Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Establishing the Link between Fibril Formation and Raman Optical Activity Spectra of Insulin

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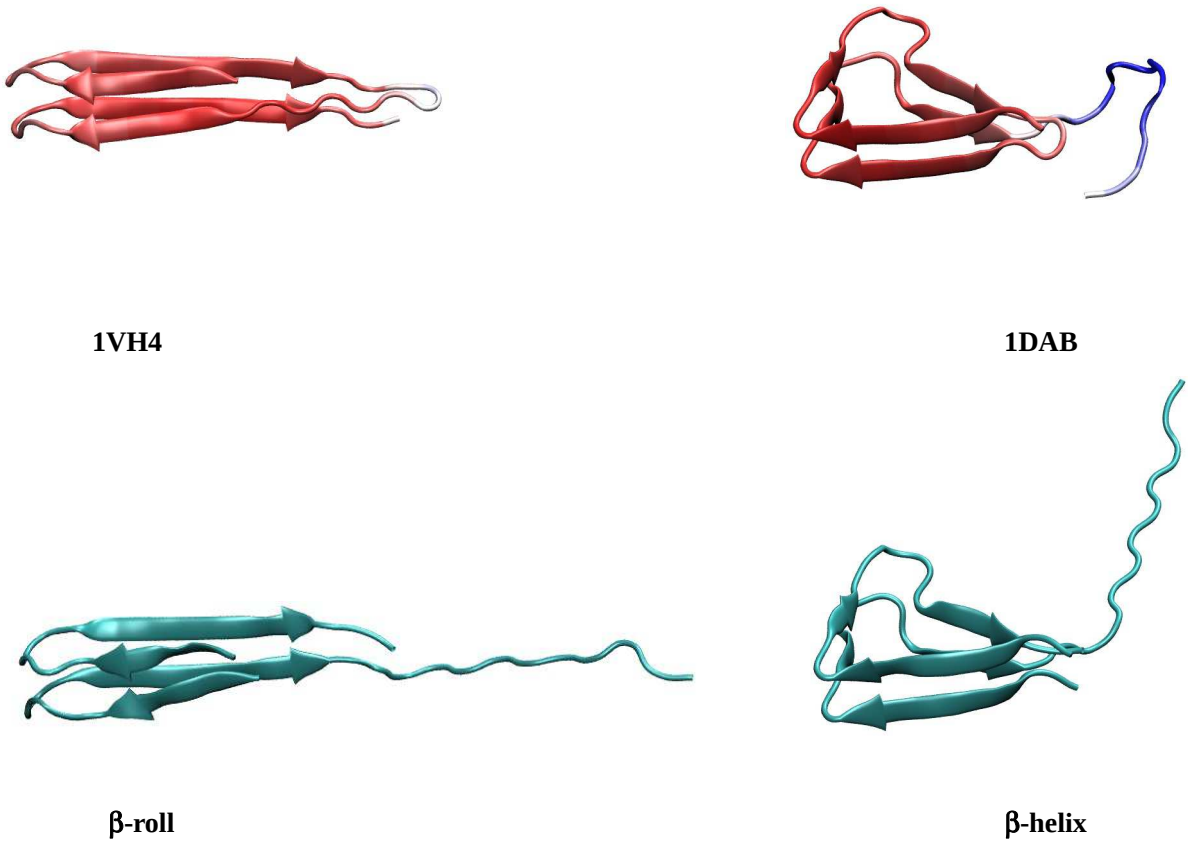

Figure S1. The mimicked parts of the 1VH4 and 1DAB proteins (top) and the two initial insulin geometries (bottom).

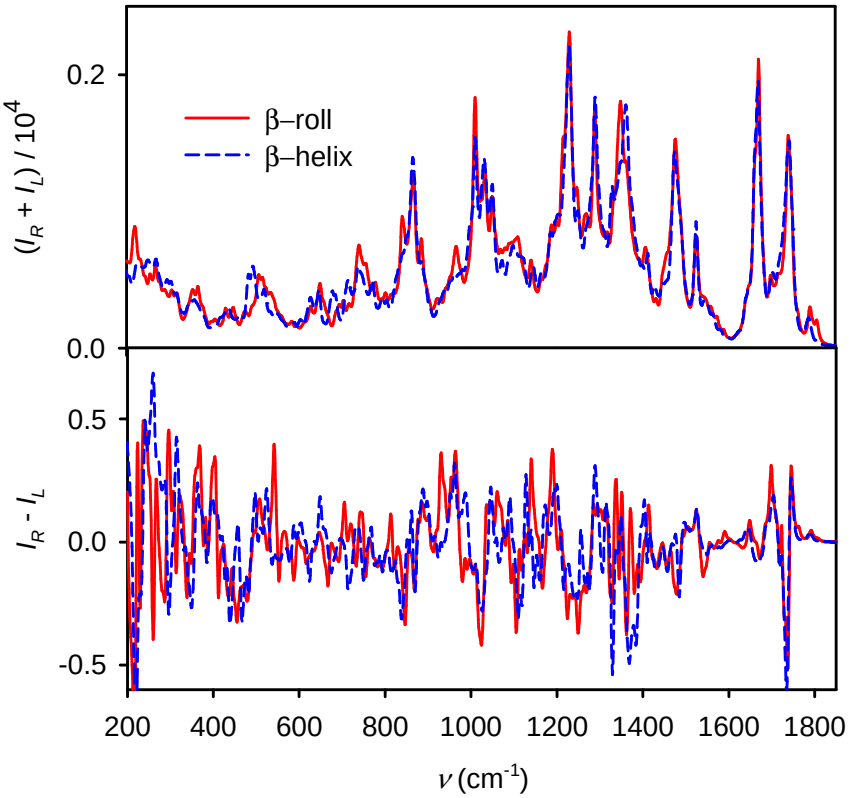

Figure S2. Raman and ROA spectra simulated for the β-roll and β-helix amyloidal conformations of insulin.

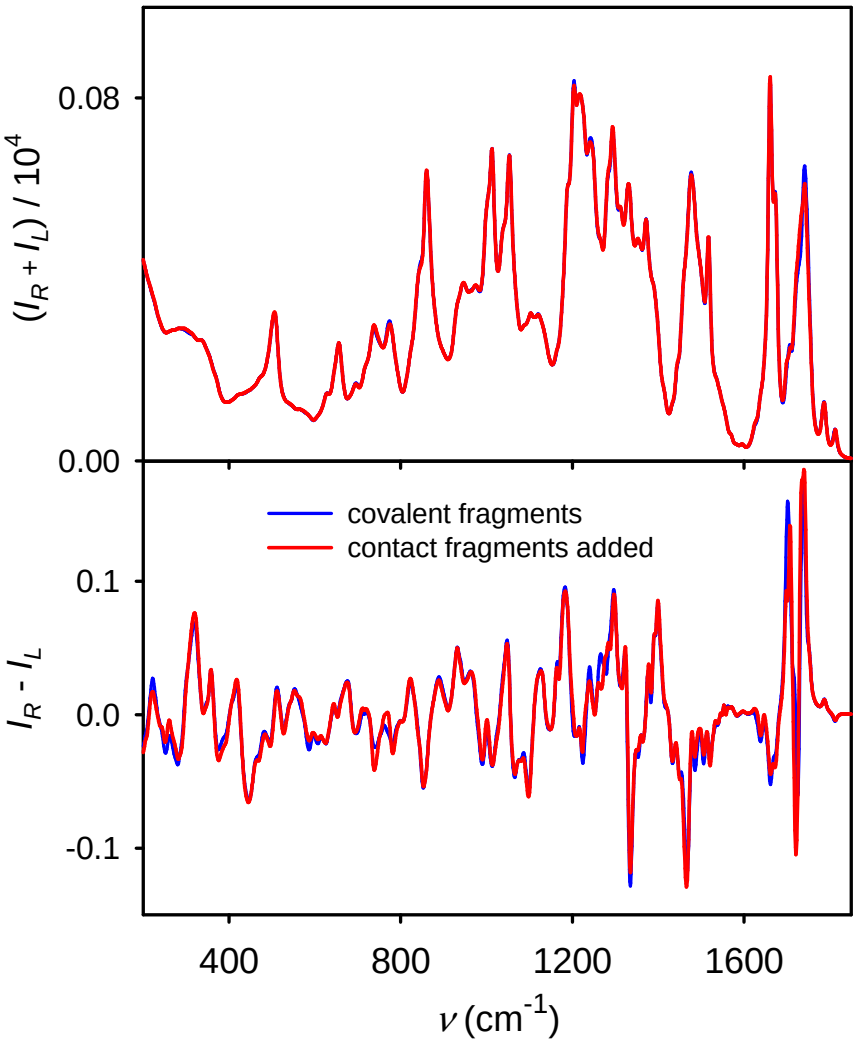

Figure S3. Insulin Raman and ROA spectra (average of 865 MD snapshots) simulated with and without fragments comprising non-covalent interactions between peptide chains.

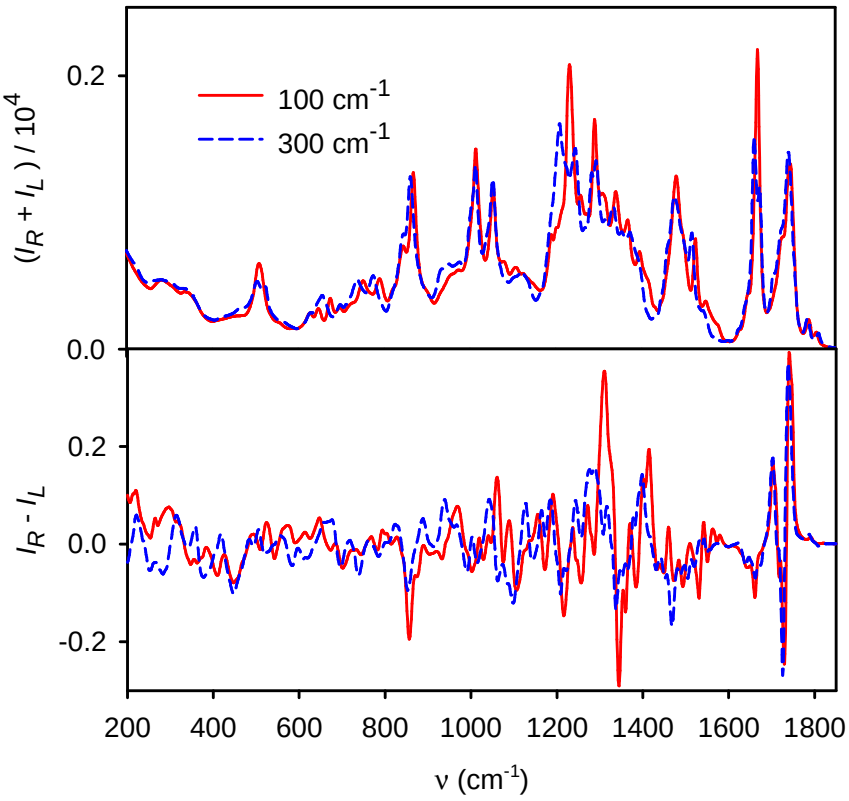

Figure S4. Raman and ROA spectra of the β-roll insulin fibril structure simulated as an average of 865 MD snapshots from fragments optimized with the lower (100 cm^{-1}, red) and higher (300 cm^{-1}, blue) normal mode frequency limit.

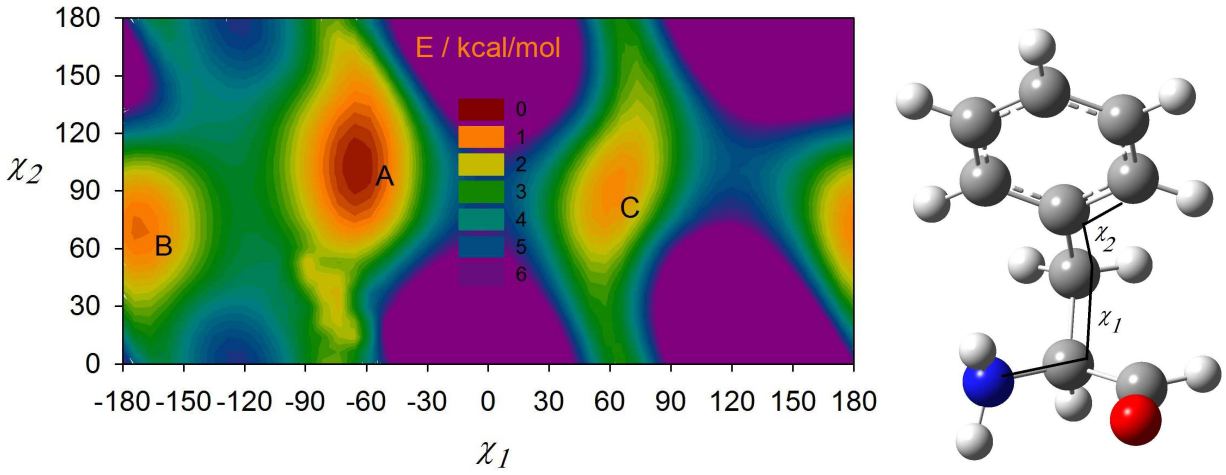

Figure S5. Calculated (B3LYP/6-311++G**/PCM) potential energy surface of the model NH_2-Phe-COH residue.

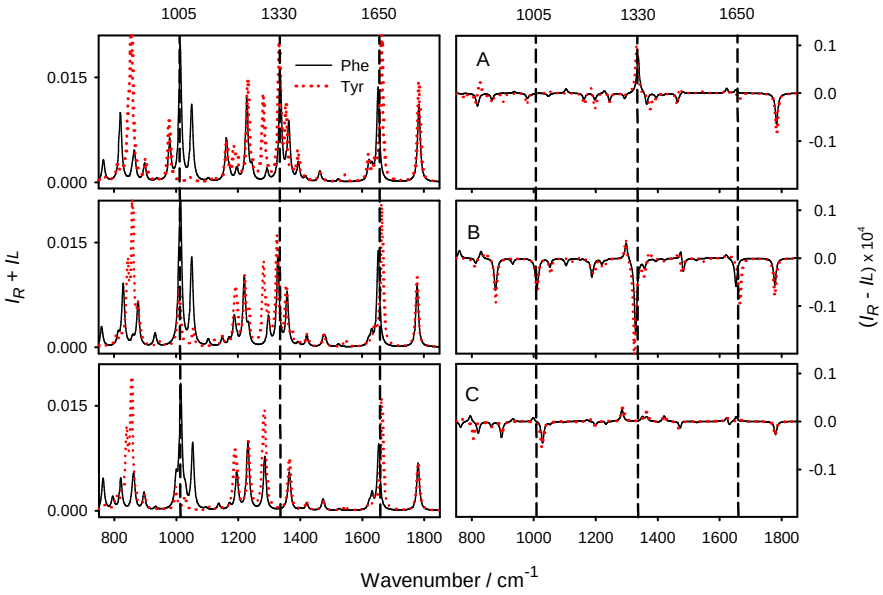

Figure S6. Calculated Raman and ROA spectra of the NH_2-Phe-COH and NH_2-Tyr-COH model molecules; the three A-C conformers are marked as in **Figure S4**.

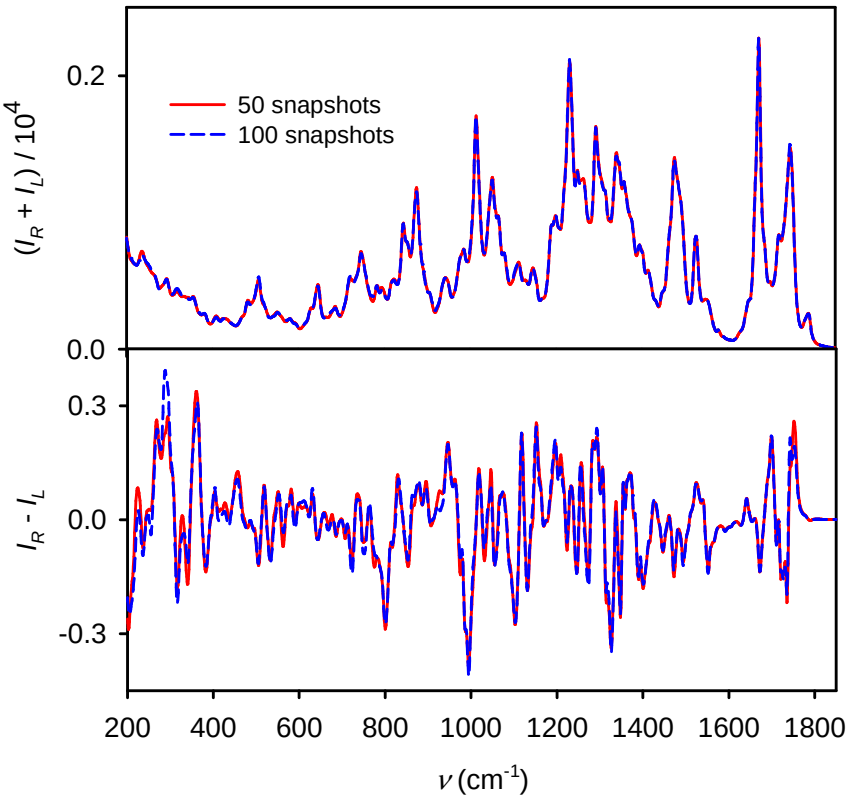

Figure S7. Raman and ROA spectra of a twisted insulin fibril (cf. **Figure 4**, τ = -6 °) obtained as averages of 50 and 100 snapshots.

Table S1. Populations (*p*, in %) and χ_1 and χ_1 angles of the three Phe and Tyr side chain conformers (**Figure S4**) in native and fibrous insulin obtained by molecular dynamics.

Conformer	χ_1 / °	χ_2 / °	*p*, native	*p*, fibril
A	-63	102	49	24
B	-173	72	31	68
C	57	92	20	8