coord_transform_to_star example

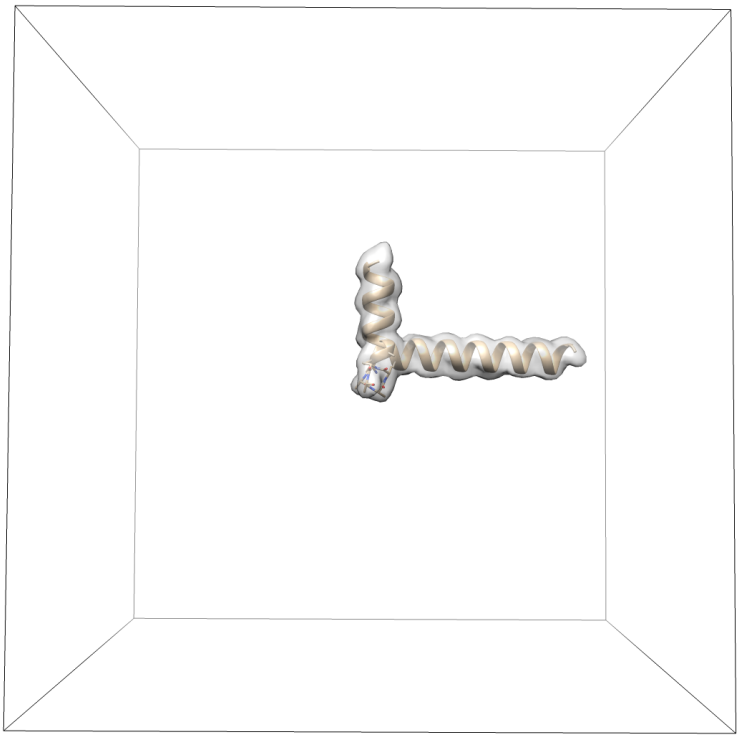
Simulated test data set of three helices of different length oriented along X (long), Y (medium), and Z (short) with the origin (0, 0, 0) at the box center.

Model: original_helix_model.pdb
Projections: original_helix_projections.mrcs (box size: 100x100)
Alignment parameters: original_helix_metadata.star

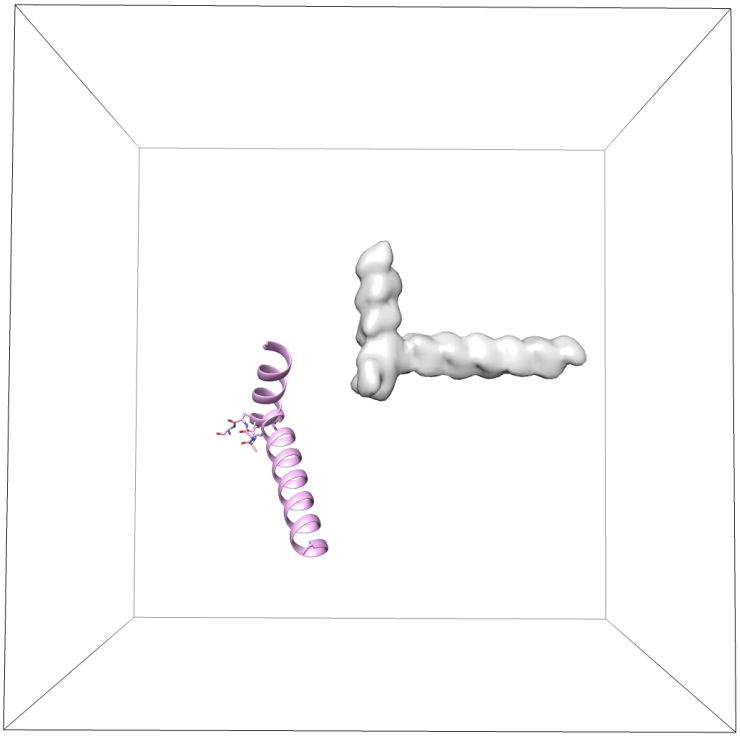
Reconstruct map with

```
relion_reconstruct --i original_helix_metadata.star --o original_helix_reconstructed.mrc --maxres 3.5
```

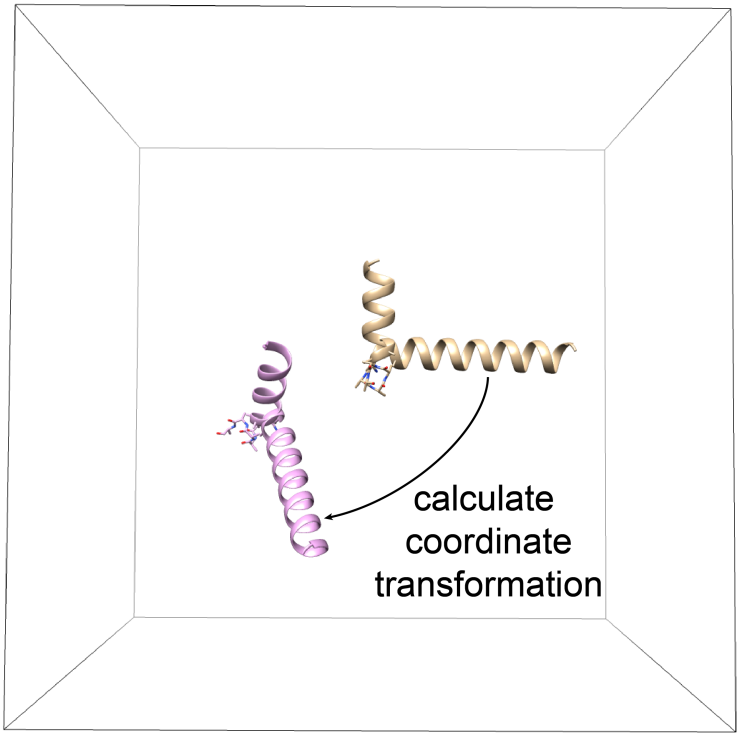
Reconstructed map: original_helix_reconstructed.mrc



Transform model: transformed_helix_model.pdb



Calculate transformation from **original_helix_model.pdb** to **transformed_helix_model.pdb**.

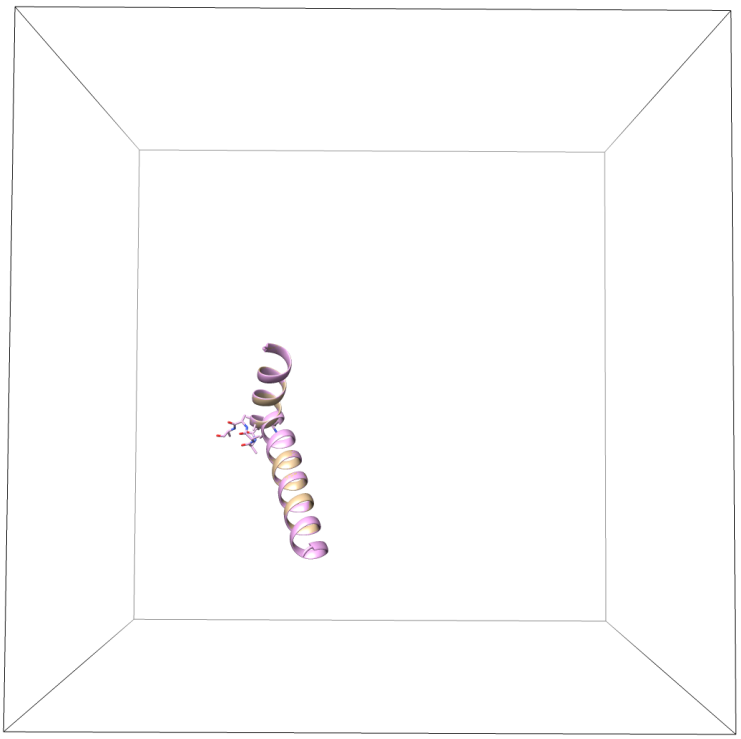


This can be done with any coordinate transformation program such as superpose (ccp4), lsqkab (ccp4), coot (SSM Superpose or LSQ superpose), or any other software that reports coordinate transformations in euler angles and an orthogonal translation in angstrom:

obtain coordinate transformation

```
superpose original_helix_model.pdb transformed_helix_model.pdb
```

Euler angles (alpha,beta,gamma): 176.372 70.352 140.038
Orthogonal translation (Angst): 54.298 32.235 -46.057



Apply transformation to particle alignment parameters. Notice that coordinate transformations are applied by rotating around the coordinate origin (0,0,0 = edge of the box) first, followed by a translation, while EM transformations align first to the box center and then rotate. Thus calculating new alignment parameters for each particle requires knowledge of the box center.

apply transformation to alignment parameters

```
./coord_transform_to_star -i original_helix_metadata.star -e 176.372 70.352 140.038 -t 54.298 32.235 -46.057 -o
transformed_helix_metadata.star -apix 1.0 -box_center 50
```

Transformed alignment parameters: transformed_helix_metadata.star

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Reconstruct map from transformed particles

```
relion_reconstruct --i transformed_helix_metadata.star --o transformed_helix_reconstructed.mrc --maxres 3.5
```

Transformed reconstructed map: transformed_helix_reconstructed.mrc