

## Supplementary material A

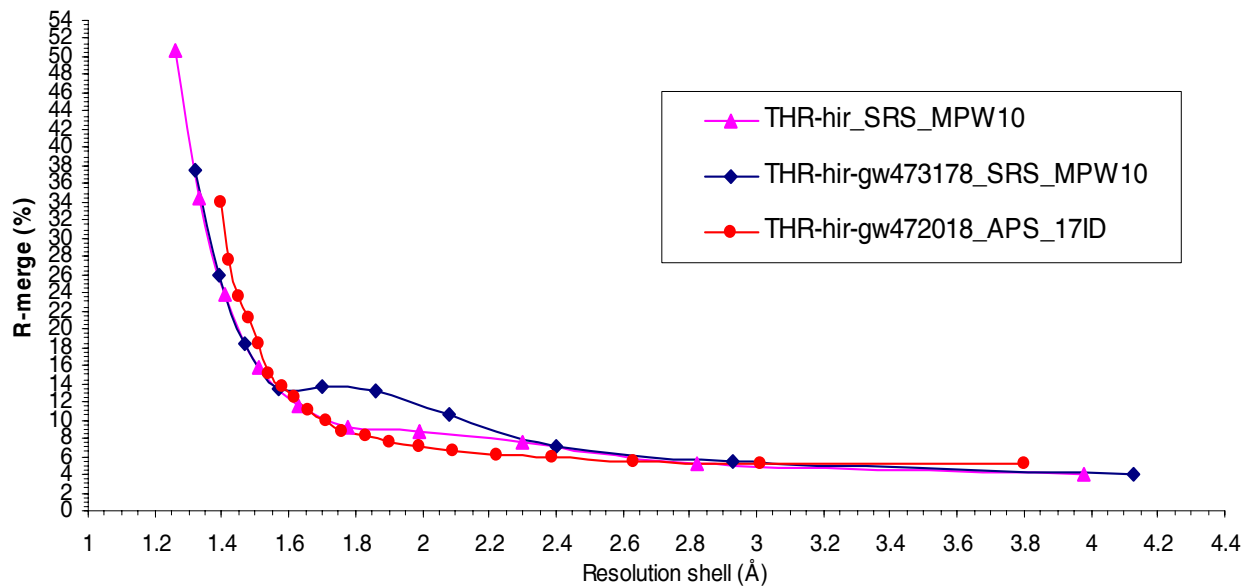


Figure 1. *R*-merge vs resolution for data sets of thrombin in a binary complex with hirugen (THR-hir) and ternary complexes with an inhibitor (gw473178 or gw472018).

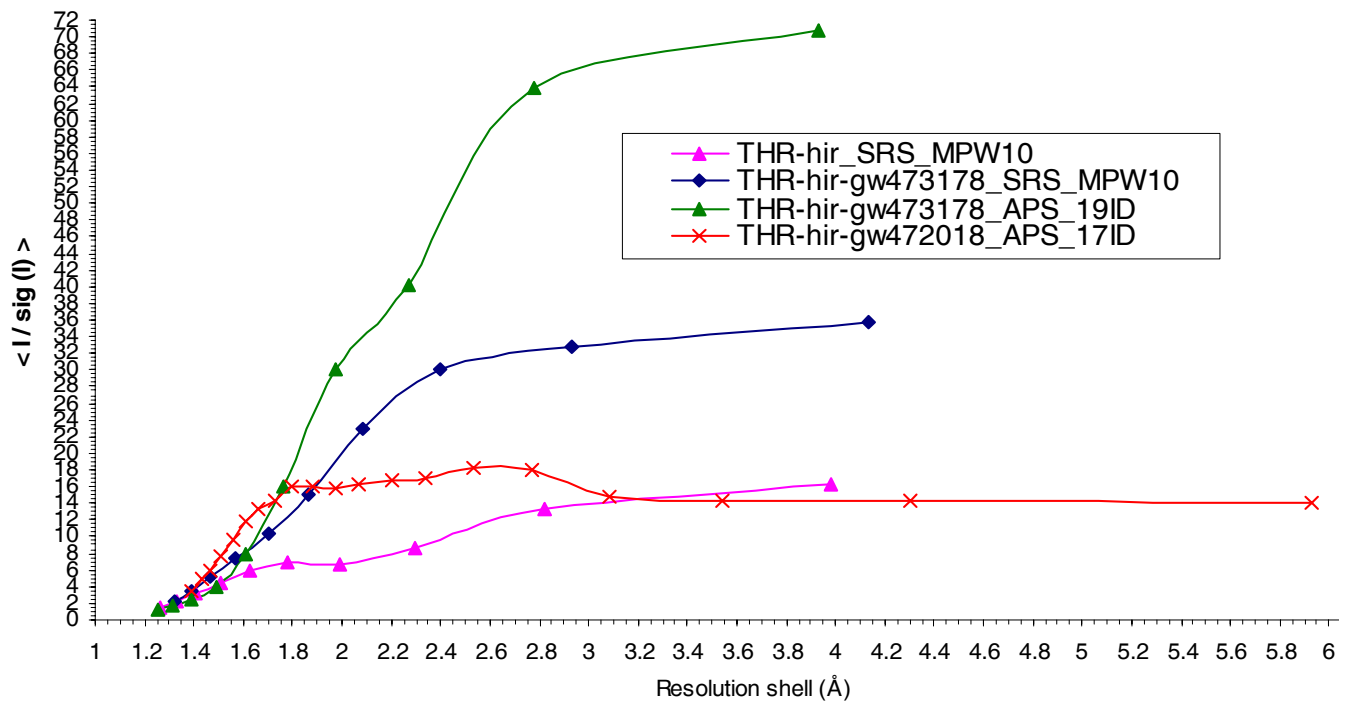


Figure 2.  $\langle I/\sigma(I) \rangle$  vs resolution for data sets of thrombin in a binary complex with hirugen (THR-hir) and ternary complexes with an inhibitor (gw473178 or gw472018).

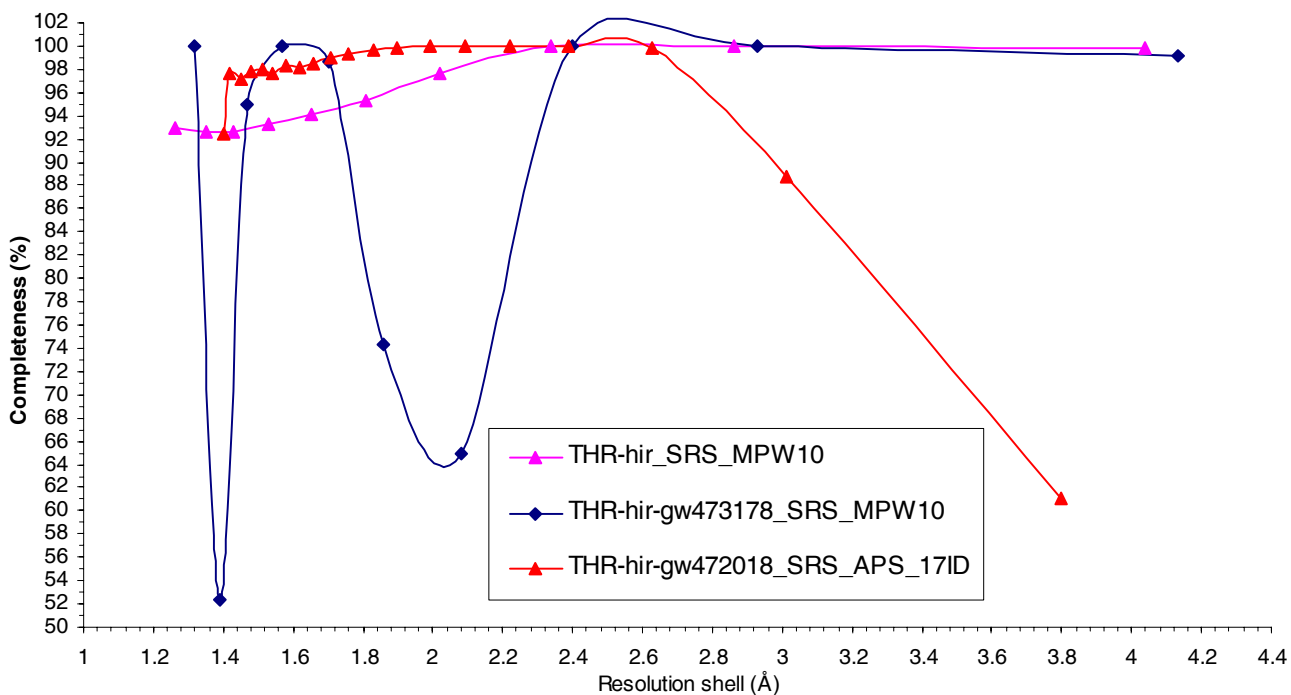


Figure 3. Completeness vs resolution for data sets of thrombin in a binary complex with hirugen (THR-hir) and ternary complexes with an inhibitor (gw473178 or gw472018). The dips in completeness for the inhibitor complex gw473178 are due to ice rings (see main text).

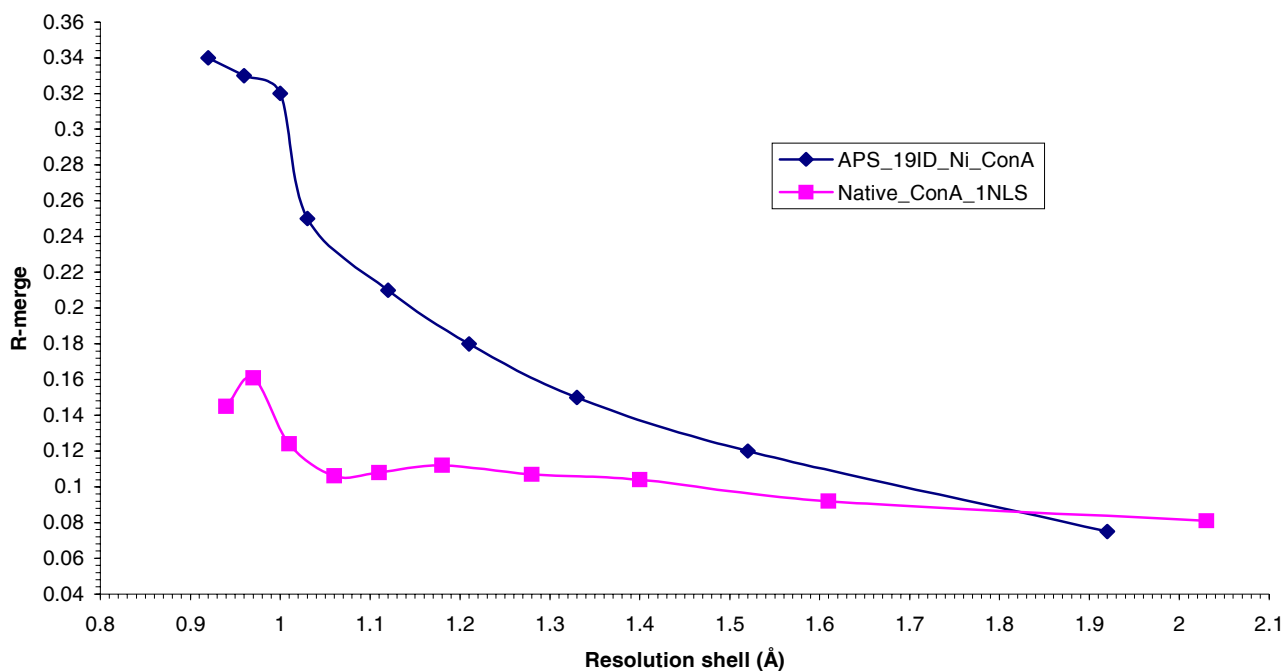


Figure 4. Rmerge versus the resolution for Ni and native (Mn,Ca) concanavalin A.

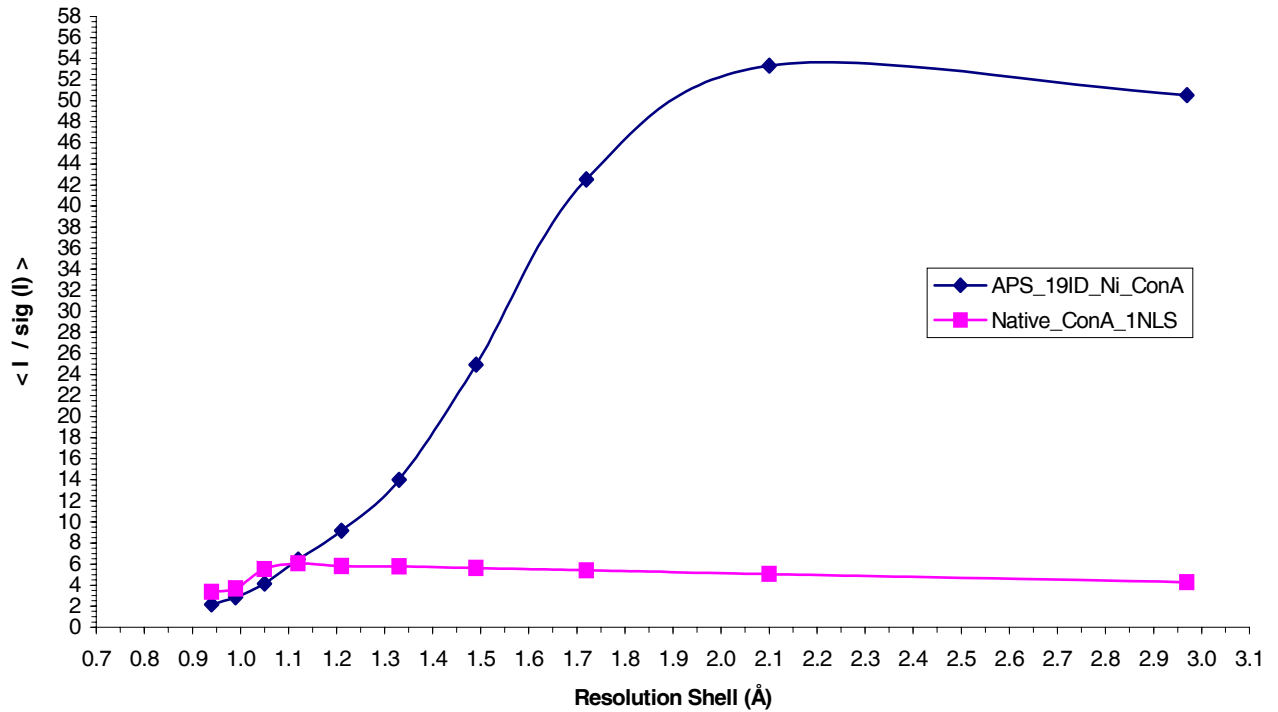


Figure 5.  $\langle I/\sigma(I) \rangle$  versus resolution for Ni and native (Mn,Ca) concanavalin A.

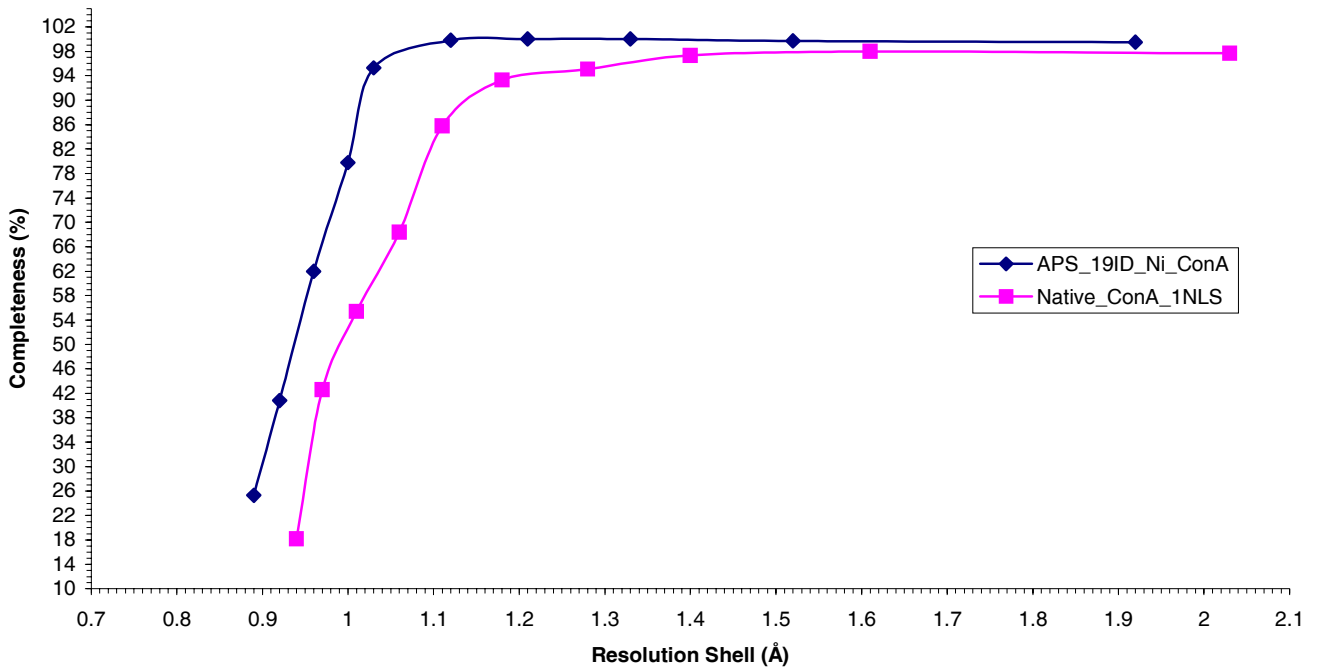


Figure 6. Completeness versus resolution for Ni and native (Mn,Ca) concanavalin A.

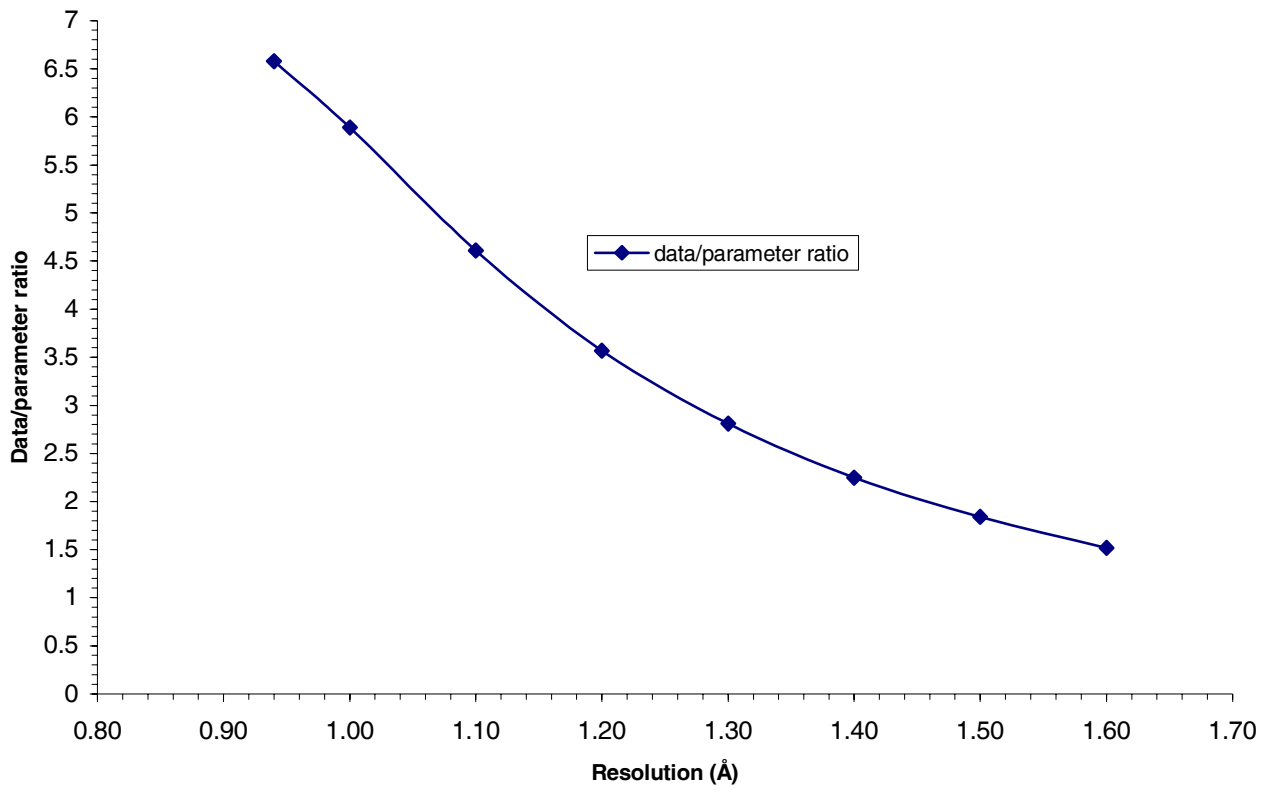


Figure 7. The data-to-parameter ratio for Ni,Ca concanavalin A.