Exploration of the structural asymmetry induced by the intrinsic flexibility of HIV-2 protease

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Supplementary Information

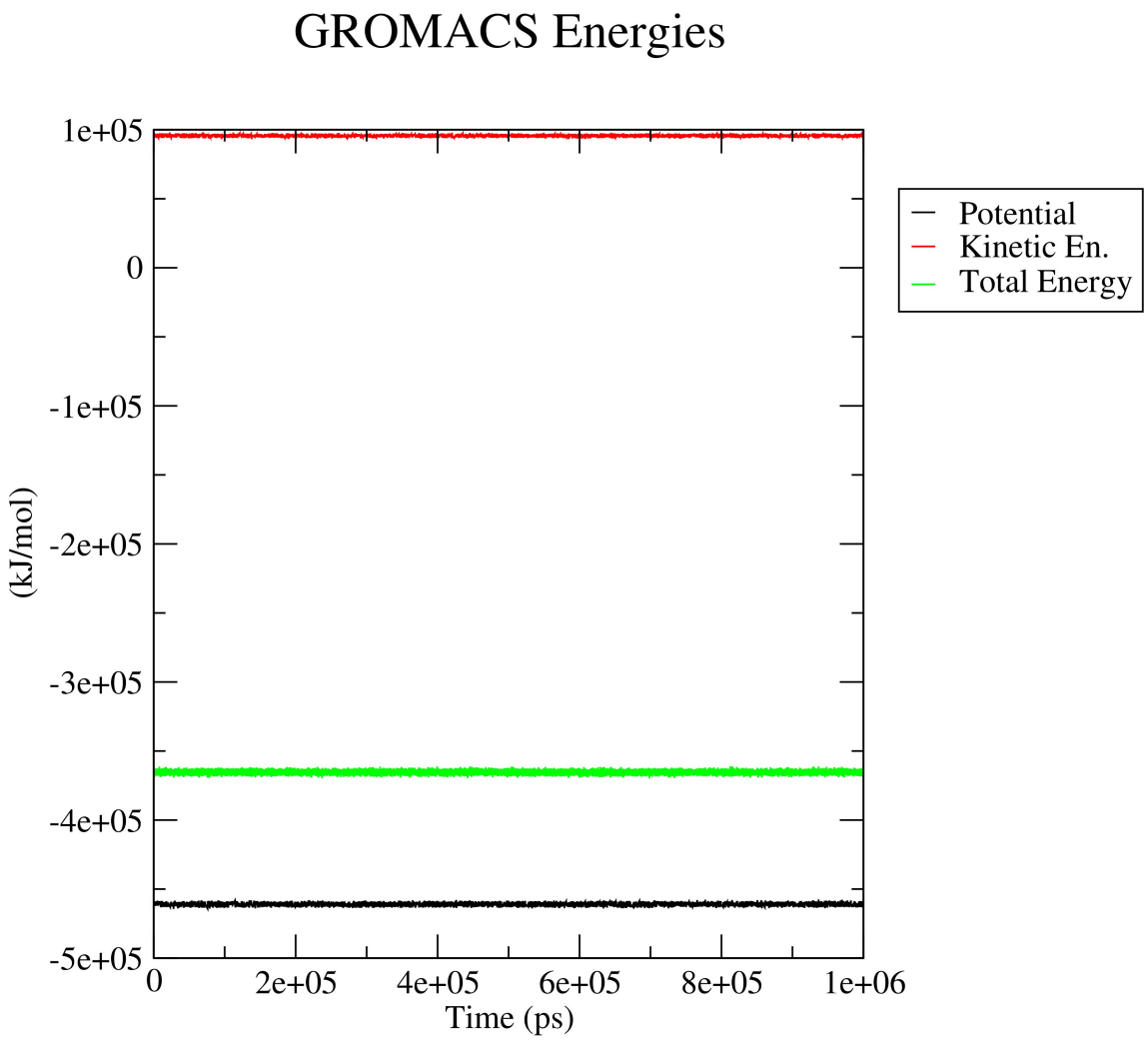


Figure S1: Evolution of the system energy over the simulation.

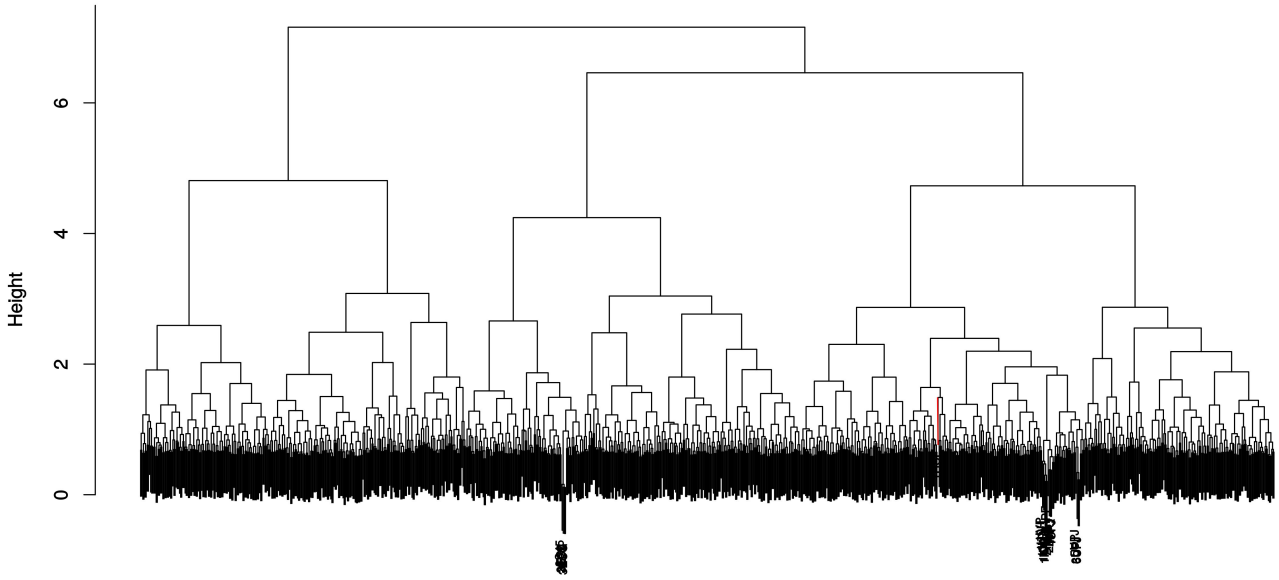


Figure S2: Hierarchical classification of MD and crystallographic structures based on their main-chain RMSD. The classification was computed using Ward aggregation method. The 1HSI structure is highlighted in red.

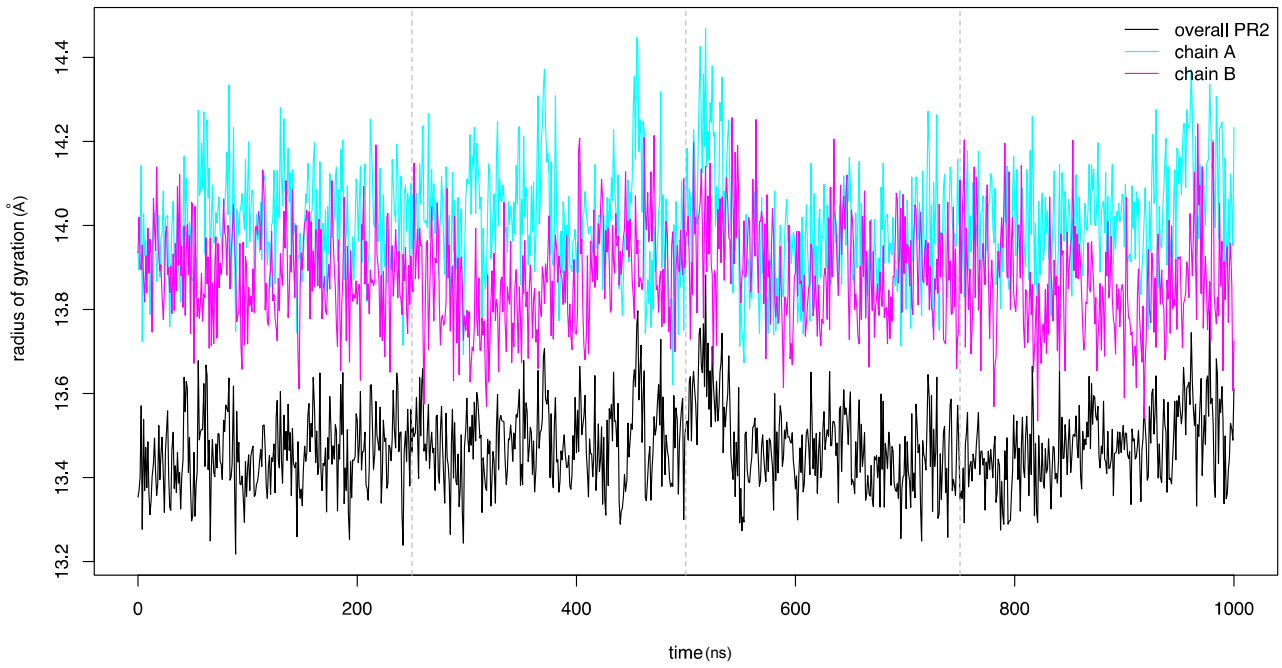


Figure S3: Evolution of the PR2 compactness over the simulation

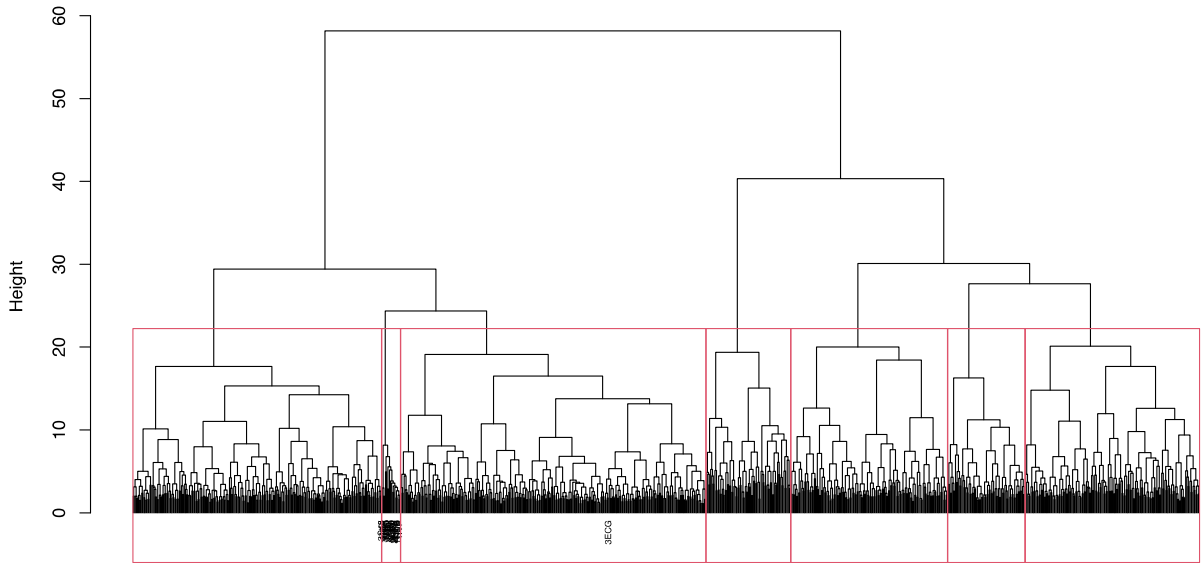


Figure S4: Classification of the 1020 structures (1001 DM structures + 19 X-ray structures) according to their local structural asymmetry. The PDB code of the 19 X-ray structures were indicated in the dendrogram.

Table S1 : Link between the global asymmetry and the composition in secondary structures

	Alpha helix	Isolated beta-bridge residue	Strand	3-10 helix	Turn	Bend	None
Average number of residues per structure	12.06 ± 1.81	4.25 ± 0.61	94.95 ± 2.93	0.11 ± 0.57	14.89 ± 2.59	26.47 ± 2.64	43.27 ± 2.97
r^*	-0.09	-0.01	-0.04	0.04	-0.01	0.10	0

R^*: Pearson's correlation coefficient between the $RMSD_{AB}$ and the number of residues in a given secondary structure state per structure.

Table S2 : Exploration of the asymmetry in terms of secondary structure in the 13 PR2 regions

	Nter	R1	Fulcrum	Catalytic site	R2	Elbow	flaps
Average $RMSD_{AB}^{reg}$ (standard deviation) in Å	1.30 (0.57)	0.87 (0.34)	1.10 (0.40)	1.17 (0.37)	1.42 (0.59)	1.75 (0.60)	1.46 (0.38)
Number of residues that are assigned in different	0	0	0	6	5	2	6

secondary structure states in at least 100 structures							
Size of the region (in terms of number of amino acid)	5	4	14	7	6	6	16
%	0	0	0	86	83	33	38

	Cantilever	R3	Wall	α-helix	R4	cter
Average $RMSD_{AB}^{reg}$ (standard deviation) in Å	0.97 (0.29)	0.97 (0.34)	1.19 (0.47)	0.86 (0.32)	0.69 (0.22	1.02 (0.39)
Number of residues that are assigned in different secondary structure states in at least 100 structures	0	2	1	3	1	0
Size of the region (in terms of number of amino acid)	17	4	4	9	3	4
%	0	50	25	33	33	0