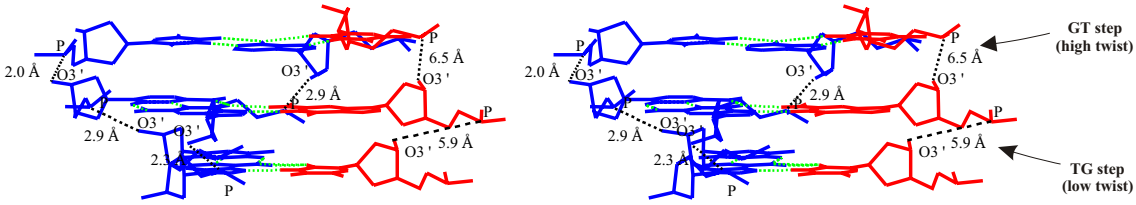

Fig. S1 Stereo diagram of a different starting model used for the MD simulation. Note the disjointed nature of all the three strands. WC duplex is coloured blue.

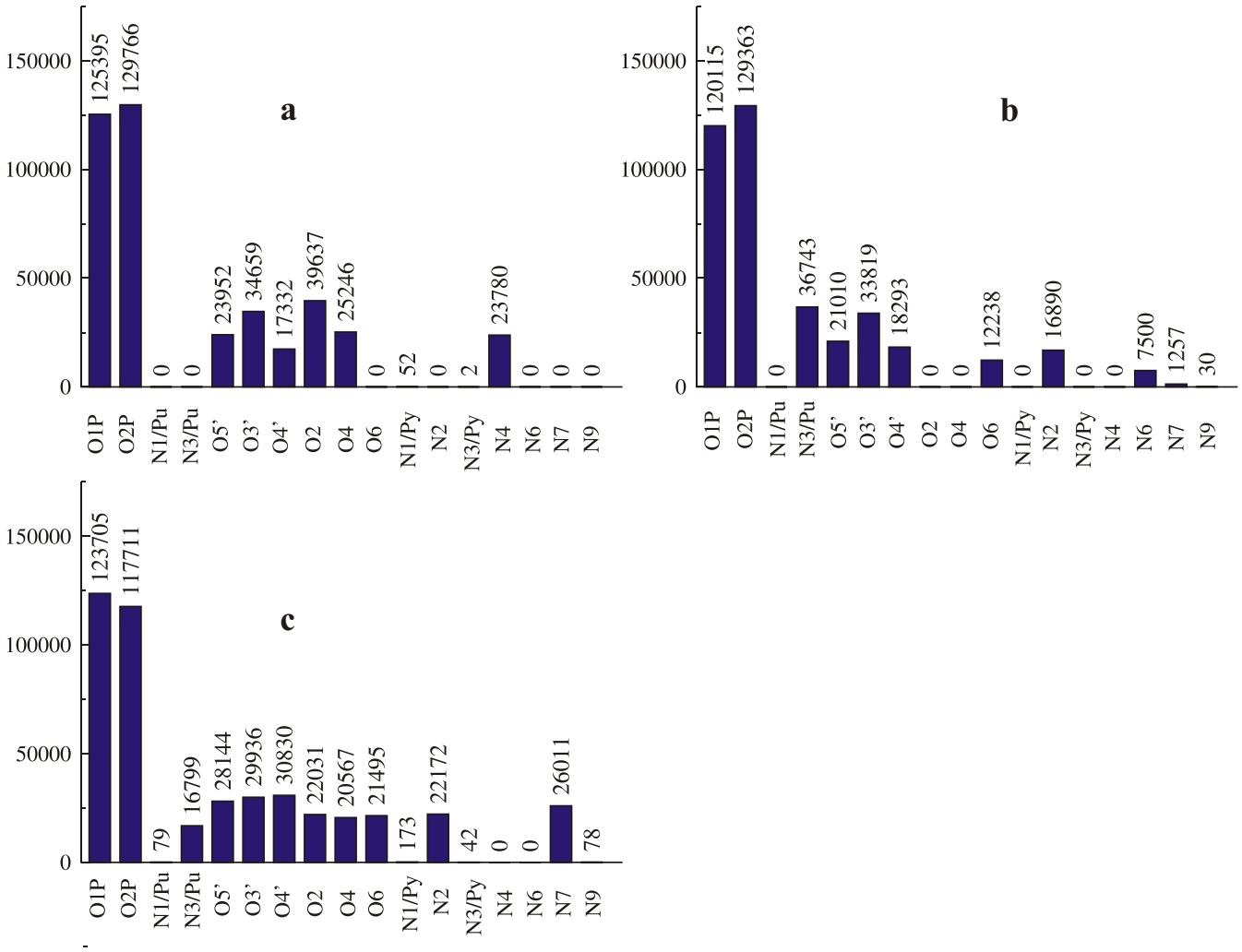

Fig. S2 Bar diagram representing the number of times (hits) the water oxygen atoms come within a distance of 3.25 Å from the backbone and base atoms to form hydrogen bonds in different strands: (a) pyrimidine & (b) purine of the WC duplex and (c) RH. Total number hits calculated over the entire trajectory for the structures taken at 1ps interval is shown on the top of each bar.

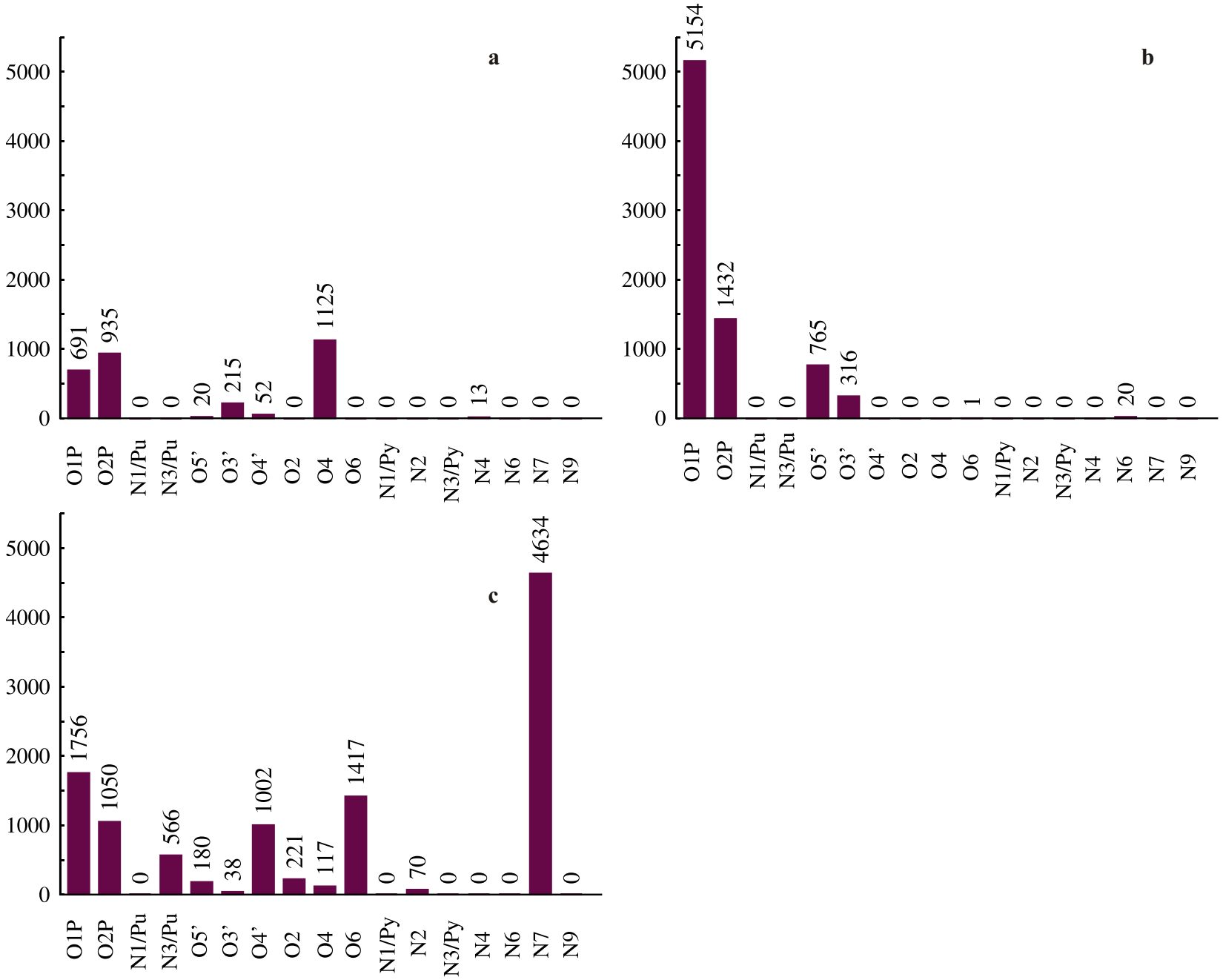

Fig. S3 Bar diagram representing the number of times (hits) the Na^+ ions come within a distance of 3.25 Å from the backbone and base atoms of the different strands: (a) pyrimidine & (b) purine of the WC duplex and (c) RH. Total number hits calculated over the entire trajectory for the structures taken at 1ps interval is shown on the top of each bar.

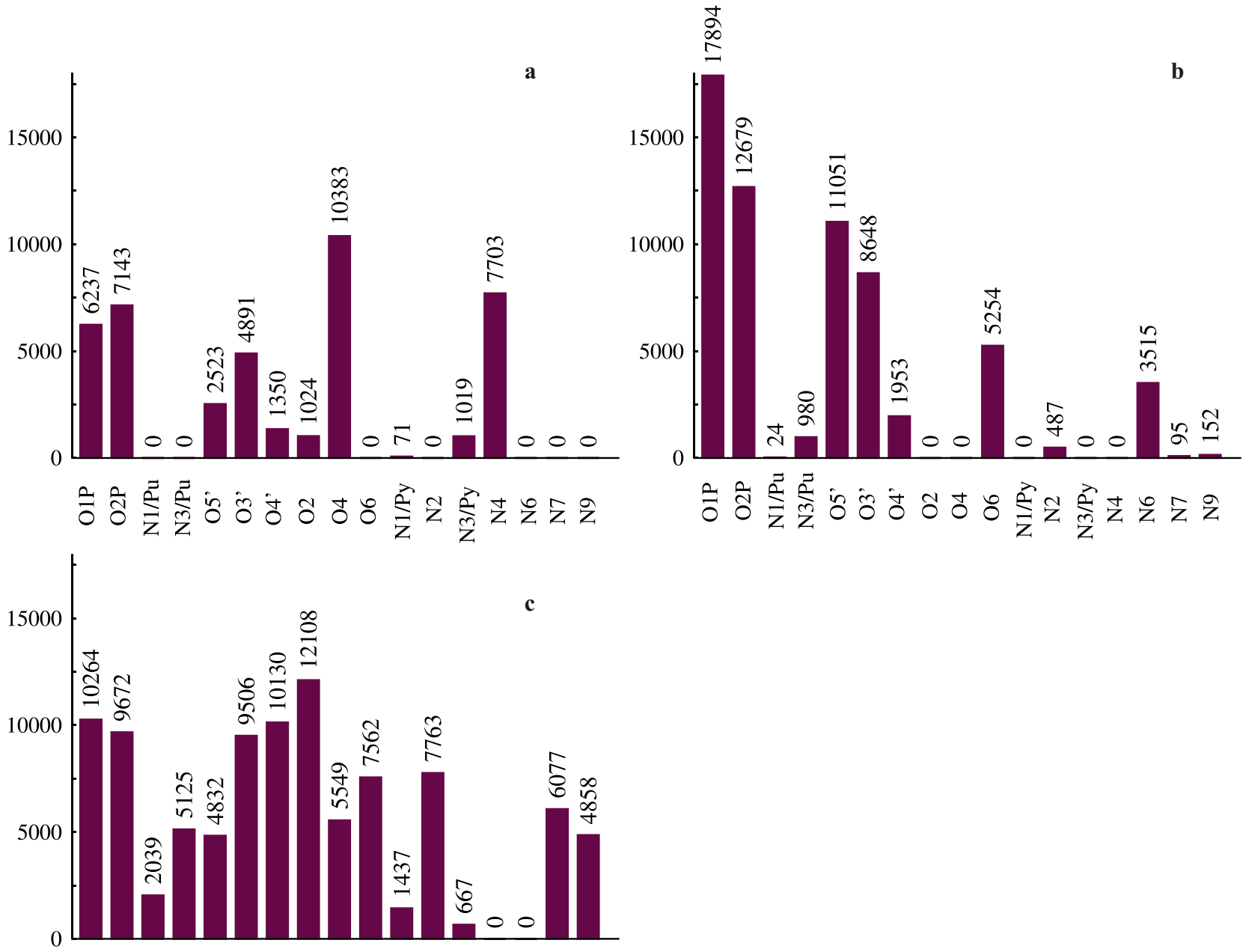

Fig. S4 Bar diagram representing the number of times (hits) the Na^+ ions come within 3.25-5 Å distance from the backbone and base atoms of the different strands: (a) pyrimidine & (b) purine of the WC duplex and (c) RH. Total number hits calculated over the entire trajectory for the structures taken at 1ps interval is shown on the top of each bar.

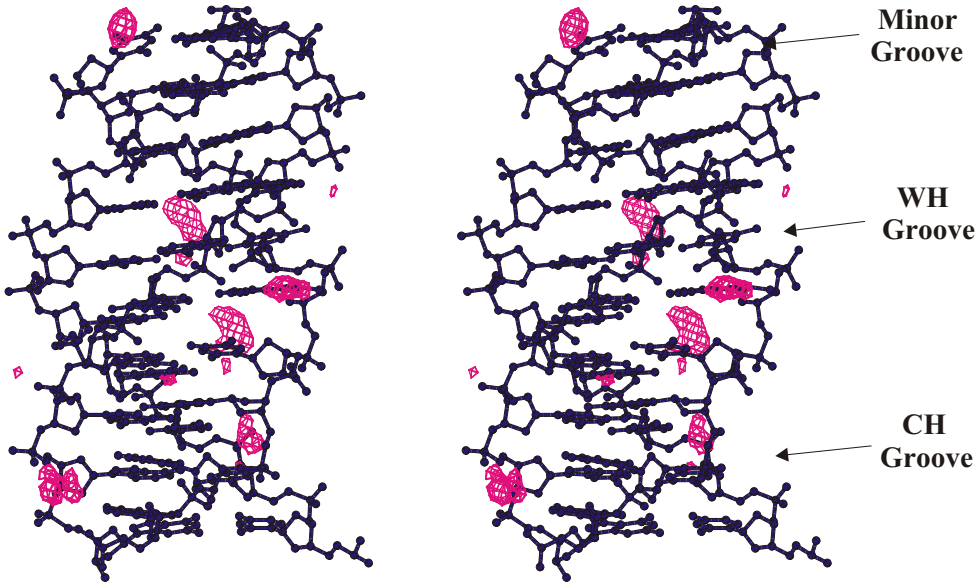

Fig. S5 Ion density contoured at 12 hits / 0.5 Å^3 around the central 10mer of the average structure of the antiparallel $(G_*GC/T_*AT)_7$ DNA triplex.