

M2BP (1by2) and Hepsin (1p57 – Chain A)

From practical session 2
Structural Bioinformatics
Msc Bioinformatics
Birkbeck College

Version still not fully tested and working. Only calculates 20 positions per second.

Alignment Report:

Value calculated = Optimised report

Initial Value=228127

Optimising for 1:1:1:1

Tripod 1=A=(21.492,12.511,2.01) B=(18.043,38.829,25.066) C=(31.099,20.559,15.54)

Tripod 2=A=(-29.537,-1.125,17.562) B=(10.417,12.67,-1.893) C=(-23.269,12.988,-8.071)

Transformation 1=

Translate: (-21.492,-12.511,-2.01)

Rotate XY:97.4661

Rotate YZ:90

Rotate XZ:-6.27744e+66

Transformation 2=

Translate: (29.537,1.125,-17.562)

Rotate XY:19.0484

Rotate YZ:234.661

Rotate XZ:-6.27744e+66

RMSD Value = 20751.8

Best RMSD Chosen as :

Optimising for 5:1:7:1

Tripod 1=A=(18.267,13.326,3.867) B=(18.043,38.829,25.066) C=(31.099,20.559,15.54)

Tripod 2=A=(-28.242,-2.366,12.448) B=(10.417,12.67,-1.893) C=(-23.269,12.988,-8.071)

Transformation 1=

Translate: (-18.267,-13.326,-3.867)

Rotate XY:90.5032

Rotate YZ:90

Rotate XZ:-6.27744e+66

Transformation 2=

Translate: (28.242,2.366,-12.448)

Rotate XY:21.253

Rotate YZ:223.645

Rotate XZ:-6.27744e+66

RMSD Value = 17248.5

Optimised report: RMSD Value=17248.5

Chimera Pictures

