

### Protein validation:

1. Find a structure of cytochrome P450 (in PDBe), which is obtained using X-ray and has the worst quality.
2. Obtain information about structure quality for a rhodostomin (PDB ID 4rqg), specifically:
  - How many clashes are there in the structure?
  - Which atom clashes are the closest?
  - How many bond length outliers are in the structure?
  - Which bond length outlier is the highest?
  - How many bond angle outliers are in the structure?
  - Which bond angle outlier is the highest?Note: Use PDB validation reports for 4rqg.
3. Protein Data Bank Europe uses summary quality criteria to summarize validation information about the structure. The summary criteria are: Clashscore, Ramachandran outliers, sidechain outliers, RSRZ outliers.  
Obtain summary criteria for oxy-hemoglobine in methanol (PDB ID 1lfz).

### Ligand validation:

1. Validate all the ligands in the nipah G attachment glycoprotein (PDB ID 3d12). Detect which of them have missing atoms or wrong chirality and describe where the validation issues are (which ligand and which atom).
2. Validate a molecule LMG in Plant Photosystem I (PDB ID 2wsc). Detect which atoms are missing.
3. Validate a molecule of  $\alpha$ -carotene (BCR) in Photosystem I (PDB ID 4rku). Detect which atoms within the ring of this molecule are missing.
4. Detect all estradiol (EST) ligands in Protein Data Bank which have chirality error.
5. Validate biotin (BTN) from 50S Complex (PDB ID 1kqs) and detect which atom is substituted.
6. Validate all sialic acids from PDB and identify the atoms of this molecule at which chirality errors occur.
7. Validate all samples of these testosterone derivatives: 5-beta-dihydrotestosterone (BDT), 5-alpha-dihydrotestosterone (DHT), epi-testosterone (FFA), testosterone (TES) and testosterone hemisuccinate (TH2). Detect if there are any samples with chirality errors.