

The files and scripts within this folder belong to the Supplementary Material of the paper:

Devising Bone Molecular Models at the Nanoscale: From Usual Mineralized Collagen Fibrils to the First Bone Fibers including Hydroxyapatite in the Extra-Fibrillar Volume

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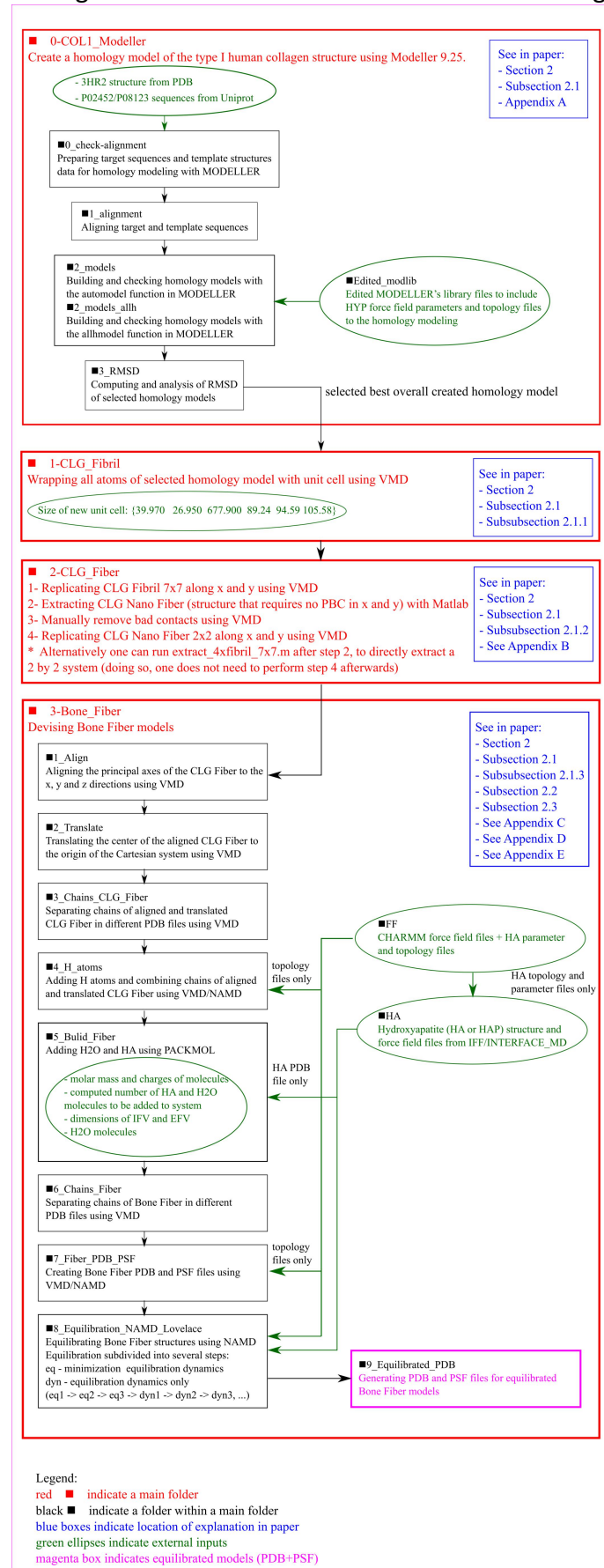
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The paper, together with these files, aims to provide a detailed prescription on how to devise all-atom bone molecular models at the nanoscale that include hydroxyapatite in the extra-fibrillar volume, resembling fibers in bones.

Tips:

- To understand the details of the modeling process, please read the paper (including Appendices) and the README files in each folder thoroughly.
 - Follow the folders in increasing order, i.e., 0-COL1_Modeller first, and 3-Bone_Filer at last.
 - Each README file informs the INPUT/OUTPUT of each step and describes how that specific step can be performed/reproduced.
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The figure below shows a flowchart of the modeling process of our Bone Fiber model.



Content of each folder:

◆ 0-COL1_Modeller

See Section 2. Devising Bone at the Nanoscale

See Subsection 2.1. Devising the Simulation Box

See Appendix A – Building Homology Models of Human Type-I Collagen using MODELLER 9.25

Files used to create a homology model of the type I human collagen structure using Modeller 9.25.

Descriptive README files.

■ 0_check-alignment

Preparing target sequences and template structures data for homology modeling with MODELLER

■ 1_alignment

Aligning target and template sequences

■ 2_models

Building and checking homology models with the automodel function in MODELLER

■ 2_models_allh

Building and checking homology models with the allhmodel function in MODELLER

■ 3_RMSD

Computing and analysis of RMSD of selected homology models

■ Edited_modlib

Edited MODELLER's library files to include HYP force field parameters and topology files to the homology modeling

See <https://salilab.org/modeller/tutorial/> for further details on homology/comparative modeling of protein three-dimensional structures with MODELLER.

◆ 1-CLG_Fibril

See Section 2. Devising Bone at the Nanoscale

See Subsection 2.1. Devising the Simulation Box

See Subsubsection 2.1.1. CLG Fibril

Devising CLG Fibril - Compressing/Wrapping homology model in Unit Cell (UC)

Files used to devise CLG Fibril model, i.e., to wrap all atoms in predefined unit cell using VMD.

Descriptive README file.

◆ 2-CLG_Fiber

See Section 2. Devising Bone at the Nanoscale

See Subsection 2.1. Devising the Simulation Box

See Subsubsection 2.1.2. CLG Fiber

See Appendix B – CLG Fiber

Devising the CLG Fiber - Replicating CLG Fibril, Extracting CLG Nano Fiber, and Replicating CLG Nano Fiber

Files used to devise CLG NanoFiber model.

Files used to replicate CLG Fibril along x and y directions using VMD.

Files used to extract from a structure that requires no PBC in x and y using Matlab.

Files used to devise CLG Fiber model.

Files used to replicate CLG NanoFiber along x and y directions using VMD.

Descriptive README file.

◆ 3-Bone_Fiber

See Section 2. Devising Bone at the Nanoscale

See Subsection 2.1. Devising the Simulation Box

See Subsubsection 2.1.3. Bone Fiber

See Subsection 2.3. Minimization and Equilibration

See Appendix C – Bone Fiber

Files used to devise Bone Fiber models.

■ 1_Align

Aligning the principal axes of the model to the x, y and z directions using VMD

■ 2_Translate

Translating the center of the model to the origin of the Cartesian system using VMD

■ 3_Chains_CLG_Fiber

Separating chains of aligned and translated CLG Fiber in different PDB files using VMD

■ 4_H_atoms

Adding H atoms to aligned and translated CLG Fiber using VMD/NAMD

■ 5_Bulid_Fiber

See Appendix D – Mass fraction calculation

Adding H₂O and HA using PACKMOL

■ 6_Chains_Fiber

Separating chains of Bone Fiber in different PDB files using VMD

■ 7_Fiber_PDB_PSF

Creating Bone Fiber PDB and PSF files using VMD/NAMD

■ 8_Equilibration_NAMD_Lovelace

Equilibrating Bone Fiber structures using NAMD

■ 9_Equilibrated_PDB

Generating PDB and PSF files for equilibrated Bone Fiber models

■ FF

See Subsection 2.2. Force Fields

CHARMM force field files + HA parameter and topology files

■ HA

See Appendix E – HA structure and FF files

Hydroxyapatite (HA or HAP) structure and force field files from IFF/INTERFACE_MD

Descriptive README files.

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CITE:

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