

Supplementary Data

Insertion of Oxidized Nucleotide Triggers Rapid DNA Polymerase Opening

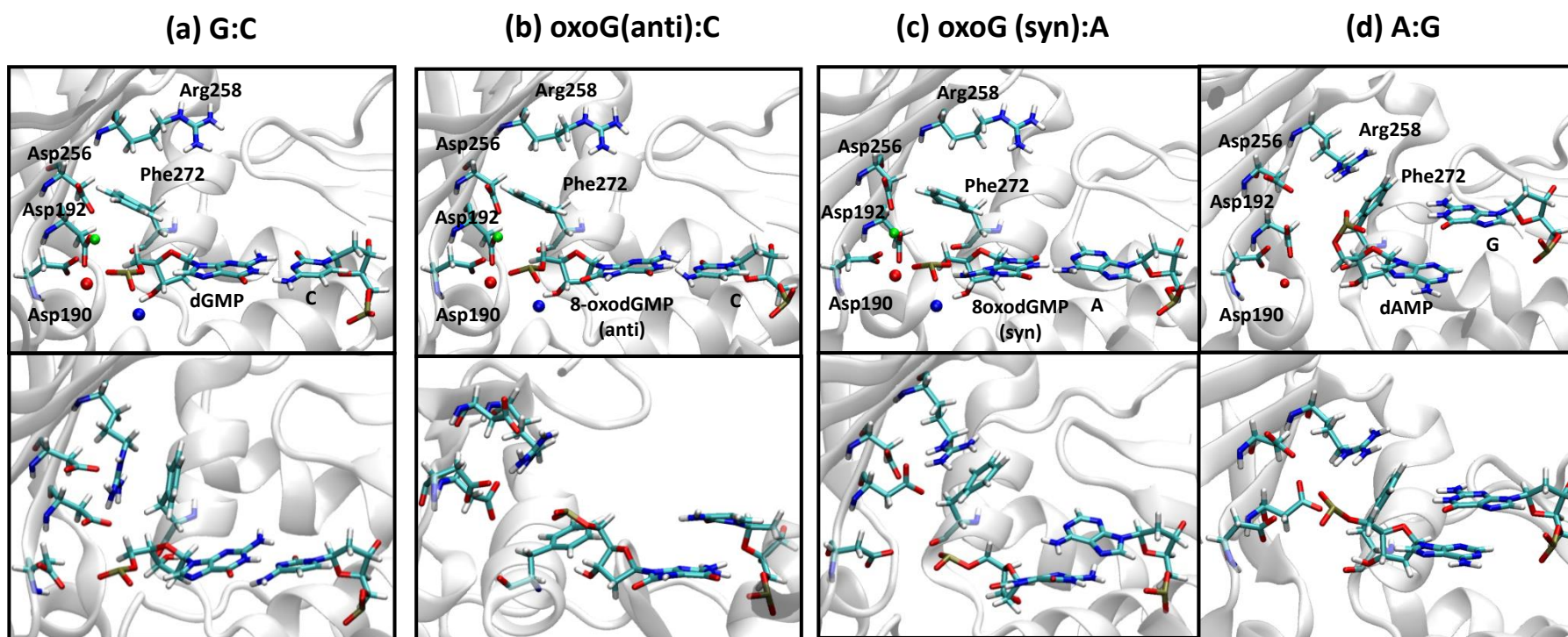
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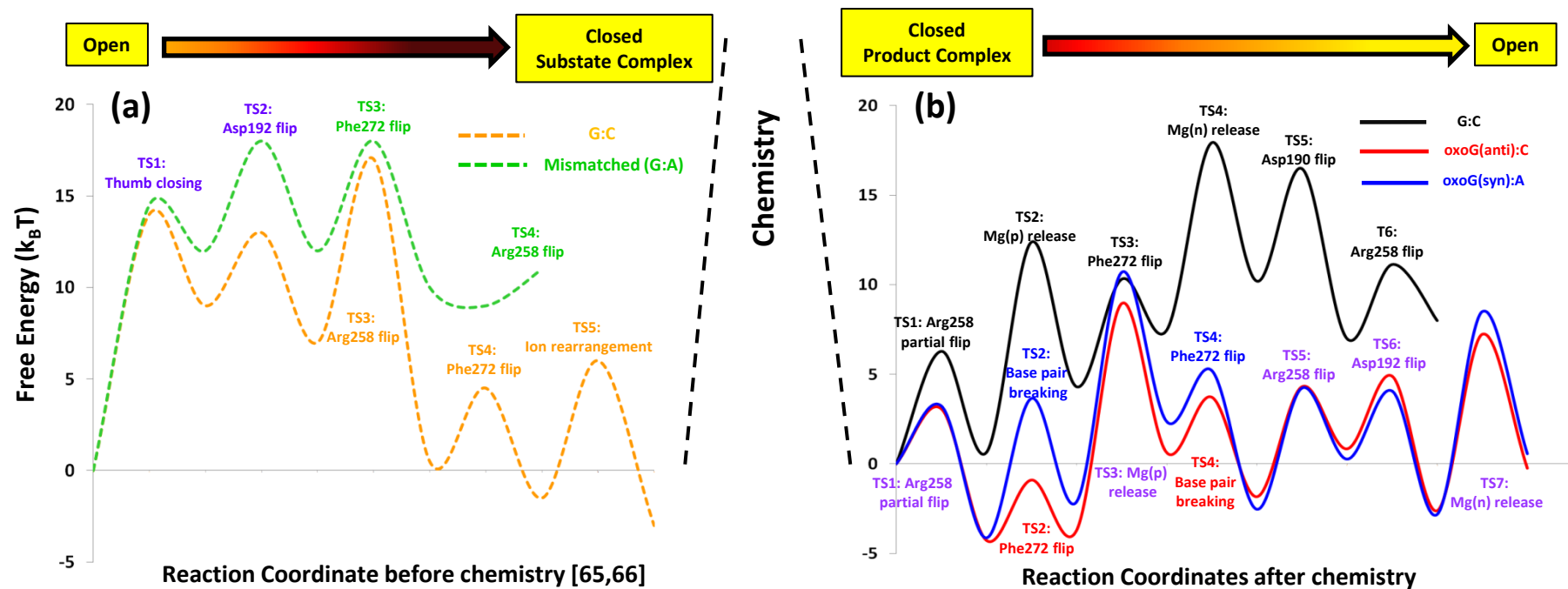
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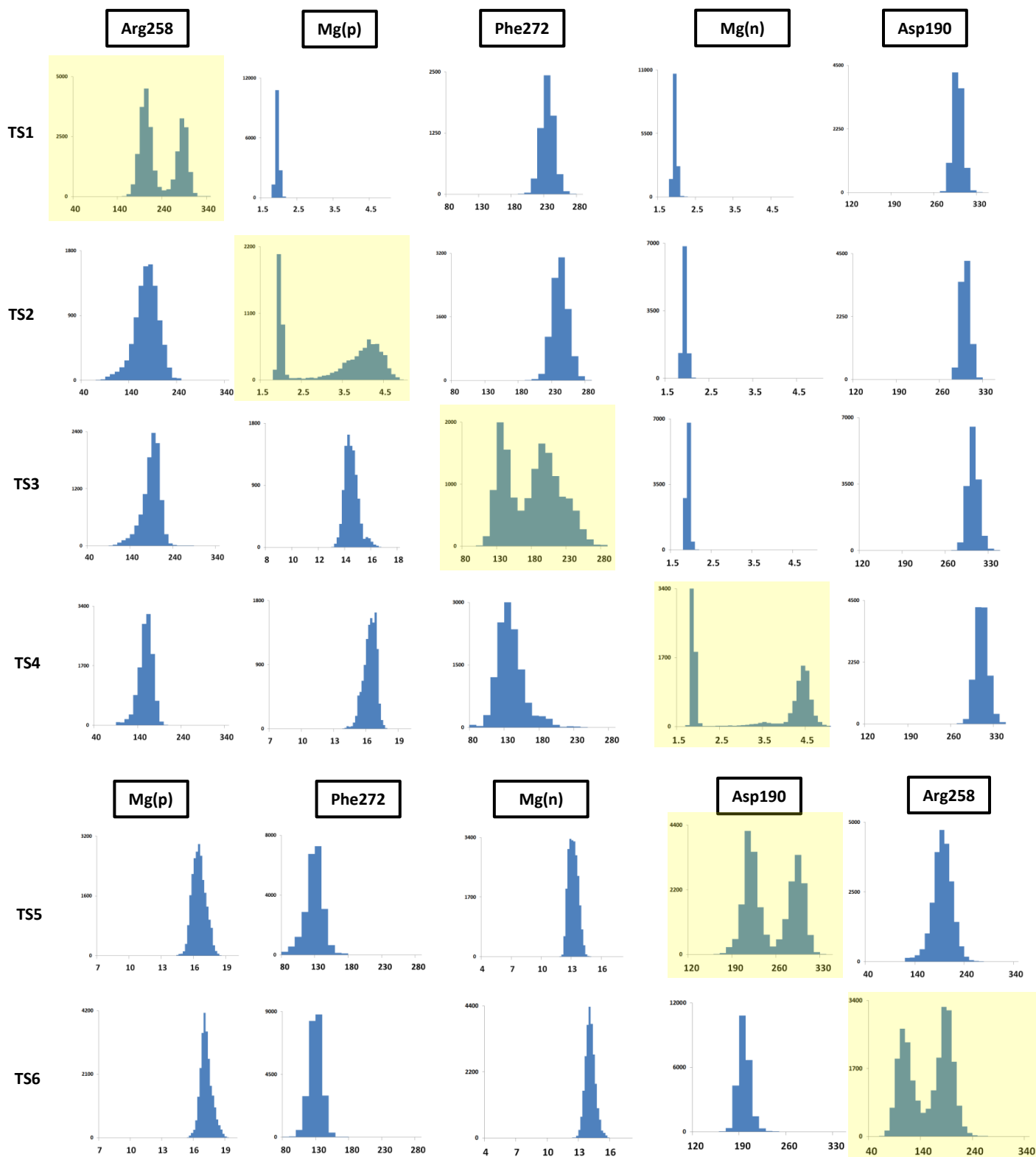
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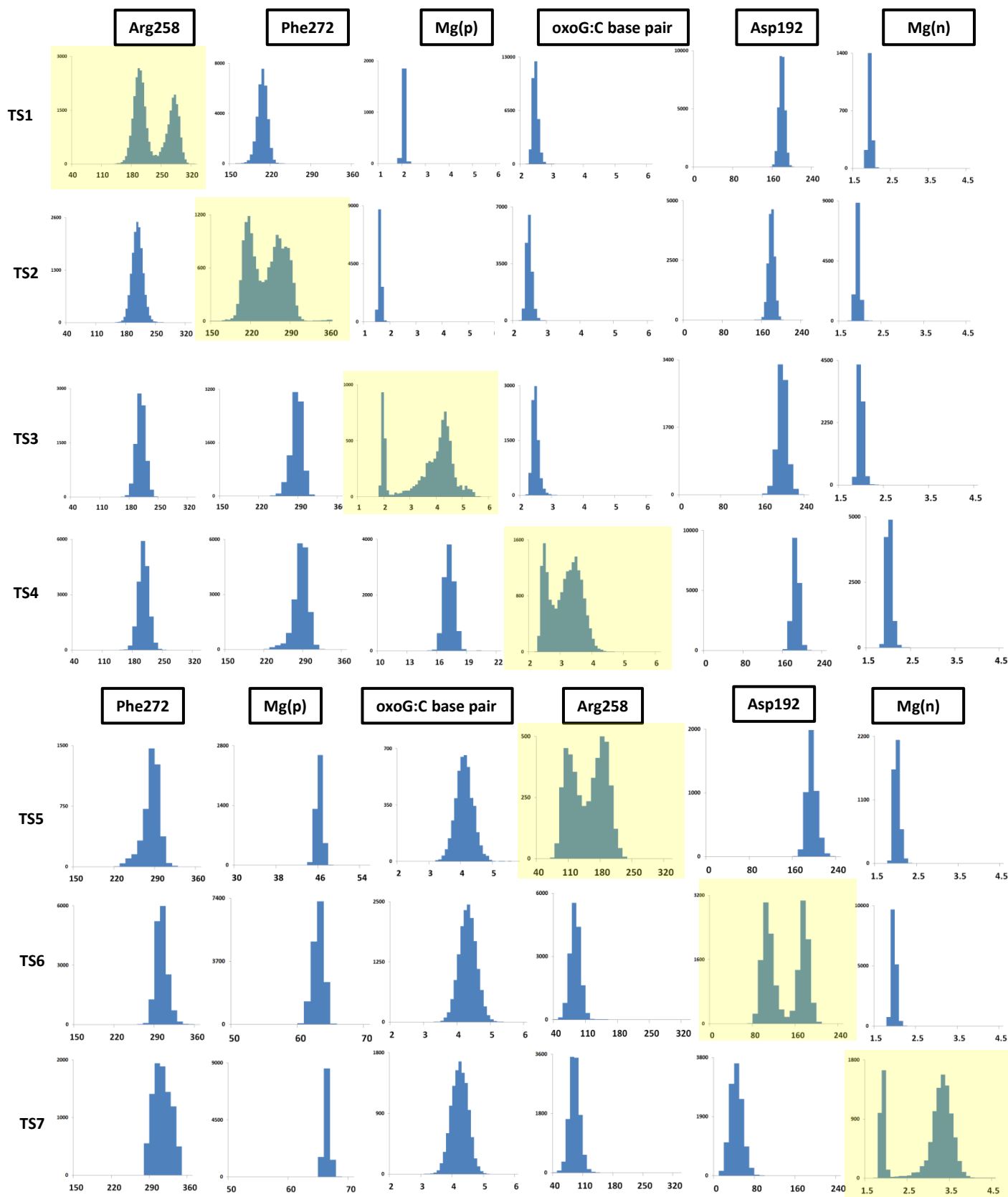
Supplementary Figure S1 The closed (upper panels) and open (lower panels) conformations of (a) G:C pol- β , (b) oxoG(anti):C pol- β system, (c) oxoG(syn):A pol- β system, and (d) A:G mismatched pol- β system. For each system, corresponding X-ray structure is minimized and equilibrated by regular MD simulations. Blue, red and green spheres are Mg(p), Mg(n) and Na_c ions, respectively. To simplify figures, PP_i is omitted from each structure.



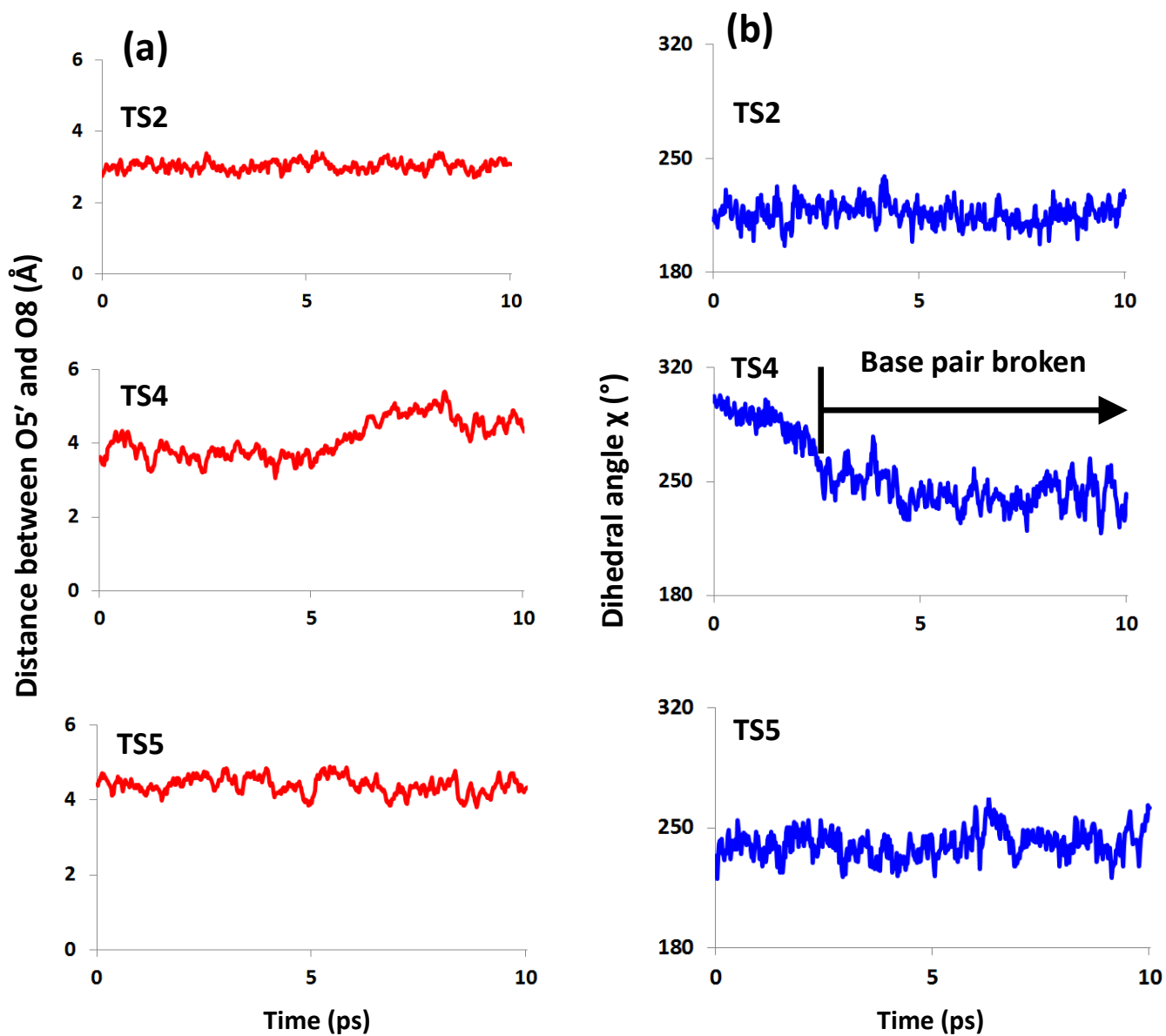
Supplementary Figure S2. The free energy profiles of (a) the G:C (orange dashed line) and mismatched G:A (green dashed line) pol- β systems before chemistry reported previously [65, 66] and (b) the G:C (black line), oxoG(anti):C (red line), and oxoG(syn):A (blue line) pol- β systems after chemistry as completed in this work. The identical transition states of two oxoG systems and G:C and mismatched systems before chemistry are indicated with violet.



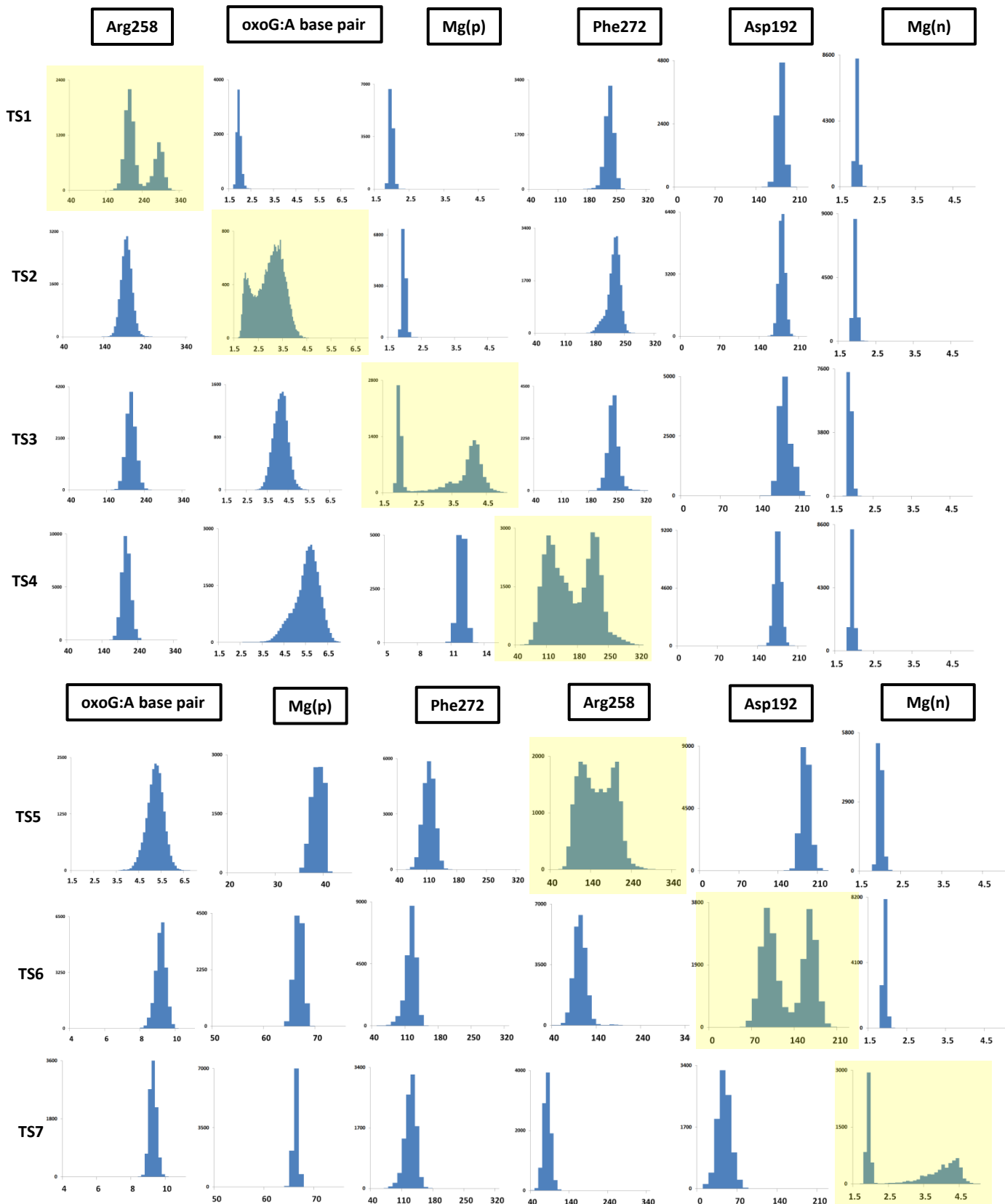
Supplementary Figure S3 Probability distribution of the order parameters for each transition state in opening conformational pathway for the G:C pol-β system. Since Arg258 is associated with two transition states (TS1 and TS6), the probability distributions of Arg258 in the last two rows (TS5 and TS6) are arranged as the last column. The bimodal plots corresponding transition events are highlighted with yellow.



Supplementary Figure S4 Probability distribution of the order parameters for each transition state in opening conformational pathway for the oxoG(anti):C pol- β system. Since Arg258 is associated with two transition states (TS1 and TS5), the probability distributions of Arg258 in the last three rows (TS5 to TS7) are arranged as the 4th column. The bimodal plots corresponding transition events are highlighted with yellow.



Supplementary Figure S5 Distributions of (a) the distance between O5' and O8, and (b) the dihedral angle χ of the oxoG (anti):C pol- β system during TS2 (before the Mg(p) dissociation), TS4 (during the Mg(p) dissociation) and TS5 (after the Mg(p) dissociation).



Supplementary Figure S6 Probability distribution of the order parameters for each transition state in opening conformational pathway for the oxoG(syn):A pol-β system. Since Arg258 is associated with two transition states (TS1 and TS5), the probability distributions of Arg258 in the last three rows (TS5 to TS7) are arranged as the 4th column. The bimodal plots corresponding transition events are highlighted with yellow.