

Strong translational NCS leads to space group ambiguity or how close inspection of data can rescue structures. Two examples from SSGCID

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Two data sets collected for the Seattle Structural Genomics Center for Infectious Disease (SSGCID) showed very clean statistics without any clear indications for data set pathologies.

For target ElanA.00692.a.B1 a hexamer was expected in the asymmetric unit. All six copies could only be found by using a locked rotation function. Despite convincing Molecular Replacement scores the refinement of the resulting model did not converge. An alternative processing in tP instead of tI yielded a data set with similar quality. Two hexamers could now be found, and the structure refined well. Translational NCS yielding a native Patterson peak of 40% of the origin peak is the likely culprit for the space group ambiguity.

For target ElmeA.00825.a.B1 two monomers were expected in the asymmetric unit. Despite very convincing Molecular Replacement scores the resulting model did not refine. Close inspection of the data led to an alternatively processed data set with a duplication of the length of the C-axis. Four molecules could now be found, and the structure refined well. Translational NCS yielding a native Patterson peak of 60% of the origin peak is the likely culprit for the space group ambiguity.