Q&A Report September 9, 2021

Q What is so special about Ile/Val residues that they get their own Ramachandran plot?

A Physically, it's because they're branched at the beta carbon. The extra (bulky) carbon in proximity to the backbone adds some extra limitation to its mobility. But ultimately, they were split into a separate distribution because the statistics gathered from tens of thousands of high-res examples showed that they *follow* a different distribution.

Q Can you apply molcular symmetry to helical structures ?

A live answered

Q Something of a tangent, but I was wondering if you have considered VR or AR functionality with Coot at all, considering that Nvidia Stereo is getting harder and harder to purchase

A live answered

Q Hi, I liked using HOLE implemented in Coot and woner Coot1.0 has updated visulaization of the results from HOLE. I had use other software to show the hollow hole earlier.

A It's on my todo list - relatively close to the top. I will write it up in a blog post.

Q does the map resampling influence position of centre of single blobs, e.g. like waters?

A I image that it might do - but at the 0.01A level or so.

Q Also, where can we find the code if we want to try compiling Coot python3?

A https://github.com/pemsley/coot/tree/gtk3
That contains a build-it-3-3 script.

Q I might be out of date but I was wondering if there is now one and only coot version for both Cristallography and CryoEM? I was used to use coot through ccpem suite since it had features absent from coot downloaded through ccp4 suite…

A There are 2 versions (new/unreleased old/released, rather than based on x-ray vs cryo-EM). CCP4 are more conservative than CCP-EM abou which version they distribute (CCP4 use releases, CCP-EM use pre-releases).

Q Woud there be a recording of the presenter's screen from the other side? As the mouse moves fast and don't show in the current video

A I didn't record it. I intend to make a YouTube video along the same lines as the presentation.

Q The text is scrolling by quickly, but I can see statistics on the model geometry after refinement. Are fit to density statistics also presented? CC between obs and calc maps, for example?

A Not on the fly - seems like a good idea though.

Q Are you seeing more issues with transmembrane segments in ISOLDE?

A live answered

Q Isolde is amazing tool for refinement of high resolution cryo-EM reconstructions but recently we had a problem to figure out how to shift amino acid register using Isolde. Is it possible and can you show this tool?

A live answered

Q Is there optimal range of resolution or requirements for the map to expect the good result? I woner if ISOLDE could work fo the poor map region like loop or linker regions.

A live answered

Q How do you introduce monosaccharides into the protein chain in ISOLDE?

A live answered

Q Any issues using ISOLDE with metal ion containing proteins?

A From https://isolde.cimr.cam.ac.uk/what-isolde/ "Currently, ISOLDE handles only residues that are in the standard AMBER protein and nucleic acid forcefields, plus water and most metal ions. Other species are not yet supported (but progress is being made)."

Q What tools do you recommend for docking of multichains to fit the map?
A live answered
Q How does Haruspex handle glycans?
A live answered
Q Did you find difference in False Positives between secondary structure elements? Were true helices identified as sheets more frequently than vice versa for ex?
A live answered
Q Can Haruspex annotate single-stranded RNA?
A live answered
Q Any recommendation for the resolution needed for Haruspex to be successful. I beleive it was trained using 4 A or better structures, so does that mean you need 4 A or better for it to work relaibly?

A live answered
Q During your preprocessing step, are the high and low intensity data standarized or the u-net is trained without the standarizing them
A live answered
Q *standardized
A live answered
Q I was wondering if 3-10 helix could be detected.
A live answered
Q Is it possible for users to provide multiple models to ARP/wARP findmysequence and have it check their correctness/p-value as opposed to using ARP/wARP to predict models?
A live answered
Q Does that mean you can get the sequence based on the 3 or 4 angstrom map without knowing the ground truth of sequence?
A live answered
Q I have 3.4 A map of ion channel, homotetramer, where there is only a torsional symmetry, making monomers assume 2 or even 4 different comformations. Size ~450 kD. Is ARP/wARP handle that?

A live answered
Q Speaking of hydrogens, for many of the programs do they add hydrogens at pH 7.4? What if we're doing structures at below 6.5 or above 8.5?
A live answered
Q In very hydrophobic environment like tranmembrane region, perhaps one should assume amino acids are protohnated?
A live answered
Q Can't Cablam outliers also be optimized in phenix?
A live answered
Q What if there no clashes.. For aminoacids that inclu both N and O such as Asn/Gln that could form hydrogen bond or electrostatical interactions, should we decide which atom (N or O) to be assigned manually or is there any software considering chemical interactions?
A live answered
Q For ISOLDE, should we donwnload just plugin?
A not answered
Q or newest version of ChimeraX?
A Download and install ChimeraX 1.2.5, then install via Tools/More Tools...