

MAPPING THE PROTEIN WORLD: OVER 1500 BIOMOLECULAR STRUCTURES SOLVED ON-LINE AT EMBL-HAMBURG

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Macromolecular structure determination is an important task in biology because of the intimate relation between the structure and function of biological molecules. This requires good quality X-ray diffraction data and is itself a complex and a multi-step computational process. Several structure-determination software pipelines have been assembled worldwide with different goals and degrees of

built-in automation. However, the best validation of an X-ray diffraction experiment is the arrival at an interpretable density map and a partial structure in a short period of time, ideally during or just after the data collection. Such on-line data evaluation pipeline, Auto-Rickshaw, has been developed at EMBL-Hamburg and has helped to determine over 1500 novel protein structures.