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Electrostatic energy of transfer and macrobond analyses of intermolecular interactions and hydration effects in protein crystals in a low ionic environment

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ABSTRACT

We developed an electrostatic energy of transfer (EET) analysis applicable to periodic boundary condition, including a nonrectangular unit cell. It was applied to monoclinic ribonuclease A crystallized with ethanol as a precipitant. Macrobond analysis was also carried out. Owing to the low ionic strength of the solvent region, atomic EET values were non-negligible even at long-distance points. Most of the molecular EET values—defined as the individual contribution of each surrounding molecule—were positive. The inclusion of the molecular EET values of hydration water molecules reduced the repulsive force, and the evaluation of hydration effects in protein crystals was found to be imperative.

Keywords

A1. Electrostatic energy; A1. Hydration water; A2. Growth from solution; B1. Biological macromolecules

1. Introduction

Understanding the crystallization of proteins is a key aspect of elucidating protein function because crystallographic analysis is the most effective tool with which to obtain details about the three-dimensional structure of proteins. Until now, however, crystallization processes have remained unclear despite experimental [1] and theoretical [2–5] efforts.

We have been conducting experimental and theoretical investigations of the crystal growth of proteins to understand crystallization processes in the context of intermolecular interactions and the correlation between