

The list of PDB files used in our study are available at url http://genome.jouy.inra.fr/~jumartin/kaksi/sup_data/

- *Ref set*: Ref_list.txt,
- *HRes set*: HRes_list.txt,
- *MRes set*: MRes_list.txt,
- *LRes set*: LRes_list.txt,
- *NMR set*: NMR_list.txt.

No that these are the final lists, i.e., PDB files that are successfully processed by all assignment programmes and correctly post-processed. PDB files lacking the HELIX and SHEET fields are removed.