Each Supplementary Data Set includes an instruction file, which should be used in conjunction with the protocol in the main paper.

i. The source of the data and corresponding publications are described

ii. The main objective is to describe the input and output of certain steps in the protocol, and where corresponding files can be found.

iii. Each instruction file further contains a section discussing the evaluation and selection of the best model, case specific comments and visualization of the structure and mapped cross-links.

Furthermore, each data set includes folders containing the input and output files used and generated during the described modeling procedure. These are the files referred to in the instruction file. The folders are labeled with sequential letters, corresponding to the order that they appear in the protocol.