

	PDB	CHARMM22	CHARMM19	Amber
ILE Cδ	CD1	CD	CD	CD1
HIS prot Nδ	HIS	HSD	HIS	HID
HIS prot Nϵ	HIS	HSE	HSD	HIE
N-terminus	1H/2H/3H	HT1/HT2/HT3	HT1/HT2/HT3	H1/H2/H3
C-terminus	O/OXT	OT1/OT2	OT1/OT2	O/OXT
Hydrogens	1HB/2HB	HB1/HB2	-	HB2/HB3
CYS S-S	CYS	CYS	CYS	CYX