

PROJECT: Structural Analysis and Clustering of VDR Crystal Structures

Objective: Analyze and classify all VDR structures to understand conformational variations and their relationship with ligands, using torsion angles and secondary structure analysis

Target data to be used:

1. All VDR crystal structures from PDB
2. Associated ligand information
3. Resolution data for each structure
4. Structure quality metrics

Approach:

1. Calculate torsion angles for all weighted structures
2. Perform clustering analysis
3. Analyze secondary structure elements
4. Correlate structural variations with ligand properties

Analysis components:

1. Torsion Angle Analysis:
 - Resolution-weighted comparison of Phi/Psi, Chi, Omega angles
2. Structure Clustering:
 - Hierarchical, K-means clustering
 - Cluster validation and outlier identification
3. Secondary Structure Analysis:
 - DSSP calculations, SSE composition
 - Conservation patterns, Domain organization
4. Additional Analyses:
 - Principal Component Analysis
 - Normal Mode Analysis
 - Hydrogen bond networks
 - SASA calculations?
 - Electrostatic potential mapping?
 - Evolutionary sequence analysis?

Potential outcomes:

1. Classification of VDR conformational states
2. Understanding of ligand-dependent structural changes
3. Identification of conserved structural motifs
4. Correlation between structure and function
5. Insights into protein flexibility
6. Structure-ligand relationship patterns
7. Discovery of novel conformational states

Skills gained:

1. Protein structure analysis
2. Clustering techniques
3. Secondary structure prediction
4. Data normalization methods and statistical analysis
5. Programming (Python/BioPython)
6. Structural bioinformatics
7. Machine learning application
8. Data visualization