

**SI Table 2.** Heavy atoms assigned to the chemical groups of the amino acid side-chains.

AA	Chemical groups							
	<i>Aromatic rings</i>	<i>Hydroxyl group</i>	<i>Thiol group</i>	<i>Carboxyl</i>	<i>Aliphatic carbons</i>	<i>Amine</i>	<i>Amide</i>	<i>Guanidine</i>
CYS			SG					
ASP				CG OD1 OD2				
GLU				CD OE1 OE2				
PHE					CG CD1 CD2 CE1 CE2 CZ			
HIS					CG CD2 NE2 CE1 ND1			
ILE					CD1 CG1 CG2			
LYS						NZ		
LEU					CD1 CD2 CG			
MET			SD CE					
ASN							CG OD1 ND2	
GLN							CD OE1 NE2	
ARG								CZ NE NH1 NH2
SER		OG						

THR		OG1
VAL		CG1 CG2
TRP	CG (1) CD1 (1) NE1 (1) CE2 (1) CD2 (1) CE2 (2) CD2 (2) CE3 (2) CZ3 (2) CH2 (2) CZ2 (2)	
TYR	CG CD1 CD2 CE1 CE2 CZ	OH