

Volume 78 (2022)

Supporting information for article:

Putting AlphaFold models to work with phenix.process_predicted_model and ISOLDE

Robert D. Oeffner, Tristan I. Croll, Claudia Millán, Billy K. Poon, Christopher J. Schlicksup, Randy J. Read and Tom C. Terwilliger

S1. AlphaFold prediction of PDB ID: 7LW7

In section 8 we remark on some of the low confidence areas of the *AlphaFold* prediction of the UniProt id: Q9H790 corresponding to the PDB ID:7LW7. The *AlphaFold* Protein Structure Database contains structural predictions of the human proteome. In anticipation of future improvements to *AlphaFold* the structures in that database may not remain static over time. The *AlphaFold* prediction of the UniProt id: Q9H790 corresponding to PDB ID:7LW7 and the associated PAE matrix at the time of writing is therefore made available as supplementary material.

S2. AlphaFold prediction of PDB ID: 6L5L and 6j09

The *PHENIX* Colab notebook *AlphaFold* predictions of the amino acid sequence corresponding to the structures with PDB ID: 6L5L and 6j09 discussed in section 7 produces coordinate files (.pdb) and associated PAE matrix files (.jsn). All files are available as supplementary material.

S3. Additional video

The ChimeraX ISOLDE video mentioned in section 7.4 is available as supplementary material.