



STRUCTURAL
BIOLOGY

Volume 78 (2022)

Supporting information for article:

A recurring packing contact in crystals of InIB pinpoints functional binding sites in the internalin domain and the B repeat

Christina Geerds, Willem M. Bleymüller, Timo Meyer, Christiane Widmann and Hartmut H. Niemann

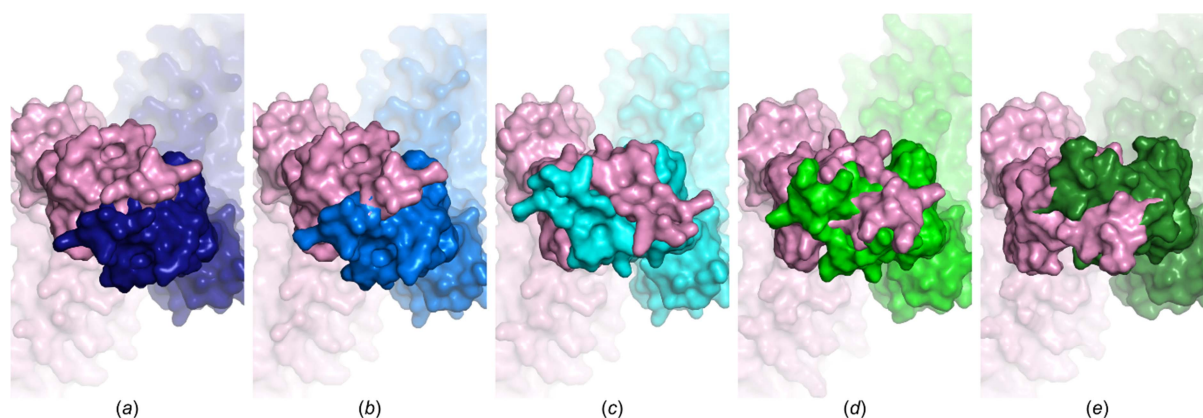


Figure S1 Clashes of two B repeats upon overlaying two InlB₃₉₂ molecules with the internalin domains in the full-length InlB dimer shown in Fig. 5. The view is from the top along the 2-fold axis of the dimer (rotated by 90° relative to the view in Fig. 5 along the horizontal axis). One chain of all InlB₃₉₂ structures was aligned with the grey monomer of full-length InlB as shown in Fig. 5. This chain is coloured as in Fig. 1, i.e. chains *A*, *B*, and *C* of InlB₃₉₂_wt are shown in dark blue, blue and cyan, respectively; crystal forms I and II of InlB₃₉₂_T332E are shown in green and dark green, respectively. A second chain of all InlB₃₉₂ structures was aligned with the pink monomer of full-length InlB as shown in Fig. 5. This second chain of InlB₃₉₂ is shown in pink in all cases. (a) InlB₃₉₂_wt, chain *A*. (b) InlB₃₉₂_wt, chain *B*. (c) InlB₃₉₂_wt, chain *C*. (d) InlB₃₉₂_T332E, crystal form I. (e) InlB₃₉₂_T332E, crystal form II.