Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for Computational Investigation of Copper-Mediated Conformational Changes in α-Synuclein Dimer, Savva and Platts

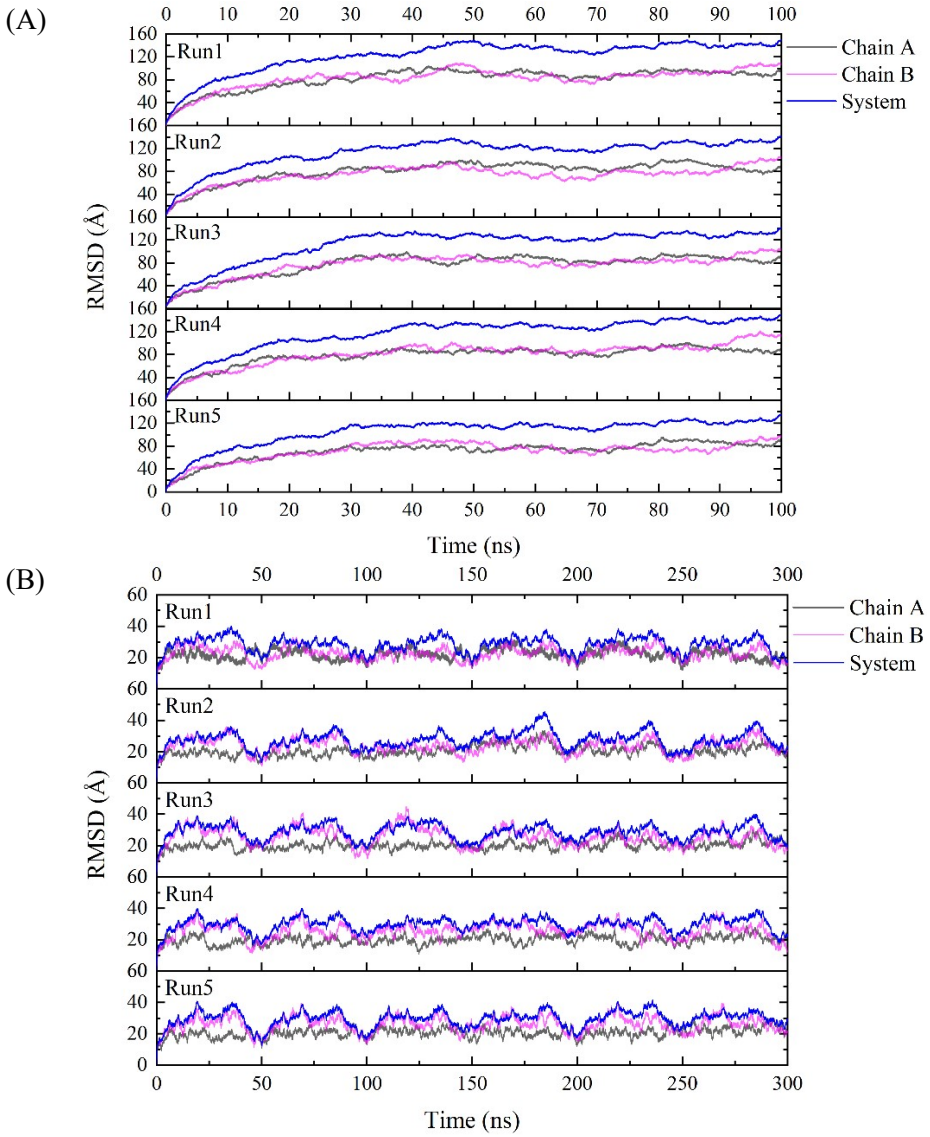


Figure S1 Plots of the RMSD in each of the runs, for the steps involved in (A) the equilibration of the Cu-bound dimer, and (B) the production data used to assess its behaviour. The values were calculated with respect to the first frame of each run.

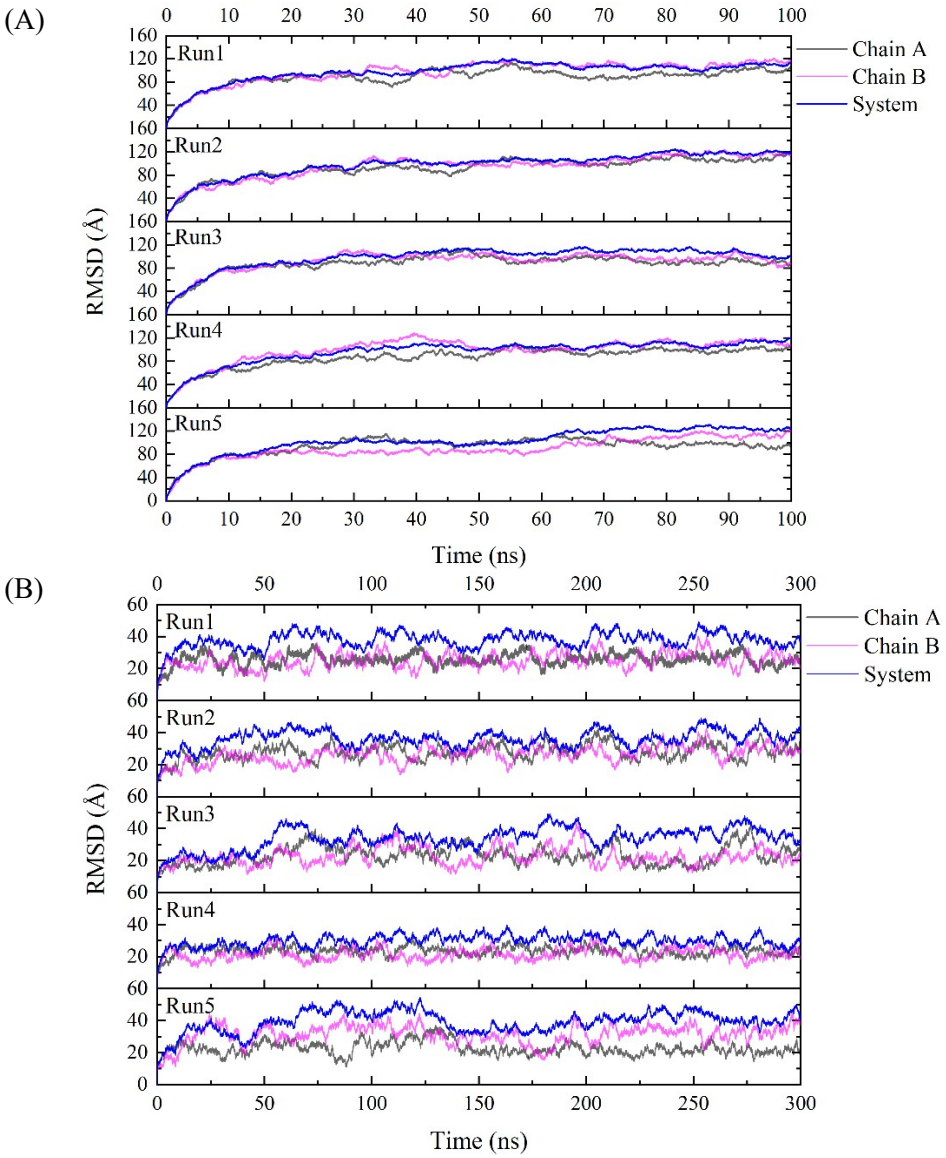


Figure S2 Plots of the RMSD in each of the runs, for the steps involved in (A) the equilibration of the metal-free dimer, and (B) the production data used to assess its behaviour. The values were calculated with respect to the first frame of each run.

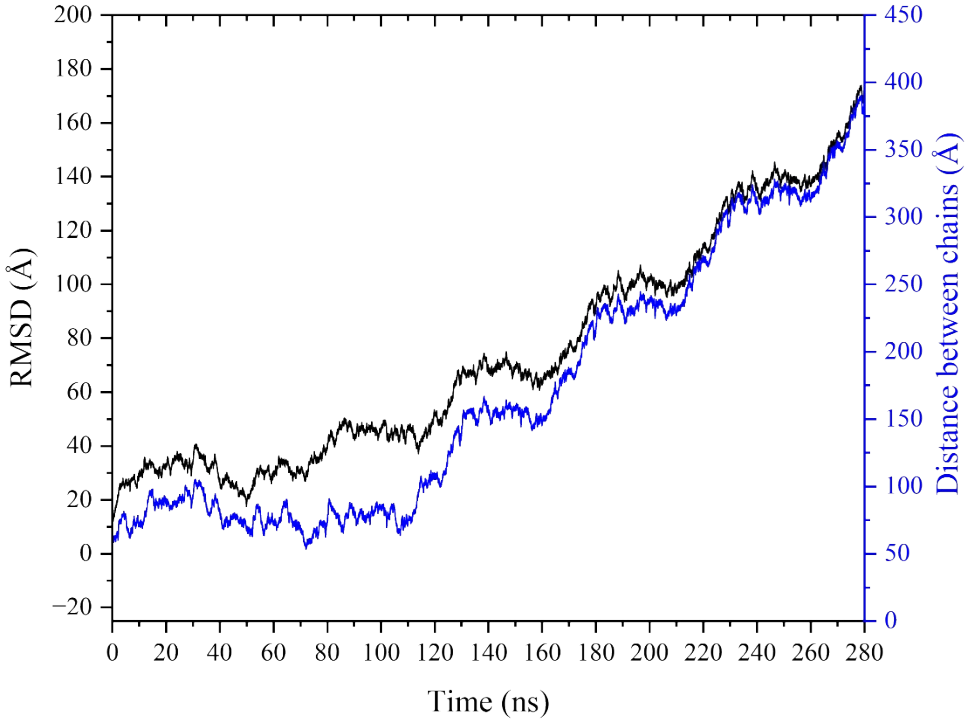


Figure S3 Plot of RMSD (black) and distance between the centre of mass of the two chains (blue) in the metal-free system, from aMD simulations.

Table S1 Detailed secondary structure percentages of the three main regions of the metal-free αS-dimer.

Region	β-character (%)	α-character (%)	Other (%)
Chain A			
N-terminal	4.77	24.94	70.29
NAC	15.31	21.70	63.00
C-terminal	0.43	20.66	78.91
Total	6.01	22.75	71.24
Chain B			
N-terminal	3.84	22.01	74.14
NAC	9.40	22.20	68.40
C-terminal	0.37	21.37	78.27
Total	4.11	21.85	74.03

Table S2 Detailed secondary structure percentages of the three main regions of the Cu-bound αS-dimer.

Region	β-character (%)	α-character (%)	Other (%)
Chain A			
N-terminal	7.70	17.96	74.34
NAC	13.98	24.92	61.10
C-terminal	0.42	21.48	78.10
Total	6.93	20.83	72.24
Chain B			
N-terminal	8.67	19.27	72.06
NAC	12.55	21.88	65.57
C-terminal	0.33	21.24	78.42
Total	6.96	20.56	72.48

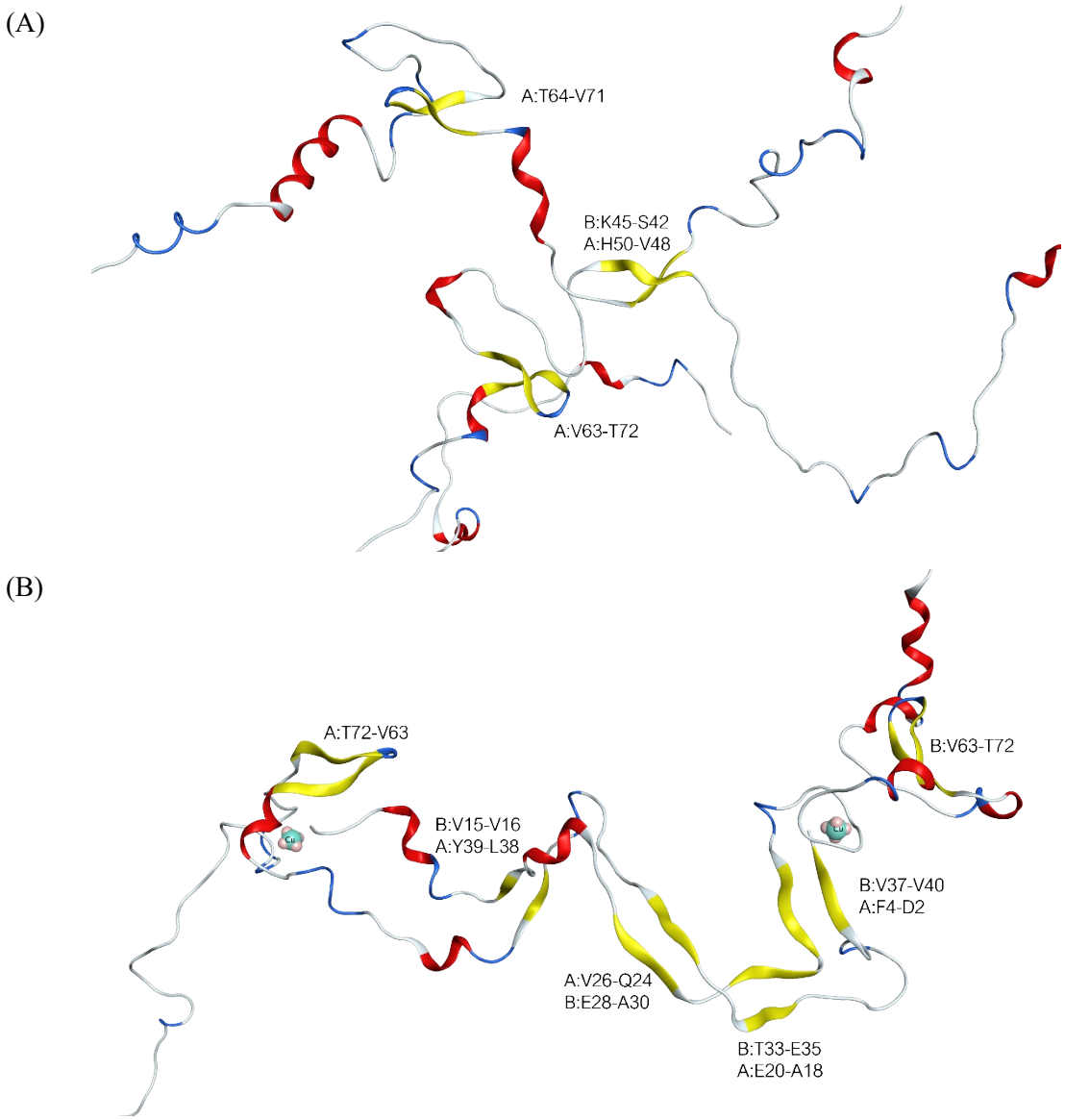


Figure S4 Snapshot of two random frames (#40,000) from the (A) metal-free and (B) Cu-bound dimers, with labelled residues involved in the β-strands (yellow) going from top to bottom, and left to right.

Table S3 Clusters from the two dimer systems, created using PCA of the cartesian coordinates of Cα.

Cluster#	Frames in Cluster (out of total 150,000)
Metal-free dimer	
1	44,808
2	460
3	41
Cu- bound dimer	
1	39,981
2	3,751
3	2,045
4	52

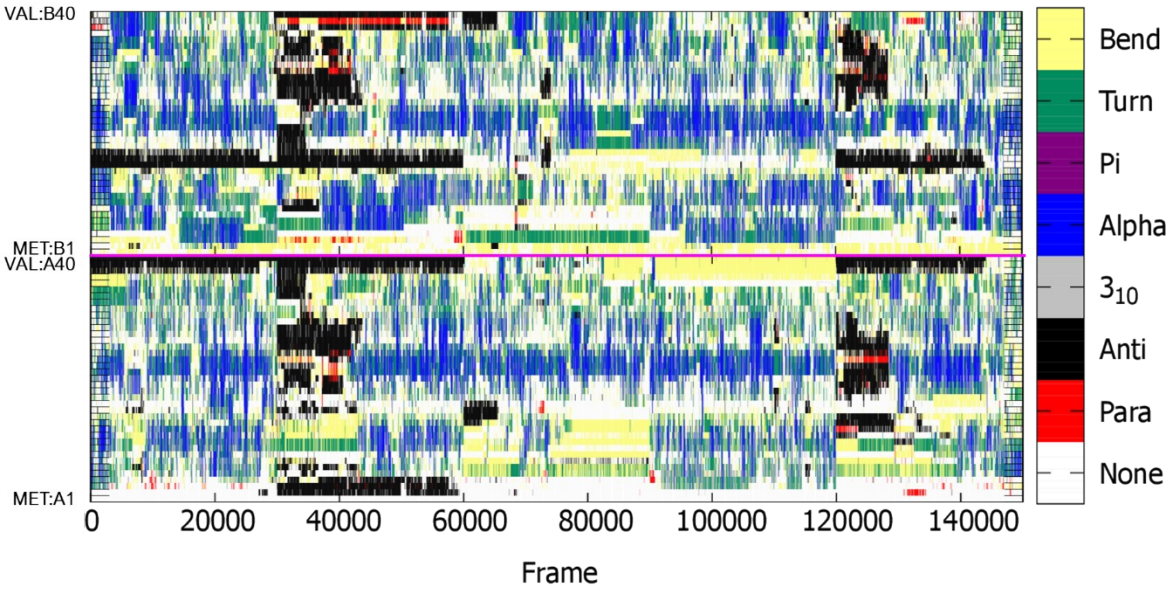
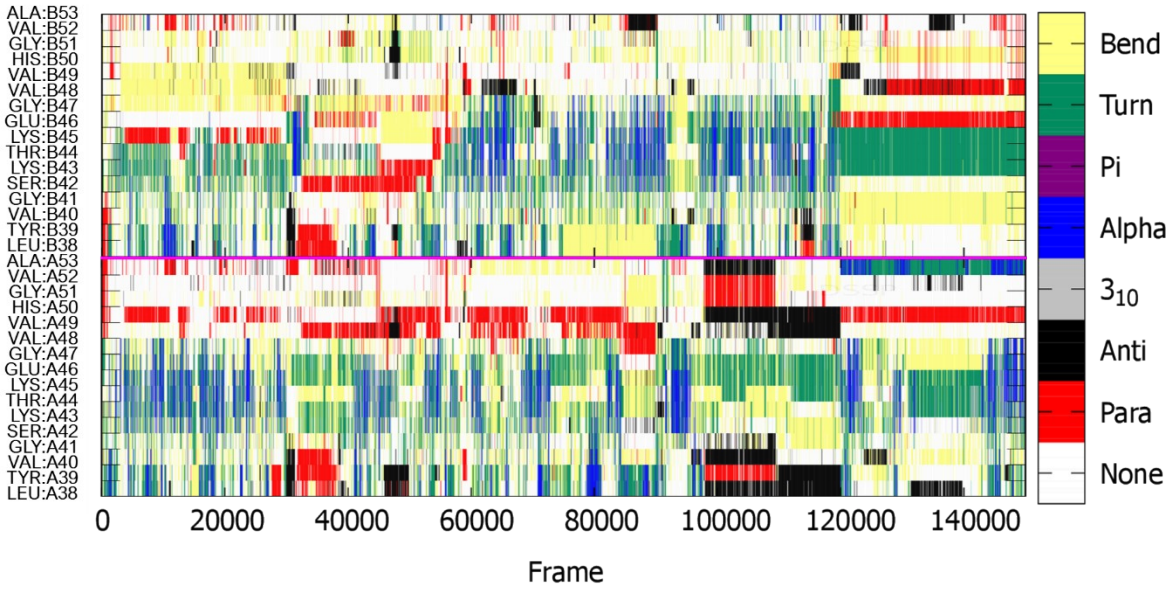


Figure S5 Evolution of secondary structural elements of each of residues M1-V40 in the two chains of the Cu-bound dimer. The pink line separates the two chains.

(A)



(B)

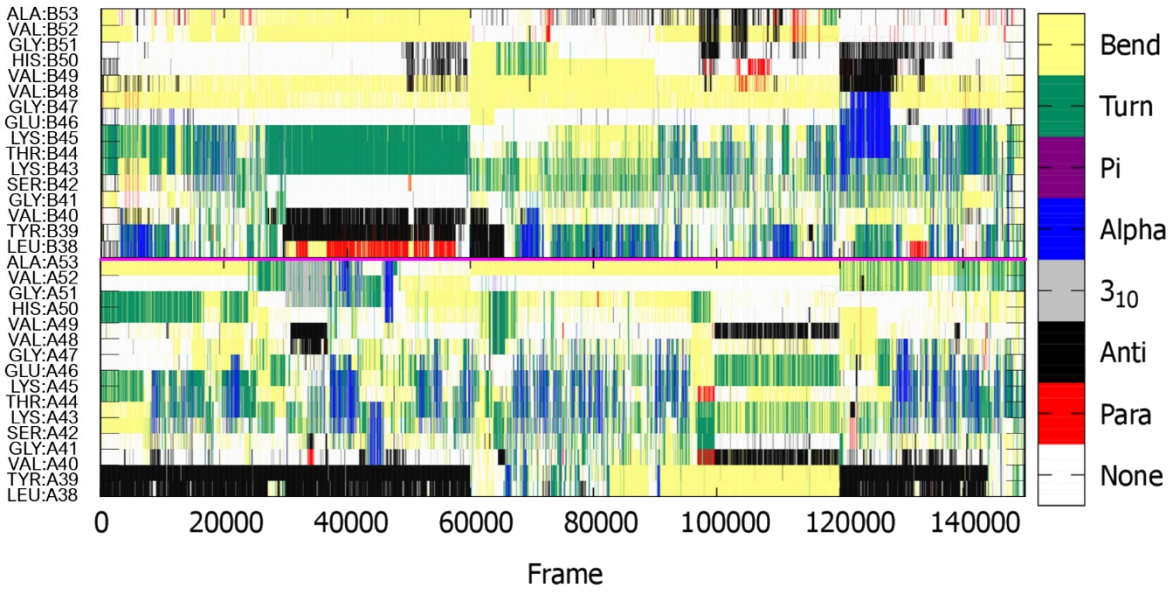


Figure S6 Evolution of secondary structural elements of each of residues L38-A53 in the two chains of the (A) metal-free and (B) Cu-bound dimers. The pink line separates the two chains.

Table S4 Mean and standard deviation of distance between Cu and centre of mass of selected residues (Å)

	Mean	Sd
M1A	3.77	0.18
D2A	3.19	0.43
H50B	2.39	0.16
M1B	3.89	0.34
D2B	3.24	0.43
H50A	5.35	2.45