Table S1. Cross-check validation report of homology models

Cross-check	Ramachandran plot statistics by PROCHECK					
	2Z81		1O77		2Z5V	
	X-ray	**HM**[a]	**X-ray**	**HM**	**X-ray**	**HM**
Most favored regions	82.9	86.4	81.4	88.5	75.4	86.6
Additionally allowed regions	16.7	10.2	17.1	9.2	23.8	11.8
Generously allowed regions	0.4	2.6	1.6	0.8	0.8	0.8
Disallowed regions	0.0	0.8	0	1.5	0	0.8

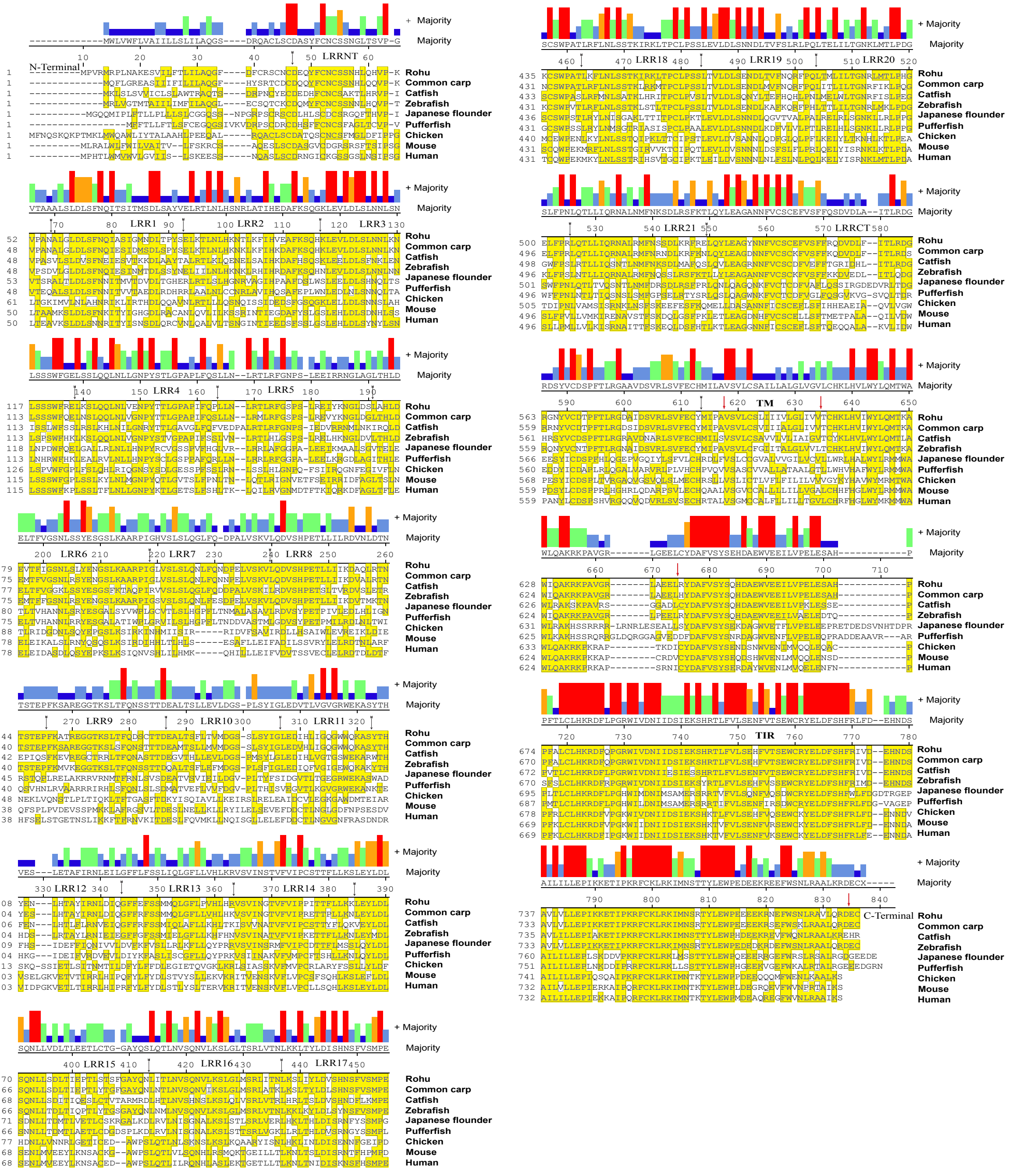
[a] HM- homology models

Table S2. List of predicted binding sites in rohu TLR2-ECD

Binding sites	**Amino acids**
B1	Thr273, Leu276, Val278, Ser304, Leu311
B2	Lys236, Arg241, Glu247, Phe275, Val278,
B3	Lys168, Leu177, Phe182, Leu187, Ser194, Leu206, Leu223
B4	Ala534, Gly535, Asn537, Val540, Leu555, Val567
B5	Asn392, Leu396, Ser399, Tyr421, Asp423, Phe444, Ser448, Ser469
B6	Ser245, Thr248, Lys258, Leu272, Val278, Asp280
B7	Ile487, Thr495, Leu496, Met517, Asn519, Asp522
B_{mouse}	Asn318, Asp320, Gly323, Gln332, His341, Gly348, Val350

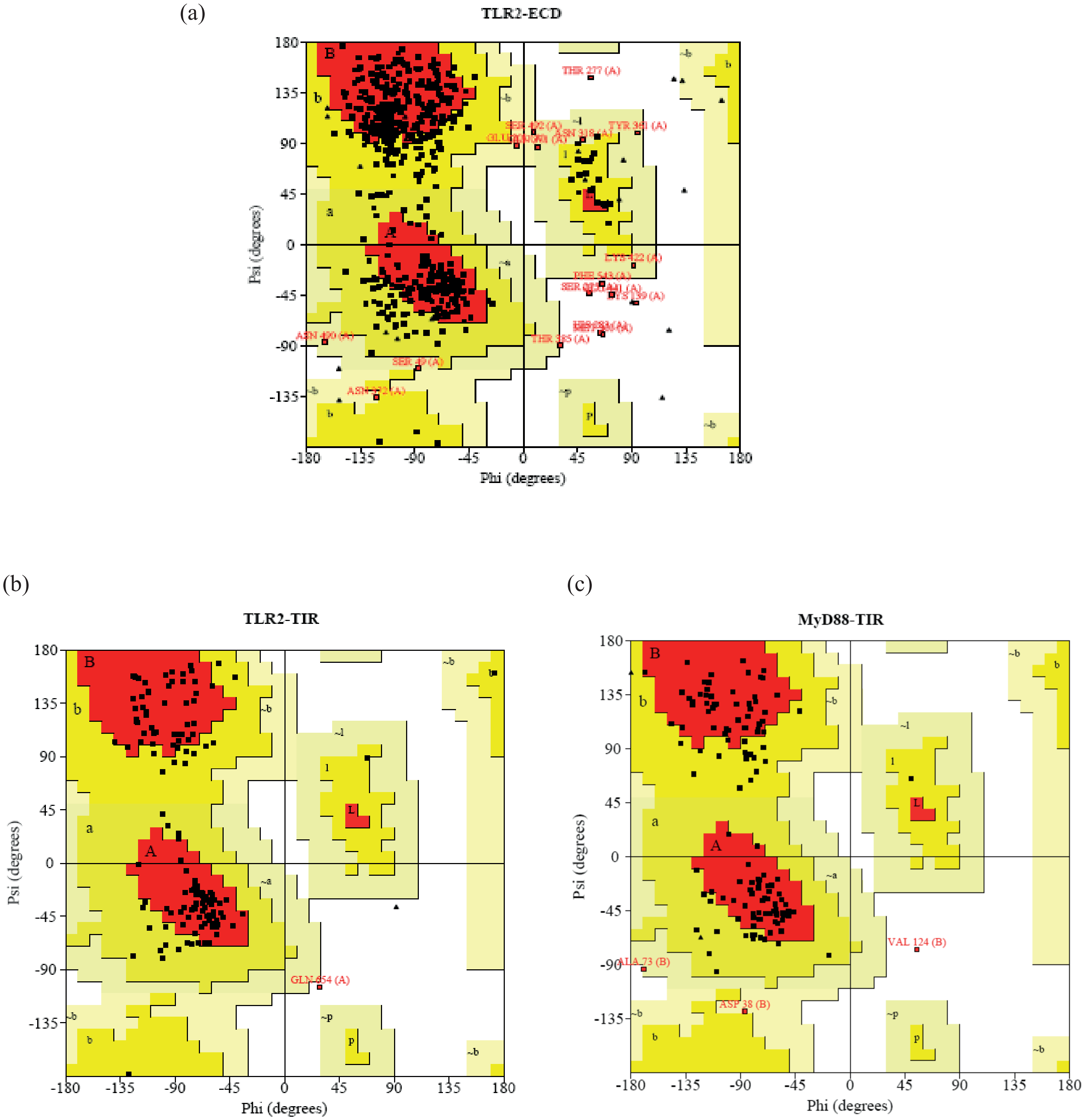
Table S3. The predicted interface residues in TLR2-TIR and MyD88-TIR domains

	TLR2-TIR	**MyD88-TIR**
cons-PPISP	H672, A676, C678, D683, F684, P686, G687, R688, W689, V691, D692, I694, D696, I698, S701, R719, L722, S725, H726, R728, H733, S736	C44, V45, A49, S50, E51, L52, E54, K55, R56, R59, K79, F80, L82, S83, L84, C85, P86, W127, R129, L130, K133, S136, L137
PatchDock	R645, Y646, V650, S651,Q685, I698, E699, K700, S701, H702, T704, L722, H726, F727, R728, I729, D731, H733, N734, D735	A81, L82, S83, L84, P86, G87, T88, H89, S90, K91, R92, L109, R110, F111, C115, D116, T118, R119, Q123, S121, F126
InterProSurf	D646, D647, I663, V665, P666, F675, A676, L677, I690, V691, D692, I694, S701, H702, R703, S725, H726, F727, R728, I729, V738, P751, L767, E768	C9, S11, H17, E18, K21, C33, F35, V39, W46, T47, F76, Q77, F80, L82, S83, H89, P104, F105, L109, R110, F111, I114, C115, D116, W125, F126, W127, I128, R129, A131, L135, S136

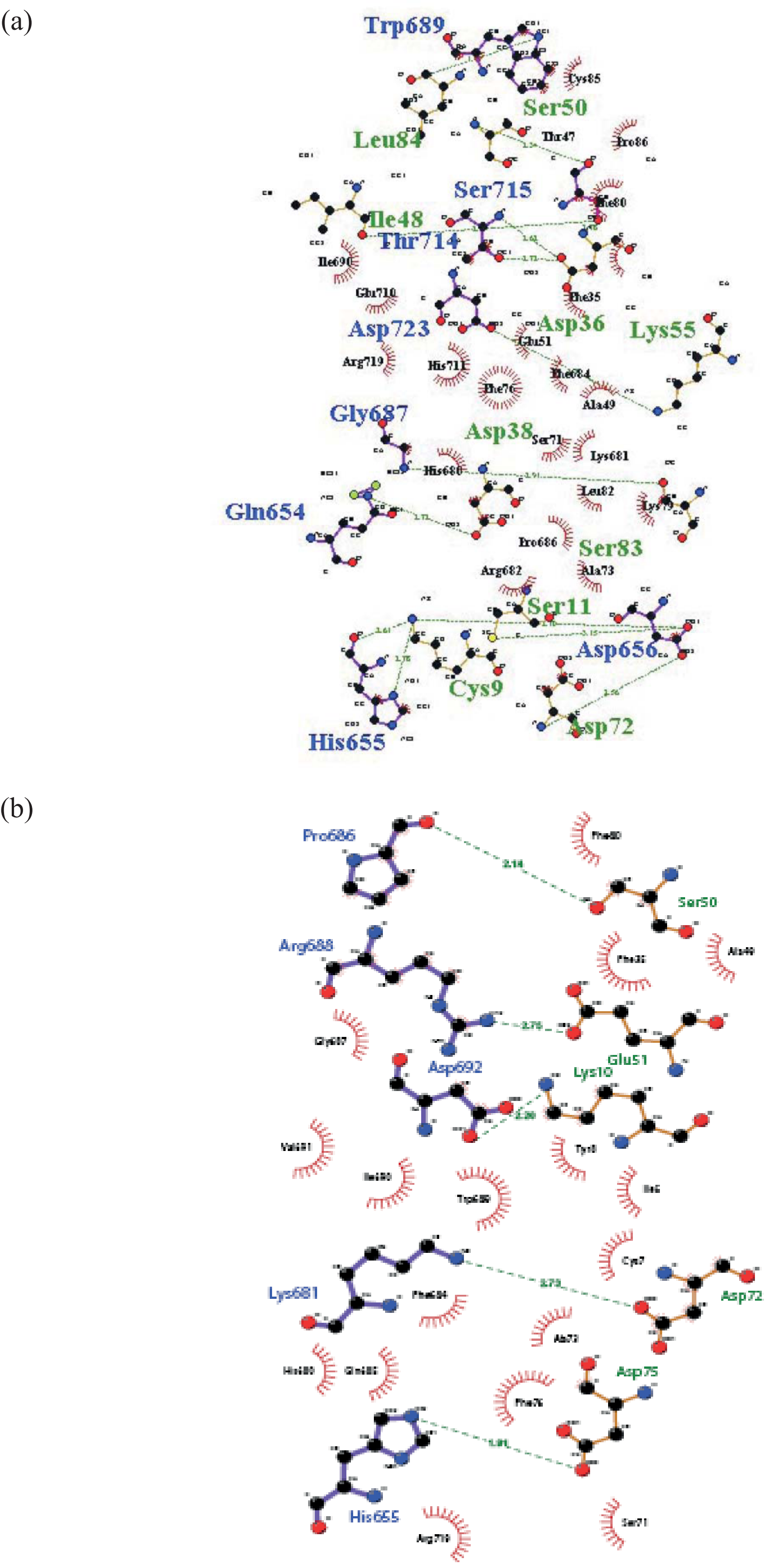


Supplementary figure 1. Multiple sequence alignment of rohu TLR2 with other species by MegAlign program

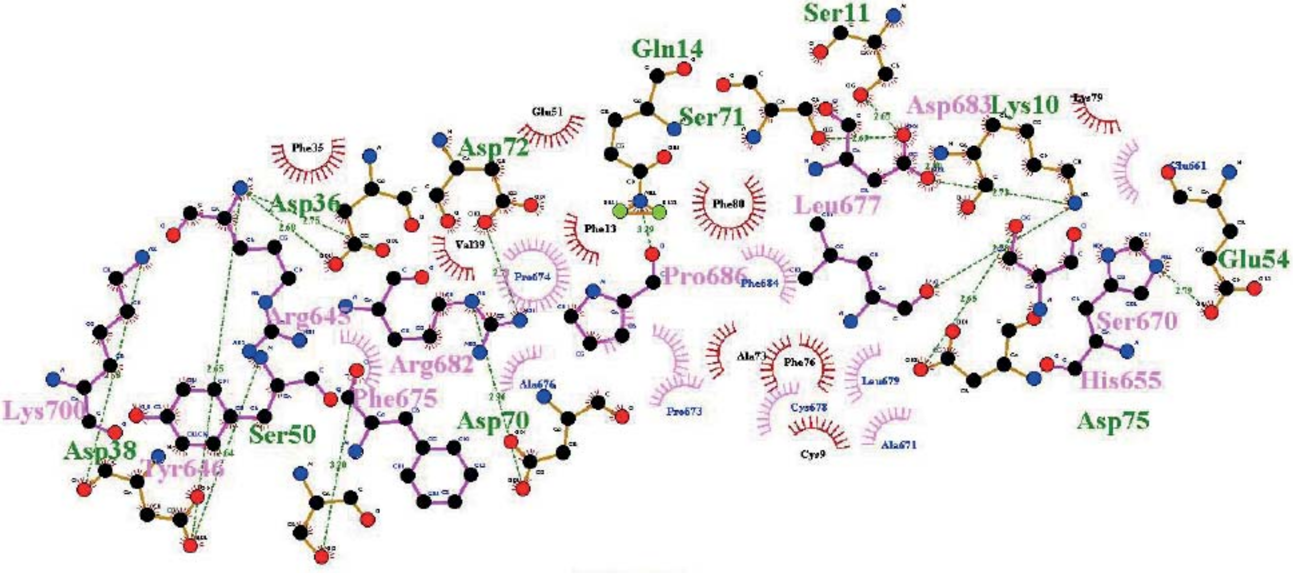
N-termini, C-termini, LRR, trans-membrane (TM) and TIR domain regions are labeled. Conserved residues are shown inside yellow box. Majority axis represents the highest occurrence of a residue in a column.



Supplementary Figure 2.
Ramachandran plot analysis of (a) TLR2-ECD, (b) TLR2-TIR and (c) MyD88-TIR model. The plot was calculated in PROCHECK program



Supplementary Figure 3.
DIMPLOT analysis of interaction between TLR2-TIR and MyD88-TIR domains (a) HADDOCK analysis and (b) ZDOCK analysis



Supplementary Figure 4.

The DIMPLOT analysis of TLR2-TIR and MyD88-TIR complex after 10 ns of MDS