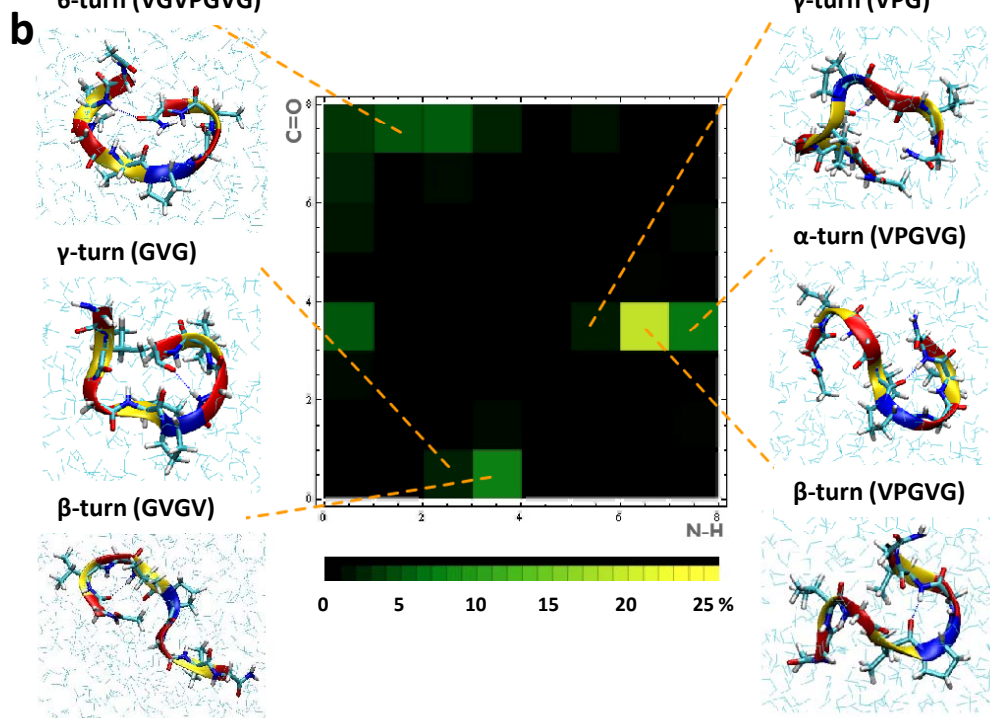
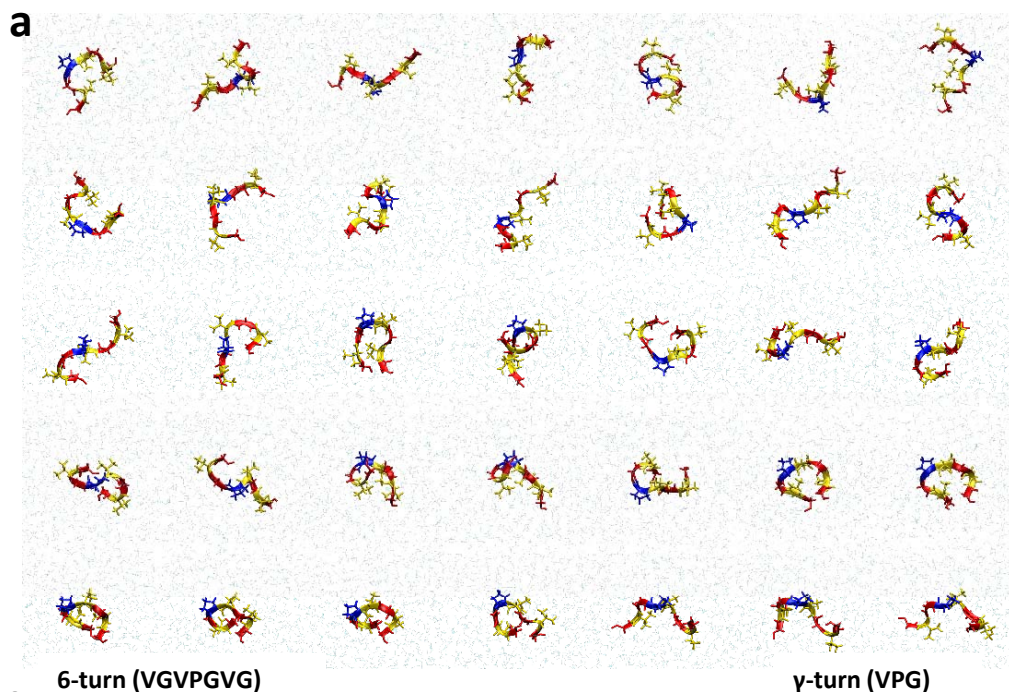
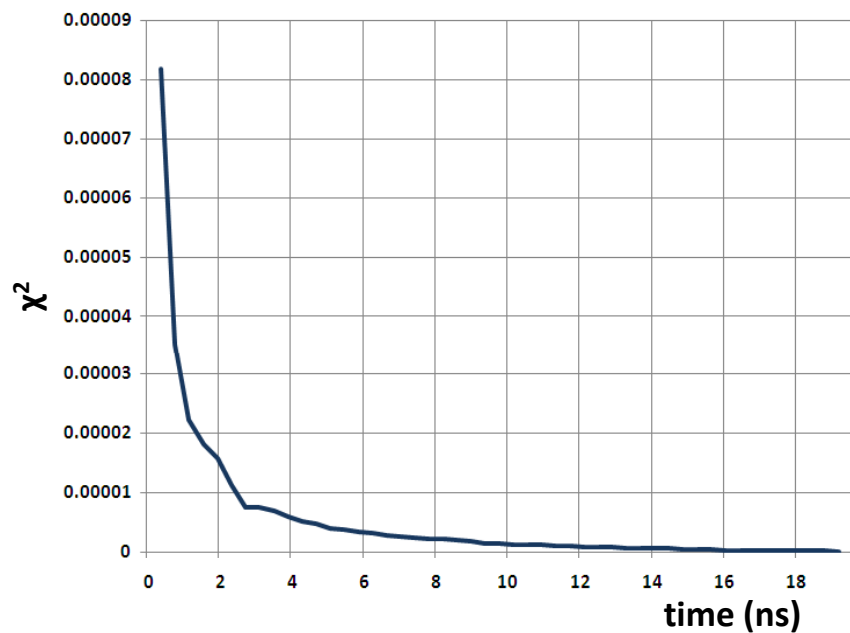
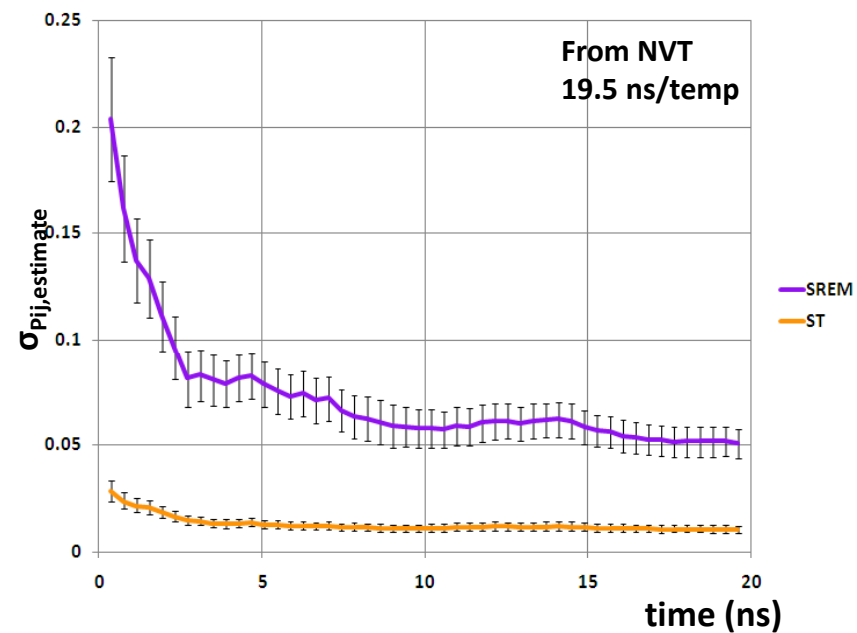
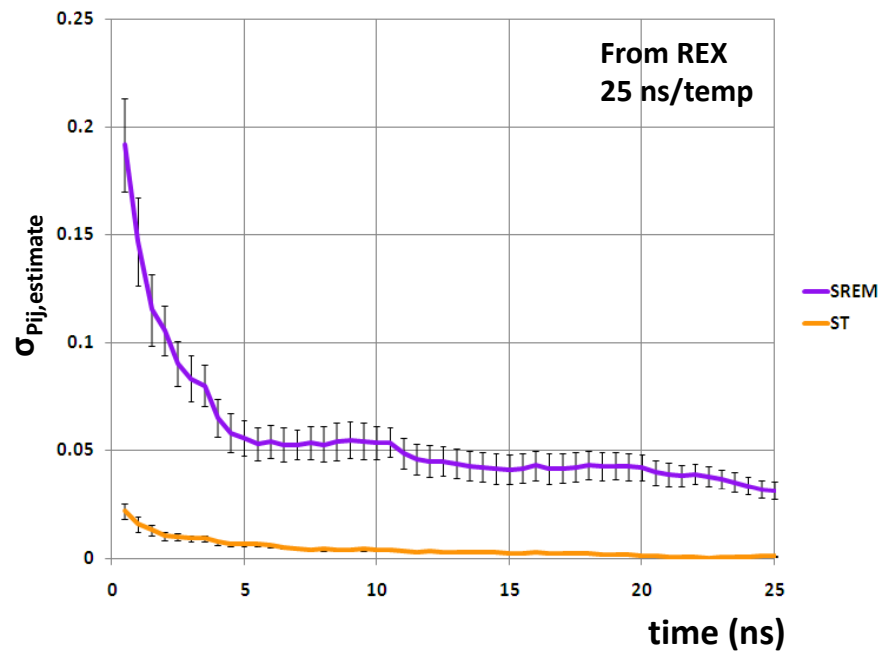
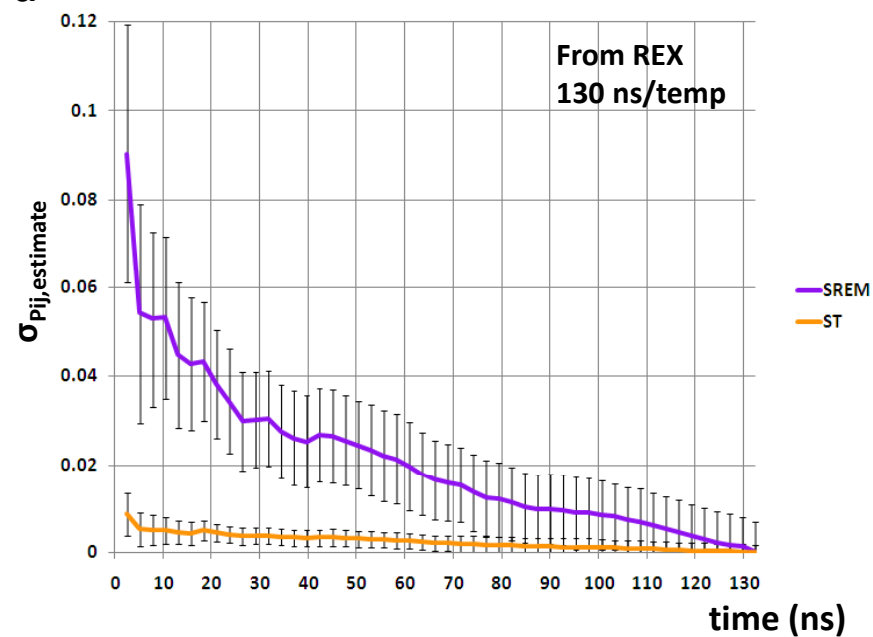
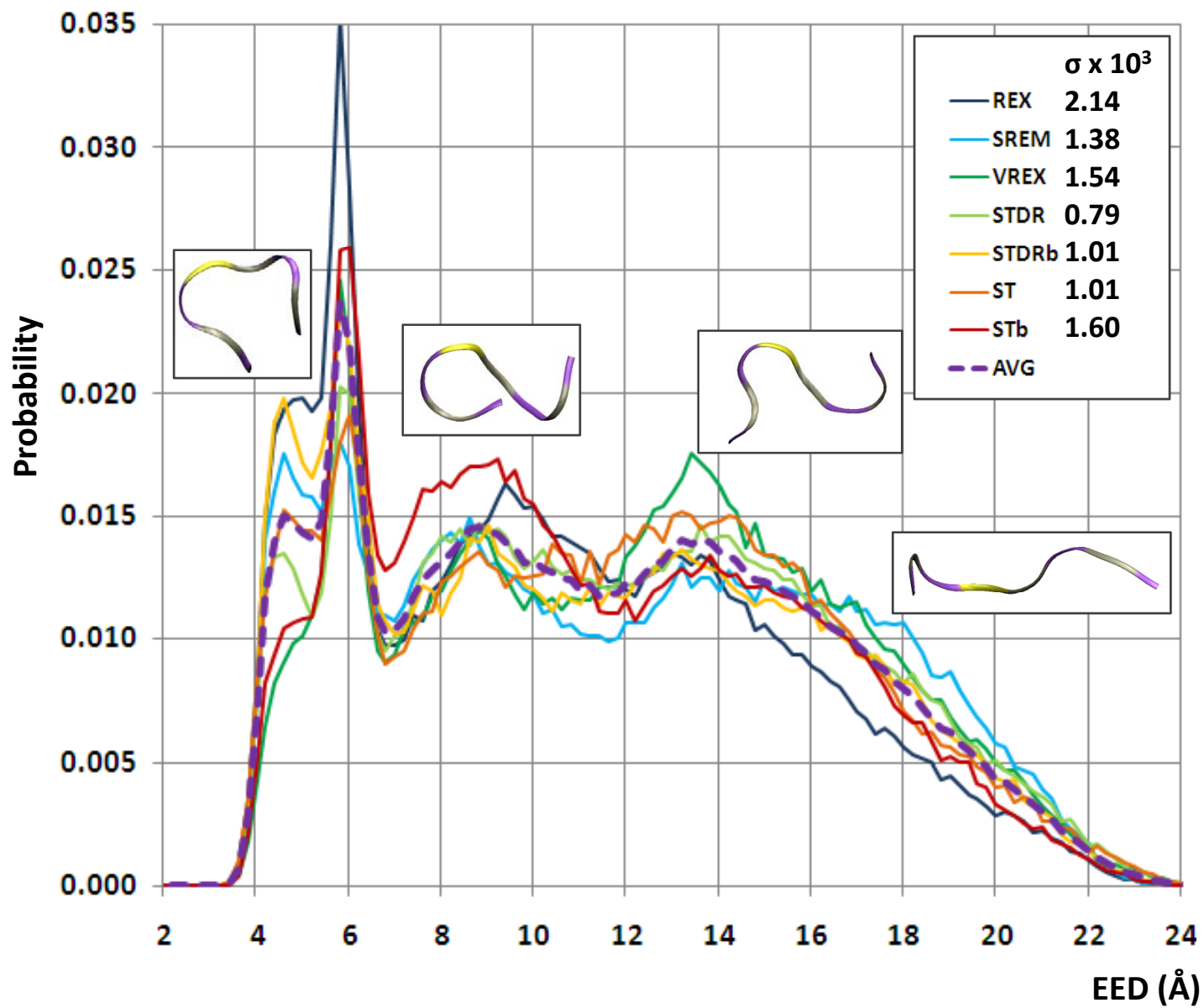


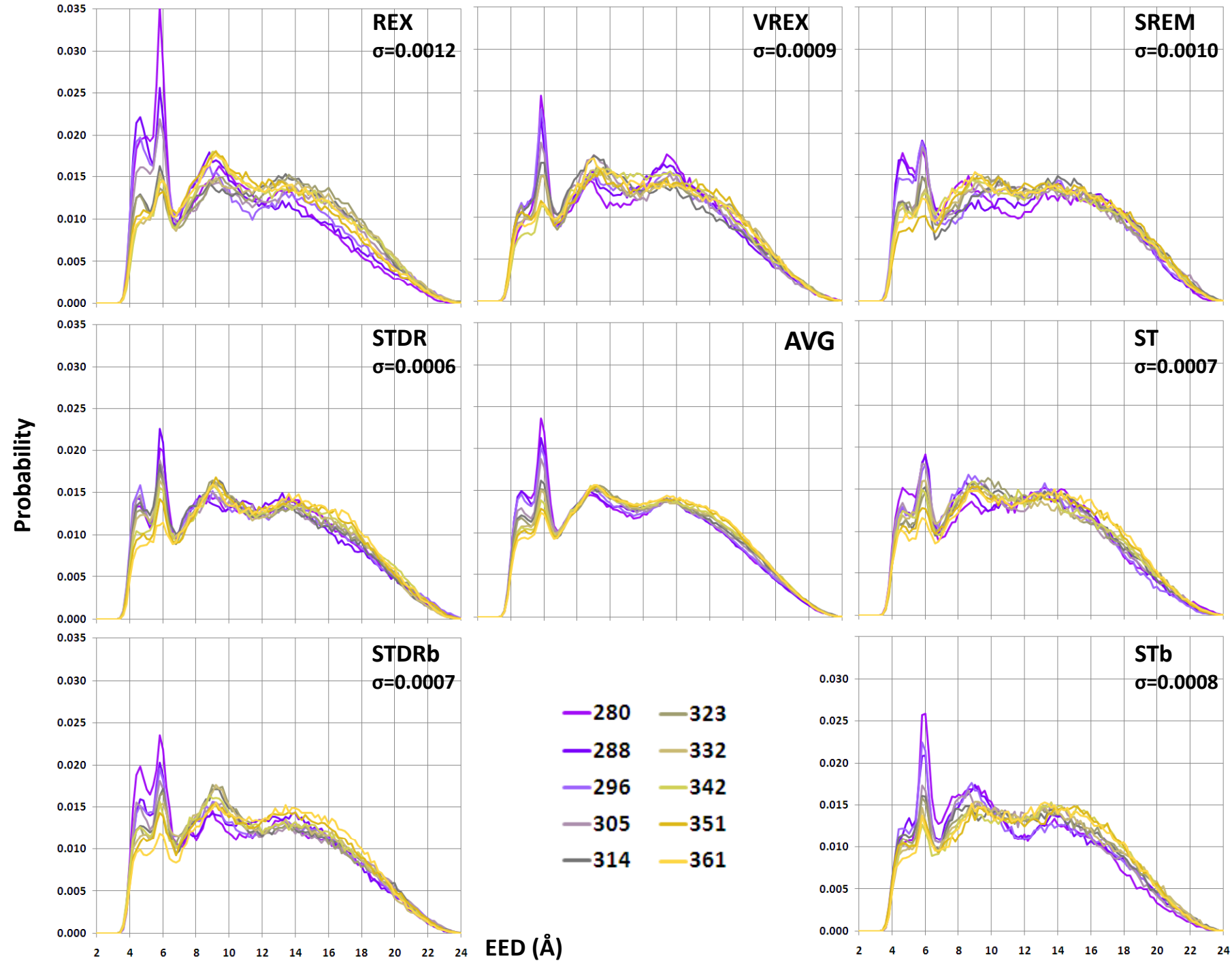
Implementation Issue	REX	SREM	VREX	STDR	ST
Scalable to any number of CPU's (even one CPU)?					
Algorithm readily accommodates a fluctuating number of CPU's?					
Efficiency impaired by inhomogeneity of CPU's?					
Performance severely affected by CPU failure?					
Initial calculation of weight factors, potential energy distribution functions or potential energy lists required?					

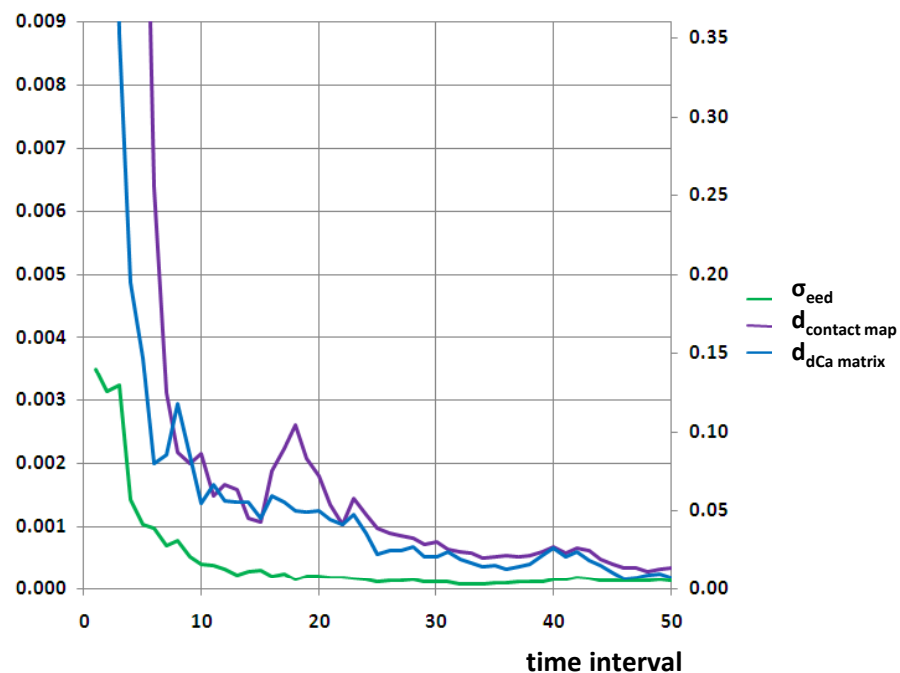
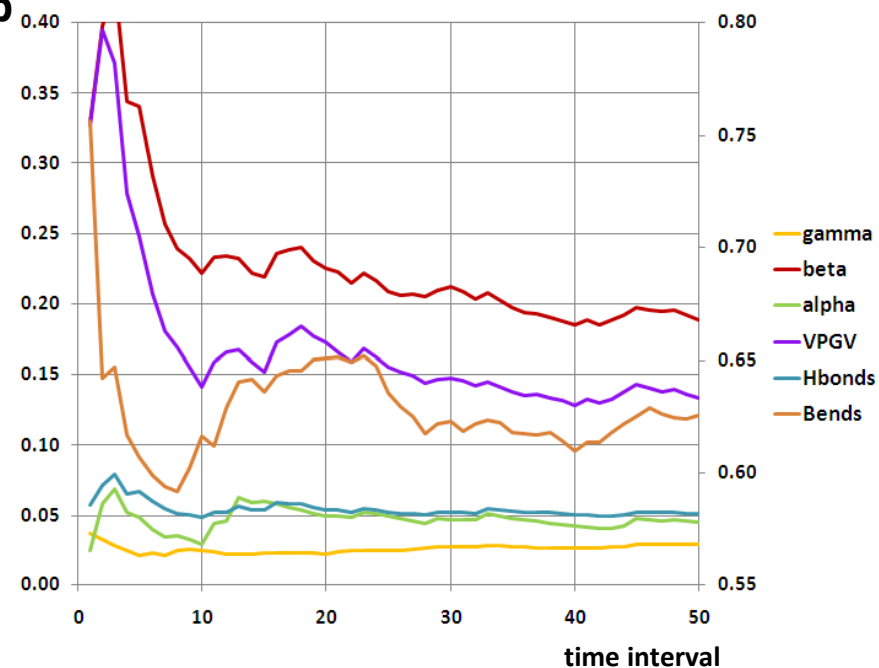
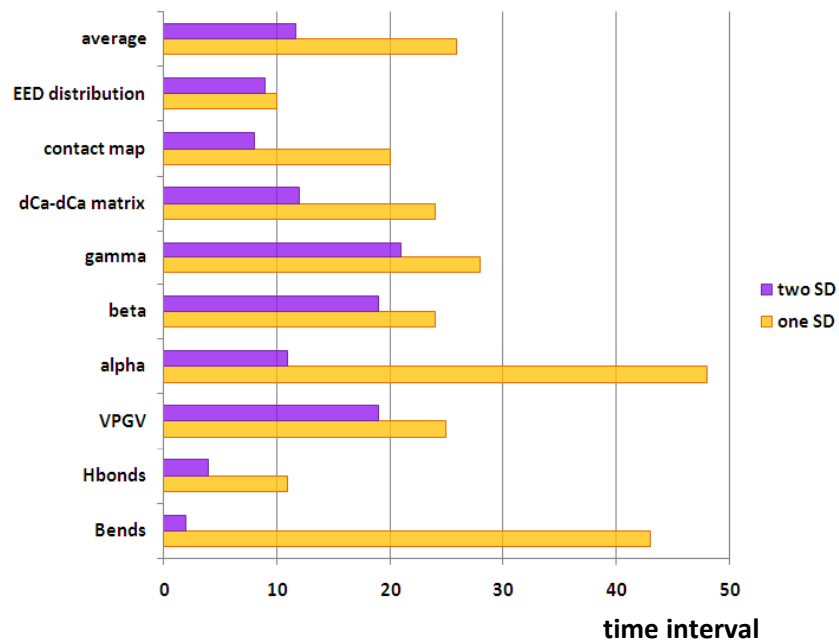
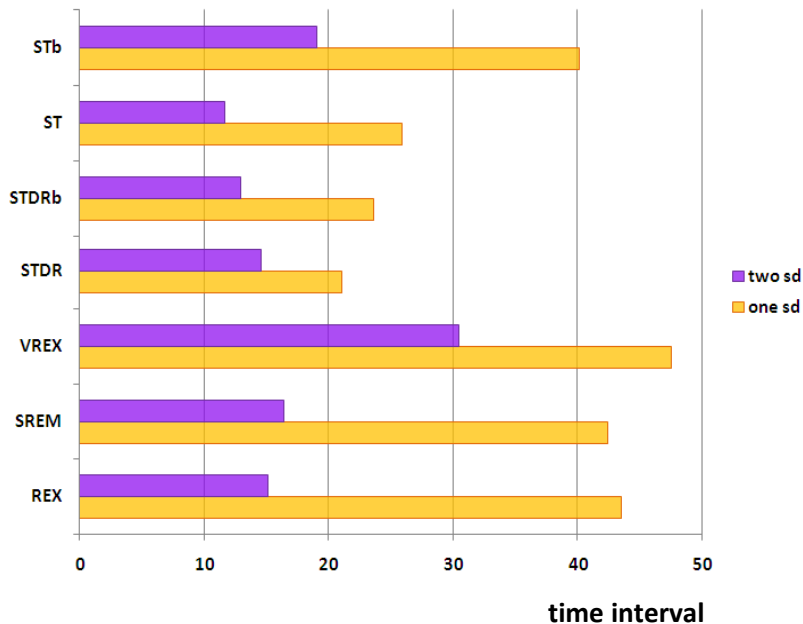
Property	REX	VREX	SREM	STDR	STDRb	ST	STb
Acceptance Ratio	0.237	0.241	0.248	0.378	0.376	0.463	0.404
Replica Speed (distance/time)	0.058	0.050	0.051	0.058	0.059	0.065	0.065
Mean Free Path	0.322	0.245	0.255	0.402	0.402	0.431	0.445
Diffusion Coefficient	0.208	0.181	0.156	0.195	0.196	0.246	0.249
Average Deviation from Sampling Homogeneity	0	6.62%	12.61%	2.50%	2.98%	3.81%	17.40%
Composite Score (a normalized linear combination)	0.793	0.700	0.679	0.874	0.876	0.984	0.940

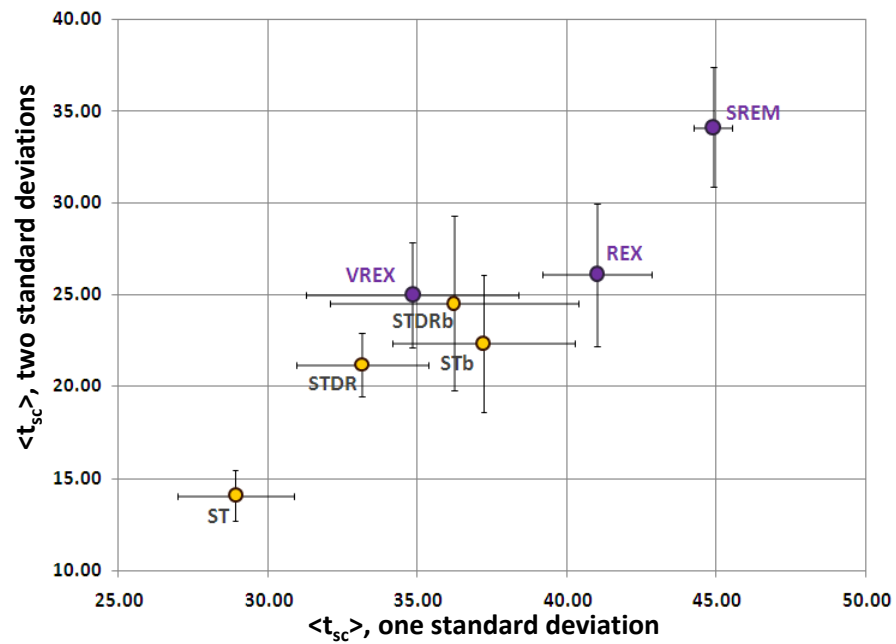
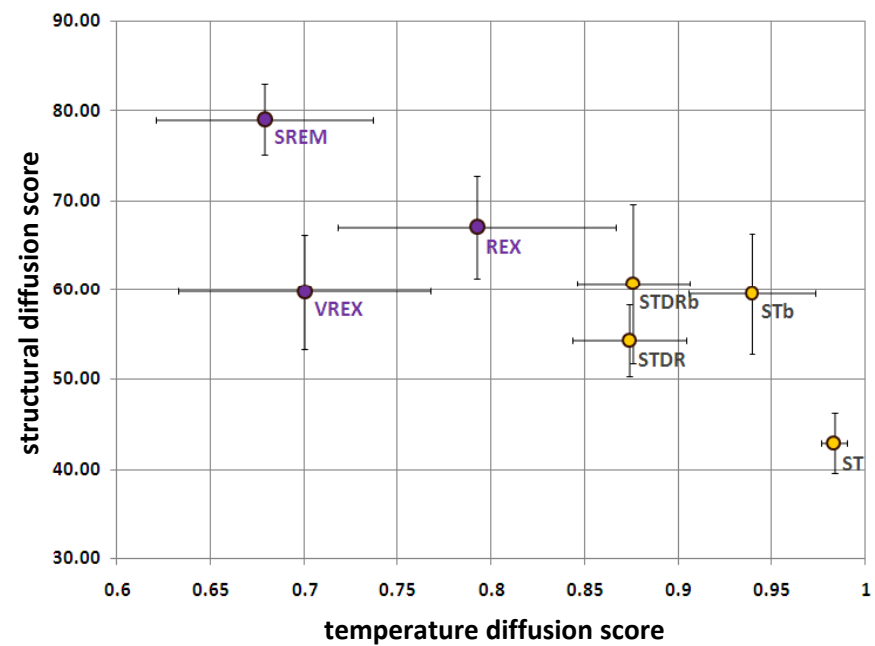


a**b****c****d**



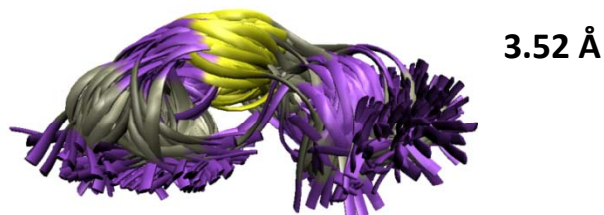


a**b****c****d**

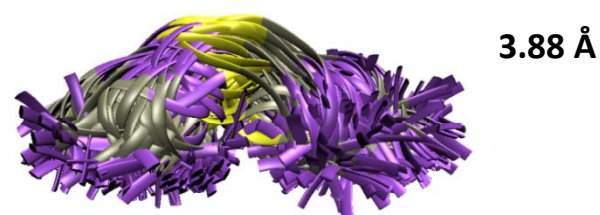
a**b**

STDR

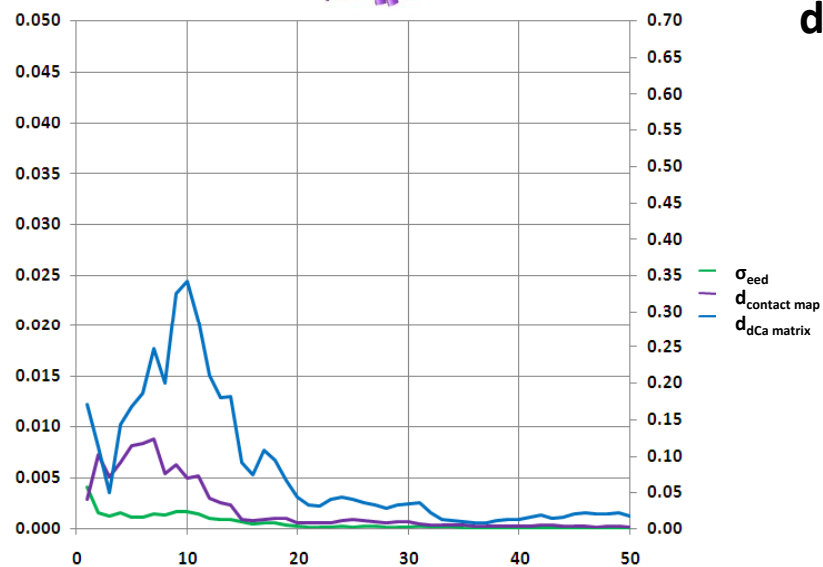
a



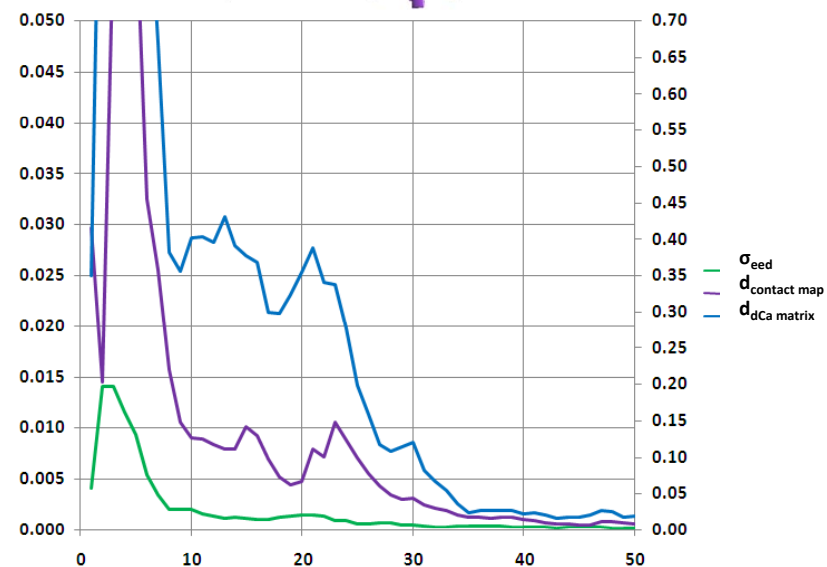
b



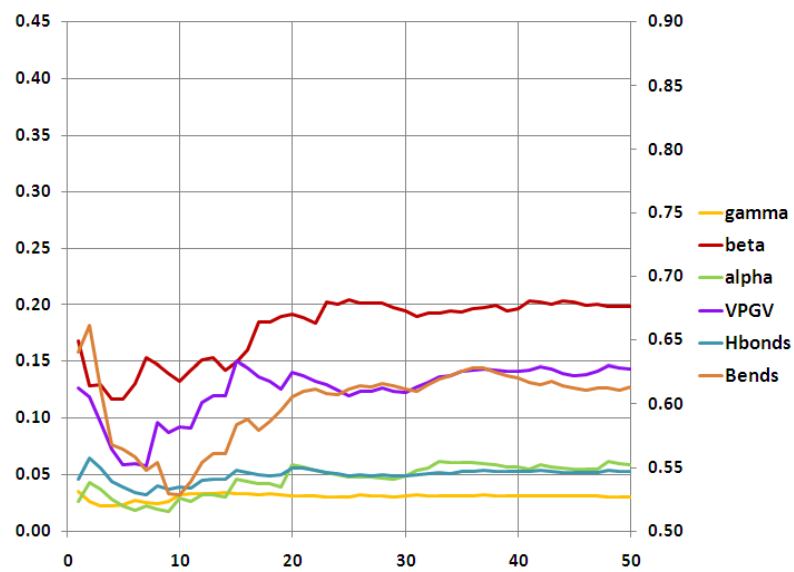
c



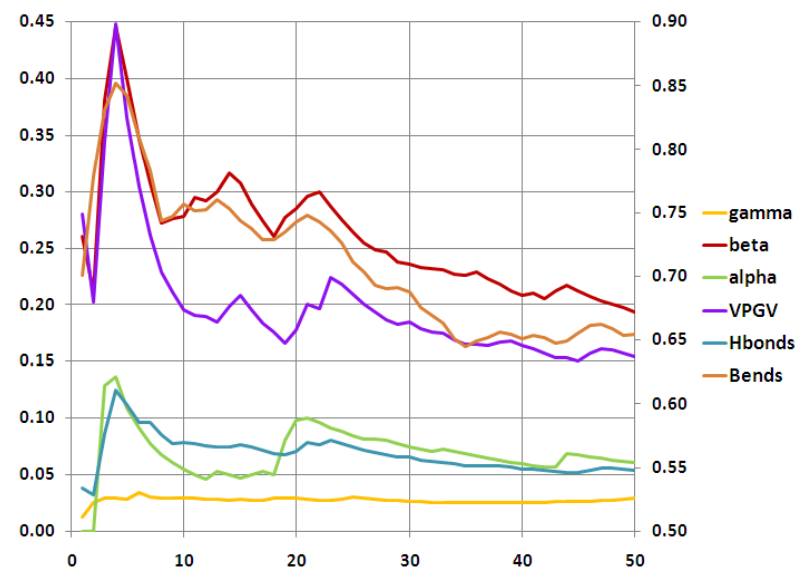
d



e



f

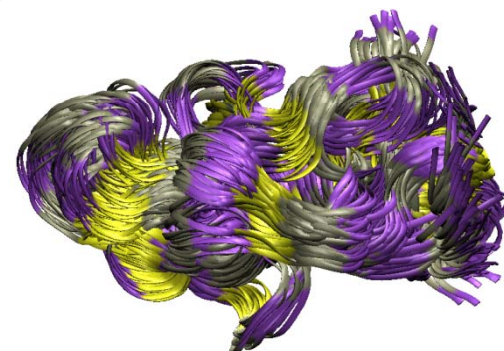


a

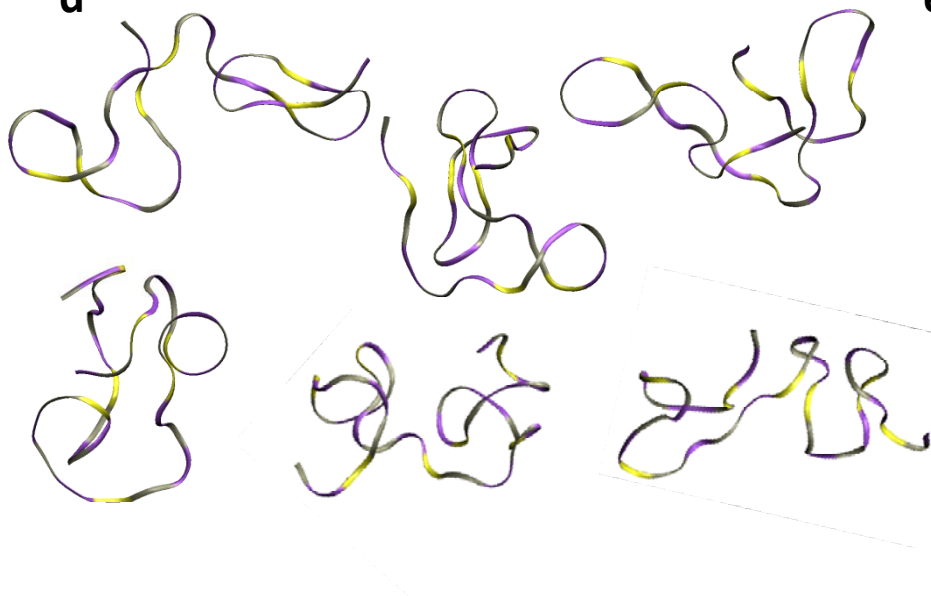
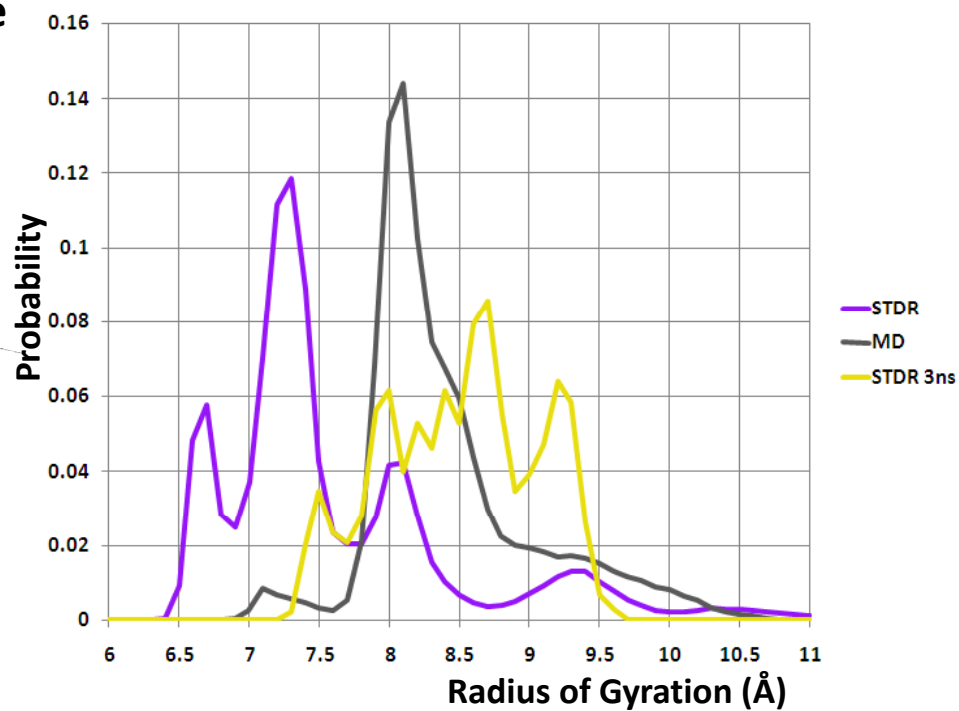
Conventional MD (200ns)
1.66 Å

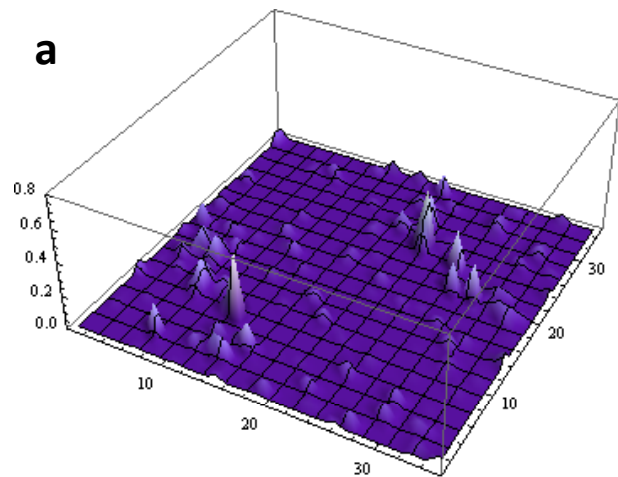
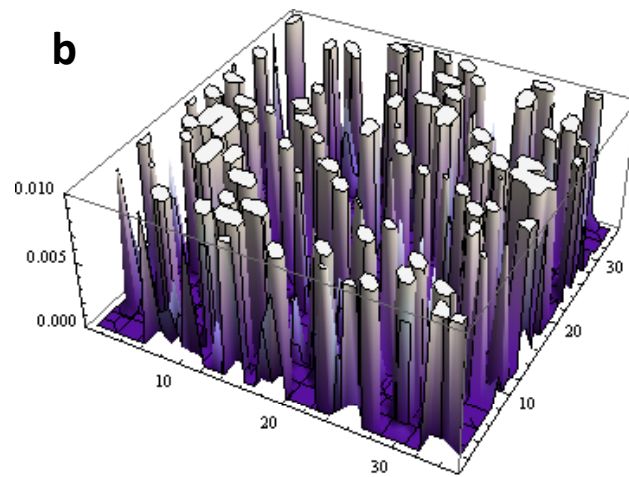
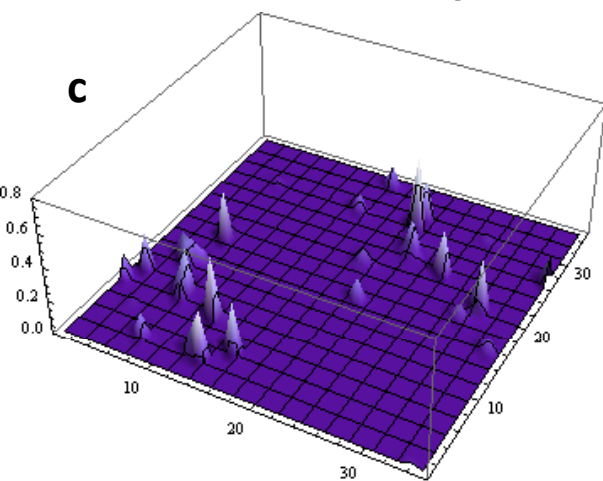
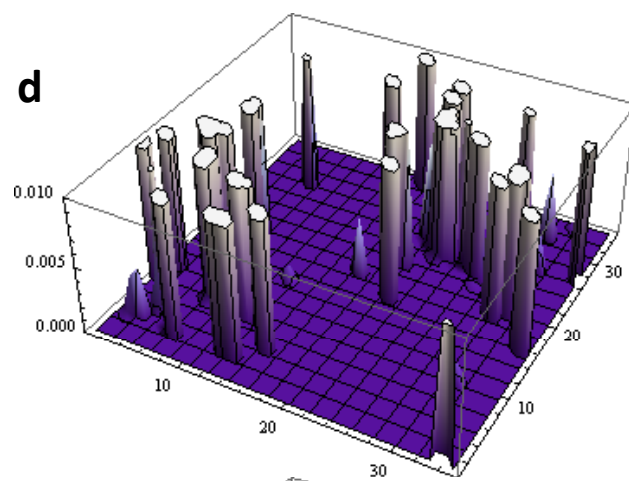
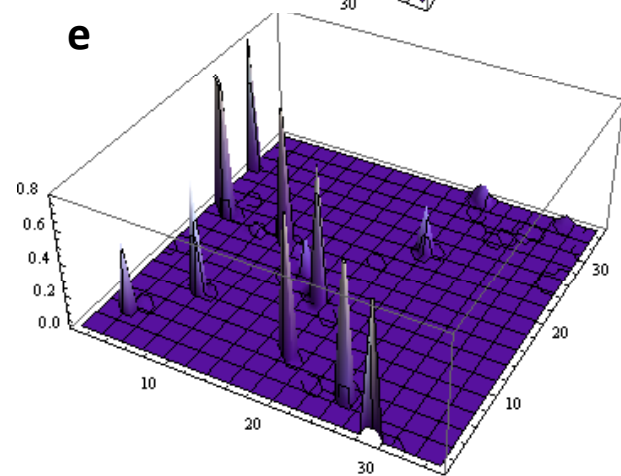
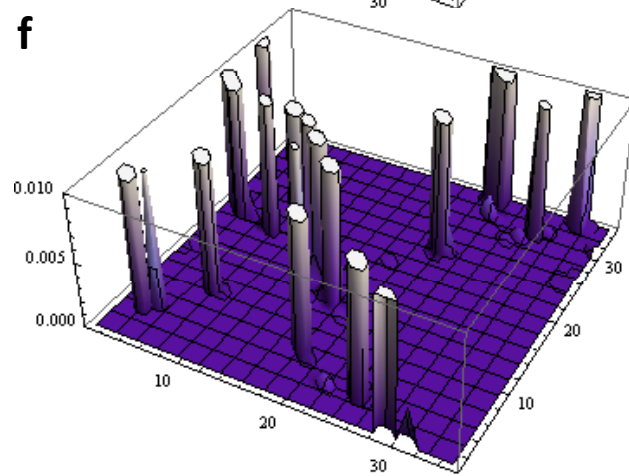
b

STDR (all data)
8.40 Å

c

STDR (3ns)
6.16 Å

d**e**

a**b****c****d****e****f**

Supplementary Material

Exponentially-Space Temperature Lists (in K)

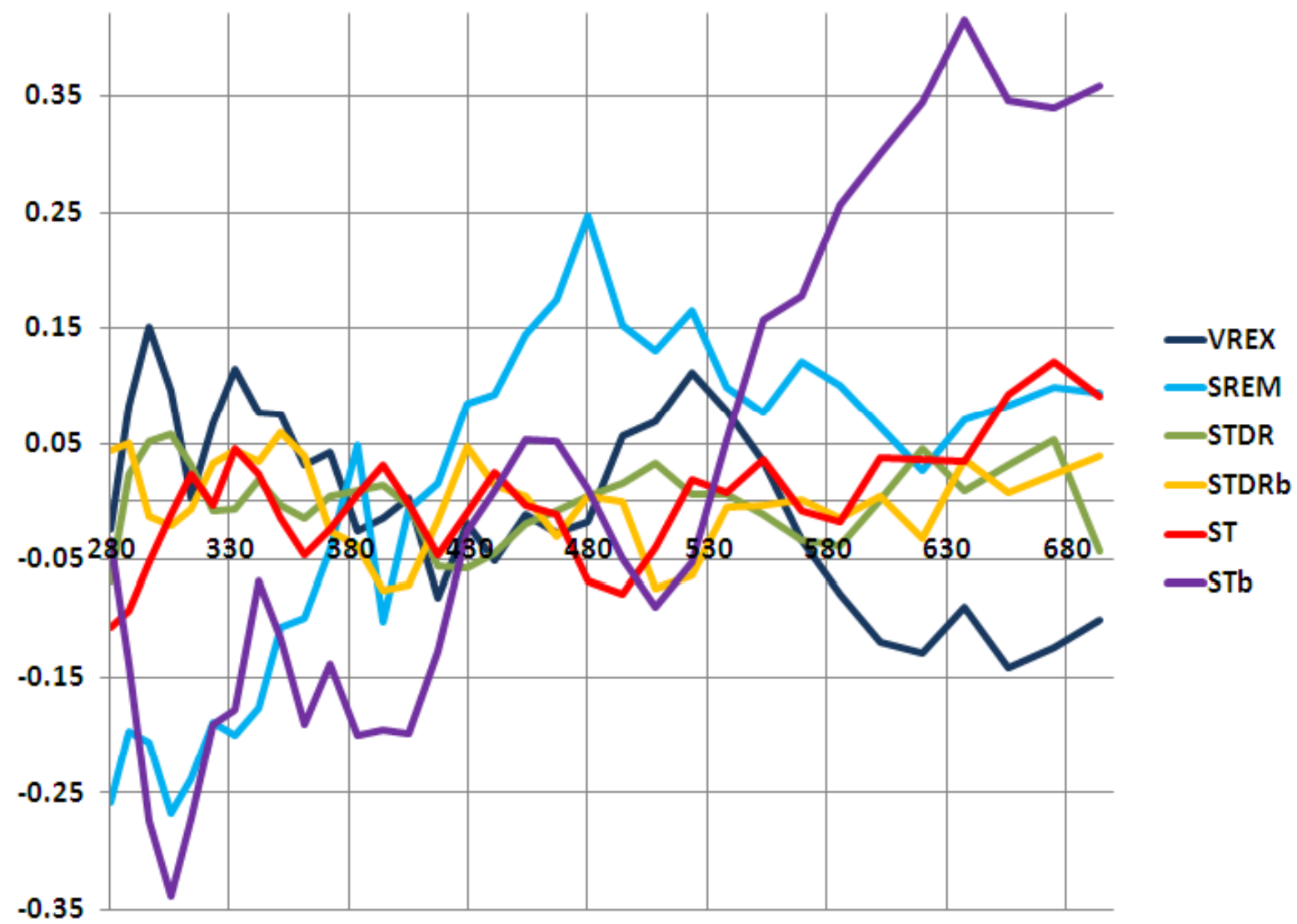
Temperature list for the octamer (33 temperatures):

280, 288, 296, 305, 314, 323, 332, 342, 351, 361, 372, 383, 394, 405, 417, 429, 441, 454, 467, 480, 494, 508, 523, 538, 553, 569, 585, 602, 620, 637, 656, 675, 694

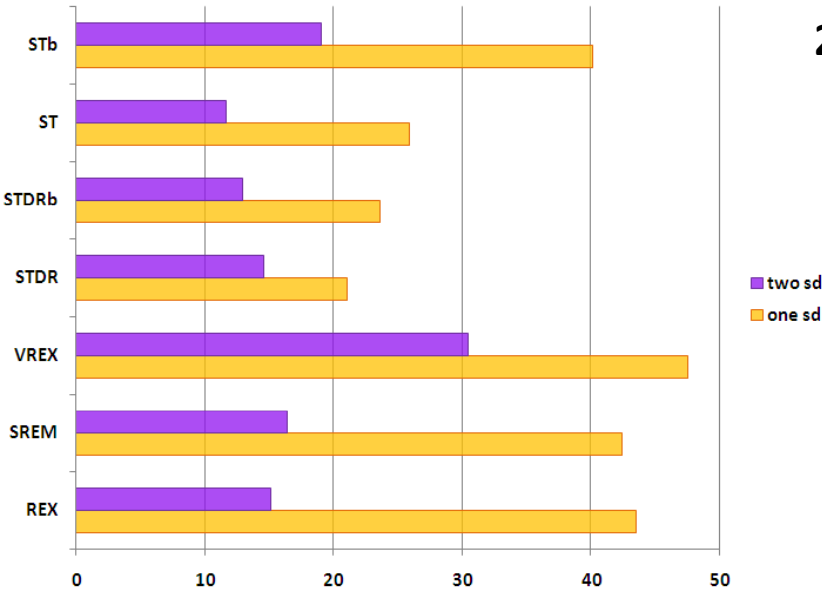
Temperature list for the 35-mer (70 temperatures):

261, 265, 268, 272, 276, 280, 284, 288, 292, 296, 300, 305, 309, 314, 318, 323, 327, 332, 337, 342, 346, 351, 356, 361, 367, 372, 377, 383, 388, 394, 399, 405, 411, 417, 422, 429, 435, 441, 447, 454, 460, 467, 473, 480, 487, 494, 501, 508, 515, 523, 530, 538, 545, 553, 561, 569, 577, 585, 594, 602, 611, 620, 628, 637, 647, 656, 665, 675, 684, 694

FIGURE S1: Deviation from Sampling Homogeneity

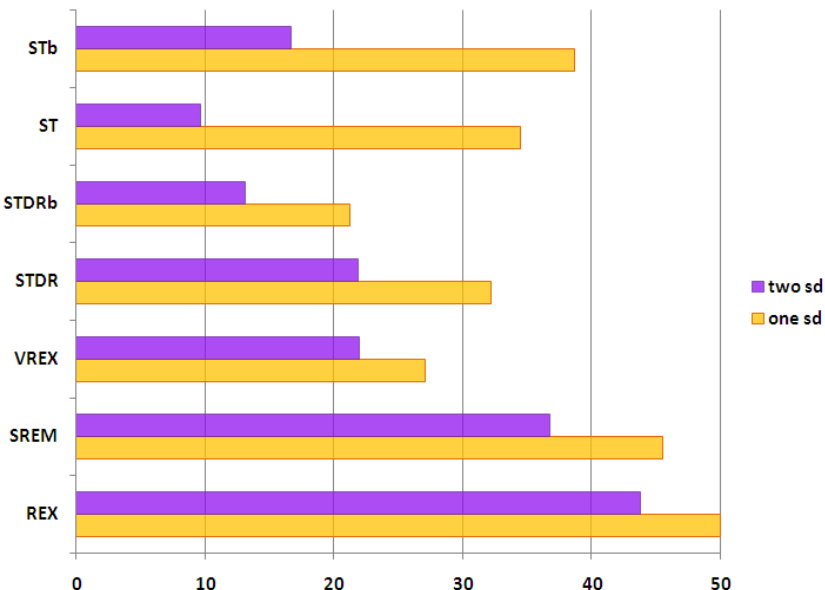


280K



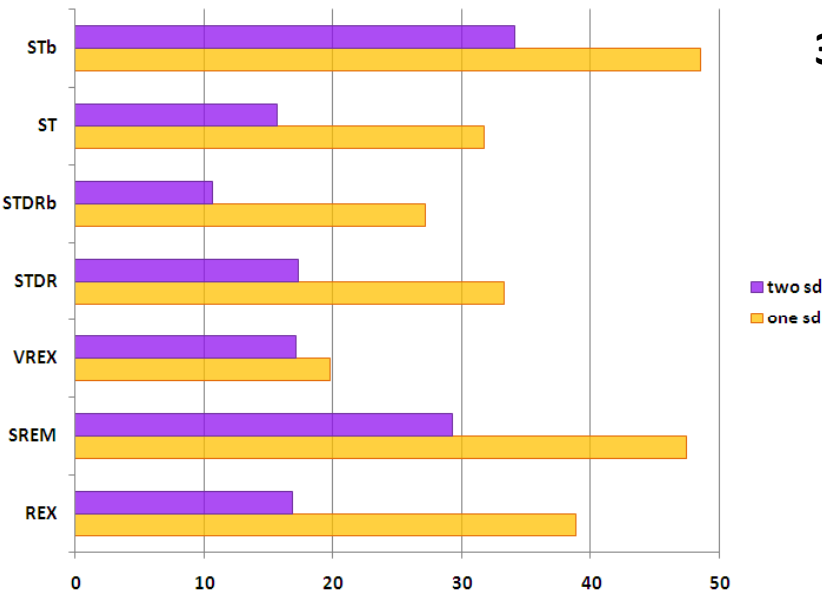
ONE SD: STDR, STDRb, ST, STb, SREM, REX, VREX
TWO SD: ST, STDR, STDRb, REX, SREM, STb, VREX

288K



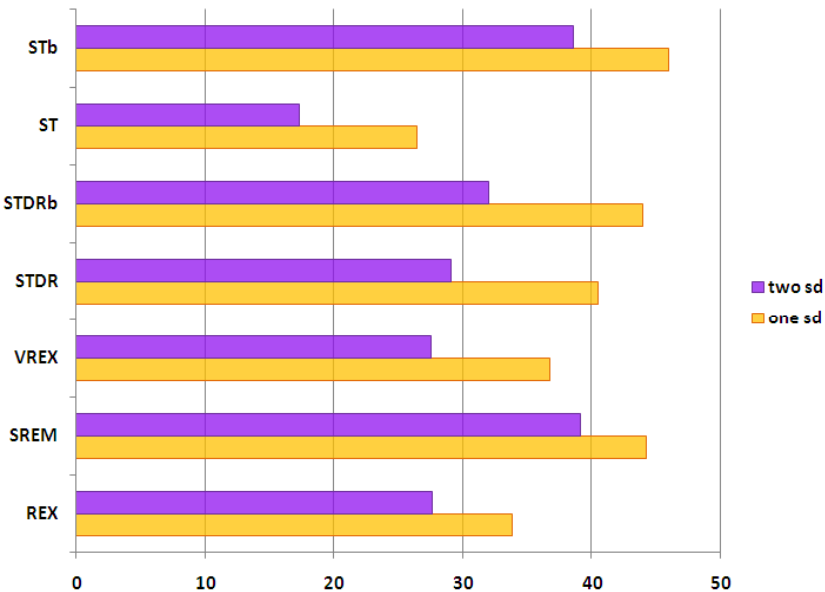
ONE SD: STDRb, VREX, STDR, ST, STb, SREM, REX
TWO SD: ST, STDRb, STb, STDR, VREX, SREM, REX

296K



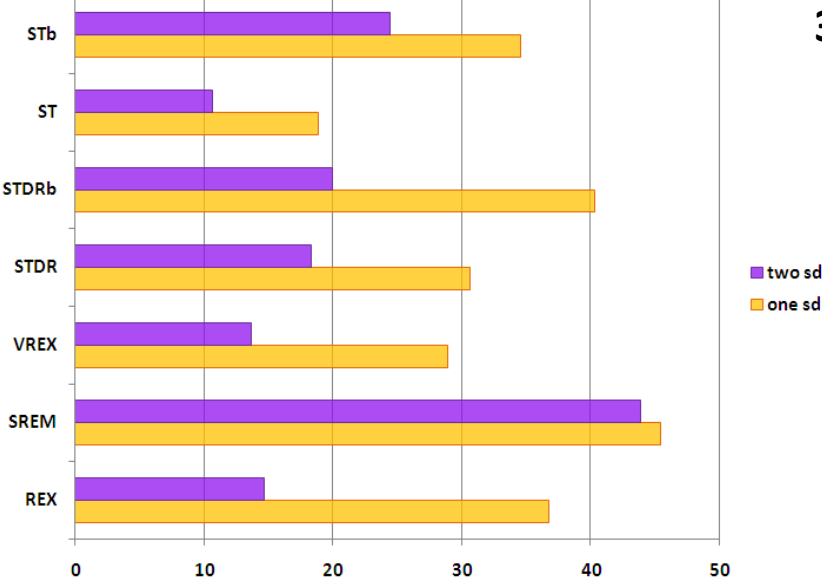
ONE SD: VREX, STDRb, ST, STDR, REX, SREM, STb
TWO SD: STDRb, ST, REX, VREX, STDR, SREM, STb

305K



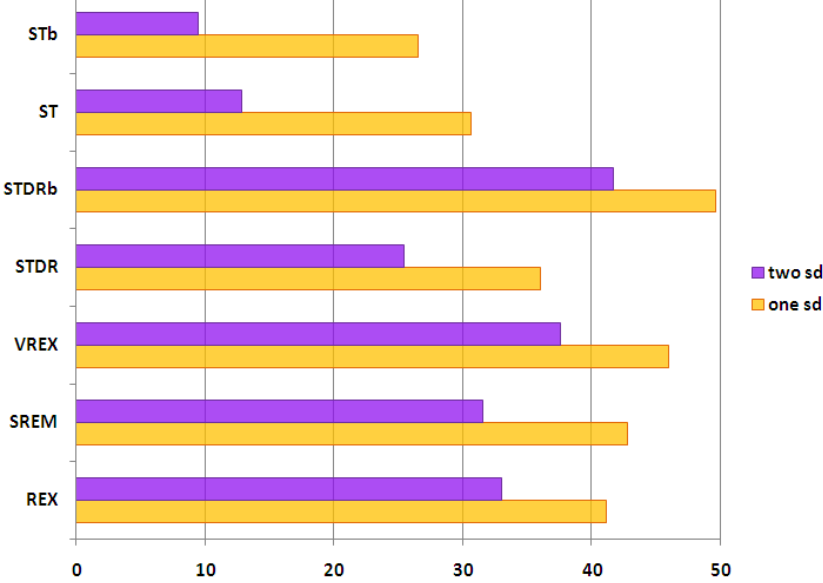
ONE SD: ST, REX, VREX, STDR, STDRb, SREM, STb
TWO SD: ST, VREX, REX, STDR, STDRb, STb, SREM

314K



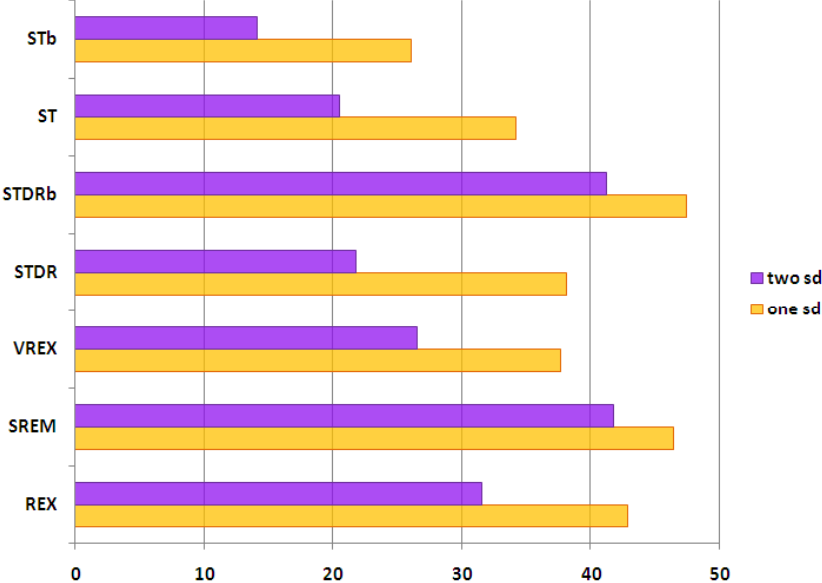
ONE SD: ST, VREX, STDR, STb, REX, STDRb, SREM
TWO SD: ST, VREX, REX, STDR, STDRb, STb, SREM

323K



ONE SD: STb, ST, STDR, REX, SREM, VREX, STDRb
TWO SD: STb, ST, STDR, SREM, REX, VREX, STDRb

332K



ONE SD: STb, ST, VREX, STDR, REX, SREM, STDRb
TWO SD: STb, ST, STDR, VREX, REX, STDRb, SREM

FIGURE S3, A: Structural Convergence at Multiple Temperatures, 2d Plot

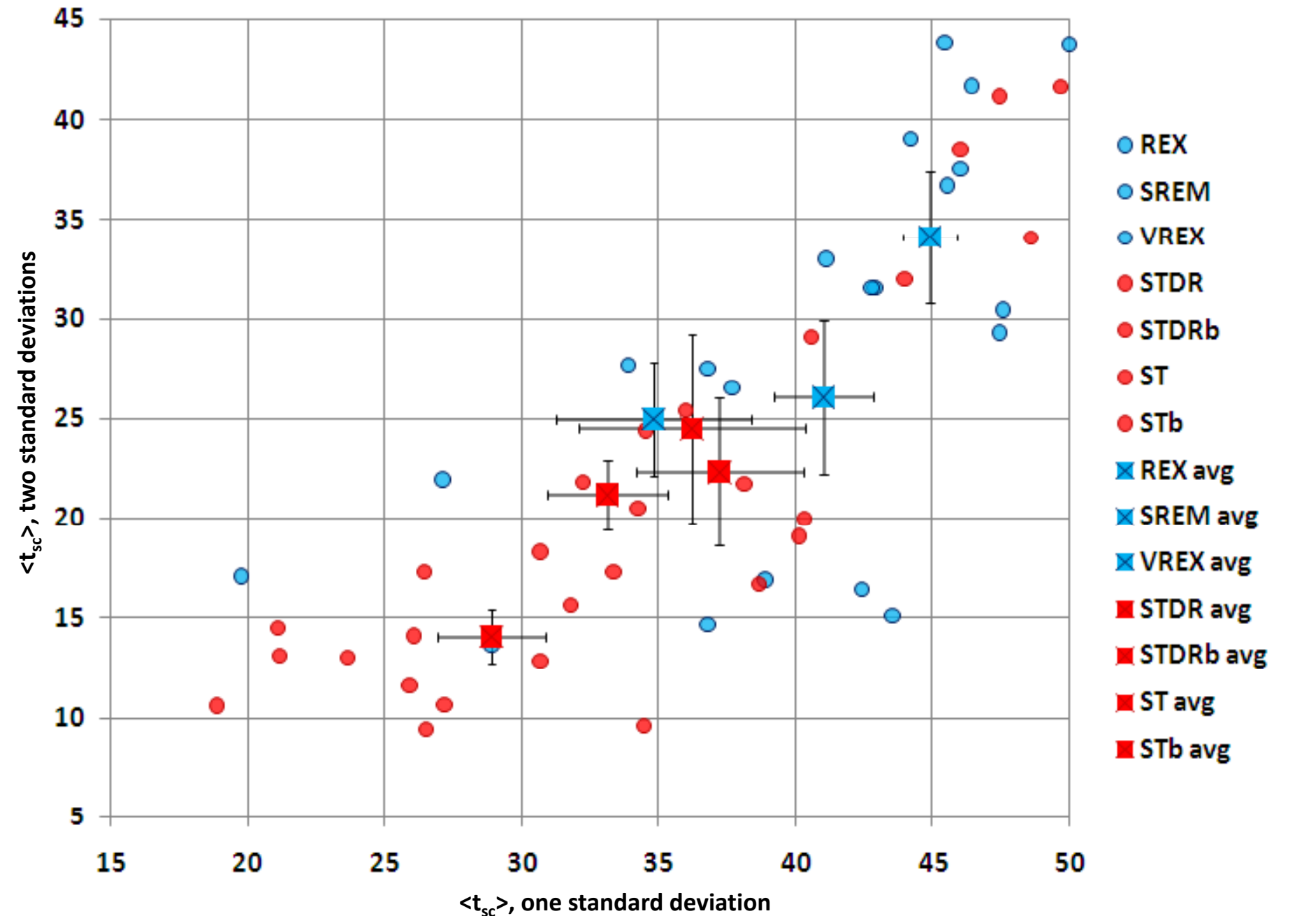


FIGURE S3, B: Structural Convergence at Multiple Temperatures, 2d Plot

