

# ASP's for non-hydrogen solvent accessible surface area in A<sup>2</sup>.

#	Key	ID	Radius	ASP	Type	Comment
APOLAR	SC	1.91	1.000	C_ALI		# aliphatic -CH <sub>2</sub> , -CH <sub>3</sub> in side chains
APOLAR	SC	1.87	1.000	C_ARO		# aromatic =CH- & =CC- in Phe, Tyr, Trp, His and SULFUR
POLAR	SC	1.87	1.000	C_C=O		# C=O in carboxyl and carbonyl and C=N in Arg
POLAR	SC	1.76	1.000	N_AMI		# Nitrogens
POLAR	BB	1.76	1.000	N_POS		# Nitrogens in LYS and ARG
POLAR	SC	1.74	1.000	O_OXY		# Oxygens
POLAR	BB	1.74	1.000	O_OH-		# Hydroxy Oxygens
POLAR	BB	1.70	1.000	O_NEG		# Oxygens
UNKNOWN	SC	0.00	0.000	UNKN_		# unknown atom type; do not change!

# This is the RAE-3 GETAREA library of AA Aliphatic Cs

RESIDUE	ANY	0
RESIDUE	ALA	1
CB	C_ALI	
RESIDUE	ARG	3
CB	C_ALI	
CG	C_ALI	
CD	C_ALI	
RESIDUE	ASN	1
CB	C_ALI	
RESIDUE	ASP	1
CB	C_ALI	
RESIDUE	CYS	1
CB	C_ALI	
RESIDUE	GLN	2
CB	C_ALI	
CG	C_ALI	
RESIDUE	GLU	2
CB	C_ALI	
CG	C_ALI	
RESIDUE	GLY	0
RESIDUE	HIS	4
CB	C_ALI	
CG	C_ARO	
CD2	C_ARO	
CE1	C_ARO	
RESIDUE	ILE	4
CB	C_ALI	
CG1	C_ALI	

CG2 C\_ALI  
CD1 C\_ALI  
RESIDUE LEU 4  
CB C\_ALI  
CG C\_ALI  
CD1 C\_ALI  
CD2 C\_ALI  
RESIDUE LYS 4  
CB C\_ALI  
CG C\_ALI  
CD C\_ALI  
CE C\_ALI  
RESIDUE MET 3  
CB C\_ALI  
CG C\_ALI  
CE C\_ALI  
RESIDUE PHE 7  
CB C\_ALI  
CG C\_ARO  
CD1 C\_ARO  
CD2 C\_ARO  
CE1 C\_ARO  
CE2 C\_ARO  
CZ C\_ARO  
RESIDUE PRO 3  
CB C\_ALI  
CG C\_ALI  
CD C\_ALI  
RESIDUE SER 1  
CB C\_ALI  
RESIDUE THR 2  
CB C\_ALI  
CG2 C\_ALI  
RESIDUE TRP 9  
CB C\_ALI  
CG C\_ARO  
CD1 C\_ARO  
CD2 C\_ARO  
CE2 C\_ARO  
CE3 C\_ARO  
CZ2 C\_ARO  
CZ3 C\_ARO  
CH2 C\_ARO

RESIDUE TYR 7

CB C\_ALI

CG C\_ARO

CD1 C\_ARO

CD2 C\_ARO

CE1 C\_ARO

CE2 C\_ARO

CZ C\_ARO

RESIDUE VAL 3

CB C\_ALI

CG1 C\_ALI

CG2 C\_ALI