

## **Shockwave induced damage of a protein by void collapse**

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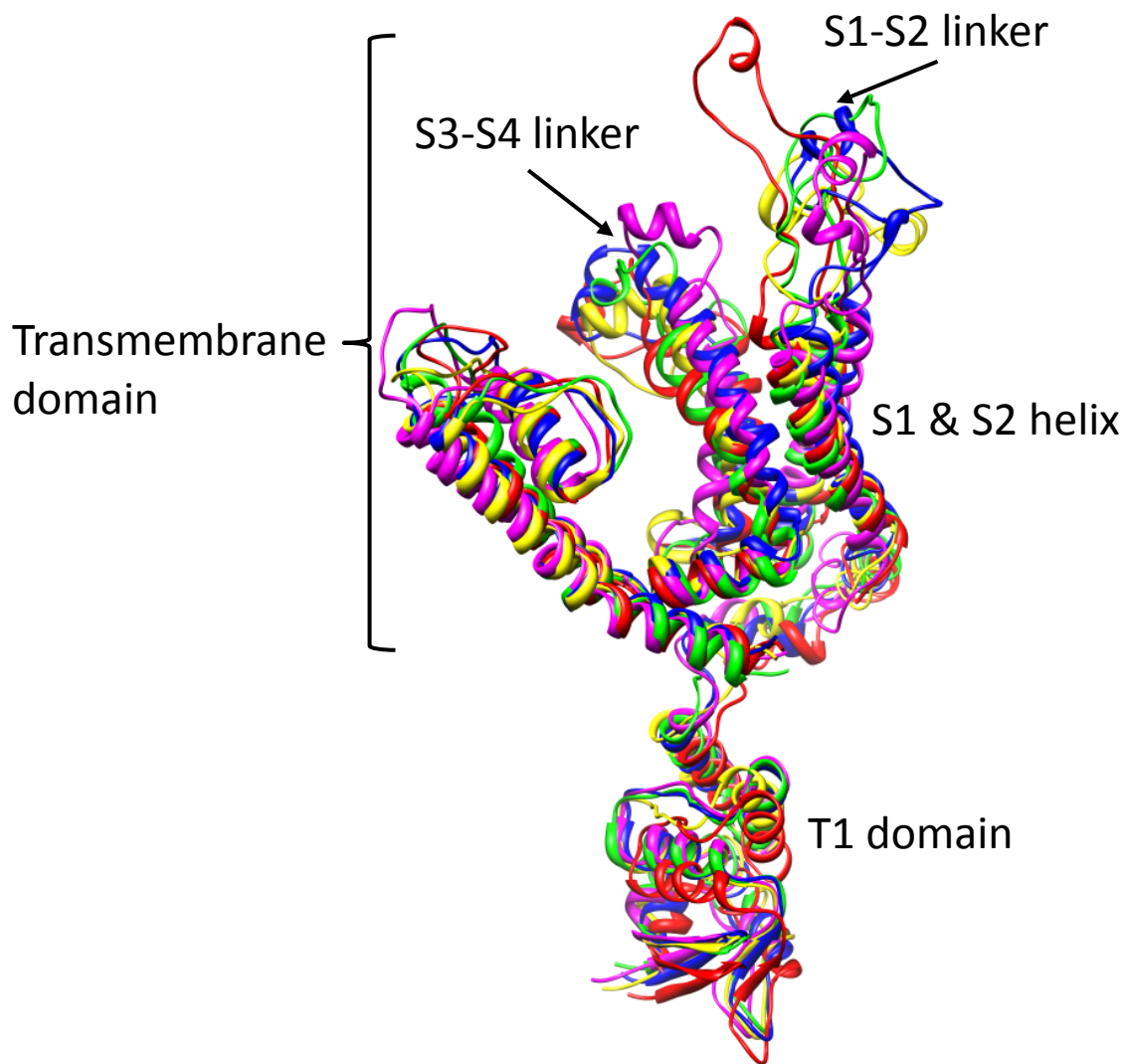


Figure S1. Overlay of the subunits of Kv1.2 in the initial structure from equilibrium NPT dynamics relative to the crystal structure (red). Subunits A, B, C, and D are colored in green, blue, violet, and yellow, respectively. The S3-S4 linker in subunit C (violet) has shifted position and the first helical turn in S4 has been lost causing larger deviations from the crystal structure.

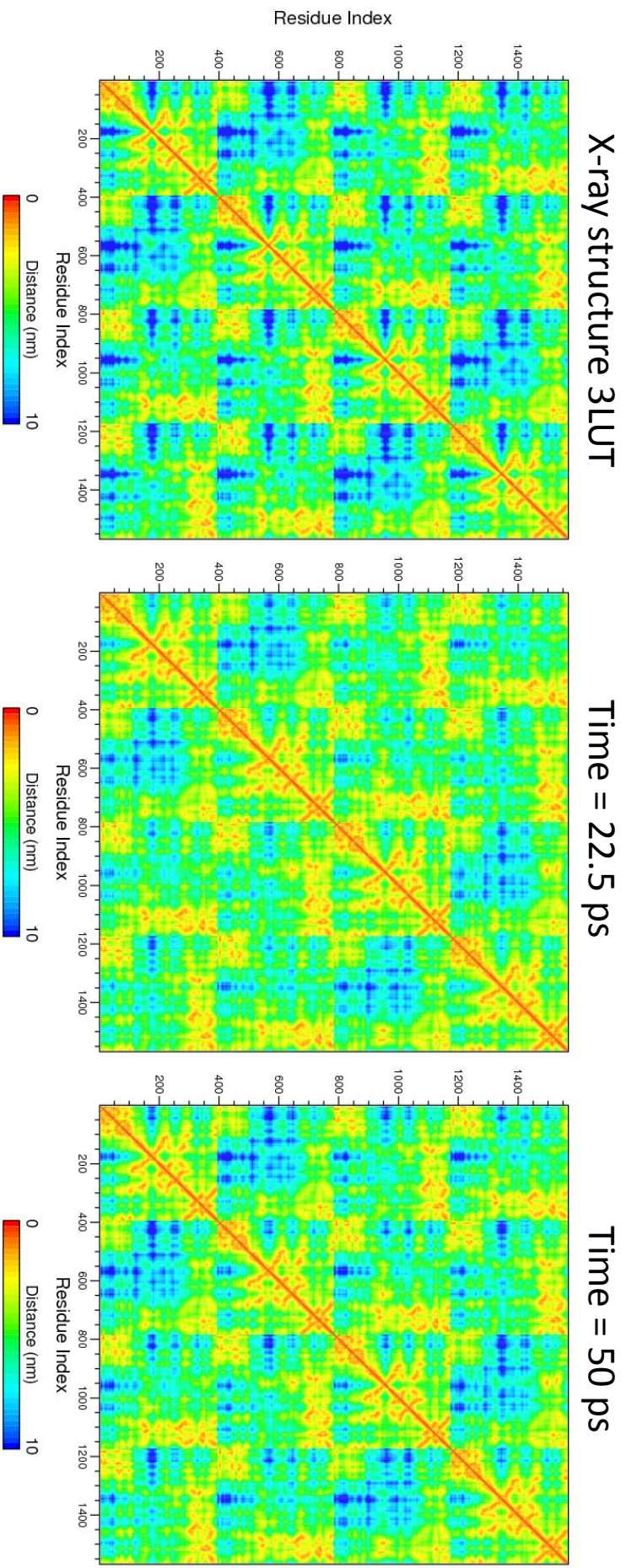


Figure S2. Distance matrices of the alpha carbons calculated for the crystal structure of Kv1.2 (3LUT) and from the shockwave simulations at times 22.5 and 50 ps (1000 m/s and no void). The plots for 22.5 and 50 ps are the average distances from the 5 individual simulations. At 22.5 ps, compression of Kv1.2 can be seen as the distances beyond 10 nm (blue) disappear. Distant features that were lost at 22.5 ps begin to reappear at 50 ps. Subunits A, B, C, and D correspond to residues 1-390, 391-780, 781-1170, 1171-1560, respectively on these plots.

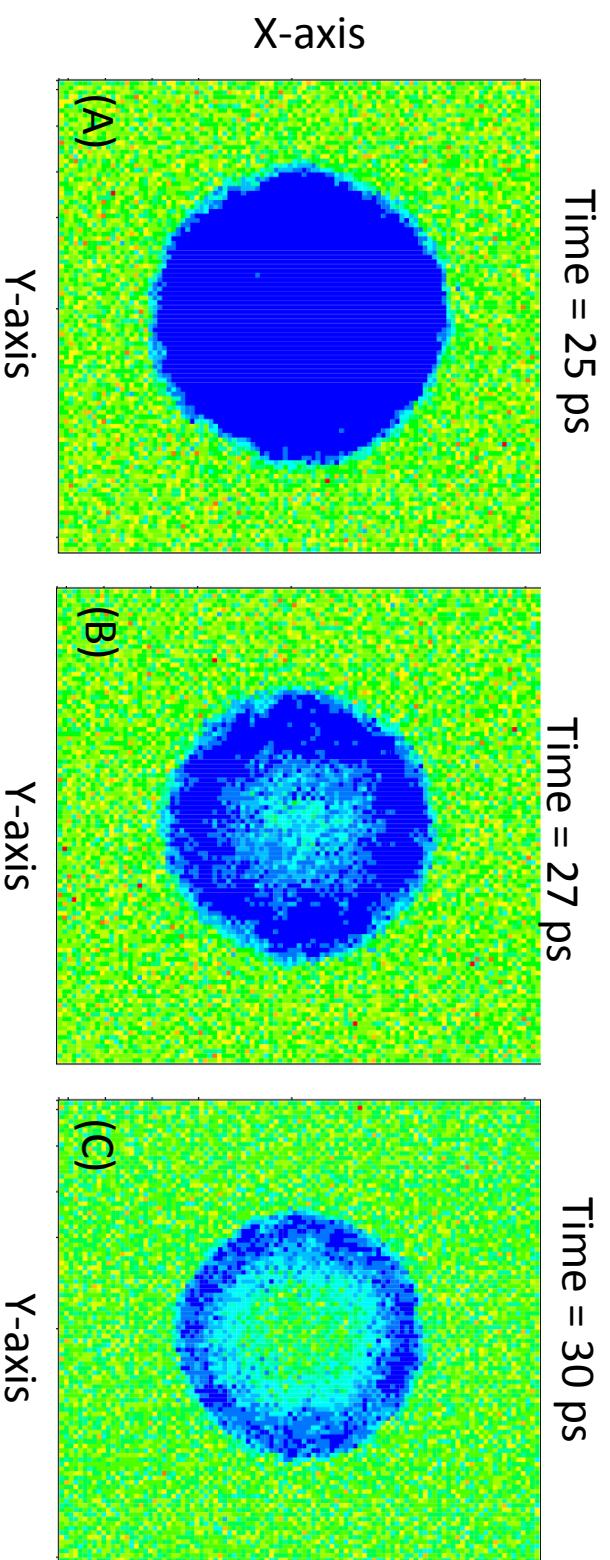


Figure S3. Cross sectional slices of the solvent density during the shockwave simulation at 500 m/s. The blue area corresponds to an absence of solvent. The development of the nanojet can be seen as it passes through the center of the void. The nanojet is caused by the shockwave collapsing the void on one side and allowing solvent to travel rapidly through the void without resistance from the medium.

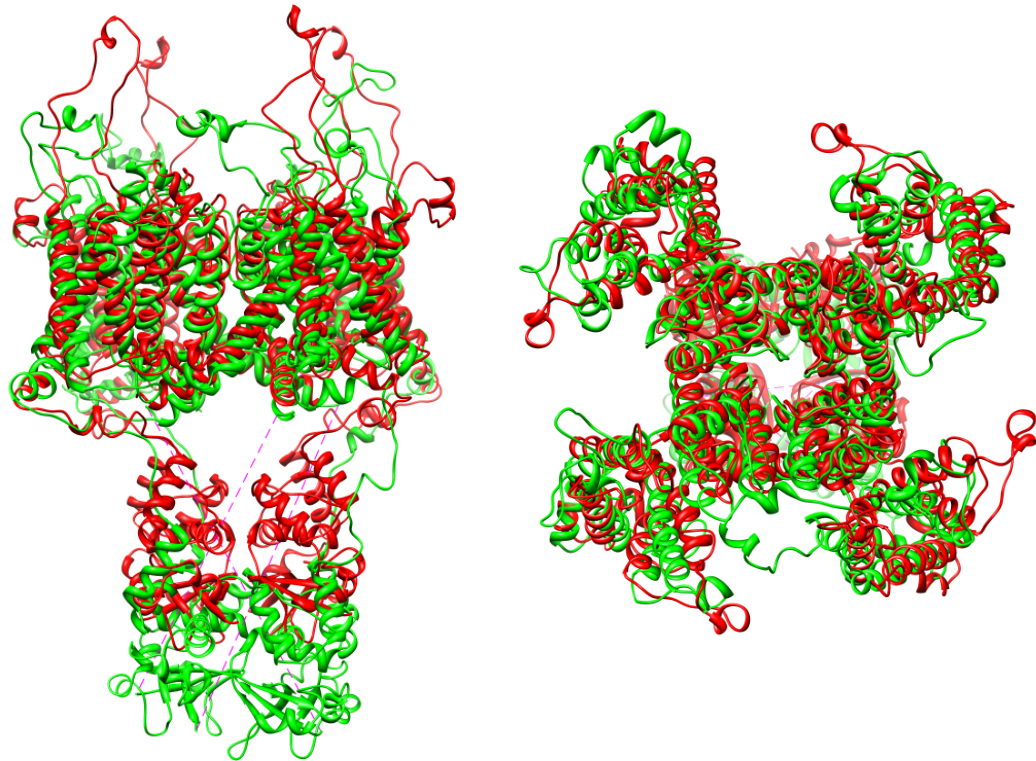


Figure S4. Overlay of the crystal structure of Kv1.2 (3LUT) with the structure of the ion channel at 1.6 ns during the void collapse simulation (no shockwave). This overlay was done only on the transmembrane domain and excluded the T1 domain (residues 32-135), S1-S2 linker (residues 185-219), and S3-S4 linker (residues 270 to 290). The structured regions of the protein shown minimal changes due to void collapse but the linker region between the transmembrane domain and the T1 domains is highly elongated and the two domains separate during the void collapse.