

## Inventory of the candidate atoms for the hydrophobic interaction analysis

**Table A. Inventory of the candidate atoms for the hydrophobic interaction analysis.** The atom names correspond to the nomenclature of the CHARMM36 force field.

Residue/lipid	Candidate atoms
ALA	CA HA CB HB1 HB2 HB3
ARG	CA HA CB HB1 HB2 CG HG1 HG2
ASN	CA HA CB HB1 HB2
ASP	CA HA CB HB1 HB2
CYS	CA HA CB HB1 HB2
GLN	CA HA CB HB1 HB2 CG HG1 HG2
GLU	CA HA CB HB1 HB2 CG HG1 HG2
GLY	CA HA1 HA2
HSD	CA HA CB HB1 HB2
HSE	CA HA CB HB1 HB2
HSP	CA HA CB HB1 HB2 CG
ILE	CA HA CB HB CG1 HG11 HG12 CG2 HG21 HG22 HG23 CD HD1 HD2 HD3
LEU	CA HA CB HB1 HB2 CG HG CD1 HD11 HD12 HD13 CD2 HD21 HD22 HD23
LYS	CA HA CB HB1 HB2 CG HG1 HG2 CD HD1 HD2 CE HE1 HE2
MET	CA HA CB HB1 HB2 CG HG1 HG2 CE HE1 HE2 HE3
PHE	CA HA CB HB1 HB2 CG CD1 HD1 CD2 HD2 CE1 HE1 CE2 HE2 CZ HZ
PRO	CA HA CB HB1 HB2 CD HD1 HD2 CG HG1 HG2
SER	CA HA CB HB1 HB2
THR	CA HA CB HB CG2 HG21 HG22 HG23
TRP	CA HA CB HB1 HB2 CG CD1 HD1 CD2 CE3 HE3 CZ3 HZ3 CH2 HH2 CZ2 HZ2
TYR	CA HA CB HB1 HB2 CG CD1 HD1 CD2 HD2 CE1 HE1
POPC/POPE	C23 H3R H3S C24 H4R H4S C25 H5R H5S C26 H6R H6S C27 H7R H7S C28 H8R H8S C29 H9I C210 H10I C211 H11R H11S C212 H12R H12S C213 H13R H13S C214 H14R H14S C215 H15R H15S C216 H16R H16S C217 H17R H17S C218 H18R H18S H18T C33 H3X H3Y C34 H4X H4Y C35 H5X H5Y C36 H6X H6Y C37 H7X H7Y C38 H8X H8Y C39 H9X H9Y C310 H10X H10Y C311 H11X H11Y C312 H12X H12Y C313 H13X H13Y C314 H14X H14Y C315 H15X H15Y C316 H16X H16Y H16Z
DOPC/DOPE	C12 C11 H11A H11B C1 HA HB C2 HS C22 H2R H2S C3 HX HY C32 H2X H2Y C23 H3R H3S C24 H4R H4S C25 H5R H5S C26 H6R H6S C27 H7R H7S C28

H8R H8S C29 C210 C211 H11R H11S C212 H12R H12S C213 H13R H13S C214  
H14R H14S C215 H15R H15S C216 H16R H16S C217 H17R H17S C218 H18R  
H18S H18T C33 H3X H3Y C34 H4X H4Y C35 H5X H5Y C36 H6X H6Y C37  
H7X H7Y C38 H8X H8Y C39 C310 C311 H11X H11Y C312 H12X H12Y C313  
H13X H13Y C314 H14X H14Y C315 H15X H15Y C316 H16X H16Y C317 H17X  
H17Y C318 H18X H18Y H18Z

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PSM

C4S H4S C5S H5S C6S H6S H6T C7S H7S H7T C8S H8S H8T C9S H9S H9T  
C10S H10S H10T C11S H11S H11T C12S H12S H12T C13S H13S H13T C14S  
H14S H14T C15S H15S H15T C16S H16S H16T C17S H17S H17T C18S H18S  
H18T H18U C3F H3F H3G C4F H4F H4G C5F H5F H5G C6F H6F H6G C7F H7F  
H7G C8F H8F H8G C9F H9F H9G C10F H10F H10G C11F H11F H11G C12F  
H12F H12G C13F H13F H13G C14F H14F H14G C15F H15F H15G C16F H16F  
H16G H16H

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CHOL

C4 H4A H4B C5 C6 H6 C7 H7A H7B C8 H8 C14 H14 C15 H15A H15B C16 H16A  
H16B C17 H17 C13 C18 H18A H18B H18C C12 H12A H12B C11 H11A H11B  
C9 H9 C10 C19 H19A H19B H19C C1 H1A H1B C2 H2A H2B C20 H20 C21  
H21A H21B H21C C22 H22A H22B C23 H23A H23B C24 H24A H24B C25 H25  
C26 H26A H26B H26C C27 H27A H27B H27C

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