

**S5 Text. Binary cross entropy loss function for training TripletRes in CASP13.**

The loss function is defined as the sum of cross entropy over all the residue pairs of the training proteins:

$$\mathcal{L}_{bin} = - \sum_{t=1}^T y_t \log(p_t) + (1 - y_t) \log(1 - p_t) \quad (\text{A})$$

Here,  $T$  is the total number of residue pairs in the training set.  $y_t = 1$  if the distance of  $t$ -th residue pair of native structure is below  $8\text{\AA}$ ; otherwise  $y_t = 0$ .  $p_t$  is the predicted probability that the  $t$ -th residue pair forms a contact.