

***'All that glitters is not gold': High-resolution crystal structures of ligand-protein complexes need not always represent confident binding poses.***

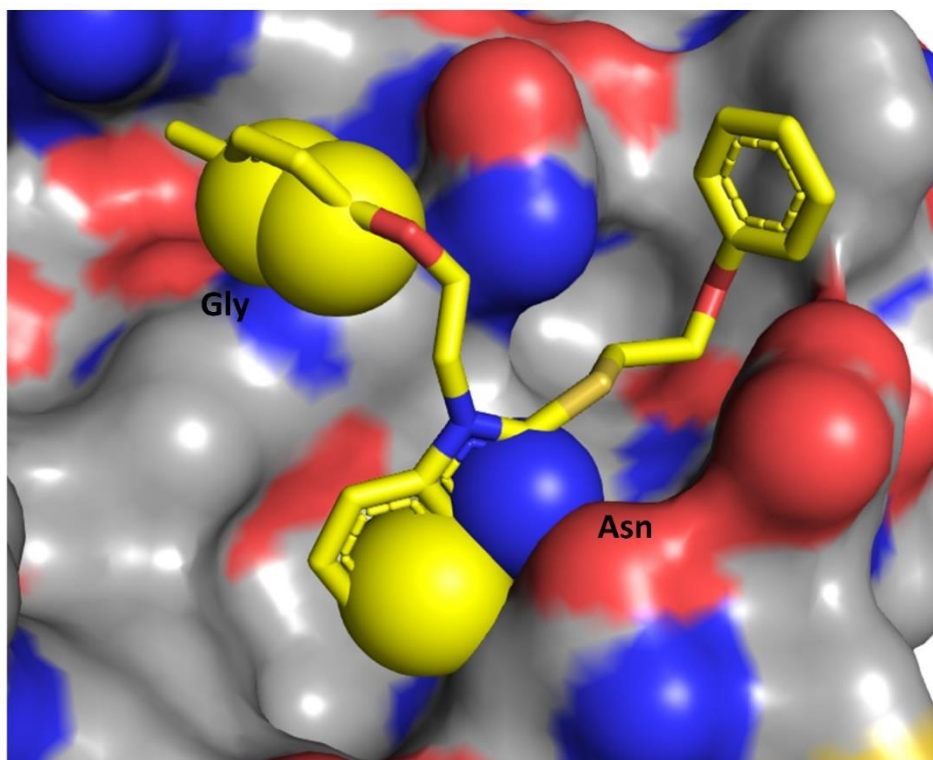
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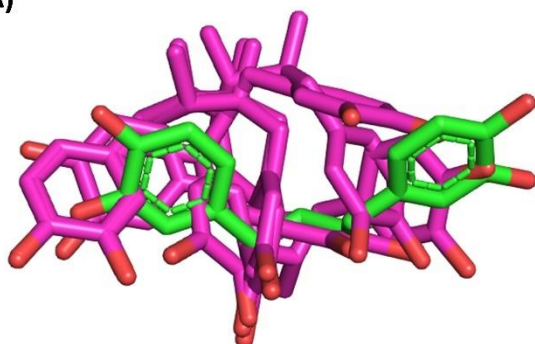
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**Supplementary Figures:**

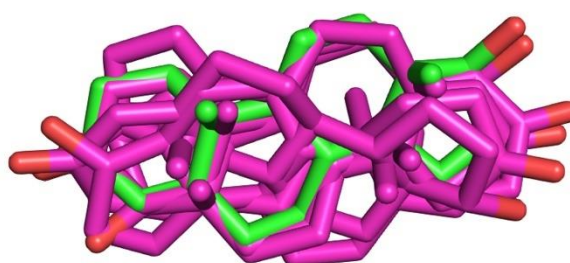


**Figure S1: Interatomic 'Bad' clashes between four ligand atoms of L4 and two protein residues (Gly and Asn).** Five steric clashes between four ligand atoms and two protein residues are observed with atomic overlaps: 0.696, 0.704, 0.772, 0.604, and 0.585.

**(A)**



**(B)**



**Figure S2: Superposition of re-docked (magenta) poses of ligands on their respective bound pose (green) reported in C1. (A) L1 and (B) L'. This is a representative example. Similar results have been observed for the other structures discussed in case study-1 (section 2.3.1).**