

Supplement to “Ranking predicted protein structures  
with support vector regression”

Jian Qiu

Department of Genome Sciences  
University of Washington  
Seattle, WA, USA

Will Sheffler

Department of Genome Sciences  
University of Washington  
Seattle, WA, USA

David Baker

Department of Biochemistry  
Department of Genome Sciences  
University of Washington  
Seattle, WA, USA

William Stafford Noble

Department of Genome Sciences  
Department of Computer Science and Engineering  
University of Washington  
Seattle, WA, USA

Feature	Description
T32S3	pairwise atomic potential
bk_tot-rep	full atom score without backbone H-bonds or repulsion
bup	buried unsatisfied polar groups
cb	C beta atom density solvation
co	contact order
env	residue burial preference
fa_atr	full atom attractive potential
fa_prob	full atom torsion angle preference
gsolt	surface area solvation
hb_lrbb	long range backbone hydrogen bonds
hb_sc	side chain hydrogen bonds
hb_srbb	short range backbone hydrogen bonds
hs	helix/sheet packing score
mGDT	median GDT_TS
mMS	median MaxSub
mTM	median TM
mrmsd	median RMSD
num_residues	number of residues
pair	residue-based pairwise potential
rama	phi/psi torsion angle preference
rg	radius of gyration
sasa	solvent accessible surface area
sasapack	packing quality score
sheet	beta strand arrangement score
vdw	van der waals repulsion

Table 1: **The features included in the training.**

Feature	Description	Weight
T32S3	pairwise atomic potential	3.695
num_residues	number of residues	3.026
env	residue burial preference	2.931
fa_prob	torsion angle preference	2.799
hb_lrbb	long range backbone hydrogen bonds	2.567
sasapack	packing quality score	2.208
sasa	solvent accessible surface area	2.097
pair	residue-based pairwise potential	1.952
hb_srbb	short range backbone hydrogen bonds	0.510
co	contact order	0.396
sheet	beta strand arrangement score	0.211
hb_sc	side chain hydrogen bonds	0.106

Table 2: **The weights of the features in the SVR score without consensus-based features.**