From: Axel Brunger
To: CCP4BB@JISCMAIL.AC.UK
Subject: Re: [ccp4bb] FW: [ccp4bb] Resolution and distance accuracies
Date: Thursday, December 23, 2010 6:20:35 PM

Dear Gerard,

Actually, for some of the tests we turned off the DEN network restraints for the last two refinement macrocycles, so, at least for these particular cases, the DEN method truly found a better minimum rather than forcing the system to the higher resolution structure.

Cheers,
Axel

On Dec 23, 2010, at 3:04 PM, Gerard Bricogne wrote:

> Dear Bernhard,
>
> I must say that I find the "super-resolution" claims in this paper a bit of a conjuring trick. If the final refined model has greater accuracy than one would expect from the resolution of the data it has been refined against, it is because that extra accuracy has been lifted from the higher resolution data that were used to refine the structure on the basis of which
> the elastic network restraints were created.
>
> Should we then say that we achieve super-resolution whenever we refine
> a macromolecular structure using Engh & Huber restraints, because these enable us to achieve distance accuracies comparable with those in the small
> molecules structures in the Cambridge Structural Database?
>
> Perhaps I have missed an essential point of this paper.
>
> With best wishes,
>
> Gerard.
>
> --
> On Thu, Dec 23, 2010 at 12:25:26PM -0800, Bernhard Rupp (Hofkristallrat a.D.) wrote:
>
>> Oops I am outdated: Axel just emailed me that he describes an improved
>>
>> coordinate estimate beyond the Rayleigh criterion in his recent paper

Schroder GF, Levitt M, & Brunger AT (2010) Super-resolution biomolecular

crystallography with low-resolution data. Nature 464(7292), 1218-1222.

For the deformable elastic network (DEN) refinement, see his ref 14

Schroder GF, Brunger AT, & Levitt M (2007) Combining efficient

conformational sampling with a deformable elastic network model facilitates

structure refinement at low resolution. Structure 15(12), 1630-1641.

BR

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