Abstract Submitted for the MAR13 Meeting of The American Physical Society

Investigating the nature of folded protein structure with the aid of crystalline and amorphous models¹ DENIZ TURGUT, OSMAN OKAN, ANGEL GARCIA, RAHMI OZISIK, Rensselaer Polytechnic Institute — Threedimensional structure of a protein is closely tied with its function. Understanding the folded shape of a protein provides crucial information both in identifying the function and engineering custom proteins that will perform desired functions. In the current work, based on the symmetries present in the local neighborhood of residues in the folded protein structure, we investigated the possibility of creating protein-like structures from crystalline and amorphous models. Parameters like Radial Distribution Function and Bond Orientational Order Parameter [Steinhardt PJ, Nelson DR, Ronchetti M, Phys Rev B 1983, 28, 784] were used to identify the similarities between the created model structures and over 400 folded protein structures. The results show both similarities and differences between folded protein structures and those obtained from crystalline or amorphous models.

¹This work was partially supported by NSF DUE-1003574.

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Date submitted: 09 Nov 2012

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