Atom Type	num (173)	Vol. (Å^3)	Radii (Å)	Comments	Protein Atoms
C3H0s	20	8.72	1.61	carbonyl carbons with branching (mainchain carbonyls from residues with a C_β, so no gly carbon)	ALA_C,ARG_C,ASN_C,ASP_C,CSS_C,CYS_C,GLN_C,GLU_C,HIS_C,ILE_C,LEU_C, LYS_C,MET_C,PHE_C,PRO_C,SER_C,THR_C,TRP_C,TYR_C,VAL_C
C3H0b	13	9.70	1.61	carboxyl and carbonyl carbons w/o branching (side chain and glycine's) and aromatic carbons w/o hydrogen	ARG_CZ,ASN_CG,ASP_CG,GLN_CD,GLU_CD,GLY_C,HIS_CG,PHE_CG,TRP_CD2, TRP_CE2,TRP_CG,TYR_CG,TYR_CZ
C4H1s	18	13.17	1.88	aliphatic carbons with one hydrogen and branching from all three heavy atom bonds	ARG_CA,ASN_CA,ASP_CA,CSS_CA,CYS_CA,GLN_CA,GLU_CA,HIS_CA,ILE_CA, LEU_CA,LYS_CA,MET_CA,PHE_CA,SER_CA,THR_CA,TRP_CA,TYR_CA,VAL_CA
C4H1b	6	14.35	1.88	aliphatic carbons with one hydrogen and no branching through at least one heavy atom bond	ALA_CA,ILE_CB,LEU_CG,PRO_CA,THR_CB,VAL_CB
C3H1s	8	20.44	1.76	small aromatic carbons with one hydrogen	HIS_CD2,HIS_CE1,PHE_CD1,TRP_CD1,TYR_CD1,TYR_CD2,TYR_CE1,TYR_CE2
C3H1b	8	21.28	1.76	big aromatic carbons with one hydrogen	PHE_CD2,PHE_CE1,PHE_CE2,PHE_CZ,TRP_CE3,TRP_CH2,TRP_CZ2,TRP_CZ3
C4H2s	21	23.19	1.88	aliphatic carbons with two hydrogens, small	ARG_CB,ARG_CD,ARG_CG,ASN_CB,ASP_CB,GLN_CB,GLN_CG,GLU_CB,GLU_CG, GLY_CA,HIS_CB,LEU_CB,LYS_CB,LYS_CD,LYS_CG,MET_CB,PHE_CB,PRO_CD, SER_CB,TRP_CB,TYR_CB
C4H2b	7	24.26	1.88	aliphatic carbons with two hydrogens, big	CSS_CB,CYS_CB,ILE_CG1,LYS_CE,MET_CG,PRO_CB,PRO_CG
C4H3u	9	36.73	1.88	aliphatic carbons with three hydrogens, i.e. methyl groups	ALA_CB,ILE_CD1,ILE_CG2,LEU_CD1,LEU_CD2,MET_CE, THR_CG2,VAL_CG1,VAL_CG2
N3H0u	1	8.65	1.64	imide nitrogens (only member is Pro N)	PRO_N
N3H1s	20	13.62	1.64	amide nitrogens with one hydrogen (all other mainchain N's)	ALA_N,ARG_N,ASN_N,ASP_N,CSS_N,CYS_N,GLN_N,GLU_N,GLY_N,HIS_N,ILE_N, LEU_N,LYS_N,MET_N,PHE_N,SER_N,THR_N,TRP_N,TYR_N,VAL_N
N3H1b	4	15.72	1.64	amide nitrogens with one hydrogen (on sidechains)	ARG_NE,HIS_ND1,HIS_NE2,TRP_NE1
N3H2u	4	22.69	1.64	all amide nitrogens with 2 hydrogens (only on sidechains)	ARG_NH1,ARG_NH2,ASN_ND2,GLN_NE2
N4H3u	1	21.41	1.64	amide nitrogen charged, with 3 hydrogens	LYS_NZ
O1H0u	27	15.91	1.42	all oxygens in carboxyl or carbonyl groups (no distinction made between oxygens in carboxyl group)	ALA_O,ARG_O,ASN_O,ASN_OD1,ASP_O,ASP_OD1,ASP_OD2,CSS_O,CYS_O, GLN_O,GLN_OE1,GLU_O,GLU_OE1,GLU_OE2,GLY_O,HIS_O,ILE_O,LEU_O,LYS_O, MET_O,PHE_O,PRO_O,SER_O,THR_O,TRP_O,TYR_O,VAL_O
O2H1u	3	17.98	1.46	all hydroxyl atoms	SER_OG,THR_OG1,TYR_OH
S2H0u	2	29.17	1.77	sulfurs with no hydrogens	CSS_SG,MET_SD
S2H1u	1	36.75	1.77	sulfurs with one hydrogen	CYS_SG