Structure, Volume *22*

Supplemental Information

Molecular Basis of the Dynamic Structure of the TIM23 Complex in the Mitochondrial Intermembrane Space

Rakhi Bajaj, Łukasz Jaremko, Mariusz Jaremko, Stefan Becker, and Markus Zweckstetter

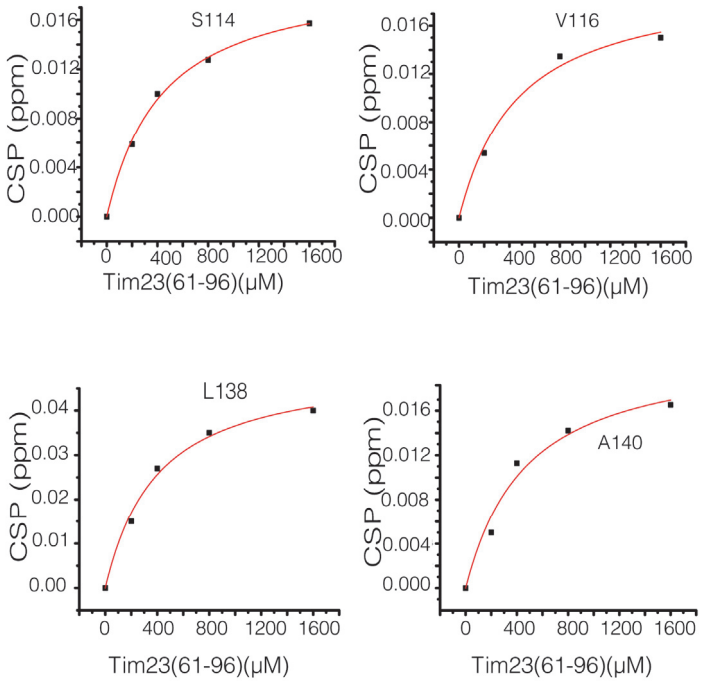

Figure S1, related to Figure 3. Residue-specific binding curves for Tim21^{IMS} residues obtained upon titration with Tim23 (61-96). The normalized average chemical shift perturbation (CSP), Δ_{HN}, was calculated as $\Delta_{HN}=\{[(\delta_N/5)^2 + (\delta_H)^2]/2\}^{1/2}$.

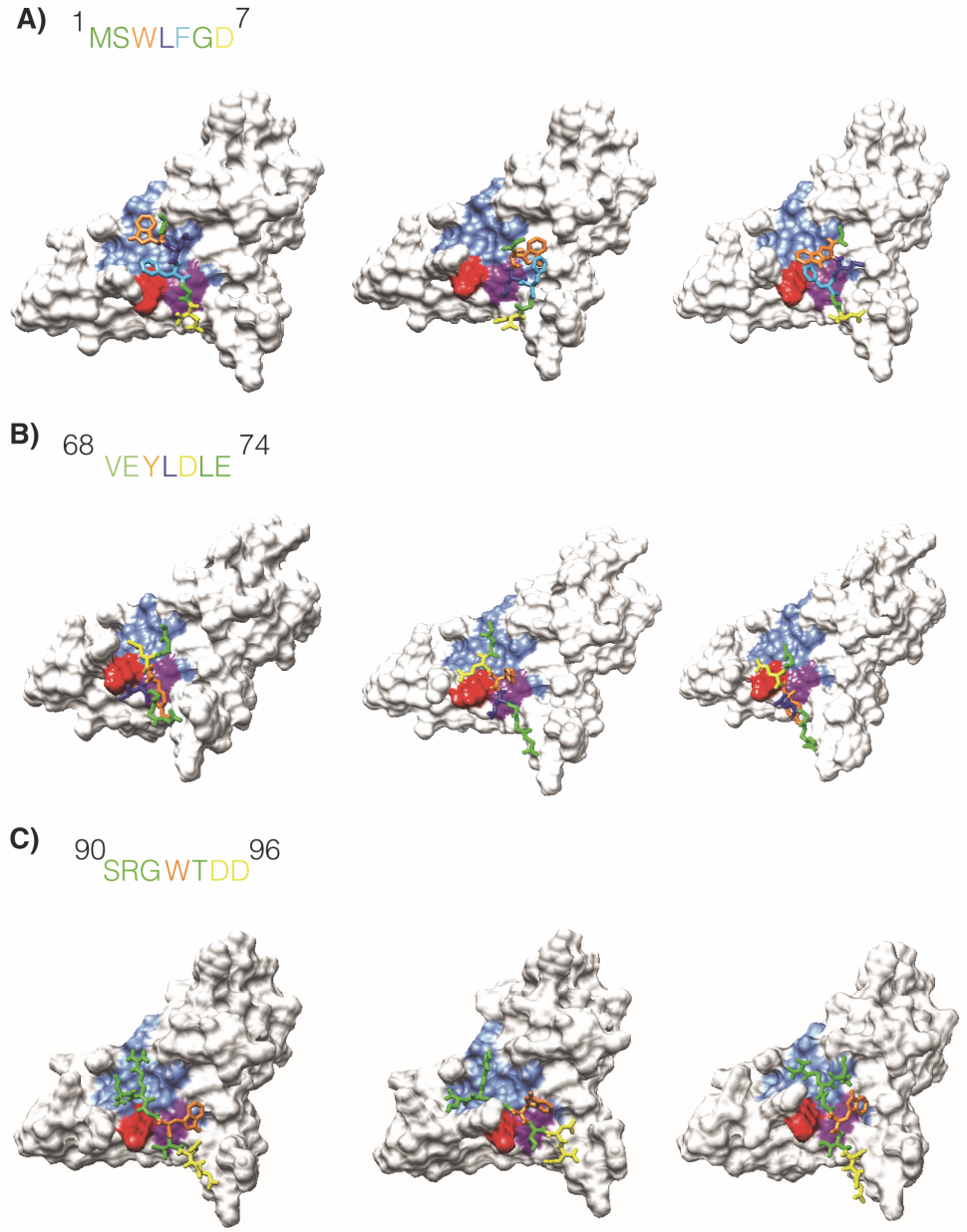

Figure S2, related to Figure 5. Additional conformers of the Tim23^{IMS}-Tim21^{IMS} complex obtained by NMR-driven flexible peptide docking. **(A)**, **(B)** and **(C)** show the lowest energy conformers of the top 2-4 clusters (the top 1 cluster is shown in Figure 4) for each of the 7-residue motifs of Tim23 in complex with Tim21^{IMS} (white surface). On top of each panel, the primary sequence of the Tim23 motif is shown. Tim23 residues in complex with Tim21^{IMS} are represented as sticks and color coded. The side chains of the key residues of Tim21, K139 and Y141, are shown in red and purple, respectively. Other Tim21 residues that showed chemical shift perturbation are marked blue.

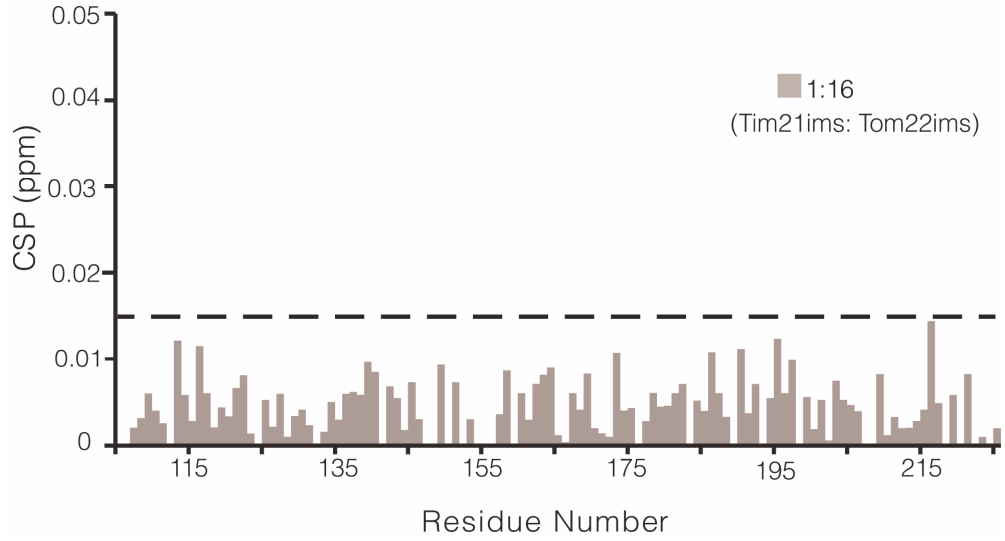

Figure S3, related to Figure 7. Chemical shift perturbation (CSP) in a 2D ^{15}N-^{1}H HSQC spectrum of Tim21^{IMS} upon addition of a 16-fold excess of Tom22^{IMS}. All changes were below the error estimate.