Residue depth exemplified by means of graphical representation (PyMOL)

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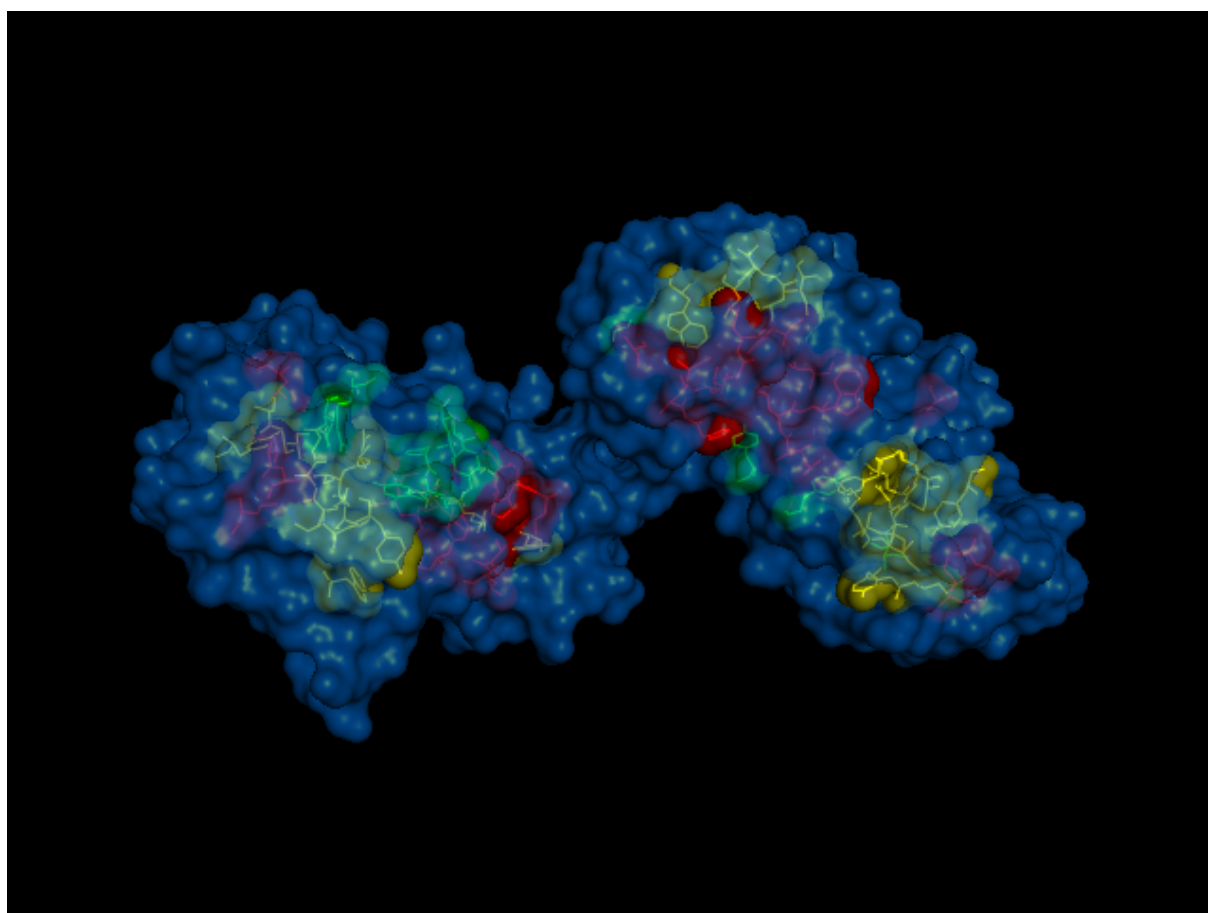
Cutoff of 3 Angstroms :

Figure 1 : Surface representation of 2za4. A residue depth cutoff of 3A is used. There can be seen core residues in transparency.
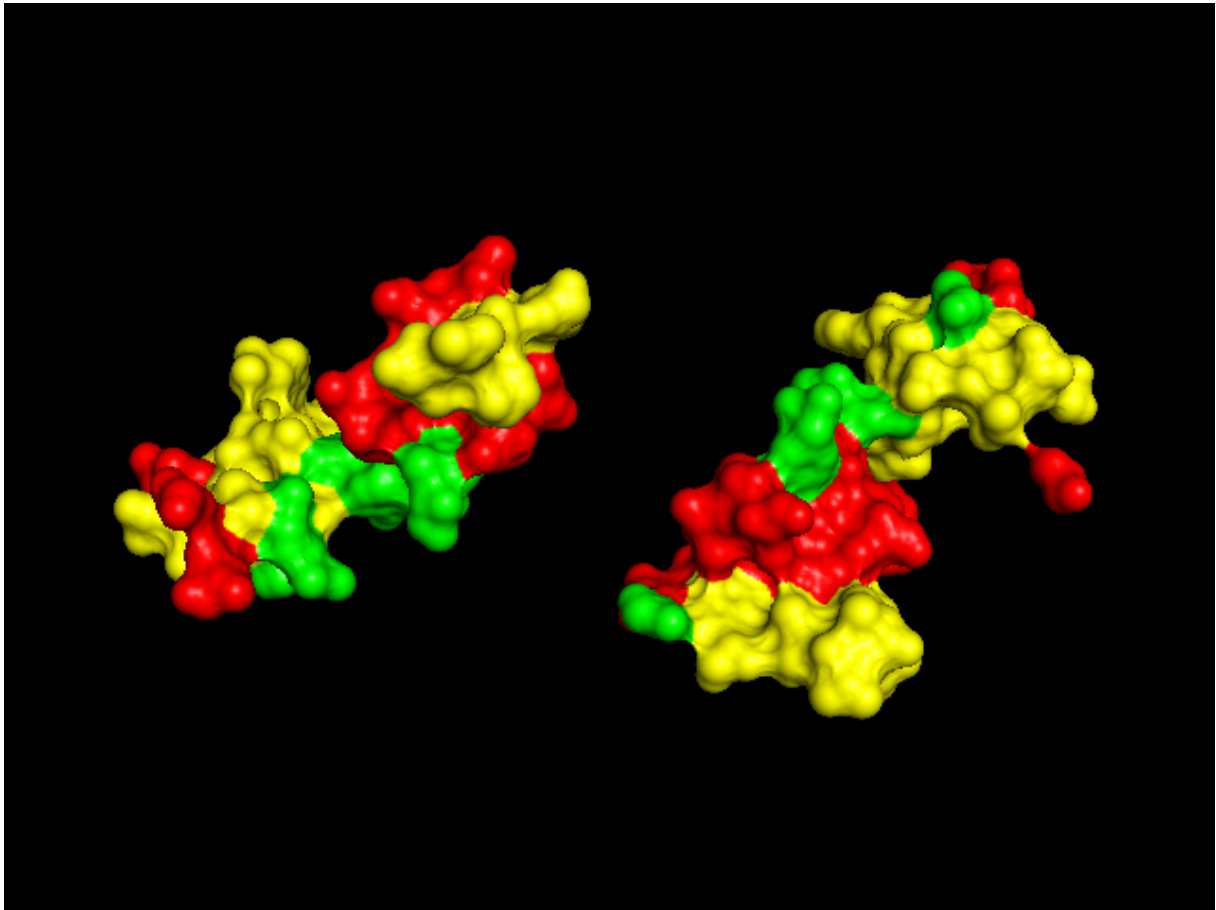
Figure 2 : Surface representation of 2za4's core residues. A focus on the core is shown here. As we increase the cutoff, we are going to notice that the surface of core residues gets smaller.
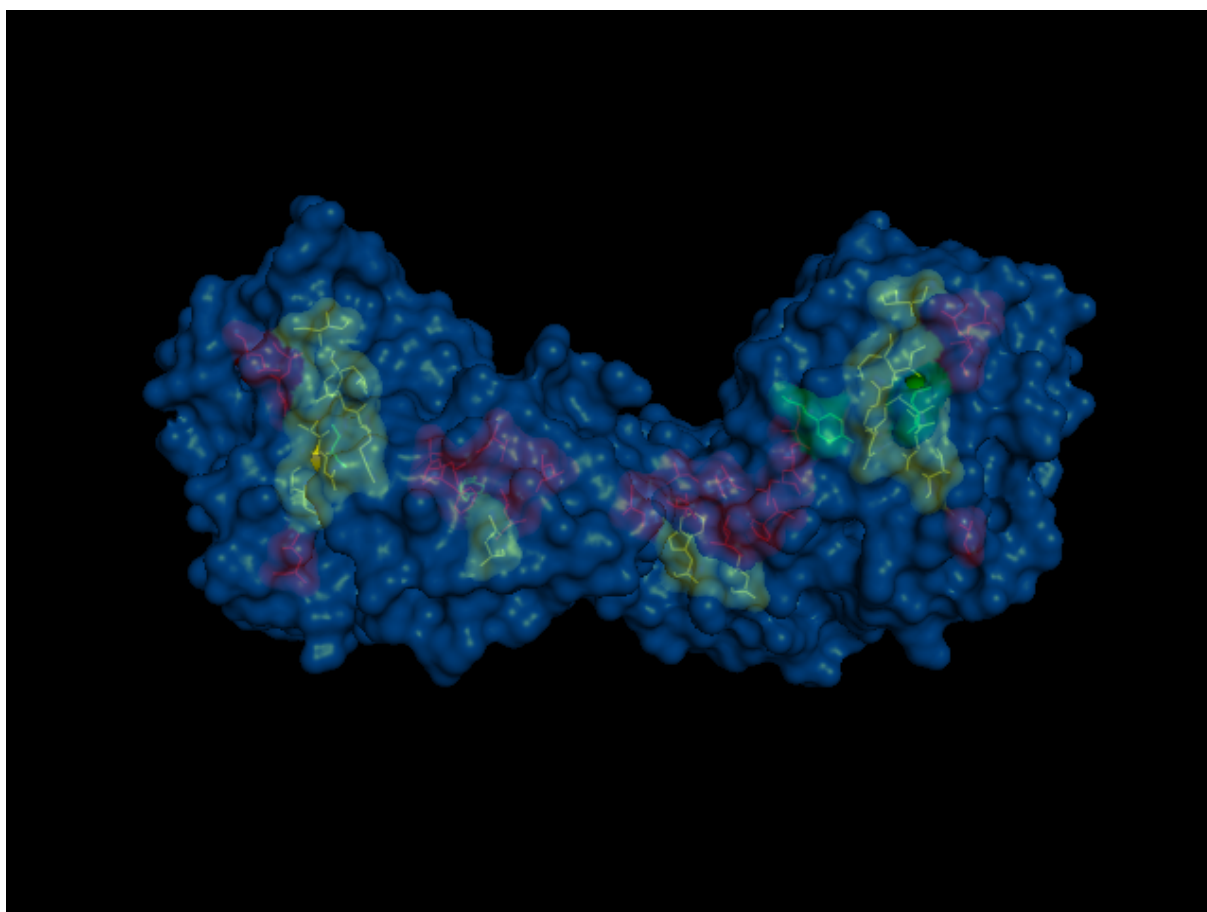
Cutoff of 4 Angstroms :

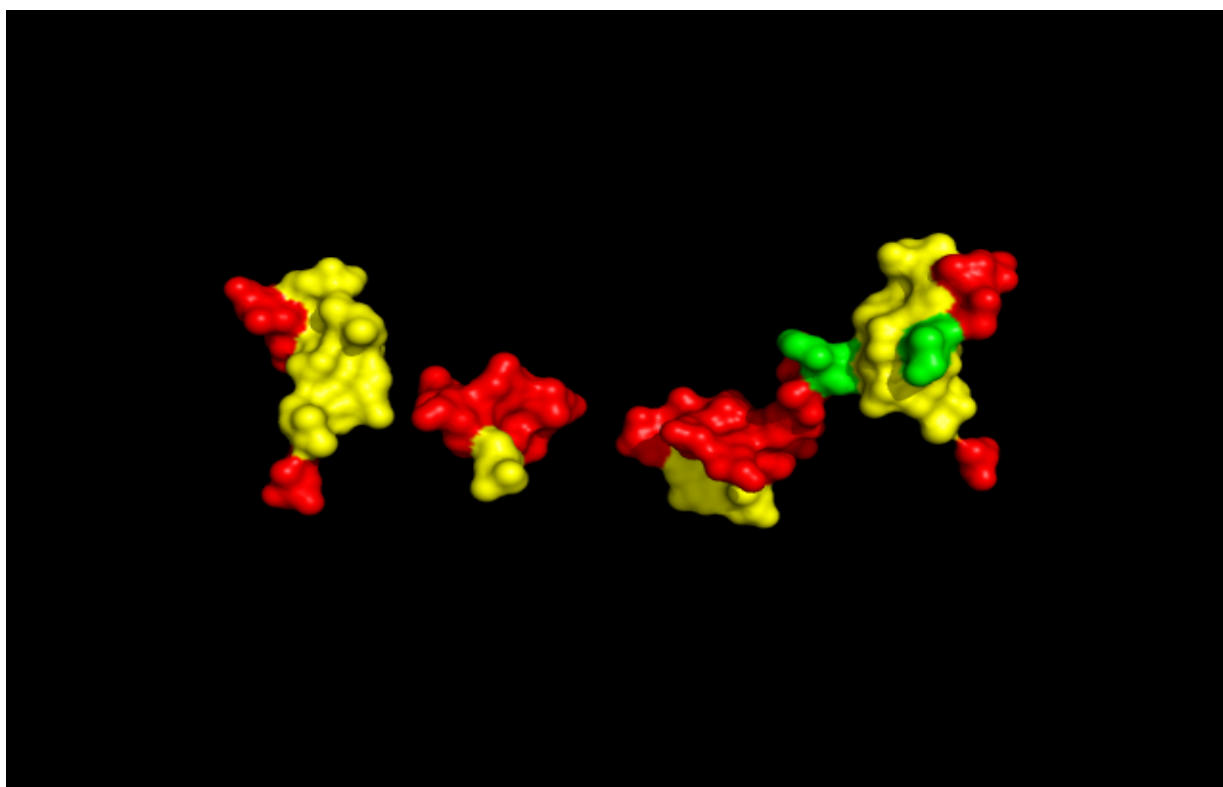Figure 3 : Surface representation of 2za4

Figure 4 : Surface representation of 2za4's core residues.
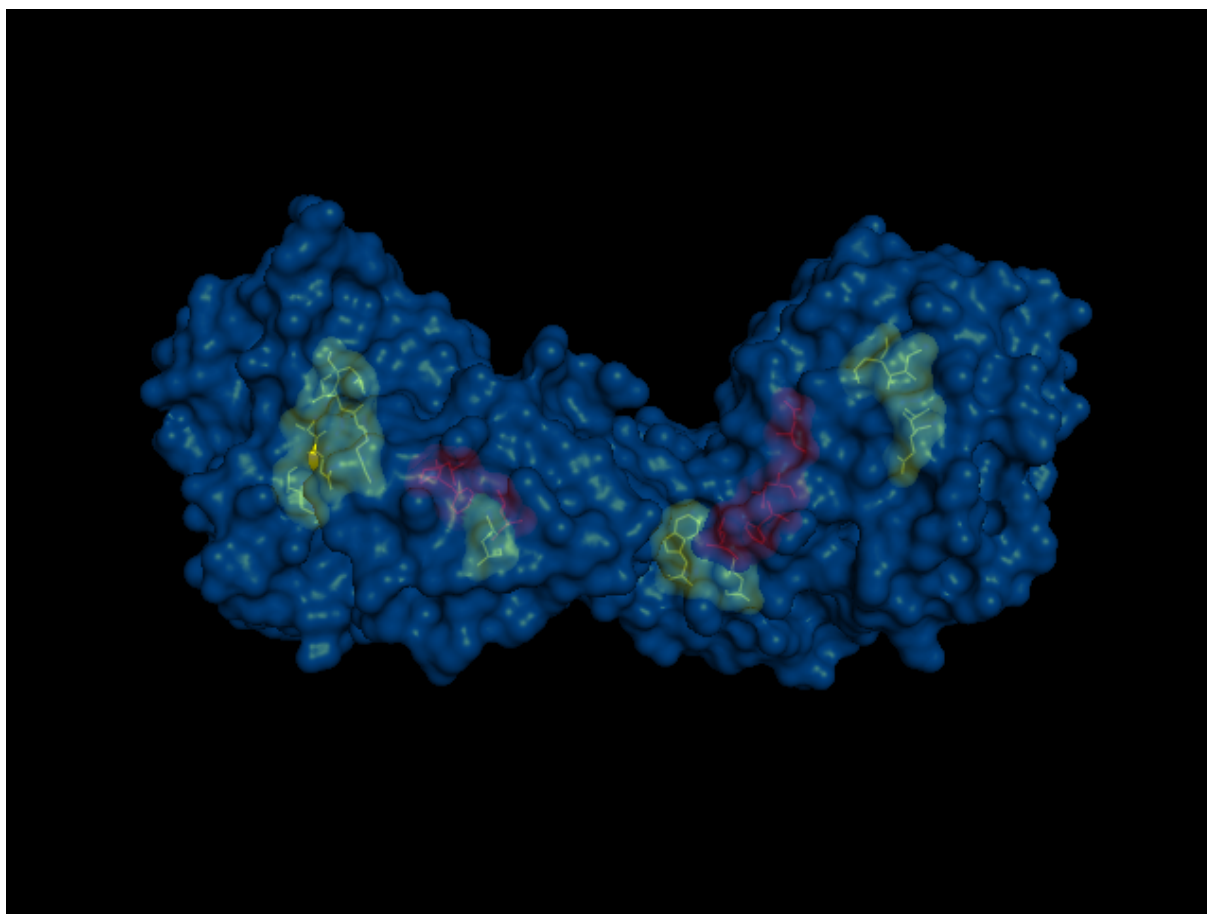
Cutoff of 5 Angstroms :

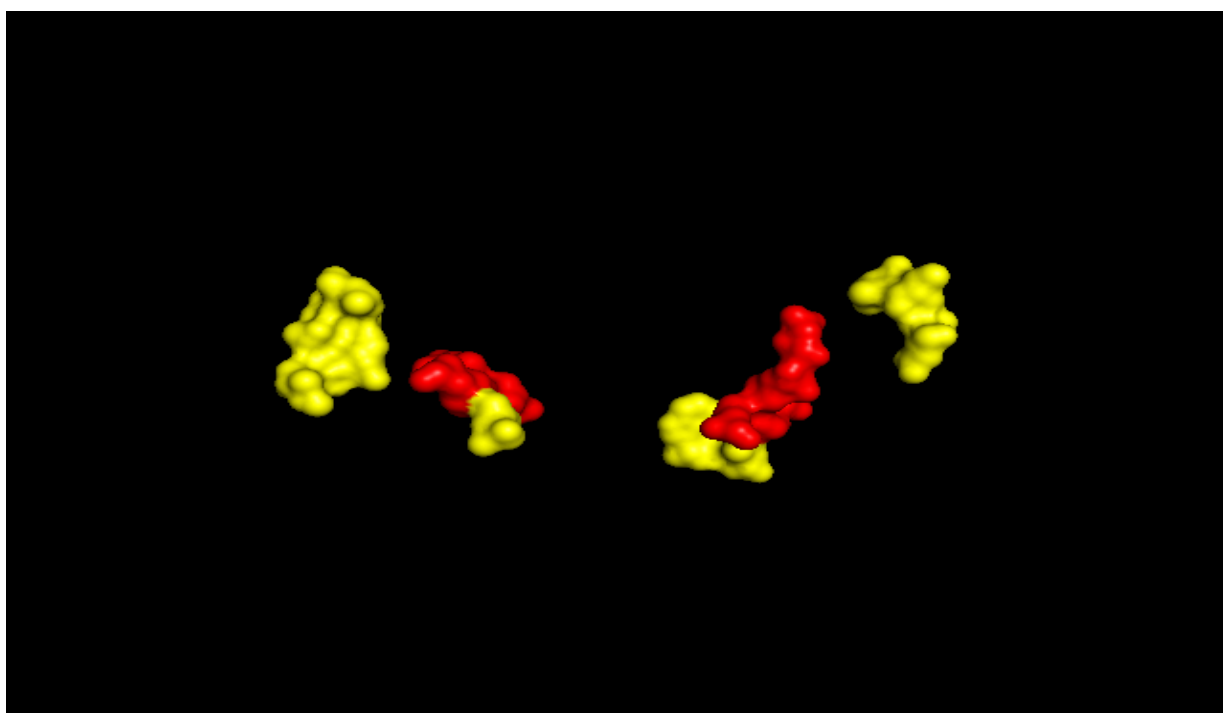Figure 5 : Surface representation of 2za4

Figure 6 : Surface representation of 2za4's core residues.

Observations :
The more the residue depth is high, the more that minimizes false negatives (that is to say, residues that are expected to be at the surface but not captured because of a low cutoff). On a flip side, false negatives are increased (residues considered at the surface whereas they belong to the core protein). In fact, false positives just cause the calculation time to be longer. A balance has to be adopted by means of molecular visualizations.
On a side note, we need to distinguish between fibrous and globular proteins.
The first type of protein has nearly all its residues at the surface, thus the residue depth is not relevant.
However, the residue depth is more germane to a globular protein where surface and core residues can be easily seperaed.