Inferring 3D chromatin structure using a multiscale approach based on quaternions – Supplementary Material

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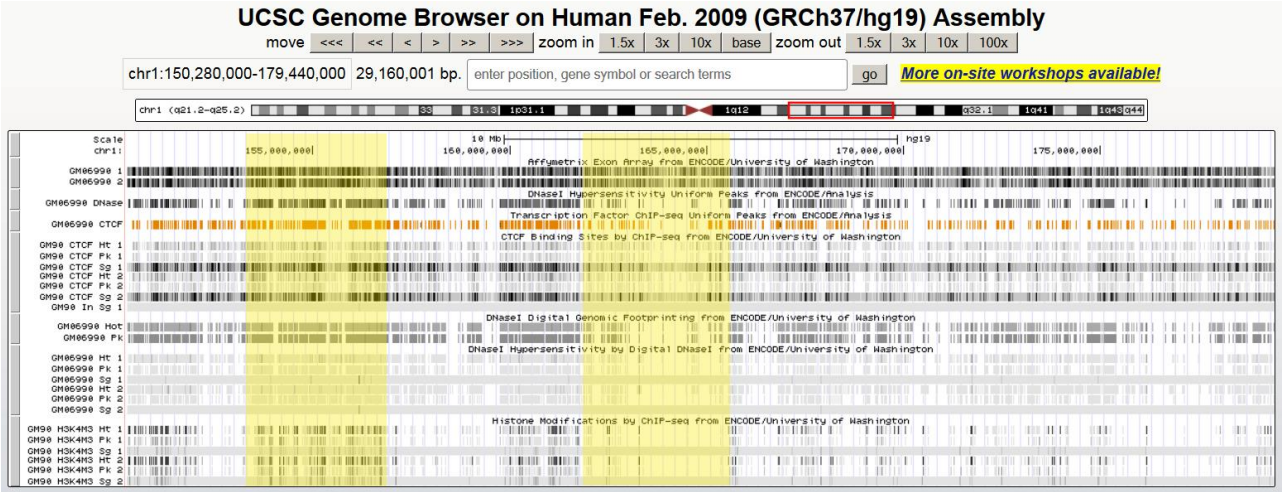
Data for a 30 Mbp stretch of Chromosome 1, long arm, from lymphoblastoid cell line GM06990 were retrieved for both the Hi-C [8] and the expression experiments (ENCODE). Two stretches of about 3.5 Mbp were selected as representative of, respectively, highly and poorly expressed genomic regions (see figure below):
Highly expressed: from q = 153.3 Mbp to q = 156.8 Mbp,
Poorly expressed: from q = 162 Mbp to q = 165.5 Mbp.

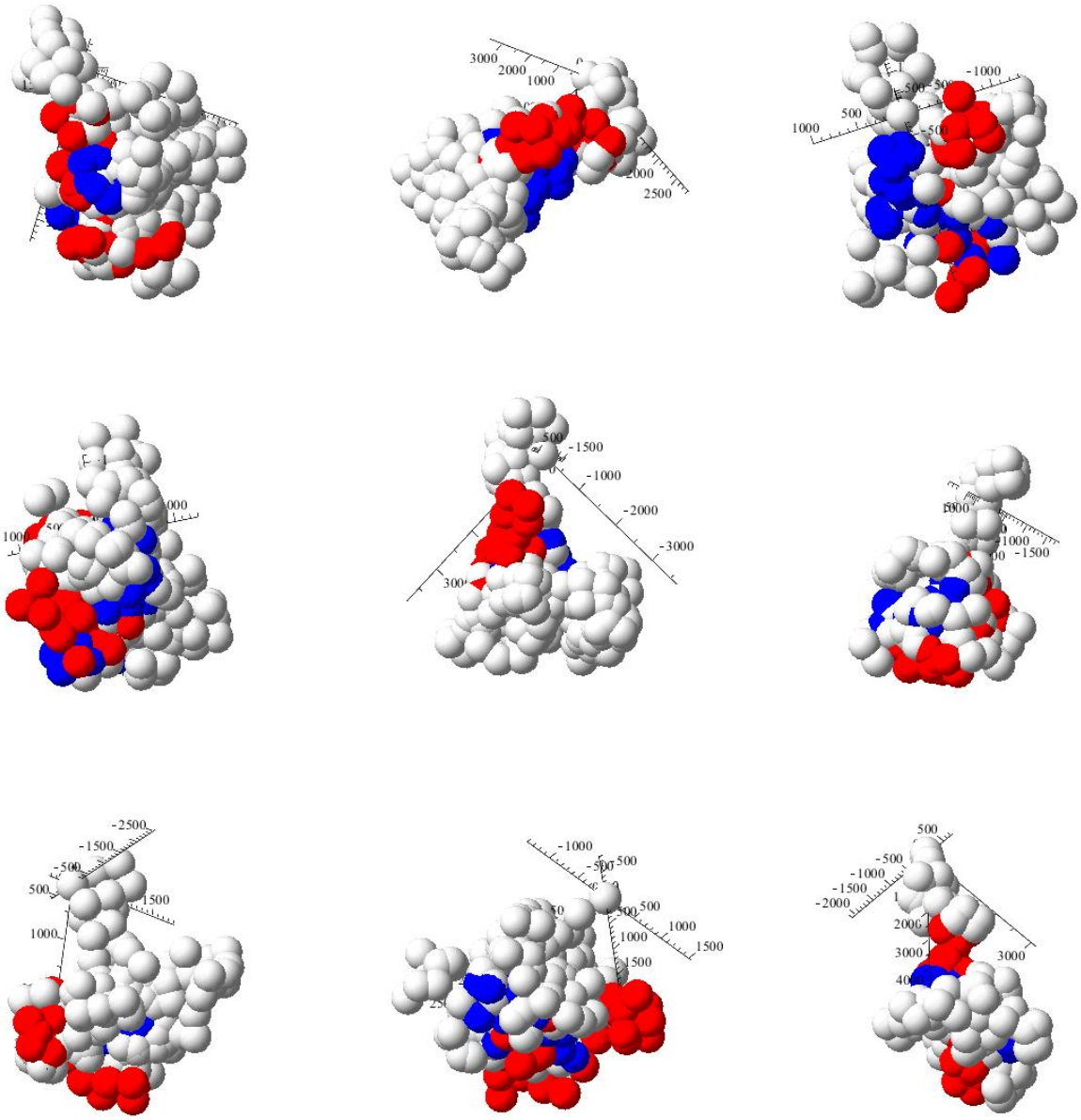


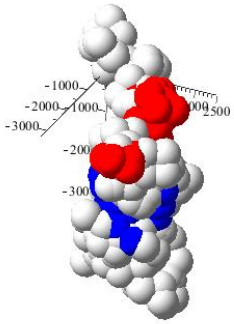
Applying our algorithm we obtained 40 configurations. For each configuration, we calculated the mean-square Euclidean distances between pairs of loci as functions of their genomic distance in the high and low expression regions (see Fig. 4 of main text). The ratio ρ between the integral of the functions obtained for the two regions is reported in Table 1.

Two clusters were identified, defined by the threshold value $\rho = 2$. Those with $\rho > 2$ (meaning that the span of the highly expressed region is at least twice as much as the poorly expressed counterpart) show a peculiar pear-like shape, clearly recognizable in the plots below.

Table 1: Ratios ρ of the 40 configurations	
Configuration	**Ratio ρ**
1	1.99
2	1.03
3	1.13
4	1.72
5	**2.51**
6	0.89
7	**5.66**
8	**3.36**
9	1.19
10	0.85
11	1.15
12	1.89
13	**2.41**
14	**2.92**
15	**3.28**
16	1.37
17	**3.03**
18	**2.46**
19	0.64
20	0.47
21	0.69
22	1.11
23	0.63
24	**3.11**
25	1.62
26	**4.02**
27	**2.72**
28	1.49
29	1.34
30	**3.85**
31	1.54
32	1.82
33	0.54
34	**2.26**
35	1.73
36	**2.72**
37	1.19
38	**2.49**
39	0.92
40	**4.05**

Final configurations with ρ > 2, “pear like” conformation (5-7-8-13-14-15-17-18-24-26-27-30-34-36-38-40):

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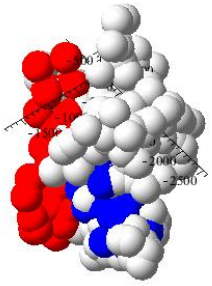
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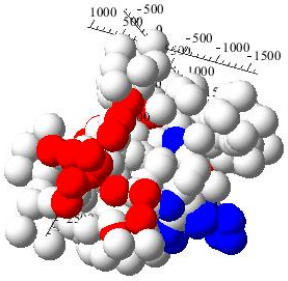
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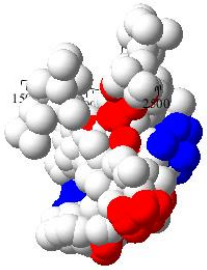

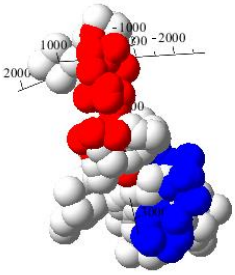
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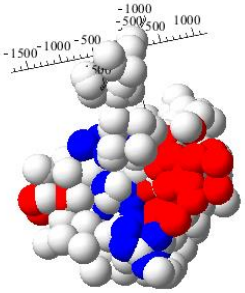
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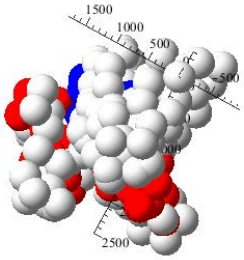
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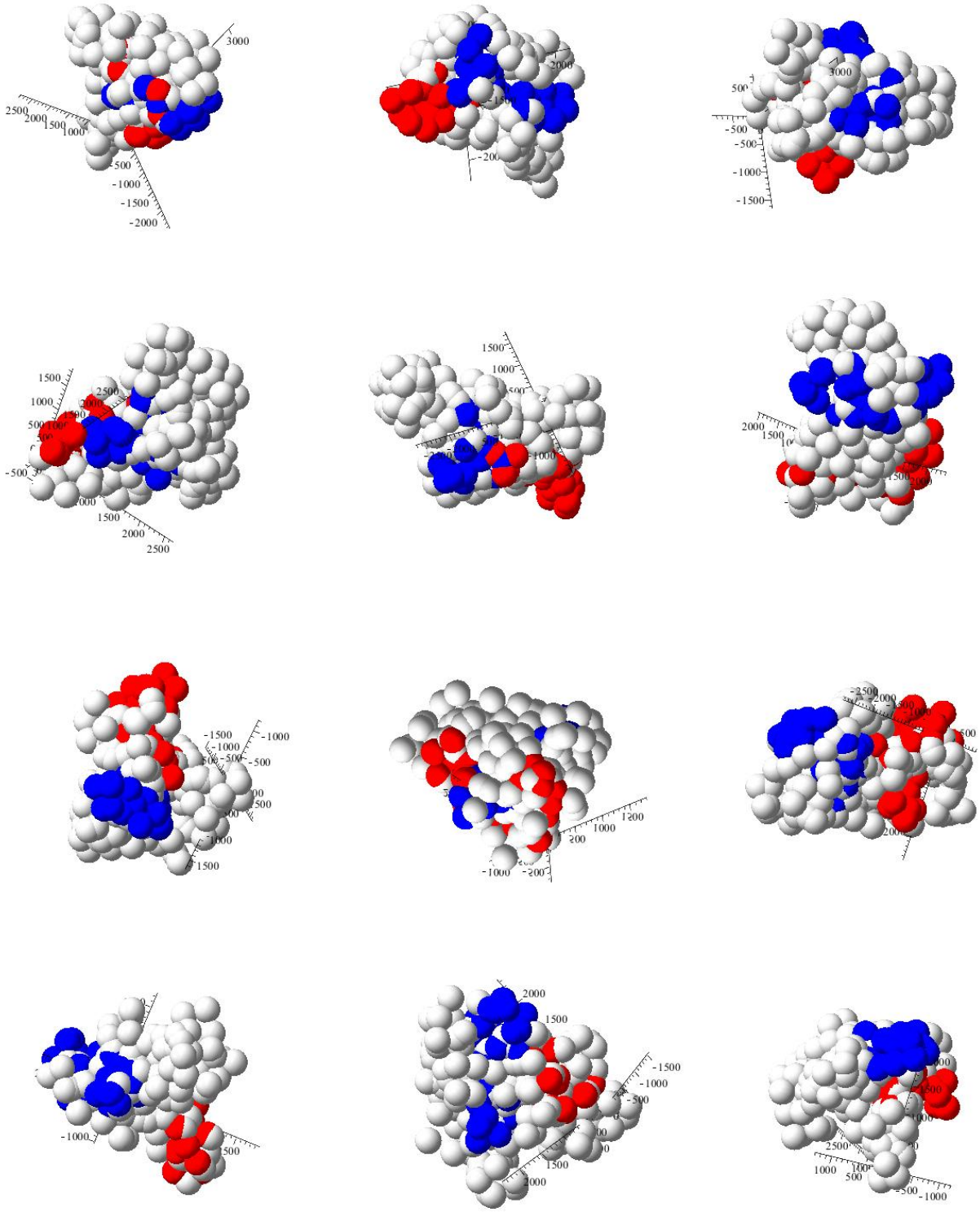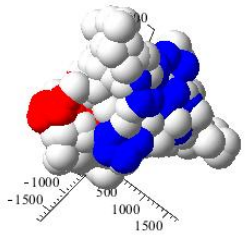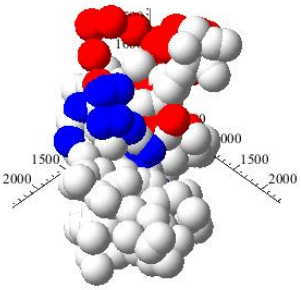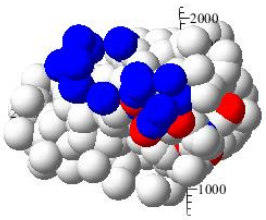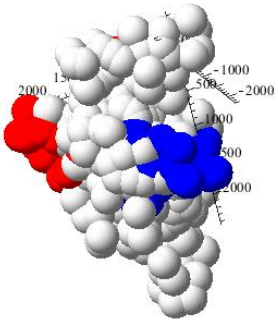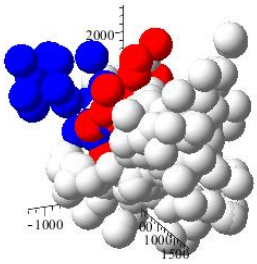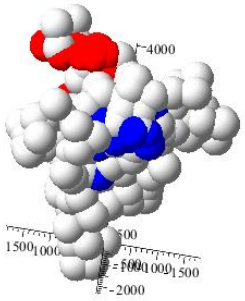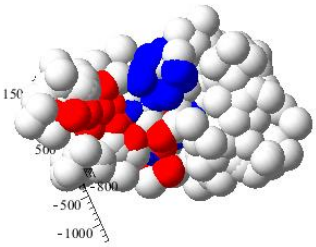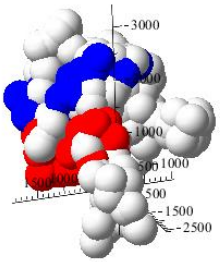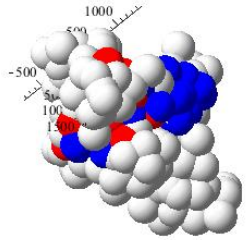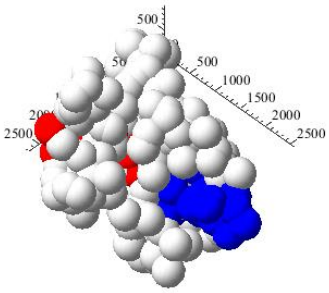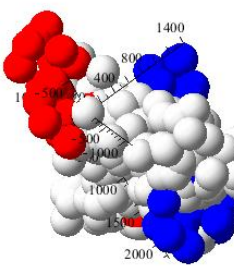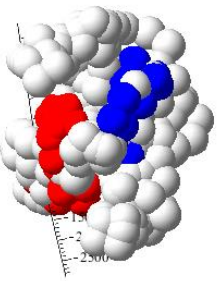
Final configurations with $\rho < 2$, “globular” conformation (1-2-3-4-6-9-10-11-12-16-19-20-21-22-23-25-28-29-31-32-33-35-37-39):