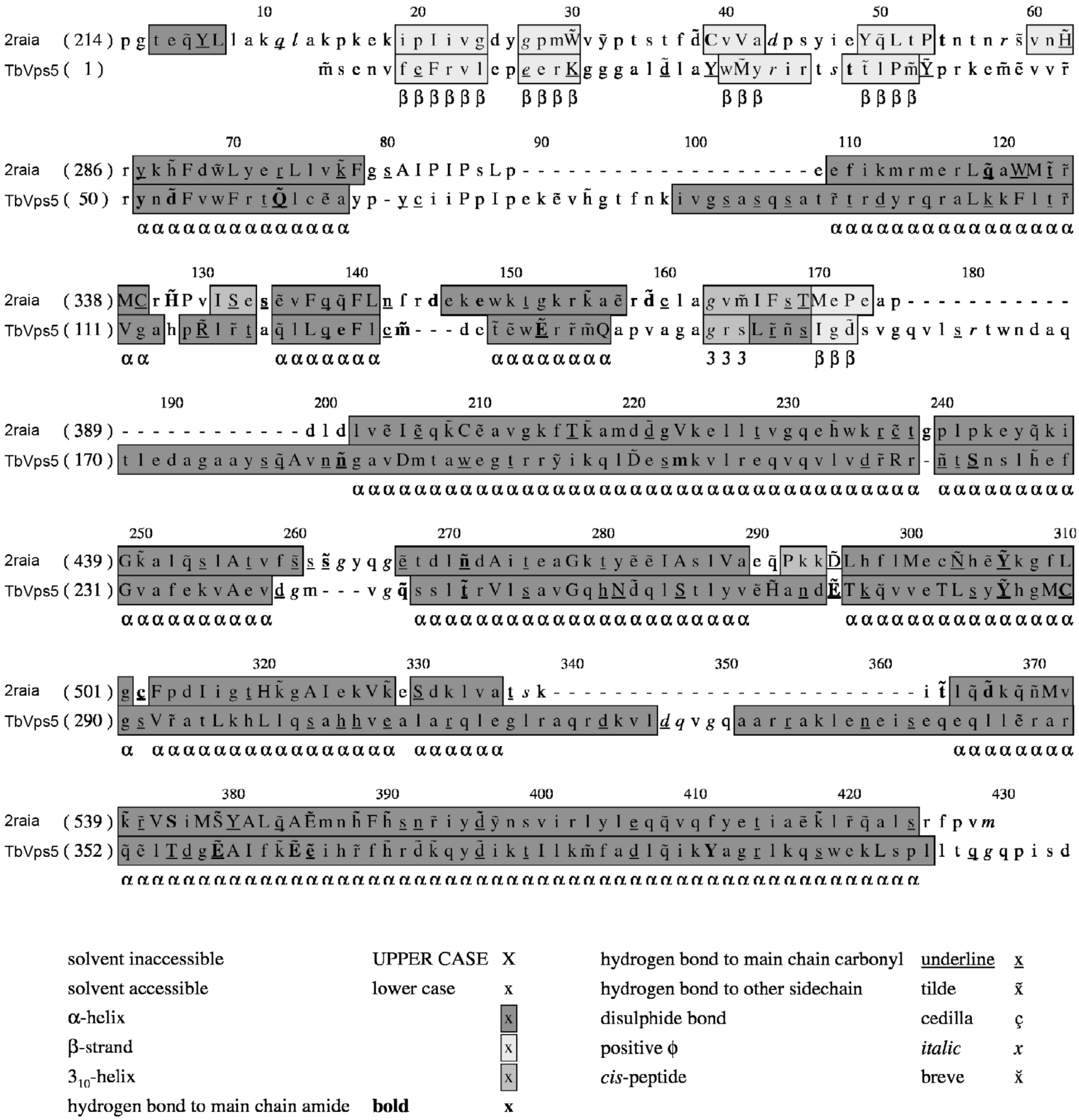
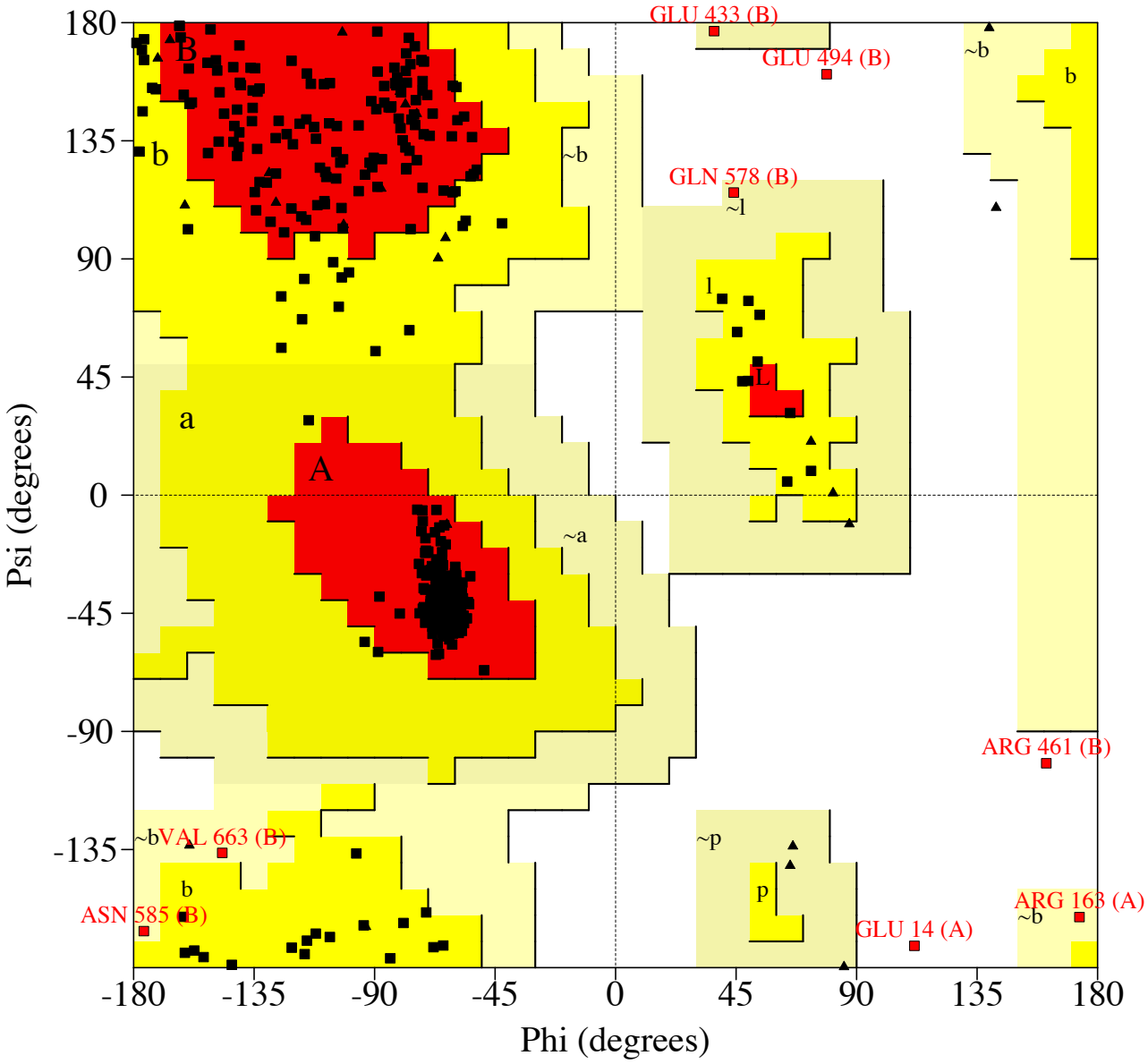

2raia
TbVps5
solvent inaccessible UPPER CASE X
solvent accessible lower case x
α-helix
β-strand
3₁₀-helix
hydrogen bond to main chain amide bold x
hydrogen bond to main chain carbonyl underline x
hydrogen bond to other sidechain tilde x̃
disulphide bond cedilla ç
positive ϕ italic x
cis-peptide breve x̆

Ramachandran Plot
TbVps5 dimer



Plot statistics

Residues in most favoured regions [A,B,L]	704	92.1%
Residues in additional allowed regions [a,b,l,p]	52	6.8%
Residues in generously allowed regions [~a,~b,~l,~p]	5	0.7%
Residues in disallowed regions	3	0.4%
Number of non-glycine and non-proline residues	764	100.0%
Number of end-residues (excl. Gly and Pro)	4	
Number of glycine residues (shown as triangles)	48	
Number of proline residues	22	
Total number of residues	838	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

As an extra validation check to the TbVps5 model, we examined the conservation of the interactions observed at the dimeric interfaces of the crystal structure of sorting nexin-9 (SNX9; PDB-Id: 2RAI) and the theoretical model of TbVps5. We obtained alignments by BLAST searches in the non-redundant database using the amino acid sequences of the crystal structure of SNX9 and TbVps5. In the case of the BLAST search with the Snx9 sequence, the alignment included SNX9, SNX18 and SNX33 amino acid sequences, while in the case of the BLAST search with the TbVps5 sequence, the alignment included SNX1 and SNX2 amino acid sequences. We accepted those other nexins in order to reduce the number of conserved residues obtained in the alignment. Then, we matched those equivalent residues, from both sorting nexins, making interactions in both dimeric interfaces with those that have high degree of conservation in both BLAST families. Equivalent residues are those residues located in similar positions in the 3D structures of the two proteins which can be identified as aligned residues in an amino acid sequence alignment of the two proteins. Even with the reduced amount of conservation obtained in the BLAST alignment, due to the acceptance of other homologous sorting nexins, several equivalent residues that make interactions in both dimers and are also conserved in both families are obtained. Table 1 shows those equivalent residues, the type of interactions they are involved in and the type of conservation observed. When residues make several different types of interactions, only those that are similar in the two dimeric structures are presented in the table. The high degree of conservation observed in the residues involved in dimerization in both the crystal structure of SNX9 and the theoretical model of TbVps5 is a good indication that TbVps5 may exist as a dimer with a dimeric structure close to that observed in the model.

Table 1.

SNX9			TbVps5		
Residue	**Interaction type**	**Conservation**	**Residue**	**Interaction type**	**Conservation**
L416	Hydrophobic	Hydrophobic amino acid	L209	Hydrophobic	Hydrophobic amino acid
R246	Salt bridge	Positive amino acid	R219	Induced dipole	Always arginine
I438	Hydrophobic	Hydrophobic amino acid	F230	Hydrophobic	Hydrophobic amino acid
L460	Hydrophobic	Always leucine but one Phe	L249	Hydrophobic	Always leucine
H556	Hydrophobic	Polar amino acid	H369	Hydrophobic	Polar amino acid
R559	Salt bridge	Always arginine	K372	Salt bridge	Positive amino acid
N564	Hydrophobic and polar	Polar amino acid	K377	Hydrophobic and polar	Positive amino acid
I567	Hydrophobic	Hydrophobic amino acid	L380	Hydrophobic	Hydrophobic amino acid
Y570	Hydrophobic	Aromatic amino acid	F383	Hydrophobic	Aromatic amino acid