

## Supplementary Information

### Collision induced unfolding and molecular dynamics simulations of norovirus capsid dimers reveal strain-specific stability profiles

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Table S1: CIU50 for all selected charge states.

CIU50 Norwalk [V]			
21+	22+	23+	24+
56.21	51.03	43.25	11.20
90.57	70.76	69.25	68.42
	90.11		

CIU50 Kawasaki [V]			
21+	22+	23+	24+
73.72	72.01	51.57	39.78
	70.88	67.17	65.37
			76.43

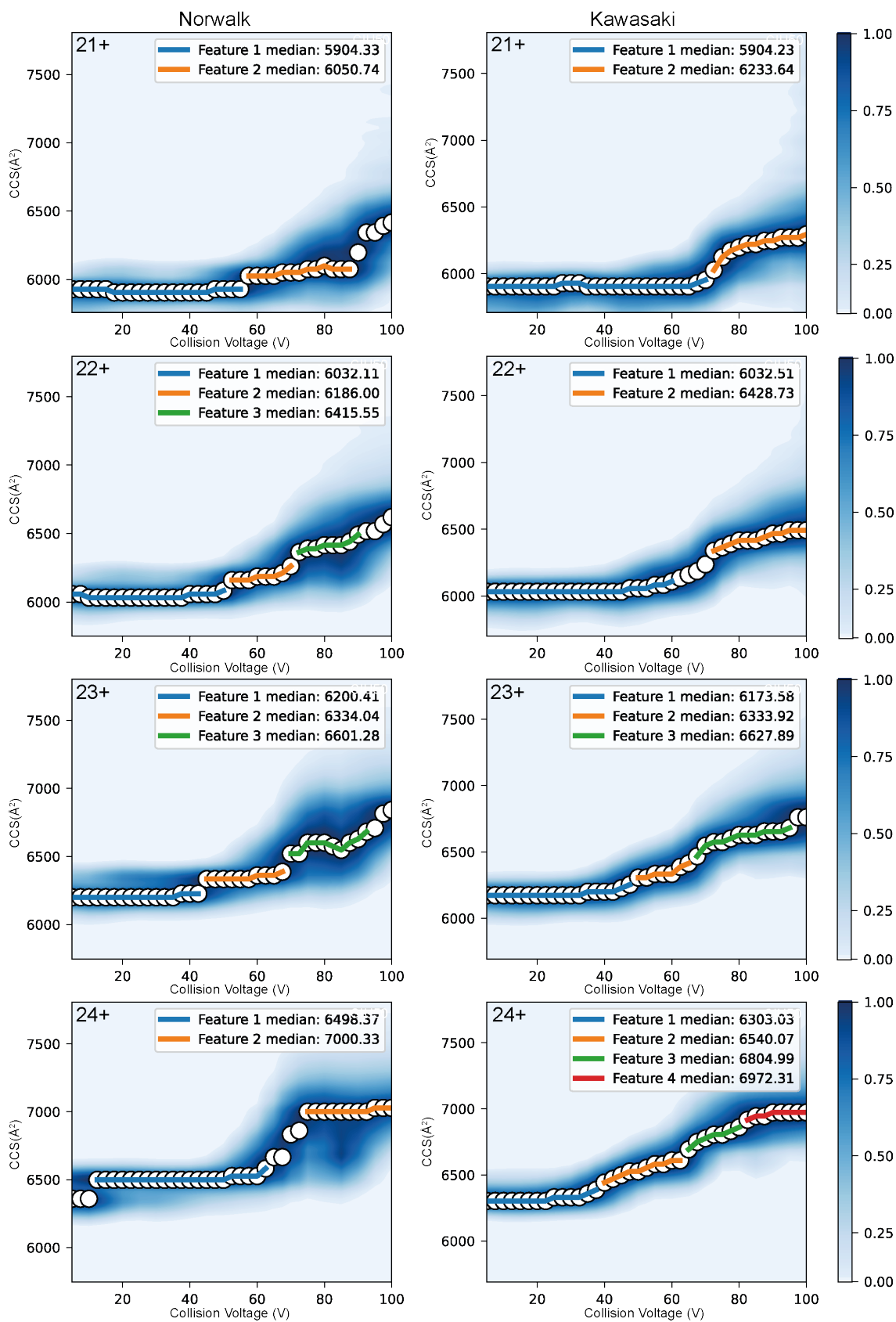


Figure S1: Distinct features according to CIU Suite2 for all selected charge states.

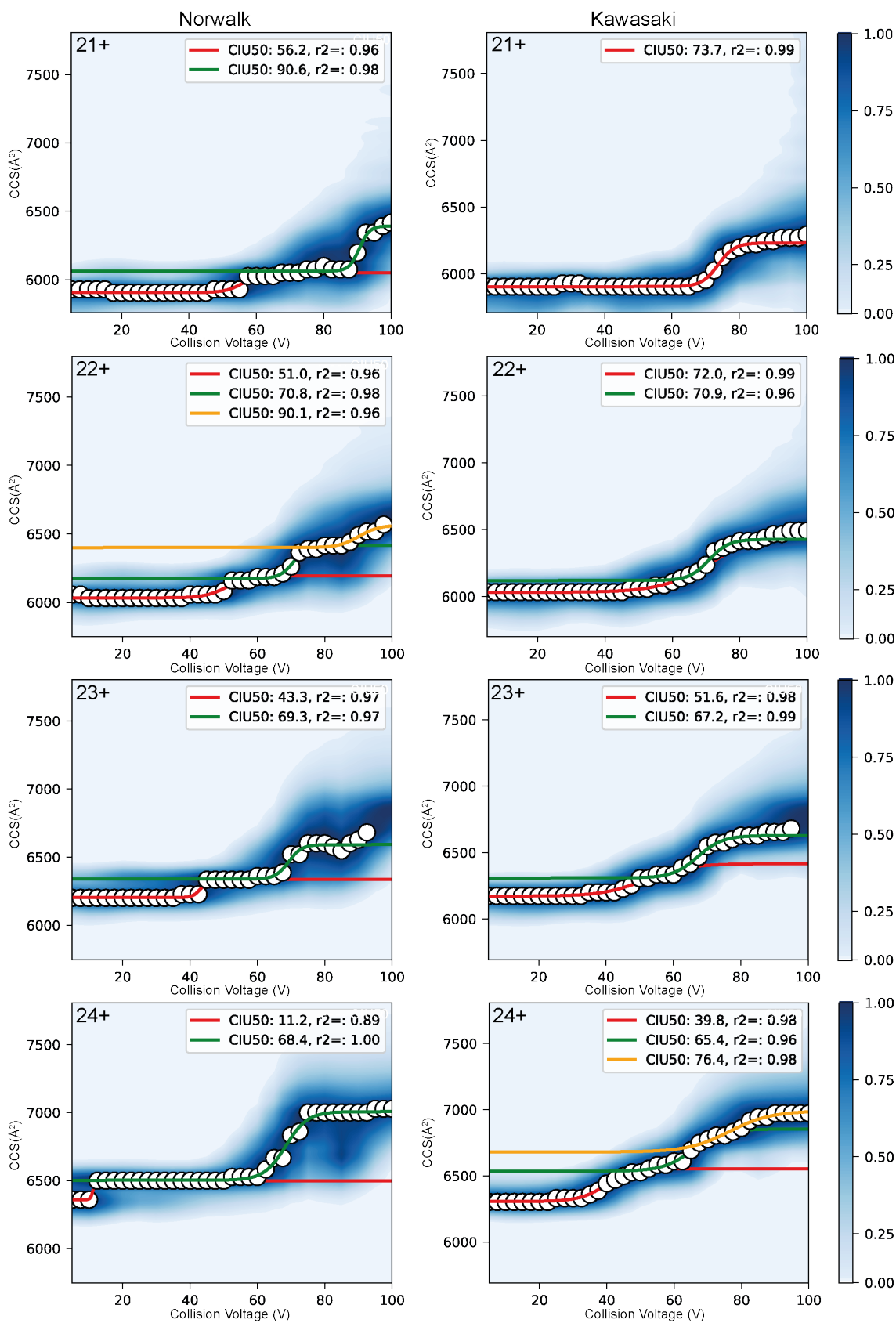


Figure S2: Conformational transitions according to CIU Suite2 for all selected charge states.

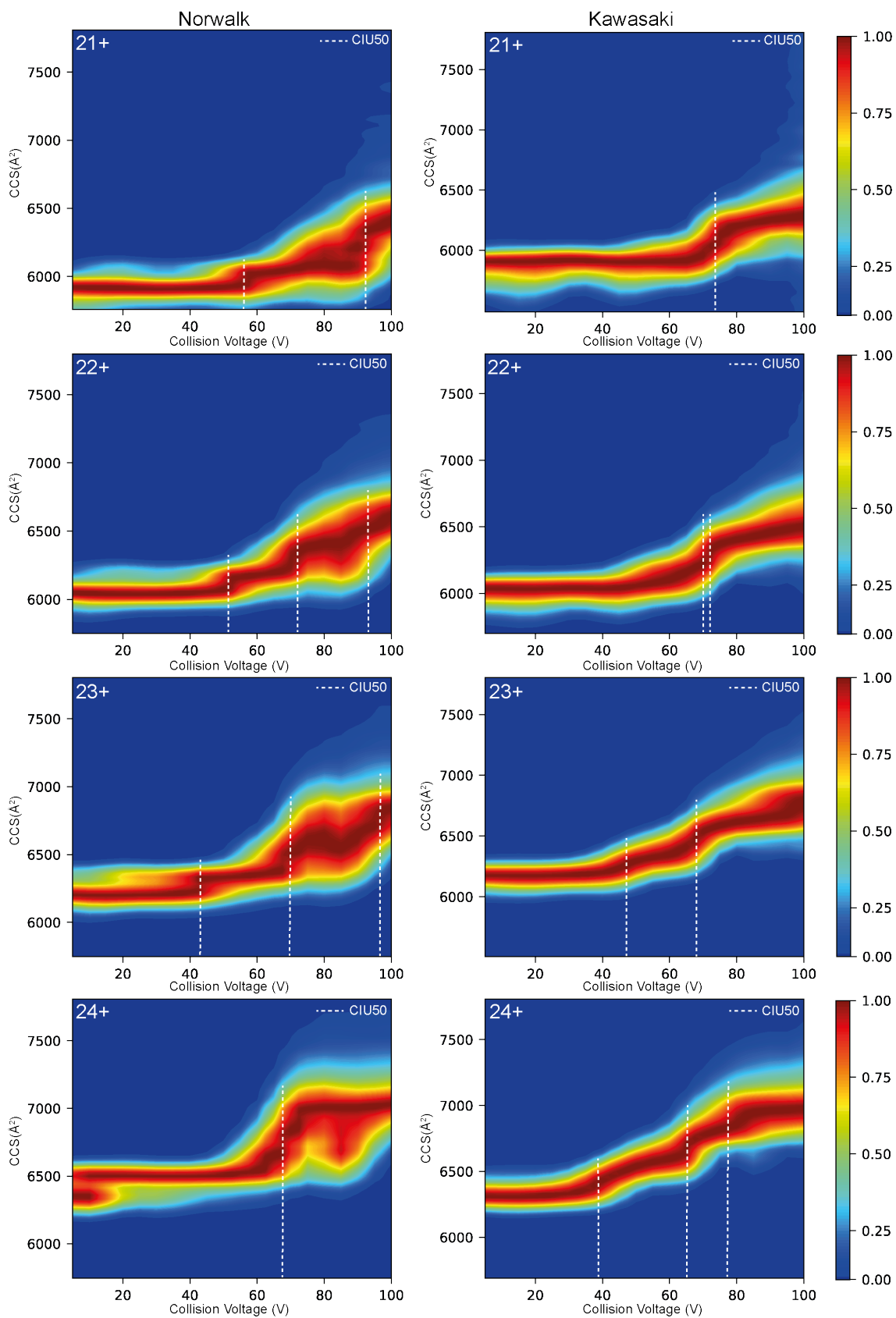


Figure S3: CIU fingerprints and CIU50 for all selected charge states.

Table S2: **Average CCS per time slots.** Comparing the average CCS per time slot for simulations at a specific temperature, one can see that unfolding seems to take place at higher temperatures. The CCS values are given with their corresponding standard error, followed by the standard error of the mean. Interestingly, Norwalk strain dimers increase in CCS notably at 700 K, whereas Kawasaki strain dimers only by 1 %. At higher temperatures the increase of CCS over the defined time slots becomes even more evident by the reported average values, where the CCS increases by 17 to 22 % for the dimers.

Time slots	Average CCS [ $\text{\AA}^2$ ] for Norwalk per time slot					
	300 K	400 K	500 K	600 K	700 K	900 K
Time slot 1	5216 ( $\pm 82, 8$ )	5235 ( $\pm 78, 7$ )	5273 ( $\pm 165, 16$ )	5436 ( $\pm 144, 14$ )	5870 ( $\pm 214, 20$ )	7762 ( $\pm 519, 49$ )
Time slot 2	5179 ( $\pm 80, 7$ )	5186 ( $\pm 81, 7$ )	5219 ( $\pm 172, 16$ )	5365 ( $\pm 154, 14$ )	5996 ( $\pm 194, 18$ )	8458 ( $\pm 420, 38$ )
Time slot 3	5170 ( $\pm 86, 8$ )	5166 ( $\pm 67, 6$ )	5200 ( $\pm 161, 15$ )	5349 ( $\pm 156, 14$ )	6135 ( $\pm 193, 18$ )	8795 ( $\pm 460, 38$ )
Time slot 4	5157 ( $\pm 82, 8$ )	5154 ( $\pm 56, 5$ )	5183 ( $\pm 151, 14$ )	5388 ( $\pm 158, 14$ )	6253 ( $\pm 189, 17$ )	8987 ( $\pm 460, 42$ )
Time slot 5	5145 ( $\pm 80, 7$ )	5146 ( $\pm 61, 6$ )	5174 ( $\pm 150, 14$ )	5375 ( $\pm 158, 15$ )	6386 ( $\pm 210, 19$ )	9012 ( $\pm 493, 45$ )
Time slot 6	5144 ( $\pm 76, 7$ )	5137 ( $\pm 68, 6$ )	5166 ( $\pm 132, 12$ )	5376 ( $\pm 146, 14$ )	6477 ( $\pm 193, 18$ )	9109 ( $\pm 453, 43$ )

Time slots	Average CCS [ $\text{\AA}^2$ ] for Kawasaki per time slot					
	300 K	400 K	500 K	600 K	700 K	900 K
Time slot 1	5197 ( $\pm 52, 5$ )	5233 ( $\pm 53, 5$ )	5209 ( $\pm 84, 8$ )	5201 ( $\pm 94, 9$ )	5335 ( $\pm 106, 10$ )	6741 ( $\pm 418, 39$ )
Time slot 2	5172 ( $\pm 57, 5$ )	5188 ( $\pm 47, 4$ )	5140 ( $\pm 79, 7$ )	5118 ( $\pm 78, 7$ )	5320 ( $\pm 123, 11$ )	7474 ( $\pm 378, 35$ )
Time slot 3	5165 ( $\pm 52, 5$ )	5174 ( $\pm 47, 4$ )	5104 ( $\pm 67, 6$ )	5095 ( $\pm 61, 6$ )	5345 ( $\pm 143, 13$ )	7815 ( $\pm 349, 32$ )
Time slot 4	5168 ( $\pm 55, 5$ )	5157 ( $\pm 49, 5$ )	5086 ( $\pm 68, 6$ )	5090 ( $\pm 84, 8$ )	5380 ( $\pm 160, 15$ )	8085 ( $\pm 400, 37$ )
Time slot 5	5161 ( $\pm 53, 5$ )	5148 ( $\pm 41, 4$ )	5072 ( $\pm 68, 6$ )	5096 ( $\pm 86, 8$ )	5387 ( $\pm 141, 13$ )	8215 ( $\pm 357, 33$ )
Time slot 6	5159 ( $\pm 51, 5$ )	5142 ( $\pm 44, 4$ )	5068 ( $\pm 63, 6$ )	5089 ( $\pm 87, 8$ )	5388 ( $\pm 159, 15$ )	8287 ( $\pm 299, 28$ )

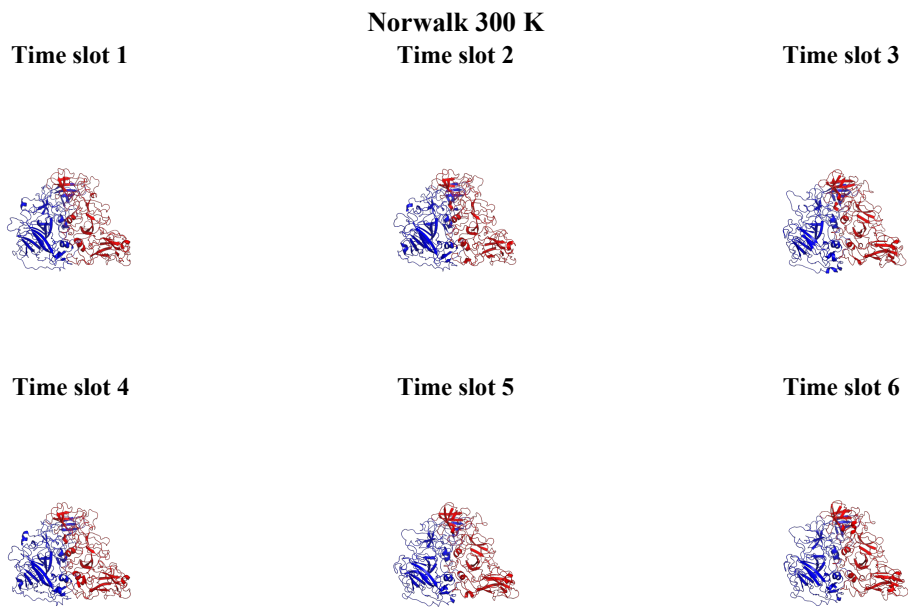


Figure S4: **Representative structures for Norwalk dimers per region at 300 K.**

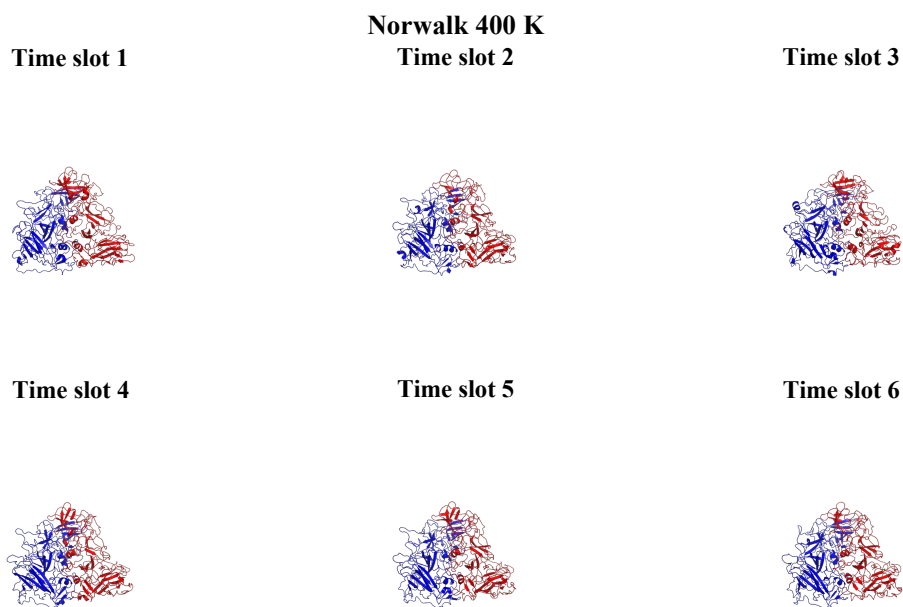


Figure S5: **Representative structures for Norwalk dimers per region at 400 K.**

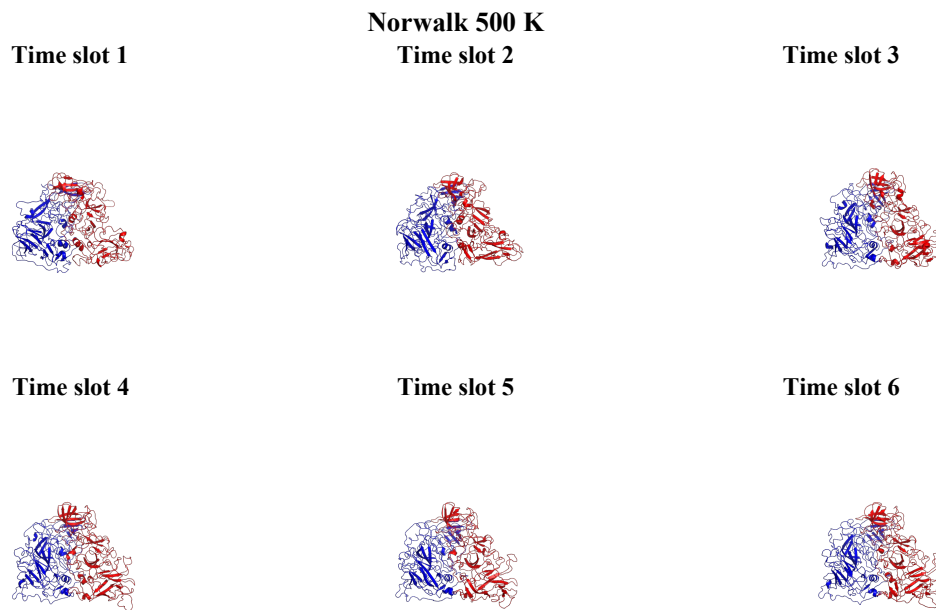


Figure S6: **Representative structures for Norwalk dimers per region at 500 K.**

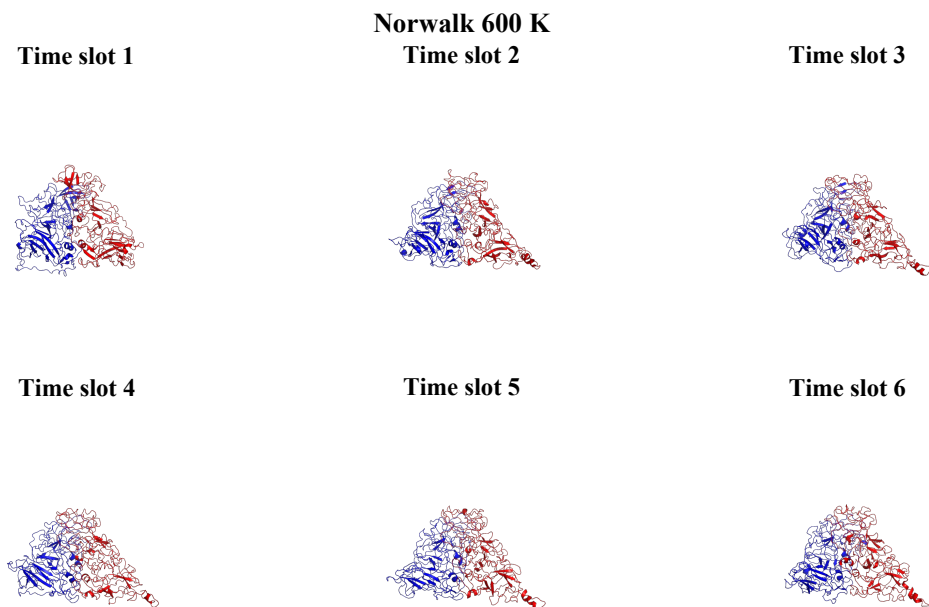


Figure S7: **Representative structures for Norwalk dimers per region at 600 K.**

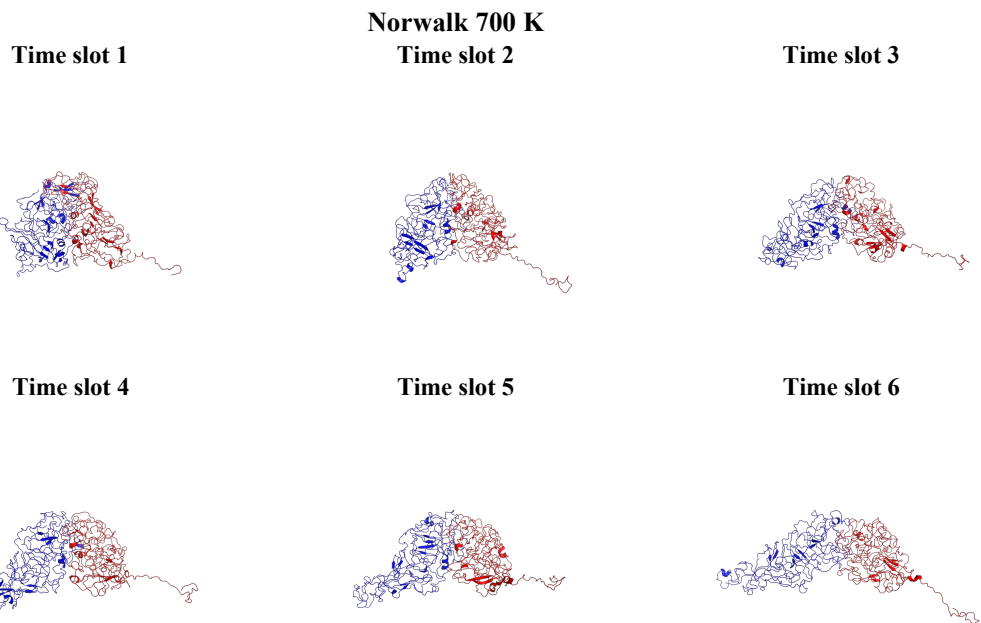


Figure S8: **Representative structures for Norwalk dimers per region at 700 K.**

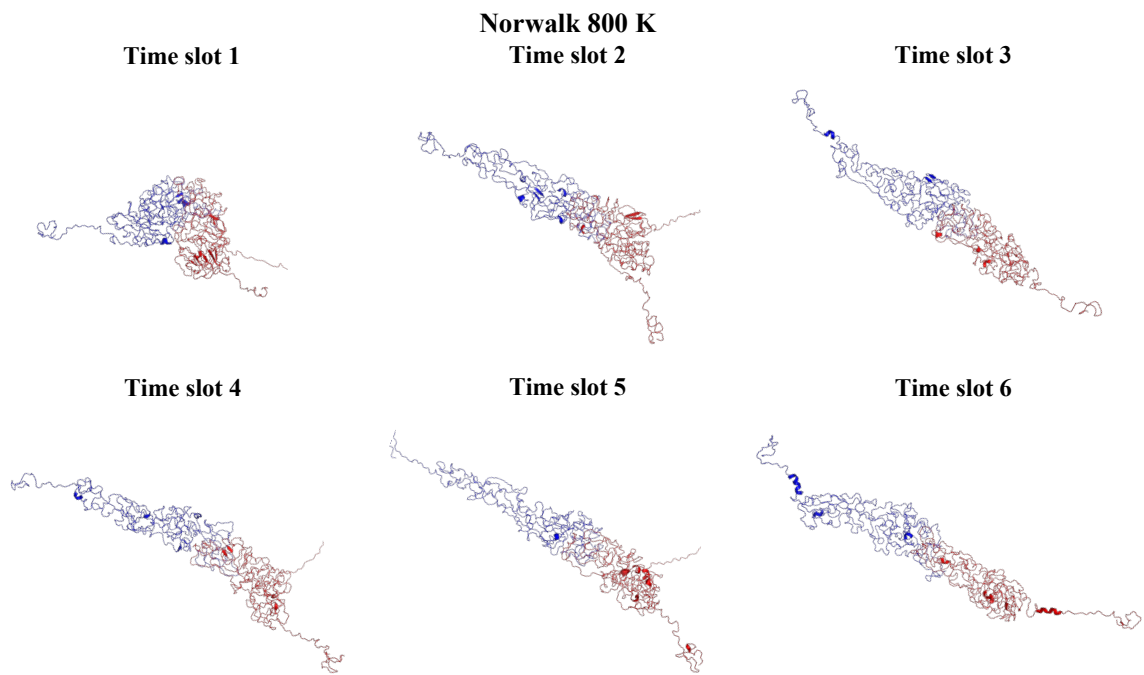


Figure S9: **Representative structures for Norwalk dimers per region at 800 K.**



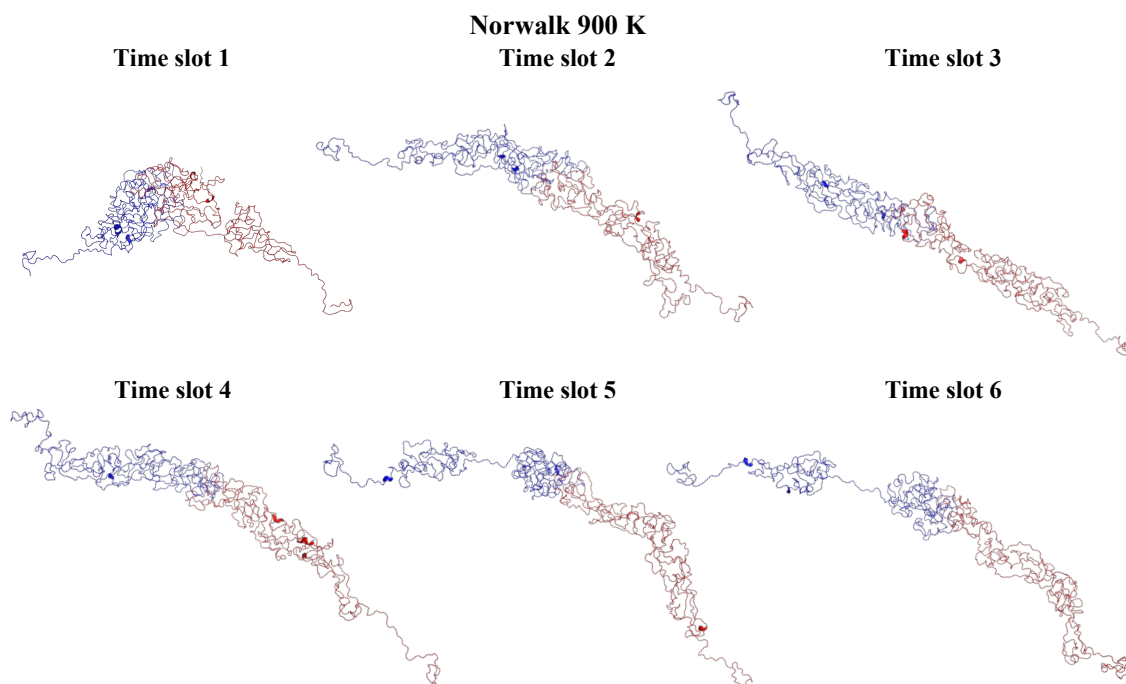


Figure S10: **Representative structures for Norwalk dimers per region at 900 K.**

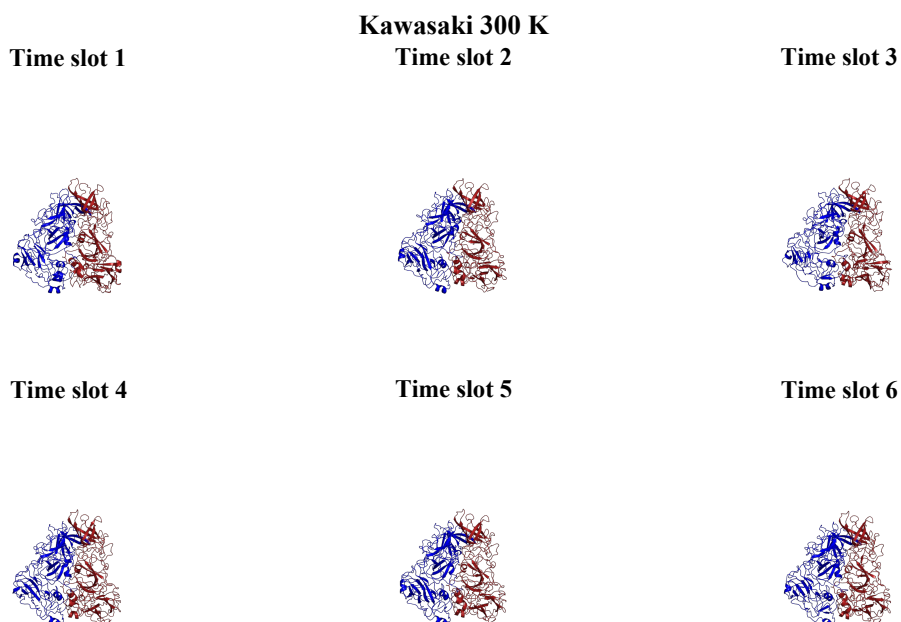


Figure S11: **Representative structures for Kawasaki dimer per region at 300 K.**

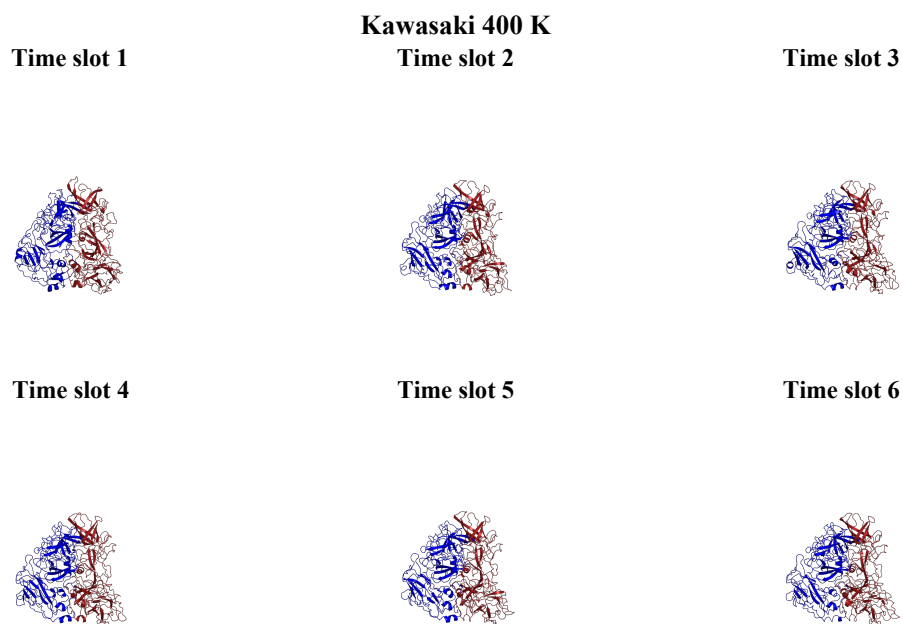


Figure S12: **Representative structures for Kawasaki dimers per region at 400 K.**

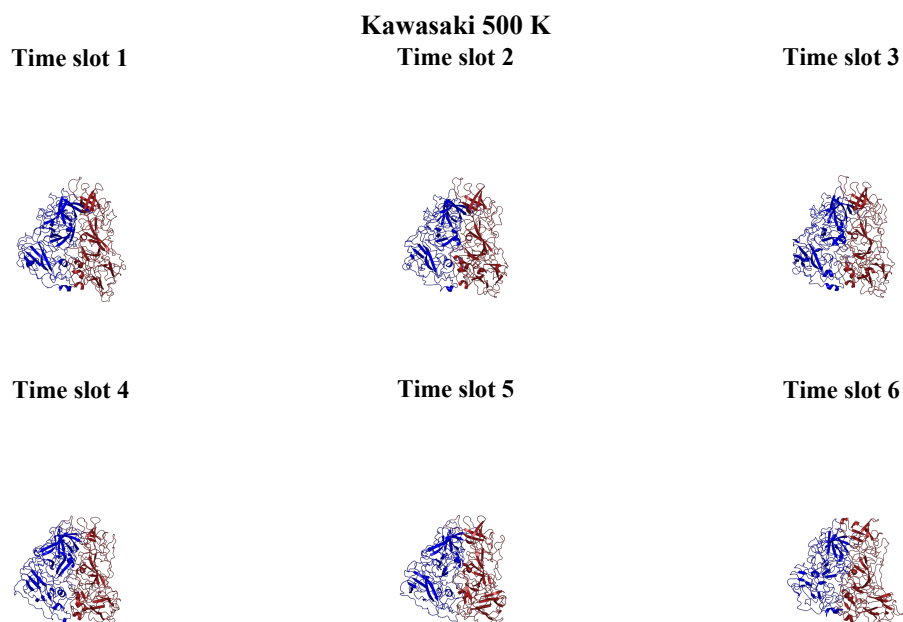


Figure S13: **Representative structures for Kawasaki dimers per region at 500 K.**

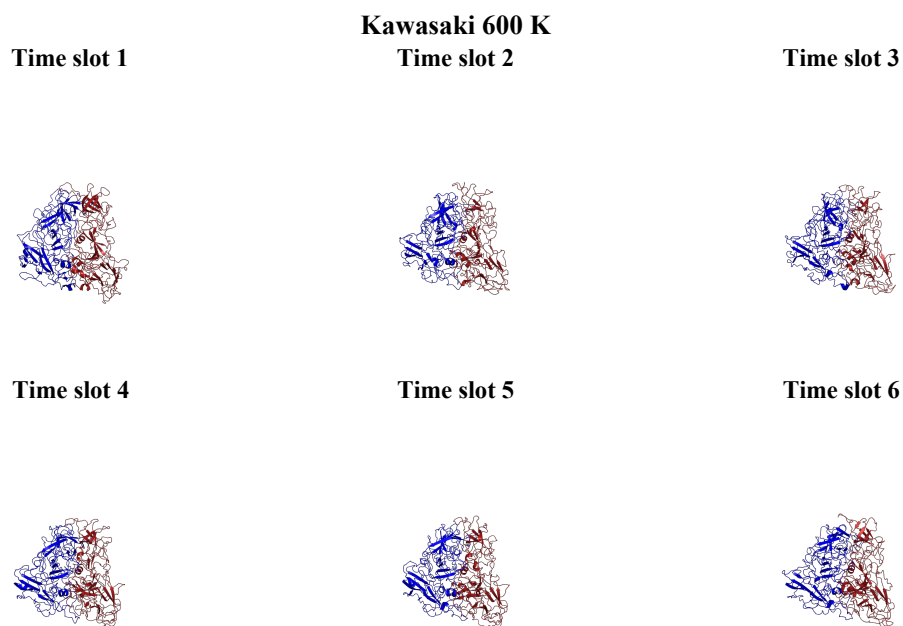


Figure S14: Representative structures for Kawasaki dimers per region at 600 K.

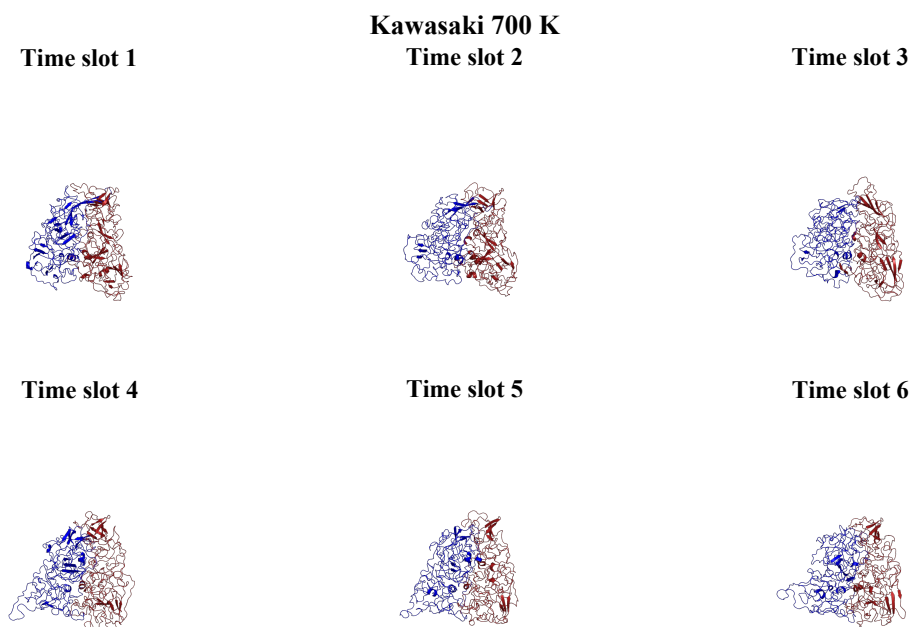


Figure S15: Representative structures for Kawasaki dimers per region at 700 K.

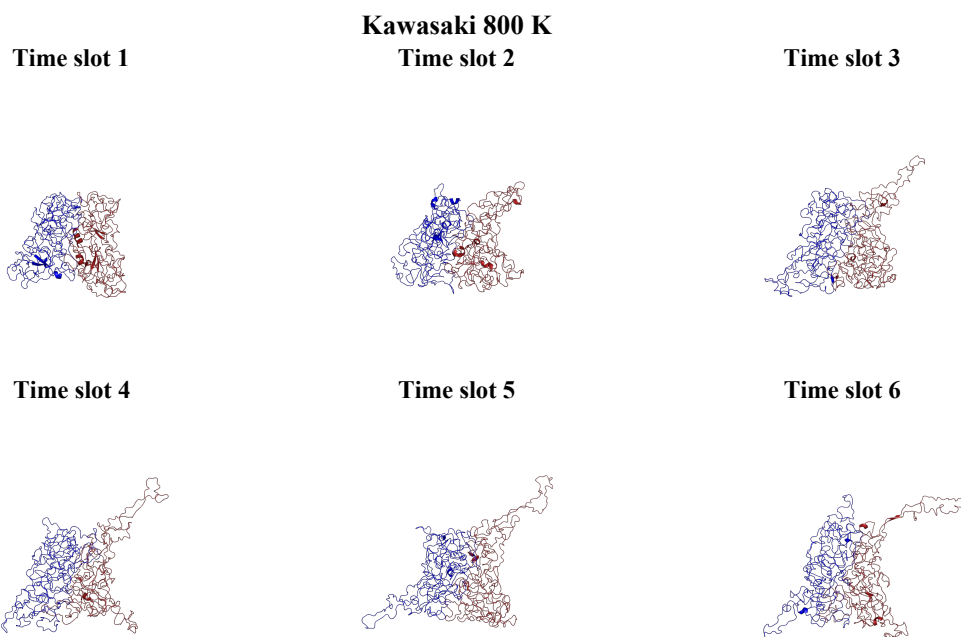


Figure S16: Representative structures for Kawasaki dimers per region at 800 K.

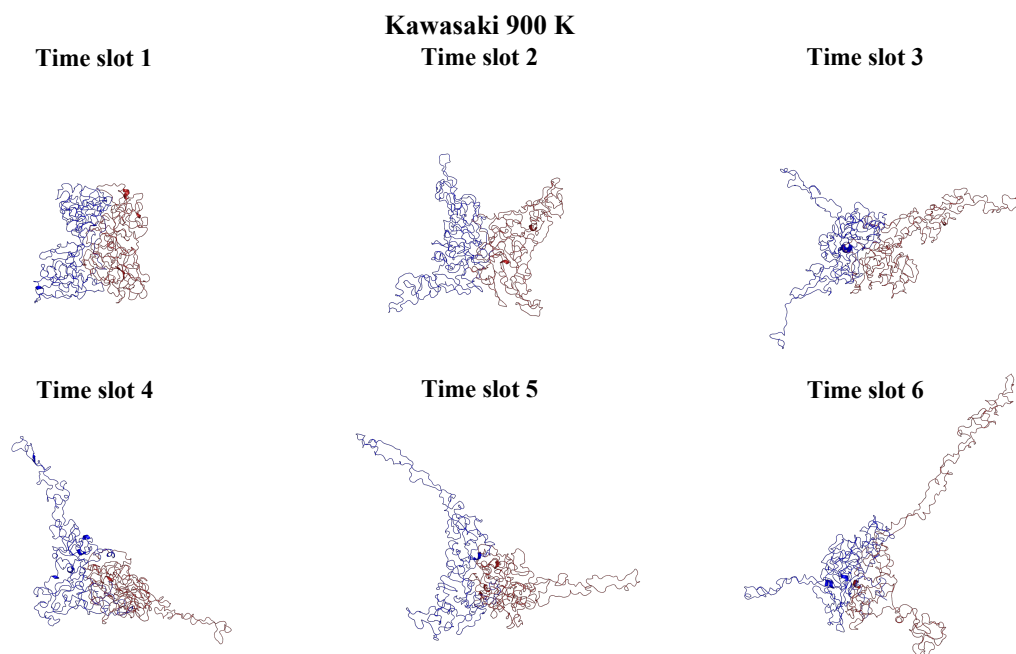


Figure S17: Representative structures for Kawasaki dimers per region at 900 K.

### Norwalk 300 K

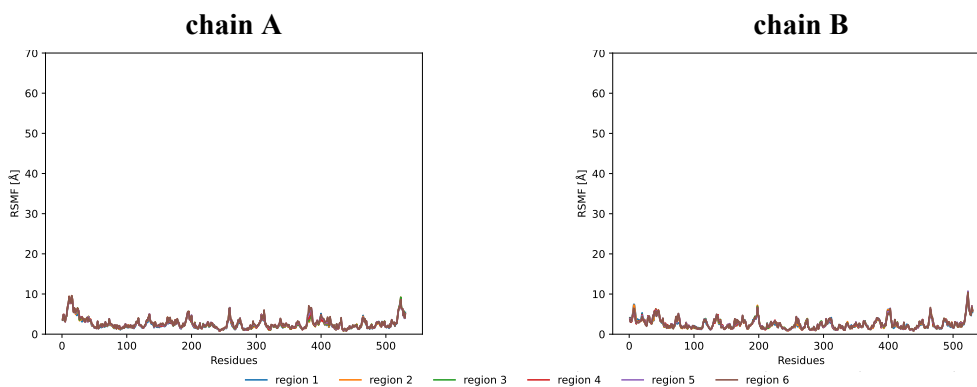


Figure S18: RMSF for Norwalk dimers per region at 300 K.

### Norwalk 400 K

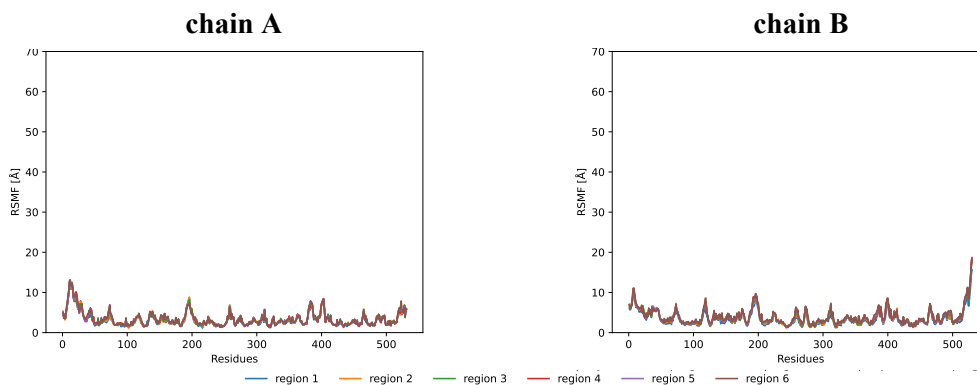


Figure S19: RMSF for Norwalk dimers per region at 400 K.

### Norwalk 500 K

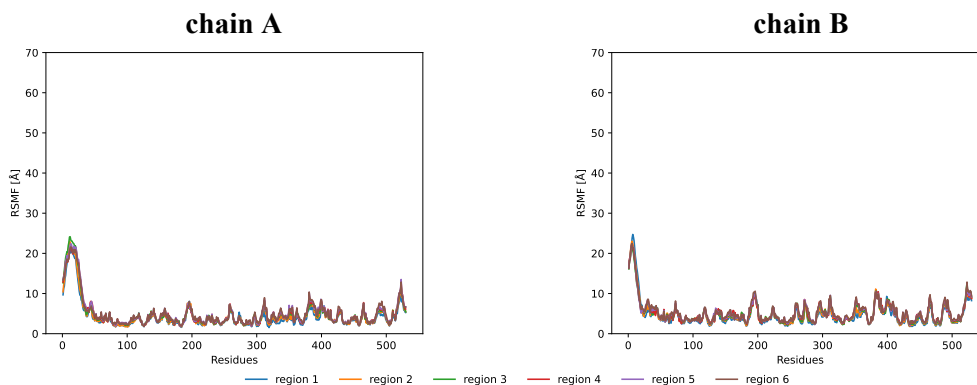


Figure S20: RMSF for Norwalk dimers per region at 500 K.

### Norwalk 600 K

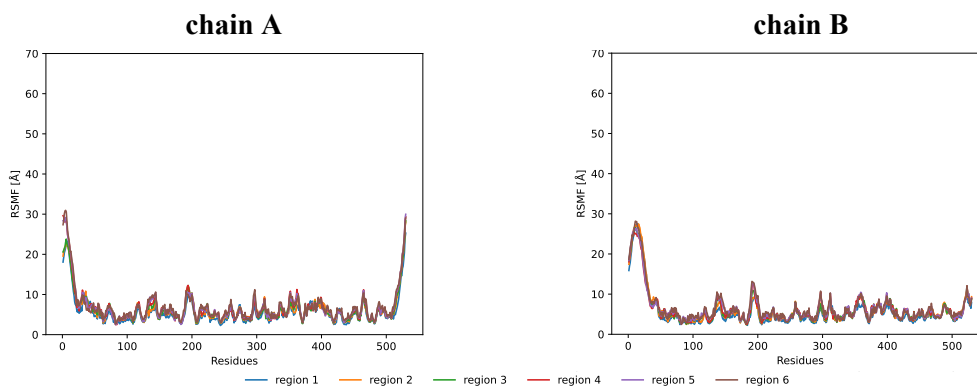


Figure S21: RMSF for Norwalk dimers per region at 600 K.

### Norwalk 700 K

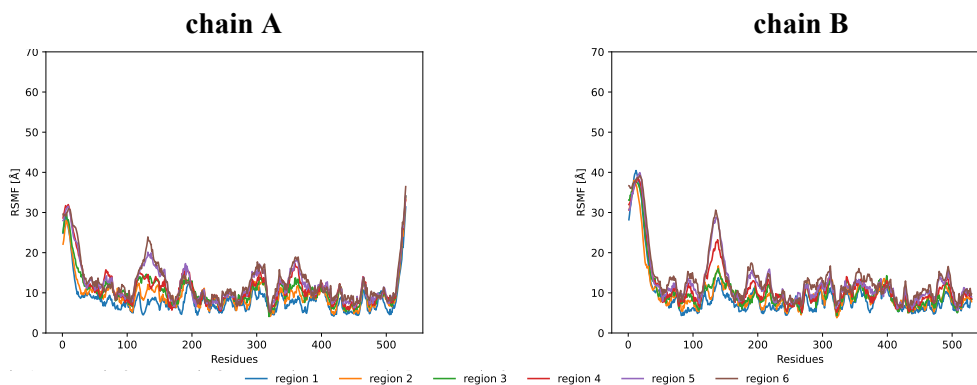


Figure S22: RMSF for Norwalk dimers per region at 700 K.

### Norwalk 800 K

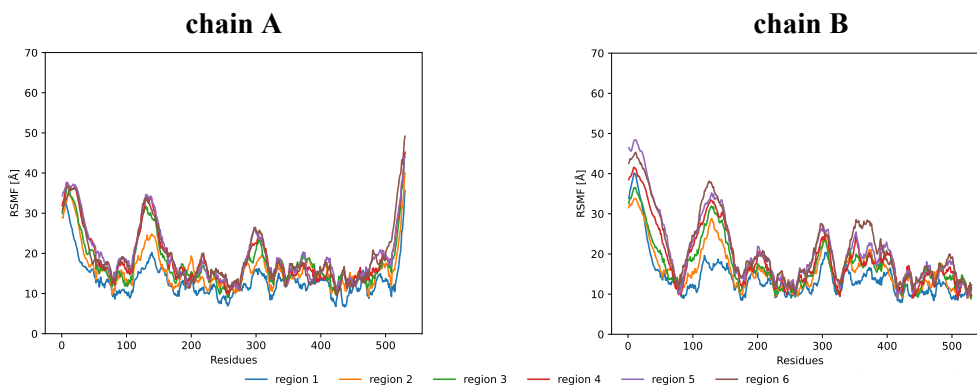


Figure S23: RMSF for Norwalk dimers per region at 800 K.

### Norwalk 900 K

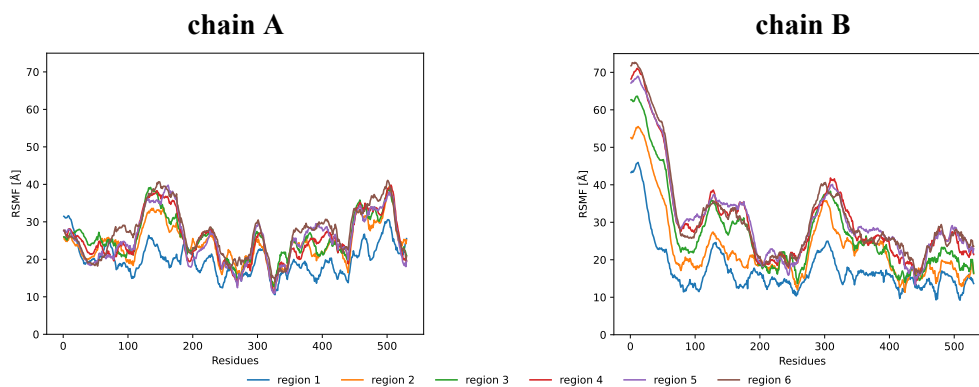


Figure S24: RMSF for Norwalk dimers per region at 900 K.

### Kawasaki 300 K

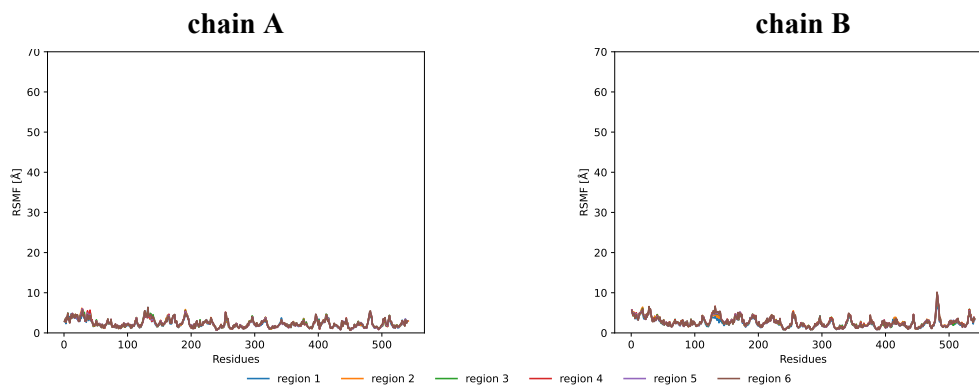


Figure S25: RMSF for Kawasaki dimers per region at 300 K.

### Kawasaki 400 K

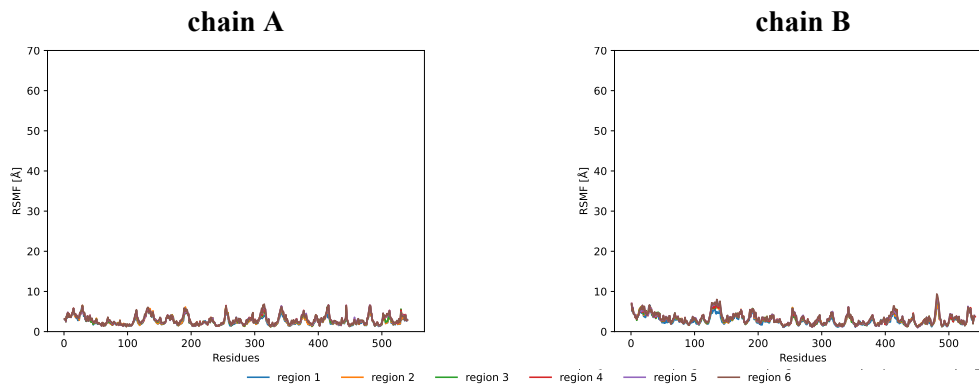


Figure S26: RMSF for Kawasaki dimers per region at 400 K.

### Kawasaki 500 K

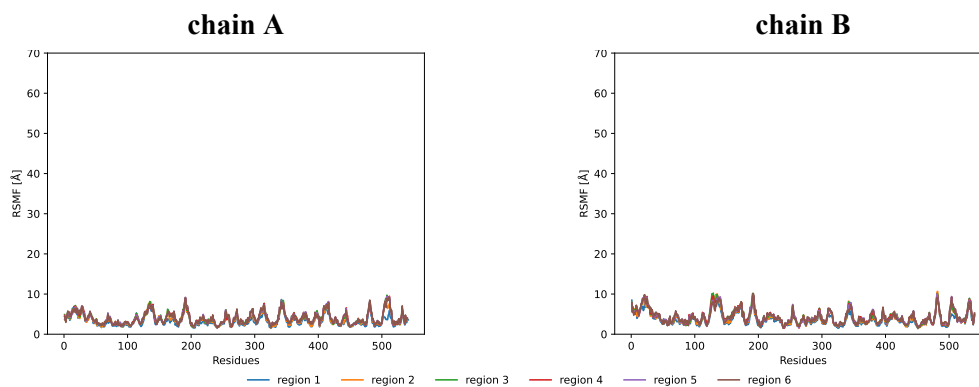


Figure S27: RMSF for Kawasaki dimers per region at 500 K.

### Kawasaki 600 K

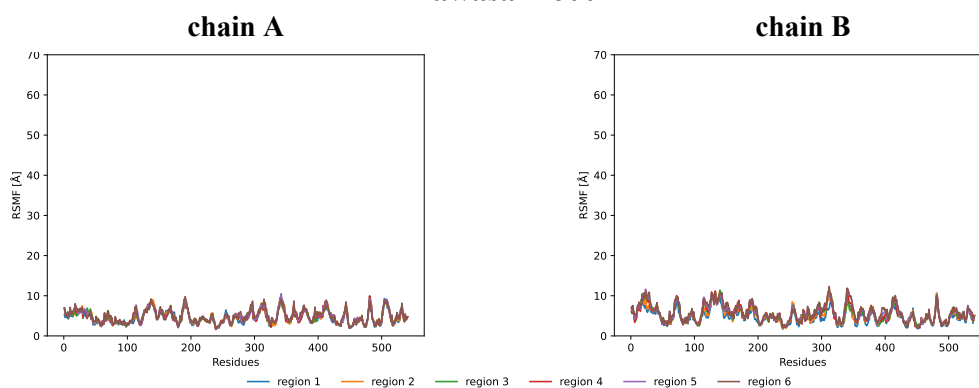


Figure S28: RMSF for Kawasaki dimers per region at 600 K.

### Kawasaki 700 K

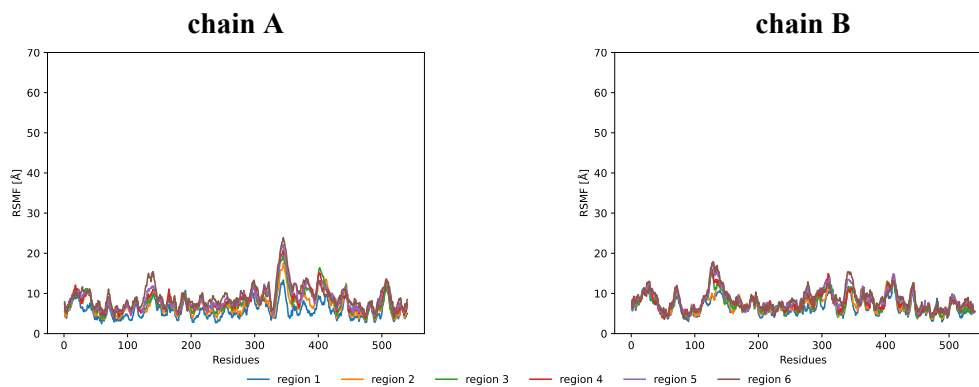


Figure S29: RMSF for Kawasaki dimers per region at 700 K.



## Kawasaki 800 K

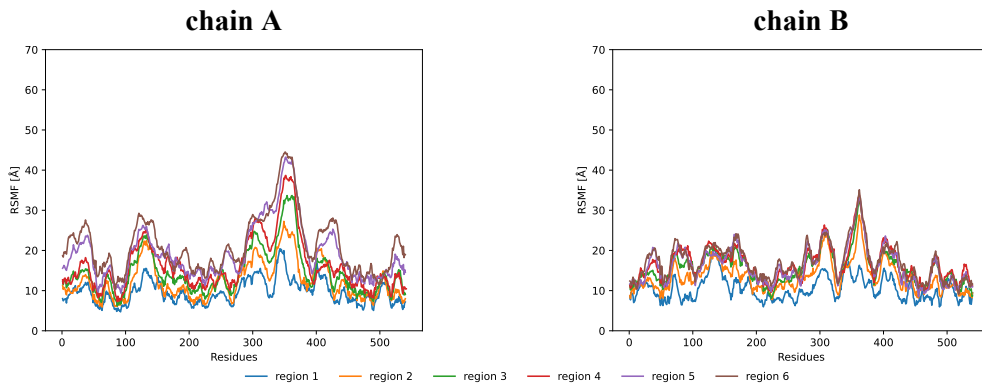


Figure S30: RMSF for Kawasaki dimers per region at 800 K.

## Kawasaki 900 K

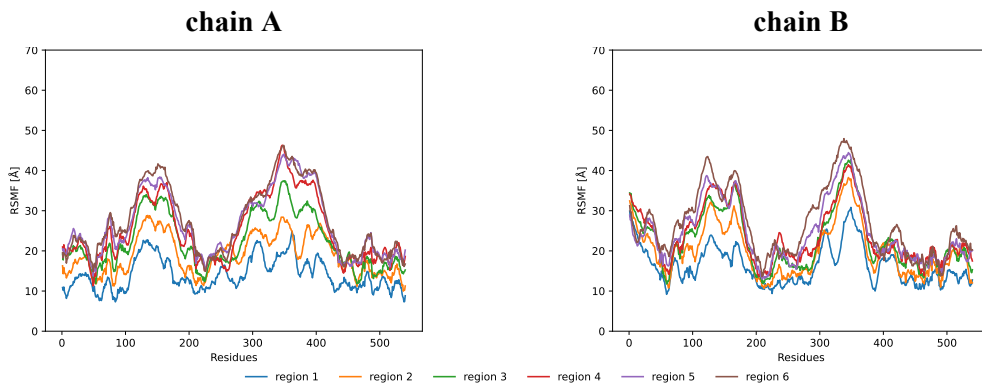


Figure S31: RMSF for Kawasaki dimers per region at 900 K.

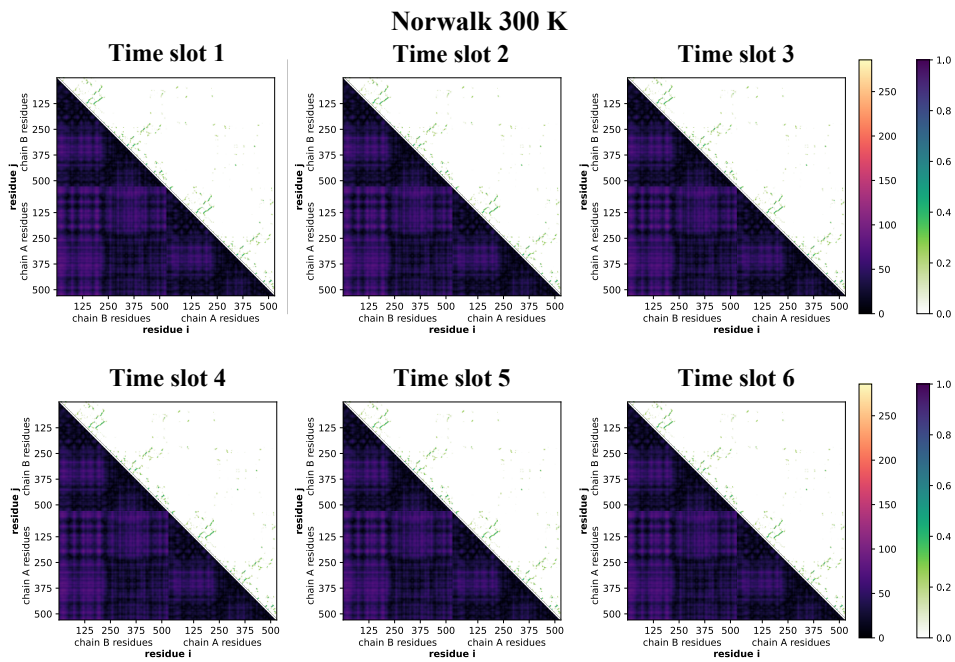


Figure S32: Average distance and contacts for Norwalk dimers per region at 300 K.

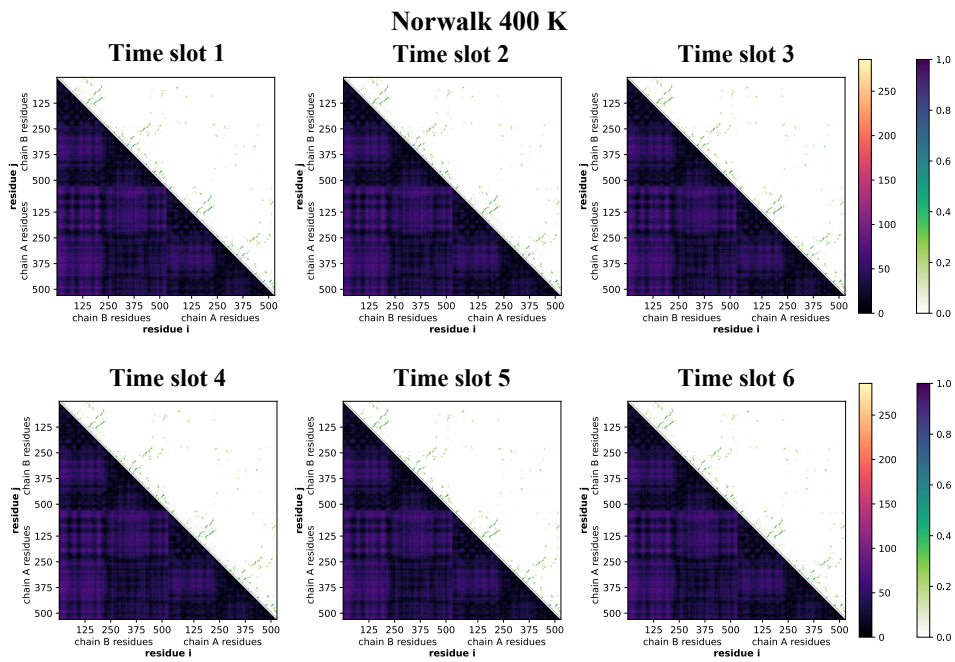


Figure S33: Average distance and contacts for Norwalk dimers per region at 400 K.

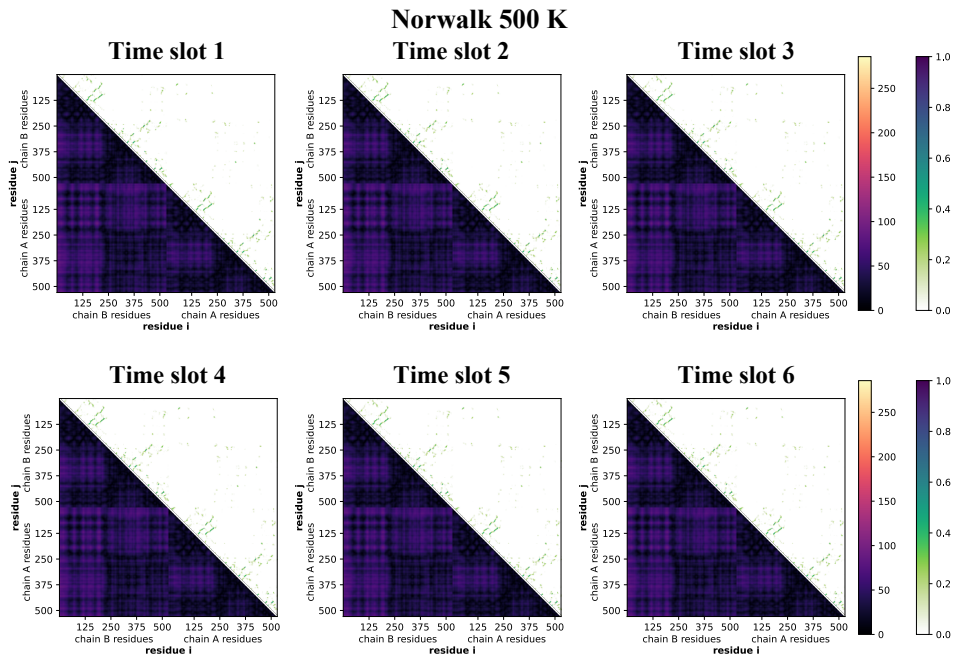


Figure S34: Average distance and contacts for Norwalk dimers per region at 500 K.

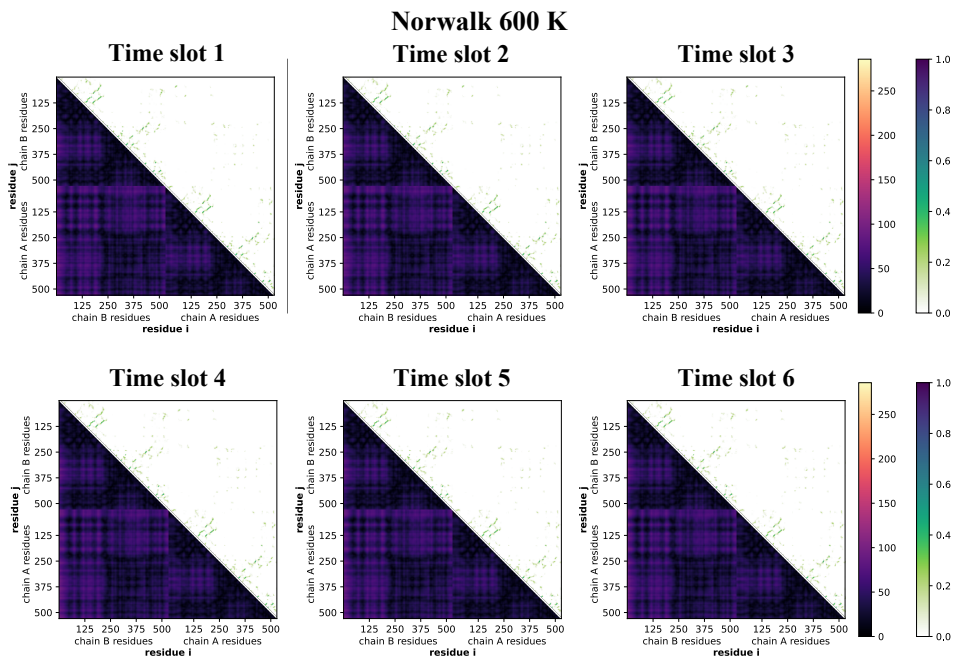


Figure S35: Average distance and contacts for Norwalk dimers per region at 600 K.

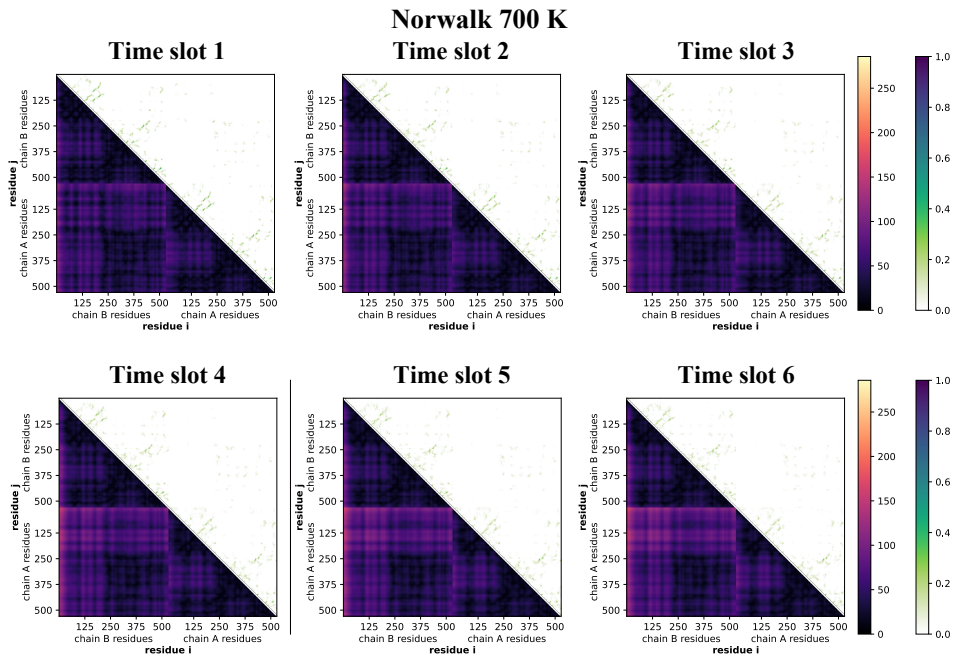


Figure S36: Average distance and contacts for Norwalk dimers per region at 700 K.

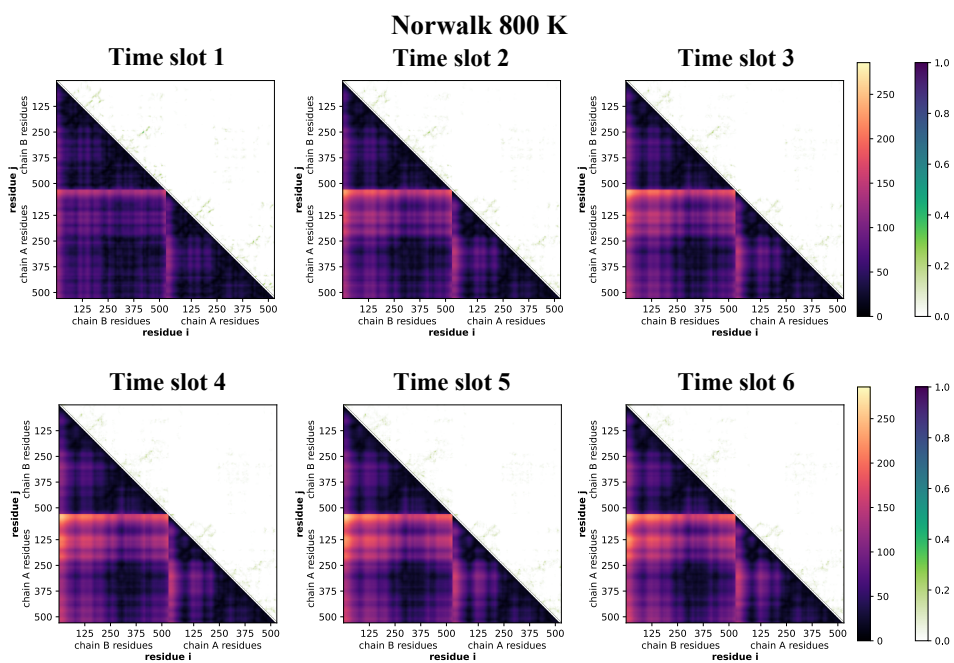


Figure S37: Average distance and contacts for Norwalk dimers per region at 800 K.

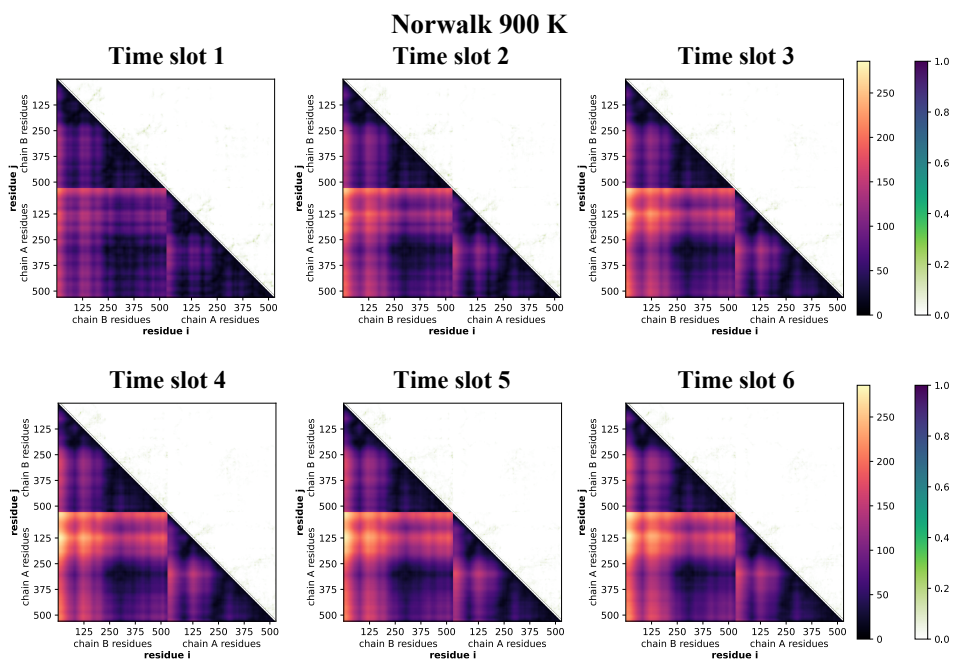


Figure S38: Average distance and contacts for Norwalk dimers per region at 900 K.

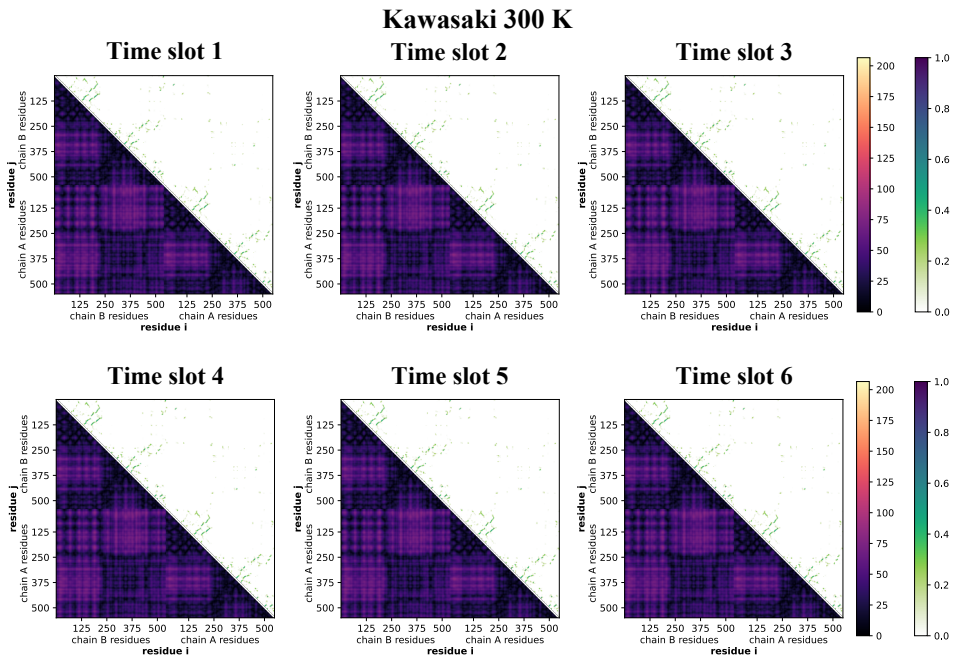


Figure S39: Average distance and contacts for Kawasaki dimers per region at 300 K.

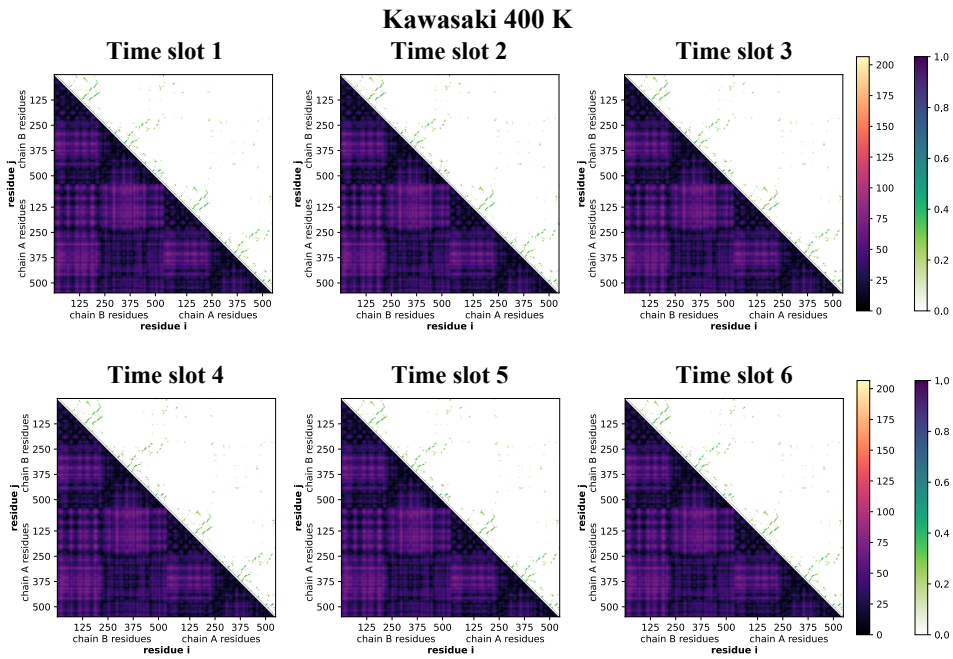


Figure S40: Average distance and contacts for Kawasaki dimers per region at 400 K.

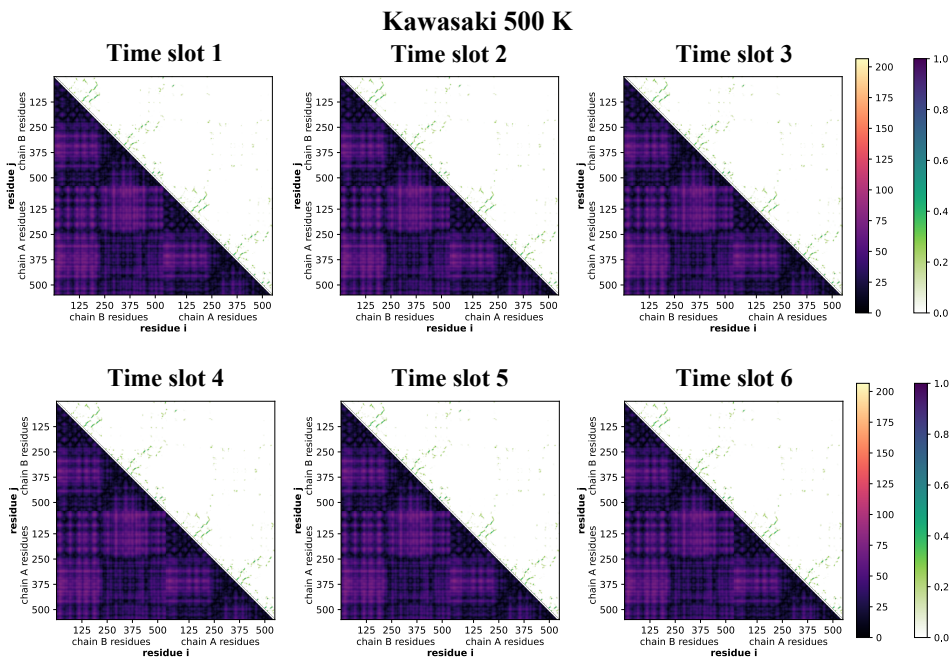


Figure S41: Average distance and contacts for Kawasaki dimers per region at 500 K.

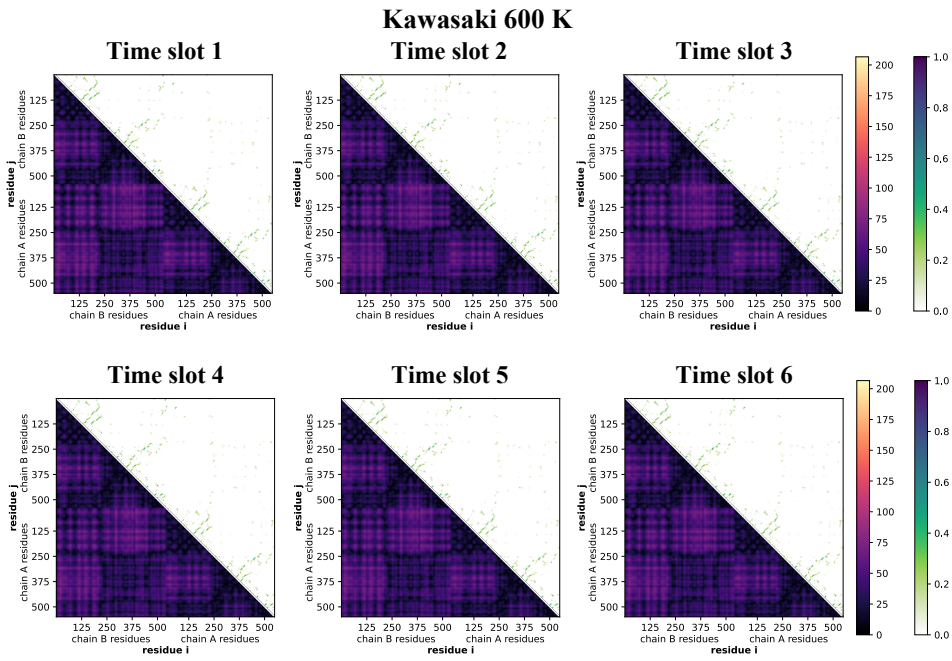


Figure S42: Average distance and contacts for Kawasaki dimers per region at 600 K.

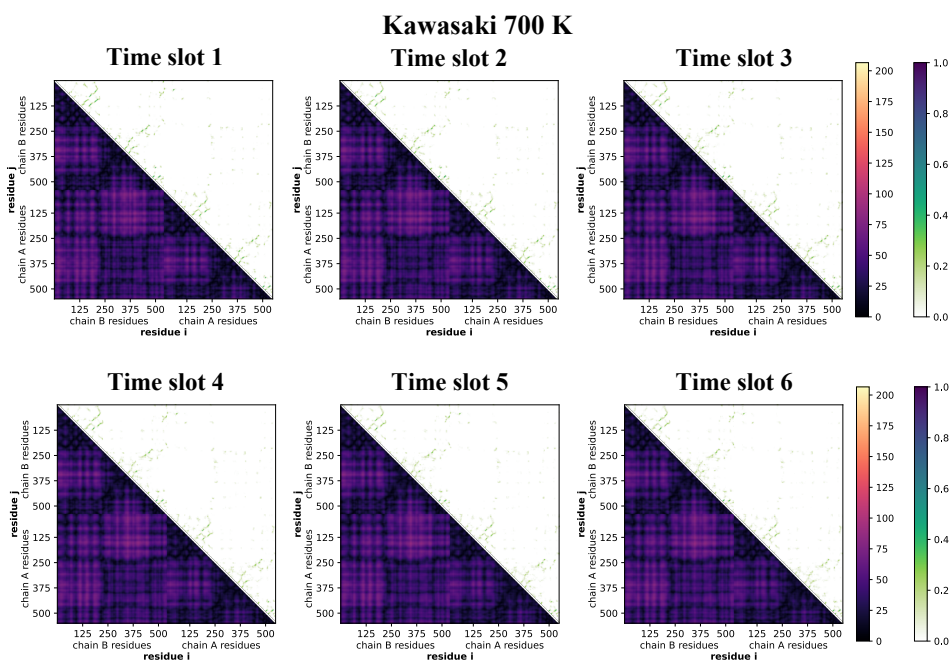


Figure S43: Average distance and contacts for Kawasaki dimers per region at 700 K.

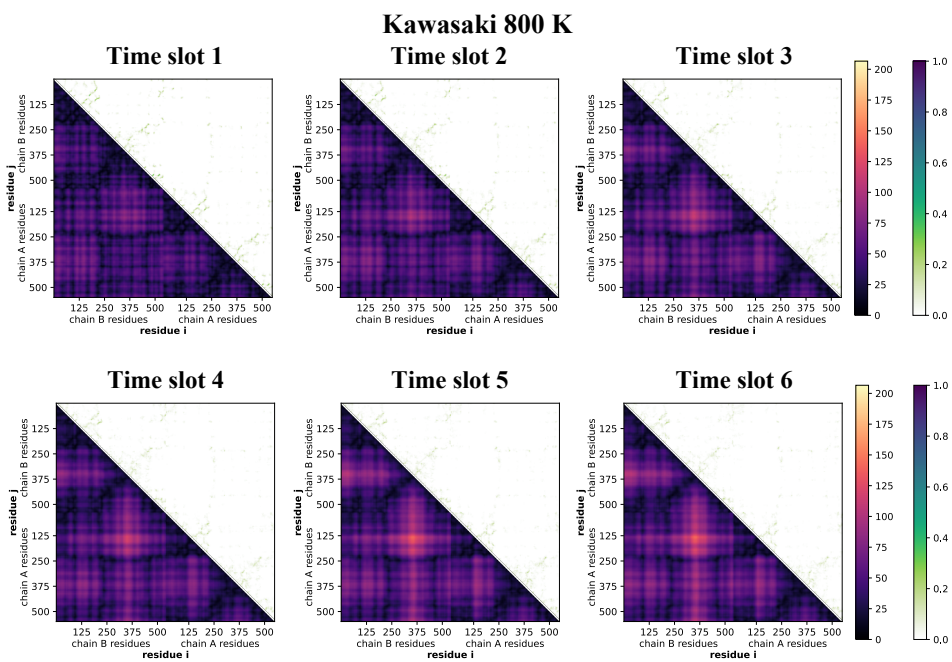


Figure S44: Average distance and contacts for Kawasaki dimers per region at 800 K.

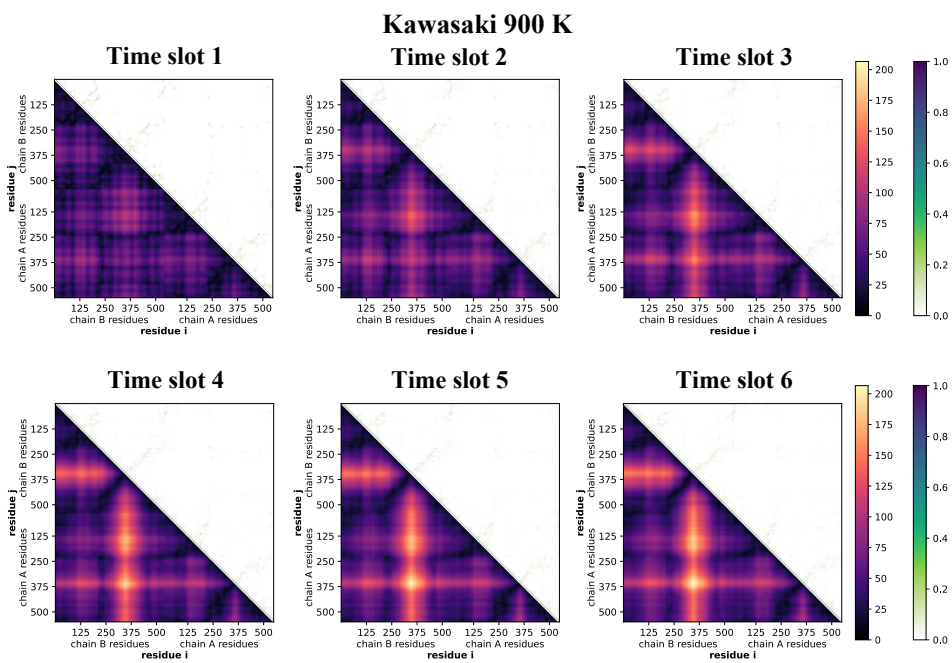


Figure S45: Average distance and contacts for Kawasaki dimers per region at 900 K.