

Violations of restraints from six different cells

	restraints from					
	cell 1	cell 2	cell 3	cell 4	cell 5	cell 6
ensemble based on cell 1	0.0	64.5	73.2	71.1	69.8	69.0
cell 2	73.2	0.0	74.5	79.6	70.8	71.0
cell 3	75.5	68.9	0.0	79.0	70.3	69.1
cell 4	70.6	65.2	73.7	0.0	68.8	69.6
cell 5	73.4	68.8	72.5	79.3	0.0	71.7
cell 6	76.1	68.3	77.6	79.1	72.1	0.0

Table S3: Percentage of restraints from different cells (columns) that are violated in structure ensembles (rows) with a tolerance of $a/8$.