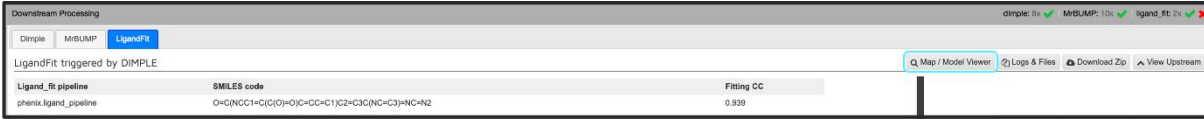


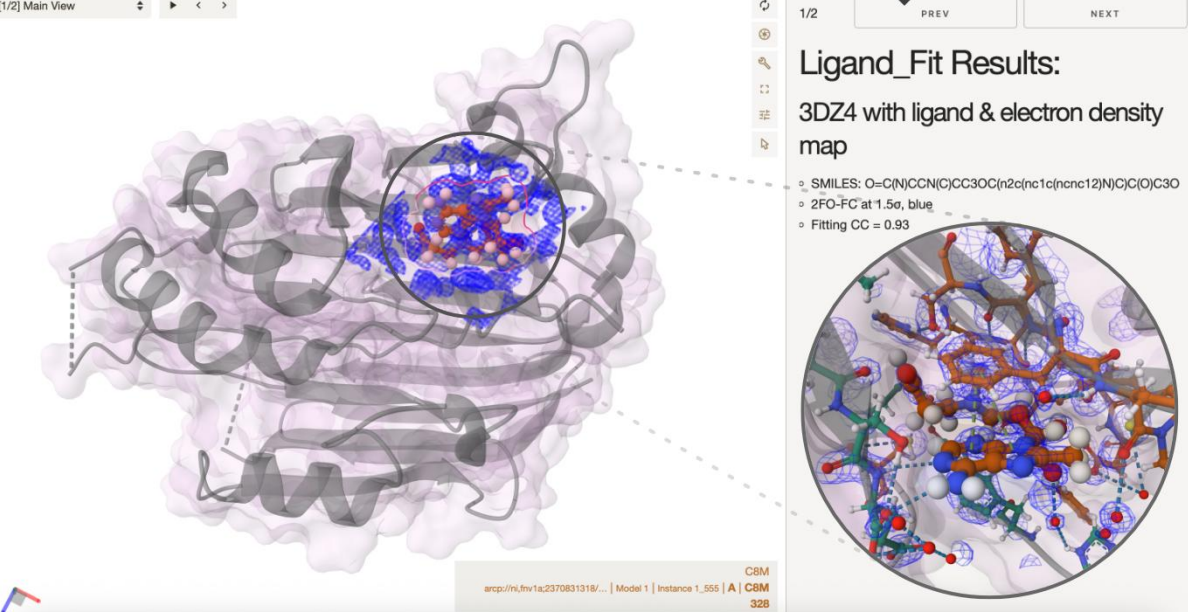
Ligand fitting pipeline

A new addition to the downstream processing pipelines at Diamond, 'ligand_fit' is now triggered following a dimple job for a given data collection, whenever a SMILES code for the ligand is entered in ISPyB. Under the hood, it is running phenix.ligand_pipeline, an automation system combining Xtrriage, Phaser, eLBOW, phenix.refine, AutoBuild, and LigandFit, capable of producing a near-finished structure of a protein-ligand complex starting from minimal inputs, and often significantly reducing the manual effort required for more difficult structures.

The pipeline works best for high occupancy ligands and is accompanied with a new Map/Model Viewer to quickly review the results from your ligand experiment. Read more about the pipeline in the phenix documentation:

(https://phenix-online.org/documentation/reference/ligand_pipeline.html)

(a) 

(b) 

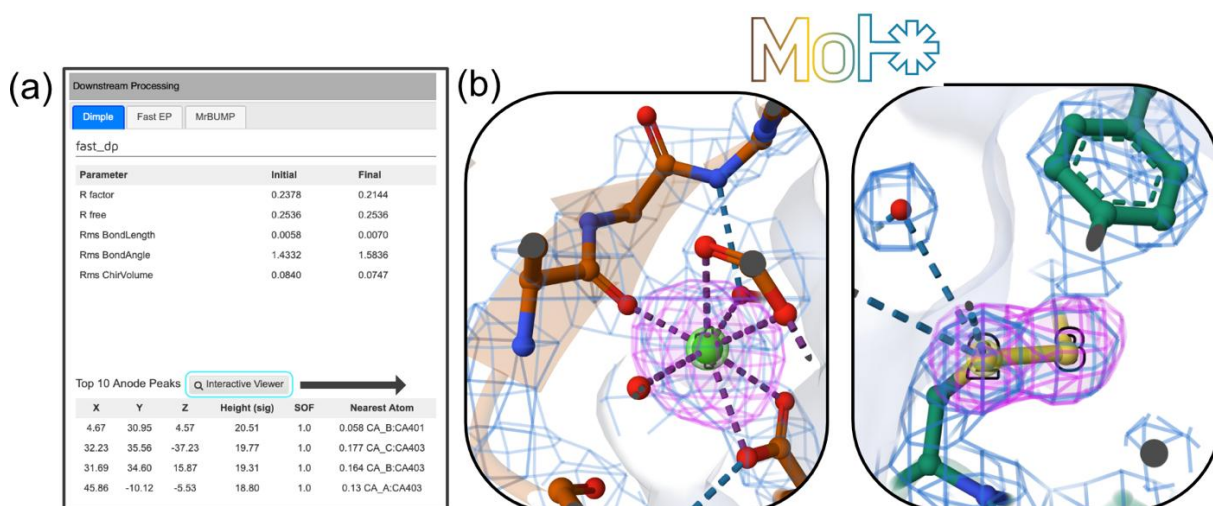
(a) Synchweb display for the ligand_fit pipeline and accompanying Map/Model Viewer button. (b) Auto-generated interactive Molstar visualisation summary of the successful ligand fitting results.

ANODE map viewer

Dimple, run as part of the downstream processing at Diamond, can also find blobs in anomalous difference maps, generated with SHELX/ANODE. ANODE detects the locations of anomalous scatterers such as heavy atoms, halides and metals.

An 'Interactive Viewer' button and panel has been added under the Dimple tab of the downstream processing section in Synchweb, showing information regarding the strongest peaks found in the generated ANODE map.

The interactive viewer displays the locations of the strongest peaks in the anomalous difference map (applying a cutoff of 4σ), ordered by peak height for quick review. By navigating with the 'Next, Previous' buttons inside the viewer, individual peak locations can be inspected more closely, along with the non-covalent interactions and the 2Fo-Fc map around the region of interest. You can also download a copy of the html ('anode.html') in the 'Logs & Files' to share your results.



(a) Updated Dimple information panel in Synchweb showing the top 10 peaks in the ANODE map and a button to launch an interactive Molstar viewer. (b) Example snapshots taken from inside the interactive viewer, displaying non-covalent interactions in a calcium binding site of Thermolysin (left panel) and a disulphide bond in Thaumatin (right panel). Anomalous difference map contoured at 3σ (magenta), 2Fo-Fc map 1.5σ (blue).

References

- https://phenix-online.org/documentation/reference/ligand_pipeline.html
- Thorn, A. & Sheldrick, G. M. ANODE: anomalous and heavy-atom density calculation (2011). *J. Appl. Cryst.* 44, 1285-1287.
- Midlik, A et al. MolViewSpec: a Mol* extension for describing and sharing molecular visualizations, *NAR* (2025), [gkaf370](https://doi.org/10.1093/nar/gkaf370), <https://doi.org/10.1093/nar/gkaf370>

4. El Omari K, Forsyth I, Duman R, Orr CM, Mykhaylyk V, Mancini EJ, Wagner A. Utilizing anomalous signals for element identification in macromolecular crystallography. *Acta Crystallogr D Struct Biol.* 2024 Oct 1;80(Pt 10):713-721. doi: 10.1107/S2059798324008659. Epub 2024 Sep 18.