

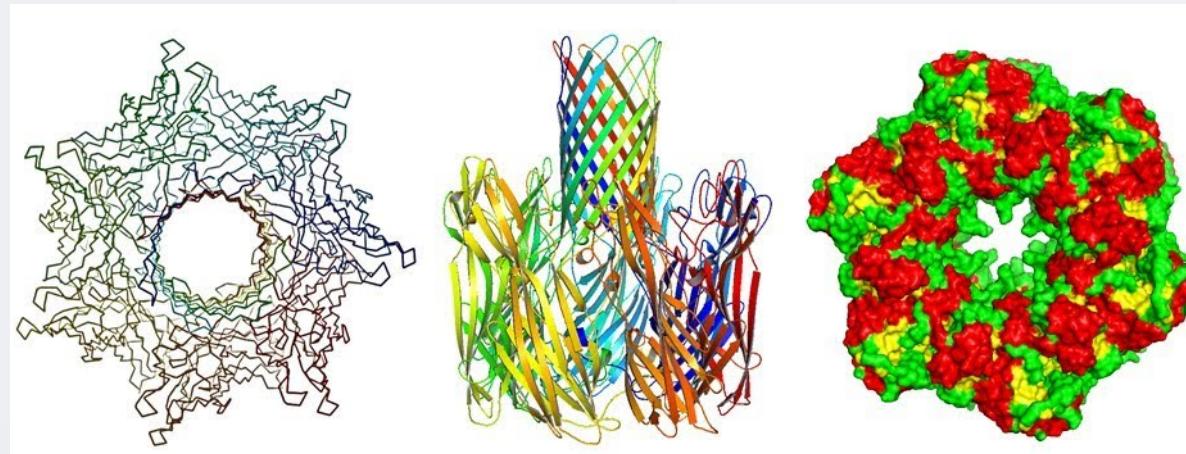
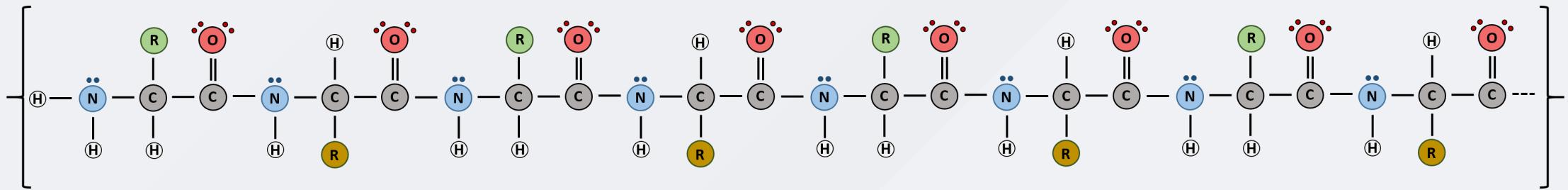
# How AlphaFold was made possible

## Overview of talk

1. Protein structures
2. MSAs
3.  $SE(3)$  Equivariance
4. The model
5. Future perspectives

Disclaimer: The discussed parts of AF are extremely cherry-picked

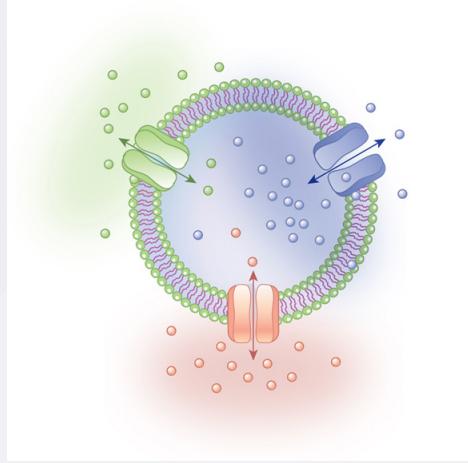
# 1. Protein structure prediction



## 2. Using MSAs

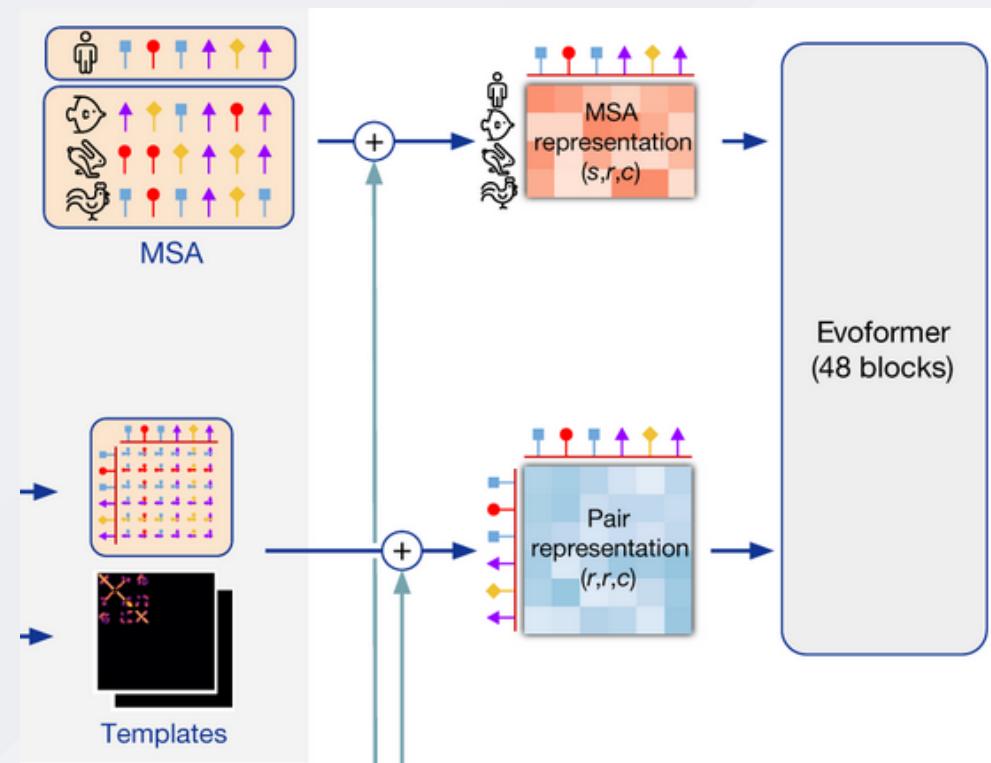


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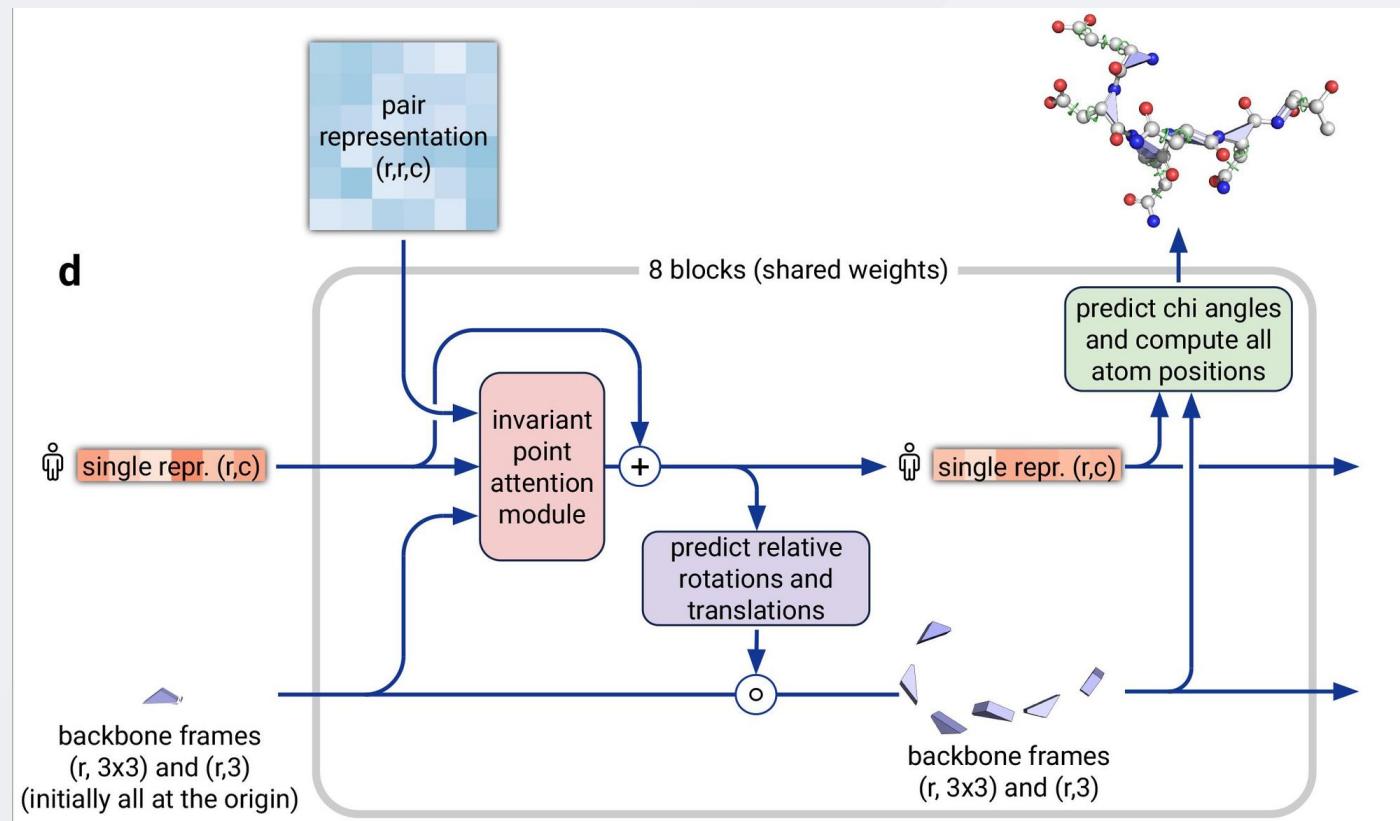
## 2. Using MSAs

Given to model as multi-dimensional input



# 3. Grounding in 3D space

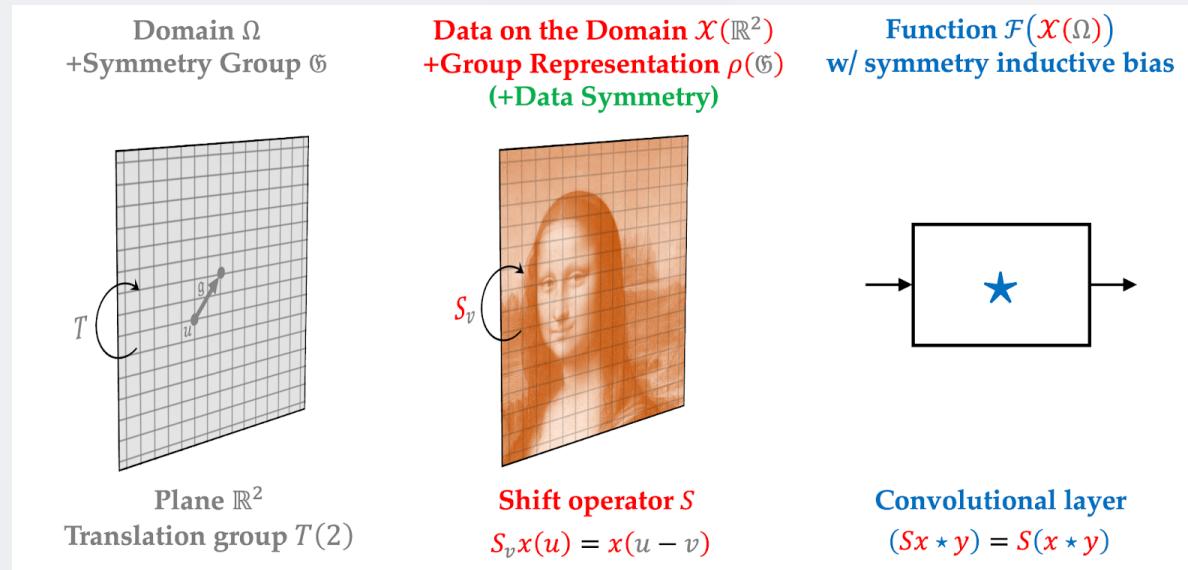
AlphaFold works by refining 3D coordinates of every amino acid



# 3. Grounding in 3D space

Geometric intuition:

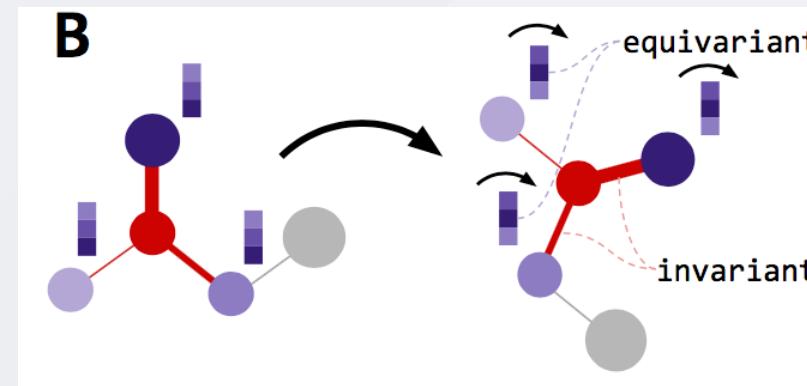
Convolutions are **equivariant** to translations  $T(2)$



### 3. Grounding in 3D space

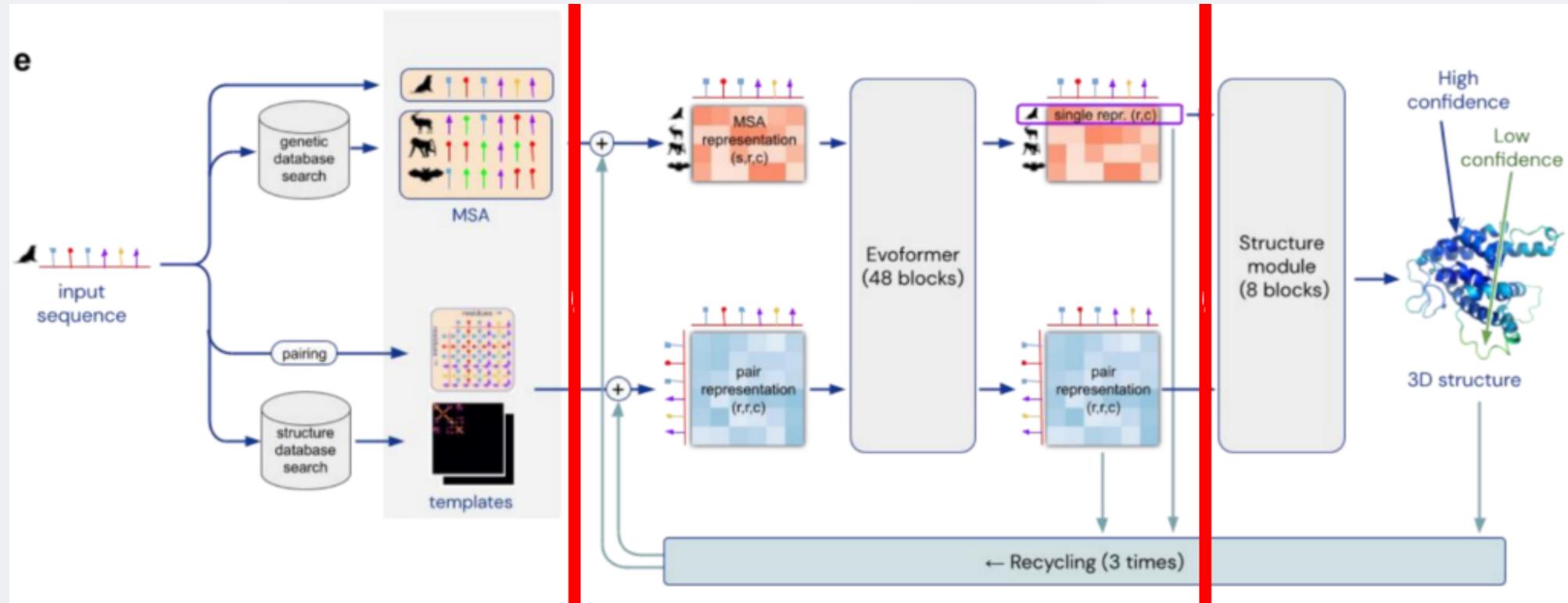
Geometric intuition:

Similarly, operations on molecules should be **equivariant** to  $SE(3)$ , which includes translations and rotations in 3D euclidean space.



Through modified self-attention (transformer)

# 4. Putting it together



# What's next

Learning interactions: Deep learning 🤝 Structural/physical models

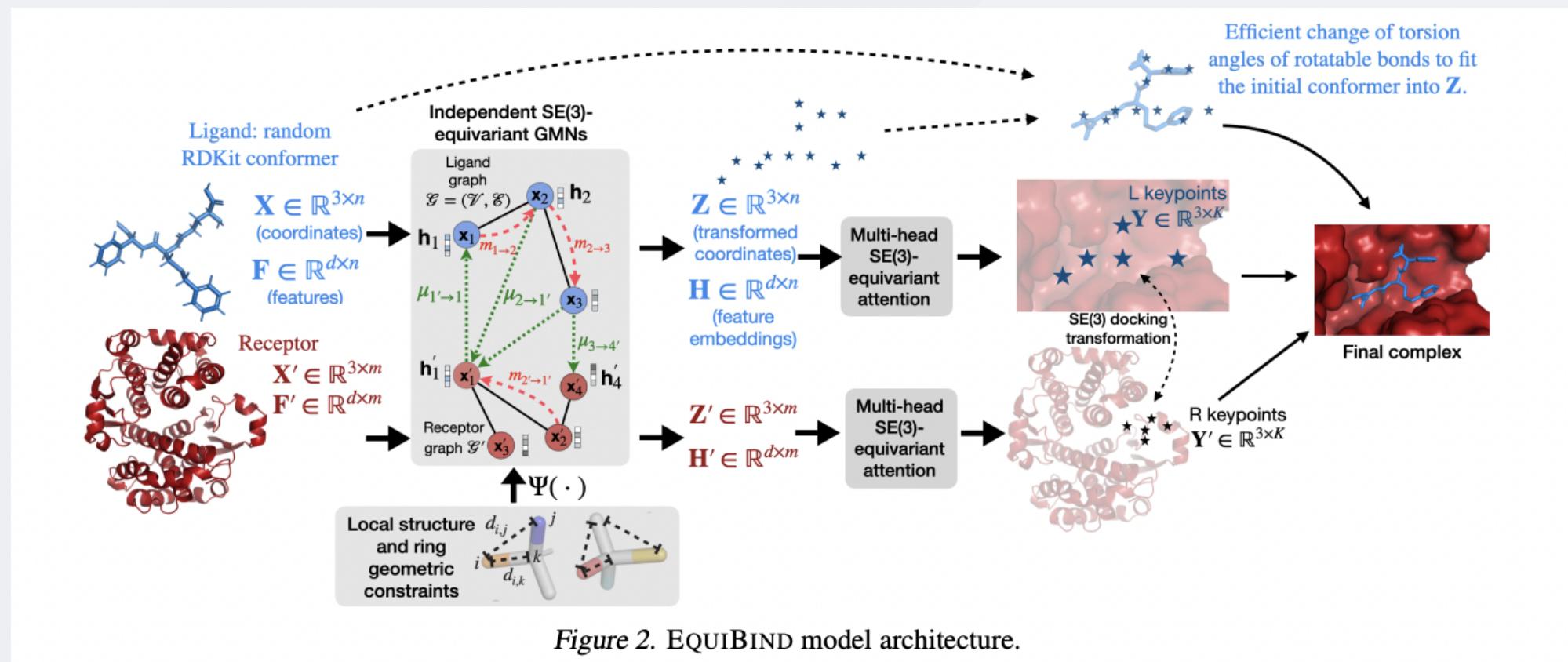


Figure 2. EQUIBIND model architecture.