

C, N, O, ...

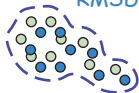
Atom elements

(x, y, z) ...

Atom coordinates

Basic input features

$\text{RMSD} \leq 2 \text{ \AA} ?$



Near-native pose

Ligand pose classification

PoseFGS

Native ligand atom

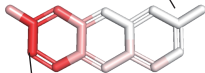
Decoy ligand atom



Atom deviations

Fine-grained supervision task

Bad local pose



Good local pose

Atom-level interpretation