

Supplementary Information

Charge Interactions Modulate the Encounter Complex Ensemble of Two Differently Charged Disordered Protein Partners of KIX

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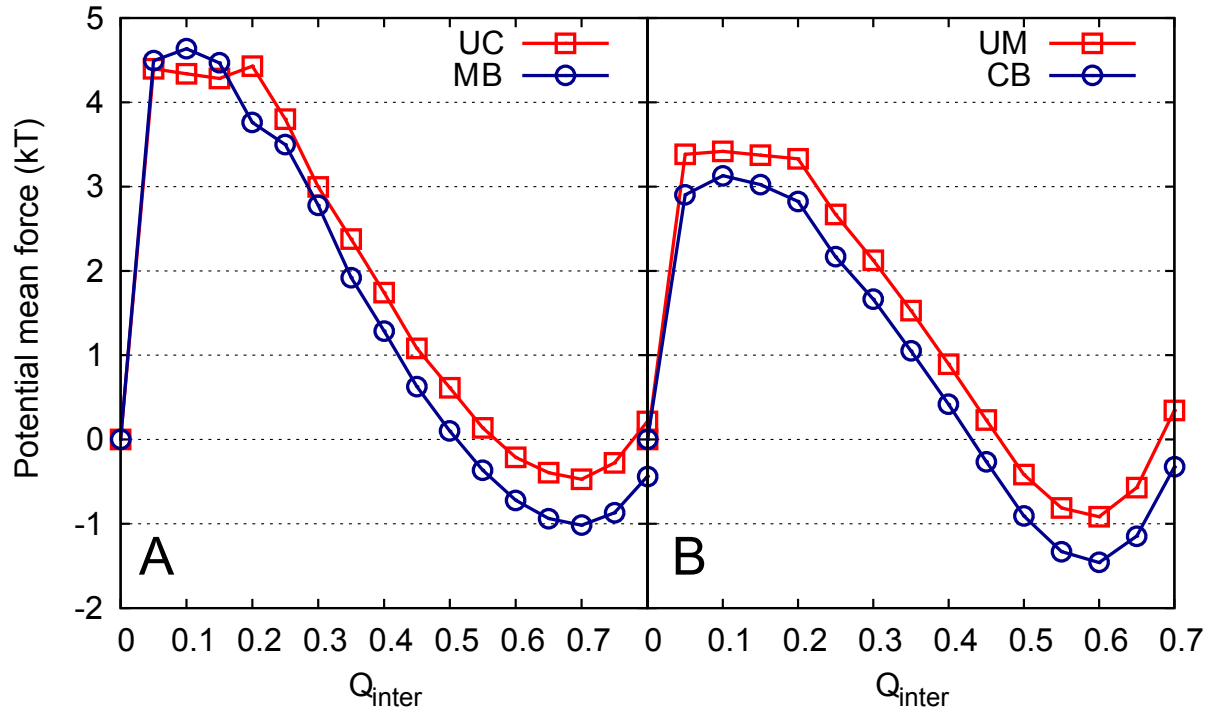


Fig. S1 The free energy curve of cMyb binding sub-processes without and with the second ligand (UC and MB, A) and MLL sub-processes without and with the second ligand (UM and CB, B) as a function of Q_{inter} . For better visualization, the free energy of unbound states are relocated to 0.

References

- [1] R. Giri, A. Morrone, A. Toto, M. Brunori and S. Gianni, *Proceedings of the National Academy of Sciences of the United States of America*, 2013, **110**, 14942–14947.

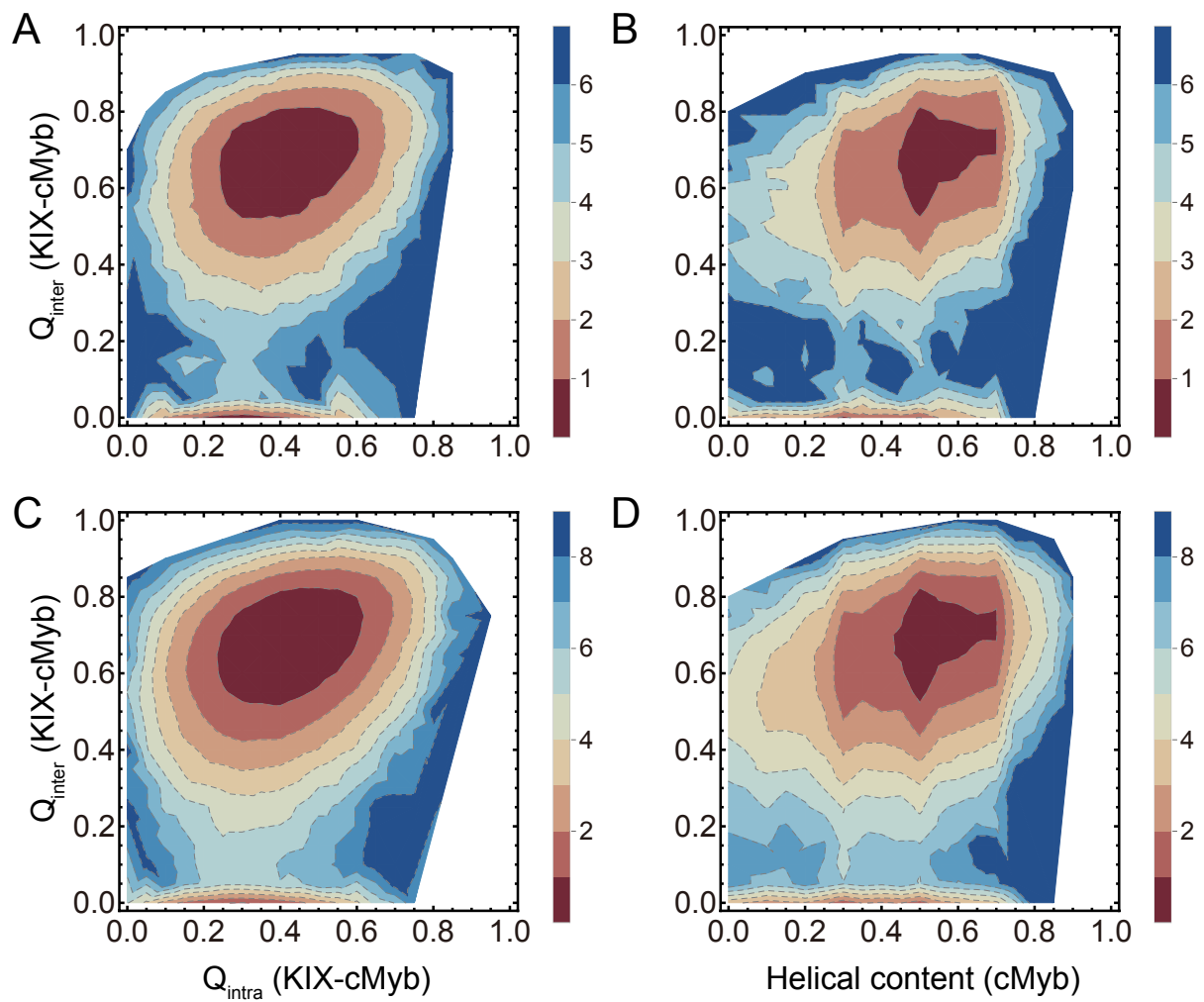


Fig. S2 The free energy profiles of cMyb folding-binding in UC (A and B) and MB (C and D) sub-processes. The reaction coordinates are the Q_{inter} between KIX and cMyb, the helical content of cMyb, and the Q_{intra} of cMyb. The free energy is in unit of kT.

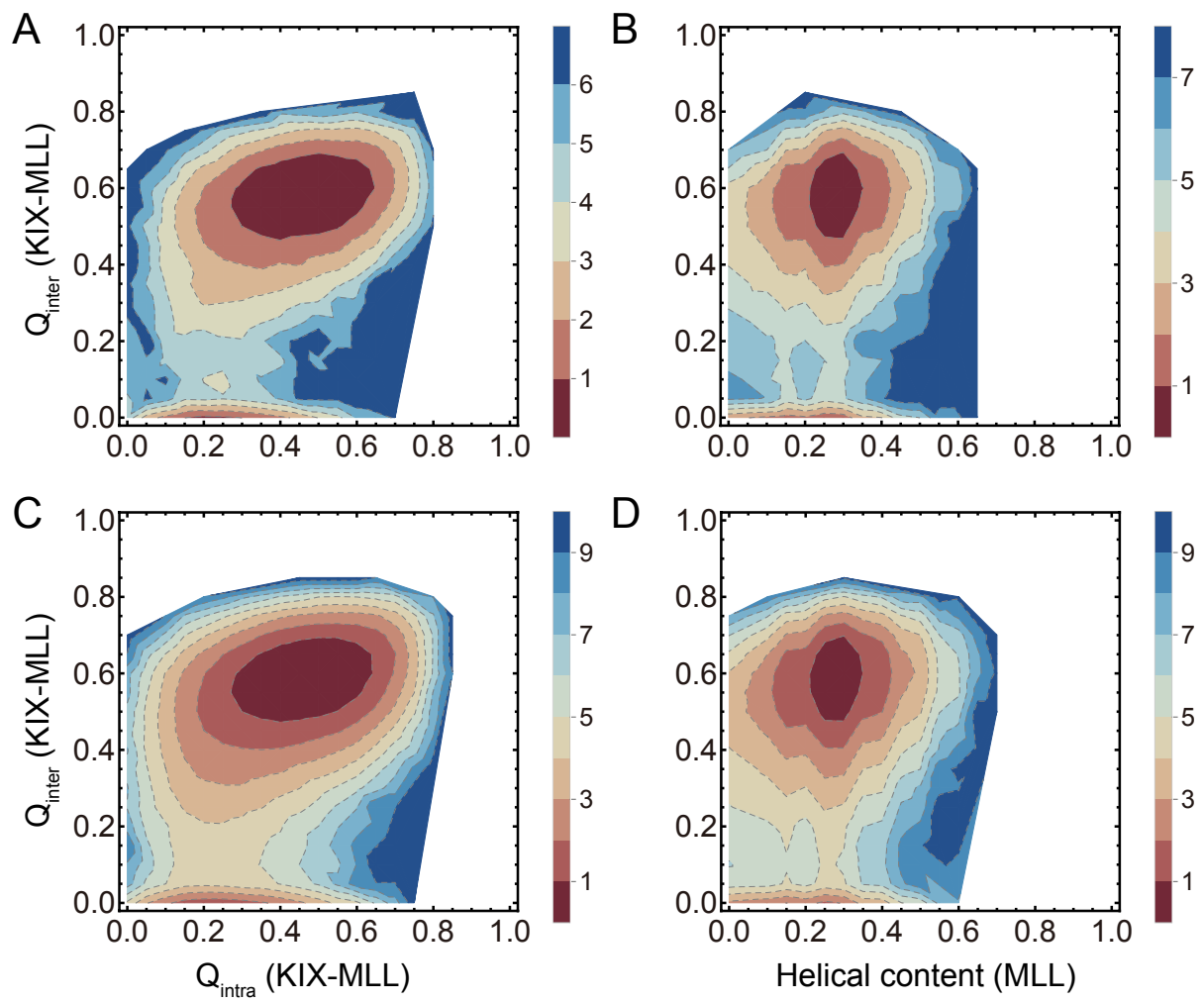


Fig. S3 The free energy profiles of MLL folding-binding in UM (A and B) and CB (C and D) sub-processes. The reaction coordinates are the Q_{inter} between KIX and MLL, the helical content of MLL, and the Q_{intra} of MLL. The free energy is in unit of kT.

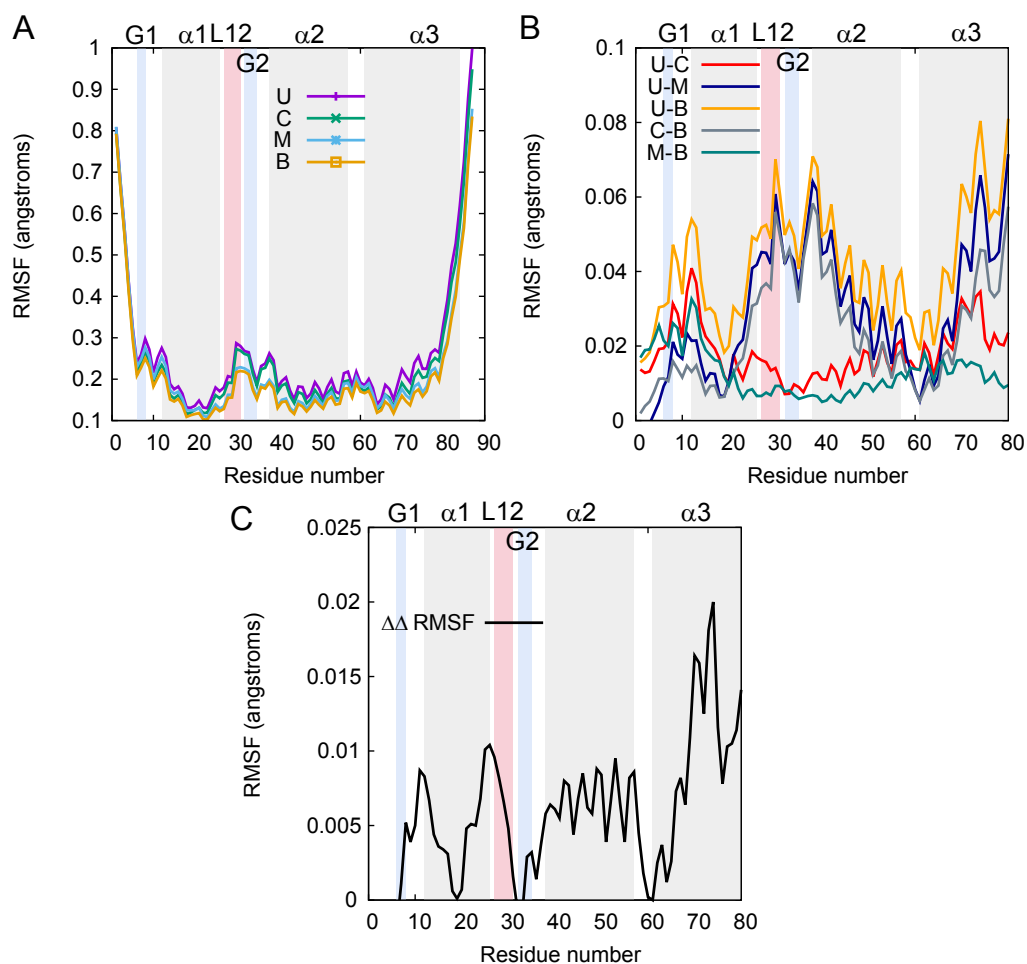


Fig. S4 (A) The RMSF of KIX at different states, with respect to the structure 2AGH. (B) The RMSF difference between U and other states, between B and other states. (C) The contribution of the first bound ligand on RMSF ($\Delta\Delta$ RMSF). The C-terminus of KIX is highly flexible with high RMSF values. Thus we do not show the RMSF difference data after residue 80. Important secondary structure components are labeled in these two panels.

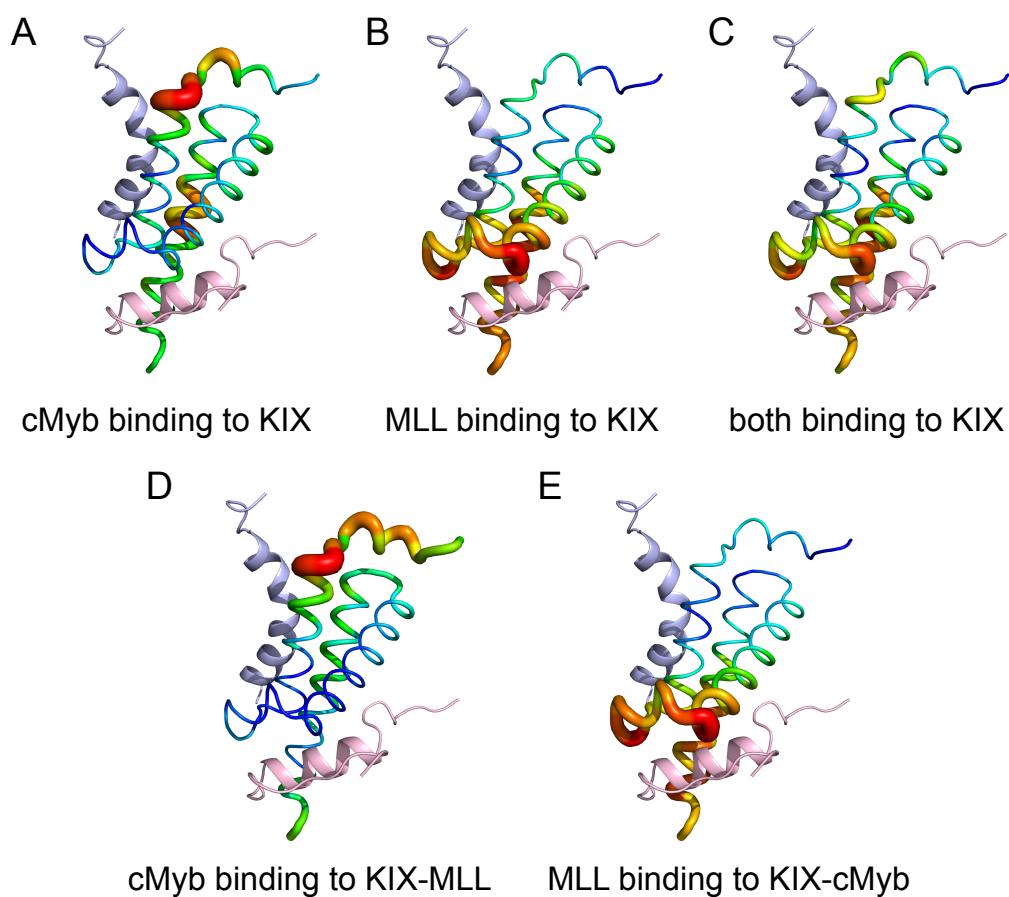


Fig. S5 The RMSF difference factor map of KIX between U and C states (A), U and M states (B), U and B states (C), M and B states (D), C and B states (E). Blue color corresponds to the lowest RMSF difference value in KIX and red to the highest. Ligands cMyb and MLL are illustrated in pale blue and pink cartoons. The RMSF difference data of KIX after residue 80 are not shown in this figure.

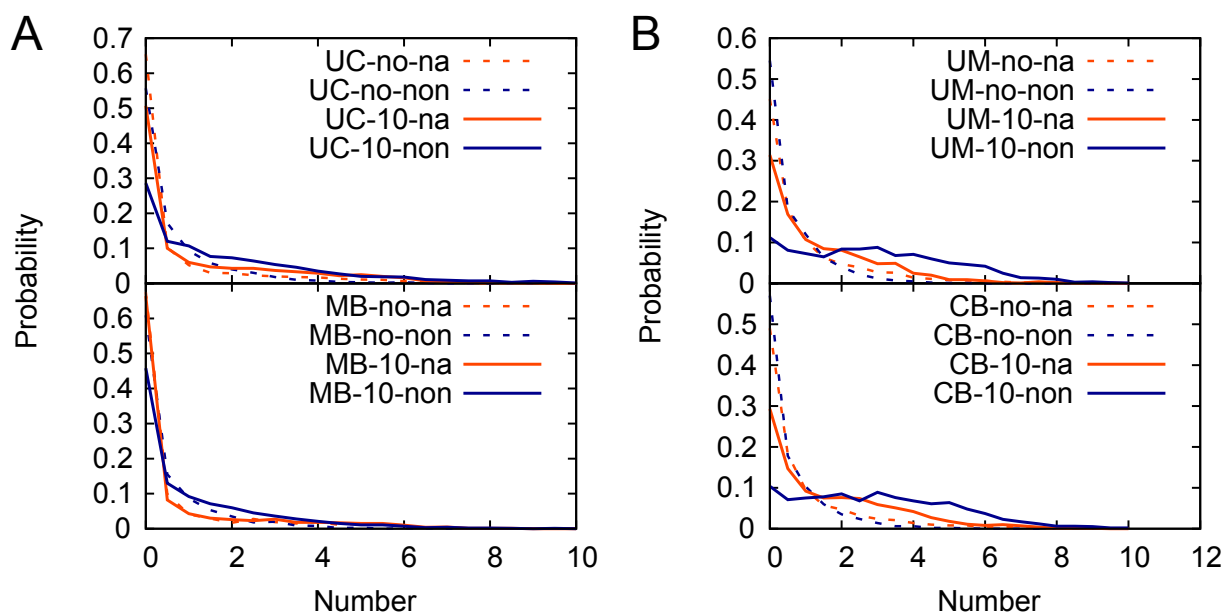


Fig. S6 The distribution of the number of inter-chain native contacts (orange) and non-native opposite-charged contacts (purple) within the encounter complex of cMyb binding sub-processes (UC and MB, A) and MLL binding sub-processes (UM and CB, B). The data at 10 mM ion strength is drawn in solid lines and that without charges in dashed lines.

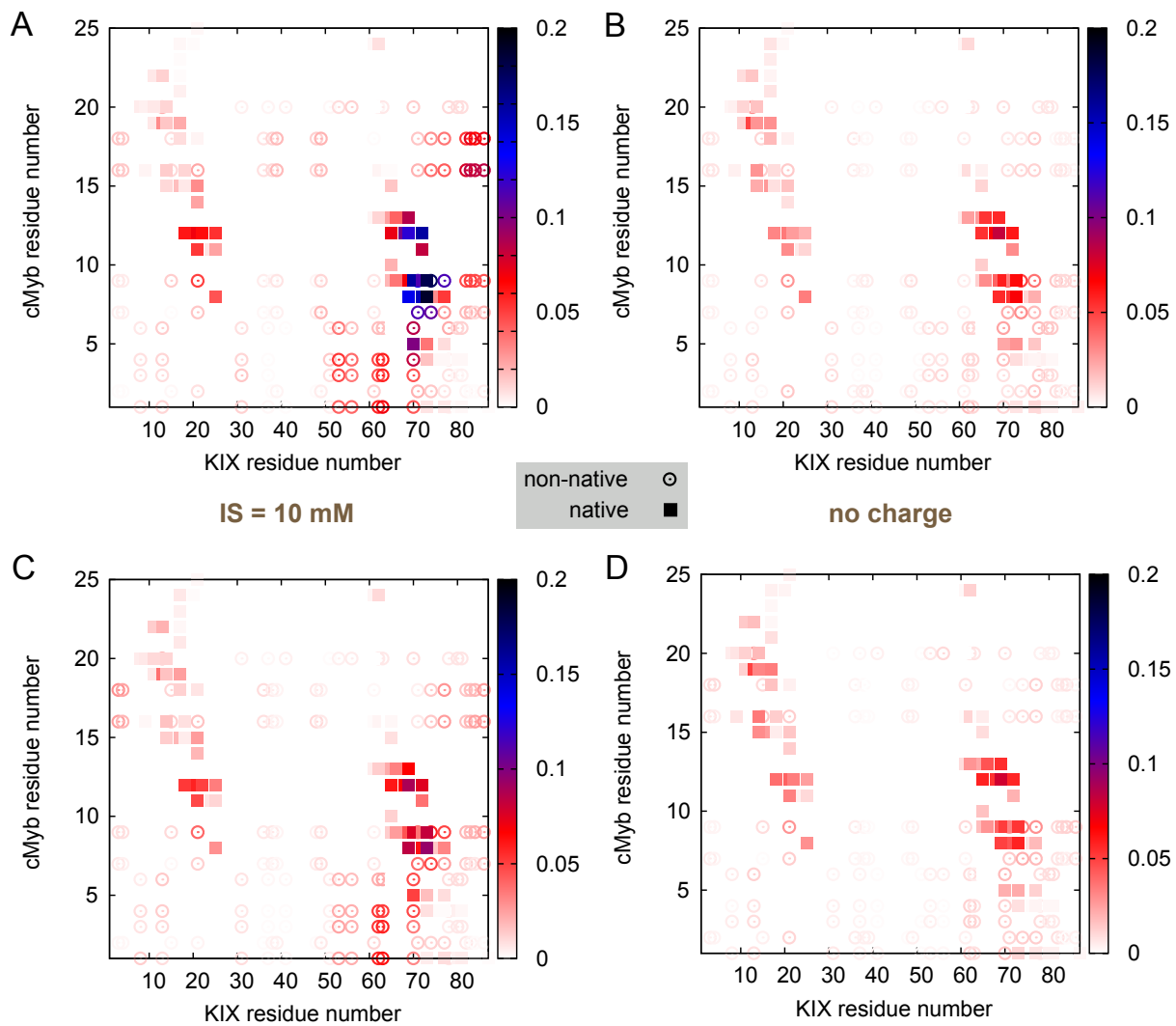


Fig. S7 Contact map of inter-chain native contacts and non-native opposite-charged contacts at the encounter state of cMyb binding sub-processes (UC (A and C) and MB (B and D)). Native contacts are illustrated as squares, non-native contacts are illustrated as circles.

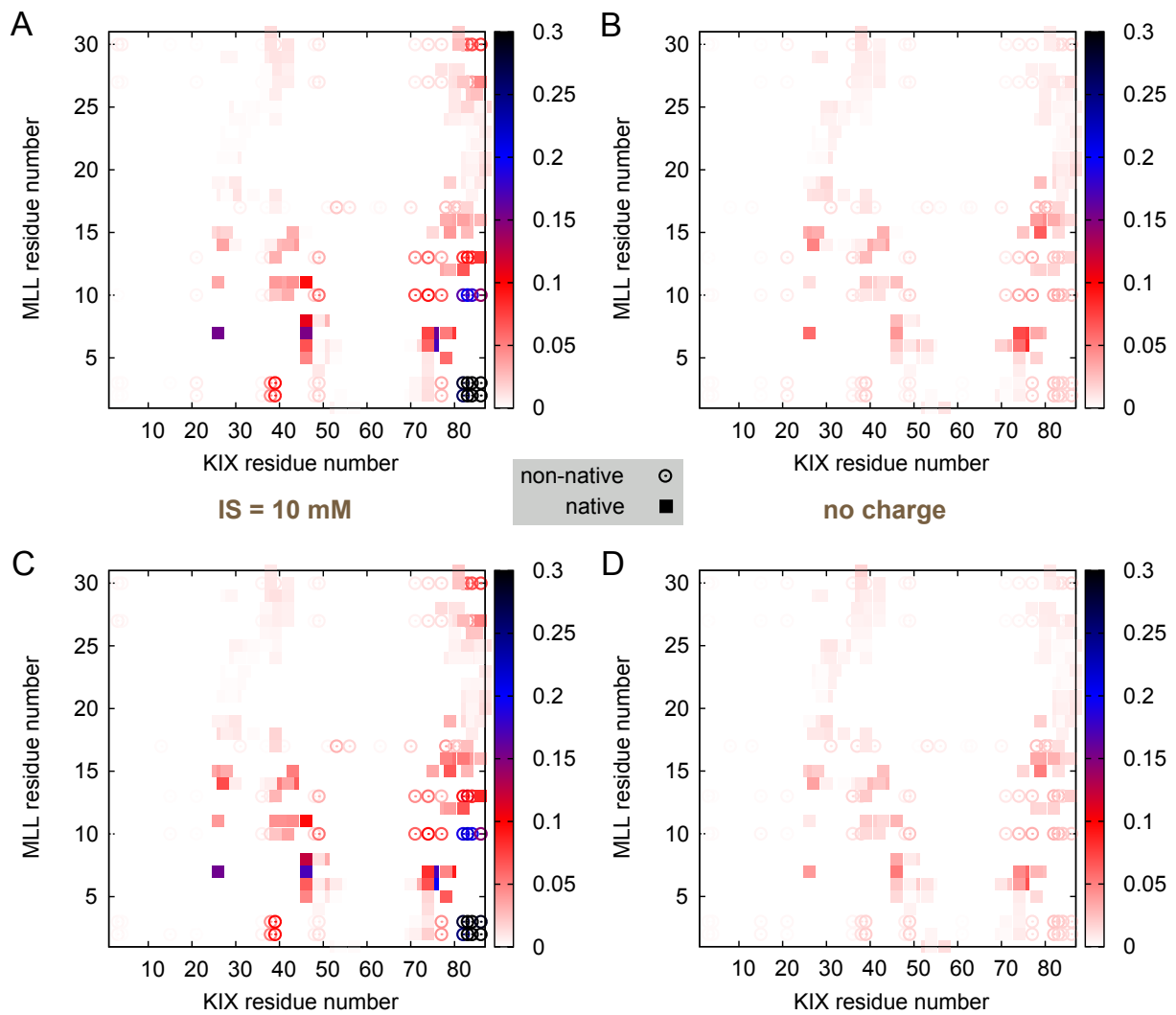


Fig. S8 Contact map of inter-chain native contacts and non-native opposite-charged contacts at the encounter state of MLL binding sub-processes (UM (A and C) and CB (B and D)). Native contacts are illustrated as squares, non-native contacts are illustrated as circles.

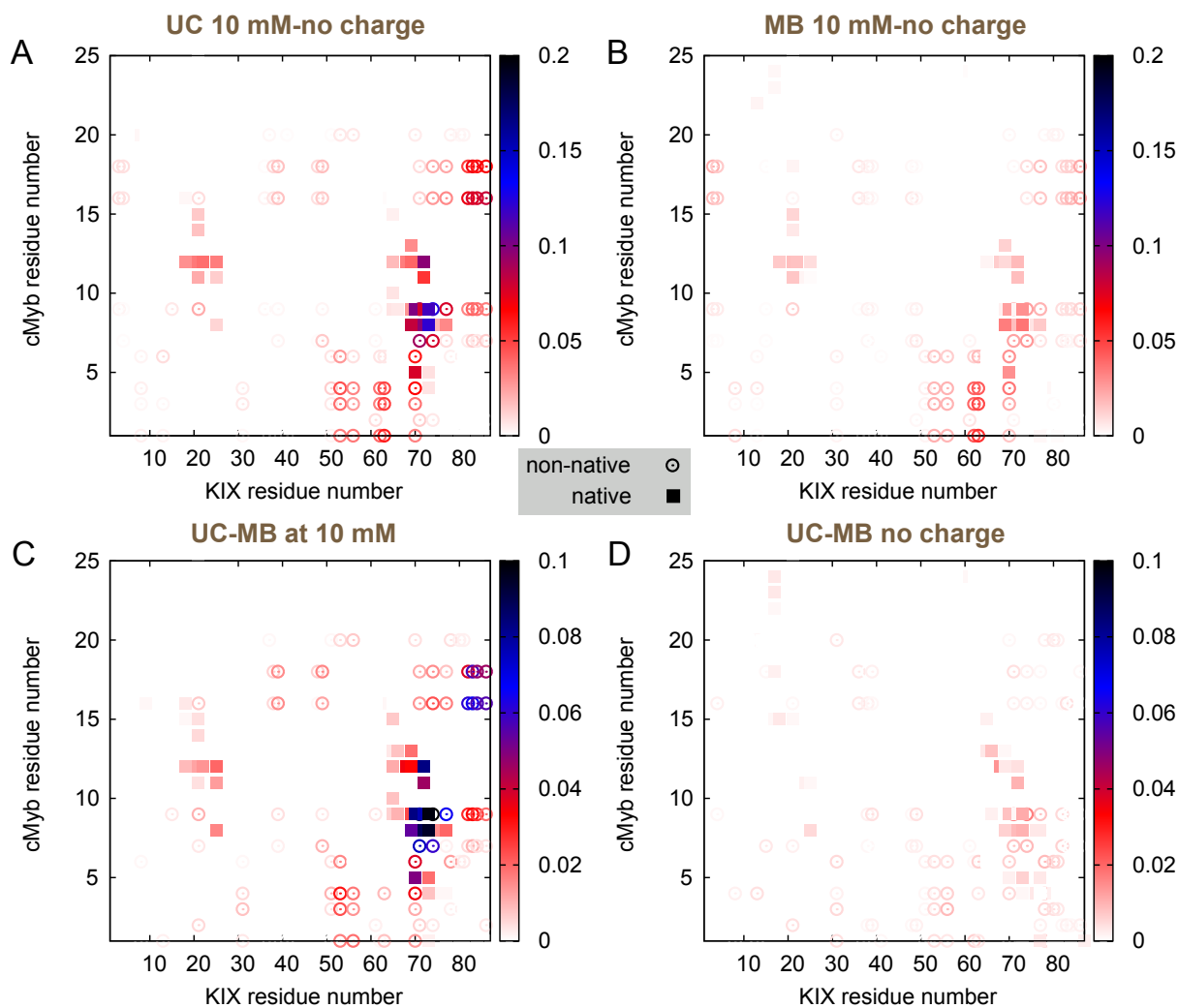


Fig. S9 Difference maps of inter-chain native contacts and non-native opposite-charged contacts at the encounter state of cMyb binding: (A) UC contact map at 10 mM – UC contact map without charges; (B) MB contact map at 10 mM – MB contact map without charges; (C) UC contact map at 10 mM – MB contact map at 10 mM; (D) UC contact map without charges – MB contact map without charges.

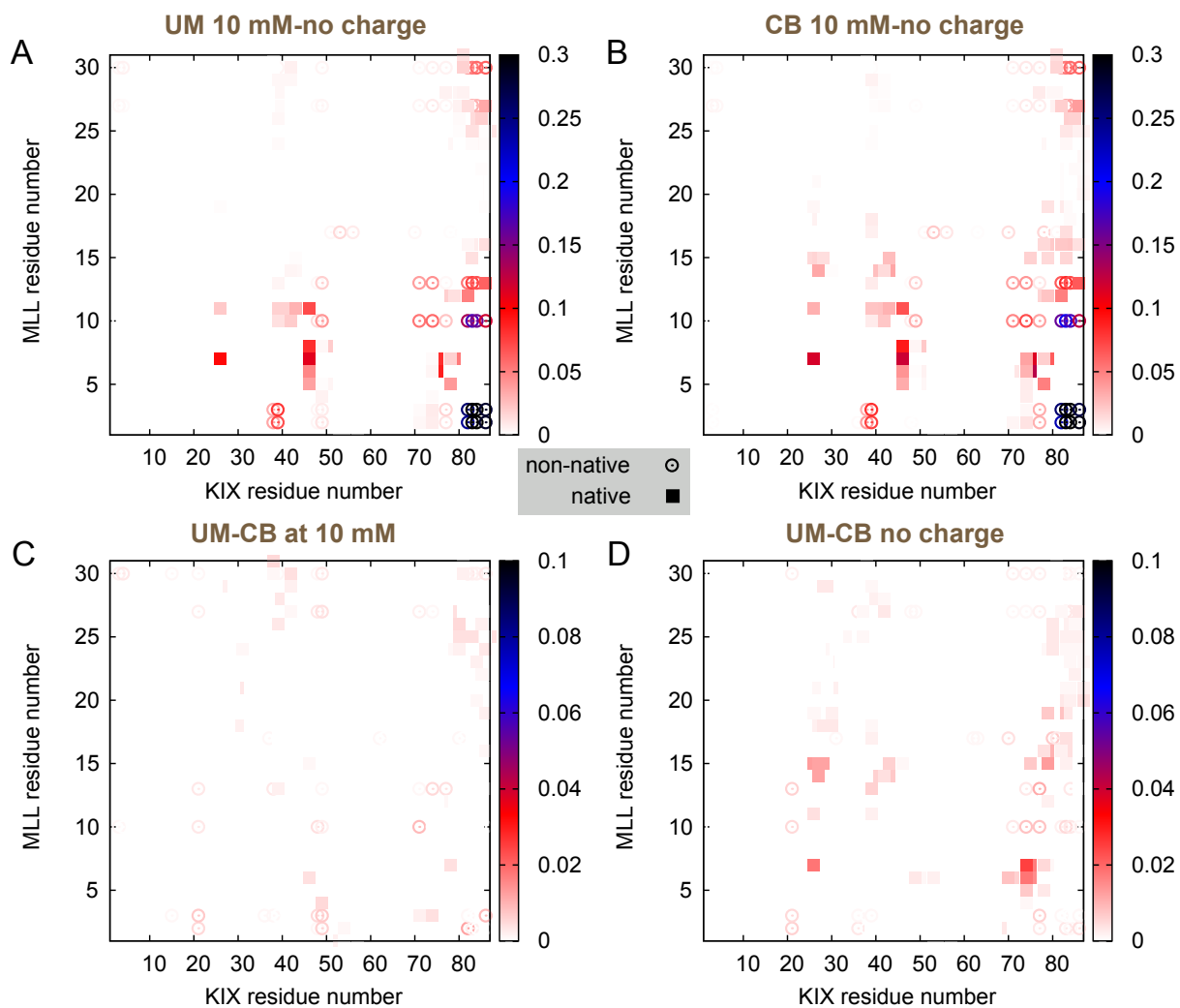


Fig. S10 Difference maps of inter-chain native contacts and non-native opposite-charged contacts at the encounter state of MLL binding: (A) UM contact map at 10 mM – UM contact map without charges; (B) CB contact map at 10 mM – CB contact map without charges; (C) UM contact map at 10 mM – CB contact map at 10 mM; (D) UM contact map without charges – CB contact map without charges.

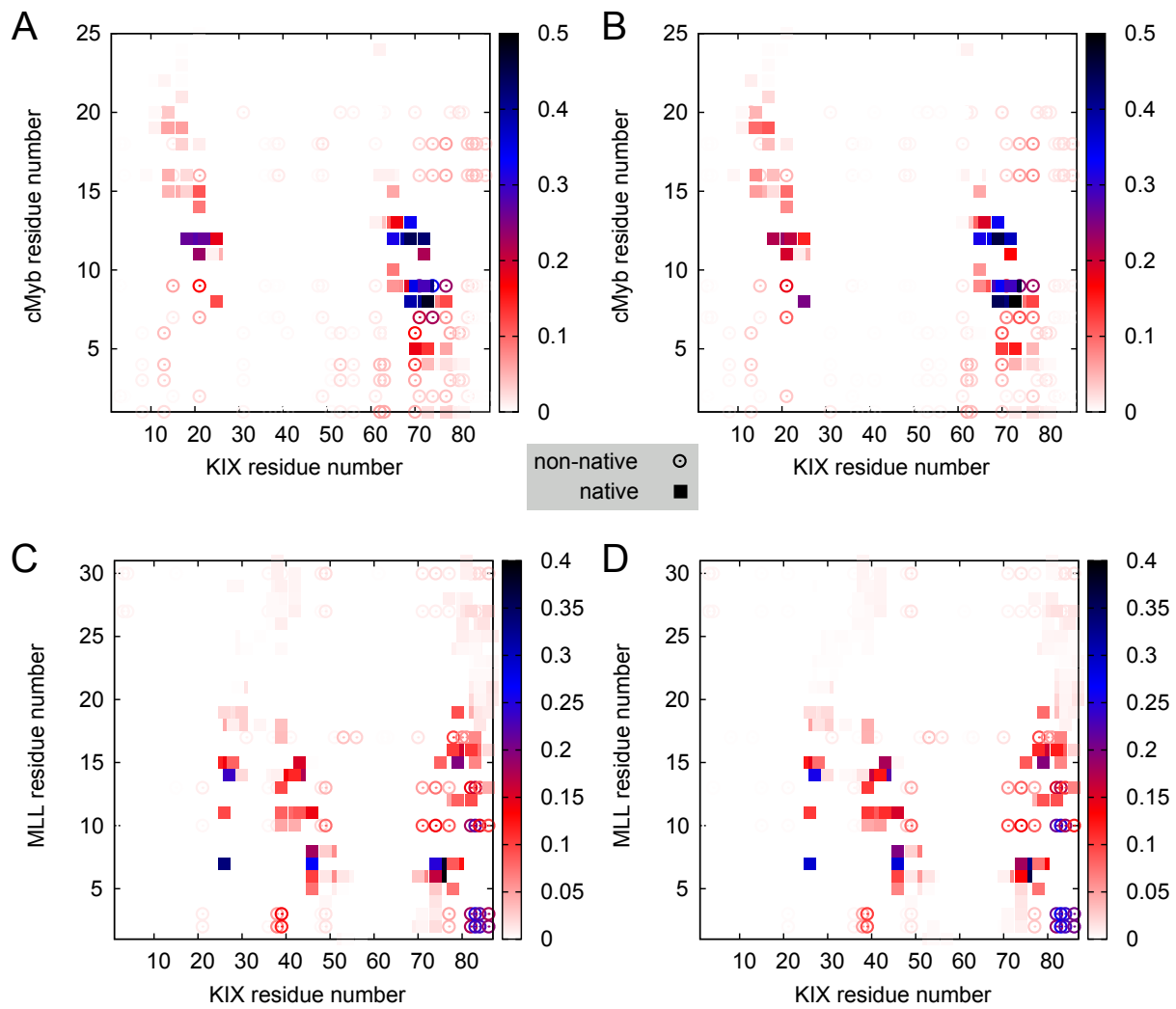


Fig. S11 Contact map of inter-chain native contacts and non-native opposite-charged contacts at the transition state of UC (A), MB (B), UM (C), and CB (D) binding sub-processes. The ionic strength is set to 150 mM according to the experimental condition. Native contacts are illustrated as squares, non-native contacts are illustrated as circles.

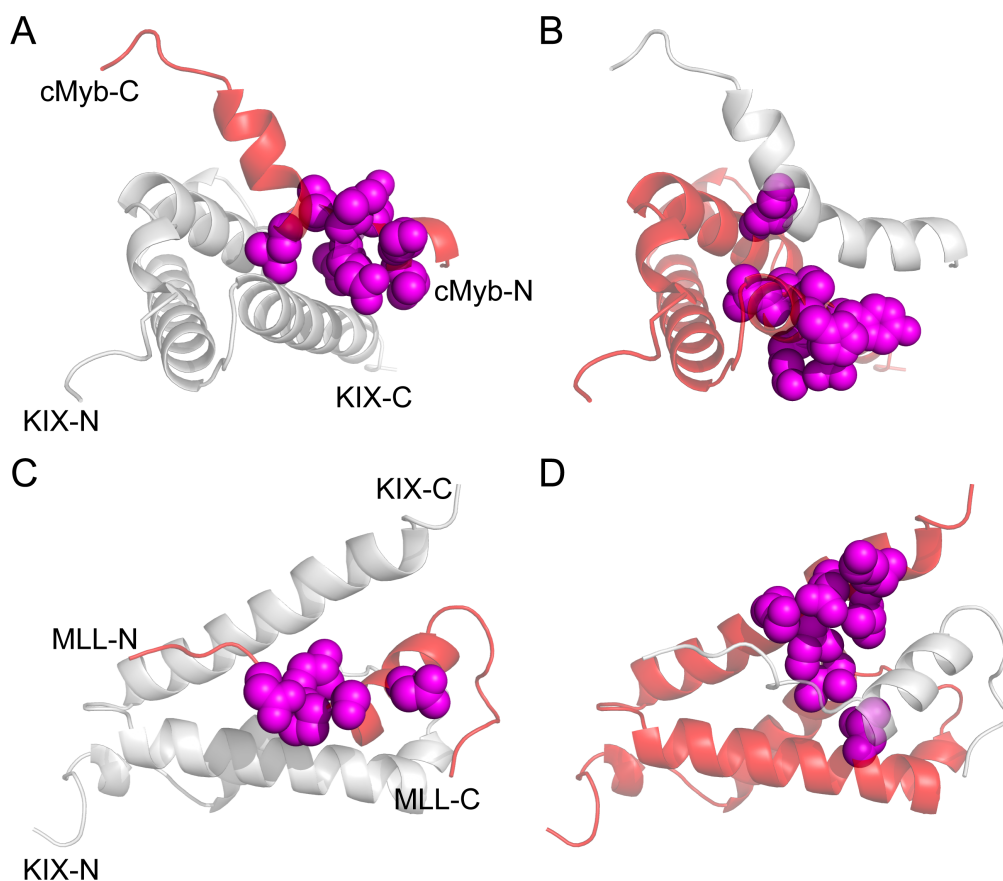


Fig. S12 Φ -value analysis on the binding process of KIX and cMyb (A and B) as well as KIX and MLL (C and D). Φ -values are colored as that in Ref¹, weak, $0 < \Phi < 0.3$ are represented in red; medium, $0.3 < \Phi < 0.7$ are represented in magenta; high, $0.7 < \Phi < 1$ are represented in blue. For the binding process of KIX and cMyb, residues I5–L12 of cMyb and residues K21, H65–L66, A68–Y73 of KIX have medium Φ -values. For the binding process of KIX and MLL, residues N5, L7–S9, D13 of MLL and residues I26, L43, K74–I75, E78–L79, K82 of KIX have medium Φ -values.

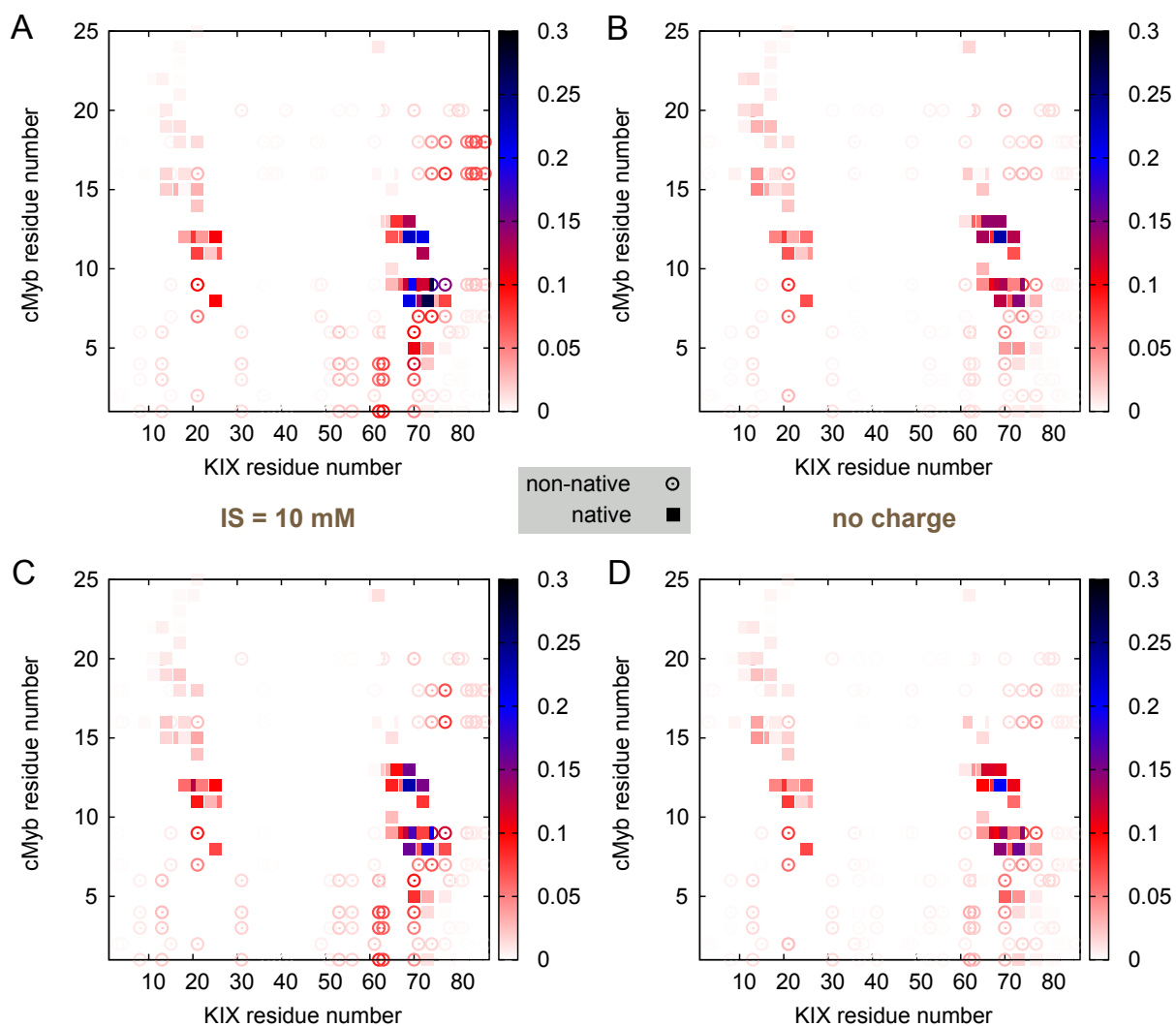


Fig. S13 Contact map of inter-chain native contacts and non-native opposite-charged contacts in cMyb successful encounter complex (UC (A and B) and MB (C and D)).

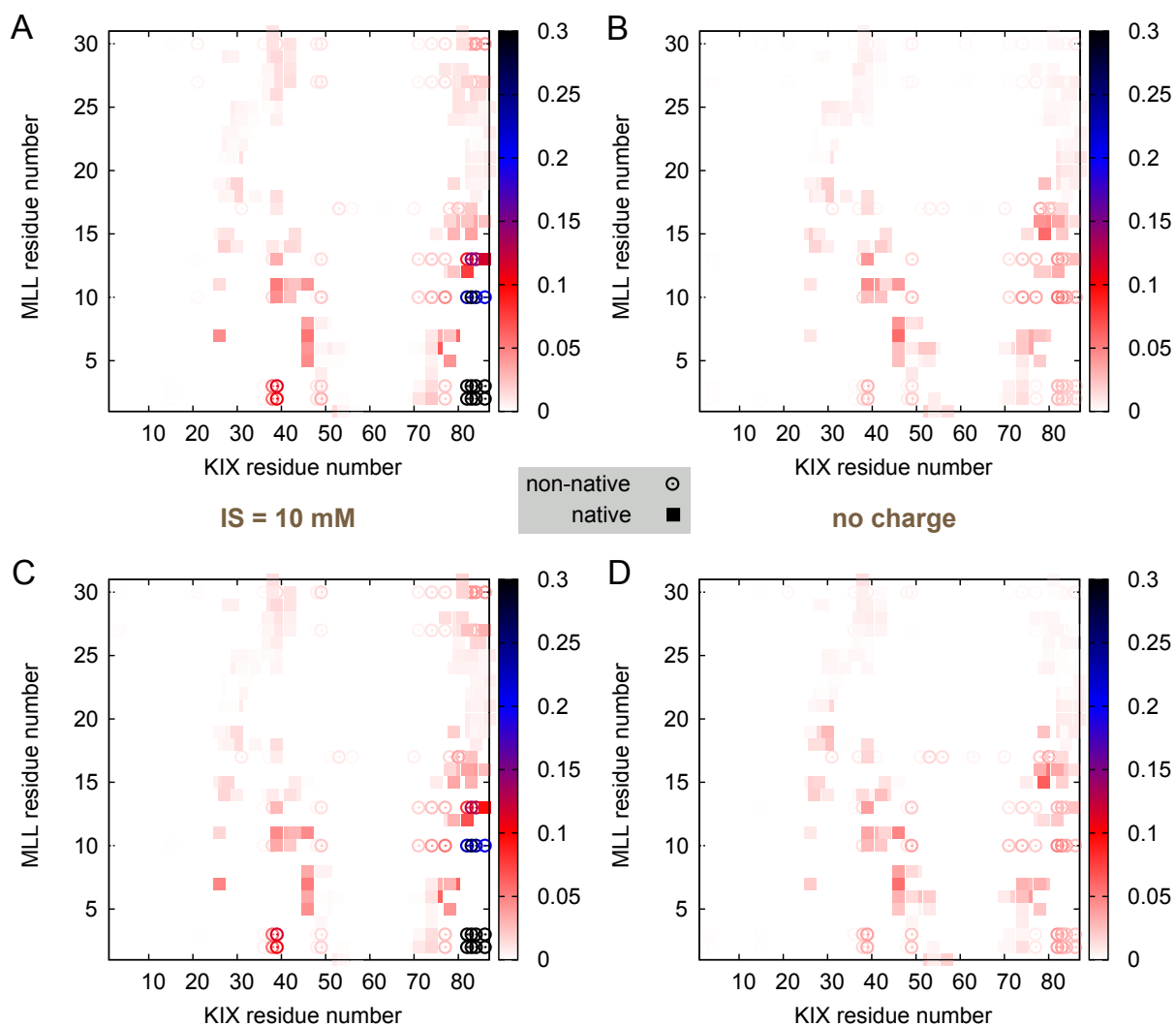


Fig. S14 Contact map of inter-chain native contacts and non-native opposite-charged contacts in MLL successful encounter complex (UM (A and B) and CB (C and D)).

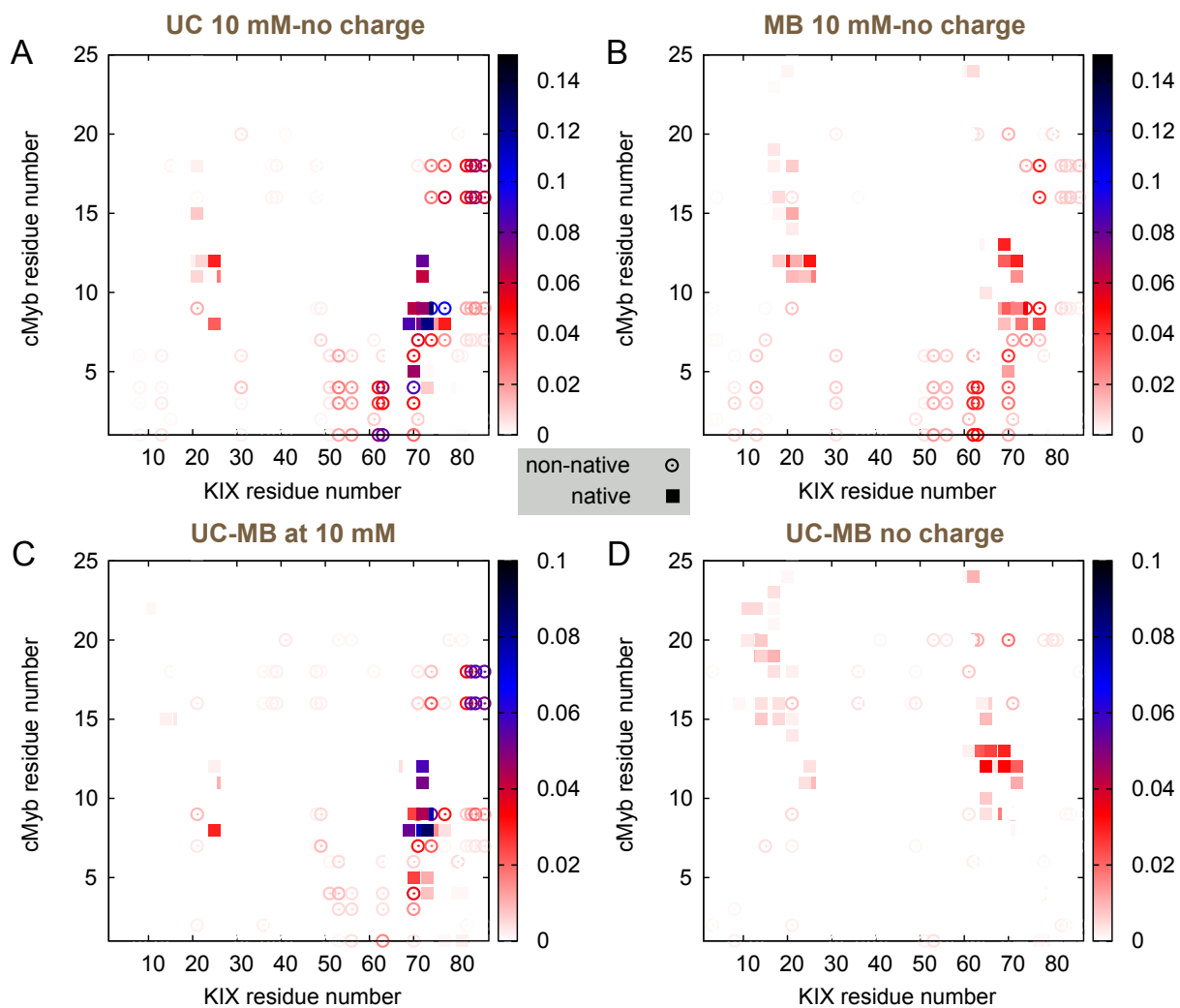


Fig. S15 Difference maps of inter-chain native contacts and non-native opposite-charged contacts in the successful encounter complex of cMyb binding (UC and MB): (A) UC contact map at 10 mM – UC contact map without charges; (B) MB contact map at 10 mM – MB contact map without charges; (C) UC contact map at 10 mM – MB contact map at 10 mM; (D) UC contact map without charges – MB contact map without charges.

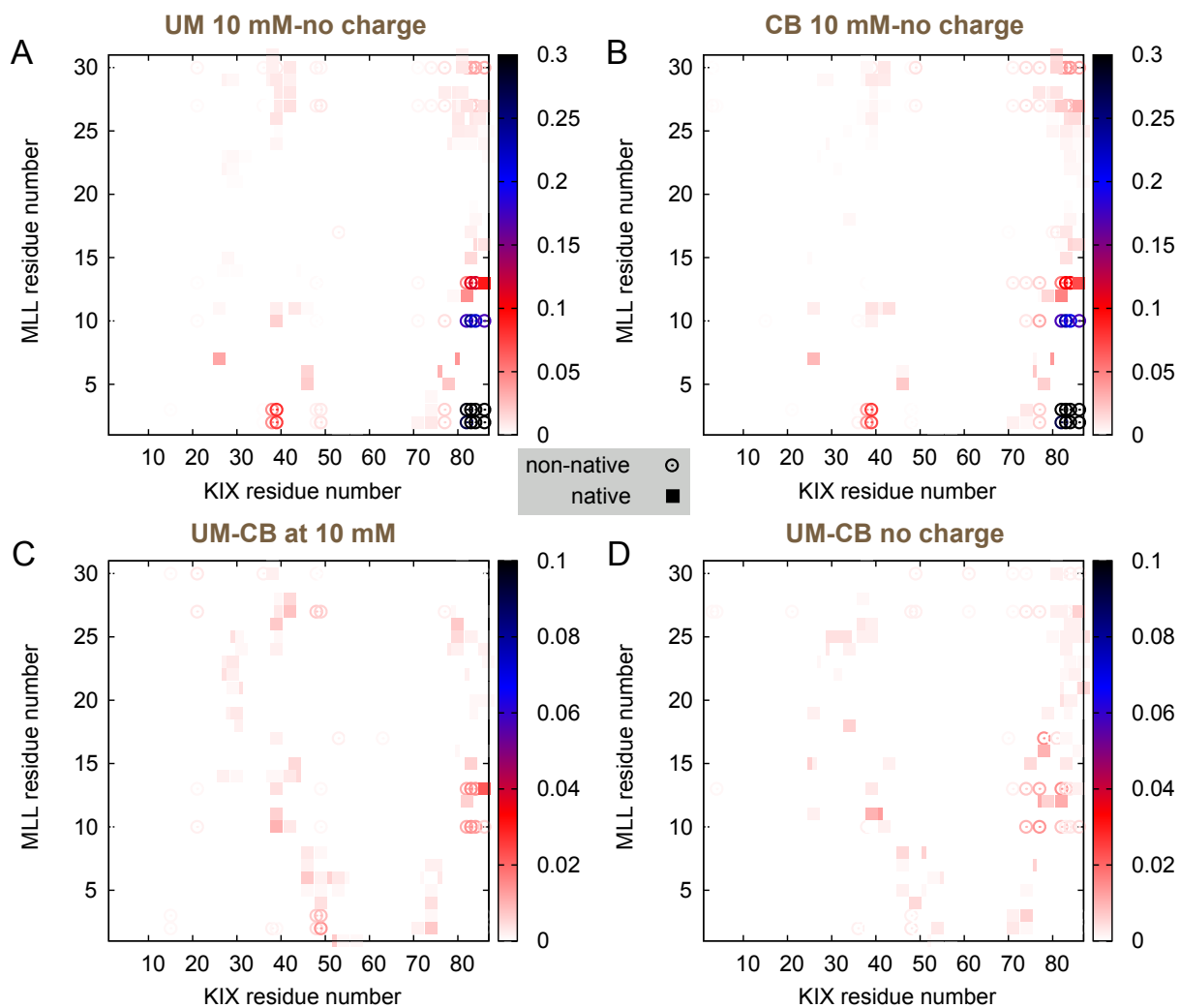


Fig. S16 Difference maps of inter-chain native contacts and non-native opposite-charged contacts in the successful encounter complex of MLL binding (UM and CB): (A) UM contact map at 10 mM – UM contact map without charges; (B) CB contact map at 10 mM – CB contact map without charges; (C) UM contact map at 10 mM – CB contact map at 10 mM; (D) UM contact map without charges – CB contact map without charges.

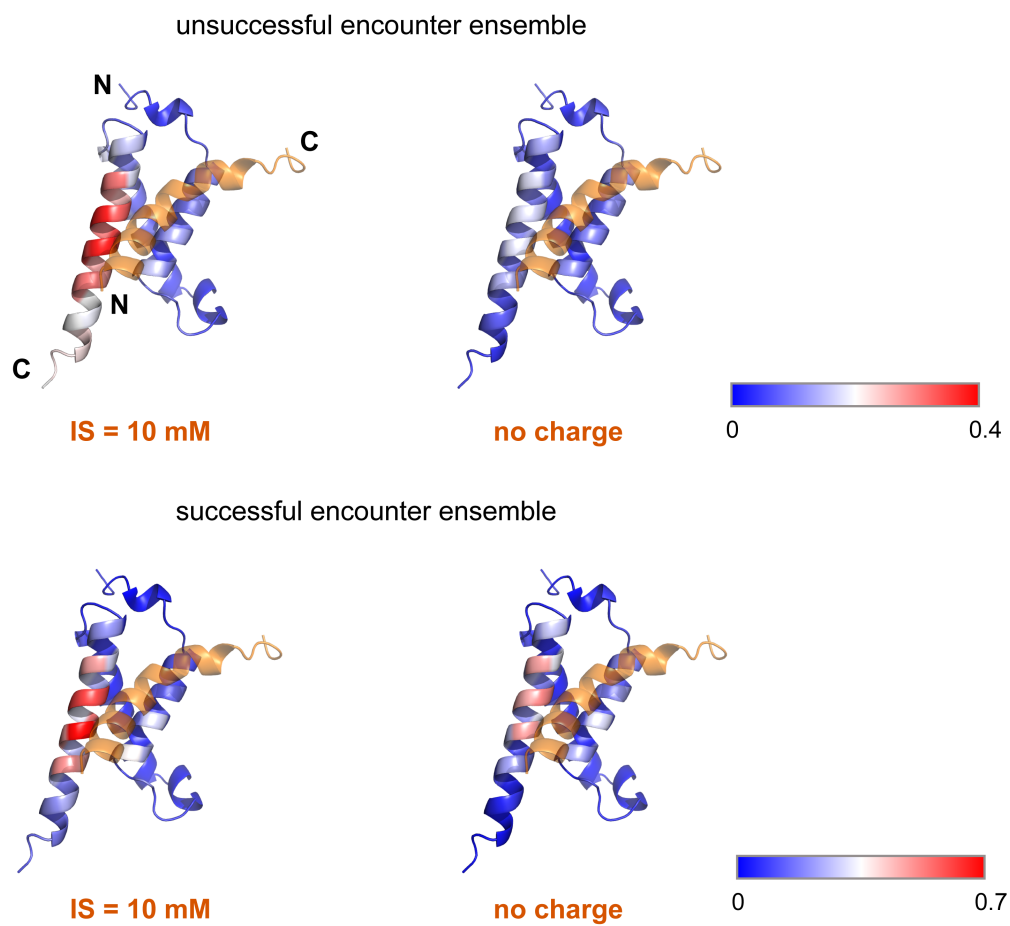


Fig. S17 Distribution of inter-molecular interactions on the surface of KIX during the binding processes with cMyb. KIX is colored based on the probability of each residue in contact with the binding partner cMyb. cMyb molecule is illustrated with orange cartoon.

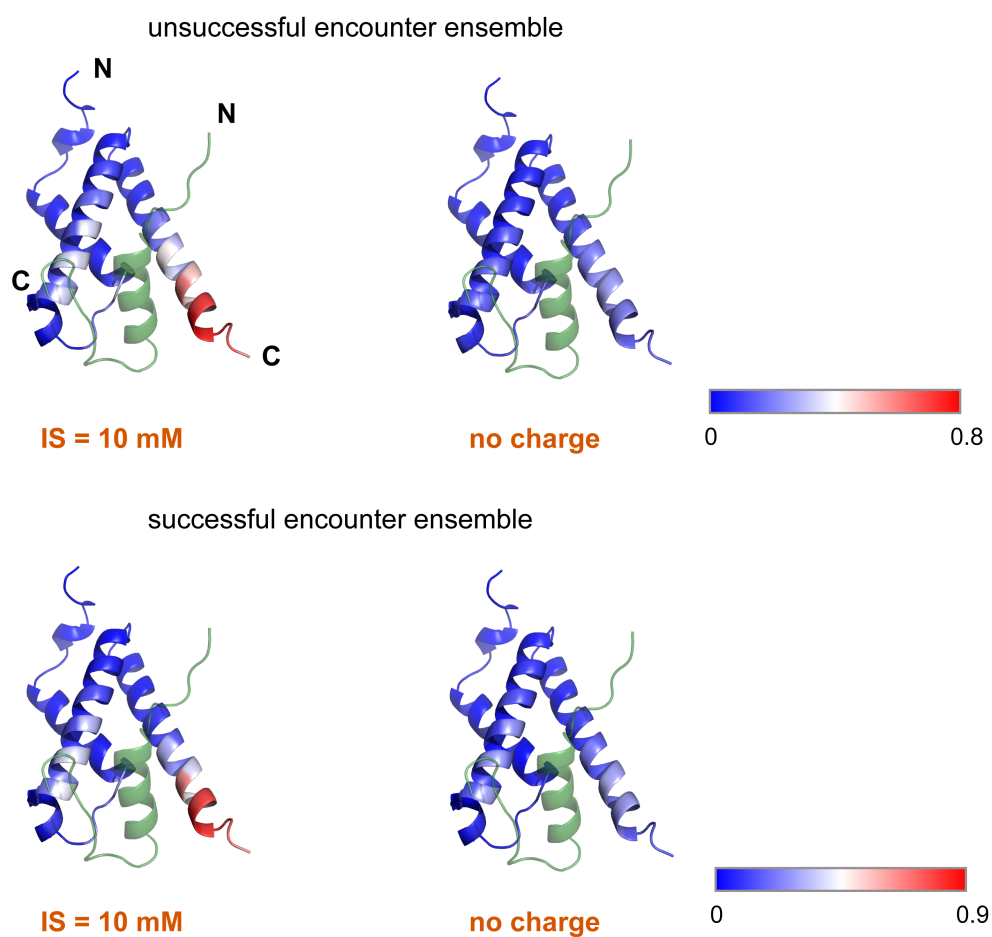


Fig. S18 Distribution of inter-molecular interactions on the surface of KIX during the binding processes with MLL. KIX is colored based on the probability of each residue in contact with the binding partner MLL. MLL molecule is illustrated with green cartoon.