2%	HID_32@O	SER_26@N
0.16%	HID_32@O	TYR_43@OH
0.12%	HID_32@O	LYS_27@NZ
0.08%	HID_32@O	GLN_21@NE2
0.08%	HID_32@NE2	ASN_29@ND2
0.06%	HID_32@O	LYS_27@NZ
0.04%	HID_32@O	ASN_29@ND2
0.04%	HID_32@NE2	ASP_28@N
0.04%	HID_32@NE2	GLY_25@N
0.04%	HID_32@NE2	LYS_27@NZ
0.04%	HID_32@ND1	VAL_33@N
0.04%	HID_32@O	GLN_3@N
0.04%	HID_32@O	ASN_29@N
0.04%	HID_32@NE2	LYS_27@NZ
0.02%	HID_32@O	GLN_3@NE2
0.02%	HID_32@NE2	SER_26@OG
0.02%	HID_32@O	GLY_5@N
0.02%	HID_32@O	GLN_10@NE2
0.02%	HID_32@NE2	ASN_29@ND2
0.02%	HID_32@NE2	GLN_40@NE2
0.02%	HID_32@ND1	GLN_40@NE2
0.02%	HID_32@NE2	ASN_29@N
0.02%	HID_32@NE2	GLY_37@N

(εε) isomer

Donor HIS 268

P	Acceptor	Donor
0.86%	HIE_2@ND1	HIE_2@N
0.4%	GLY_6@O	HIE_2@NE2
0.34%	GLY_7@O	HIE_2@NE2
0.2%	VAL_42@O	HIE_2@NE2
0.1%	GLN_10@O	HIE_2@NE2
0.1%	GLN_10@OE1	HIE_2@NE2
0.08%	PRO_45@O	HIE_2@NE2
0.08%	ASP_16@OD1	HIE_2@NE2
0.06%	ILE_11@O	HIE_2@NE2
0.06%	VAL_9@O	HIE_2@NE2
0.06%	PRO_45@OXT	HIE_2@NE2
0.06%	VAL_42@O	HIE_2@N
0.06%	SER_38@O	HIE_2@NE2

0.06%	TYR_43@O	HIE_2@NE2
0.04%	ILE_30@O	HIE_2@NE2
0.04%	PRO_45@O	HIE_2@N
0.04%	PRO_45@OXT	HIE_2@N
0.04%	GLN_40@O	HIE_2@NE2
0.04%	VAL_39@O	HIE_2@NE2
0.04%	LYS_8@O	HIE_2@NE2
0.02%	PRO_34@O	HIE_2@NE2
0.02%	ASP_16@OD1	HIE_2@N
0.02%	ASP_16@OD2	HIE_2@NE2
0.02%	ASN_13@OD1	HIE_2@N
0.02%	TYR_43@OH	HIE_2@NE2
0.02%	ASP_16@OD2	HIE_2@N
0.02%	SER_22@O	HIE_2@NE2
0.02%	ILE_41@O	HIE_2@N
0.02%	LYS_44@O	HIE_2@NE2
0.02%	LYS_27@O	HIE_2@NE2
0.02%	HIE_32@O	HIE_2@NE2
0.02%	LYS_14@O	HIE_2@NE2
0.02%	ILE_41@O	HIE_2@NE2
0.02%	SER_26@O	HIE_2@NE2

Acceptor HIS 268

P	Acceptor	Donor
3.86%	HIE_2@ND1	GLN_3@N
2.16%	HIE_2@O	GLN_3@NE2
0.86%	HIE_2@ND1	HIE_2@N
0.16%	HIE_2@O	GLN_3@NE2
0.06%	HIE_2@O	TYR_43@OH
0.06%	HIE_2@O	LYS_1@NZ
0.06%	HIE_2@O	LYS_1@NZ
0.06%	HIE_2@O	LYS_1@NZ
0.04%	HIE_2@ND1	TYR_43@OH
0.02%	HIE_2@O	GLY_36@N

Donor HIS 299

P	Acceptor	Donor
2.16%	ASN_29@O	HIE_32@N
1.48%	ILE_30@O	HIE_32@N
1.36%	ASN_29@OD1	HIE_32@N
0.88%	HIE_32@ND1	HIE_32@N
0.58%	ASP_28@O	HIE_32@N

0.56%	LEU_17@O	HIE_32@N
0.3%	SER_38@O	HIE_32@NE2
0.26%	GLN_21@O	HIE_32@NE2
0.24%	PRO_45@O	HIE_32@NE2
0.22%	SER_22@OG	HIE_32@NE2
0.2%	GLN_40@OE1	HIE_32@N
0.18%	GLY_36@O	HIE_32@NE2
0.18%	SER_22@O	HIE_32@NE2
0.18%	GLN_21@OE1	HIE_32@NE2
0.16%	PRO_45@OXT	HIE_32@NE2
0.12%	ASP_16@OD2	HIE_32@NE2
0.12%	ASP_28@OD1	HIE_32@NE2
0.12%	GLN_40@OE1	HIE_32@NE2
0.12%	ILE_41@O	HIE_32@NE2
0.12%	GLN_10@OE1	HIE_32@NE2
0.1%	ASN_29@OD1	HIE_32@NE2
0.08%	ASP_28@OD2	HIE_32@NE2
0.08%	ASN_29@O	HIE_32@NE2
0.08%	LYS_14@O	HIE_32@NE2
0.08%	CYS_24@O	HIE_32@NE2
0.06%	PRO_4@O	HIE_32@N
0.06%	PRO_4@O	HIE_32@NE2
0.06%	LYS_27@O	HIE_32@NE2
0.04%	SER_26@O	HIE_32@NE2
0.04%	SER_18@O	HIE_32@N
0.04%	ASN_13@O	HIE_32@NE2
0.04%	SER_18@O	HIE_32@NE2
0.04%	SER_38@OG	HIE_32@NE2
0.04%	LEU_17@O	HIE_32@NE2
0.04%	GLY_25@O	HIE_32@N
0.04%	SER_18@OG	HIE_32@NE2
0.04%	VAL_42@O	HIE_32@N
0.02%	ILE_11@O	HIE_32@NE2
0.02%	GLN_40@O	HIE_32@NE2
0.02%	ASN_19@O	HIE_32@N
0.02%	GLN_10@O	HIE_32@NE2
0.02%	VAL_20@O	HIE_32@NE2
0.02%	ASP_16@O	HIE_32@NE2
0.02%	ASN_19@OD1	HIE_32@NE2
0.02%	SER_26@OG	HIE_32@NE2
0.02%	ASP_16@OD1	HIE_32@NE2
0.02%	VAL_39@O	HIE_32@NE2
0.02%	GLY_37@O	HIE_32@NE2
0.02%	LYS_44@O	HIE_32@NE2
0.02%	TYR_43@OH	HIE_32@N

0.02%	LYS_23@O	HIE_32@NE2
0.02%	GLY_7@O	HIE_32@N
0.02%	LYS_23@O	HIE_32@N
0.02%	GLY_25@O	HIE_32@NE2
0.02%	GLN_40@O	HIE_32@N
0.02%	GLN_21@OE1	HIE_32@N

Acceptor HIS 299

P	Acceptor	Donor
2.1%	HIE_32@ND1	VAL_33@N
1.16%	HIE_32@O	SER_26@OG
0.88%	HIE_32@ND1	HIE_32@N
0.5%	HIE_32@O	TYR_43@OH
0.32%	HIE_32@O	ASN_29@ND2
0.28%	HIE_32@ND1	SER_26@OG
0.14%	HIE_32@O	GLY_25@N
0.14%	HIE_32@O	SER_26@N
0.1%	HIE_32@O	GLN_21@NE2
0.08%	HIE_32@O	SER_18@OG
0.08%	HIE_32@ND1	SER_38@OG
0.08%	HIE_32@O	ILE_41@N
0.08%	HIE_32@O	GLY_7@N
0.08%	HIE_32@ND1	GLN_21@NE2
0.06%	HIE_32@O	TYR_43@N
0.06%	HIE_32@O	LYS_31@NZ
0.04%	HIE_32@O	GLY_5@N
0.04%	HIE_32@O	ASN_19@ND2
0.04%	HIE_32@ND1	ASN_29@ND2
0.04%	HIE_32@ND1	ASN_29@ND2
0.04%	HIE_32@O	ASN_29@ND2
0.04%	HIE_32@O	LYS_31@NZ
0.04%	HIE_32@O	GLN_40@NE2
0.02%	HIE_32@O	LYS_27@N
0.02%	HIE_32@O	LYS_8@NZ
0.02%	HIE_32@O	LYS_23@NZ
0.02%	HIE_32@ND1	TYR_43@OH
0.02%	HIE_32@O	GLN_10@NE2
0.02%	HIE_32@O	HIE_2@NE2
0.02%	HIE_32@O	LYS_27@NZ
0.02%	HIE_32@ND1	GLN_40@NE2
0.02%	HIE_32@O	LYS_31@NZ
0.02%	HIE_32@ND1	GLN_21@NE2
0.02%	HIE_32@ND1	SER_26@N
0.02%	HIE_32@O	LYS_23@NZ

0.02%	HIE_32@O	SER_38@OG
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($\delta\epsilon$) isomer

Donor HIS 268

P	Acceptor	Donor
13.78%	GLN_3@O	HID_2@ND1
1.48%	HID_2@O	HID_2@ND1
0.5%	LYS_1@O	HID_2@ND1
0.16%	PRO_34@O	HID_2@ND1
0.06%	PRO_45@OXT	HID_2@ND1
0.04%	ASP_16@OD1	HID_2@ND1
0.04%	GLY_6@O	HID_2@ND1
0.04%	PRO_45@O	HID_2@ND1
0.02%	GLN_10@OE1	HID_2@ND1
0.02%	GLY_35@O	HID_2@ND1
0.02%	ASP_16@OD2	HID_2@ND1
0.02%	LYS_31@O	HID_2@N
0.02%	VAL_42@O	HID_2@ND1
0.02%	GLN_3@OE1	HID_2@ND1
0.02%	HIE_32@O	HID_2@ND1
0.02%	GLN_3@OE1	HID_2@N
0.02%	CYS_24@O	HID_2@ND1
0.02%	LYS_31@O	HID_2@ND1

Acceptor HIS 268

P	Acceptor	Donor
1.48%	HID_2@O	HID_2@ND1
1.1%	HID_2@O	GLN_3@NE2
0.08%	HID_2@O	GLN_3@NE2
0.06%	HID_2@O	LYS_1@NZ
0.04%	HID_2@O	TYR_43@OH
0.04%	HID_2@NE2	TYR_43@OH
0.04%	HID_2@ND1	GLN_3@N
0.02%	HID_2@O	GLY_36@N
0.02%	HID_2@NE2	GLY_36@N
0.02%	HID_2@NE2	LYS_44@NZ
0.02%	HID_2@O	LYS_1@NZ
0.02%	HID_2@O	LYS_1@NZ

Donor HIS 299

P	Acceptor	Donor
1.6%	GLN_40@OE1	HIE_32@NE2
0.9%	GLY_36@O	HIE_32@NE2
0.74%	ILE_30@O	HIE_32@N
0.74%	ASN_29@O	HIE_32@N
0.68%	ASN_29@OD1	HIE_32@N
0.6%	HIE_32@ND1	HIE_32@N
0.28%	GLY_37@O	HIE_32@NE2
0.1%	TYR_43@O	HIE_32@NE2
0.06%	ASP_16@OD2	HIE_32@NE2
0.04%	SER_18@OG	HIE_32@NE2
0.04%	ASP_28@OD1	HIE_32@NE2
0.04%	GLN_21@OE1	HIE_32@NE2
0.04%	GLN_3@OE1	HIE_32@N
0.04%	LYS_27@O	HIE_32@NE2
0.04%	ASP_16@OD1	HIE_32@NE2
0.04%	ASP_28@OD2	HIE_32@NE2
0.04%	LYS_23@O	HIE_32@NE2
0.04%	SER_18@O	HIE_32@NE2
0.04%	GLN_21@O	HIE_32@NE2
0.02%	ILE_41@O	HIE_32@N
0.02%	PRO_4@O	HIE_32@NE2
0.02%	LYS_14@O	HIE_32@NE2
0.02%	VAL_39@O	HIE_32@NE2
0.02%	ILE_12@O	HIE_32@NE2
0.02%	ILE_41@O	HIE_32@NE2
0.02%	GLY_25@O	HIE_32@NE2
0.02%	ASN_13@OD1	HIE_32@NE2
0.02%	SER_22@OG	HIE_32@NE2
0.02%	ASP_28@O	HIE_32@NE2
0.02%	SER_38@O	HIE_32@NE2
0.02%	ASN_29@OD1	HIE_32@NE2
0.02%	ASP_28@O	HIE_32@N
0.02%	SER_26@OG	HIE_32@NE2

Acceptor HIS 299

P	Acceptor	Donor
1.58%	HIE_32@ND1	VAL_33@N
0.66%	HIE_32@ND1	GLN_40@NE2
0.6%	HIE_32@ND1	HIE_32@N

0.12%	HIE_32@ND1	GLN_40@NE2
0.08%	HIE_32@ND1	SER_38@OG
0.06%	HIE_32@O	SER_26@OG
0.04%	HIE_32@O	SER_22@OG
0.04%	HIE_32@O	GLY_36@N
0.04%	HIE_32@O	LYS_31@NZ
0.04%	HIE_32@O	ASN_19@ND2
0.04%	HIE_32@ND1	ASN_29@ND2
0.02%	HIE_32@O	SER_18@OG
0.02%	HIE_32@O	GLN_21@NE2
0.02%	HIE_32@O	HID_2@ND1
0.02%	HIE_32@O	GLN_21@NE2
0.02%	HIE_32@O	LYS_8@NZ
0.02%	HIE_32@ND1	ASN_13@N
0.02%	HIE_32@O	GLN_3@NE2
0.02%	HIE_32@O	LYS_31@NZ
0.02%	HIE_32@O	GLY_5@N
0.02%	HIE_32@O	TYR_43@OH
0.02%	HIE_32@O	LYS_14@NZ
0.02%	HIE_32@ND1	ASN_29@ND2
0.02%	HIE_32@ND1	ASN_13@ND2

(εδ) isomer

Donor HIS 268

P	Acceptor	Donor
0.5%	HIE_2@ND1	HIE_2@N
0.48%	GLY_6@O	HIE_2@NE2
0.26%	PRO_45@OXT	HIE_2@NE2
0.26%	ASP_16@OD2	HIE_2@NE2
0.18%	VAL_42@O	HIE_2@NE2
0.12%	PRO_34@O	HIE_2@NE2
0.1%	TYR_43@O	HIE_2@NE2
0.1%	ILE_41@O	HIE_2@NE2
0.08%	LEU_17@O	HIE_2@NE2
0.08%	PRO_45@O	HIE_2@NE2
0.08%	ILE_11@O	HIE_2@NE2
0.08%	VAL_9@O	HIE_2@NE2
0.06%	CYS_24@O	HIE_2@N
0.06%	GLY_7@O	HIE_2@NE2
0.04%	ASP_16@O	HIE_2@NE2
0.04%	GLY_5@O	HIE_2@NE2
0.04%	VAL_20@O	HIE_2@NE2

0.04%	SER_22@O	HIE_2@NE2
0.02%	VAL_39@O	HIE_2@NE2
0.02%	GLY_36@O	HIE_2@NE2
0.02%	SER_18@O	HIE_2@NE2
0.02%	GLN_3@OE1	HIE_2@N
0.02%	GLY_35@O	HIE_2@NE2
0.02%	LYS_8@O	HIE_2@NE2
0.02%	LYS_44@O	HIE_2@NE2
0.02%	ILE_12@O	HIE_2@NE2
0.02%	GLN_40@O	HIE_2@NE2
0.02%	LYS_23@O	HIE_2@NE2
0.02%	GLN_10@O	HIE_2@NE2
0.02%	SER_26@O	HIE_2@NE2

Acceptor HIS 268

P	Acceptor	Donor
4%	HIE_2@ND1	GLN_3@N
2.02%	HIE_2@O	GLN_3@NE2
0.5%	HIE_2@ND1	HIE_2@N
0.14%	HIE_2@O	SER_26@OG
0.04%	HIE_2@O	TYR_43@OH
0.04%	HIE_2@O	LYS_1@NZ
0.04%	HIE_2@O	GLN_3@NE2
0.02%	HIE_2@O	GLN_21@NE2
0.02%	HIE_2@O	LYS_1@NZ
0.02%	HIE_2@O	LYS_1@NZ
0.02%	HIE_2@ND1	GLN_40@NE2

Donor HIS 299

P	Acceptor	Donor
5.08%	VAL_33@O	HID_32@ND1
4.12%	ILE_30@O	HID_32@ND1
3.64%	ASP_28@OD1	HID_32@ND1
3.42%	ASP_28@OD2	HID_32@ND1
2.84%	ASP_28@O	HID_32@N
2.5%	HID_32@O	HID_32@ND1
2.46%	GLN_40@OE1	HID_32@ND1
2.06%	ASN_29@O	HID_32@N
1.5%	ASP_28@O	HID_32@ND1
1.44%	ASN_29@O	HID_32@ND1
1.2%	LYS_31@O	HID_32@ND1
0.9%	GLY_37@O	HID_32@ND1

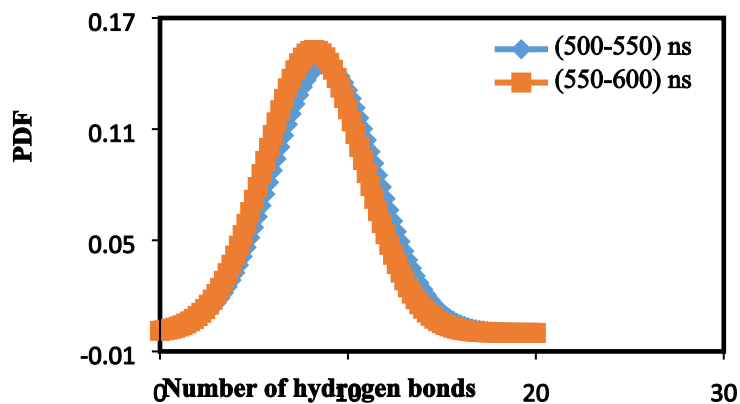
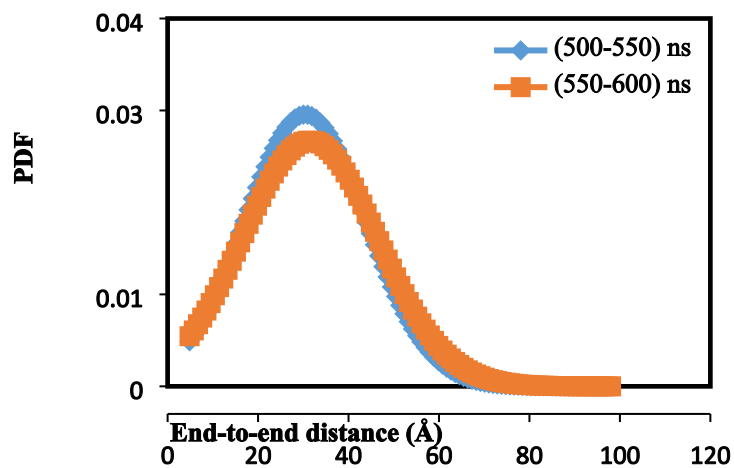
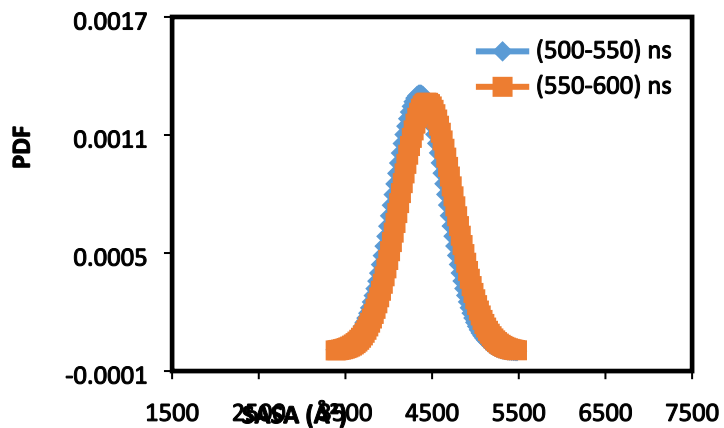
0.72%	ILE_30@O	HID_32@N
0.64%	ILE_41@O	HID_32@ND1
0.56%	GLN_40@O	HID_32@ND1
0.44%	ASN_29@OD1	HID_32@N
0.32%	SER_22@O	HID_32@ND1
0.26%	SER_38@OG	HID_32@ND1
0.26%	ASN_13@O	HID_32@ND1
0.22%	SER_26@O	HID_32@ND1
0.2%	ASN_29@OD1	HID_32@ND1
0.18%	CYS_24@O	HID_32@ND1
0.14%	TYR_43@O	HID_32@ND1
0.14%	VAL_39@O	HID_32@ND1
0.12%	VAL_20@O	HID_32@ND1
0.08%	ASN_19@O	HID_32@ND1
0.08%	VAL_42@O	HID_32@ND1
0.06%	TYR_43@OH	HID_32@ND1
0.04%	VAL_42@O	HID_32@N
0.04%	GLN_21@O	HID_32@ND1
0.04%	LYS_23@O	HID_32@ND1
0.04%	SER_18@OG	HID_32@ND1
0.04%	ASN_19@OD1	HID_32@ND1
0.04%	ASP_16@OD1	HID_32@ND1
0.04%	GLY_25@O	HID_32@ND1
0.02%	LYS_44@O	HID_32@ND1
0.02%	ILE_11@O	HID_32@ND1
0.02%	LYS_27@O	HID_32@ND1
0.02%	SER_38@O	HID_32@ND1
0.02%	VAL_33@N	HID_32@ND1
0.02%	CYS_24@O	HID_32@N

Acceptor HIS 299

P	Acceptor	Donor
2.5%	HID_32@O	HID_32@ND1
0.46%	HID_32@O	SER_26@OG
0.2%	HID_32@O	TYR_43@OH
0.12%	HID_32@O	SER_26@N
0.1%	HID_32@NE2	GLN_40@NE2
0.06%	HID_32@O	SER_22@OG
0.06%	HID_32@O	ASN_29@ND2
0.04%	HID_32@O	SER_18@OG
0.04%	HID_32@O	TYR_43@N
0.04%	HID_32@O	GLN_3@NE2
0.04%	HID_32@O	GLN_3@NE2
0.04%	HID_32@NE2	SER_26@OG

0.04%	HID_32@O	LYS_31@NZ
0.02%	HID_32@O	LYS_31@NZ
0.02%	HID_32@NE2	LYS_14@NZ
0.02%	HID_32@O	LYS_31@NZ
0.02%	HID_32@NE2	GLN_21@NE2
0.02%	HID_32@O	GLY_5@N
0.02%	HID_32@O	GLN_40@NE2
0.02%	HID_32@O	ASN_29@ND2
0.02%	HID_32@NE2	ASN_13@ND2
0.02%	HID_32@O	LYS_14@NZ
0.02%	HID_32@O	GLN_21@NE2
0.02%	HID_32@NE2	ASN_13@ND2
0.02%	HID_32@O	GLY_25@N
0.02%	HID_32@NE2	LYS_27@NZ
0.02%	HID_32@O	LYS_23@NZ

P301L ($\delta\epsilon$) Isomer



P301L ($\epsilon\epsilon$) Isomer

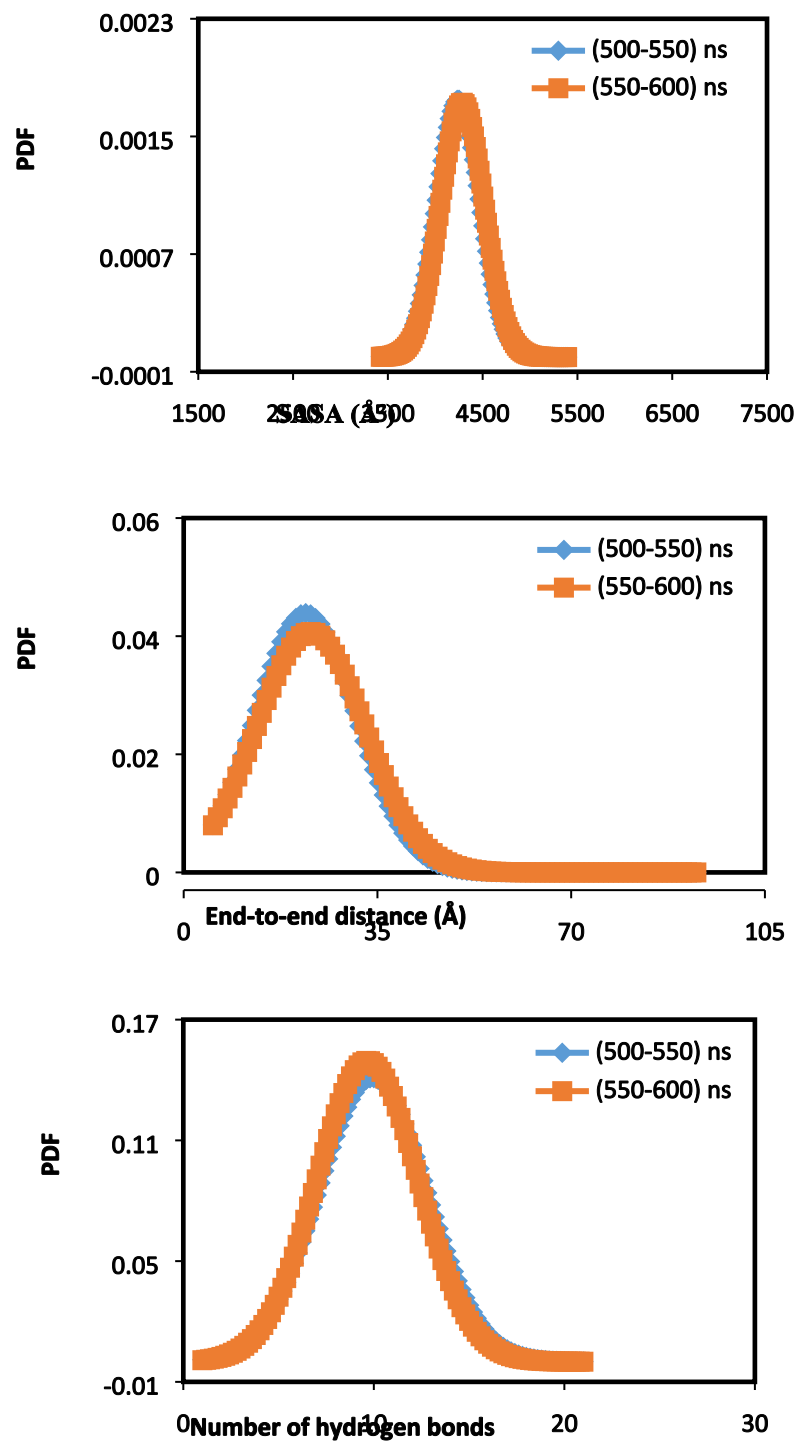


Figure S2 [A]. The convergence evaluation of P301L $\delta\epsilon$ and $\epsilon\epsilon$ isomers, at 310 K

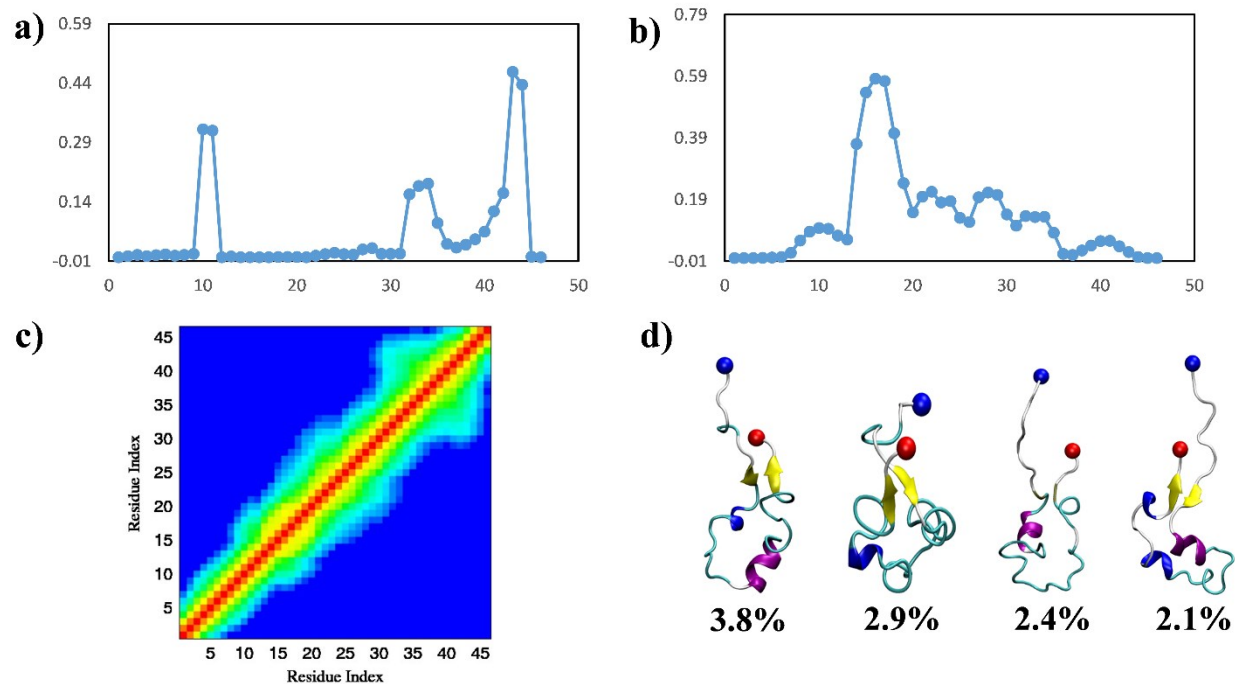


Figure S3 [A]. a) Antiparallel sheet content, b) α -helical content, c) contact map, and d) clustering of P301L $\delta\epsilon$ isomer

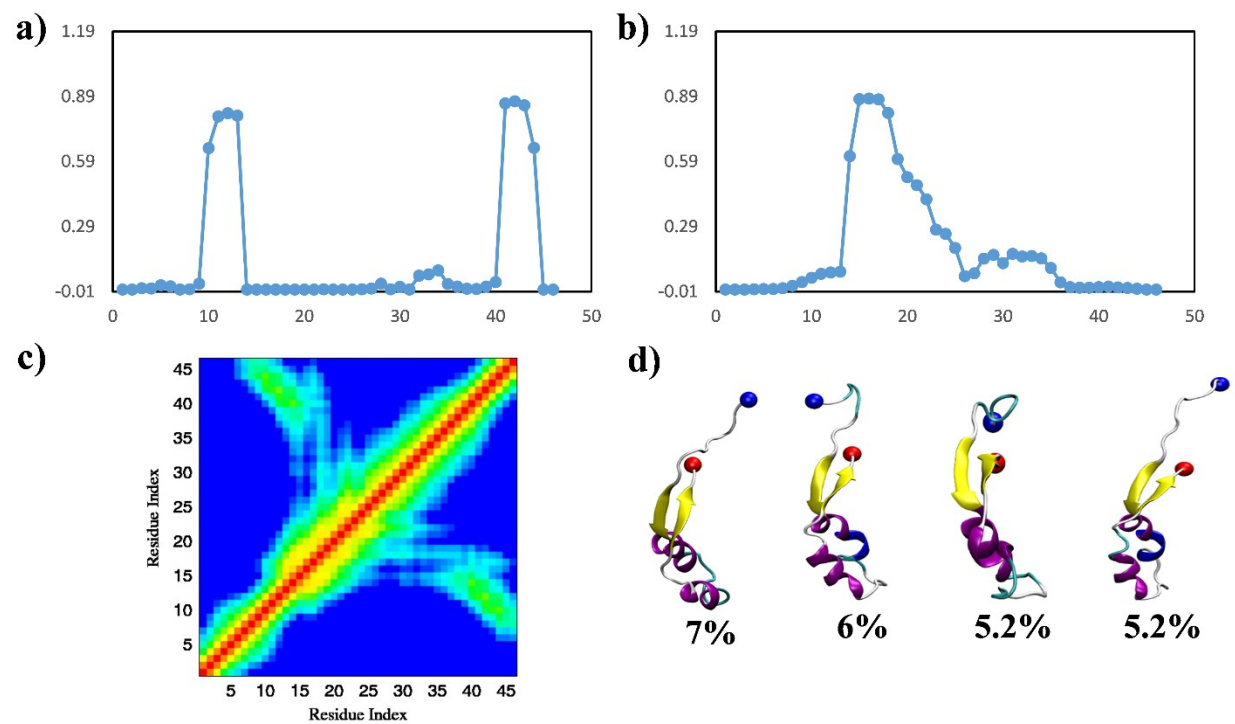


Figure S4 [A]. a) Antiparallel sheet content, b) α -helical content, c) contact map, and d) clustering of P301L $\epsilon\epsilon$ isomer