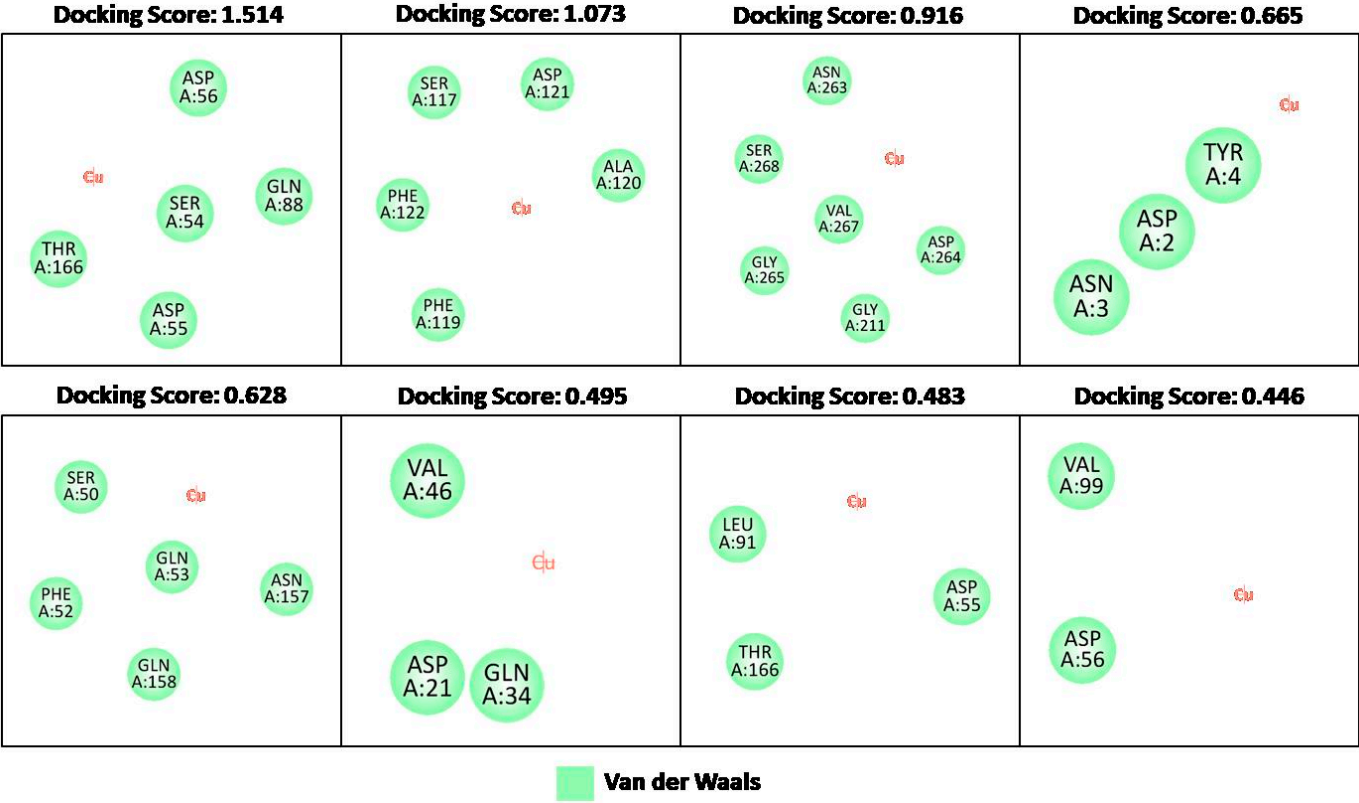


**Figure S1.** Molecular interaction diagrams of BCL with Cu<sup>2+</sup> at bind poses with all docking score values.



**Table S1.** Interacting amino acids predicted by MIB for BCL – Cu<sup>2+</sup> complex.

Docking Score	Amino Acid	Type of interaction
1.514	ASP55	Van der Waals
	ASP56	
	GLN88	
	SER54	
	THR166	
1.073	ALA120	Van der Waals
	ASP121	
	SER117	
	PHE122	
	PHE119	
0.916	ASN263	Van der Waals
	SER268	
	VAL267	
	ASP264	
	GLY265	
	GLY211	
0.665	TYR4	Van der Waals
	ASP2	
	ASN3	
0.628	SER50	Van der Waals
	PHE52	
	GLN53	
	ASN157	
	GLN158	
0.495	VAL46	Van der Waals
	ASP21	
	GLN34	
0.483	LEU91	Van der Waals
	THR166	
	ASP55	
0.446	VAL99	Van der Waals
	ASP56	
0.405	-	-