

Supporting Information

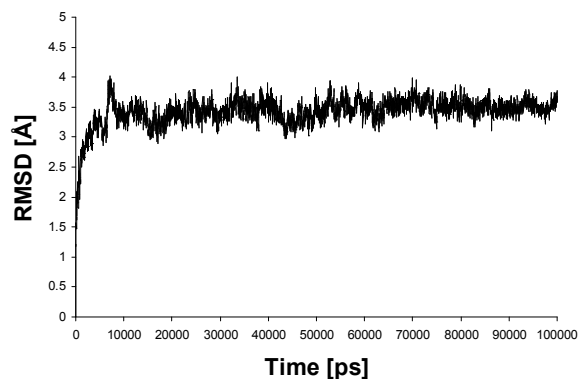


Figure S1. RMSD values in [Å] of 100ns simulation of the wild type free ALK

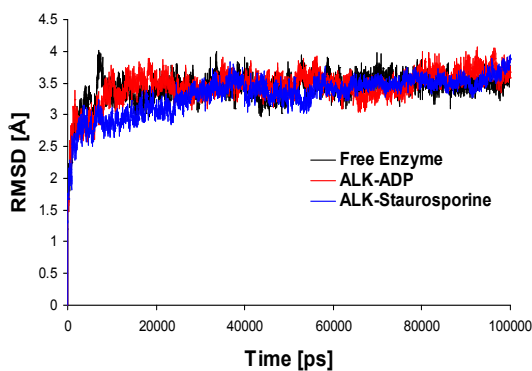
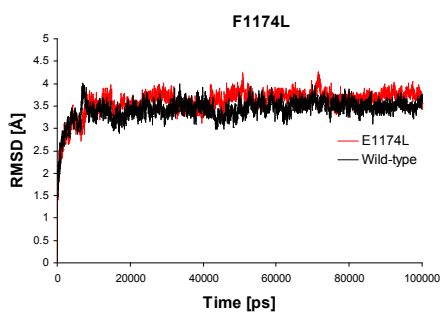
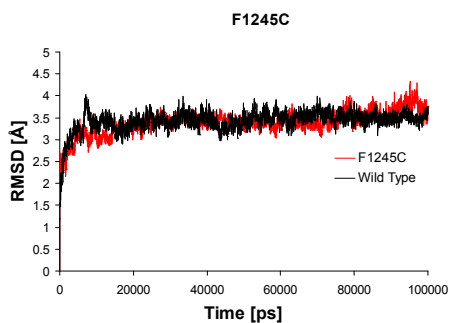


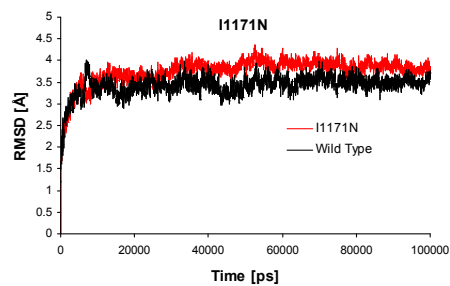
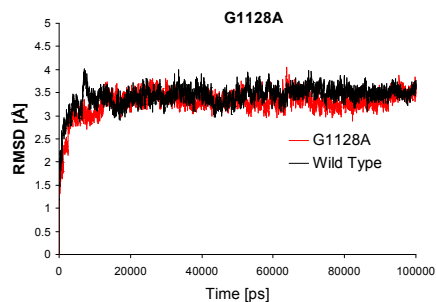
Figure S2. RMSD values in [Å] of 100ns simulation of i) wild type ALK-ADP complex (in red); ii) wild type ALK-Staurosporine Complex (in blue) in reference to the iii) wild type free enzyme ALK (in black).



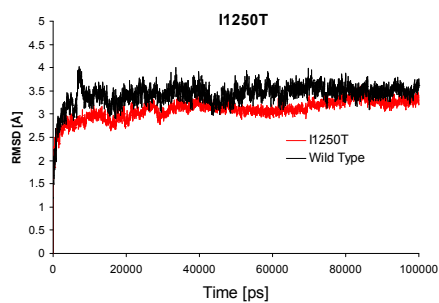
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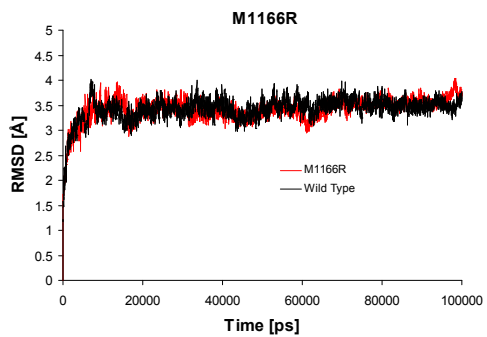
B



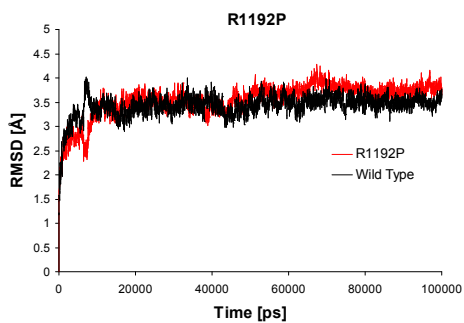
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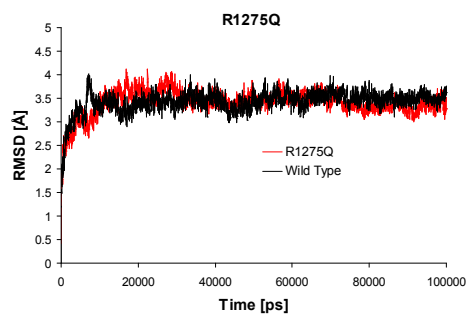
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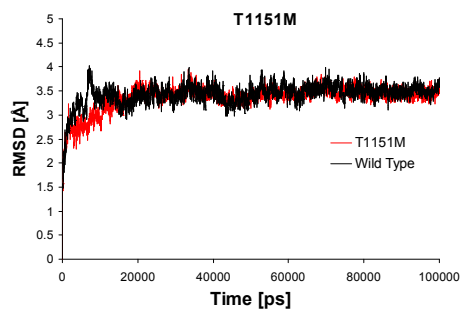
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F



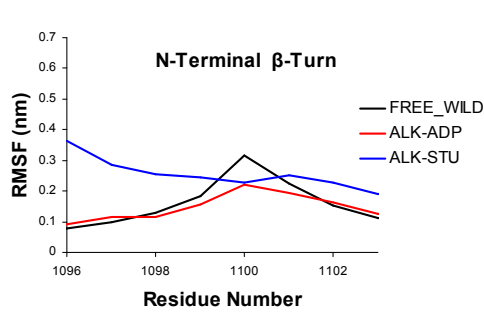
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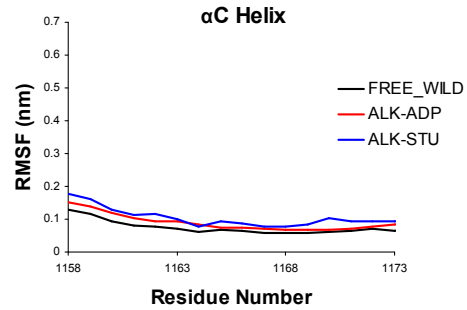
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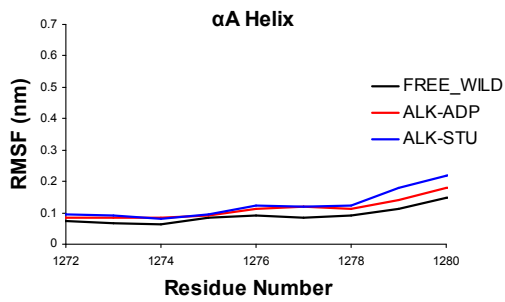
Figure S3 (A to I) RMSD values in [Å] of 100ns simulation of all activation mutation forms of the free ALK in reference to the wild type free ALK



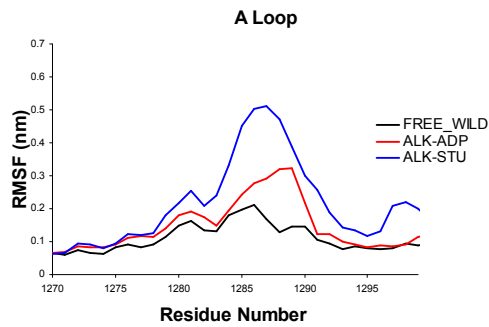
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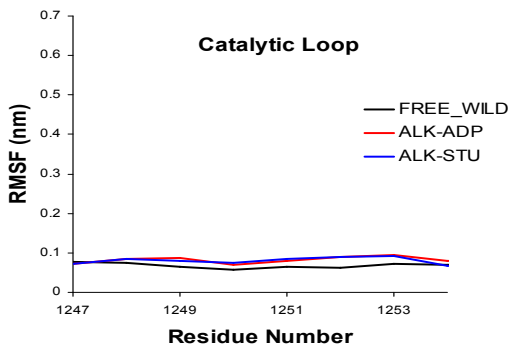
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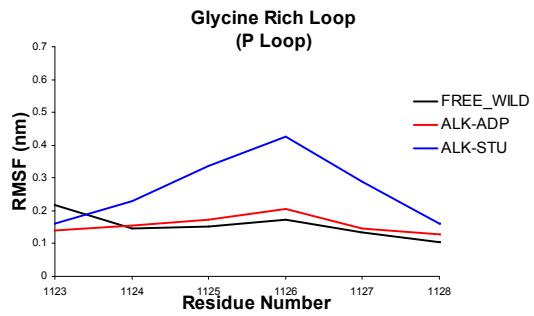
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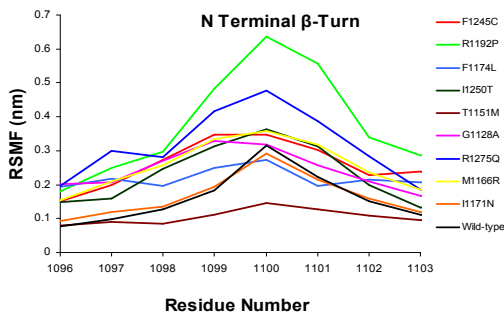


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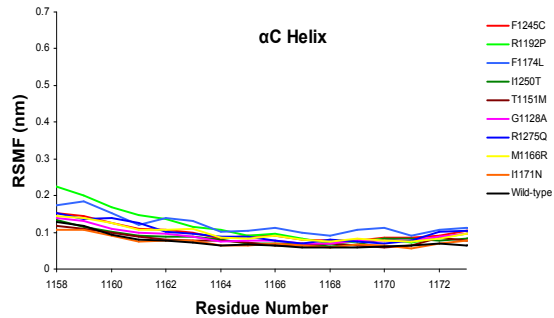


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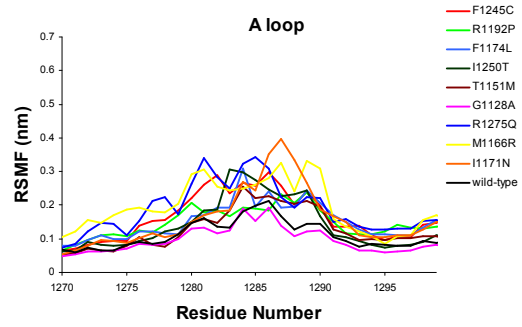
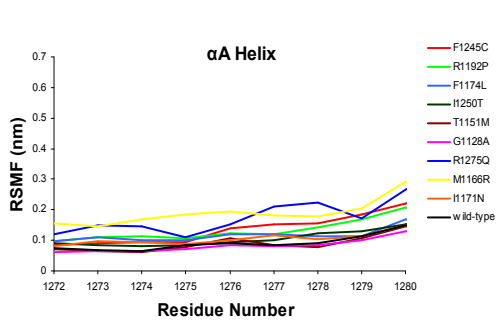
Figure S4. RMSF Values for the α C-helix, α A-helix, A-loop, catalytic loop and P-loop for ALK-ADP and ALK-Staurosporine Complexes in reference to the wild type free ALK.



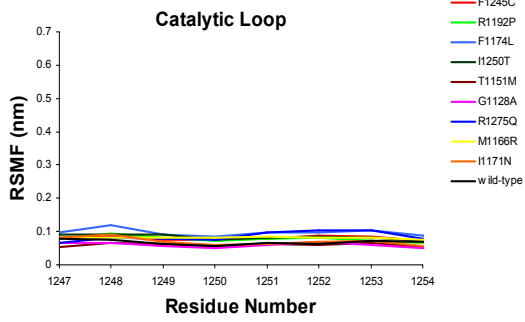
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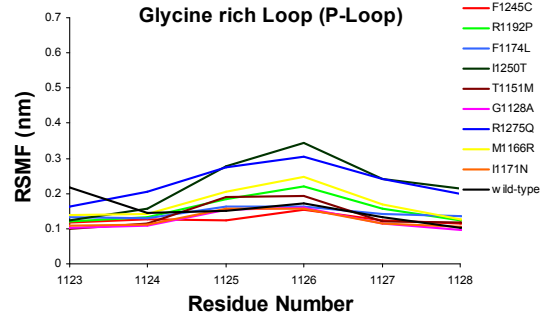
B



C



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Figure S5. RMSF Values for the α C-helix, α A-helix, A-loop, catalytic loop and P-loop for all activation mutants free ALK in reference to the wild type free enzyme.