Characterizing early drug resistance-related events using geometric ensembles from HIV protease dynamics

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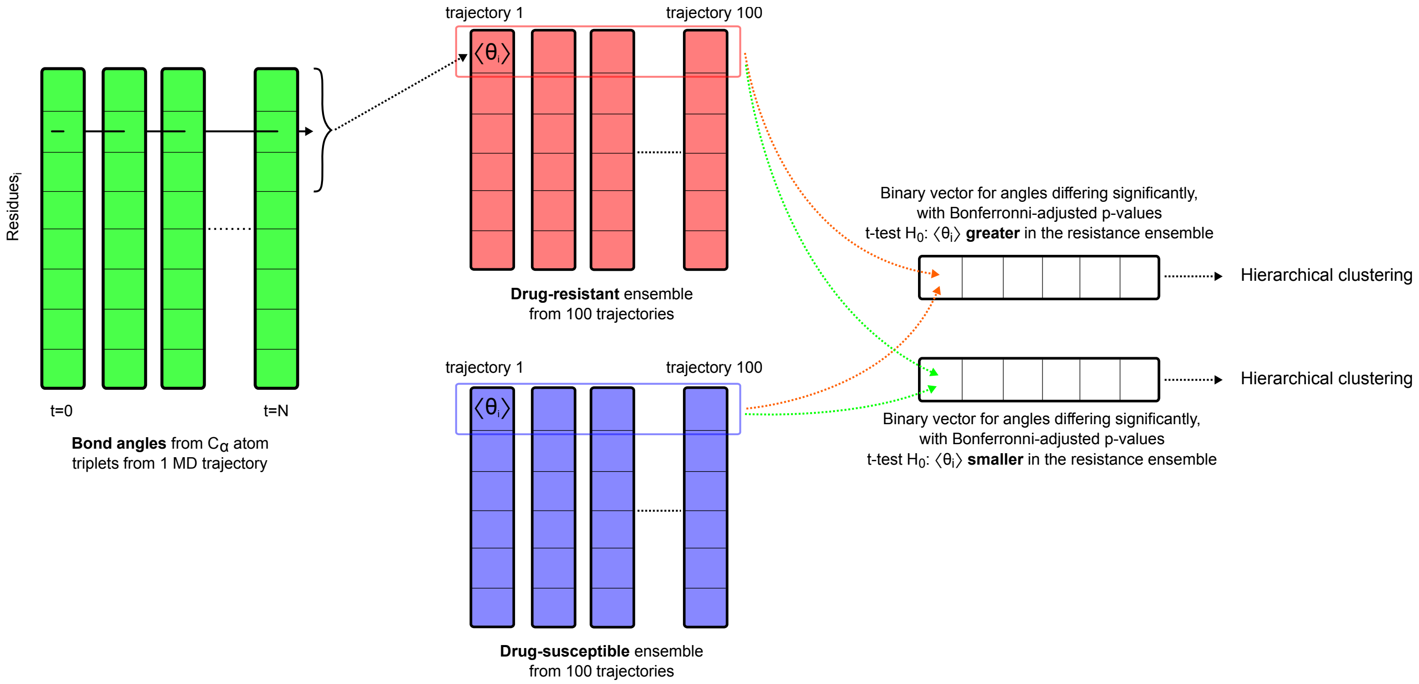
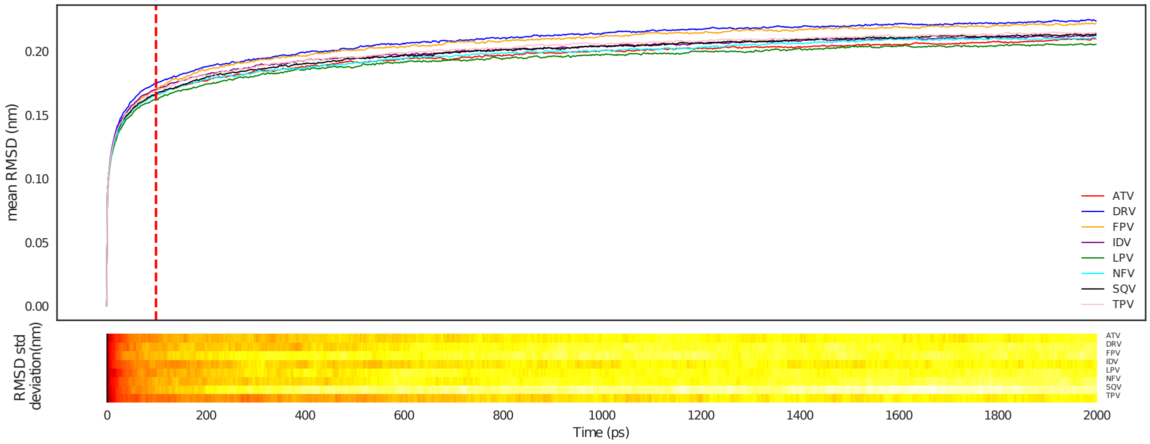
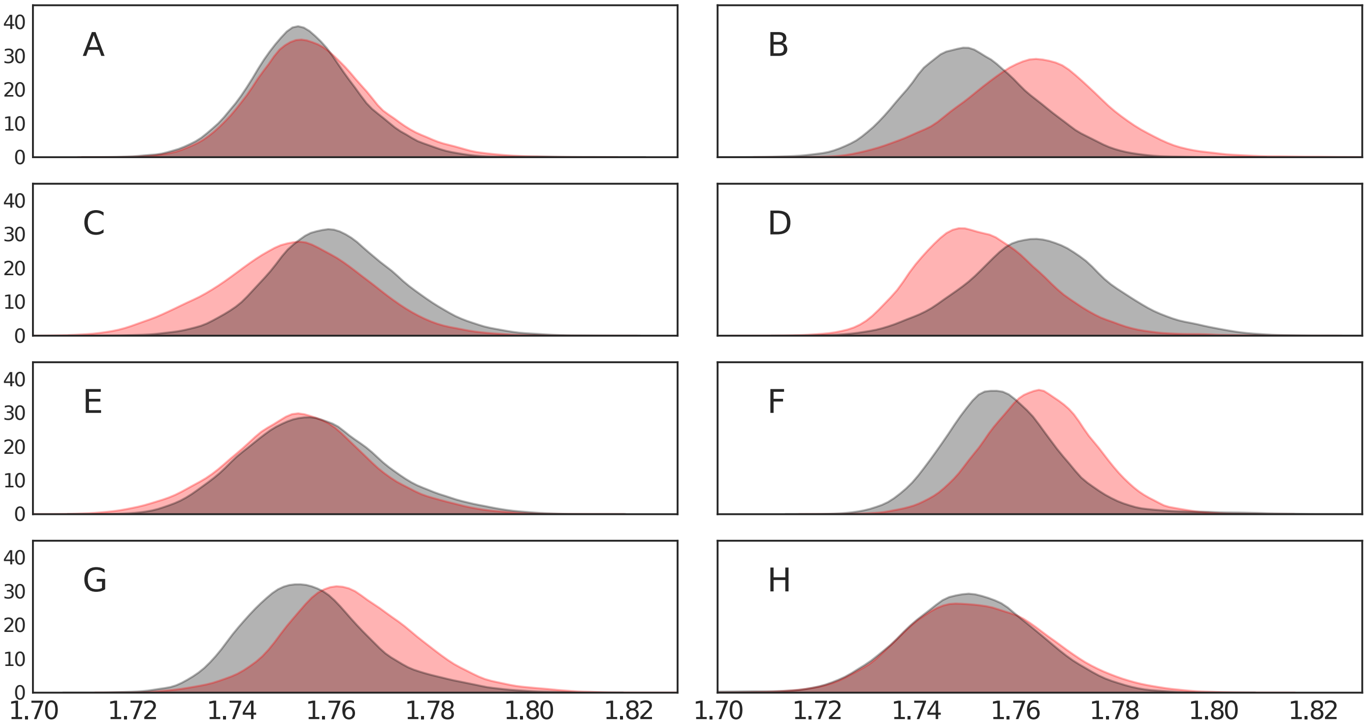


Supplementary Figure 1: Experimental layout for evaluating t-tests from C_α angles for residue triplets from MD trajectories prior to hierarchical clustering.

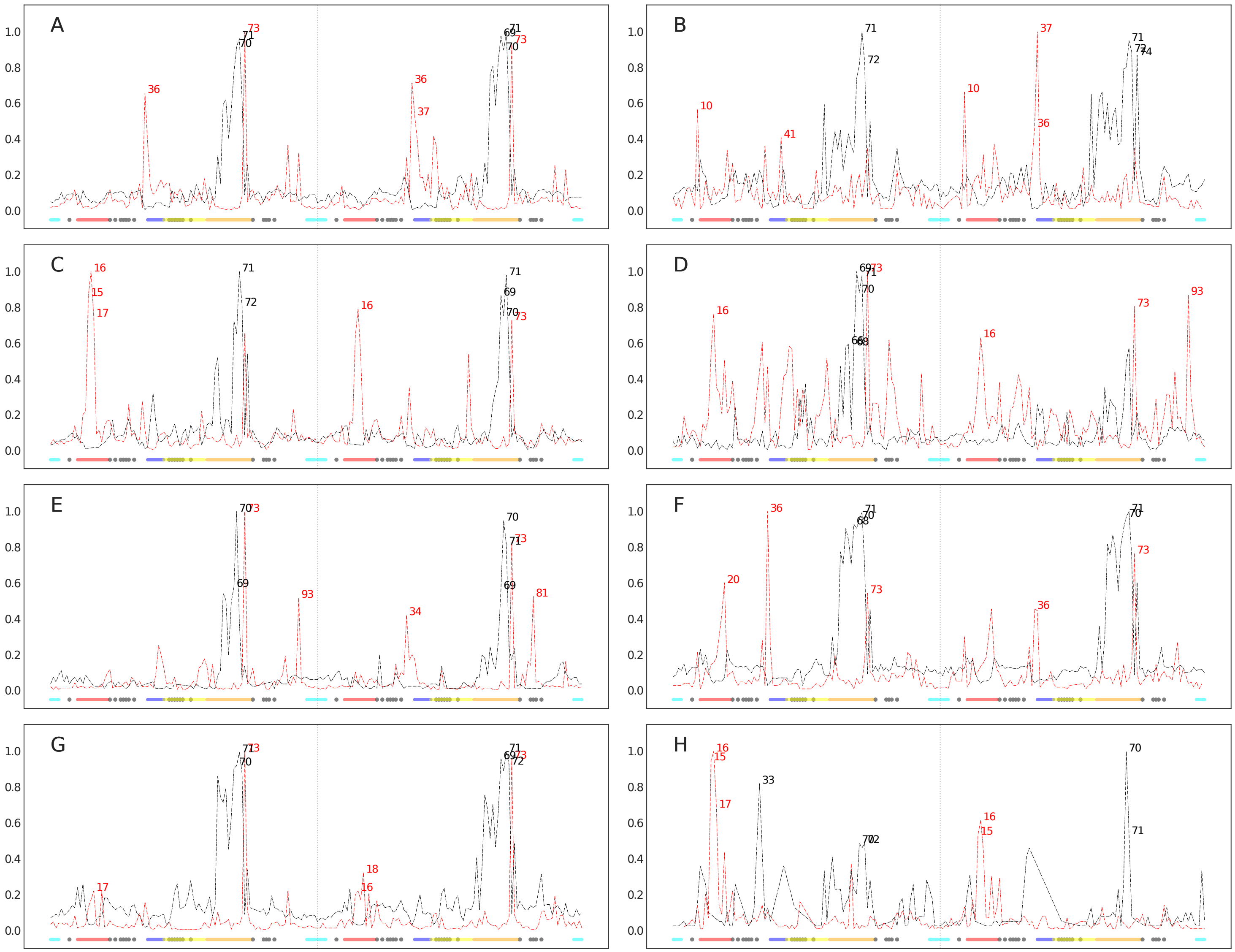


Supplementary Figure S2: Mean Cα RMSD values obtained across 200 complexes over the duration of the MD simulations for each of ATV, DRV, FPV, IDV, LPV, NFV, SQV and TPV. The red dotted line depicts the 100ps region beyond which the MD runs stabilize. At the botom, the heat map shows the standard deviations of the RMSD values for the same drugs, with higher values colored red, through yellow and white, which represent lower values.



Supplementary Figure S3: Density distributions for the radii of gyration for each HIV protease drug resistance ensemble for (A) ATV, (B) DRV, (C) FPV, (D) IDV, (E) NFV, (F) NFV, (G) SQV and (H) TPV, obtained from the replicate molecular dynamics simulations. Drug resistance ensembles are shaded in red while the susceptible ones are in grey.

Supplementary Table S4: Mutations present in each drug resistance ensemble (according to the 2017 update)
ATV
4S, **10IVF,** 11LI, 12I, 13VM, 14R, 15V, 16A, 19IV, 20RIVTM, 21D, 22V, 24IM, **32I**, **33FV**, **34Q**F, 35DNG, 36IV, 37DS, 41K, 43IT, **46LI**, 47V, **48**QV, 51A, **53L**, **54LVM**, 55RN, 57K, 58E, **60E**, 61HDN, **62V**, 63P, **64VM**, 66V, 67YFE, 69RYQ, 70E, **71IV**, 72LTVMF, **73STA**, 74PS, 75I, 76V, 77I, 79SA, 82LSTA, 83D, **84V**A, 89V, **90M**, 91S, 92K, **93LM**, 95F, 96S
DRV
10IFV, **11LI**, 12KPA, 13V, 14R, 15V, 16A, 19QV, 20RTVM, 24M, 30N, **32I**, **33F**, 34Q, 35DG, 36IVT, 37QDT, 43IQT, 46LI, **47V**, 51A, 53L, **54LM**, 55RN, 57KG, 58E, 60E, 62V, 63P, 64VM, 66V, 67WY, 69Q, 71IV, 72LVM, 73STA, 77IT, 79S, 82LA, **84V**, 85L, 88D, **89V**, 90M, 91S, 92K, 93L
FPV
10IVF, 11I, 12KDPV, 13V, 14RT, 15V, 16A, 19QTI, 20RITVM, 24M, 30N, **32I**, 33F, 35KDNG, 36LI, 37HDQTP, 41K, 43IT, **46LI**, **47V**, 48Q, 53L, **54LVM**, 55RN, 57KG, 58E, 60E, 61DN, 62V, 63P, 64LV, 66FV, 67YGFE, 68E, 69KLQ, 70TE, 71LIVT, 72LTM, **73S**T, 74PS, **76V**, 77IT, 79SA, **82**L**TA**, **84V**A, 87G, 88D, 89VM, **90M**, 91S, 92KR, 93L, 95F
IDV
4A, 7R, **10IFV**, 11I, 12KP, 13VM, 15V, 19QIPT, **20R**IT, 21D, 22V, 24M, **32I**, 33IF, 34TQ, 35DNG, **36LI**, 37SDE, 41K, 43TE, **46LI**, 47V, 48LVM, 50V, 53LY, **54TV**SACM, 57K, 58E, 60NE, 61HNE, 62V, 63P, 64VM, 66VF, 67FE, 68E, 69RYQ, **71TV**, 72LTV, **73**C**STA**, 74DS, 75I, **76V**, **77I**, **82**SFTA, 83D, **84V**A, 85V, 89V, **90M**, 92K, 93L
LPV
10IFV, 11LI, 12KP, 13V, 14R, 15V, 16A, 19IPQV, **20R**TV**M**, **24I**, 30N, **32I**, **33F**V, 34TQ, 35DAG, 36I, 37EDQTS, 41K, 43QITE, 45R, **46LI**, **47VA**, 48V, **50V**, 51A, **53L**, **54LTVMS**, 55RN, 57K, 58E, 60E, 61HE, 62V, **63P**, 64VM, 65D, 66VF, 67Y, 68E, 69Y, 70E, **71IVT**, 72TVM, **73**CSTA, 74PAS, 75I, **76V**, 77IT, 79S, **82SFTA**I, **84V**, 85LV, 87G, 88D, 89TV, **90M**, 91S, 92K, 93L, 95F
NFV
7R, **10IVF**, 11LI, 12IA, 13V, 15V, 16E, 18H, 19I, 20RIVT, 21D, 22V, 24M, 30N, 33IVFM, 35DNG, **36I**, 37DSTE, 38F, 41K, 43TN, 45R, **46LI**, 48M, 53L, 54VM, 55R, 57K, 58E, 60E, 61HNE, 62V, 63PT, 64V, 65D, 66VF, 67W, 68E, 69R, **71TV**I, 72LTV, 73STA, **77I**, **82FA**, 83D, **84V**A, 85V, **88D**, 90M, 93L
SQV
10IF, 11LI, 12IP, 13VM, 15V, 18H, 19I, 20RIVT, 21D, 22V, 24M, 32I, 33IVF, 34D, 35DNG, 36IV, 37DS, 41K, 43T, 46LI, **48**QV, 53L, **54L**V**M**, 55R, 57K, 58E, 60E, 61HN, **62V**, 63PE, 64V, 66FV, 67WFE, 69Q, **71TV**I, 72LTVM, **73S**T, 74SP, 75I, 76V, **77I**, 79A, **82A**, 83D, **84V**A, 85V, 89V, 90M, 91S, 92K, 93LM, 95V
TPV
10IV, 11LI, 12K, 13V, 14R, 15V, 16A, 19V, 20RTV, 21D, 22V, 24IM, 32I, **33F**, 34QDF, 35DG, **36IV**, 37D, **43T**, 45R, **46L**I, **47V**, 53L, **54**L**VM**, 55R, 57K, **58E**, 60E, 61HN, 62V, 63P, 64V, 66V, 70T, 71IVM, 72TVM, 73ST, **74P**, 77I, **82LT**A, **83D**, **84V**, 85L, 87G, **89VM**, 90M, 91S, 93LM



Supplementary Figure S5: Normalized degree centralities for replicate molecular dynamics simulations showing significantly larger (red lines) and smaller (black lines) distances observed in resistant ensembles for 8 FDA-approved protease inhibitor complexes, namely ATV (A), DRV (B), FPV (C), IDV (D), LPV (E), NFV (F), SQV (G) and TPV (H). The top 5 residue positions with the highest connectivities are labelled at the peaks in each graph. Inserted underneath are the functional protease residues depicted as colored dots, namely the fulcrum (red), the elbow (blue), the flap (yellow), the cantilever (orange), the interface (cyan) and the binding cavity residues (grey).

Supplementary dataset S6: HIV protease sequences used for the ensembles. Sequence headers consist of the sequence IDs and the fold resistance scores. An additional number is appended after an underscore as an internal representation of the mutant after sequence expansion.

Sequences for the ATV-resistant ensemble

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>143473_13 700.0
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>143473_15 700.0
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>115081_0 700.0
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>113192_0 700.0
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>113192_2 700.0
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>103067_1 700.0
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>145212_6 700.0
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>115065_0 700.0
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>115065_1 700.0
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Sequences for the ATV-susceptible ensemble

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>102783_2 0.4
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>102795_1 0.5
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>235727_0 0.5
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>235727_1 0.5
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>187159_1 0.5
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VLIGPTPVNIIGRNLLTQIGCTLNF
>187159_5 0.5
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>187159_29 0.5
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>187159_33 0.5
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>187159_49 0.5
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>187159_53 0.5
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>187159_57 0.5
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>187159_69 0.5
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>187159_73 0.5
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>187159_93 0.5
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>216593_0 0.4
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>216593_2 0.4
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>187159_30 0.5
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>187159_34 0.5
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>187159_38 0.5
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>187159_50 0.5
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>187159_98 0.5
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Sequences for the DRV-resistant ensemble

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Sequences for the DRV-susceptible ensemble

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Sequences for the IDV-susceptible ensemble

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Sequences for the LPV-resistant ensemble

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>117053_15 500.0
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Sequences for the LPV-susceptible ensemble

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>187173_28 0.2
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VGPTPVNIIGRNMLTQIGCTLNF
>187173_29 0.2
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GPTPVNIIGRNMLTQIGCTLNF
>187173_30 0.2
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VGPTPVNIIGRNMLTQIGCTLNF
>187173_31 0.2
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Sequences for the NFV-resistant ensemble
>107985_112 600.0
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>107985_217 600.0
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>107985_219 600.0
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>107985_220 600.0
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>107985_222 600.0
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>107985_223 600.0
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>107985_224 600.0
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>107985_225 600.0
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>107985_226 600.0
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>107985_228 600.0
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>107985_229 600.0
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>107985_241 600.0
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>107985_245 600.0
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>107985_248 600.0
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>123049_4 600.0
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>123049_5 600.0
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>143332_25 600.0
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>143332_83 600.0
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>103057_2 600.0
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>56150_0 600.0
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>56150_1 600.0
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VLVGPTPVNIIGRDLMTQLGCTLNF

Sequences for the NFV-susceptible ensemble

>81921_0 0.4
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Sequences for the TPV-susceptible ensemble

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