

Supporting Information

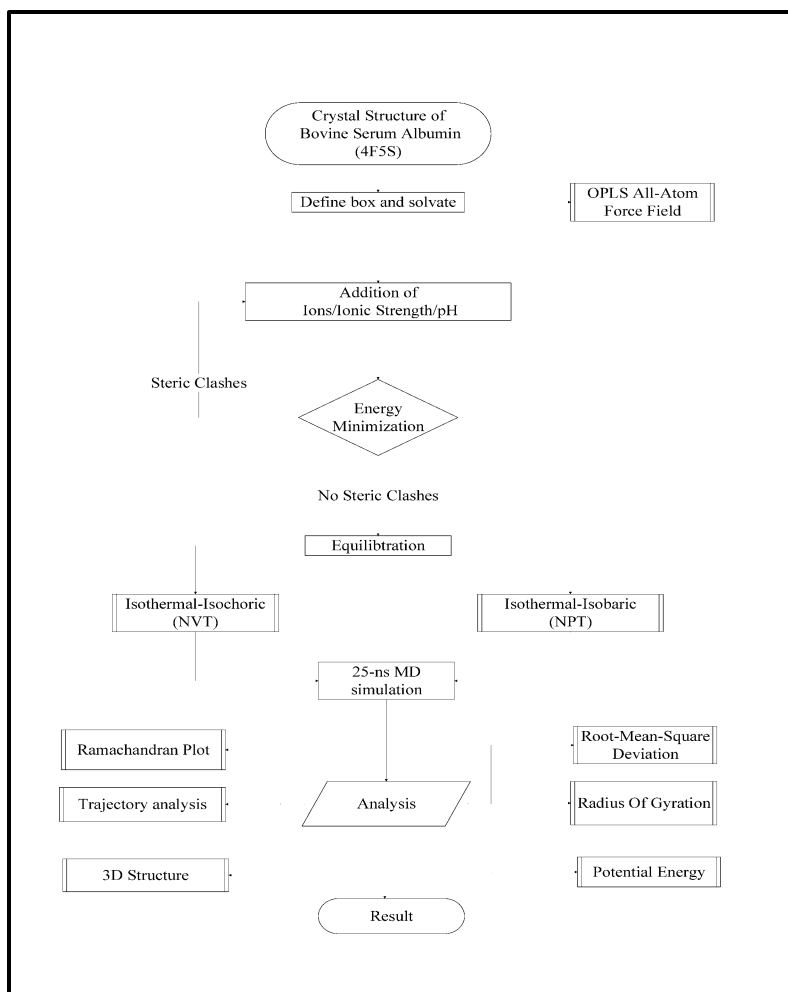


Fig S1: Simulations protocol for the role of protonation state and electrostatic charges on the conformation and dynamics of albumin structure.

Fig S2: 3D structure of BSA (4F5S.pdb)

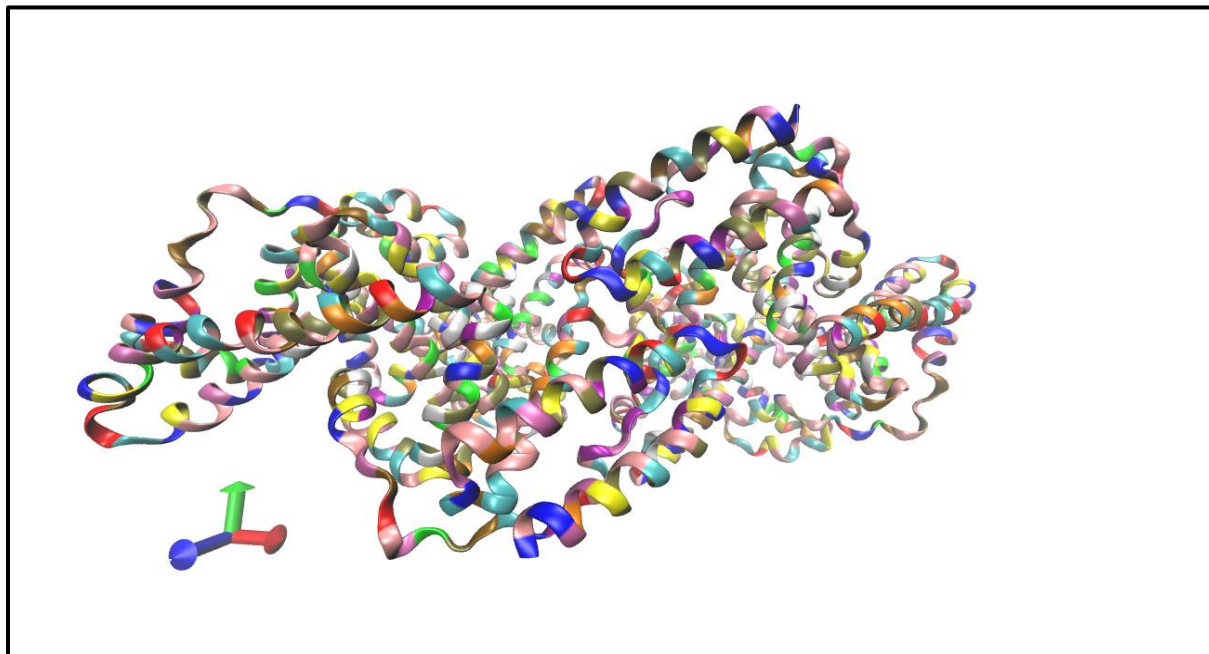


Fig S3: 3D structure of Simulated BSA at 10mM and pH 2

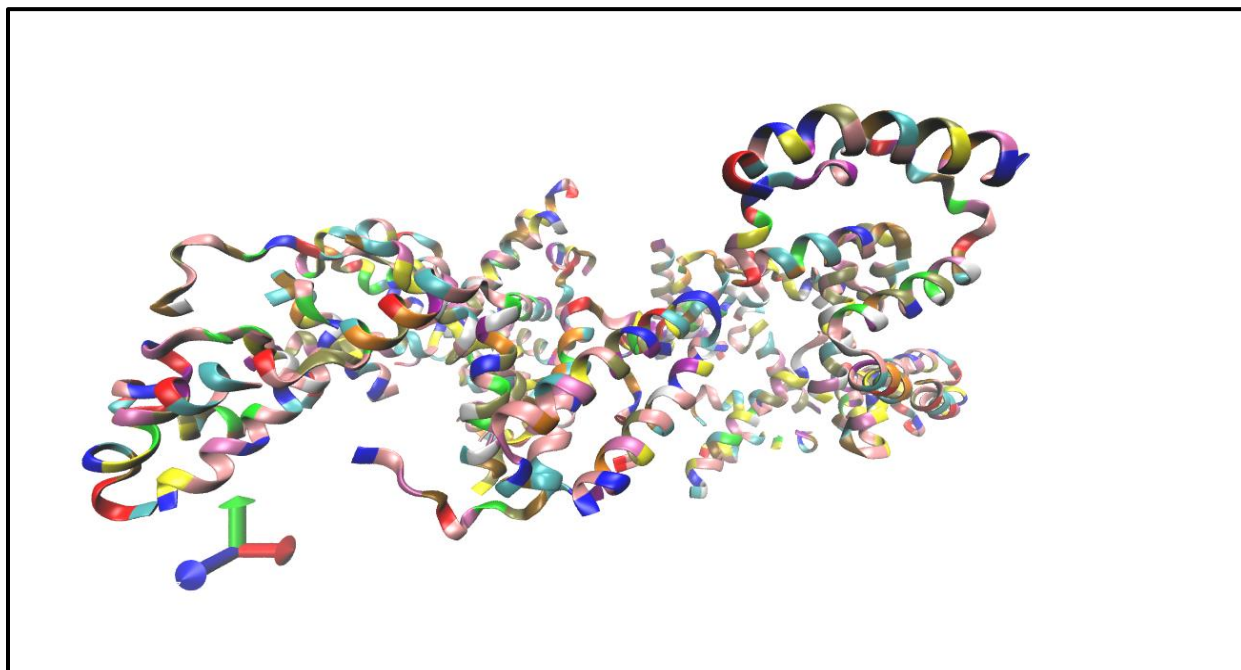


Fig S4: 3D structure of Simulated BSA at 10mM and pH 3.5

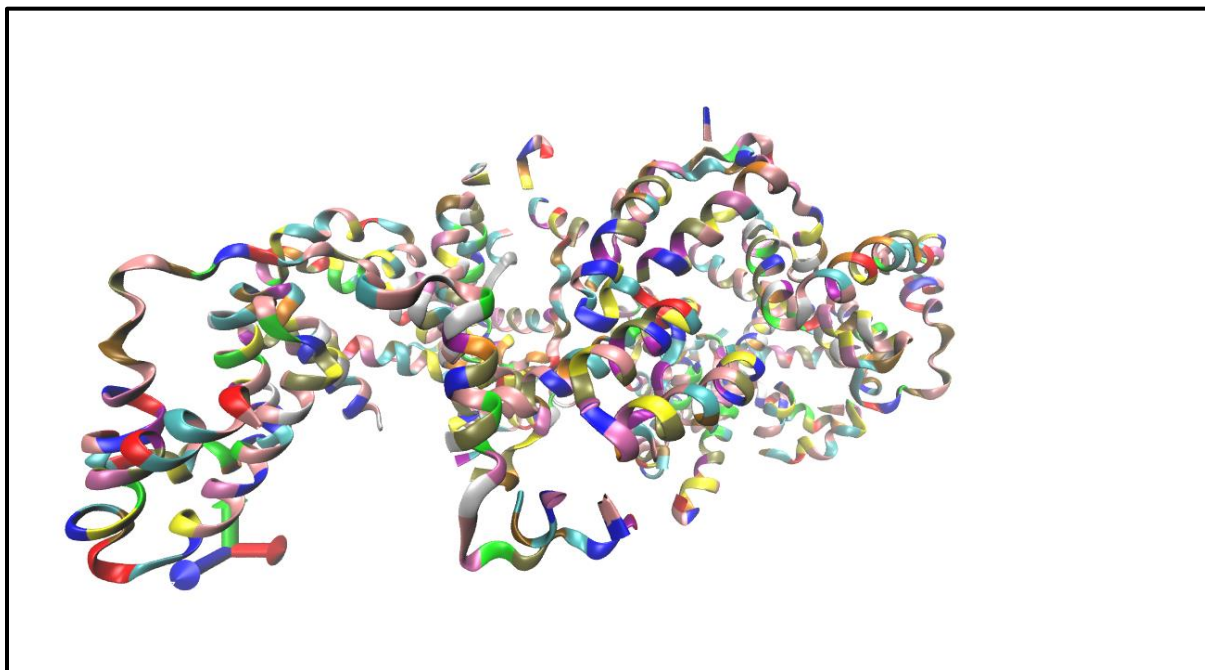


Fig S5: 3D structure of Simulated BSA at 10mM and pH 4.3

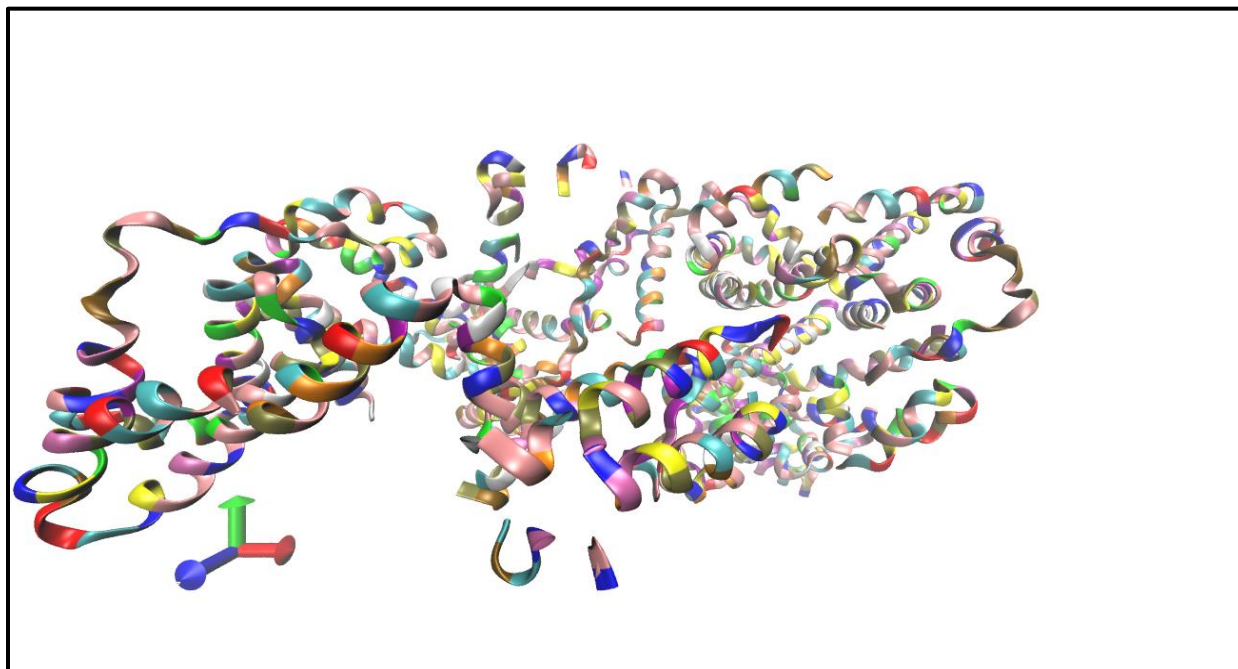


Fig S6: 3D structure of Simulated BSA at 10mM and pH 7.4

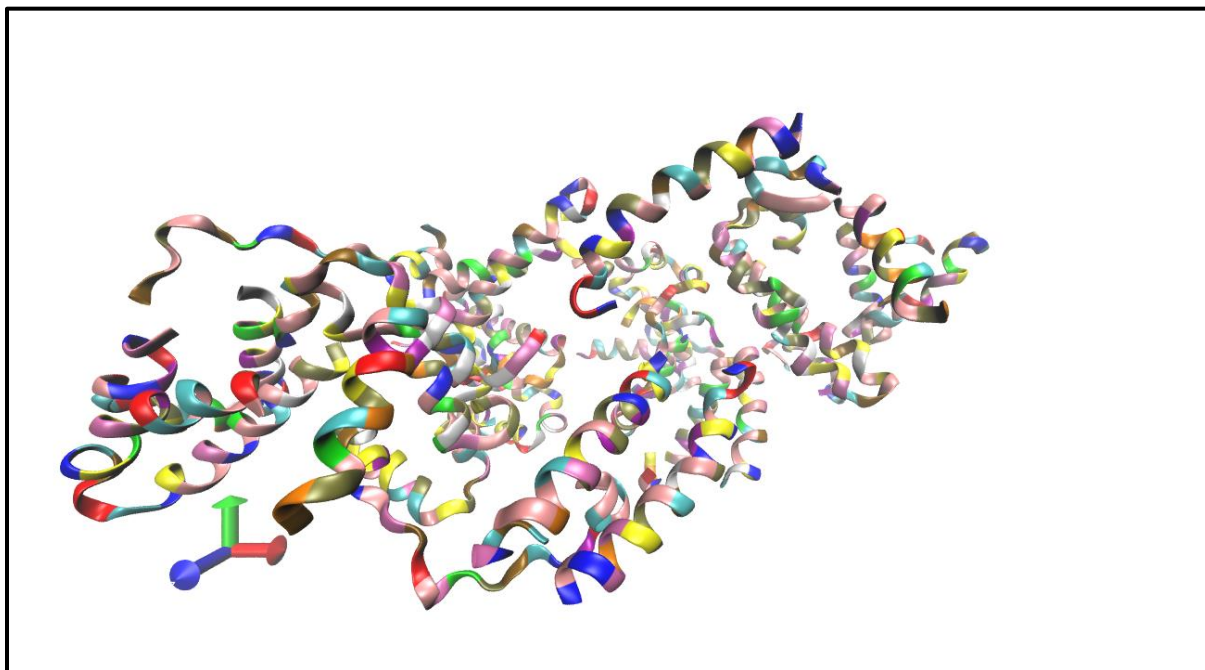


Fig S7: 3D structure of Simulated BSA at 10mM and pH 9.0

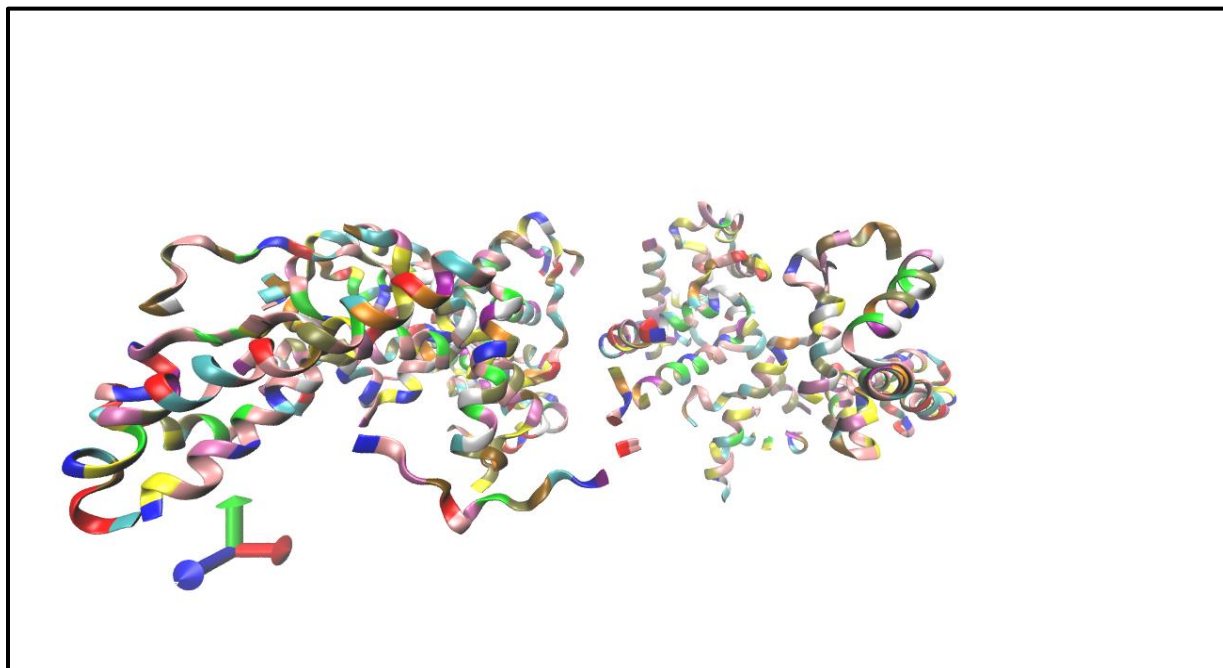


Fig S8: 3D structure of Simulated BSA at 20mM and pH 2.0

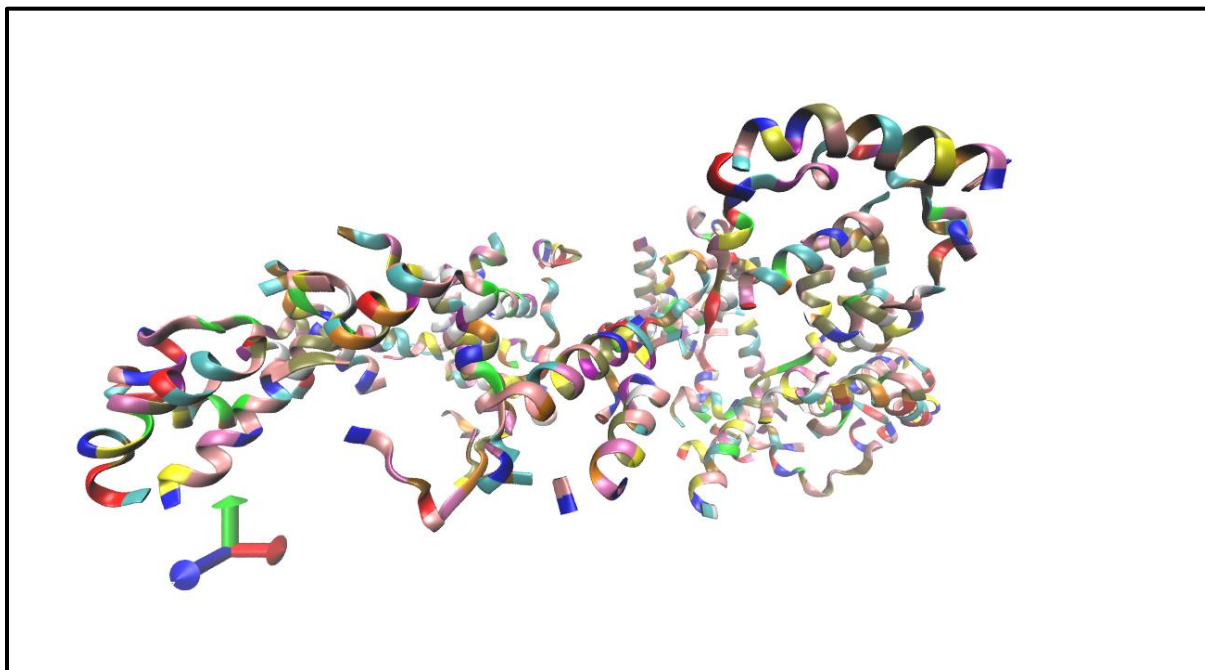


Fig S9: 3D structure of Simulated BSA at 20mM and pH 3.5

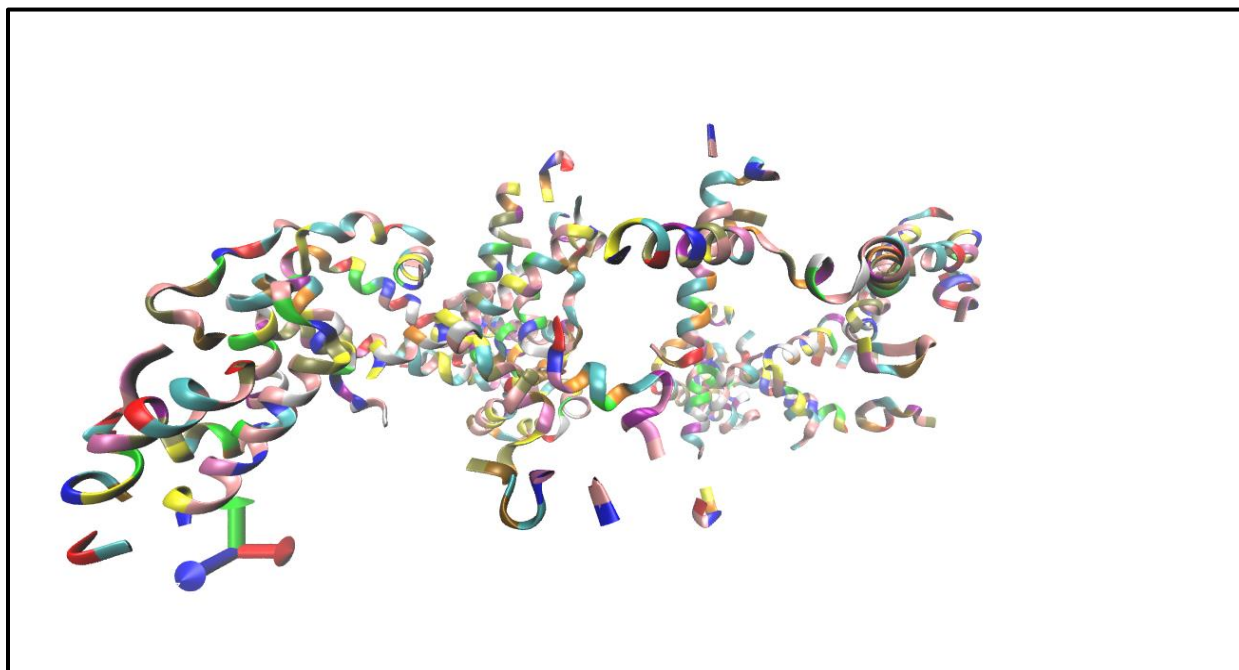


Fig S10: 3D structure of Simulated BSA at 20mM and pH 4.3

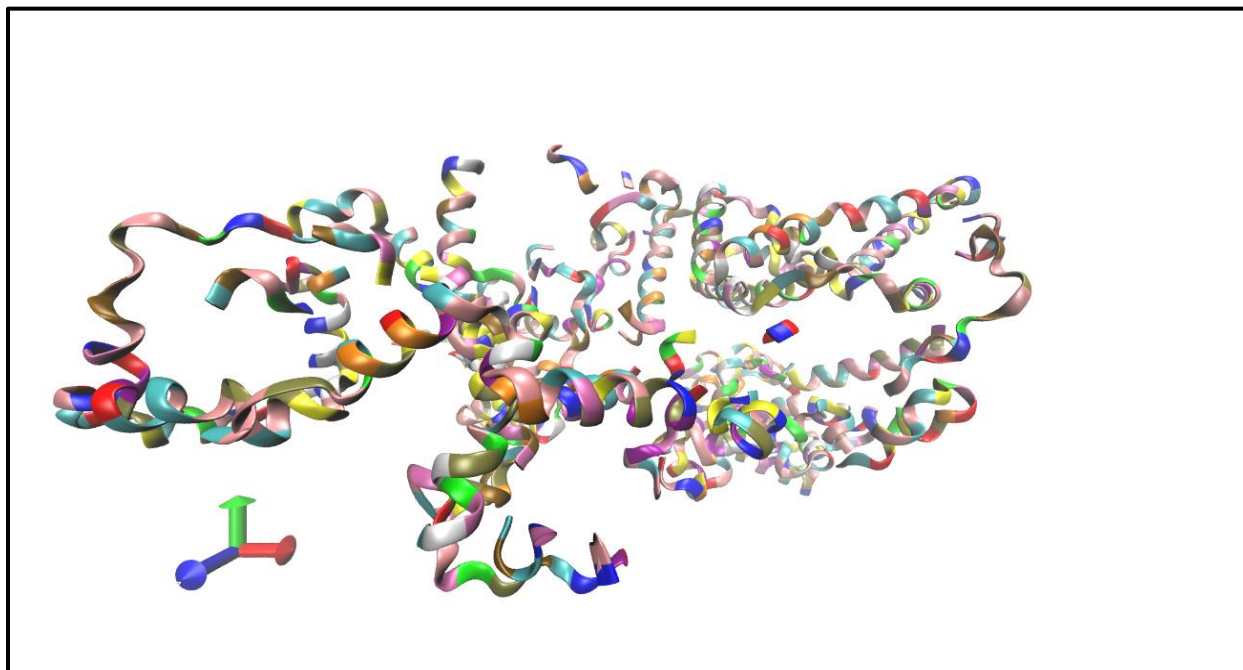


Fig S11: 3D structure of Simulated BSA at 20mM and pH 7.4

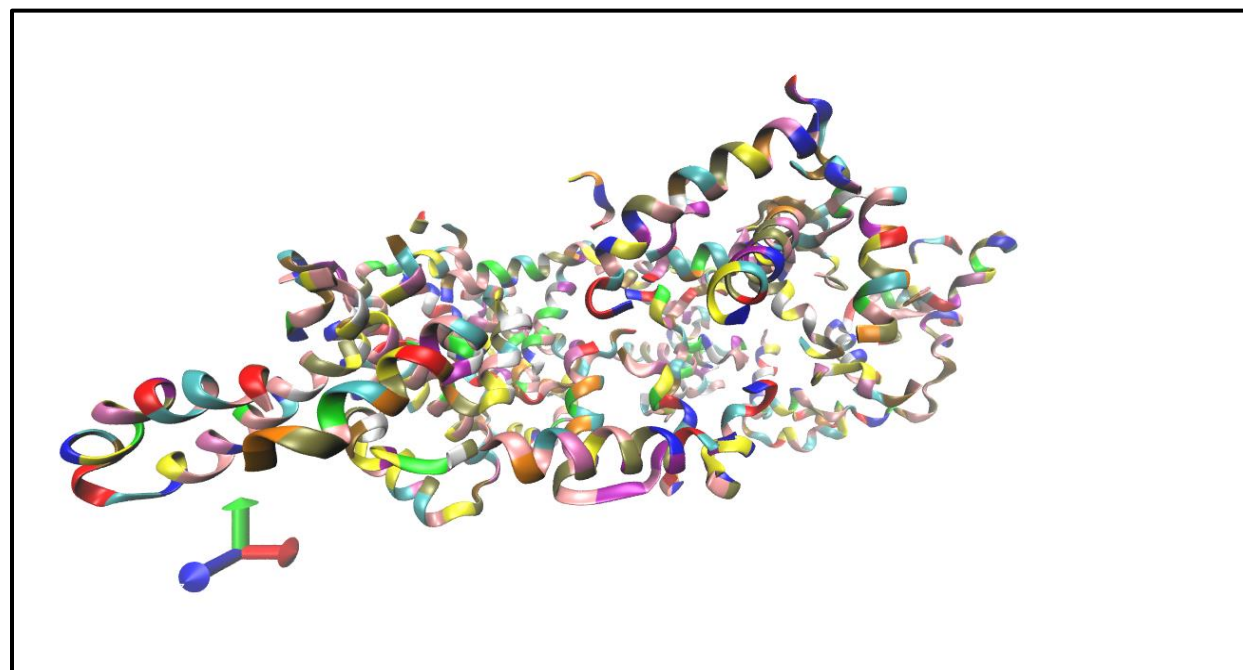


Fig S12: 3D structure of Simulated BSA at 20mM and pH 9.0

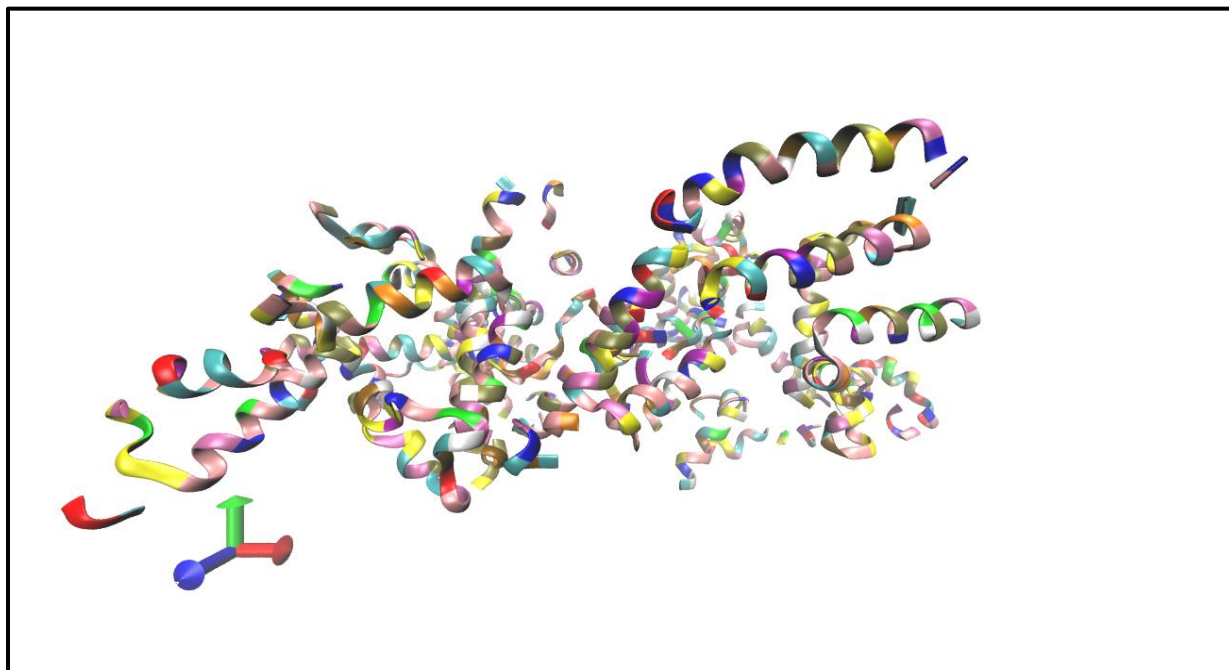


Fig S13: 3D structure of Simulated BSA at 30mM and pH 2.0

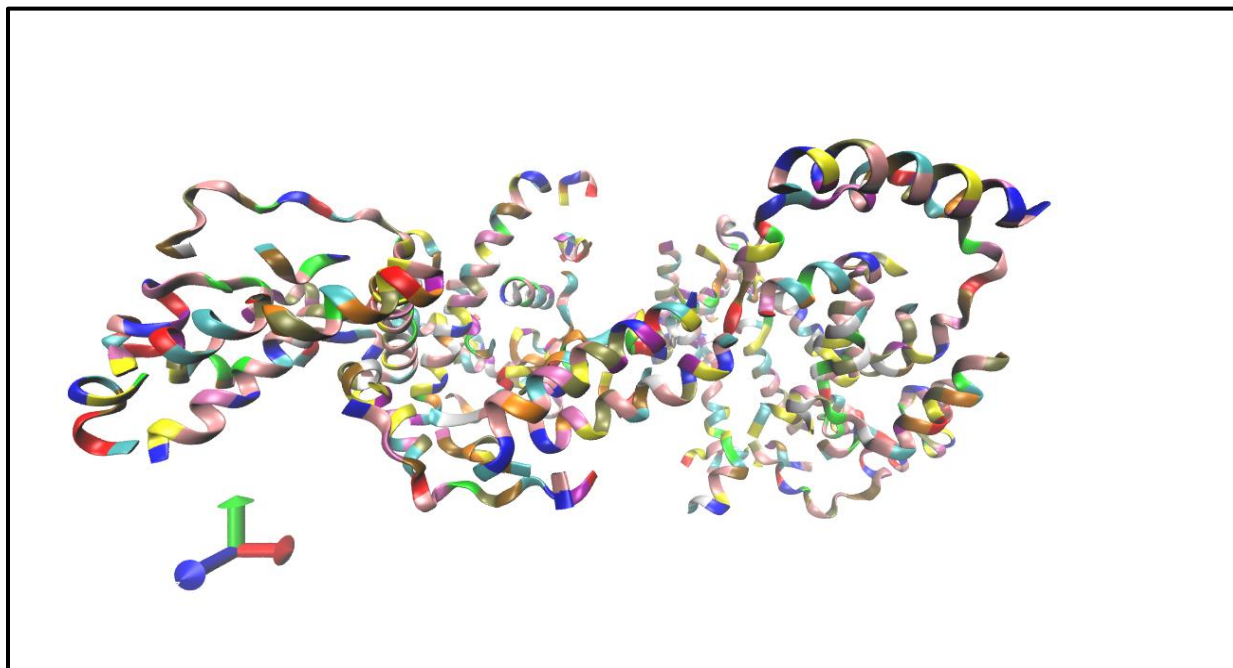


Fig S14: 3D structure of Simulated BSA at 30mM and pH 3.5

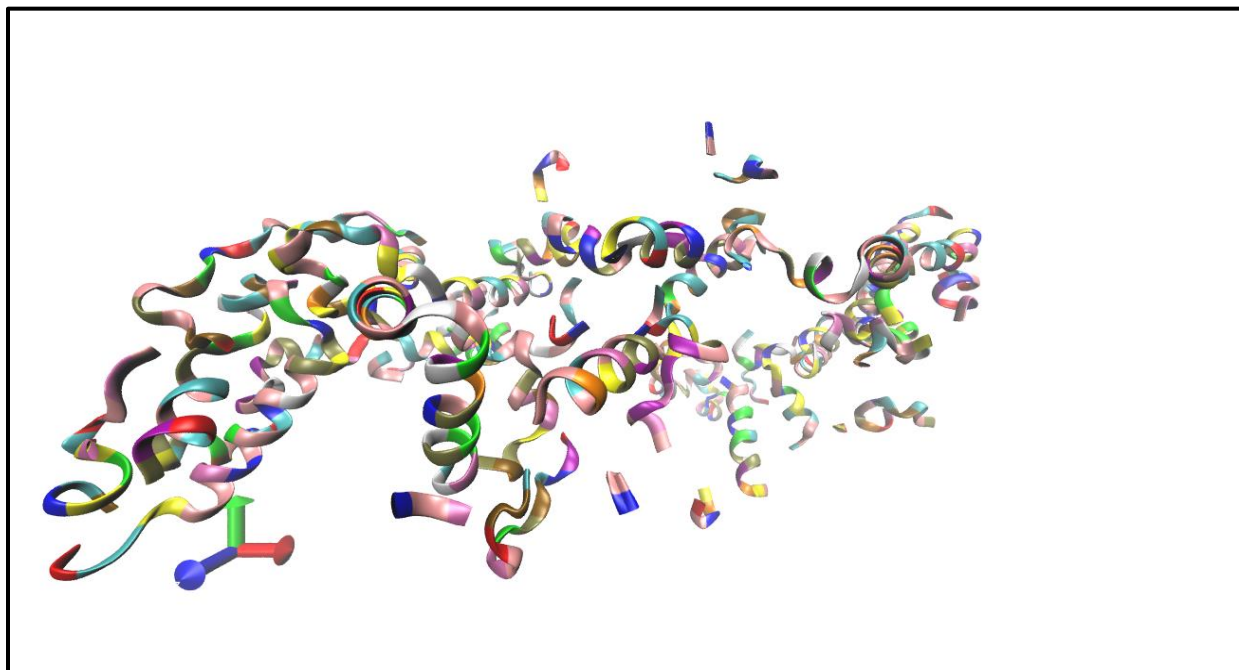


Fig S15: 3D structure of Simulated BSA at 30mM and pH 4.3

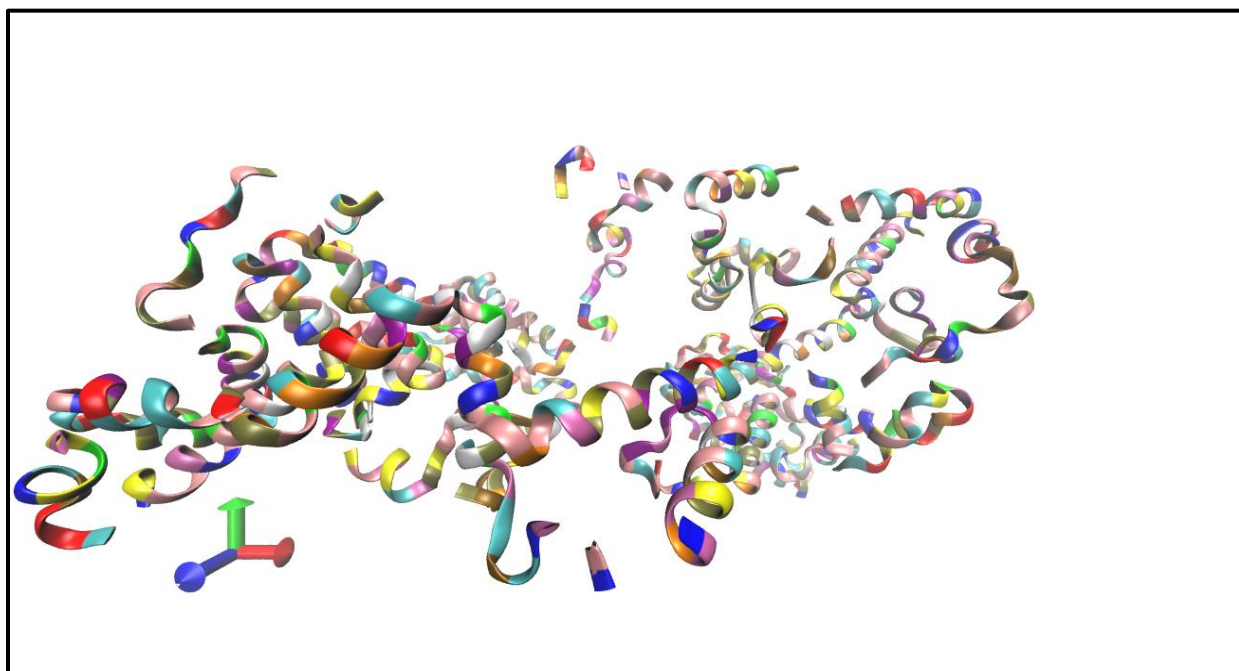


Fig S16: 3D structure of Simulated BSA at 30mM and pH 7.4

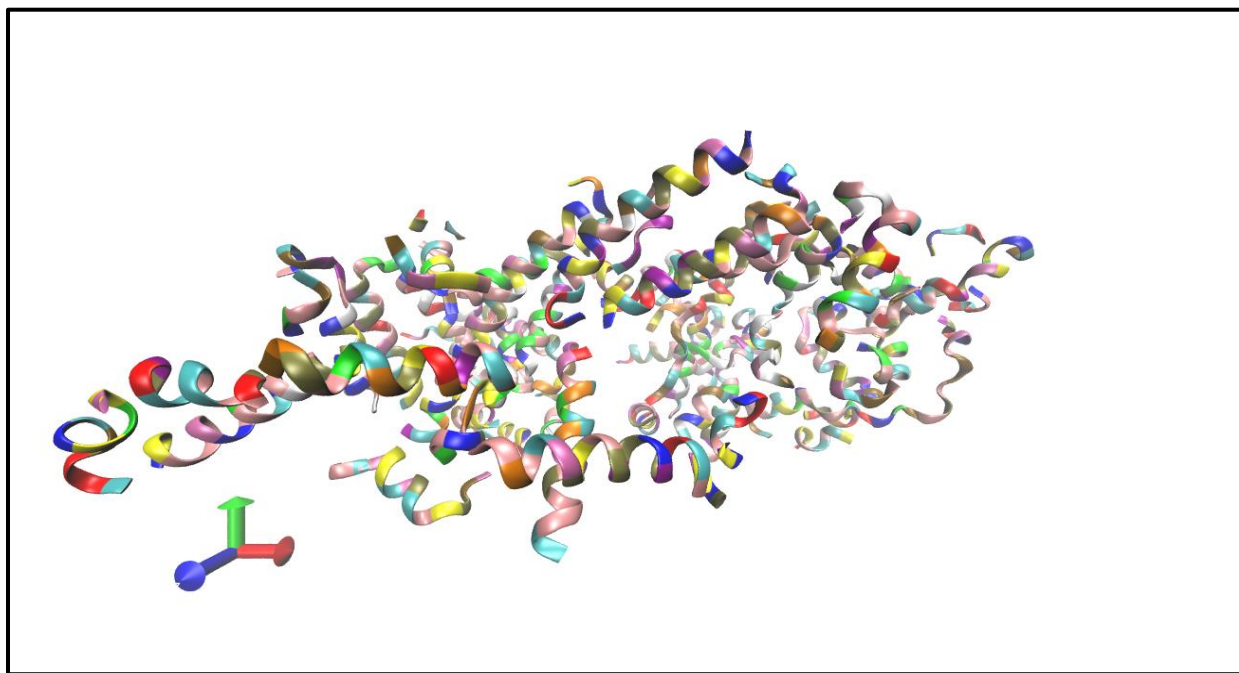


Fig S17: 3D structure of Simulated BSA at 30mM and pH 9.0

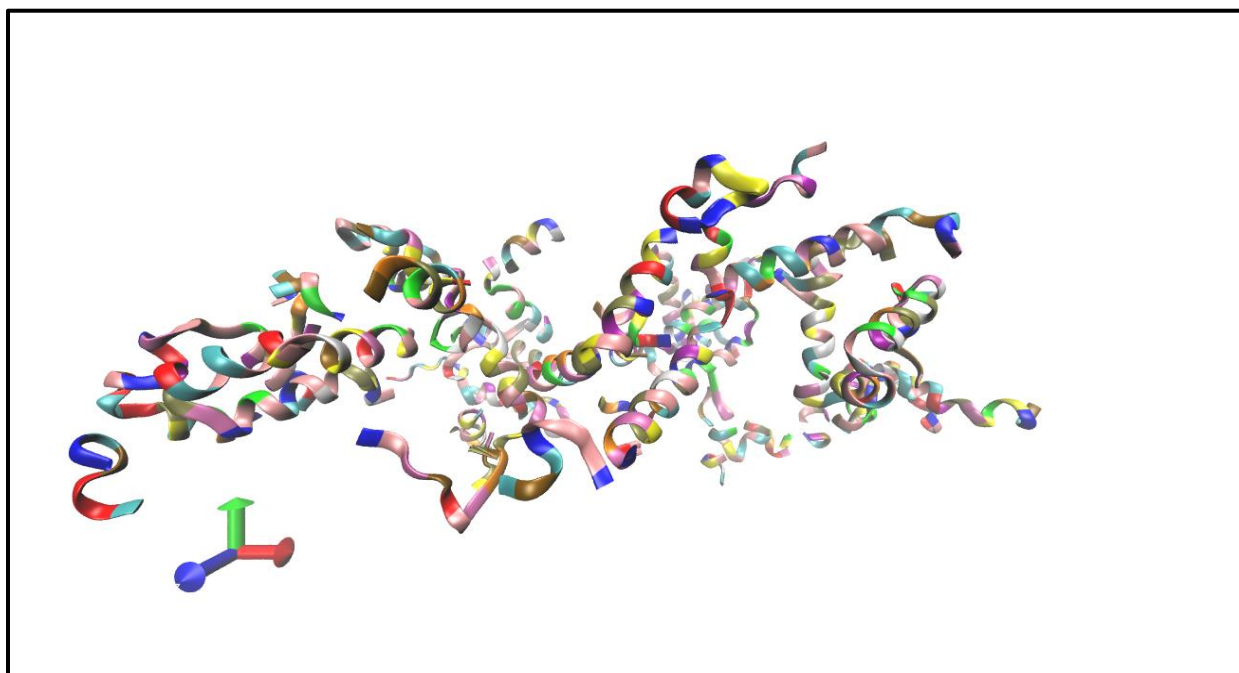


Fig S18: 3D structure of Simulated BSA at 40 mM and pH 2.0

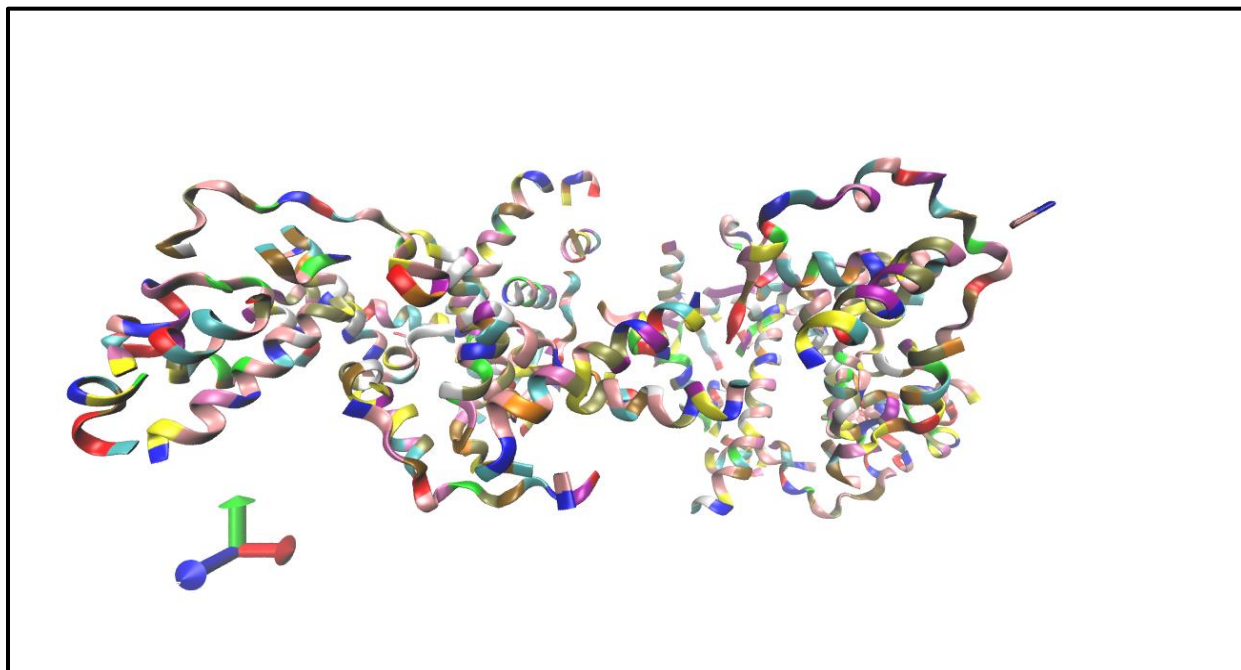


Fig S19: 3D structure of Simulated BSA at 40 mM and pH 3.5

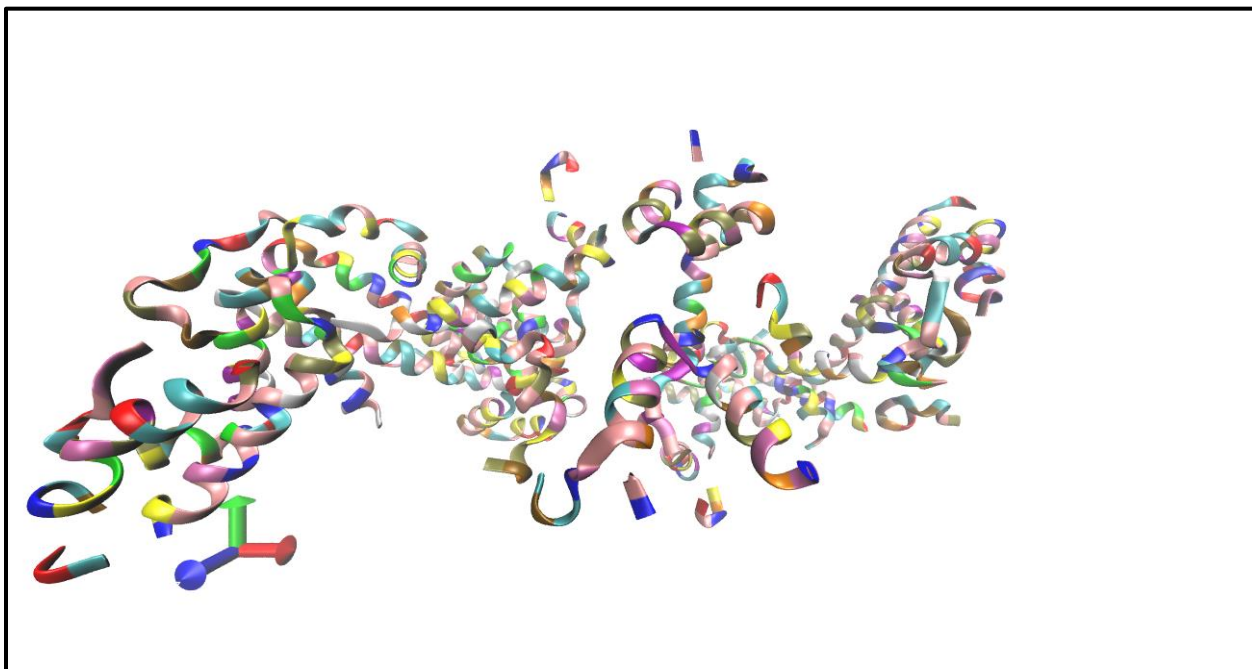


Fig S20: 3D structure of Simulated BSA at 40 mM and pH 4.3

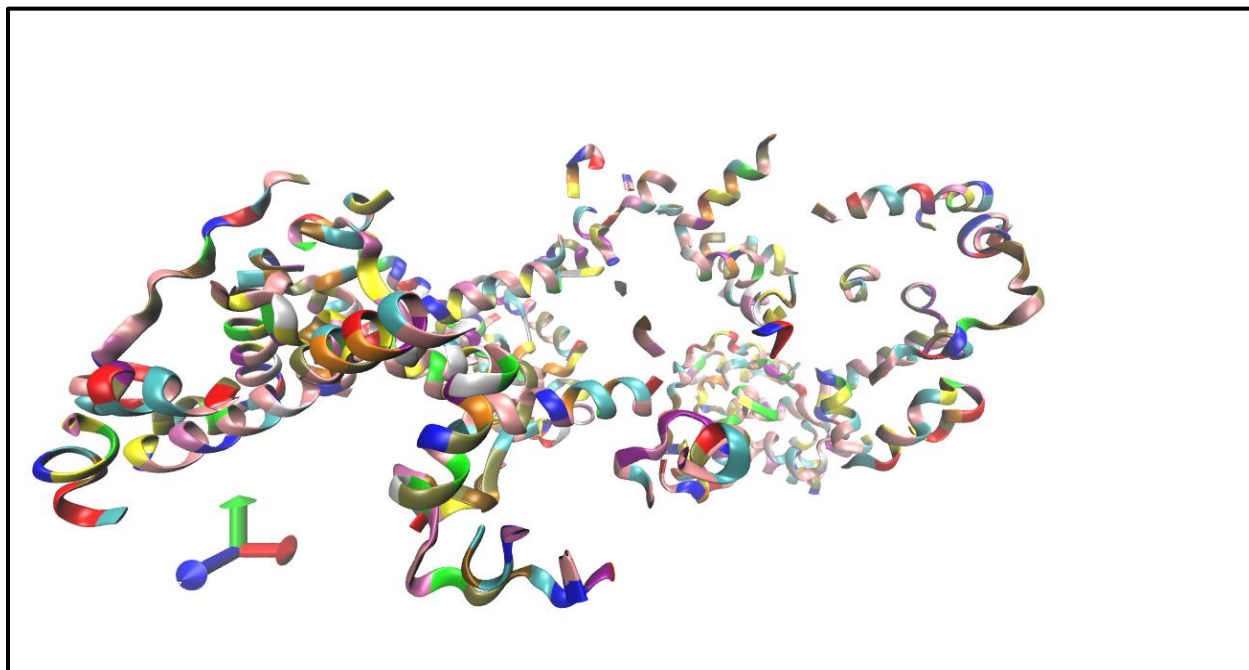


Fig S21: 3D structure of Simulated BSA at 40 mM and pH 7.4

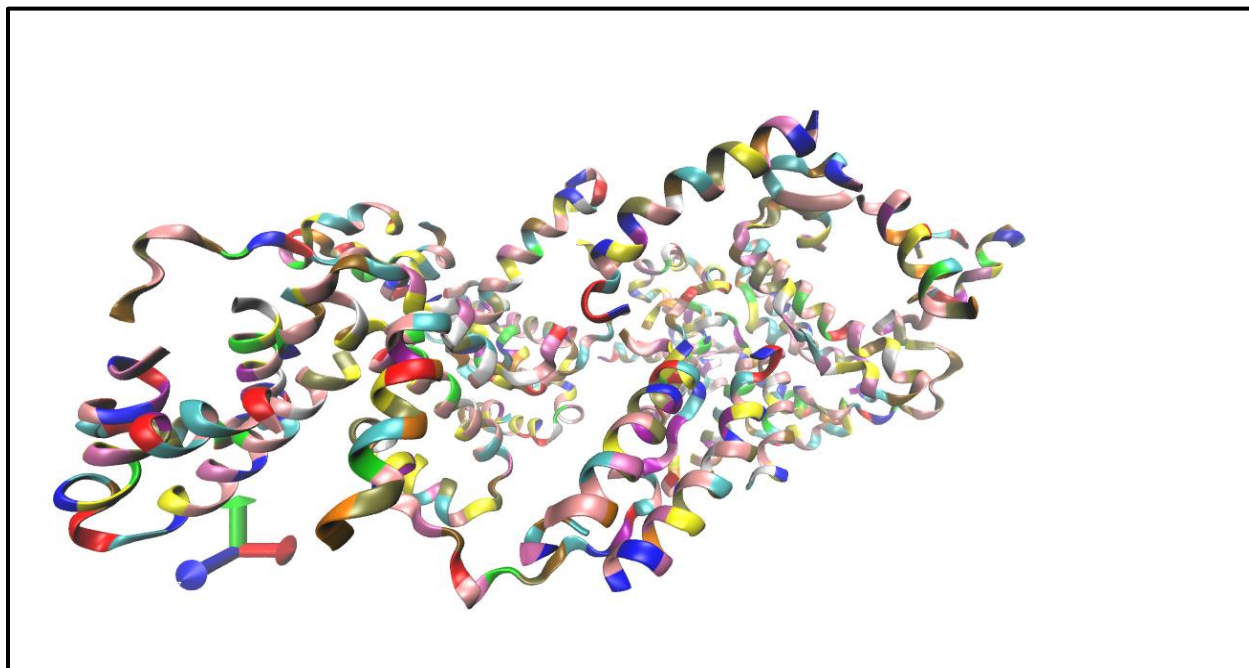


Fig S22: 3D structure of Simulated BSA at 40 mM and pH 9.0

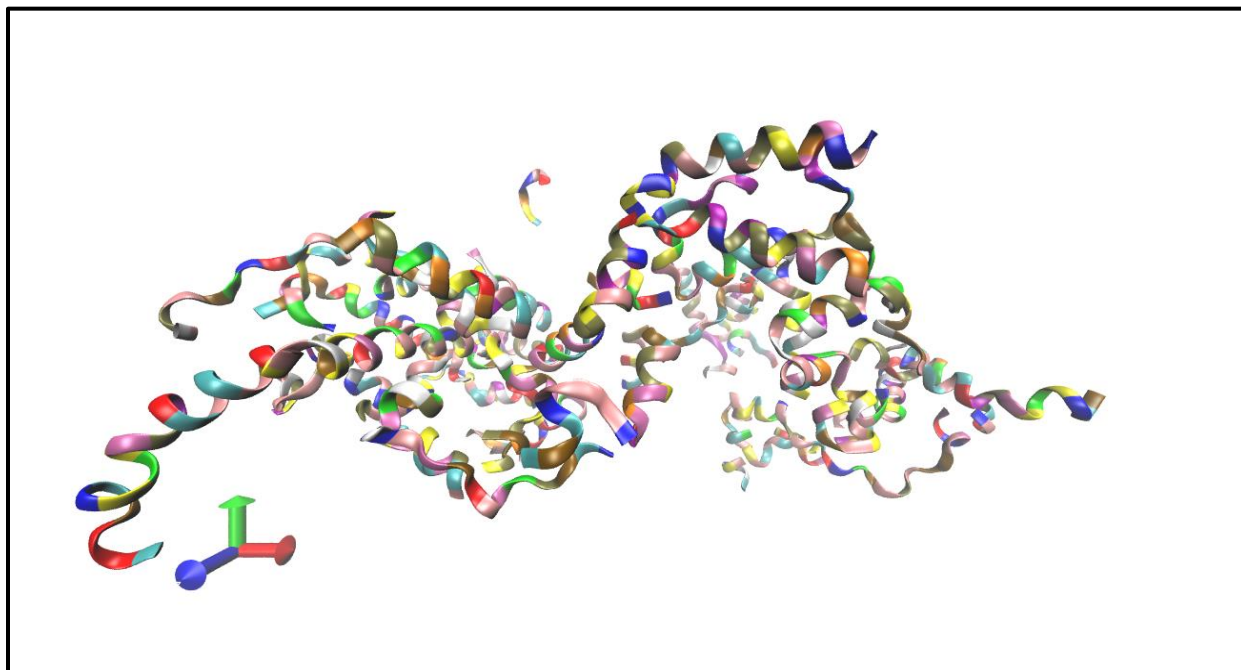


Fig S23: 3D structure of Simulated BSA at 50 mM and pH 2.0

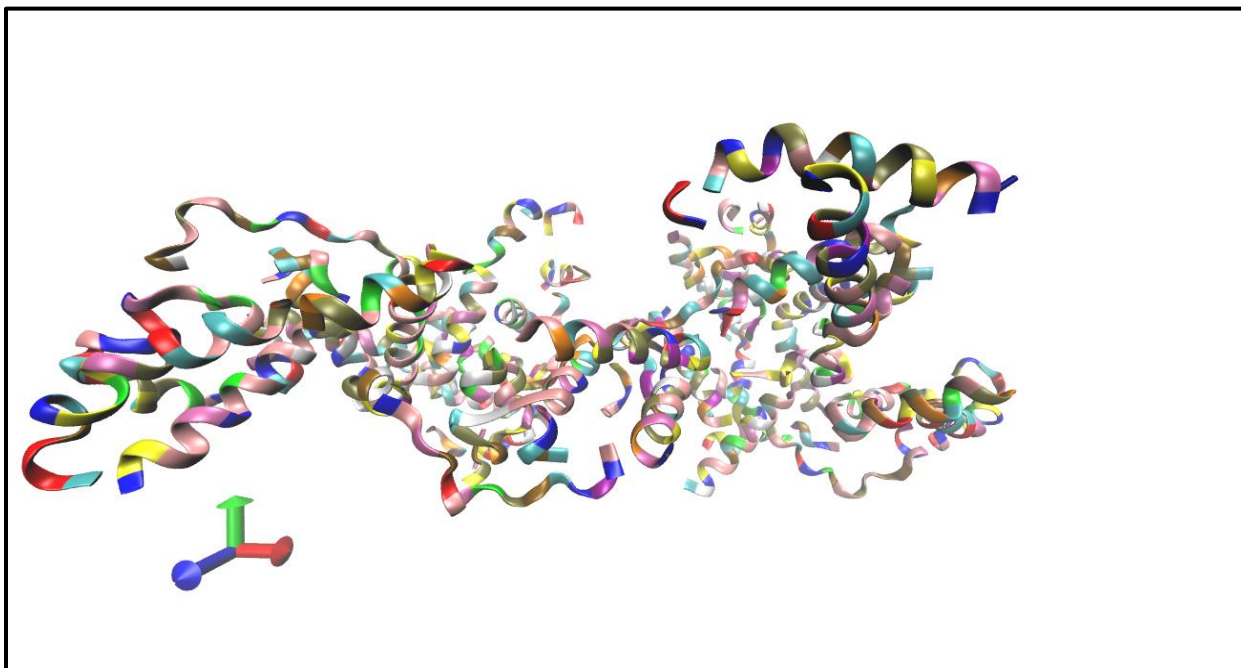


Fig S24: 3D structure of Simulated BSA at 50 mM and pH 3.5

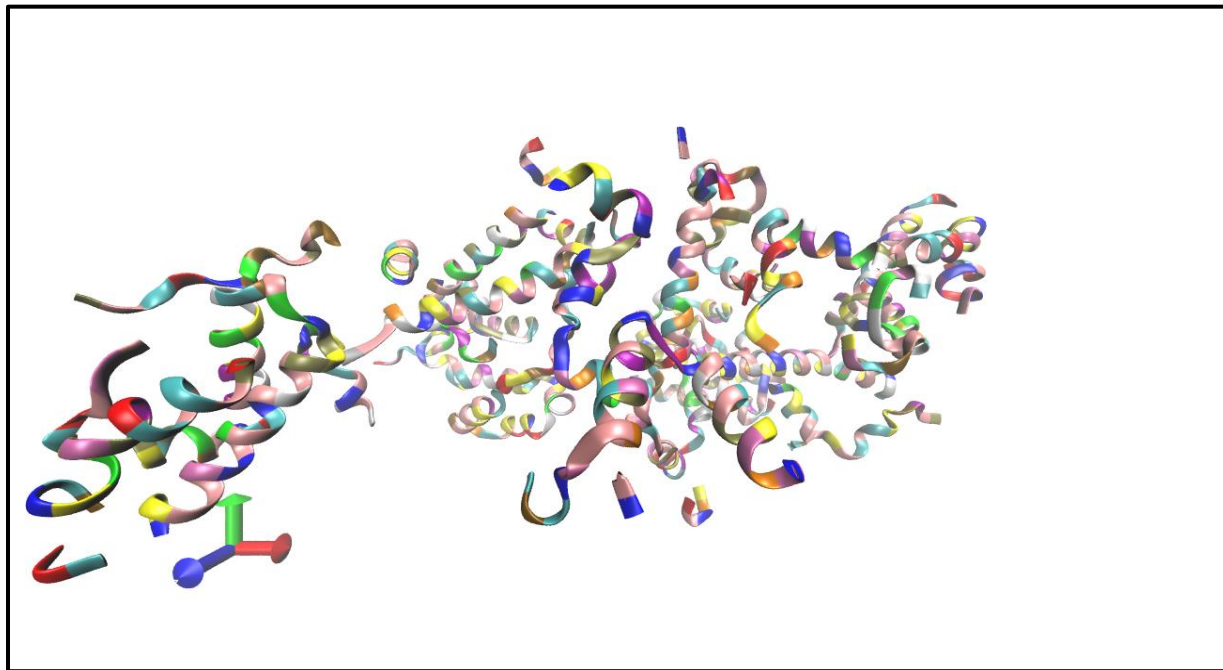


Fig S25: 3D structure of Simulated BSA at 50 mM and pH 4.3

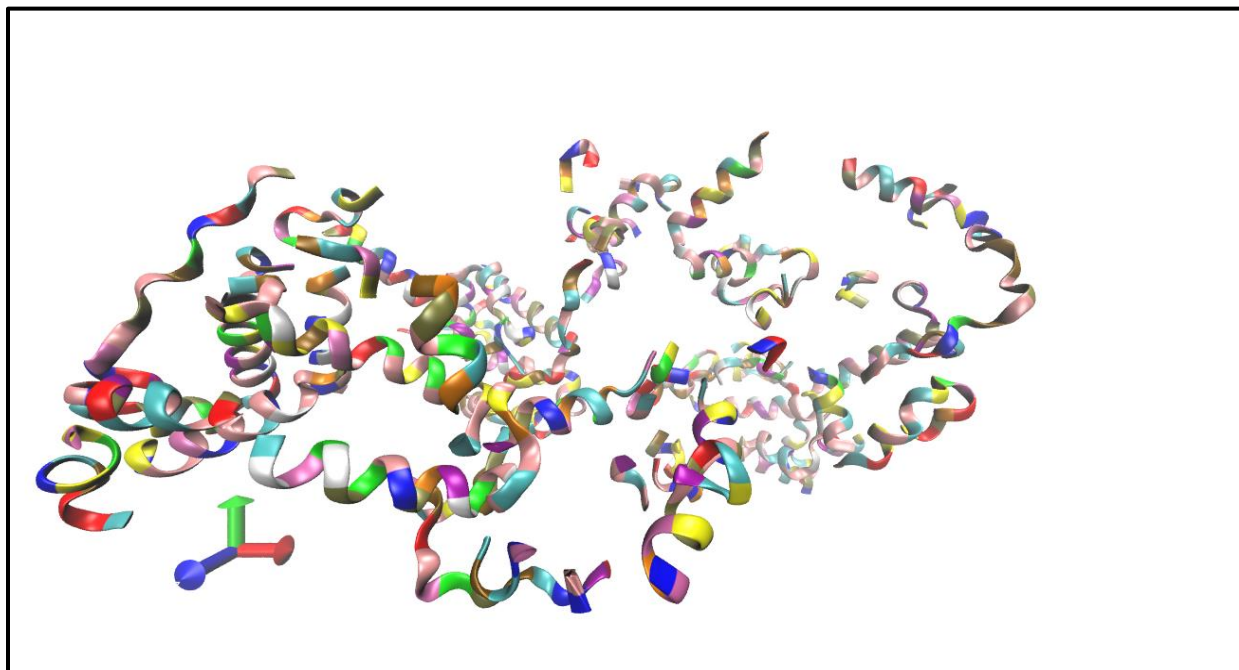


Fig S26: 3D structure of Simulated BSA at 50 mM and pH 7.4

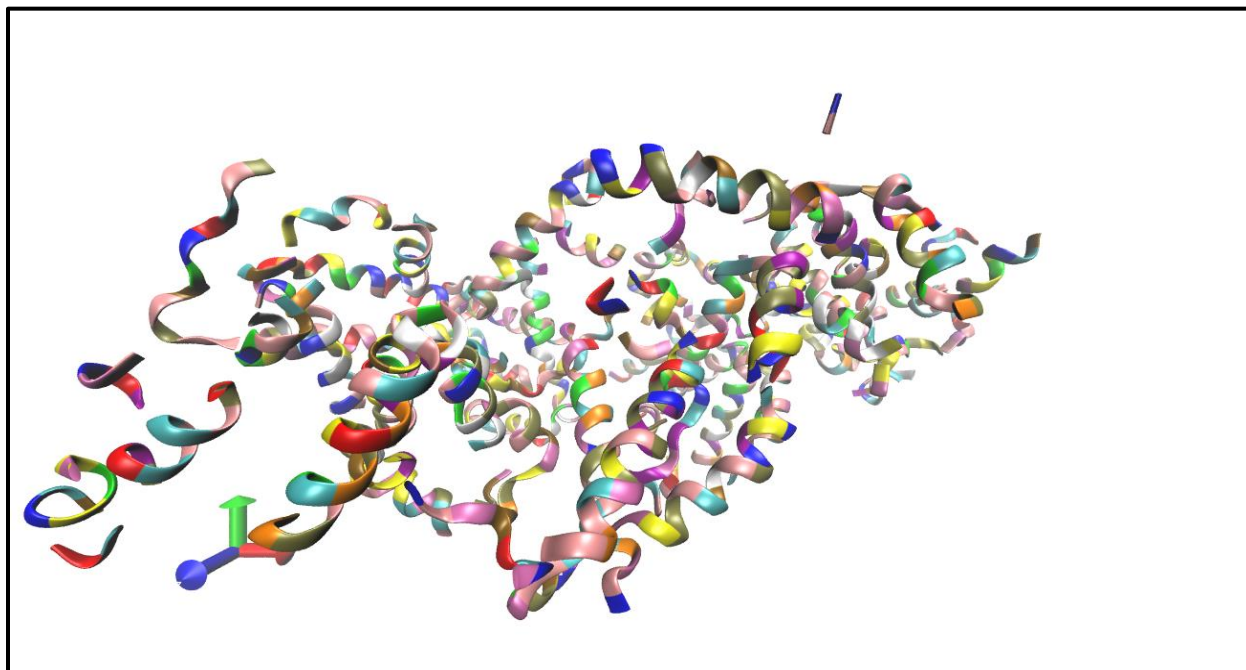


Fig S27: 3D structure of Simulated BSA at 50 mM and pH 9.0

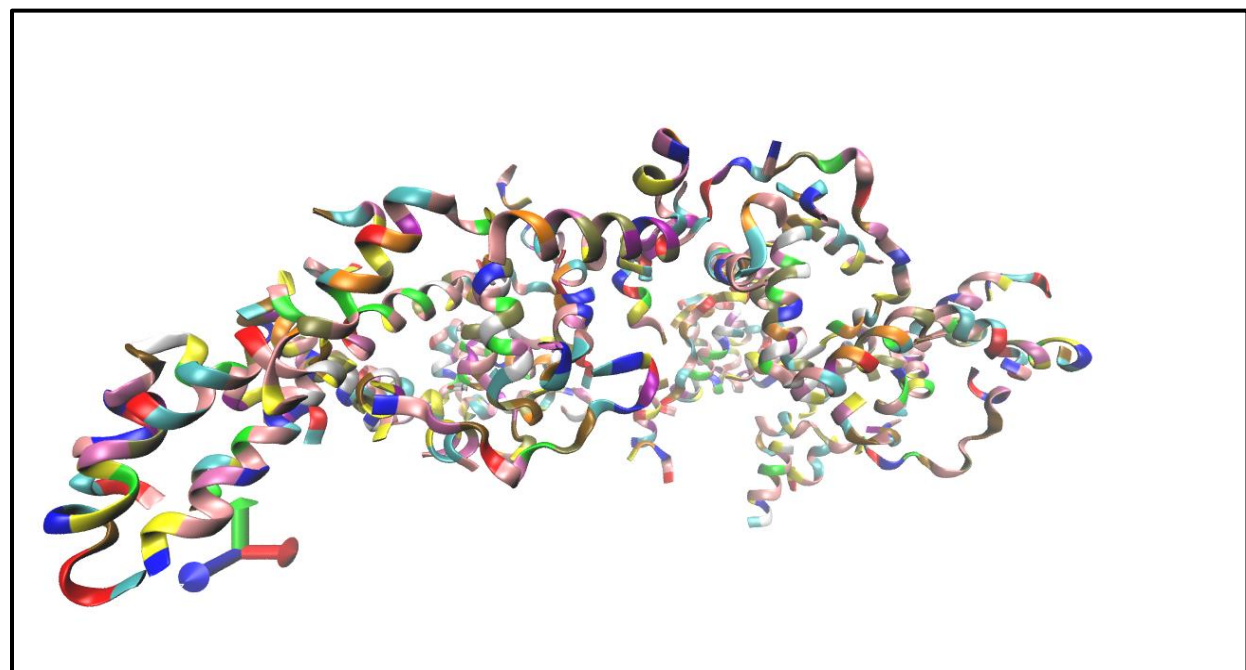


Fig S28: Ramachandran Plot of Simulated BSA at 10 mM and pH 2.0

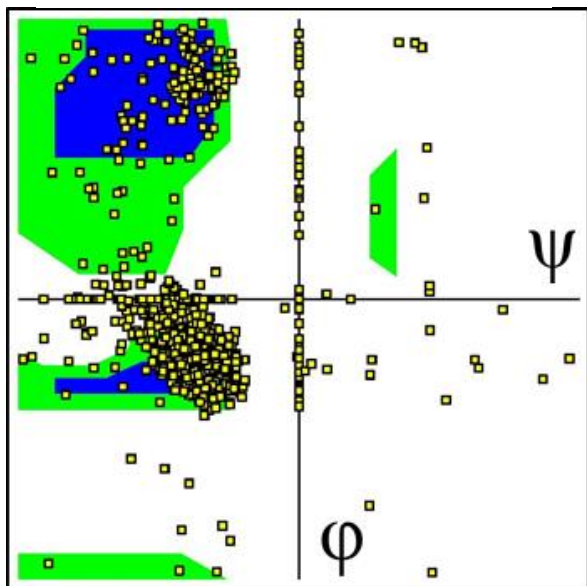


Fig S29: Ramachandran Plot of Simulated BSA at 10 mM and pH 3.5

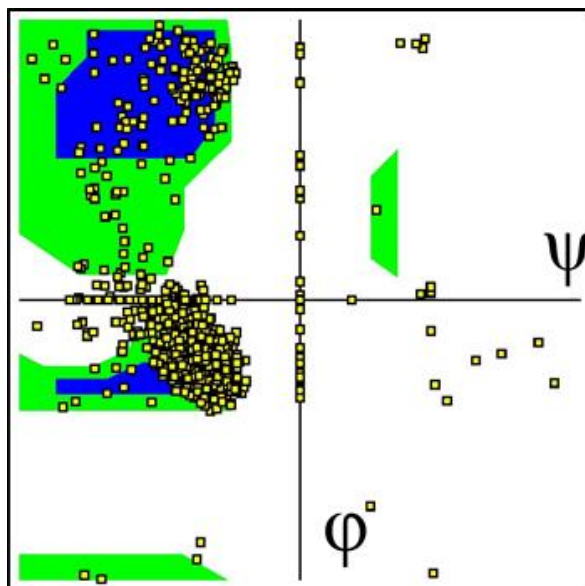


Fig S30: Ramachandran Plot of Simulated BSA at 10 mM and pH 4.3

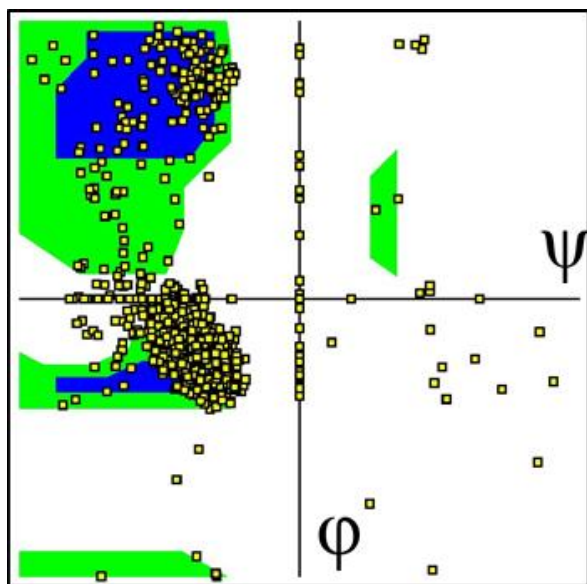


Fig S31: Ramachandran Plot of Simulated BSA at 10 mM and pH 7.4

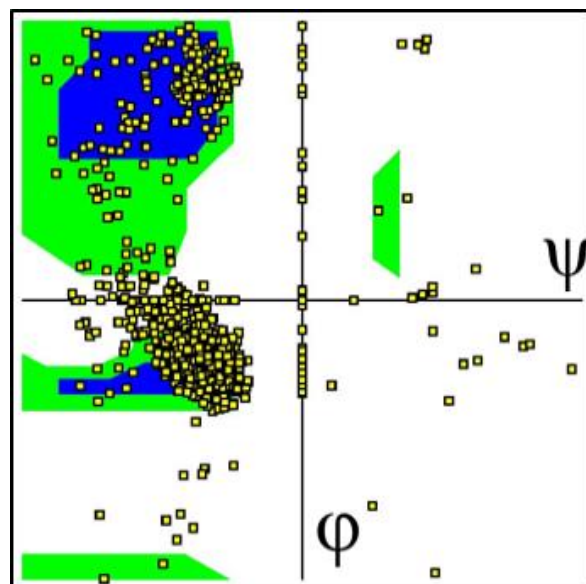


Fig S32: Ramachandran Plot of Simulated BSA at 10 mM and pH 9.0

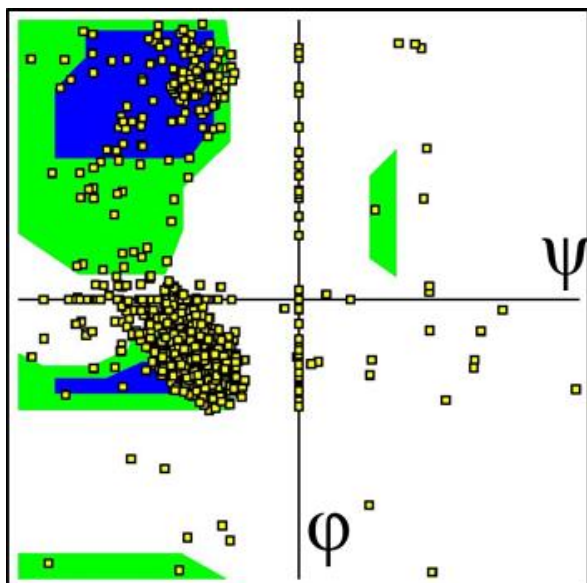


Fig S33: Ramachandran Plot of Simulated BSA at 20 mM and pH 2.0

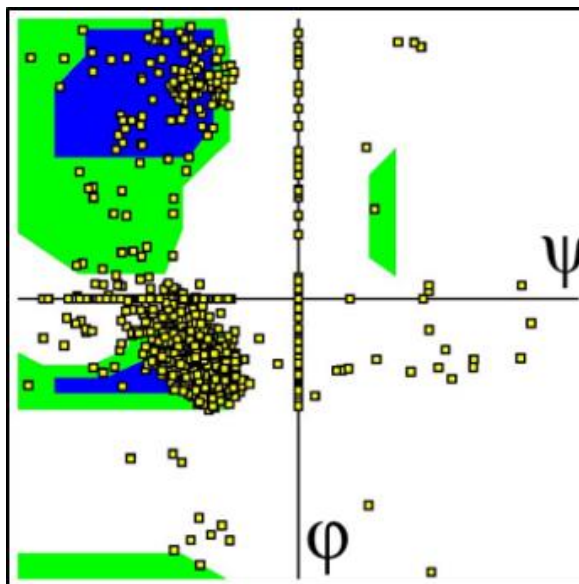


Fig S34: Ramachandran Plot of Simulated BSA at 20 mM and pH 3.5

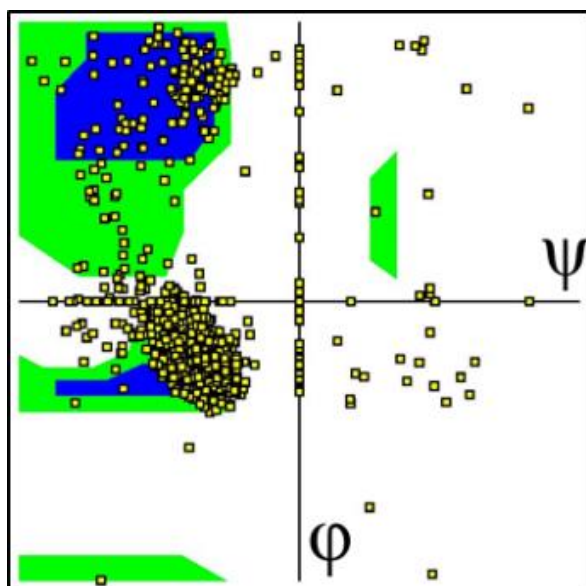


Fig S35: Ramachandran Plot of Simulated BSA at 20 mM and pH 4.3

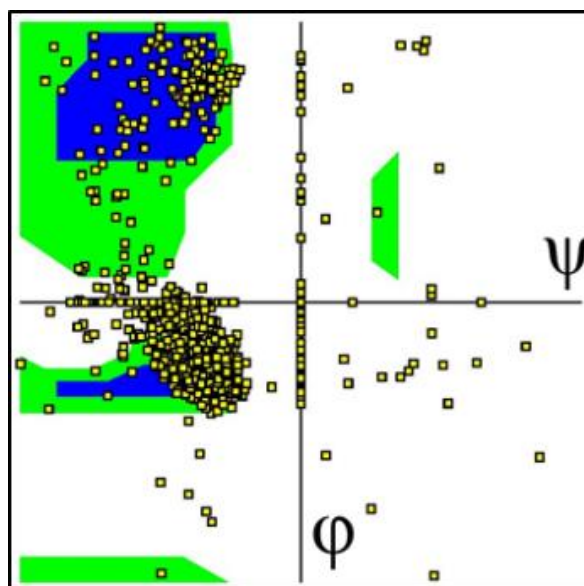


Fig S36: Ramachandran Plot of Simulated BSA at 20 mM and pH 7.4

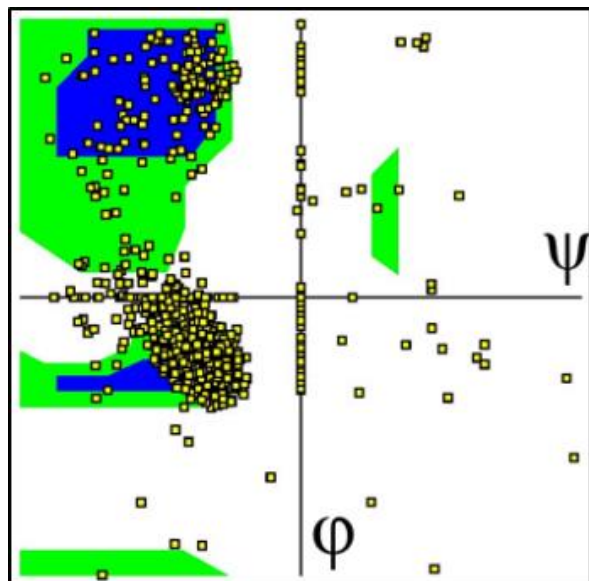


Fig S37: Ramachandran Plot of Simulated BSA at 20 mM and pH 9.0

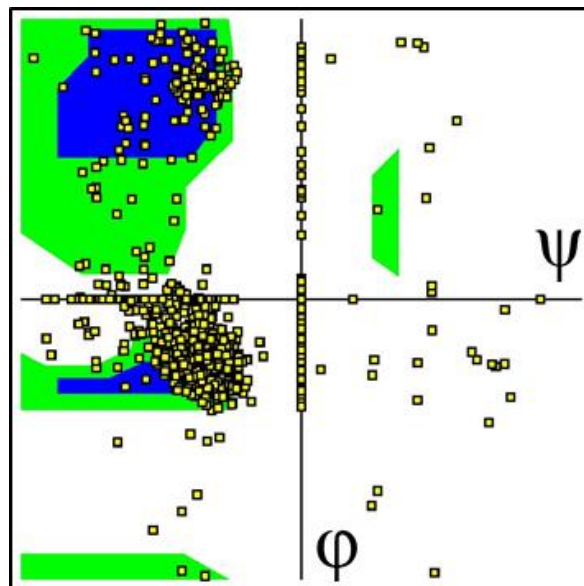


Fig S38: Ramachandran Plot of Simulated BSA at 30 mM and pH 2.0

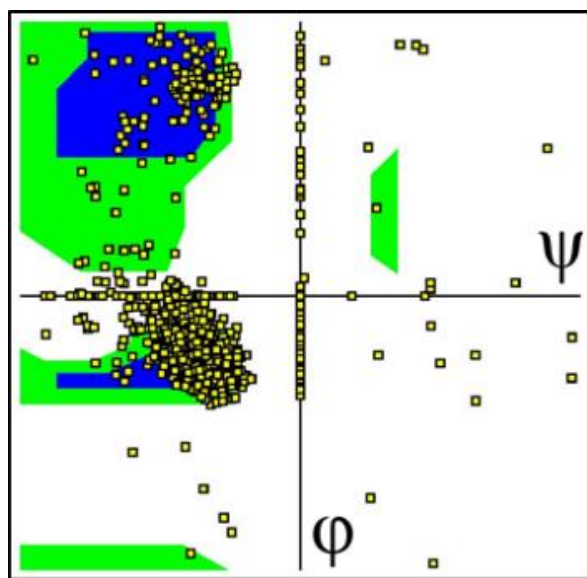


Fig S39: Ramachandran Plot of Simulated BSA at 30 mM and pH 3.5

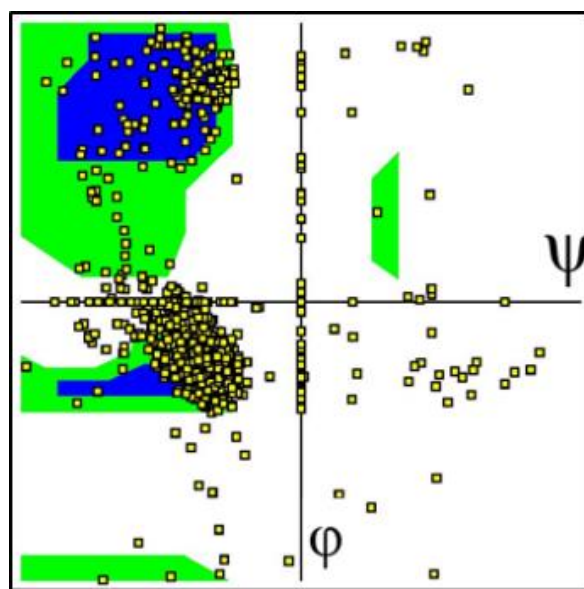


Fig S40: Ramachandran Plot of Simulated BSA at 30 mM and pH 4.3

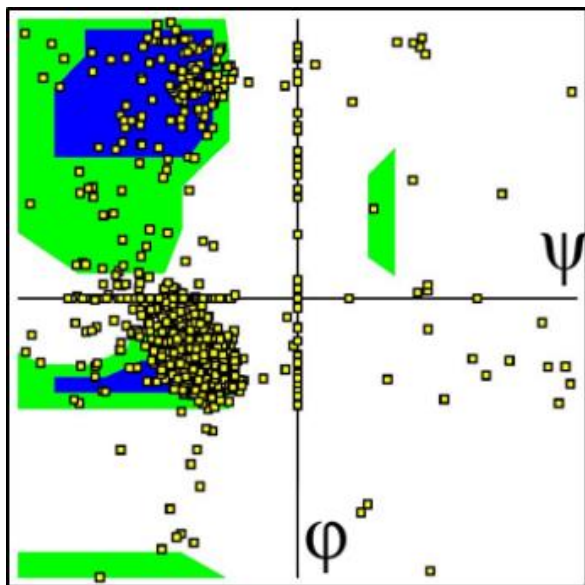


Fig S41: Ramachandran Plot of Simulated BSA at 30 mM and pH 7.4

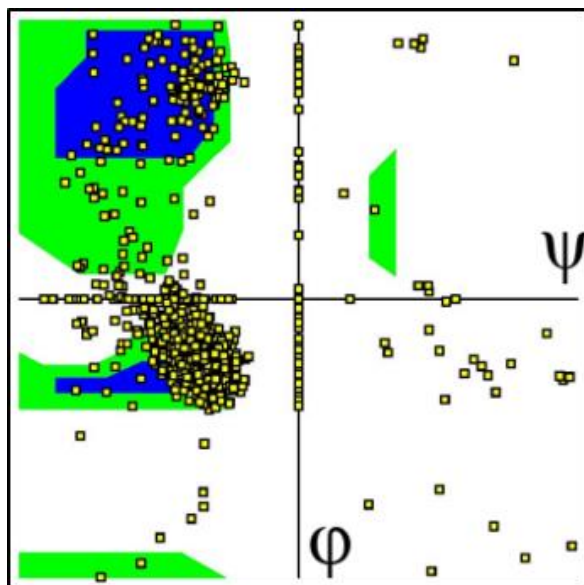


Fig S42: Ramachandran Plot of Simulated BSA at 30 mM and pH 9.0

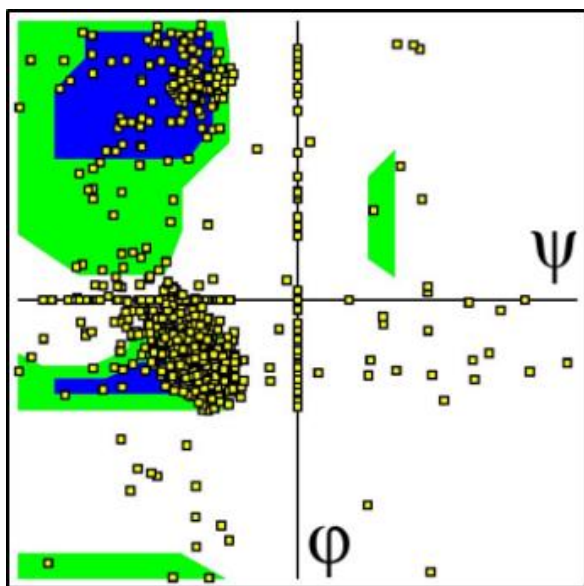


Fig S43: Ramachandran Plot of Simulated BSA at 40 mM and pH 2.0

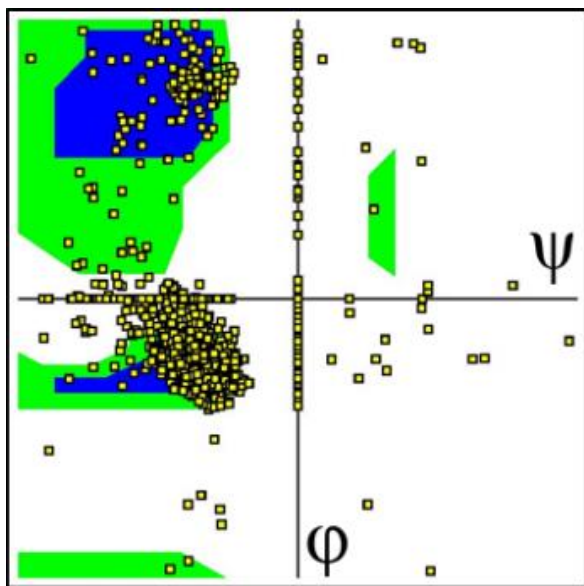


Fig S44: Ramachandran Plot of Simulated BSA at 40 mM and pH 3.5

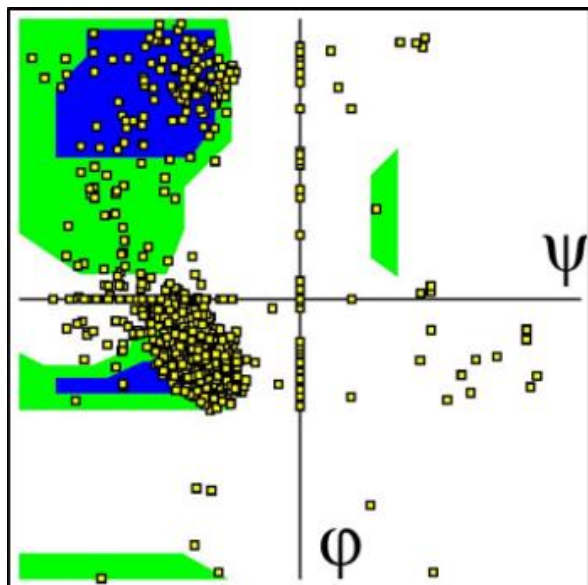


Fig S45: Ramachandran Plot of Simulated BSA at 40 mM and pH 4.3

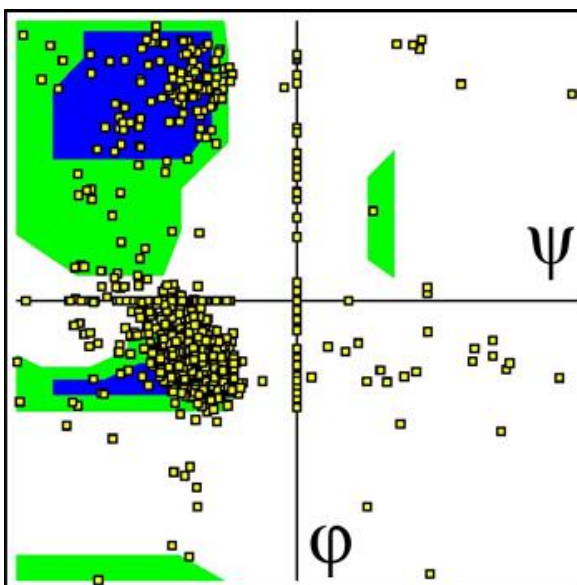


Fig S46: Ramachandran Plot of Simulated BSA at 40 mM and pH 7.4

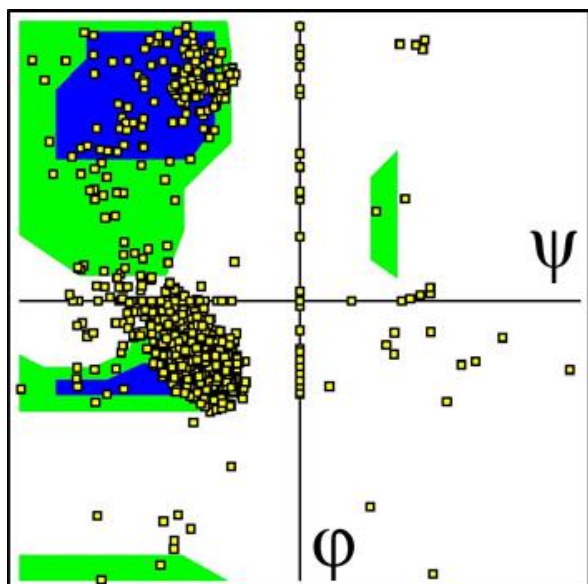


Fig S47: Ramachandran Plot of Simulated BSA at 40 mM and pH 9.0

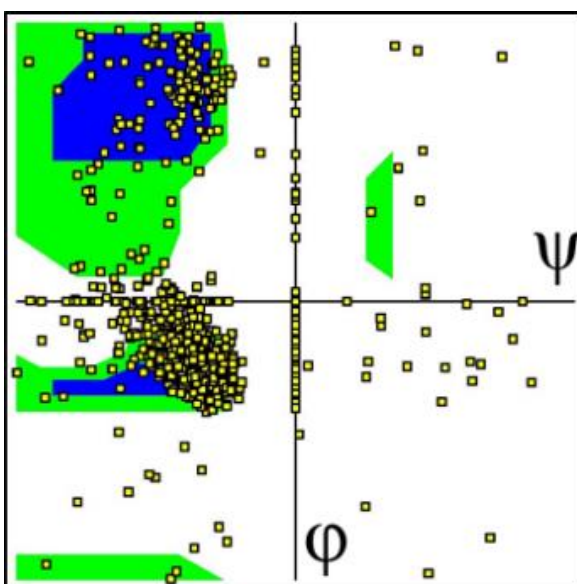


Fig S48: Ramachandran Plot of Simulated BSA at 50 mM and pH 2.0

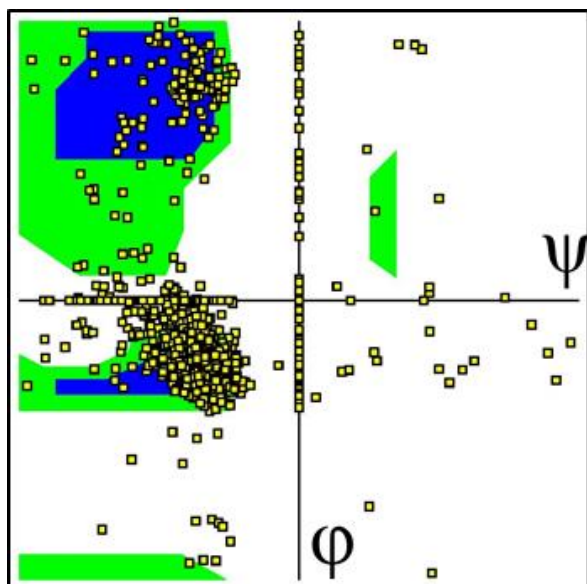


Fig S49: Ramachandran Plot of Simulated BSA at 50 mM and pH 3.5

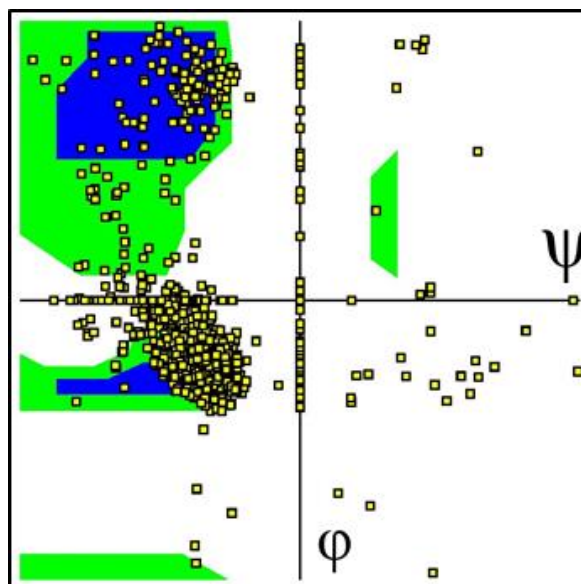


Fig S50: Ramachandran Plot of Simulated BSA at 50 mM and pH 4.3

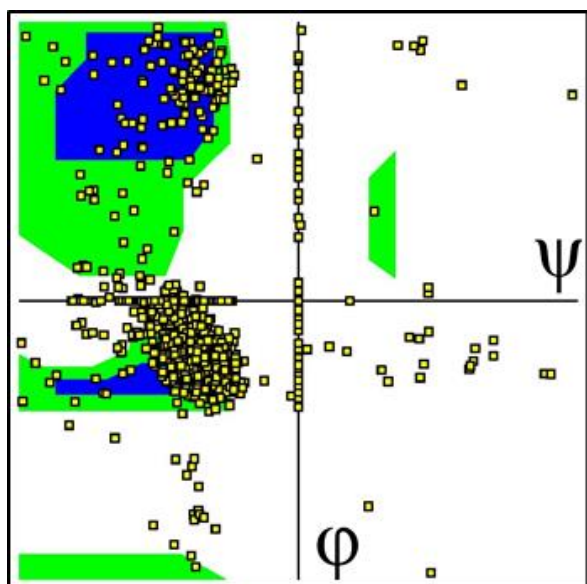


Fig S51: Ramachandran Plot of Simulated BSA at 50 mM and pH 7.4

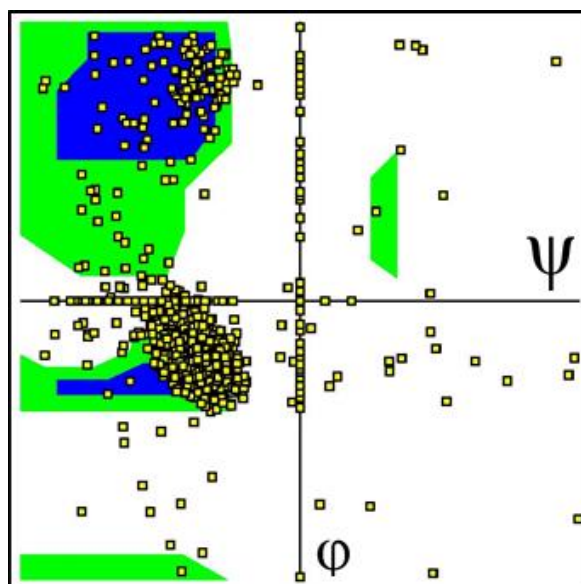


Fig S52: Ramachandran Plot of
Simulated BSA at 50 mM and pH 9.0

