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Effects of Proline Substitutions on the Thermostable LOV Domain from *Chloroflexus aggregans*

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Supplementary information

Supplementary figures S1-S6

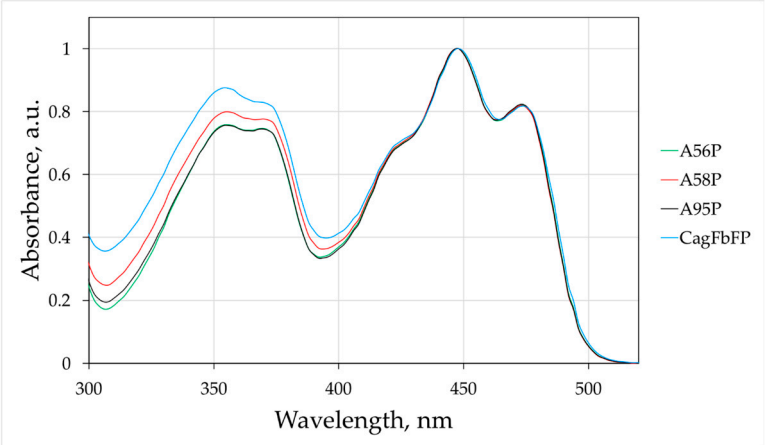

Figure S1. Normalized absorption spectra of CagFbFP and its proline-substituted variants.

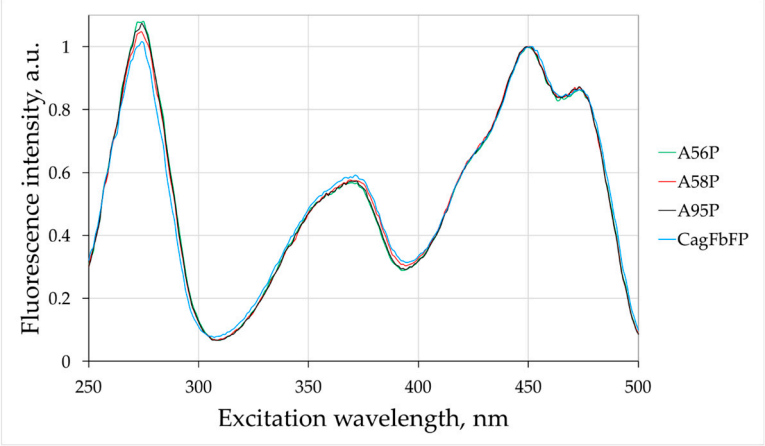

Figure S2. Normalized fluorescence excitation spectra of CagFbFP and its proline-substituted variants.

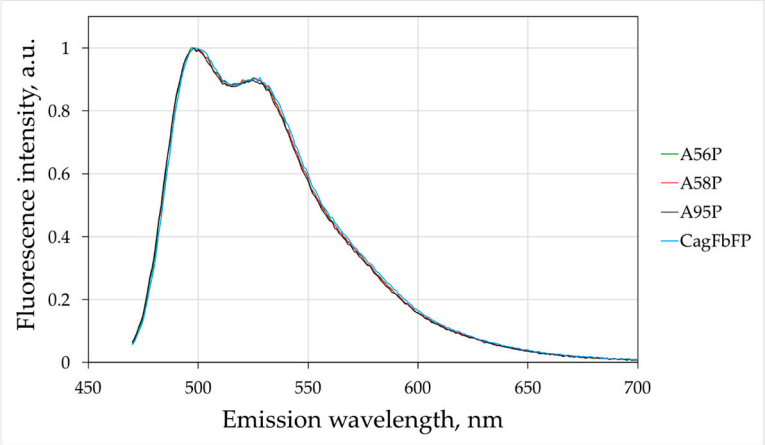

Figure S3. Normalized fluorescence emission spectra of CagFbFP and its proline-substituted variants.

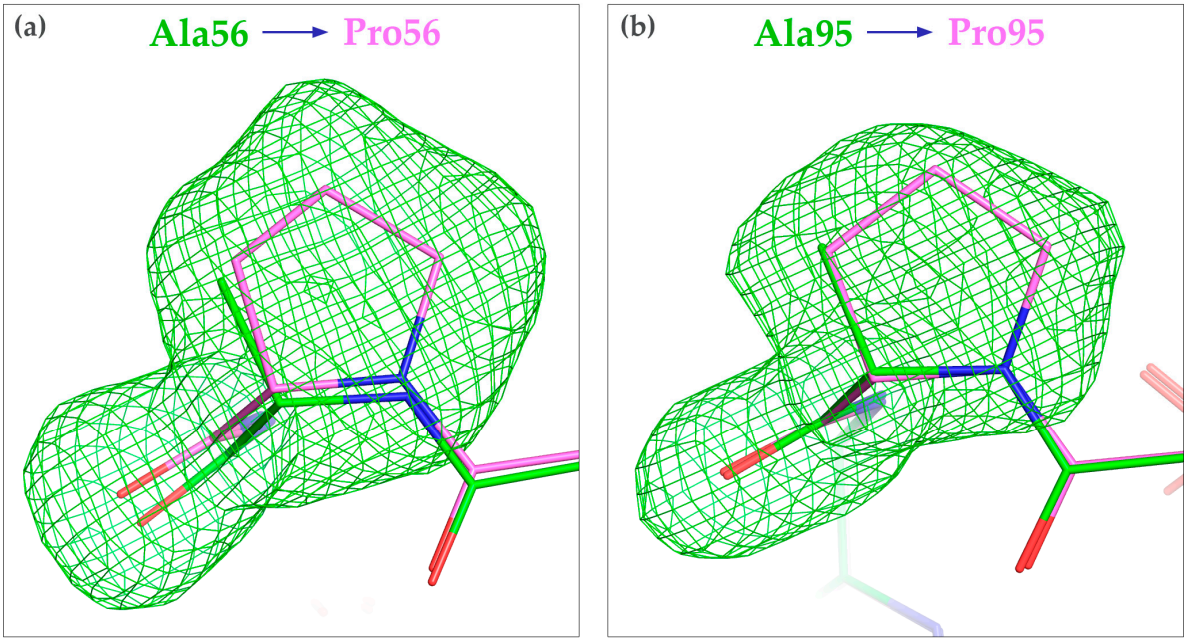

Figure S4. Omit (polder) maps for the mutants, (a) A56P and (b) A95P. The original structure of CagFbFP (PDB ID 6RHF) is shown in green, the structures of the mutants are shown in magenta. Polder electron density maps (green) are contoured at the level of 3 × r.m.s.

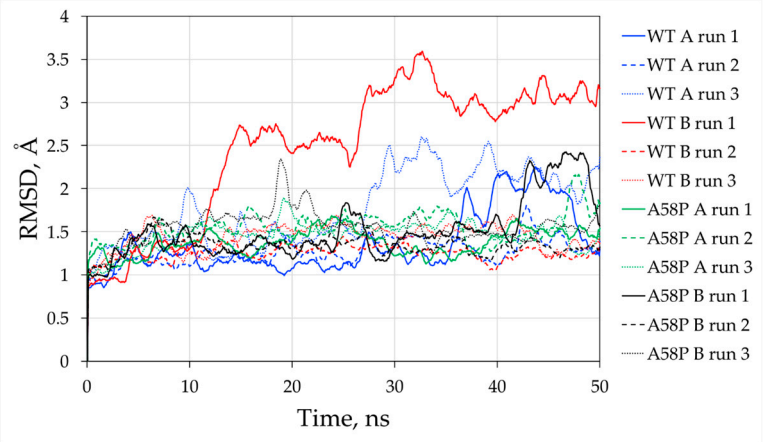

Figure S5. Root mean square deviations of backbone atom positions as a function of time. Dimers of proteins harboring the conformers A and B of the residue 58 were simulated both for the WT and A58P variants for 3 times (runs 1-3). The values were averaged over 1 ns time intervals. Some trajectories, such as WT B run 1, display relatively high overall RMSD as a consequence of displacement of one protomer relative to another one. Structures of individual protomers are conserved well in all simulations (Figure S6).

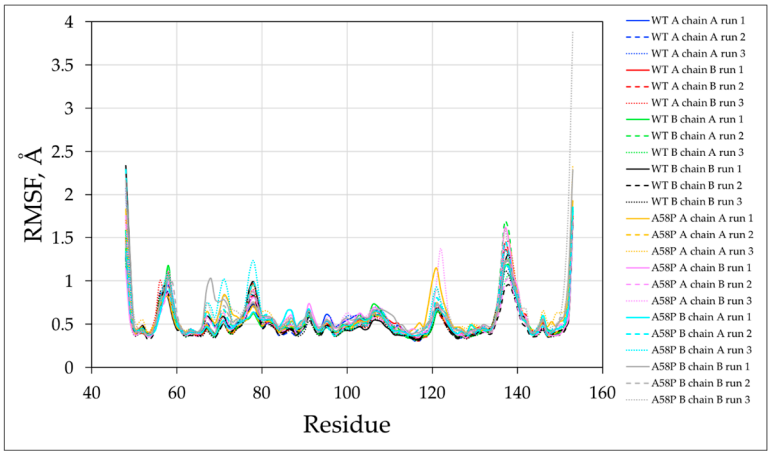

Figure S6. Root mean square fluctuations of backbone atom positions as a function of residue number during the last 40 ns of the simulations. Trajectory snapshots of each of the two protomers from each simulation were aligned and analyzed separately, and labeled chain A or chain B. No clear differences in the flexibility of different elements of the WT and A58P mutant variants are evident from the data.