

Lysozyme iodide soak SAD phasing

Files

Dataset: `iod.mtz`

Heavy atom sites: `iod_sites.pdb`

Wavelength: 1.5418 Å (Cu K α)

Composition: `hewl.seq`, 1 copy/asu

Correct structure: `hewl.pdb`

Protocol

1. Run *Phaser* in SAD mode.
2. Input iodide sites.
3. Try both heavy atom hands.
4. Use iodide for LLG map completion atom type.
5. Check the figures of merit and likelihood values for both hands. Run density modification to find out, which hand is correct.
6. Repeat the *Phaser* run (trying both heavy atom hands), but in addition to iodide, also add sulfur for LLG map completion.
7. Compare results with those from density modification.
8. Compare the sulfur sites found with the correct structure.

Lysozyme MR-assisted SAD

Files

Dataset: `lyso2001.mtz`

MR solution: `partial_model.pdb`

Wavelength: 1.5418 Å (Cu K α)

Composition: `hewl.seq`, 1 copy/asu

Correct structure: `hewl.pdb`

Protocol

1. Run *Phaser* in MR-SAD mode.
2. Input the MR solution. Leave the heavy atom sites empty.
3. Use sulfur for LLG map completion atom type.
4. Compare sulfur sites found with the molecular replacement solution and the correct structure.