**Dynamics and deformability of α-, 310- and π-helices**

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**SUPPLEMENTARY DATA**

|  |  |  |  |
| --- | --- | --- | --- |
| d1n45ad1n7ead1nazad1ng6ad1nkdad1nkga2d1nkga3d1nkiad1nq7ad1ntvad1nycad1nykad1nyta1d1nyta2d1o7iad1oboad1ogad1d1oh0ad1okia2d1omrad1oohad1p3cad1p6oad1pkhad1psrad1pvma4d1q1fad1q6za2d1q6za3d1qftad1qh4a1d1qs1a2d1r29ad1r7jad1r8sad1r8sed1riead1rocad1rttad1s8nad1sauad1sh8ad1shuxd1sjwad1szhad1t1ea2 | d1t2da1d1t2da2d1t61a1d1t61a2d1t6uad1tkea2d1tp6ad1tu7a2d1tu9ad1tuaa2d1tzvad1uaiad1ucdad1ui0ad1urrad1uscad1uxzad1v05ad1v2xad1v30ad1v37ad1v4pad1v70ad1v7rad1v8ha1d1vh5ad1vyiad1w66a1d1w7ca2d1w7ca3d1wc2a1d1whiad1wkqad1wluad1wmda1d1wn2ad1wpnad1wrmad1x46ad1xsza1d1xsza2d1y0pa3d1ypqa1d1z1sa1d1z3xa2d1z6na1 | d1zhva1d1zi8ad2nw2b1d2nw2b2d2ohwa1d2oxcad2piead2pmra1d2pv2ad2pvbad2q9oa2d2q9oa3d2qjlad2r7512d2r8oa1d2r8oa3d2rb8ad2rcqad2tnfad2tpsad2ux6ad2uyza1d2v6ka1d2v6ka2d2vhkad2vimad2w72ad2wf7ad2wy4ad2x4kad2x7kad2xhfad2xolad2xpwa1d2y78ad2yvea1d2yvea2d2z3gad2zhnad3mzfa2d3n4jad3n8iad3nerad3ni6ad3o6wa1d3obqa | d3od3a2d3otmad3p1gad3p3ca2d3p73a2d3piwad3po8ad3pwka2d3qfta2d3qvpa2d3qzmad3qzrad3qztad3r3qad3rhbad3rnjad3ry4a2d3s4ead3tnla1d3tnla2d3twyad3u81ad3us6ad3ve9ad3vl9ad3vqfad3vura2d3zqxad3ztpad3zyhad3zzsa |

**Supplementary Data 1.** *Dataset*. Provided are the SCOP ids used in the study.



**Supplementary Data 2.** *Normalized B-factor distribution*. For A) α-, B) 310- and C) π-helices.



**Supplementary Data 3.** *Relative Solvent Accessibility distribution*. For A) α-, B) 310- and C) π-helices.



**Supplementary Data 4.** *Normalized RMSf distribution*. For A) α-, B) 310- and C) π-helices.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Initial state | 100% | >90% | >50% | <25% |
| α-helix | 29.1 | 74.6 | 91.4 | 3.9 |
| 310-helix | 0.0 | 15.7 | 54.1 | 24.0 |
| π-helix | 0.0 | 0.0 | 2.4 | 97.6 |
| π-newDSSP-helix | 0.0 | 15.0 | 39.6 | 38.6 |

**Sup data 5.** *Persistence of the original helical state*. For the three type of helices is shown the frequency of residues staying in the original assigned state (100%) during the simulations with the α–, 310- and the π-helices (noted π-helices for the classical DSSP assignment and π-newDSSP-helix assigned with DSSP\_v2.2.1), the occurrence for those staying more than 90%, more than 50% and less than 25% of the simulation time.



**Sup data 6**. *Analyses of the clusters associated to α-helix*. (x-axis) is the normalized B-factors and (y-axis) is the normalized RMSf. The clusters are named in regards to their content in secondary structures (namely α1, α2, αT1, αT2 and αC). The secondary structures are shown with a gradient of colours ranging from red (100% of presence) to blue (0%). The secondary structures are disposed with α-, 310- and π-helix, β-strand, turn, bend and coil.



**Sup data 7**. *Analyses of the clusters associated to 310-helix*. The clusters are named in regards to their content in secondary structures (namely 310, 310α, 310T1, 310T2and 310c). See Sup data 6 for more details.



**Sup data 8**. *Analyses of the clusters associated to* π*-helix*. The clusters are named in regards to their content in secondary structures (namelyπ, πα1, πα2, παT and πT). See Sup data 6 for more details.