

Supplementary table 1 List of amino acid indices were used in REALoc

Accession number	Data description
ANDN920101	alpha-CH chemical shifts
ARGP820101	Hydrophobicity index
BIGC670101	Residue volume
BROC820101	Retention coefficient in TFA
BULH740101	Transfer free energy to surface
BULH740102	Apparent partial specific volume
BUNA790101	alpha-NH chemical shifts
BUNA790102	alpha-CH chemical shifts
BUNA790103	Spin-spin coupling constants 3JHalpha-NH
BURA740101	Normalized frequency of alpha-helix
BURA740102	Normalized frequency of extended structure
CHAM810101	Steric parameter
CHOP780201	Normalized frequency of alpha-helix
DAWD720101	Size
DAYM780201	Relative mutability
FASG760101	Molecular weight
GEIM800104	Alpha-helix indices for alpha/beta-proteins
GEIM800105	Beta-strand indices
GEIM800107	Beta-strand indices for alpha/beta-proteins
GOLD730101	Hydrophobicity factor
GOLD730102	Residue volume
GRART40101	Composition
GRAR740102	Polarity
GUYH850101	Partition energy
HUTJ700101	Heat capacity
HUTJ700102	Absolute entropy
HUTJ700103	Entropy of formation
ISOY800101	Normalized relative frequency of alpha-helix
ISOY800102	Normalized relative frequency of extended structure
ISOY800103	Normalized relative frequency of bend
ISOY800104	Normalized relative frequency of bend R
ISOY800107	Normalized relative frequency of double bend
ISOY800108	Normalized relative frequency of coil
JANJ780102	Percentage of buried residues
JANJ780103	Percentage of exposed residues
JANJ790101	Ratio of buried and accessible molar fractions (36)

JANJ790102	Transfer free energy
JOND750101	Hydrophobicity
JOND920101	Relative frequency of occurrence
JOND920102	Relative mutability
JUKT750101	Amino acid distribution
JUNJ780101	Sequence frequency
KANM800101	Average relative probability of helix
KANM800102	Average relative probability of beta-sheet
KANM800103	Average relative probability of inner helix
KARP850101	Flexibility parameter for no rigid neighbors
KARP850102	Flexibility parameter for one rigid neighbor
KARP850103	Flexibility parameter for two rigid neighbors
KHAG800101	The Kerr-constant increments
KLEP840101	Net charge
KRIW710101	Side chain interaction parameter
KRIW790101	Side chain interaction parameter
KRIW790102	Fraction of site occupied by water
KRIW790103	Side chain volume
KYTJ820101	Hydropathy index
LEVM760101	Hydrophobic parameter
LEVM760103	Side chain angle theta(AAR)
LEVM760105	Radius of gyration of side chain
LEVM760107	van der Waals parameter epsilon
LEWP710101	Frequency of occurrence in beta-bends
LIFS790102	Conformational preference for parallel beta-strands
MAXF760101	Normalized frequency of alpha-helix
MAXF760102	Normalized frequency of extended structure
MAXF760103	Normalized frequency of zeta R
MAXF760104	Normalized frequency of left-handed alpha-helix
MAXF760105	Normalized frequency of zeta L
MEEJ810101	Retention coefficient in NaClO4
MEEJ810102	Retention coefficient in NaH2PO4
MEIH800102	Average reduced distance for side chain
MEIH800103	Average side chain orientation angle
MIYS850101	Effective partition energy
NAGK730101	Normalized frequency of alpha-helix
NAGK730102	Normalized frequency of beta-structure
NAGK730103	Normalized frequency of coil

NAKH900101	AA composition of total proteins
NAKH900102	SD of AA composition of total proteins
NAKH900103	AA composition of mt-proteins
NAKH900108	Normalized composition from fungi and plant
NAKH920101	AA composition of CYT of single-spanning proteins
NAKH920103	AA composition of EXT of single-spanning proteins
NAKH920105	AA composition of MEM of single-spanning proteins
NAKH920108	AA composition of MEM of multi-spanning proteins
OOBM770101	Average non-bonded energy per atom
OOBM850101	Optimized beta-structure-coil equilibrium constant
OOBM850102	Optimized propensity to form reverse turn
OOBM850105	Optimized side chain interaction parameter
PRAM900101	Hydrophobicity
RACS770102	Average reduced distance for side chain
RADA880108	Mean polarity
TANS770101	Normalized frequency of alpha-helix
TANS770103	Normalized frequency of extended structure
TANS770108	Normalized frequency of zeta R
TANS770109	Normalized frequency of coil
VELV850101	Electron-ion interaction potential
ZIMJ680101	Hydrophobicity
ZIMJ680103	Polarity
ZIMJ680104	Isoelectric point
WOLR790101	Hydrophobicity index
ENGD860101	Hydrophobicity index
FASG890101	Hydrophobicity index
