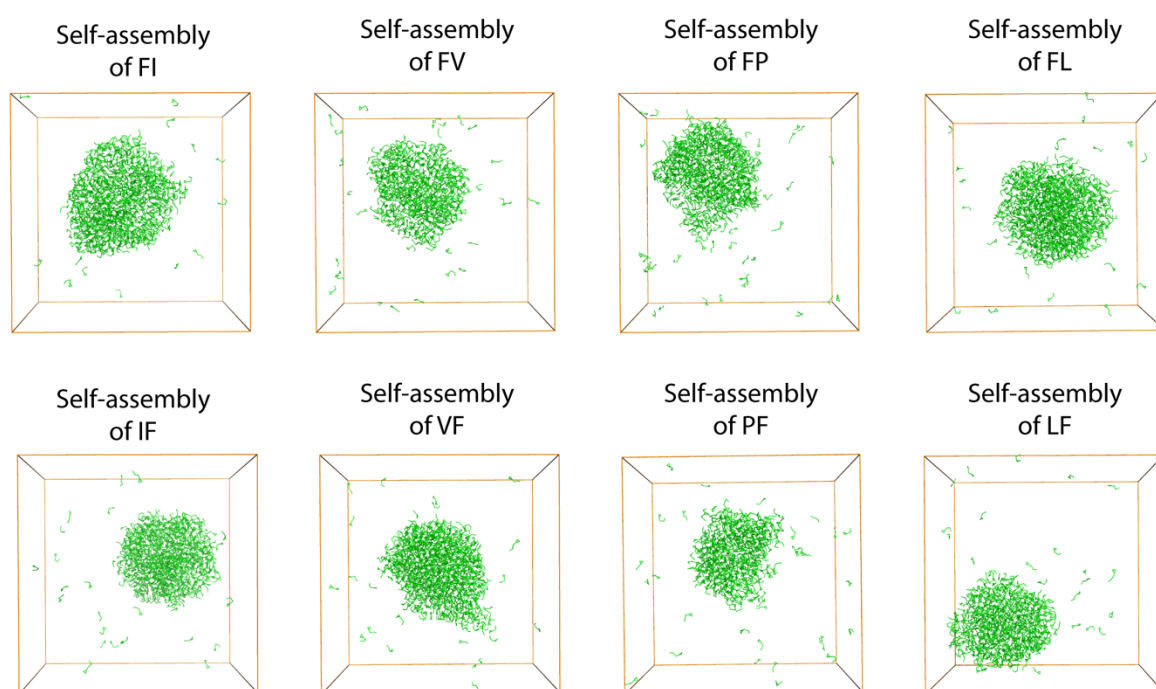


## Expanding the structural diversity of peptide assemblies by coassembling dipeptides with diphenylalanine

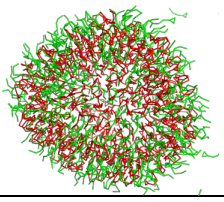
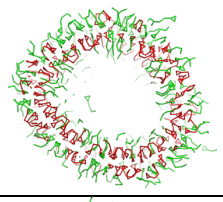
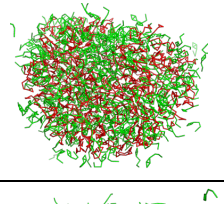
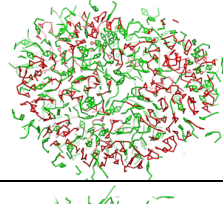
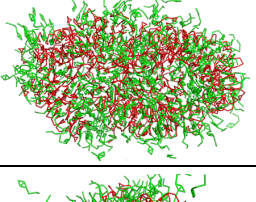
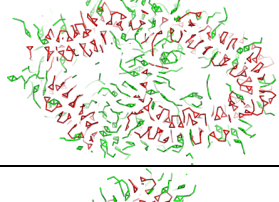
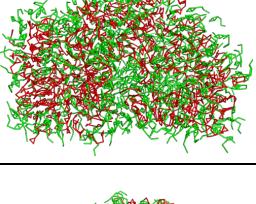
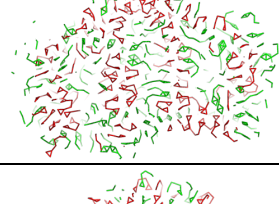
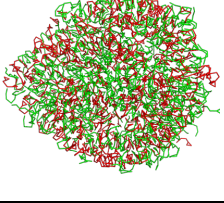
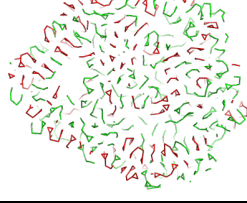
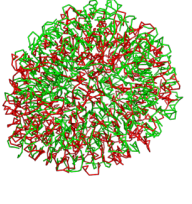
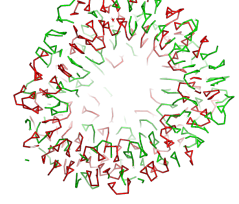
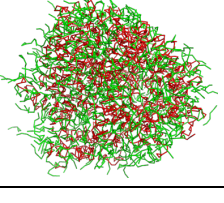
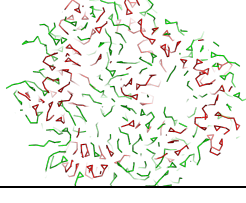
Yiming Tang, Yifei Yao and Guanghong Wei\*

Department of Physics, State Key Laboratory of Surface physics, and Key Laboratory for Computational Physical Science (Ministry of Education), Multiscale Research Institute of Complex Systems, and Collaborative Innovation Center of Advanced Microstructures (Nanjing), Fudan University, Shanghai 200433, People's Republic of China

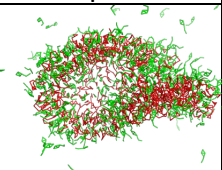
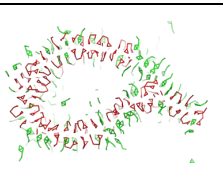
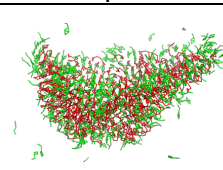
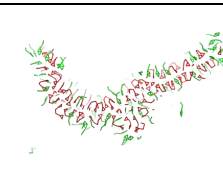
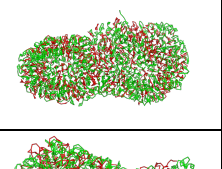
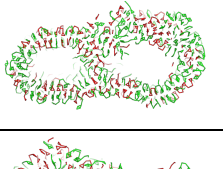
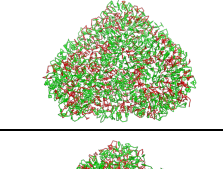
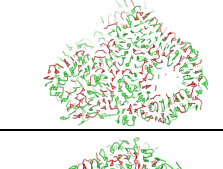
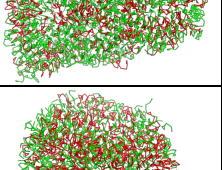
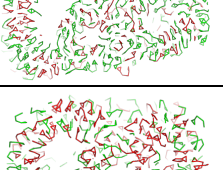
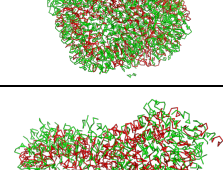
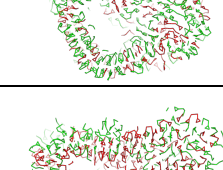
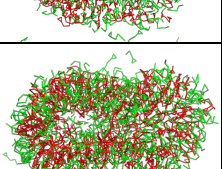
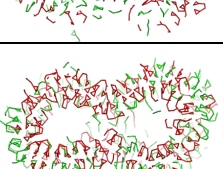
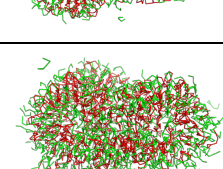
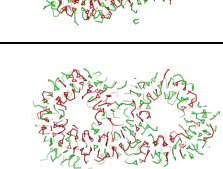
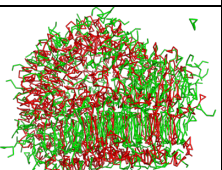
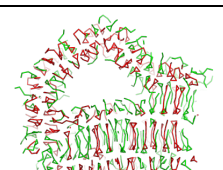
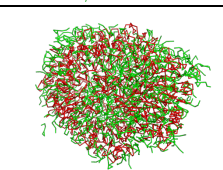
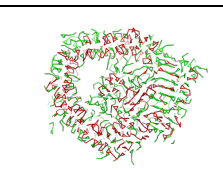
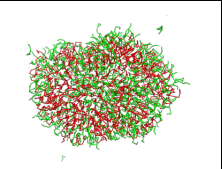
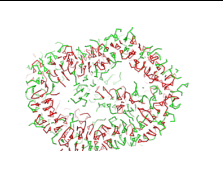
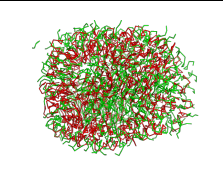
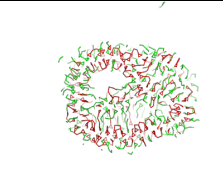
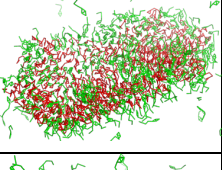
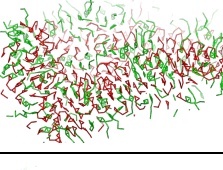
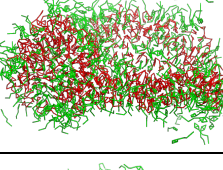
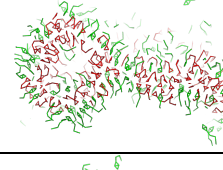
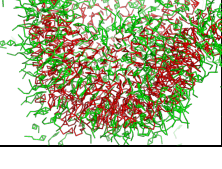
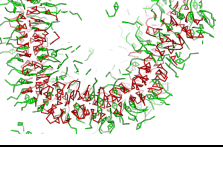
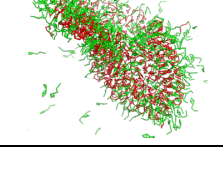
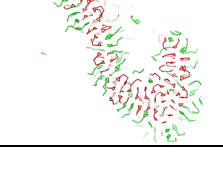




**Figure. S1. Self-assemblies of eight dipeptides that have an ability to coassemble with FF into multi-cavity nanostructures.**



**Table S1. Nanostructures formed by FF and charged aromatic dipeptides with the sidechain charges being switched off. The symbol 0 on the shoulder of charged residue indicates that the charge is switched off.**

System	Snapshot	Cross-section
FD + FF		
WE + FF		
DW + FF		
WD + FF		
FK + FF		
KF + FF		
FR + FF		

**Table S2. Single-cavity assemblies formed by coassembly of non-FF dipeptides with FF.**

Systems	MD2		MD3	
	Snapshot	Cross-section	Snapshot	Cross-section
GW + FF				
FW + FF				
WF + FF				
FM + FF				
MF + FF				
FT + FF				
TF + FF				
QW + FF				
WQ + FF				

## 2. Formation mechanisms of single-cavity coassemblies.

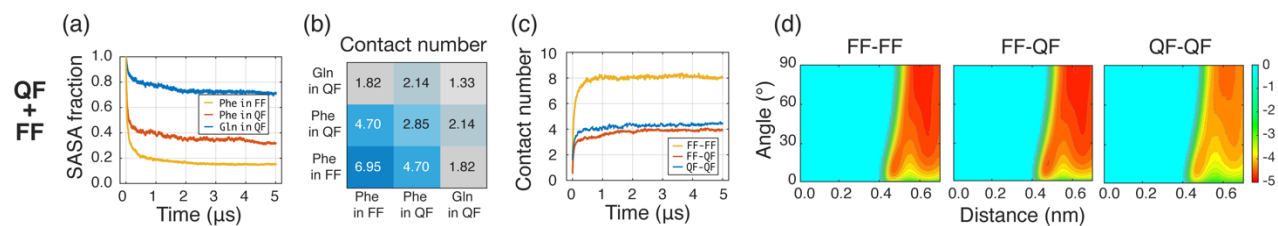


Figure S2.1. Coassembly mechanisms of QF-FF.

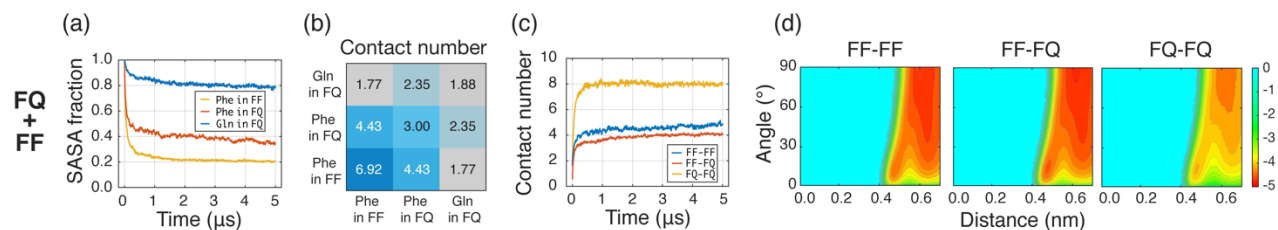


Figure S2.2. Coassembly mechanisms of FQ-FF.

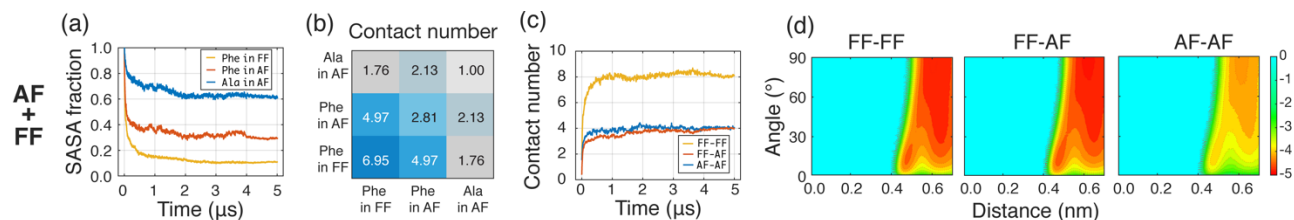


Figure S2.3. Coassembly mechanisms of AF-FF.

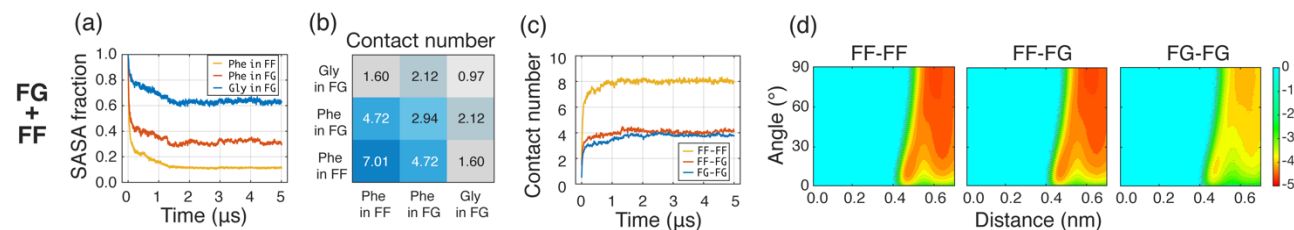


Figure S2.4. Coassembly mechanisms of FG-FF.

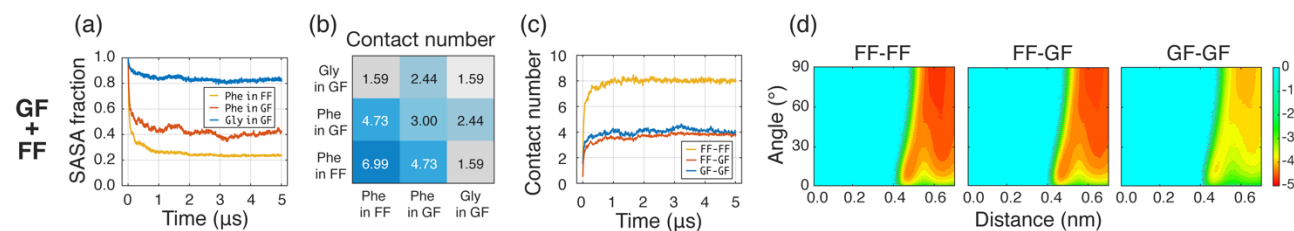


Figure S2.5. Coassembly mechanisms of GF-FF.

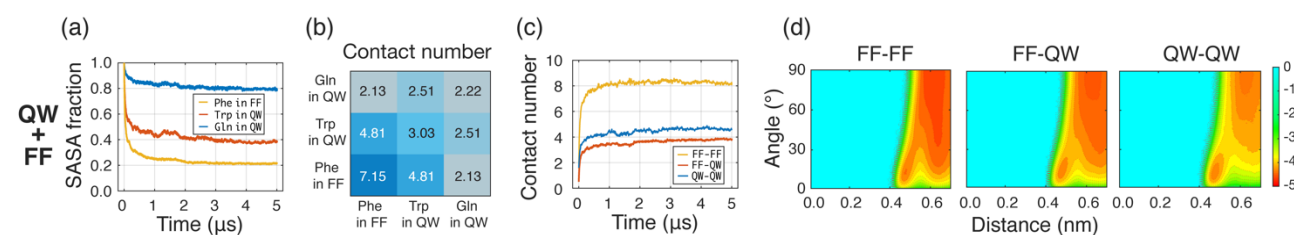
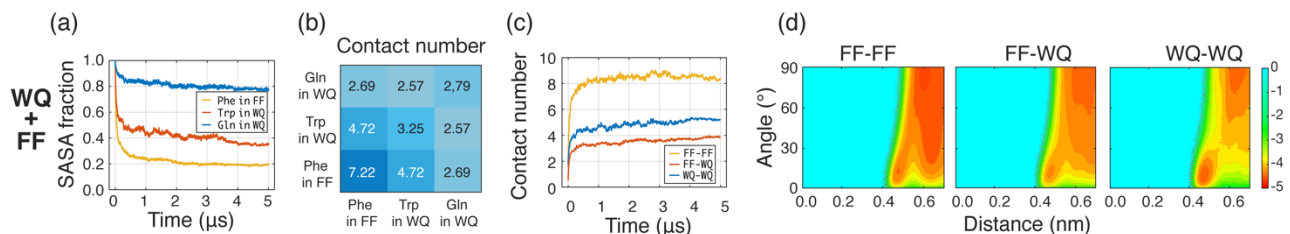
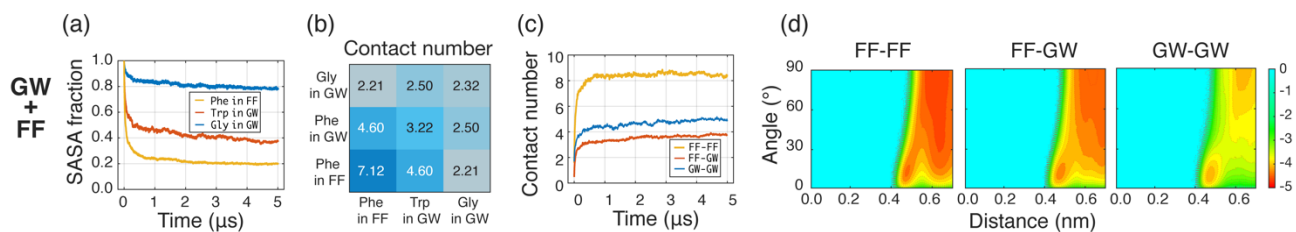


Figure S2.6. Coassembly mechanisms of QW-FF.

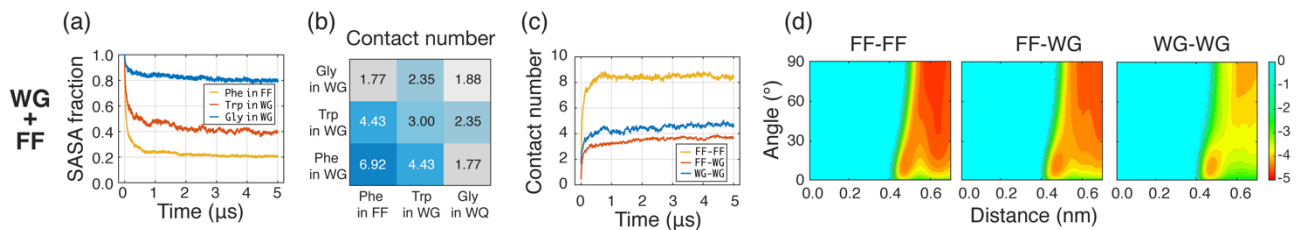




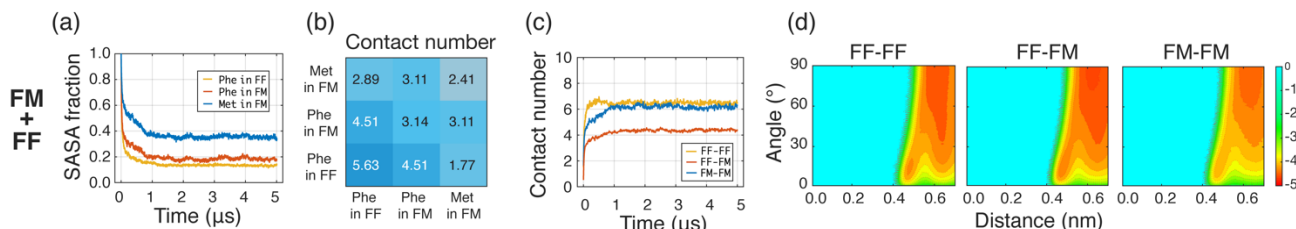
**Figure S2.7. Coassembly mechanisms of WQ-FF.**



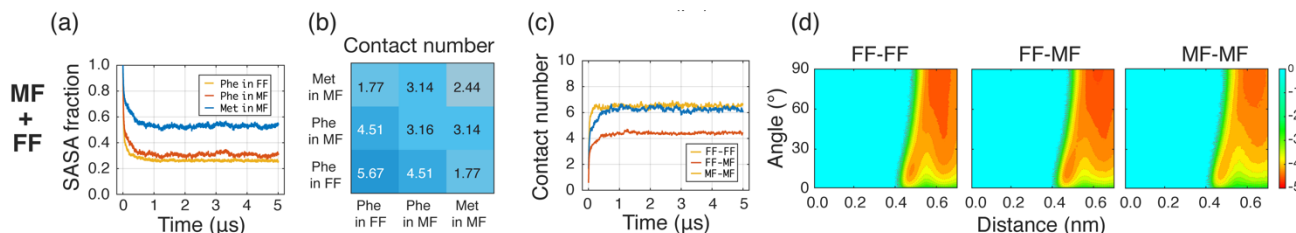
**Figure S2.8. Coassembly mechanisms of GW-FF.**



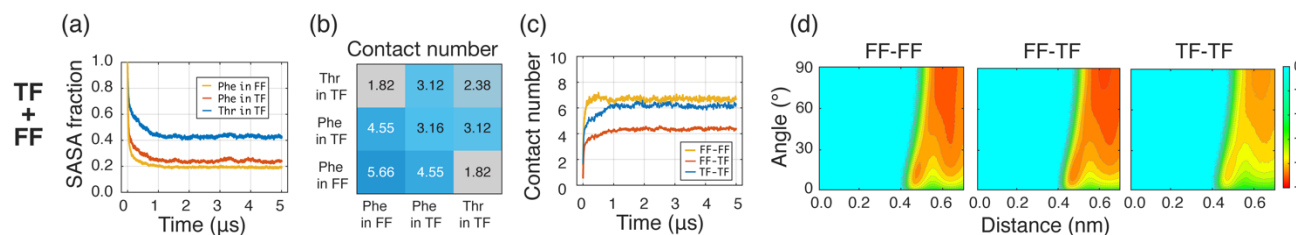
**Figure S2.9. Coassembly mechanisms of WG-FF.**



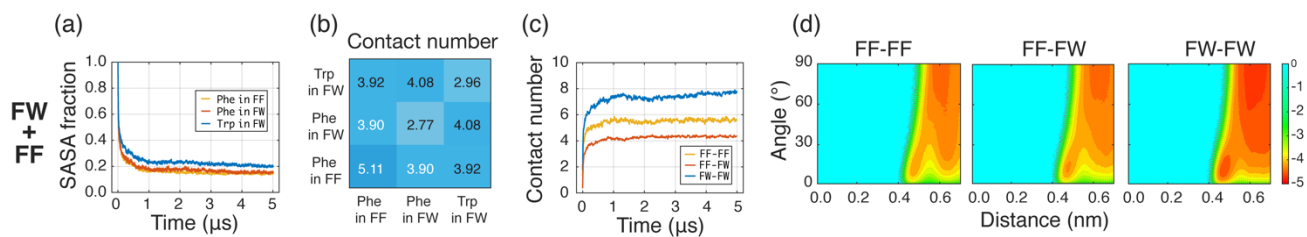
**Figure S2.10. Coassembly mechanisms of FM-FF.**



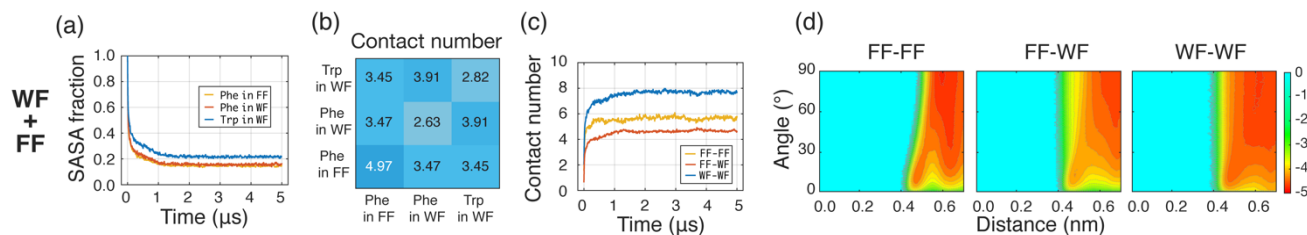
**Figure S2.11. Coassembly mechanisms of MF-FF.**



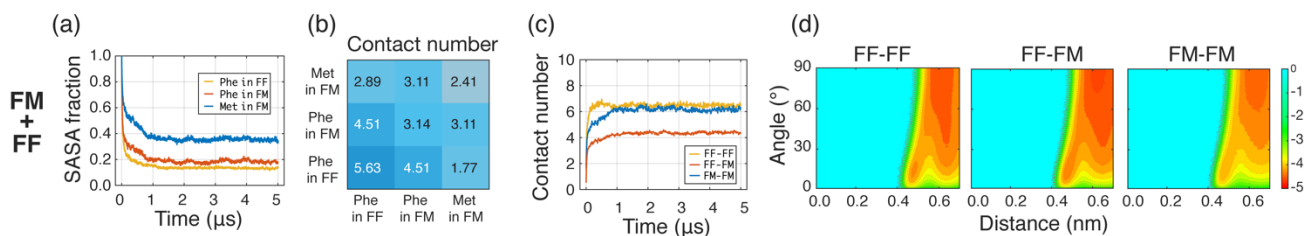
**Figure S2.12. Coassembly mechanisms of TF-FF.**



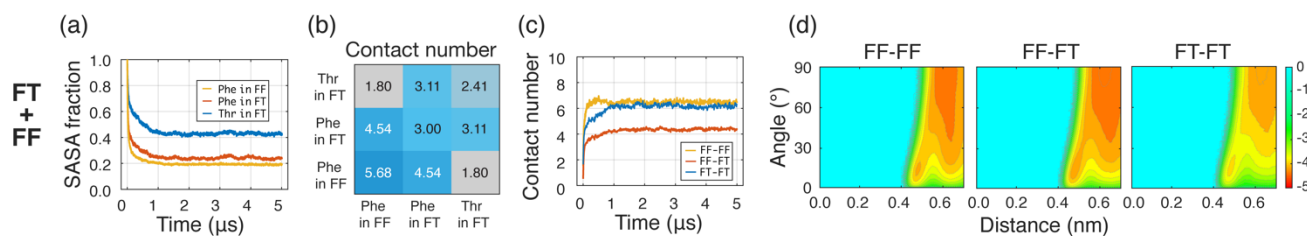
**Figure S2.13. Coassembly mechanisms of FW-FF.**



**Figure S2.14. Coassembly mechanisms of WF-FF.**

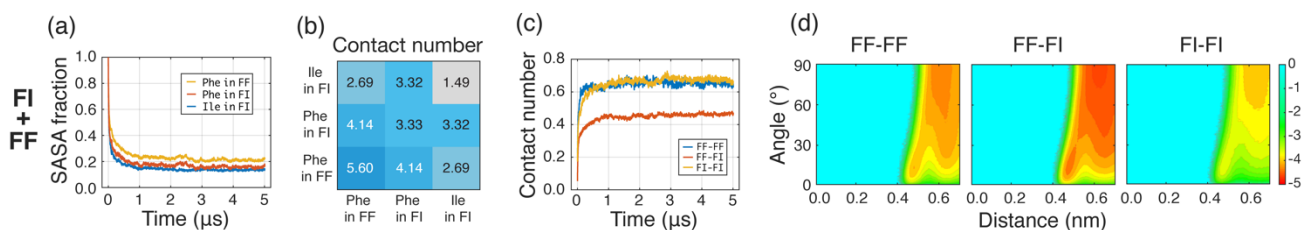


**Figure S2.15. Coassembly mechanisms of FM-FF.**

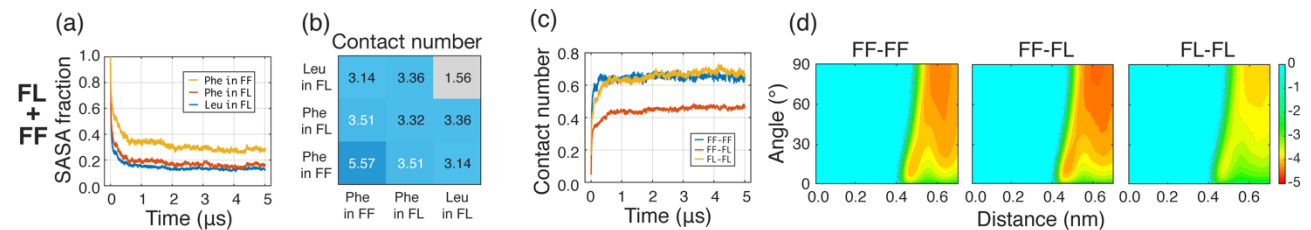
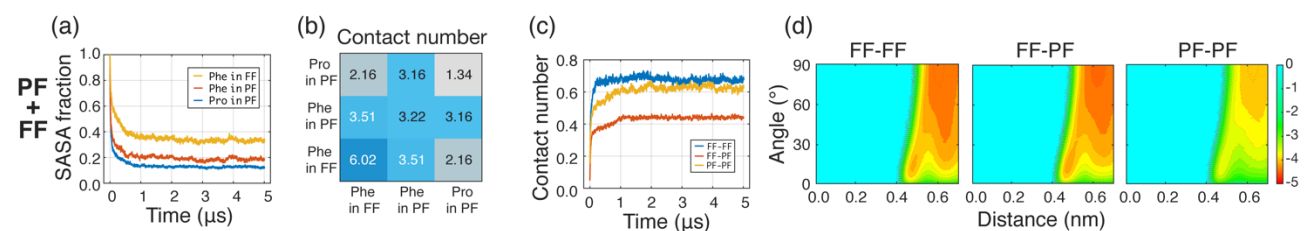
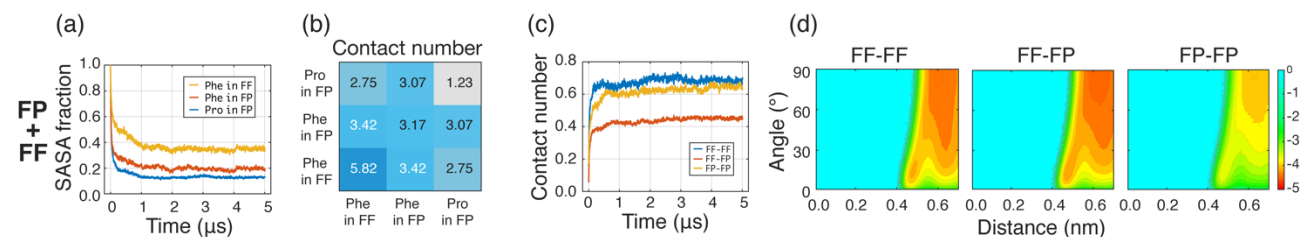
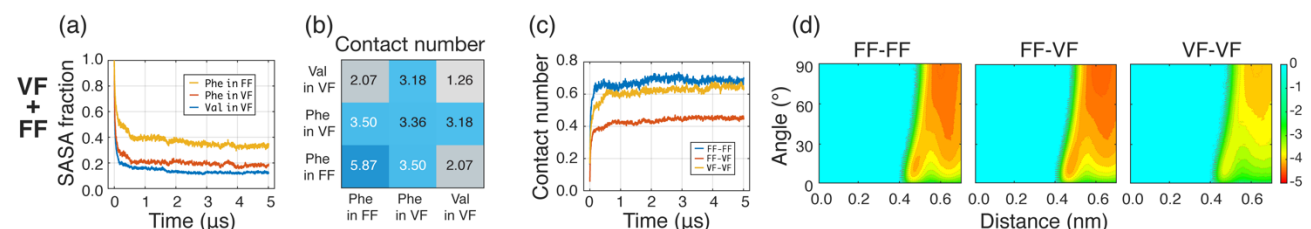
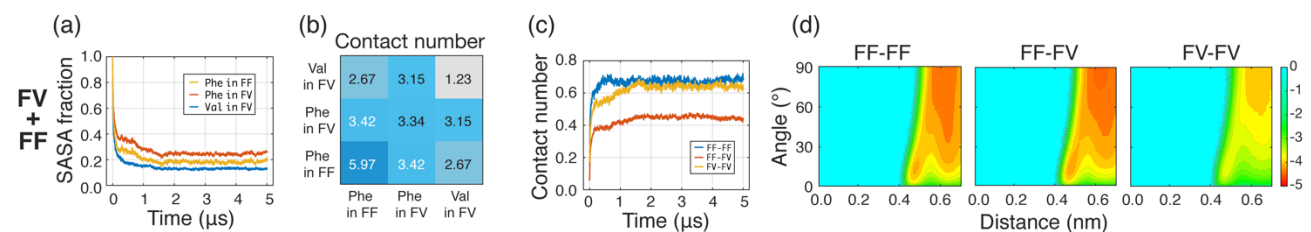
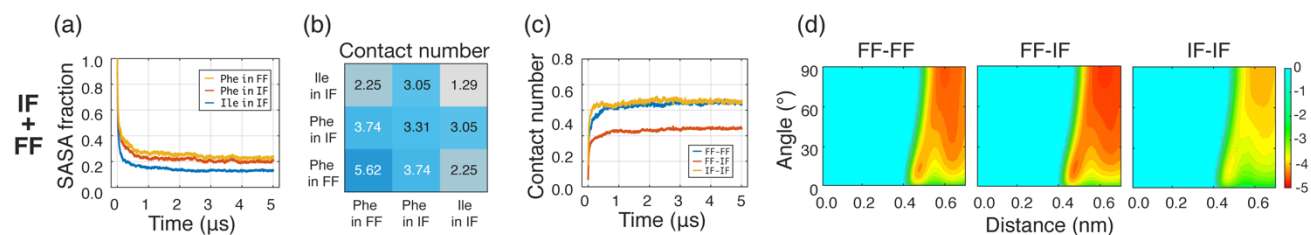


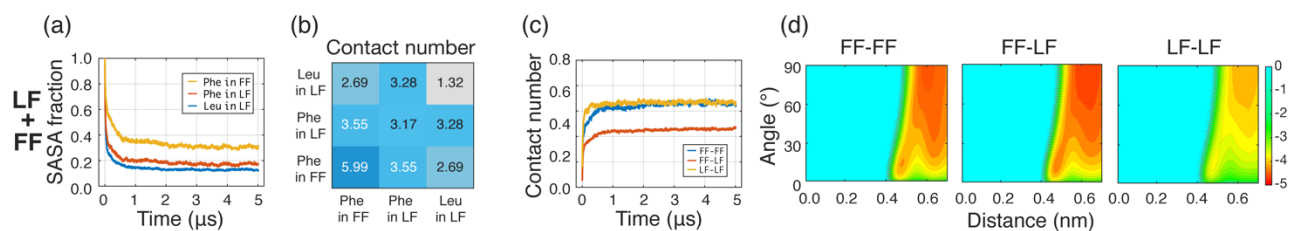
**Figure S2.16. Coassembly mechanisms of FT-FF.**

### 3. Formation mechanisms of multi-cavity coassemblies.



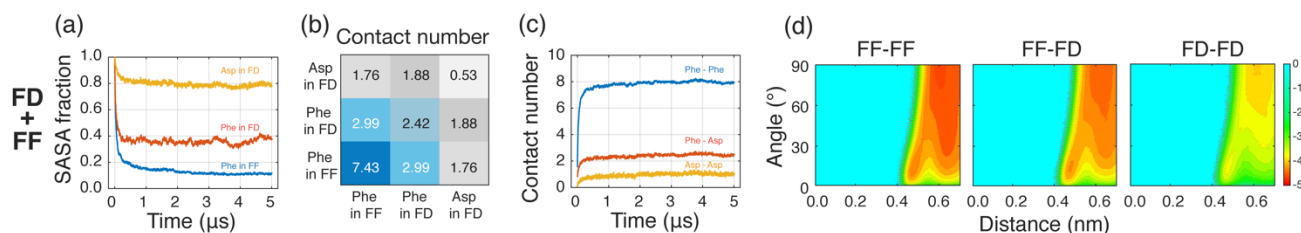
**Figure S3.1. Coassembly mechanisms of FI-FF.**



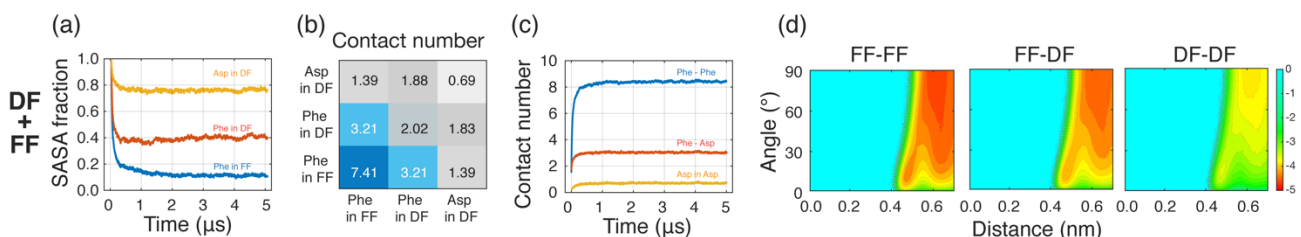


**Figure S3.8. Coassembly mechanisms of LF-FF.**

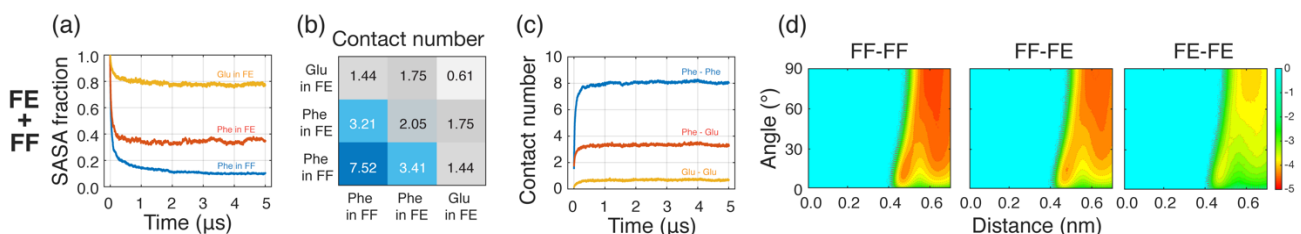
#### 4. Formation mechanisms of bilayer sheets.



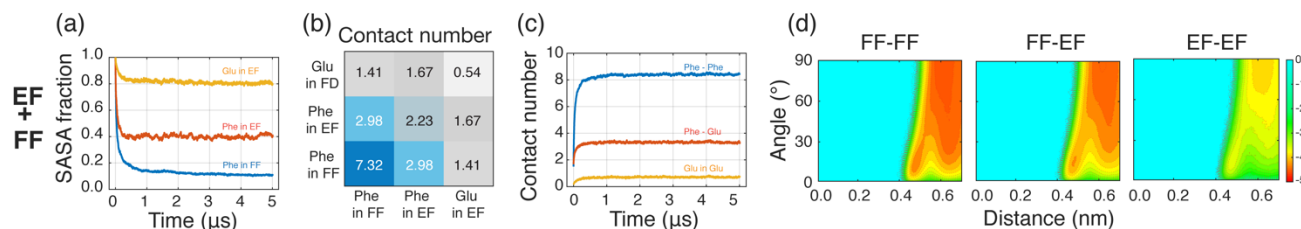
**Figure S4.1. Coassembly mechanisms of FD-FF.**



**Figure S4.2. Coassembly mechanisms of DF-FF.**

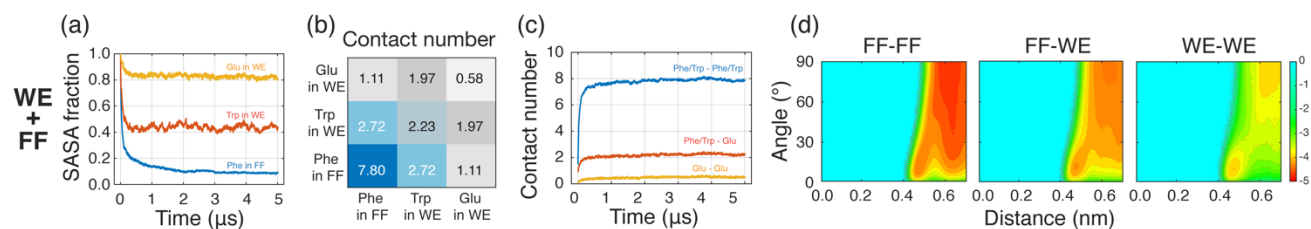


**Figure S4.3. Coassembly mechanisms of FE-FF.**

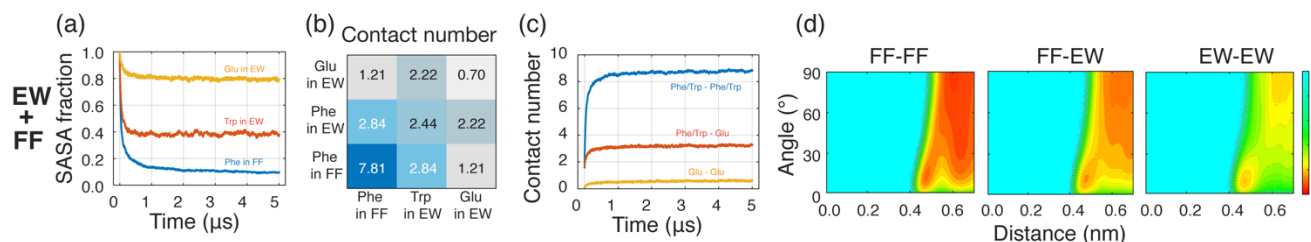


**Figure S4.4. Coassembly mechanisms of EF-FF.**

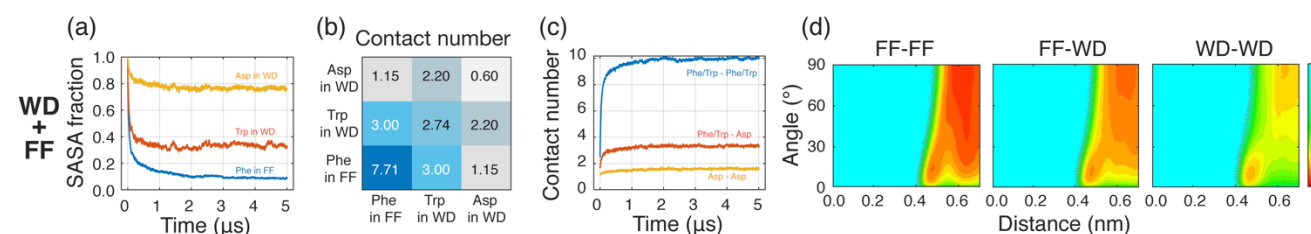




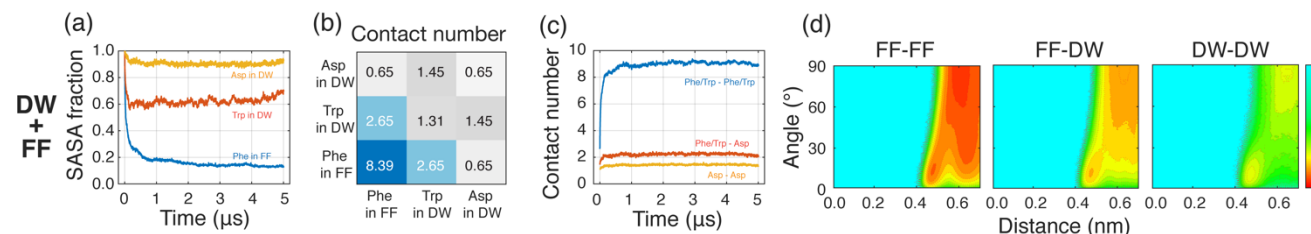
**Figure S4.5. Coassembly mechanisms of WE-FF.**



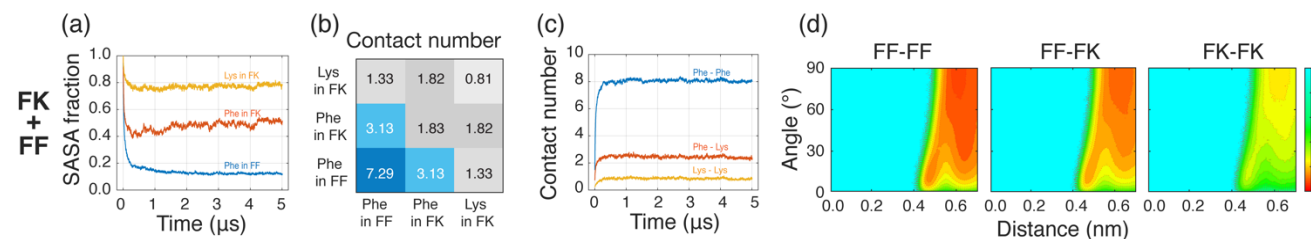
**Figure S4.6. Coassembly mechanisms of EW-FF.**



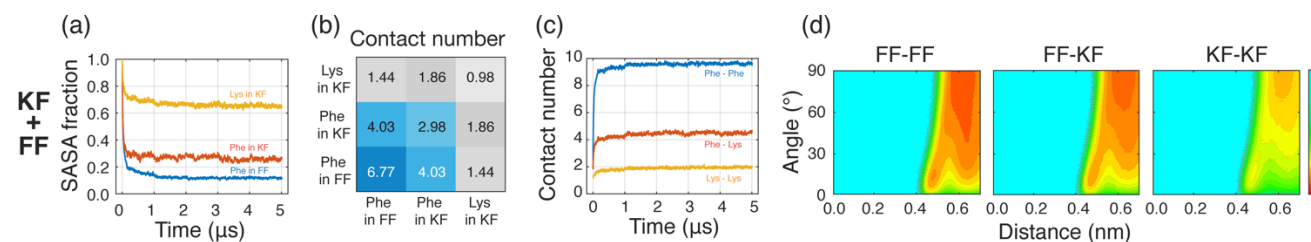
**Figure S4.7. Coassembly mechanisms of WD-FF.**



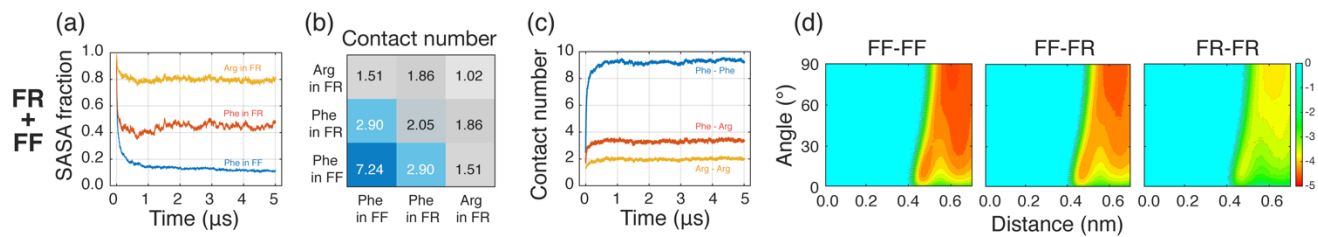
**Figure S4.8. Coassembly mechanisms of DW-FF.**



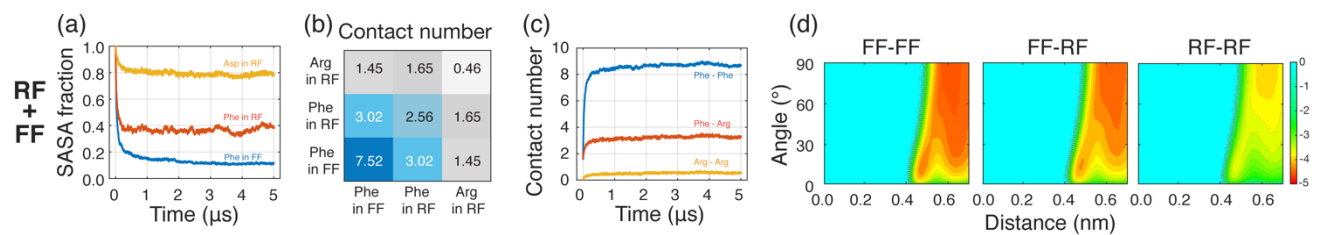
**Figure S4.9. Coassembly mechanisms of FK-FF.**



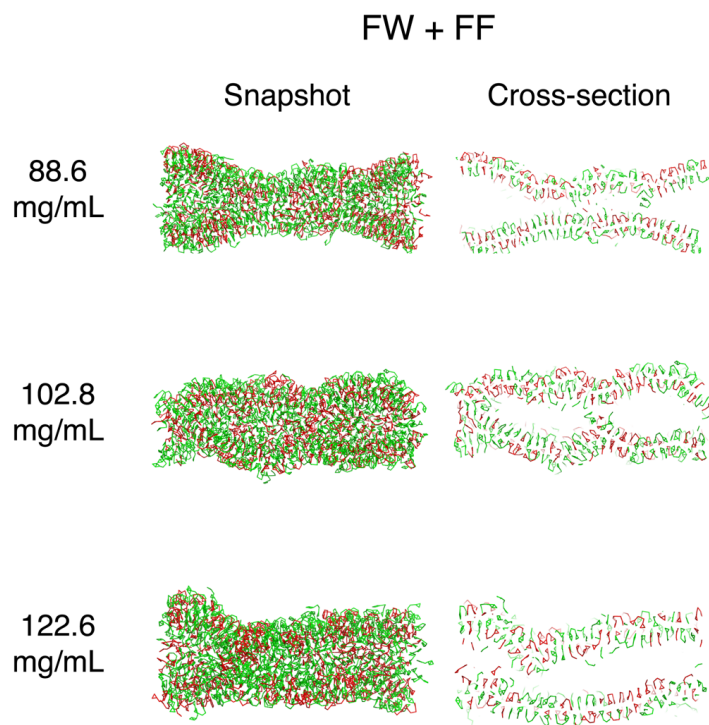
**Figure S4.10. Coassembly mechanisms of KF-FF.**



**Figure S4.11. Coassembly mechanisms of FR-FF.**



**Figure S4.12. Coassembly mechanisms of RF-FF.**



**Figure S5. Nanotubes formed by coassembly of FW with FF at high dipeptide concentrations.**