Qeios

Peer Review

Review of: "Over Half a Century of Burial of ρ, θ and ϕ in PDB"

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I am new to Queios and not really sure what I should do. Normally, when a new journal pops up in my mailbox, my SPAM filter takes care of things. This time, not. Queios is advertised as something new. I decided to give it a chance. But if their information about the concepts, etc., doesn't improve quickly, this will not only be my first but also my last refereeing for them. I understand that I am not so much supposed to ask the question of whether this article is worth publishing, but I must make suggestions on how to improve it. I will try.

The authors define another set of coordinates to describe where atoms are found in space. My first thought is that it doesn't matter how you describe the location of atoms, because in the end, they are where they are. Using 'another coordinate system' will at best make certain calculations easier or more transparent. However, people like me have learned for 50 years how to think along the lines of x, y, and z, so it will be hard to come up with a system that makes things more transparent to me by using three other coordinates than x, y, and z.

The bottom line of this article is the alternative coordinate system. But, no matter how hard I look, I do not see a good explanation of the system. Yes, there are the formulas, but then I cannot find (or I don't understand) what the parameters mean. One of the parameters is rho1, defined as the equilibrium interatomic bond length. But, if bond lengths are a function of what old-fashioned people like me would call a force field parameter, then we are not describing coordinates in another coordinate system, but adjusting them to the force

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field. Genuine differences between shorter and longer bonds would certainly get lost in translation.

Figure 1 seems set up to suggest that the ABN-SCS method was the first and is the best at doing something. But Figure 1 provides no relevant information. I would suggest that the authors take a good look at Ruben Abagyan's (and I am not him, I just happen to know about his work as I heard a seminar on it in 1992, give or take a year) ICM software. ICM does, for example, MD simulations in a non-Cartesian system that shows some resemblance (or perhaps is nearly the same as) ABN-SCS.

I frequently read sentences that feel like things get blown up very much. E.g., a sentence like (I cut and paste):
"Here in this manuscript, the ABN-SCS framework is defined as a chemically grounded geometric framework for the representation of protein structures by integrating covalent atomic bonding information with spherical coordinates. Its core principles and methodology are outlined as follows:" seems totally unnecessary. And there are many like this. If the method is good, then people will appreciate it if they understand it.

Spending one page on the explanation of how five amino acids become one pentapeptide seems a bit unnecessary.

If the x, y, z coordinates of the PDB can be mathematically converted into ABN-SCS coordinates, then I suggest the authors deposit the script somewhere and do not embark on making a PDB in the new system. (Why, look at: Babbitt PC, Bagos PG, Bairoch A, Bateman A, Chatonnet A, Chen MJ et al. (2015). Creating a specialist protein resource network: a meeting report for the protein bioinformatics and community resources retreat. Database 2015).

The many references to AI (especially to AF2; we are today at AF3, by the way) seem a bit hollow as nowhere do I find a single example.

Again, I do not know what Queios wants me to do. If this was an article for 'Bioinformatics' or 'Structure', I would reject it. But it feels that I have to make suggestions to make things better. Well, I have two suggestions:

1) Explain how the coordinate system works in a way that I can understand it

2) Don't blow up the text with big bombastic sentences; if the method is good, the article will be good, no matter how it was/is written.

Yours

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Declarations

Potential competing interests: No potential competing interests to declare.

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