Taking biological structure communications into the third dimension
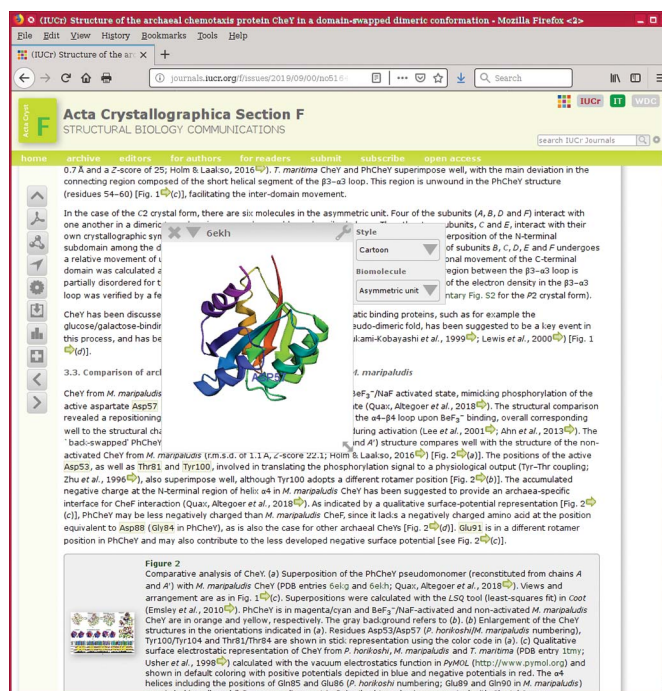
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In this issue of *Acta Crystallographica F, Structural Biology Communications*, Firth *et al.* (2019) present a text-mining tool for automatic protein-residue annotation in published papers. The tool, called *pyresid*, searches the text of an article for references to amino acids, then identifies the relevant protein and links that amino acid reference in the text to the residue in the associated PDB or mmcif file(s). In doing so, it enables the reader, at the touch of a button, to jump to the relevant part of the 3D structure.

By the time you read this, our developer, Simon Westrip, will have implemented an annotation system for all our *Acta F* articles that uses *pyresid* behind the scenes. For example, if you are reading this online, you can navigate to Mank *et al.* (2018), 'Structure of aspartate β-semialdehyde dehydrogenase from *Francisella tularensis*' or to Molina *et al.* (2018), 'Structure and stability of the human respiratory syncytial virus M2-1 RNA-binding core domain reveals a compact and cooperative folding unit'. Clicking on one of the highlighted amino acids in these articles will bring up a simple structure browser (based on 3Dmol.js; Rego & Koes, 2015), showing where the selected residue is in the 3D structure. Using the spanner icon, you can display the protein in cartoon format, stick format or ball-and-stick format. It will also allow you to hide or display water molecules and choose a white or black background. For display of the associated experimental electron density, you will need to open a specialized structure visualization program but this may be included in future versions if the annotations prove popular.

An example of an *Acta F* article (Paithankar *et al.*, 2019) annotated to show the residue Asp57.

editorial

We think our *pyresid* implementation is a good example of how integrated multimedia can enhance the reader experience, by enabling the facile location of biologically important amino acid residues in 3D structural models. We have included all *Acta F* papers to begin with and will extend the implementation to other IUCr journals as appropriate. Together with mobile phone augmented reality apps such as *Augment* (https://www.augment.com/) and *ScholAR* (https://www.ini.usc.edu/ScholAR/download.html), reading and, more importantly, *understanding* structural biology papers has never been easier!

References

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