

## Optimal clustering for quantum refinement of biomolecular structures: Q|R#4

### Autorzy

Yaru Wang

Holger Kruse

Nigel W. Moriarty

Mark P. Waller

Pavel V. Afonine

Małgorzata Biczysko

### Rok wydania

2023

### Czasopismo

Theoretical Chemistry  
Accounts

### Numer woluminu

142

### Strony

100/1-100/15

### DOI

10.1007/s00214-023-03046-0

### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

Quantum refinement (Q|R) of crystallographic or cryo-EM-derived structures of biomolecules within the Q|R project aims at using ab initio computations instead of library-based chemical restraints. An atomic model refinement requires the calculation of the gradient of the objective function. While it is not a computational bottleneck in classic refinement it is a roadblock if the objective function requires ab initio calculations. A solution to this problem adopted in Q|R is to divide the molecular system into manageable parts and do computations for these parts rather than using the whole macromolecule. This work focuses on the validation and optimization of the automatic divide-and-conquer procedure developed within the Q|R project. Also, we propose an atomic gradient error score that can be easily examined with common molecular visualization programs. While the tool is designed to work within the Q|R setting the error score can be adapted to similar fragmentation methods. The gradient testing tool presented here allows a priori determination of the computationally efficient strategy given available resources for the potentially time-expensive refinement process. The procedure is illustrated using a peptide and small protein models considering different quantum mechanical (QM) methodologies from Hartree–Fock, including basis set and dispersion corrections, to the modern semi-empirical method from the GFN-xTB family. The results obtained provide some general recommendations for the reliable and effective quantum refinement of larger peptides and proteins.

### Słowa kluczowe

Quantum refinement, Divide-and-conquer, HF, XTB

### Adres publiczny

<http://dx.doi.org/10.1007/s00214-023-03046-0>

<http://link.springer.com>

Plik został wygenerowany dnia 2026-05-05 04:52:38

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/ukD4e12>.