Notes:

**Path:**

Reference: extra\_bio\_ligands\_reference.zip

Generated Conformer: extra\_bio\_ligands\_boltz\_af3\_generated\_conformers.zip (215D\_DNA: generated by AF3; others: generated by Boltz2)

\*The 6y13\_stapled helix is removed, and replaced by 1afo because the stapled helix cannot be generated correctly by neither RDKit nor Boltz.

Collected Conformer: ATP, imatinib, from Cambridge Structure Database(CSD)

**Example for each case:**

1. 1afo\_dimer (Transmembrane domain dimer in the form of two alpha helices, extracted from NMR data )

1.a 1afo\_dimer(two helix)

Conformer: boltz\_results\_1afo\_dimer/1afo\_dimer\_model\_0.pdb

1.b 1afo\_single\_helix

Conformer: boltz\_results\_1afo\_dimer/1afo\_dimer\_model\_0\_chainB\_pH74.pdb

2. 1ln1\_DLP (Phospholipids)

2.a DLP

Conformer: boltz\_results\_1ln1\_DLP/1ln1\_DLP\_model\_0\_chainB\_pH74.pdb

3. 4csv\_imatinib (Tyrosine kinase inhibitor antineoplastic agent)

3.a imatinib

Conformer: boltz\_results\_4csv\_imatinib/4csv\_imatinib\_model\_0\_chainB\_pH74.pdb

3.b imatinib from CSD

Conformer: extra\_bio\_ligands\_CSD/ CSD\_AJIGUZ\_imatinib\_manual.pdb

4. boltz\_results\_5bvs\_EIC (unsaturated fatty acid)

4.a EIC

Conformer: boltz\_results\_5bvs\_EIC/ 5bvs\_EIC\_model\_0\_chainB\_pH74.pdb

5. boltz\_results\_6ln3\_ATP (adenosine triphosphate)

5.a ATP

Conformer: boltz\_results\_6ln3\_ATP/ 6ln3\_ATP\_model\_0\_chainB\_pH74.pdb

5.b ATP from CSD

Conformer: extra\_bio\_ligands\_CSD/CSD\_GAYLOH\_ATP\_manual.pdb (just one)

6. boltz\_results\_8w4x\_sugars (include both mannose: BGC and disaccharide: BGC\_GLC)

6.a BGC

Conformer: boltz\_results\_8w4x\_sugars/ 8w4x\_sugars\_model\_0\_chainB\_pH74.pdb

6.b BGC\_GLC

Conformer: boltz\_results\_8w4x\_sugars/ 8w4x\_sugars\_model\_0\_chainC\_pH74.pdb

7. 215D\_DNA

7.a single chain (there is only one chain in the crystal structure as reference)

Conformer: AF3\_215D\_DNA/seed-1\_sample-0/model\_chainA\_pH74.pdb