Including crystallographic symmetry in quantum-based refinement: *Q*|*R*#2

Autorzy

Min Zheng

Małgorzata Biczysko

Yanting Xu

Nigel W. Moriarty

Holger Kruse

Alexandre Urzhumtsev

Mark P. Waller

Pavel V. Afonine

Rok wydania

2020

Czasopismo

Acta Crystallographica Section D: Structural Biology

Numer woluminu

76

Strony

41-50

DOI

10.1107/s2059798319015122

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Three-dimensional structure models refined using low-resolution data from crystallographic or electron cryo-microscopy experiments can benefit from high-quality restraints derived from quantum-chemical methods. However, nonperiodic atom-centered quantum-chemistry codes do not inherently account for nearest-neighbor interactions of crystallographic symmetry-related copies in a satisfactory way. Here, these nearest-neighbor effects have been included in the model by expanding to a super-cell and then truncating the super-cell to only include residues from neighboring cells that are interacting with the asymmetric unit. In this way, the fragmentation approach can adequately and efficiently include nearest-neighbor effects. It has previously been shown that a moderately sized X-ray structure can be treated using quantum methods if a fragmentation approach is applied. In this study, a target protein (PDB entry 4gif) was partitioned into a number of large fragments. The use of large fragments (typically hundreds of atoms) is tractable when a GPU-based package such as TeraChem is employed or cheaper (semi-empirical) methods are used. The QM calculations were run at the HF-D3/6-31G level. The models refined using a recently developed semi-empirical method (GFN2-xTB) were compared and contrasted. To validate the refinement procedure for a non-P1 structure, a standard set of crystallographic metrics were used. The robustness of the implementation is shown by refining 13 additional protein models across multiple space groups and a summary of the refinement metrics is presented.

Słowa kluczowe

quantum refinement, symmetry, fragmentation, graph-based clustering, crystalography, cryo-EM, Hartree-Fock theory

Adres publiczny

http://dx.doi.org/10.1107/s2059798319015122