Structure, Volume *20*

Supplemental Information

Structures of Lysenin Reveal a Shared Evolutionary Origin for Pore-Forming Proteins And Its Mode of Sphingomyelin Recognition

Luigi De Colibus, Andreas F.-P. Sonnen, Keith J. Morris, C. Alistair Siebert, Patrizia Abrusci, Jürgen Plitzko, Vesna Hodnik, Matthias Leippe, Emanuela Volpi, Gregor Anderluh, and Robert J.C. Gilbert

Inventory of Supplemental Information

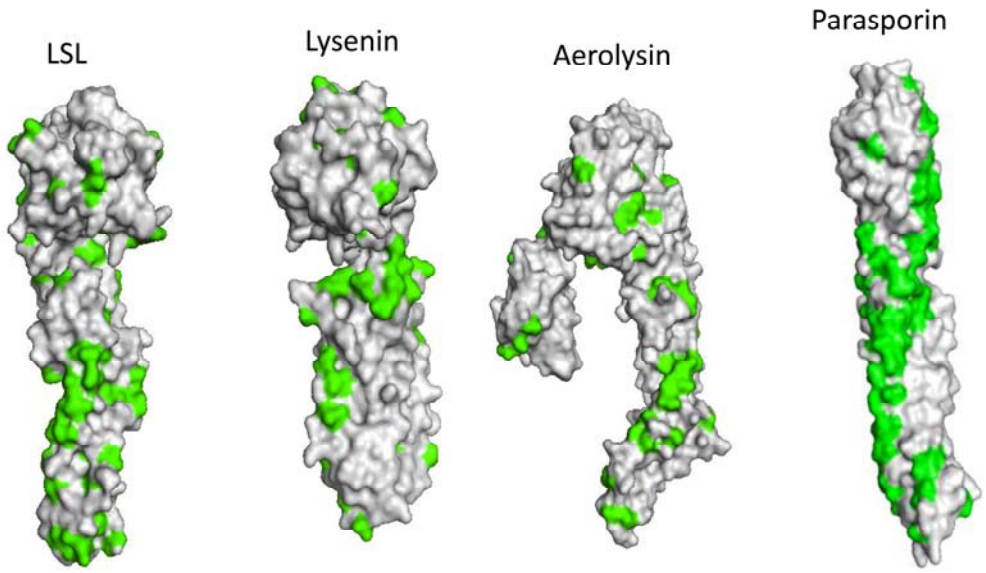

Figure S1, related to Figure 2. Surface properties of Lysenin and evolutionarily related toxins.

Surface representations to show the serine and threonine distribution (colored in green) within the structures.

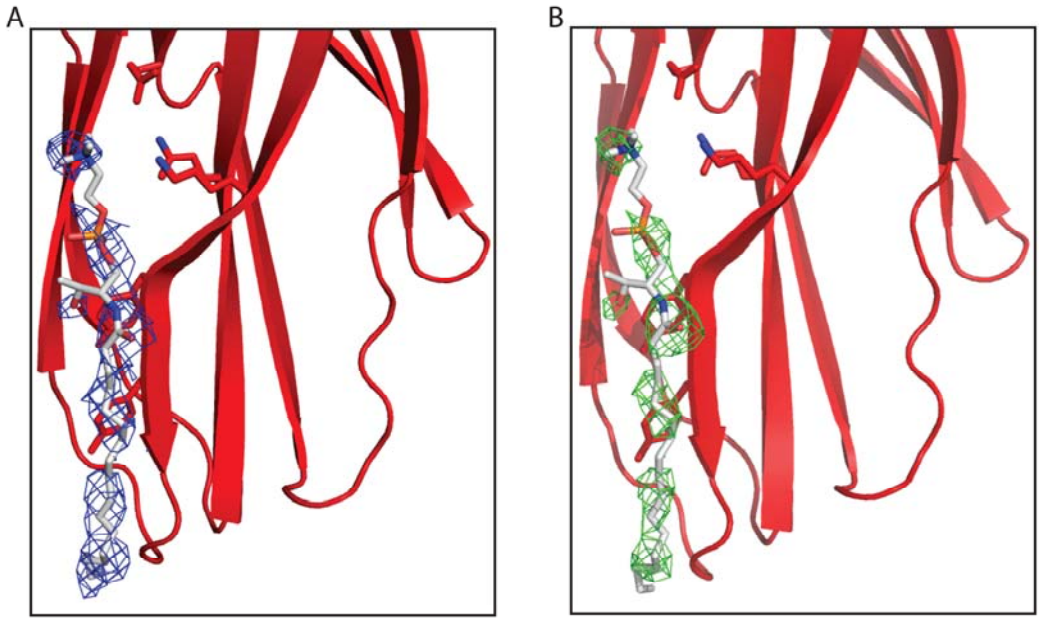

Figure S2, related to Figure 3. SM electron density map.

An omit map was calculated by removing the ligand from the model, then subjecting the model to a 2000K simulated annealing run followed by positional and B factor refinement. The resulting 2Fo-Fc (A) and Fo-Fc (B) maps are contoured respectively at 1.0 and 2.5 σ.

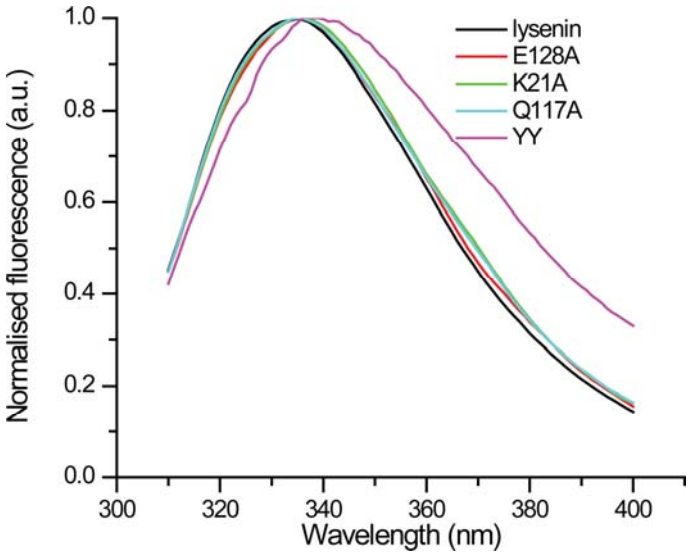

Figure S3, related to Figure 4. Fluoresce spectra of WT lysenin and its mutants.

Fluorescence emission plots of the lysenin WT, single mutants K21A, E128A, Q117A, and double mutant Y24A-Y26A.

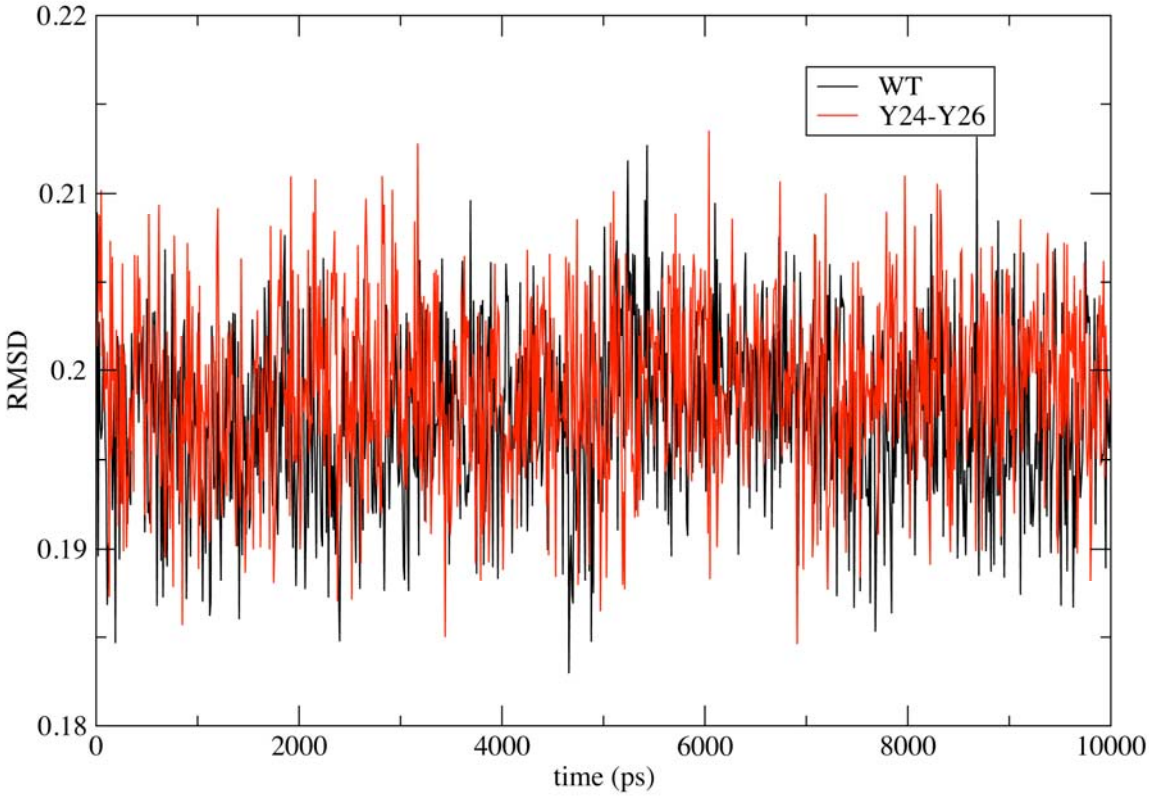

Figure S4, related to Figure 4. Molecular dynamics simulation of wild type and tyrosine double-mutant lysenin.

RMSD fluctuation of the wild type (black) and Tyr24Ala-Tyr26Ala mutant (red) lysenin over 10 ns. Both the wild type and mutant structures show the same fluctuation amplitude.

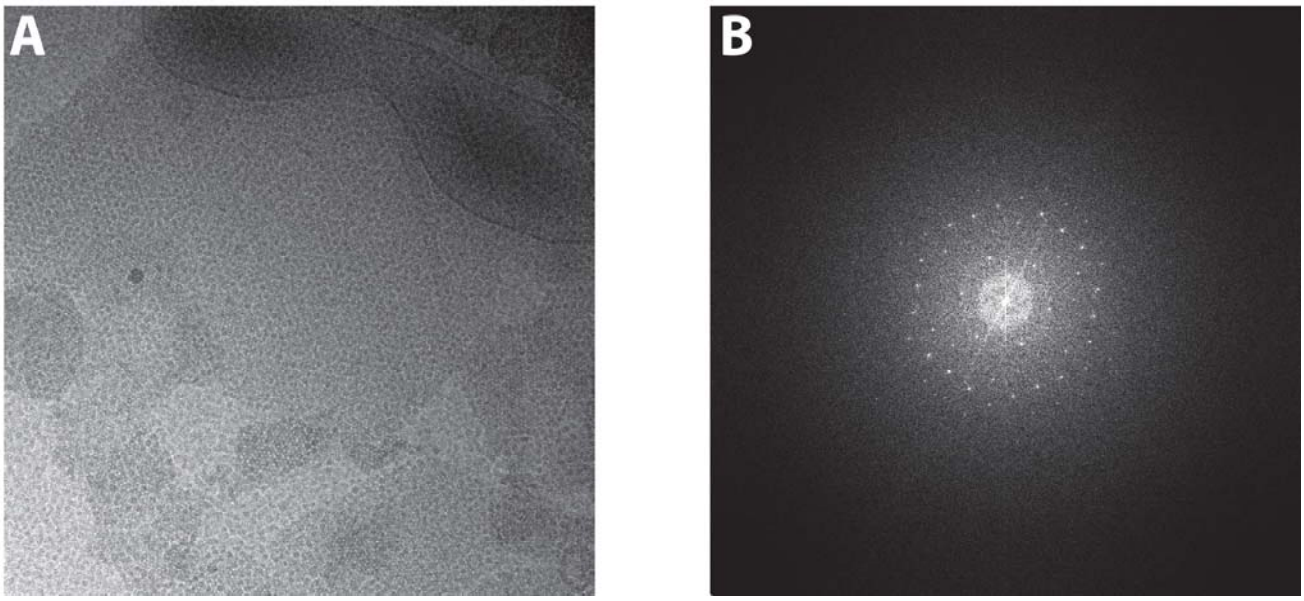

Figure S5, related to Figure 5. Two-Dimensional crystals of lysenin on liposomes

A) Lysenin 2D crystal showing the honeycomb structure.

B) Diffraction pattern for the honeycomb shown in Figure S4A.