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Supporting information for article:

The structure of the proteinaceous inhibitor PliI from *Aeromonas hydrophila* in complex with its target lysozyme

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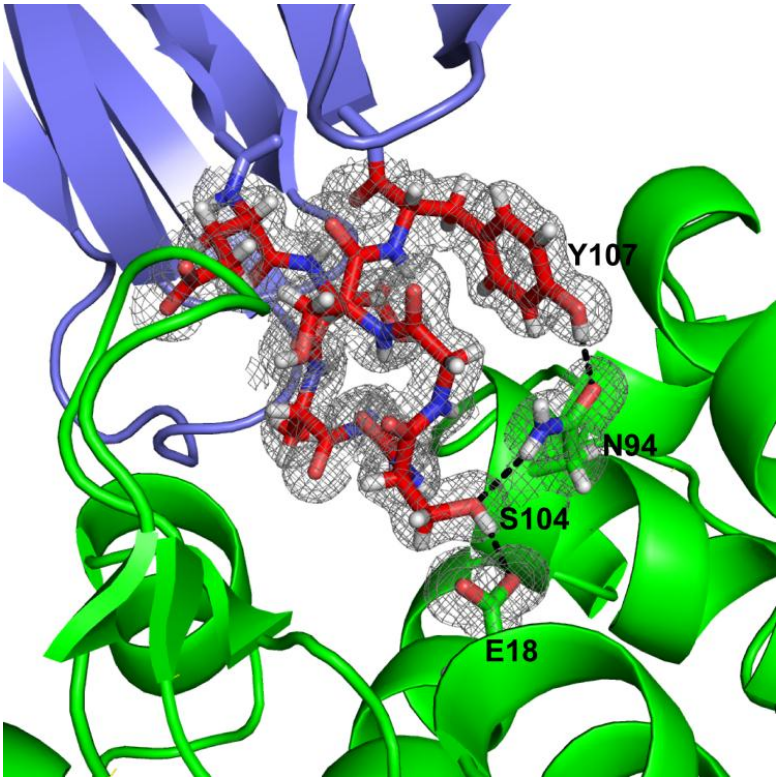

Fig. S1. Detailed conformation of loop 6 of PliI-Ac (red) which inserts into the active site of the lysozyme (green). Full atomic model including hydrogen atoms is shown together with the weighted $2F_{obs}$-F_{calc} density countoured at 0.46 e/A^3 (1.2σ).

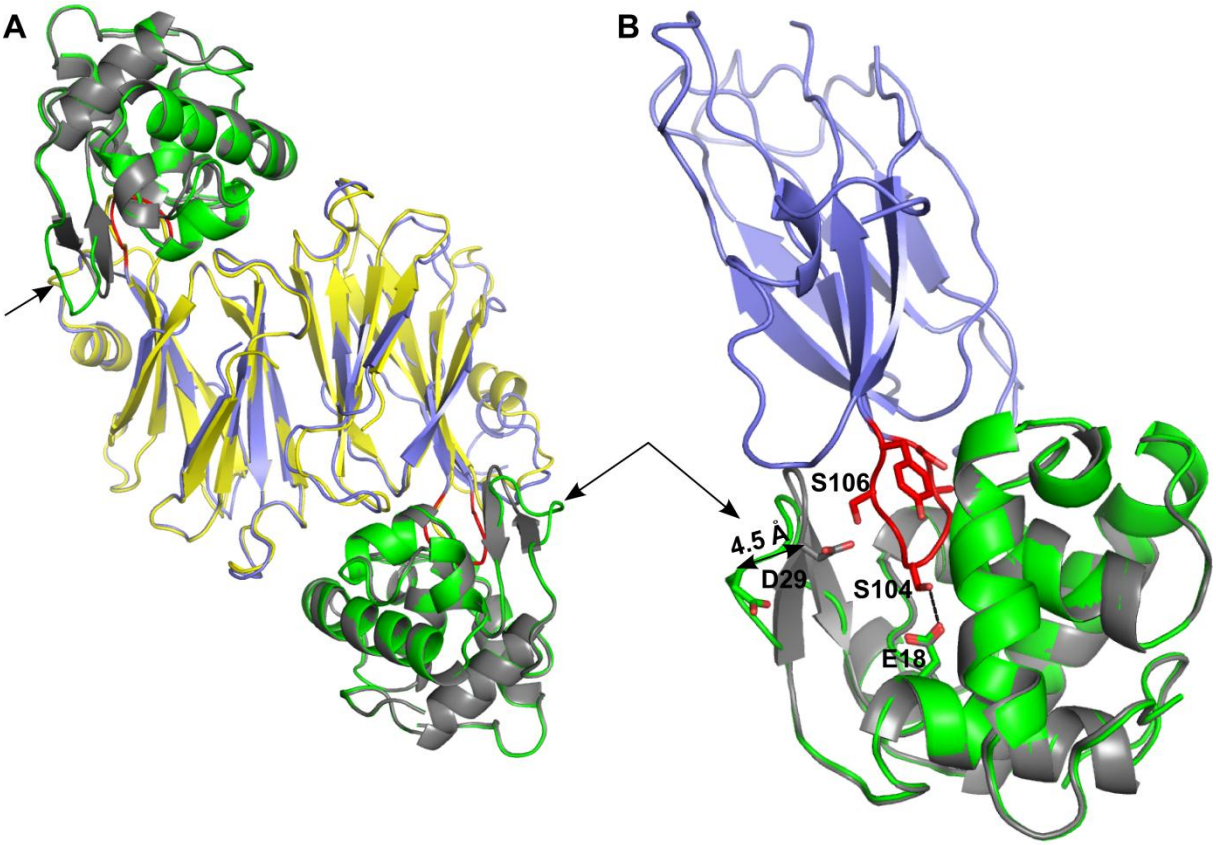

Fig S2. Conformational changes upon the complex formation. (A) Substrate-bound Ml-iLys (grey) and free PliI-Ah (yellow) were superposed on their counterparts in the inhibitory complex (green and blue with loop 6 in red, respectively). The arrows mark a local change in the Ml-iLys active site upon the inhibition by PliI-Ah. (B) A close-up on one inhibitor-lysozyme pair, rotated 90^0 with respect to panel A. The insertion of loop 6 (red) of PliI-Ah into the active site results in the outward movement of the catalytic residue Asp29 of Ml-iLys by 4.5Å (for Cα).

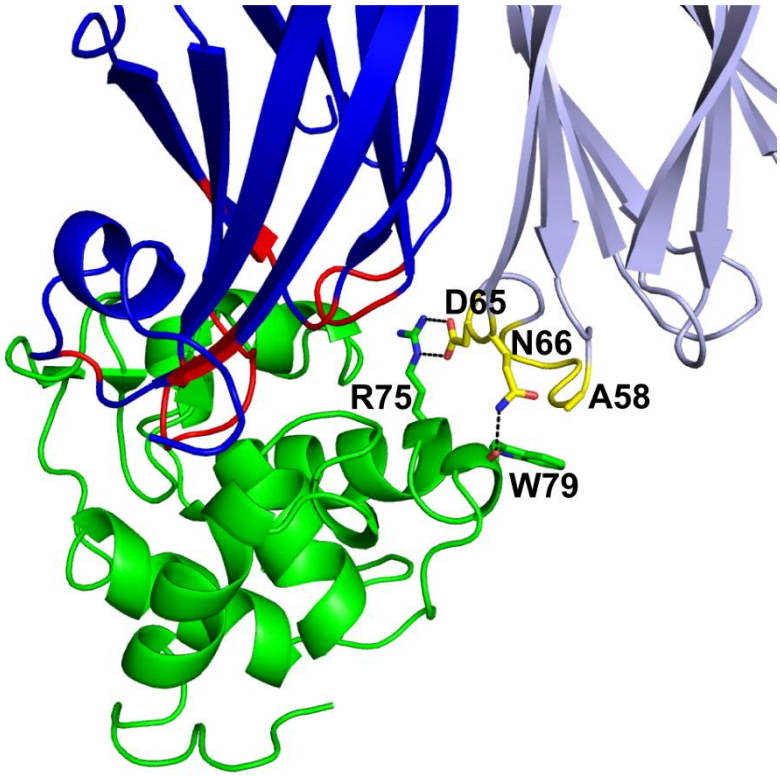

Fig. S3. Interactions at the secondary interface (yellow) between Ml-iLys (green) and the second PliI-Ah monomer (light blue). The primary interface (red) with the first PliI-Ah monomer (dark blue) is also shown.