Conformational biases of linear motifs

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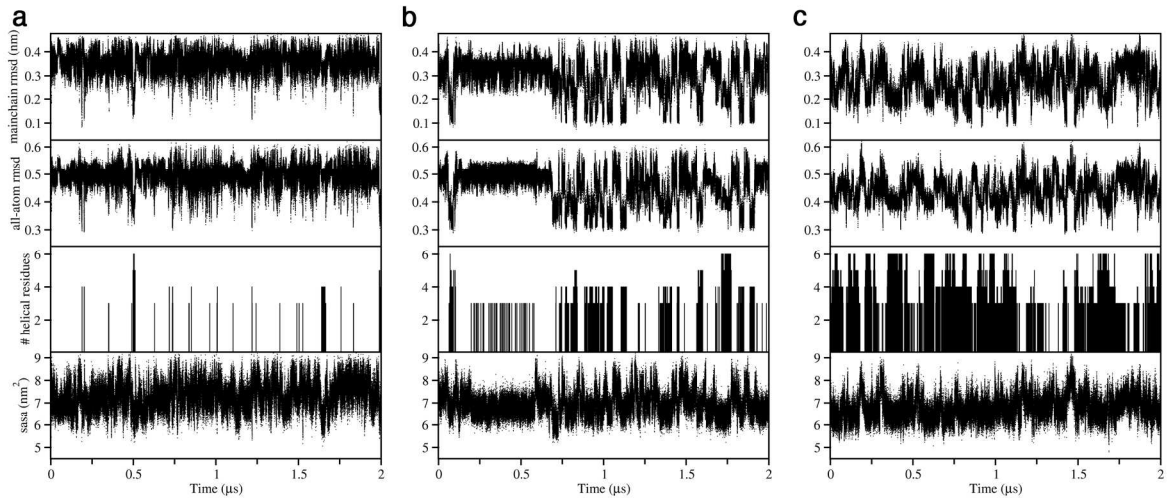

Figure S1. ExoS – 14-3-3 complexed to uncomplexed state comparison. a) GROMOS96 53a6, b) GROMOS96 54a7, and c) Amber99SB*-ILDN. Mainchain and all-atom rmsds to the complexed state and peptide helicity measurement. For the rmsd calculations, 7 residues (GLLDALD), including 28 mainchain (N, C_α, C', and CO) and 49 non-hydrogen atoms were compared. Peptide helicity was the sum of residues in all helix types (α, 3_{10}, and π) as assigned by the DSSP algorithm. Solvent accessible surface areas were calculated using the g_sas tool[1-3].

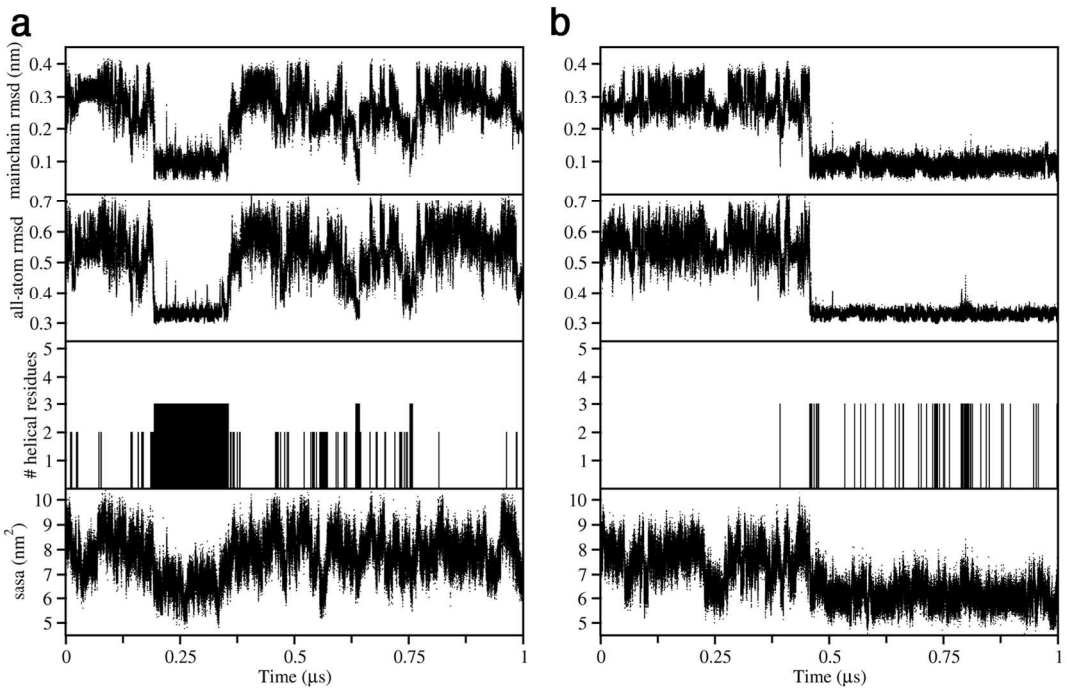

Figure S2. Amphiphysin 1 – Clathrin complexed to uncomplexed state comparison. a) GROMOS96 53a6 and b) GROMOS96 54a7. Mainchain and all-atom rmsds to the complexed state and peptide helicity measurement. For the rmsd calculations, 7 residues (TLPWDLW), including 28 mainchain (N, C_α, C', and CO) and 66 non-hydrogen atoms were compared. Peptide helicity was the sum of residues in a 3_{10} helix as assigned by the DSSP algorithm. Solvent accessible surface areas were calculated using the g_sas tool[1-3].

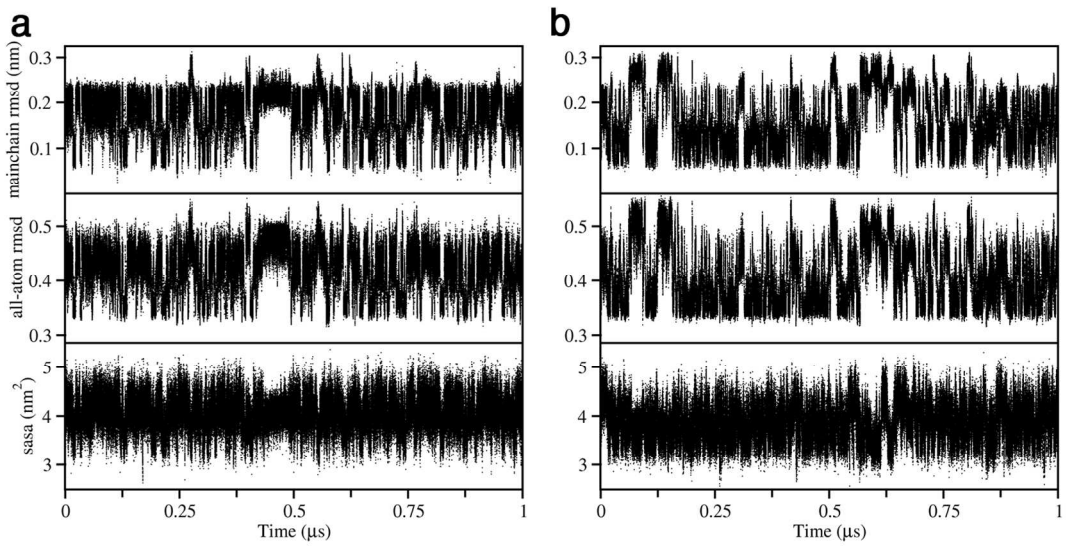

Figure S3. β-arrestin 2 – Clathrin complexed to uncomplexed state comparison. a) GROMOS96 53a6 and b) GROMOS96 54a7. Mainchain and all-atom rmsds to the complexed state. For the rmsd calculations, 5 residues (NLIEF), including 20 mainchain (N, C_α, C', and CO) and 44 non-hydrogen atoms were compared. Solvent accessible surface areas were calculated using the g_sas tool[1-3].

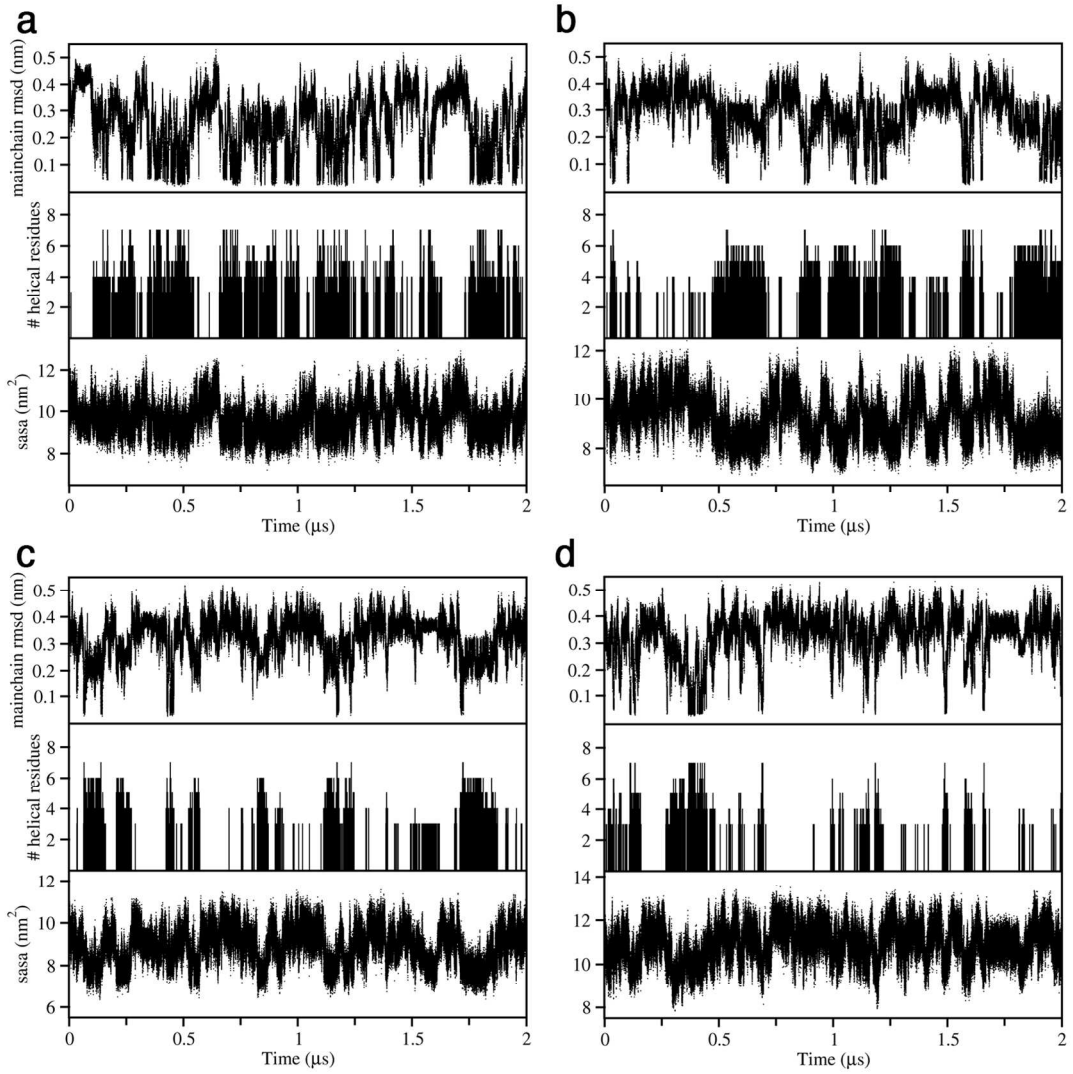

Figure S4. LxxLL motif complexed to uncomplexed state comparison for duplicate set of MD simulations. Mainchain rmsds to the RIP140 L5 complexed state structure (a, optimized peptide; b, c, d, RIP140 L6, L7 and L3 peptides, respectively). For the rmsd calculations, the corresponding mainchain atoms of the different motifs were compared to the same 9-residue (SLLLHLLKS) segment of the L5 motif, which includes 36 mainchain (N, C_α, C', and CO) atoms. Peptide helicity was the sum of residues in all helix types (α, 3_{10}, and π) as assigned by the DSSP algorithm. Solvent accessible surface areas were calculated using the g_sas tool[1-3].

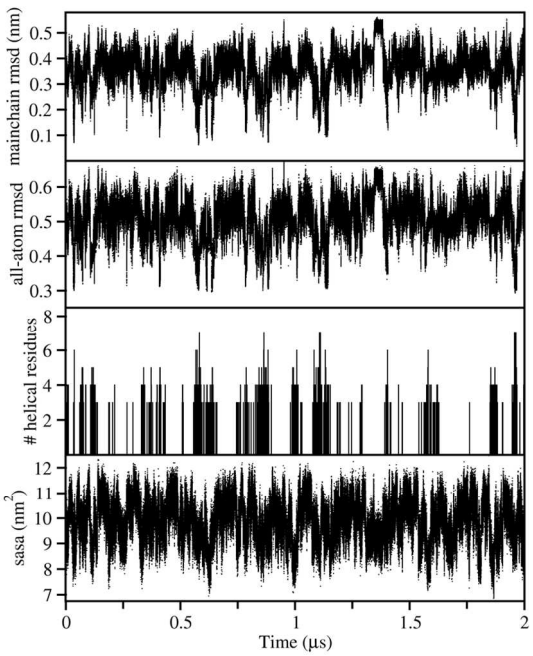

Figure S5. Tcf4 – β-catenin complexed to uncomplexed state comparison for the duplicate simulation. Mainchain and all-atom rmsds to the complexed state. For the rmsd calculations, 10 residues (DLADVKSSLV), including 40 mainchain (N, C_α, C', and CO) and 72 non-hydrogen atoms were compared. Peptide helicity was the sum of residues in all helix types (α, 3_{10}, and π) as assigned by the DSSP algorithm. Solvent accessible surface areas were calculated using the g_sas tool[1-3].

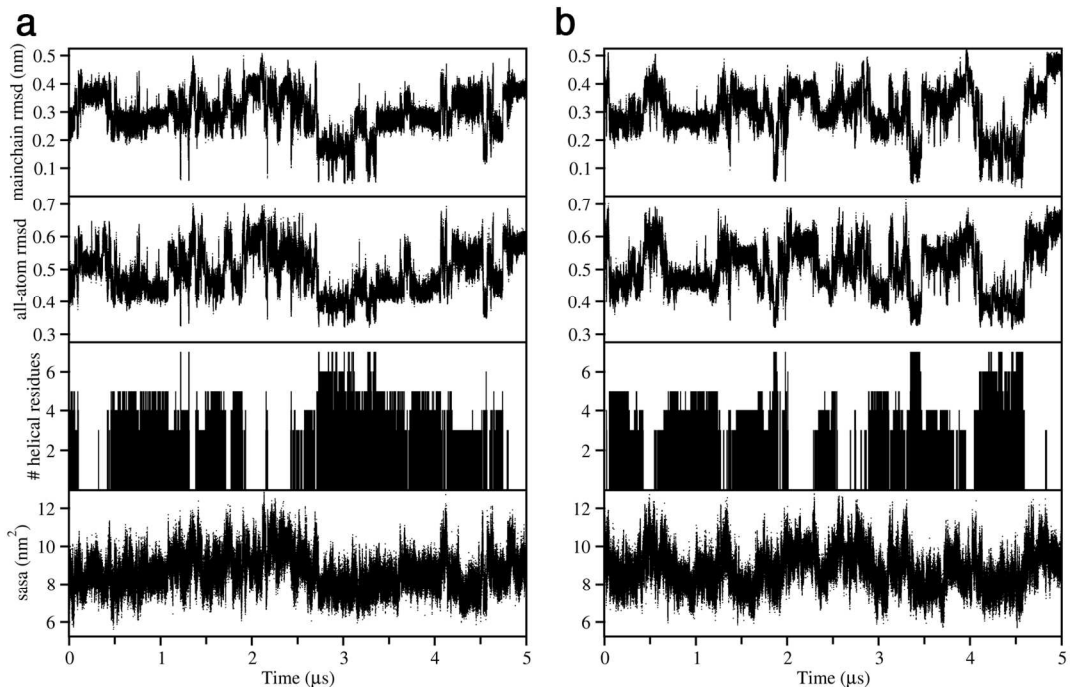

Figure S6. p53 TAD complexed to uncomplexed state comparison for the duplicate simulations. a) WT and b) P27S peptides. For the rmsd calculations, 9 residues (TFSDLWKLL), including 36 mainchain (N, C_α, C', and CO) and 79 non-hydrogen atoms were compared to the corresponding atoms in the MDM2 bound state structure[4]. Peptide helicity was the sum of residues in all helix types (α, 3_{10}, and π) as assigned by the DSSP algorithm. Solvent accessible surface area was calculated using the g_sas tool[1-3].

References

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