Supplementary Figure 1: Mean C_α protein RMSD (top) and standard deviations (bottom) for each PI ensemble

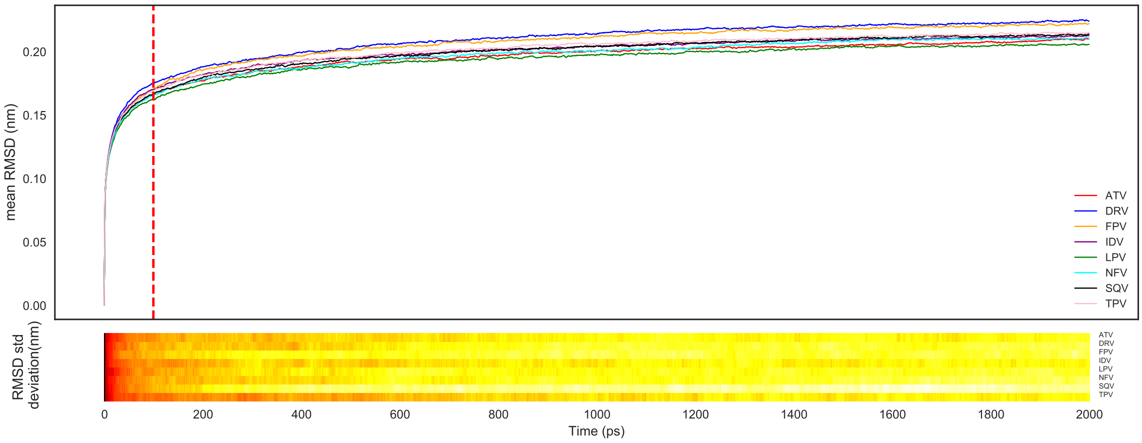

Figure S1: Mean C_α RMSD values obtained across 200 complexes over the duration of the MD simulations for each of ATV, DRV, FPV, IDV, LPV, NFV, SQV and TPV. The red dotted line depicts the 100ps region beyond which the MD runs stabilize. At the bottom, the heat map shows the standard deviations of the RMSD values for the same drugs, with higher values colored red, through yellow and white which represent lower values.

Supplementary Figure 2: Distributions of R_g values for the different PI ensembles in the replicate run.

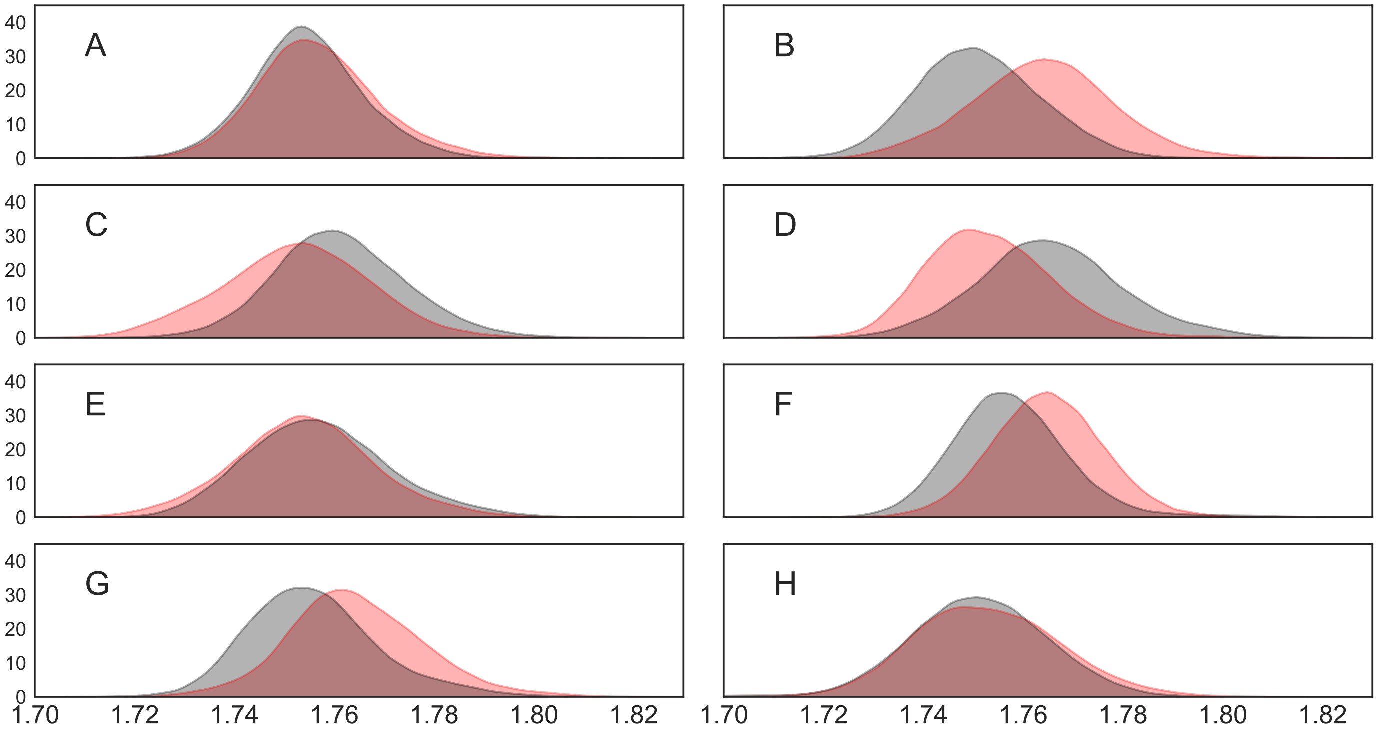

Figure S2: Density distributions for the radii of gyration for each HIV protease drug resistance ensemble for (A) ATV, (B) DRV, (C) FPV, (D) IDV, (E) LPV, (F) NFV, (G) SQV and (H) TPV, obtained from the replicate molecular dynamics simulation. Drug resistance ensembles are shaded in red while the susceptible ones are in grey.

Supplementary Table S3: 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, **11**LI, 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**, 84VA, 87G, 88D, 89VM, **90M**, 91S, 92KR, 93L, 95F
IDV
4A, 7R, **10I**FV, 11I, 12KP, 13VM, 15V, 19QIPT, **20R**IT, 21D, 22V, 24M, **32I**, 33IF, 34TQ, 35DNG, **36LI**, 37SDE, 41K, 43TE, **46LI**, 47V, 48LVM, 50V, 53LY, **54**TVSACM, 57K, 58E, 60NE, 61HNE, 62V, 63P, 64VM, 66VF, 67FE, 68E, 69RYQ, **71TV**, 72LTV, **73**CSTA, 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, **54LV**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 4: Normalized degree centralities for protease inihibitor complexes for replicate MD runs.

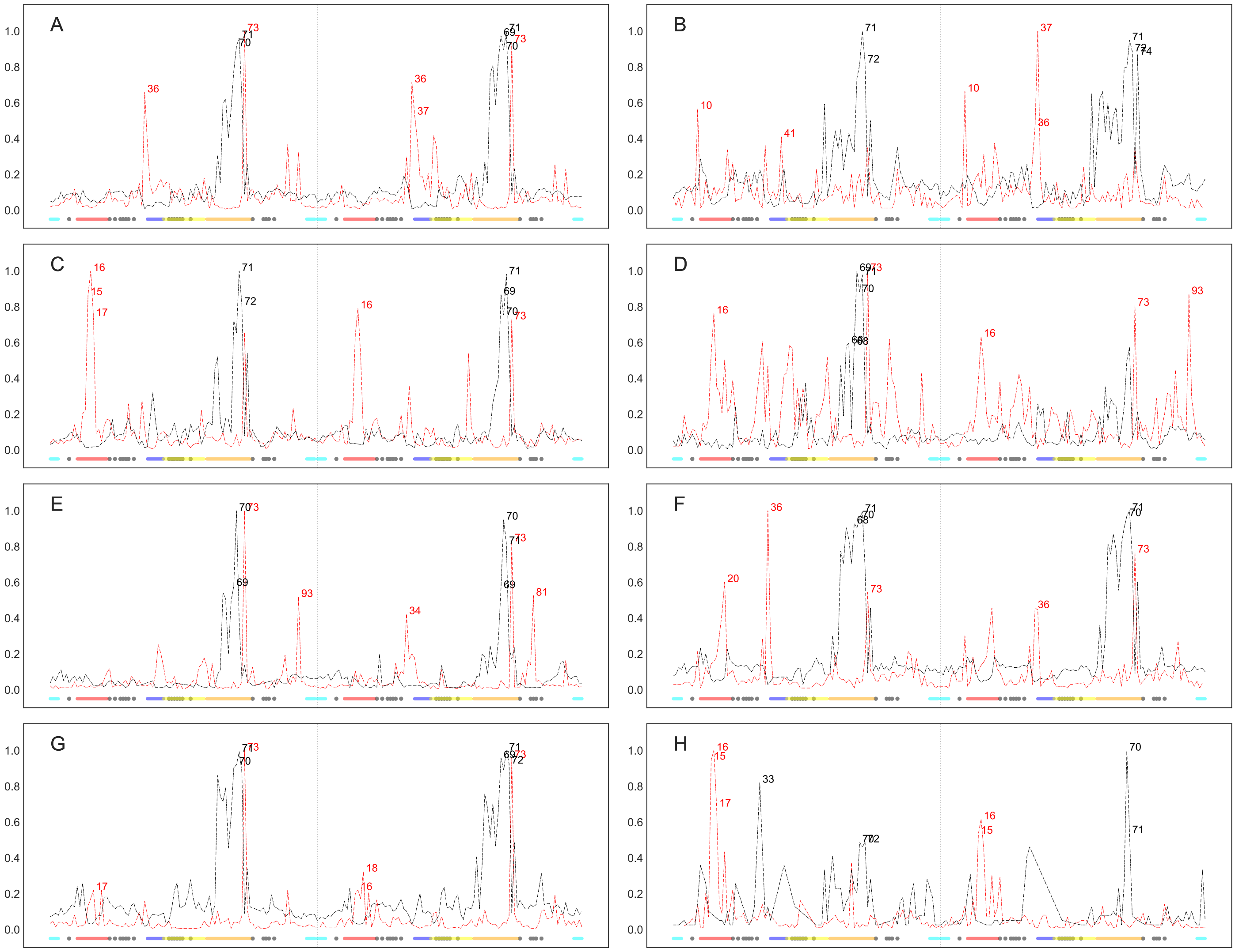

Figure. S4: Normalized degree centralities for replicate molecular dynamics simulations, showing significantly larger (red lines) and smaller (black lines) distances observed in resistant ensembles for 8 FDA-approved protease inhibitor complexes, namely ATV (A), DRV (B), FPV (C), IDV (D), LPV (E), NFV (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 S5: 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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Sequences for the ATV-susceptible ensemble
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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 FPV-resistant ensemble
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Sequences for the FPV-susceptible ensemble

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Sequences for the LPV-resistant ensemble

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PTPFNVVGRNLLTQLGCTLNF
>117053_4 500.0
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PTPFNVVGRNLLTQLGCTLNF
>117053_5 500.0
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>117053_6 500.0
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PTPFNVVGRNLLTQLGCTLNF
>117053_7 500.0
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>117053_8 500.0
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>117053_9 500.0
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PTPFNVVGRNLLTQLGCTLNF
>117053_10 500.0
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PTPFNVVGRNLLTQLGCTLNF
>117053_11 500.0
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>117053_12 500.0
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PTPFNVVGRNLLTQLGCTLNF
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>117053_14 500.0
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>117053_15 500.0
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Sequences for the LPV-susceptible ensemble

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STPVNIIGRNLLTQLGCTLNF
>102783_2 0.3
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ATPVNIIGRNLLTQLGCTLNF
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PTPVNIIGRNMLTQIGCTLNF
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PTPVNIIGRSMLTQIGCTLNF
>102782_174 0.3
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PTPVNIIGRNMLTQIGCTLNF
>102782_175 0.3
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PTPVNIIGRSMLTQIGCTLNF
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PTPVNIIGRNMLTQIGCTLNF
>102782_181 0.3
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PTPVNIIGRSMLTQIGCTLNF
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PTPVNIIGRNMLTQIGCTLNF
>102782_183 0.3
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PTPVNIIGRSMLTQIGCTLNF
>102782_188 0.3
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PTPVNIIGRSMLTQIGCTLNF
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PTPVNIIGRSMLTQIGCTLNF
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PTPVNIIGRNMLTQIGCTLNF
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PTPVNIIGRSMLTQIGCTLNF
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PTPVNIIGRSMLTQIGCTLNF
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PTPVNIIGRSMLTQIGCTLNF
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>102782_161 0.3
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PTPVNIIGRSMLTQIGCTLNF
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PTPVNIIGRNMLTQIGCTLNF
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PTPVNIIGRSMLTQIGCTLNF
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STPVNIIGRNLLTQLGCTLNF
>102782_4 0.3
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PTPVNIIGRNMLTQIGCTLNF
>102782_5 0.3
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PTPVNIIGRSMLTQIGCTLNF
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>102782_10 0.3
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>102782_11 0.3
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PTPVNIIGRSMLTQIGCTLNF
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>105308_27 0.3
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PTPTNIIGRNLLTQLGCTLNF
>105308_34 0.3
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PTPTNIIGRNLLTQIGCTLNF
>105308_35 0.3
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PTPTNIIGRNLLTQLGCTLNF
>105308_38 0.3
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>105308_63 0.3
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>75054_0 0.3
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PTPVNIIGRNLLTQIGCTLNF
>75054_2 0.3
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>75054_4 0.3
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>75054_6 0.3
PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEINLPGRWKPKMIGGIGGFIKVRQYDQITIDICGHKAIGTVLVG
PTPVNIIGRNLLTQIGCTLNF
>75054_8 0.3
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PTPVNIIGRNLLTQIGCTLNF
>75054_10 0.3
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PTPVNIIGRNLLTQIGCTLNF
>75054_12 0.3
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>75054_14 0.3
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>187173_5 0.2
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PTPVNIIGRNMLTQIGCTLNF
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>187173_11 0.2
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>187173_24 0.2
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>187173_28 0.2
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PTPVNIIGRNMLTQIGCTLNF
>187173_29 0.2
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>187173_30 0.2
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PTPVNIIGRNMLTQIGCTLNF
>187173_31 0.2
PQITLWQRPIVTVRIGGQLTEALLDTGADDTVLEDINLPGNWKPKMIGGIGGFIKVRQYDQILIEICGKKAIGTVLIG
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Sequences for the NFV-resistant ensemble

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>107985_112 600.0
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>107985_217 600.0
PQITLWQRPLIAIKIGGQIIEALLDTGADNTVLENIELPGRWKPKMIGGIGGLIKVRQYEEIPIEICGHKVTGTVLVG
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Sequences for the NFV-susceptible ensemble
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Sequences for the SQV-resistant ensemble

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Sequences for the SQV-susceptible ensemble

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