

!pip install scikit-learn !pip install umap-learn

```
In [2]: from Bio import Entrez, SeqIO
```

```
In [3]: Entrez.email = "osama2172003aladesoky.com"
query = "blaTEM AND Escherichia coli[Organism]"

retmax = 100
handle_search = Entrez.esearch(db="nucleotide", term=query, retmax=retmax)
search_results = Entrez.read(handle_search)
handle_search.close()
id_list = search_results["IdList"]
print(f" Number of retrieved sequences: {len(id_list)}")
handle_fetch = Entrez.efetch(db="nucleotide", id=id_list, rettype="fasta", retmode="text")
records = list(SeqIO.parse(handle_fetch, "fasta"))
handle_fetch.close()

print(f"Downloaded {len(records)} sequence from NCBI")
SeqIO.write(records, "tem1_sequences.fasta", "fasta")
print("The sequences were saved in a file: tem1_sequences.fasta")
print(search_results)
```

Number of retrieved sequences: 100
Downloaded 93 sequence from NCBI
The sequences were saved in a file: tem1_sequences.fasta
{'Count': '26412', 'RetMax': '100', 'RetStart': '0', 'IdList': ['3024353050', '3023638427', '3023560251', '3023536798', '3022846721', '3022725241', '3022630913', '3022630876', '3020292345', '2752880018', '2524484095', '2255885729', '1148836538', '1119795159', '1119778745', '1103820147', '757605208', '692990478', '3015430272', '2752129683', '2521722531', '1888298469', '1862746456', '1853504665', '181643663', '1816433658', '1816433652', '3012355828', '1883825494', '1866146194', '1836674118', '1816513184', '3010737428', '1848406648', '1800078768', '237640188', '1848406551', '1832836016', '410593098', '256367708', '1786223106', '2520284883', '2515153030', '1727822781', '1727822689', '1727822686', '1727822683', '1727822681', '1727822679', '1727822676', '1727822674', '1727822672', '1727822670', '1727822668', '1727822665', '1727822663', '1727822661', '1727822658', '1727822656', '1727822653', '1727822651', '1727822648', '1727822646', '1727822644', '1727822642', '1727822640', '1727822638', '1727822635', '1727822633', '1727822631', '1727822629', '1727822626', '1727822624', '1727822622', '1727822619', '1727822617', '1727822614', '1727822612', '1727822610', '1727822608', '1727822606', '1727822604', '1727822602', '1727822599', '1727822597', '1727822595', '1727822592', '1727822589', '1727822587', '1727822584', '1727822582', '1727822580', '1727822577', '1727822574', '1727822571', '1727822566', '1727822563', '1727822559', '1727822556', '1727822552'], 'TranslationSet': [{{'From': 'Escherichia coli[Organism]', 'To': '"Escherichia coli"[Organism]'}}], 'TranslationStack': [{{'Term': 'blaTEM[All Fields]', 'Field': 'All Fields', 'Count': '1', 'Explode': 'N'}, {'Term': '"Escherichia coli"[Organism]', 'Field': 'Organism', 'Count': '1', 'Explode': 'Y'}, 'AND'], 'QueryTranslation': 'blaTEM[All Fields] AND "Escherichia coli"[Organism]'}}

```
In [4]: from Bio import SeqIO
import pandas as pd
```

```
# Load sequences from a fasta file
records = list(SeqIO.parse("tem1_sequences.fasta", "fasta"))
print(f" Number of original sequences: {len(records)}")

min_len = 100
max_len = 3000
```

```

# Filter sequences by Length
filtered = [r for r in records if min_len <= len(r.seq) <= max_len]
print(f" Number of filtered sequences: {len(filtered)}")

# Save them to a new file for analysis
SeqIO.write(filtered, "filtered_sequences.fasta", "fasta")

# Save sequence lengths to a table CSV (for later visualization)
lengths = [len(r.seq) for r in filtered]
pd.DataFrame({"length": lengths}).to_csv("sequence_lengths.csv", index=False)

print(" Filtered sequences and statistical data saved")

```

Number of original sequences: 93
 Number of filtered sequences: 47
 Filtered sequences and statistical data saved

```

In [5]: import subprocess
from Bio import AlignIO
import pandas as pd

#1) Input and Output Files
input_file = "filtered_sequences.fasta"
output_file = "aligned_sequences.aln"

clustal_path = r"D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncb

#2) Run Alignment
cline = ClustalOmegaCommandline(
cmd=clustal_path,
infile=input_file,
outfile=output_file,
verbose=True,
auto=True,
force=True
)
print(" Running Alignment...")
cline()
print(" Alignment completed")

#3) Read alignment
alignment = AlignIO.read(output_file, "fasta")
L = alignment.get_alignment_length()
print(f" Alignment length: {L} column")

#4) Extract SNPs with list comprehension
snp_df = pd.DataFrame([
{
"Position": pos + 1,
"Variants": "".join(sorted(set(alignment[:, pos]) - {"-", "N"}))
}
for pos in range(L)
if len(set(alignment[:, pos]) - {"-", "N"}) > 1
])

#5) Save results

```

```
snp_df.to_csv("snp_table.csv", index=False)
print(f" {len(snp_df)} SNP mutation location identified")
```

D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-packages\Bio\Application__init__.py:39: BiopythonDeprecationWarning: The Bio.Application modules and modules relying on it have been deprecated.

Due to the on going maintenance burden of keeping command line application wrappers up to date, we have decided to deprecate and eventually remove these modules.

We instead now recommend building your command line and invoking it directly with the subprocess module.

```
warnings.warn(
    Running Alignment...
    Alignment completed
    Alignment length: 2992 column
    2850 SNP mutation location identified
```

In [6]:

```
import numpy as np
from Bio import AlignIO

# 1) Read the alignment
alignment = AlignIO.read("aligned_sequences.aln", "fasta")
L = alignment.get_alignment_length()
n = len(alignment)

# 2) Calculate π for each column in one stroke
pi_values = []
for pos in range(L):
    column = alignment[:, pos]
    freqs = np.array([column.count(b) for b in set(column) if b not in ("-", "N")]
    total = freqs.sum()
    # Here we use ternary to avoid a lengthy if block
    pi_site = 0.0 if total < 2 else 1 - np.sum((freqs/total)**2)
    pi_values.append(pi_site)

# 3) π Total
pi_total = sum(pi_values) * 2 / (n * (n - 1))

#4) Print the result
print(f"\tNumber of sequences: {n}")
print(f"\tAlignment length: {L}")
print(f"\tNucleotide diversity (π): {pi_total:.5f}")
```

Number of sequences: 47
 Alignment length: 2992
 Nucleotide diversity (π): 1.57992

In [7]:

```
import numpy as np
import matplotlib.pyplot as plt
from Bio import AlignIO

alignment = AlignIO.read("aligned_sequences.aln", "fasta")
L = alignment.get_alignment_length()
n = len(alignment)

def pi_site(column):
    freqs = np.array(
        [column.count(b) for b in set(column) if b not in ("-", "N")],
```

```

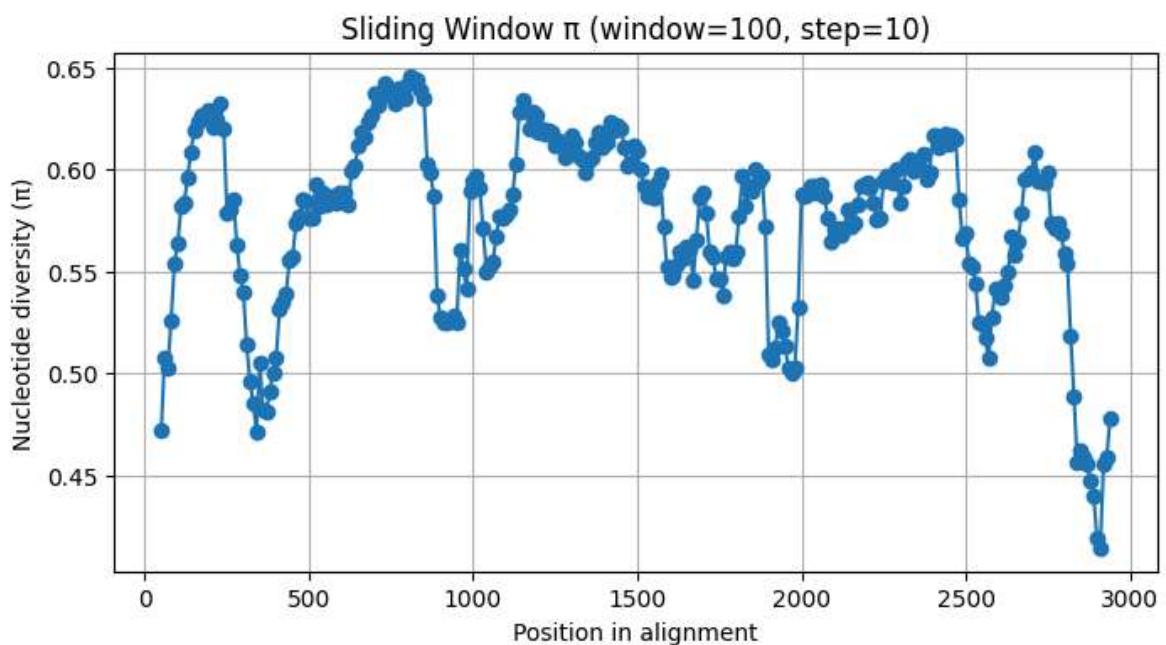
        dtype=float
    )
    total = freqs.sum()
    return 0.0 if total < 2 else 1 - np.sum((freqs/total)**2)

window_size = 100
step = 10
windows = range(0, L - window_size + 1, step)

pi_window = []
for start in windows:
    site_vals = [pi_site(alignment[:, pos]) for pos in range(start, start + wind
pi_window.append(np.mean(site_vals))

positions = [w + window_size/2 for w in windows]
plt.figure(figsize=(8, 4))
plt.plot(positions, pi_window, marker='o', linestyle='--')
plt.title("Sliding Window  $\pi$  (window=100, step=10)")
plt.xlabel("Position in alignment")
plt.ylabel("Nucleotide diversity ( $\pi$ )")
plt.grid(True)
plt.savefig("sliding_window_pi.png", dpi=300, bbox_inches='tight')
plt.show()

```



```

In [9]: import numpy as np
from sklearn.decomposition import PCA
import matplotlib.pyplot as plt

bases = ["A", "T", "G", "C"]
n, L = len(alignment), alignment.get_alignment_length()
X = np.zeros((n, L * 4), dtype=int)
for i, record in enumerate(alignment):
    for j, b in enumerate(record.seq.upper()):
        if b in bases:
            X[i, 4*j + bases.index(b)] = 1

pca = PCA(n_components=2)
coords = pca.fit_transform(X)

plt.figure(figsize=(6, 5))

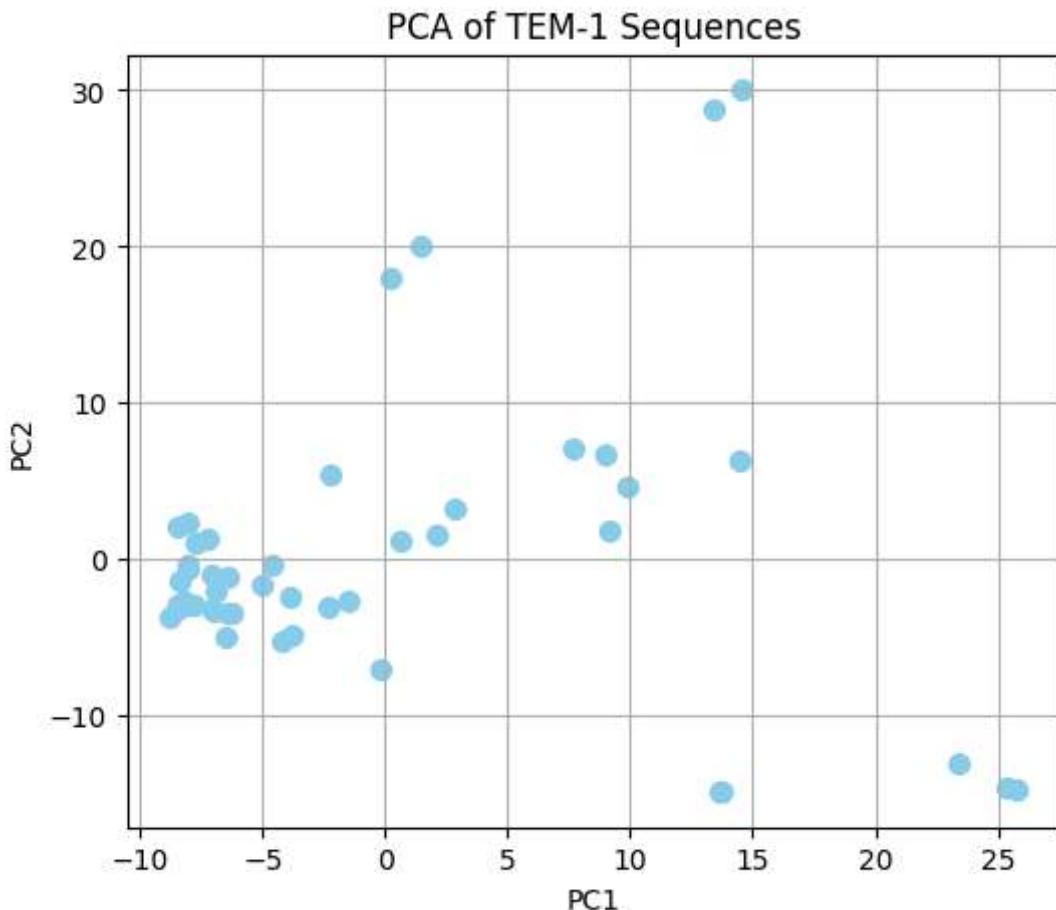
```

```

plt.scatter(coords[:, 0], coords[:, 1], c='skyblue', s=50)
plt.title("PCA of TEM-1 Sequences")
plt.xlabel("PC1")
plt.ylabel("PC2")
plt.grid(True)

plt.savefig("pca_plot.png", dpi=300, bbox_inches='tight')
plt.show()

```



In [10]:

```

import umap

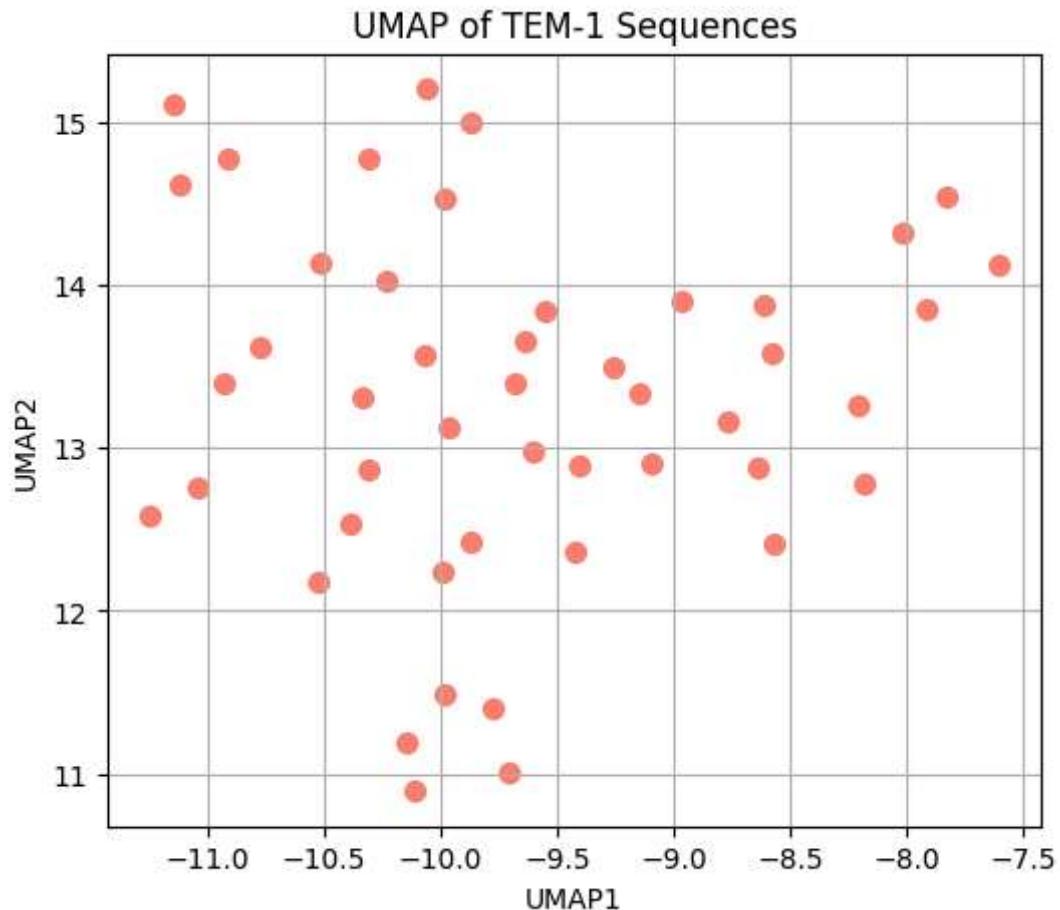
reducer = umap.UMAP(n_components=2, random_state=42)
umap_coords = reducer.fit_transform(X)

plt.figure(figsize=(6, 5))
plt.scatter(umap_coords[:, 0], umap_coords[:, 1], c='salmon', s=50)
plt.title("UMAP of TEM-1 Sequences")
plt.xlabel("UMAP1")
plt.ylabel("UMAP2")
plt.grid(True)

plt.savefig("umap_plot.png", dpi=300, bbox_inches='tight')
plt.show()

```

D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-packages\umap\umap_.py:1952: UserWarning: n_jobs value 1 overridden to 1 by setting random_state. Use no seed for parallelism.
warn(



```
In [8]: import numpy as np

pi_arr = np.array(pi_window)
high_thresh = np.percentile(pi_arr, 85)
low_thresh = np.percentile(pi_arr, 15)

high_windows = [(positions[i], pi_arr[i])
                 for i in range(len(pi_arr)) if pi_arr[i] >= high_thresh]
low_windows = [(positions[i], pi_arr[i])
                 for i in range(len(pi_arr)) if pi_arr[i] <= low_thresh]

print("High-diversity windows (pos, π):", high_windows)
print("Low-diversity windows (pos, π):", low_windows)
```

```
High-diversity windows (pos, π): [(150.0, np.float64(0.6194133913237322)), (160.0, np.float64(0.6238210764893016)), (170.0, np.float64(0.6269075174772505)), (180.0, np.float64(0.6264379117308381)), (190.0, np.float64(0.6290302638596323)), (200.0, np.float64(0.6268832566688626)), (210.0, np.float64(0.6211521322937988)), (220.0, np.float64(0.6245821096472878)), (230.0, np.float64(0.632330266394394)), (240.0, np.float64(0.6202068988747873)), (660.0, np.float64(0.6185442120759767)), (680.0, np.float64(0.6232323801244771)), (690.0, np.float64(0.6266312744831919)), (700.0, np.float64(0.6376965494430101)), (710.0, np.float64(0.6319625927550881)), (720.0, np.float64(0.6376708147035726)), (730.0, np.float64(0.6427499240856092)), (740.0, np.float64(0.6369460678619772)), (750.0, np.float64(0.6378695972206083)), (760.0, np.float64(0.6325286551339384)), (770.0, np.float64(0.6397499468792047)), (780.0, np.float64(0.6389291897791651)), (790.0, np.float64(0.6354235601745633)), (800.0, np.float64(0.6414001178458668)), (810.0, np.float64(0.6460733394148548)), (820.0, np.float64(0.6447803825109581)), (830.0, np.float64(0.6440718806194045)), (840.0, np.float64(0.6389259500240747)), (850.0, np.float64(0.6351852817527955)), (1140.0, np.float64(0.6287017844995062)), (1150.0, np.float64(0.6340242855325152)), (1160.0, np.float64(0.6293387232399913)), (1170.0, np.float64(0.6199562070030439)), (1180.0, np.float64(0.6282510797453166)), (1190.0, np.float64(0.6265910446436022)), (1200.0, np.float64(0.618444735452277)), (1210.0, np.float64(0.6201567889327153)), (1230.0, np.float64(0.6190612857510661)), (1240.0, np.float64(0.618453889347068)), (1380.0, np.float64(0.6184536447158272)), (1420.0, np.float64(0.6233475998332599)), (1430.0, np.float64(0.6194569109284191)), (1440.0, np.float64(0.6215519563573815)), (1450.0, np.float64(0.6204488580652044))]

Low-diversity windows (pos, π): [(50.0, np.float64(0.4723771762408667)), (60.0, np.float64(0.5079854528848576)), (70.0, np.float64(0.5030212506535225)), (80.0, np.float64(0.5262029329516885)), (310.0, np.float64(0.5138096412562799)), (320.0, np.float64(0.49636393261027406)), (330.0, np.float64(0.48520344391289716)), (340.0, np.float64(0.4712885428977724)), (350.0, np.float64(0.5051767737953351)), (360.0, np.float64(0.48156018544382984)), (370.0, np.float64(0.4809684585858406)), (380.0, np.float64(0.49139402259376125)), (390.0, np.float64(0.5000110029055135)), (400.0, np.float64(0.507913850106913)), (910.0, np.float64(0.525335419350331)), (920.0, np.float64(0.5251904889765712)), (930.0, np.float64(0.5256870470976335)), (950.0, np.float64(0.5252188259772815)), (1900.0, np.float64(0.5095298046412172)), (1910.0, np.float64(0.5064567723923248)), (1920.0, np.float64(0.5123639552228996)), (1930.0, np.float64(0.5247436776686999)), (1940.0, np.float64(0.521086636627455)), (1950.0, np.float64(0.5134994470844765)), (1960.0, np.float64(0.5022376548657967)), (1970.0, np.float64(0.4999185703827964)), (1980.0, np.float64(0.5026139130691981)), (2540.0, np.float64(0.5253442866213283)), (2550.0, np.float64(0.523943055985528)), (2560.0, np.float64(0.517426904330915)), (2570.0, np.float64(0.5072705465990327)), (2820.0, np.float64(0.5183374085065143)), (2830.0, np.float64(0.4887306446964537)), (2840.0, np.float64(0.45608193863459834)), (2850.0, np.float64(0.4621127240867665)), (2860.0, np.float64(0.4587638417724996)), (2870.0, np.float64(0.45584813612767455)), (2880.0, np.float64(0.4471440721277534)), (2890.0, np.float64(0.4396424165734649)), (2900.0, np.float64(0.41883981222208616)), (2910.0, np.float64(0.41428275979980106)), (2920.0, np.float64(0.4551412096612271)), (2930.0, np.float64(0.4590755584083965)), (2940.0, np.float64(0.4781480168362119))]
```

```
In [12]: active_sites = [44, 66, 104, 166]
```

```
aa_high = [int(pos/2) for pos, _ in high_windows]
aa_low = [int(pos/2) for pos, _ in low_windows]

print("Overlap with active sites (high π):",
      set(aa_high) & set(active_sites))
print("Overlap with active sites (low π):",
      set(aa_low) & set(active_sites))
```

```
Overlap with active sites (high π): set()
Overlap with active sites (low π): set()
```

```
In [13]: import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from Bio import AlignIO

alignment = AlignIO.read("aligned_sequences.aln", "fasta")
L = alignment.get_alignment_length()
window_size = 100
step = 10
windows = np.arange(0, L-window_size+1, step)
pi_window = [
    np.mean([
        0.0 if (lambda freqs: freqs.sum()<2)(freqs := np.array(
            [alignment[:, pos].count(b)
             for b in set(alignment[:, pos])
             if b not in ("-", "N")]),
            float
        )
        ) else 1 - np.sum((freqs/freqs.sum())**2)
        for pos in range(start, start+window_size)
    ])
    for start in windows
]

positions = windows + window_size/2

pi_arr = np.array(pi_window)
high_thr = np.percentile(pi_arr, 85)
low_thr = np.percentile(pi_arr, 15)

groups = ["high" if val>=high_thr
          else "low" if val<=low_thr
          else "mid"
          for val in pi_arr]

active_sites = [70, 73, 130, 166, 234, 238]

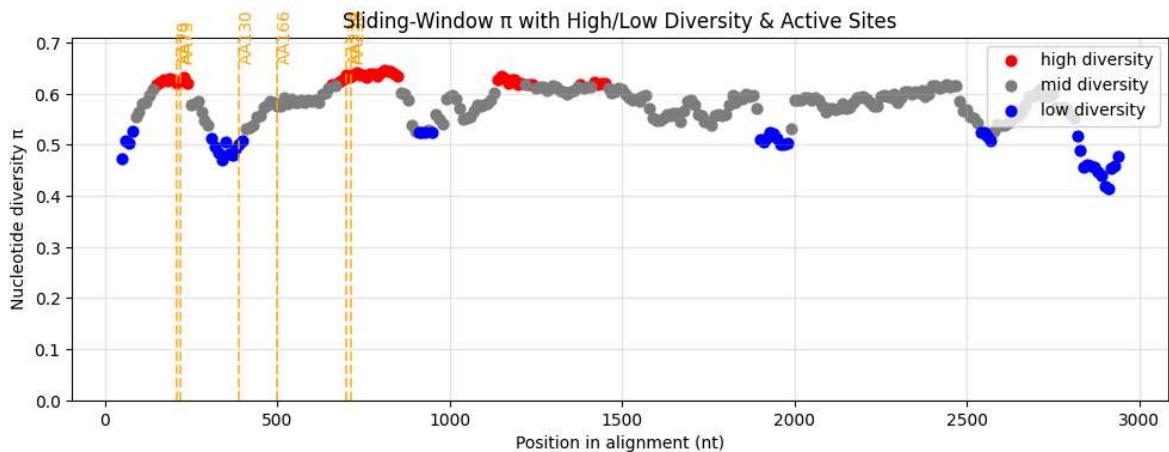
plt.figure(figsize=(10,4))
for grp, color in zip(["high", "mid", "low"], ["red", "grey", "blue"]):
    idx = [i for i, g in enumerate(groups) if g==grp]
    plt.scatter(positions[idx], pi_arr[idx],
                c=color, label=f"{grp} diversity", s=40)

for aa in active_sites:
    nuc_pos = aa * 3
    plt.axvline(nuc_pos, color='orange', linestyle='--', alpha=0.7)
    plt.text(nuc_pos, max(pi_arr)*1.02, f"AA{aa}",
              rotation=90, va='bottom', color='orange')

plt.title("Sliding-Window π with High/Low Diversity & Active Sites")
plt.xlabel("Position in alignment (nt)")
plt.ylabel("Nucleotide diversity π")
plt.legend(loc="upper right")
plt.ylim(0, max(pi_arr)*1.1)
plt.grid(alpha=0.3)

plt.tight_layout()
```

```
plt.savefig("sliding_window_pi_annotated.png", dpi=300)
plt.show()
```



```
In [14]: df = pd.DataFrame({
    "window_start": windows,
    "window_mid": positions,
    "pi": pi_arr,
    "group": groups
})

df["aa_pos_mid"] = (df["window_mid"] / 3).round().astype(int)

df["overlaps_active"] = df["aa_pos_mid"].isin(active_sites)

df.to_csv("window_pi_functional_comparison.csv", index=False)

print("Windows that intersect with functional locations:")
print(df[df["overlaps_active"]])
```

Windows that intersect with functional locations:

	window_start	window_mid	pi	group	aa_pos_mid	overlaps_active
16	160	210.0	0.621152	high	70	True
17	170	220.0	0.624582	high	73	True
34	340	390.0	0.500011	low	130	True

```
In [25]: import numpy as np
import matplotlib.pyplot as plt
from Bio import AlignIO

# 1) Load alignment
alignment = AlignIO.read("aligned_sequences.aln", "fasta")
L = alignment.get_alignment_length()
window_size = 100
step = 10
starts = np.arange(0, L - window_size + 1, step)

# 2) Compute sliding-window π
def pi_window_vals(aln, starts, w):
    vals = []
    for s in starts:
        cols = [aln[:, i] for i in range(s, s + w)]
        pi_sites = []
        for col in cols:
            freqs = np.array([
                [col.count(b) for b in set(col) if b not in ("-", "N")],
                float
            ])
            pi_sites.append(freqs.sum(0) / len(freqs))
    return pi_sites
```

```

        )
        pi_sites.append(0.0 if freqs.sum() < 2 else 1 - np.sum((freqs/freqs.
    vals.append(np.mean(pi_sites)))
return np.array(vals)

pi_vals = pi_window_vals(alignment, starts, window_size)
positions = starts + window_size/2

# 3) Categorize diversity Levels
high_thr = np.percentile(pi_vals, 85)
low_thr = np.percentile(pi_vals, 15)

colors = np.where(pi_vals >= high_thr, "red",
                  np.where(pi_vals <= low_thr, "navy", "olive"))

# 4) Active-site mapping (AA positions)
active_sites_aa = [44, 66, 104, 130, 166, 237, 238]
active_sites_nt = [aa * 3 for aa in active_sites_aa]

# 5) Plotting
fig, ax = plt.subplots(figsize=(16, 6), dpi=300)
sc = ax.scatter(positions, pi_vals, c=colors, s=60, alpha=0.8)

# annotate top 5 peaks
top5 = np.argsort(pi_vals)[-5:]
for idx in top5:
    ax.annotate(f"{pi_vals[idx]:.3f}",
                (positions[idx], pi_vals[idx]),
                textcoords="offset points", xytext=(0, 10),
                ha="center", fontsize= 10, color="darkred")

# draw active-site lines
for aa, nt in zip(active_sites_aa, active_sites_nt):
    ax.axvline(nt, color="orange", linestyle="--", linewidth=1)
    ax.text(nt, ax.get_ylim()[1]*1.02, f"AA{aa}",
            rotation=90, va="bottom", ha="center",
            fontsize=20, color="orange")

# formatting
ax.set_title("Sliding-Window π Across TEM-1 (w=100, step=10)", fontsize=16)
ax.set_xlabel("Alignment position (nt)", fontsize=20)
ax.set_ylabel("Nucleotide diversity π", fontsize=20)
ax.set_xlim(0, L)
ax.set_ylim(0, pi_vals.max()*1.15)
ax.grid(which="major", linestyle="--", alpha=0.4)
ax.grid(which="minor", linestyle=":", alpha=0.2)
ax.minorticks_on()

# custom legend
from matplotlib.lines import Line2D
legend_elements = [
    Line2D([0], [0], marker='o', color='w', label='High π', markerfacecolor='r',
    Line2D([0], [0], marker='o', color='w', label='Mid π', markerfacecolor='c',
    Line2D([0], [0], marker='o', color='w', label='Low π', markerfacecolor='n',
    Line2D([0], [0], linestyle='--', color='orange', label='Active sites')
]
ax.legend(handles=legend_elements, loc="upper right", fontsize=15)

plt.tight_layout()
# save high-res image

```

```
fig.savefig("detailed_sliding_window_pi.png", dpi=300)
plt.show()
```



In [28]: `!pip install nglview biopython`

Requirement already satisfied: nglview in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (3.1.4)
Requirement already satisfied: biopython in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (1.85)
Requirement already satisfied: ipywidgets>=8 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (8.1.7)
Requirement already satisfied: notebook>=7 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (7.4.4)
Requirement already satisfied: jupyterlab>=3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (4.4.4)
Requirement already satisfied: jupyterlab_widgets in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (3.0.15)
Requirement already satisfied: numpy in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (2.2.6)
Requirement already satisfied: comm>=0.1.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets>=8->nglview) (0.2.2)
Requirement already satisfied: ipython>=6.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets>=8->nglview) (9.4.0)
Requirement already satisfied: traitlets>=4.3.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets>=8->nglview) (5.14.3)
Requirement already satisfied: widgetsnbextension~=4.0.14 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets>=8->nglview) (4.0.14)
Requirement already satisfied: colorama in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (0.4.6)
Requirement already satisfied: decorator in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (5.2.1)
Requirement already satisfied: ipython-pygments-lexers in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (1.1.1)
Requirement already satisfied: jedi>=0.16 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (0.19.2)
Requirement already satisfied: matplotlib-inline in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (0.1.7)
Requirement already satisfied: prompt_toolkit<3.1.0,>=3.0.41 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (3.0.51)
Requirement already satisfied: pygments>=2.4.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (2.19.2)
Requirement already satisfied: stack_data in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets>=8->nglview) (0.6.3)
Requirement already satisfied: wcwidth in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from prompt_toolkit<3.1.0,>=3.0.41->ipython>=6.1.0->ipywidgets>=8->nglview) (0.2.13)
Requirement already satisfied: parso<0.9.0,>=0.8.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jedi>=0.16->ipython>=6.1.0->ipywidgets>=8->nglview) (0.8.4)
Requirement already satisfied: async-lru>=1.0.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.0.5)

Requirement already satisfied: httpx>=0.25.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (0.28.1)

Requirement already satisfied: ipykernel>=6.5.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (6.29.5)

Requirement already satisfied: jinja2>=3.0.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (3.1.6)

Requirement already satisfied: jupyter-core in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (5.8.1)

Requirement already satisfied: jupyter-lsp>=2.0.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.2.6)

Requirement already satisfied: jupyter-server<3,>=2.4.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.16.0)

Requirement already satisfied: jupyterlab-server<3,>=2.27.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.27.3)

Requirement already satisfied: notebook-shim>=0.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (0.2.4)

Requirement already satisfied: packaging in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (25.0)

Requirement already satisfied: setuptools>=41.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (80.9.0)

Requirement already satisfied: tornado>=6.2.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (6.5.1)

Requirement already satisfied: anyio>=3.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (4.9.0)

Requirement already satisfied: argon2-cffi>=21.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (25.1.0)

Requirement already satisfied: jupyter-client>=7.4.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (8.6.3)

Requirement already satisfied: jupyter-events>=0.11.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.12.0)

Requirement already satisfied: jupyter-server-terminals>=0.4.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.5.3)

Requirement already satisfied: nbconvert>=6.4.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (7.16.6)

Requirement already satisfied: nbformat>=5.3.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (5.10.4)

Requirement already satisfied: overrides>=5.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (7.7.0)

Requirement already satisfied: prometheus-client>=0.9 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.22.1)

Requirement already satisfied: pywinpty>=2.0.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.0.15)

Requirement already satisfied: pyzmq>=24 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (27.0.0)

Requirement already satisfied: send2trash>=1.8.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.8.3)

Requirement already satisfied: terminado>=0.8.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.18.1)

Requirement already satisfied: websocket-client>=1.7 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.8.0)

Requirement already satisfied: babel>=2.10 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (2.17.0)

Requirement already satisfied: json5>=0.9.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (0.12.0)

Requirement already satisfied: jsonschema>=4.18.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (4.25.0)

Requirement already satisfied: requests>=2.31 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (2.32.4)

Requirement already satisfied: idna>=2.8 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from anyio>=3.1.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (3.10)

Requirement already satisfied: sniffio>=1.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from anyio>=3.1.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.3.1)

Requirement already satisfied: argon2-cffi-bindings in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from argon2-cffi>=21.1->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (21.2.0)

Requirement already satisfied: certifi in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from httpx>=0.25.0->jupyterlab>=3->nglview) (2025.7.14)

Requirement already satisfied: httpcore==1.* in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from httpx>=0.25.0->jupyterlab>=3->nglview) (1.0.9)

Requirement already satisfied: h11>=0.16 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from httpcore==1.*->httpx>=0.25.0->jupyterlab>=3->nglview) (0.16.0)

Requirement already satisfied: debugpy>=1.6.5 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipykernel>=6.5.0->jupyterlab>=3->nglview) (1.8.15)

Requirement already satisfied: nest-asyncio in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipykernel>=6.5.0->jupyterlab>=3->nglview) (1.6.0)

Requirement already satisfied: psutil in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipykernel>=6.5.0->jupyterlab>=3->nglview) (7.0.0)

Requirement already satisfied: MarkupSafe>=2.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jinja2>=3.0.3->jupyterlab>=3->nglview) (3.0.2)

Requirement already satisfied: attrs>=22.2.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema>=4.18.0->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (25.3.0)

Requirement already satisfied: jsonschema-specifications>=2023.03.6 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema>=4.18.0->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (2025.4.1)

Requirement already satisfied: referencing>=0.28.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema>=4.18.0->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (0.36.2)

Requirement already satisfied: rpds-py>=0.7.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema>=4.18.0->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (0.26.0)

Requirement already satisfied: python-dateutil>=2.8.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-client>=7.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.9.0.post0)

Requirement already satisfied: platformdirs>=2.5 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-core->jupyterlab>=3->nglview) (4.3.8)

Requirement already satisfied: pywin32>=300 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-core->jupyterlab>=3->nglview) (311)

Requirement already satisfied: python-json-logger>=2.0.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (3.3.0)

Requirement already satisfied: pyyaml>=5.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (6.0.2)

Requirement already satisfied: rfc3339-validator in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.1.4)

Requirement already satisfied: rfc3986-validator>=0.1.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.1.1)

Requirement already satisfied: fqdn in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.5.1)

Requirement already satisfied: isoduration in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (20.11.0)

Requirement already satisfied: jsonpointer>1.13 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (3.0.0)

Requirement already satisfied: rfc3987-syntax>=1.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.1.0)

Requirement already satisfied: uri-template in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.3.0)

Requirement already satisfied: webcolors>=24.6.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (24.11.1)

Requirement already satisfied: beautifulsoup4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (4.13.4)

Requirement already satisfied: bleach!=5.0.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from bleach[css]!=5.0.0->

nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (6.2.0)
Requirement already satisfied: defusedxml in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.7.1)
Requirement already satisfied: jupyterlab-pygments in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.3.0)
Requirement already satisfied: mistune<4,>=2.0.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (3.1.3)
Requirement already satisfied: nbclient>=0.5.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.10.2)
Requirement already satisfied: pandocfilters>=1.4.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.5.1)
Requirement already satisfied: webencodings in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from bleach!=5.0.0->bleach[css]!=5.0.0->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.5.1)
Requirement already satisfied: tinyccs2<1.5,>=1.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from bleach[css]!=5.0.0->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.4.0)
Requirement already satisfied: fastjsonschema>=2.15 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbformat>=5.3.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.21.1)
Requirement already satisfied: six>=1.5 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from python-dateutil>=2.8.2->jupyter-client>=7.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.17.0)
Requirement already satisfied: charset_normalizer<4,>=2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from requests>=2.31->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (3.4.2)
Requirement already satisfied: urllib3<3,>=1.21.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from requests>=2.31->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (2.5.0)
Requirement already satisfied: lark>=1.2.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from rfc3987-syntax>=1.1.0->jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.2.2)
Requirement already satisfied: cffi>=1.0.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from argon2-cffi-bindings->argon2-cffi>=21.1->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.17.1)
Requirement already satisfied: pycparser in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from cffi>=1.0.1->argon2-cffi-bindings->argon2-cffi>=21.1->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.22)
Requirement already satisfied: soupsieve>1.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from beautifulsoup4->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.7)
Requirement already satisfied: typing-extensions>=4.0.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from beautifulsoup4->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (4.14.1)
Requirement already satisfied: arrow>=0.15.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from isoduration->jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.3.0)
Requirement already satisfied: types-python-dateutil>=2.8.10 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from arr

```
w>=0.15.0->isoduration->jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0
->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.9.0.20250708)
Requirement already satisfied: executing>=1.2.0 in d:\osama\biotec\bioinformatics
\mutation_structural_analysis_ncbi\venv\lib\site-packages (from stack_data->ipython>=6.1.0->ipywidgets>=8->nglview) (2.2.0)
Requirement already satisfied: asttokens>=2.1.0 in d:\osama\biotec\bioinformatics
\mutation_structural_analysis_ncbi\venv\lib\site-packages (from stack_data->ipython>=6.1.0->ipywidgets>=8->nglview) (3.0.0)
Requirement already satisfied: pure-eval in d:\osama\biotec\bioinformatics\mutati
on_structural_analysis_ncbi\venv\lib\site-packages (from stack_data->ipython>=6.
1.0->ipywidgets>=8->nglview) (0.2.3)

WARNING: Ignoring invalid distribution ~umpy (D:\Osama\biotec\Bioinformatics\muta
tion_structural_analysis_ncbi\venv\Lib\site-packages)
WARNING: Ignoring invalid distribution ~umpy (D:\Osama\biotec\Bioinformatics\muta
tion_structural_analysis_ncbi\venv\Lib\site-packages)
WARNING: Ignoring invalid distribution ~umpy (D:\Osama\biotec\Bioinformatics\muta
tion_structural_analysis_ncbi\venv\Lib\site-packages)
```

In [29]: `jupyter-nbextension enable nglview --py --sys-prefix`

'jupyter-nbextension' is not recognized as an internal or external command,
operable program or batch file.

In [30]: `jupyter labextension install nglview-js-widgets`

(Deprecated) Installing extensions with the jupyter labextension install command
is now deprecated and will be removed in a future major version of JupyterLab.

Users should manage prebuilt extensions with package managers like pip and conda,
and extension authors are encouraged to distribute their extensions as prebuilt p
ackages

D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-p
ackages\jupyterlab\debuglog.py:54: UserWarning: An error occurred.

warnings.warn("An error occurred.")

D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-p
ackages\jupyterlab\debuglog.py:55: UserWarning: ValueError: Please install Node.js
and npm before continuing installation. You may be able to install Node.js from y
our package manager, from conda, or directly from the Node.js website ([https://no
dejs.org](https://no
dejs.org)).

warnings.warn(msg[-1].strip())

D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-p
ackages\jupyterlab\debuglog.py:56: UserWarning: See the log file for details: C:\U
sers\osama\AppData\Local\Temp\jupyterlab-debug-ylwdwbx8.log

warnings.warn(f"See the log file for details: {log_path!s}")

In [31]: `%pip install nglview biopython ipywidgets`

Requirement already satisfied: nglview in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (3.1.4)
Requirement already satisfied: biopython in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (1.85)
Requirement already satisfied: ipywidgets in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (8.1.7)
Requirement already satisfied: notebook>=7 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (7.4.4)
Requirement already satisfied: jupyterlab>=3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (4.4.4)
Requirement already satisfied: jupyterlab_widgets in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (3.0.15)
Requirement already satisfied: numpy in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nglview) (2.2.6)
Requirement already satisfied: comm>=0.1.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets) (0.2.2)
Requirement already satisfied: ipython>=6.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets) (9.4.0)
Requirement already satisfied: traitlets>=4.3.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets) (5.1.4.3)
Requirement already satisfied: widgetsnbextension~=4.0.14 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipywidgets) (4.0.14)
Requirement already satisfied: colorama in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (0.4.6)
Requirement already satisfied: decorator in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (5.2.1)
Requirement already satisfied: ipython-pygments-lexers in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (1.1.1)
Requirement already satisfied: jedi>=0.16 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (0.19.2)
Requirement already satisfied: matplotlib-inline in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (0.1.7)
Requirement already satisfied: prompt_toolkit<3.1.0,>=3.0.41 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (3.0.51)
Requirement already satisfied: pygments>=2.4.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (2.19.2)
Requirement already satisfied: stack_data in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipython>=6.1.0->ipywidgets) (0.6.3)
Requirement already satisfied: wcwidth in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from prompt_toolkit<3.1.0,>=3.0.41->ipython>=6.1.0->ipywidgets) (0.2.13)
Requirement already satisfied: parso<0.9.0,>=0.8.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jedi>=0.16->ipython>=6.1.0->ipywidgets) (0.8.4)
Requirement already satisfied: async-lru>=1.0.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.0.5)
Requirement already satisfied: httpx>=0.25.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview)

ew) (0.28.1)
Requirement already satisfied: ipykernel>=6.5.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (6.29.5)
Requirement already satisfied: jinja2>=3.0.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (3.1.6)
Requirement already satisfied: jupyter-core in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (5.8.1)
Requirement already satisfied: jupyter-lsp>=2.0.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.2.6)
Requirement already satisfied: jupyter-server<3,>=2.4.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.16.0)
Requirement already satisfied: jupyterlab-server<3,>=2.27.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (2.27.3)
Requirement already satisfied: notebook-shim>=0.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (0.2.4)
Requirement already satisfied: packaging in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (25.0)
Requirement already satisfied: setuptools>=41.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (80.9.0)
Requirement already satisfied: tornado>=6.2.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab>=3->nglview) (6.5.1)
Requirement already satisfied: anyio>=3.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (4.9.0)
Requirement already satisfied: argon2-cffi>=21.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (25.1.0)
Requirement already satisfied: jupyter-client>=7.4.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (8.6.3)
Requirement already satisfied: jupyter-events>=0.11.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.12.0)
Requirement already satisfied: jupyter-server-terminals>=0.4.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.5.3)
Requirement already satisfied: nbconvert>=6.4.4 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (7.16.6)
Requirement already satisfied: nbformat>=5.3.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (5.10.4)
Requirement already satisfied: overrides>=5.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (7.7.0)
Requirement already satisfied: prometheus-client>=0.9 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.22.1)
Requirement already satisfied: pywinpty>=2.0.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,

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>=2.4.0->jupyterlab>=3->nglview) (2.0.15)
Requirement already satisfied: pyzmq>=24 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (27.0.0)
Requirement already satisfied: send2trash>=1.8.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.8.3)
Requirement already satisfied: terminado>=0.8.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.18.1)
Requirement already satisfied: websocket-client>=1.7 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.8.0)
Requirement already satisfied: babel>=2.10 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (2.17.0)
Requirement already satisfied: json5>=0.9.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (0.12.0)
Requirement already satisfied: jsonschema>=4.18.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (4.25.0)
Requirement already satisfied: requests>=2.31 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (2.32.4)
Requirement already satisfied: idna>=2.8 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from anyio>=3.1.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (3.10)
Requirement already satisfied: sniffio>=1.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from anyio>=3.1.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.3.1)
Requirement already satisfied: argon2-cffi-bindings in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from argon2-cffi>=21.1->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (21.2.0)
Requirement already satisfied: certifi in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from httpx>=0.25.0->jupyterlab>=3->nglview) (2025.7.14)
Requirement already satisfied: httpcore==1.* in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from httpx>=0.25.0->jupyterlab>=3->nglview) (1.0.9)
Requirement already satisfied: h11>=0.16 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from httpcore==1.*->httpx>=0.25.0->jupyterlab>=3->nglview) (0.16.0)
Requirement already satisfied: debugpy>=1.6.5 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipykernel>=6.5.0->jupyterlab>=3->nglview) (1.8.15)
Requirement already satisfied: nest-asyncio in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipykernel>=6.5.0->jupyterlab>=3->nglview) (1.6.0)
Requirement already satisfied: psutil in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from ipykernel>=6.5.0->jupyterlab>=3->nglview) (7.0.0)
Requirement already satisfied: MarkupSafe>=2.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jinja2>=3.0.3->jupyterlab>=3->nglview) (3.0.2)
Requirement already satisfied: attrs>=22.2.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema>=4.18.0->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (25.3.0)
Requirement already satisfied: jsonschema-specifications>=2023.03.6 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (fr
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om jsonschema>=4.18.0->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (202
5.4.1)
Requirement already satisfied: referencing>=0.28.4 in d:\osama\biotec\bioinformat
ics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema>=4.
18.0->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (0.36.2)
Requirement already satisfied: rpds-py>=0.7.1 in d:\osama\biotec\bioinformatics\m
utation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema>=4.18.0-
>jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (0.26.0)
Requirement already satisfied: python-dateutil>=2.8.2 in d:\osama\biotec\bioinfor
matics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-cl
ient>=7.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.9.0.post0)
Requirement already satisfied: platformdirs>=2.5 in d:\osama\biotec\bioinformatic
s\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-core->ju
pyterlab>=3->nglview) (4.3.8)
Requirement already satisfied: pywin32>=300 in d:\osama\biotec\bioinformatics\mut
ation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-core->jupyter
lab>=3->nglview) (311)
Requirement already satisfied: python-json-logger>=2.0.4 in d:\osama\biotec\bioin
formatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-
events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (3.3.0)
Requirement already satisfied: pyyaml>=5.3 in d:\osama\biotec\bioinformatics\muta
tion_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-events>=0.11.0-
->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (6.0.2)
Requirement already satisfied: rfc3339-validator in d:\osama\biotec\bioinformatic
s\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-events>=
0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.1.4)
Requirement already satisfied: rfc3986-validator>=0.1.1 in d:\osama\biotec\bioinf
ormatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jupyter-e
vents>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.1.1)
Requirement already satisfied: fqdn in d:\osama\biotec\bioinformatics\mutation_st
ructural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nongpl]>=4.
18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview
) (1.5.1)
Requirement already satisfied: isoduration in d:\osama\biotec\bioinformatics\muta
tion_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-nong
pl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->ngl
view) (20.11.0)
Requirement already satisfied: jsonpointer>1.13 in d:\osama\biotec\bioinformatics
\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-
nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3
->nglview) (3.0.0)
Requirement already satisfied: rfc3987-syntax>=1.1.0 in d:\osama\biotec\bioinform
atics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-
nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterl
ab>=3->nglview) (1.1.0)
Requirement already satisfied: uri-template in d:\osama\biotec\bioinformatics\mut
ation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[format-non
gpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3-
>nglview) (1.3.0)
Requirement already satisfied: webcolors>=24.6.0 in d:\osama\biotec\bioinformatic
s\mutation_structural_analysis_ncbi\venv\lib\site-packages (from jsonschema[forma
t-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=
3->nglview) (24.11.1)
Requirement already satisfied: beautifulsoup4 in d:\osama\biotec\bioinformatics\m
utation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->j
upyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (4.13.4)
Requirement already satisfied: bleach!=5.0.0 in d:\osama\biotec\bioinformatics\mu
tation_structural_analysis_ncbi\venv\lib\site-packages (from bleach[css]!=5.0.0->
nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (6.2.0)
Requirement already satisfied: defusedxml in d:\osama\biotec\bioinformatics\mutat
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ion_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.7.1)
Requirement already satisfied: jupyterlab-pygments in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.3.0)
Requirement already satisfied: mistune<4,>=2.0.3 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (3.1.3)
Requirement already satisfied: nbclient>=0.5.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.10.2)
Requirement already satisfied: pandocfilters>=1.4.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.5.1)
Requirement already satisfied: webencodings in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from bleach!=5.0.0->bleach[css]!=5.0.0->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (0.5.1)
Requirement already satisfied: tinyccs2<1.5,>=1.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from bleach[css]!=5.0.0->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.4.0)
Requirement already satisfied: fastjsonschema>=2.15 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from nbformat>=5.3.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.21.1)
Requirement already satisfied: six>=1.5 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from python-dateutil>=2.8.2->jupyter-client>=7.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.17.0)
Requirement already satisfied: charset_normalizer<4,>=2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from requests>=2.31->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (3.4.2)
Requirement already satisfied: urllib3<3,>=1.21.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from requests>=2.31->jupyterlab-server<3,>=2.27.1->jupyterlab>=3->nglview) (2.5.0)
Requirement already satisfied: lark>=1.2.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from rfc3987-syntax>=1.1.0->jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.2.2)
Requirement already satisfied: cffi>=1.0.1 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from argon2-cffi-bindings->argon2-cffi>=21.1->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.17.1)
Requirement already satisfied: pycparser in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from cffi>=1.0.1->argon2-cffi-bindings->argon2-cffi>=21.1->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.22)
Requirement already satisfied: soupsieve>1.2 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from beautifulsoup4->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.7)
Requirement already satisfied: typing-extensions>=4.0.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from beautifulsoup4->nbconvert>=6.4.4->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (4.14.1)
Requirement already satisfied: arrow>=0.15.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from isoduration->jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (1.3.0)
Requirement already satisfied: types-python-dateutil>=2.8.10 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from arrow>=0.15.0->isoduration->jsonschema[format-nongpl]>=4.18.0->jupyter-events>=0.11.0->jupyter-server<3,>=2.4.0->jupyterlab>=3->nglview) (2.9.0.20250708)
```

Requirement already satisfied: executing>=1.2.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from stack_data->ipython>=6.1.0->ipywidgets) (2.2.0)
Requirement already satisfied: asttokens>=2.1.0 in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from stack_data->ipython>=6.1.0->ipywidgets) (3.0.0)
Requirement already satisfied: pure-eval in d:\osama\biotec\bioinformatics\mutation_structural_analysis_ncbi\venv\lib\site-packages (from stack_data->ipython>=6.1.0->ipywidgets) (0.2.3)
Note: you may need to restart the kernel to use updated packages.

WARNING: Ignoring invalid distribution ~umpy (D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-packages)
WARNING: Ignoring invalid distribution ~umpy (D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-packages)
WARNING: Ignoring invalid distribution ~umpy (D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-packages)

```
In [1]: import nglview as nv
print("nglview version:", nv.__version__)
```

nglview version: 3.1.4

D:\Osama\biotec\Bioinformatics\mutation_structural_analysis_ncbi\venv\Lib\site-packages\nglview__init__.py:12: UserWarning: pkg_resources is deprecated as an API. See https://setuptools.pypa.io/en/latest/pkg_resources.html. The pkg_resources package is slated for removal as early as 2025-11-30. Refrain from using this package or pin to Setuptools<81.

```
import pkg_resources
```

```
In [2]: from Bio.PDB import PDBList
```

```
pdbl = PDBList()
pdbl.retrieve_pdb_file("1ZG4", pdir=".", file_format="pdb")
```

Downloading PDB structure '1zg4'...

```
Out[2]: '.\\pdb1zg4.ent'
```

```
In [15]: from Bio.PDB import PDBList, PDBParser
import os
```

```
pdbl = PDBList()
pdbl_path = pdbl.retrieve_pdb_file(
    "1ZG4",
    pdir=".",
    file_format="pdb"
)
print("The file was downloaded to:", pdbl_path)
```

```
base = os.path.basename(pdbl_path)           # e.g. 'pdb1zg4.ent'
if base.startswith("pdb") and base.endswith(".ent"):
    new_name = "1zg4.pdb"
    os.rename(pdbl_path, new_name)
    pdbl_path = new_name
    print(" Renamed to:", pdbl_path)
```

```
parser = PDBParser(QUIET=True)
structure = parser.get_structure("TEM1", pdbl_path)
print(" The structure was successfully loaded from:", pdbl_path)
```

```
import nglview as nv
view = nv.show_biopython(structure)
view.clear_representations()
view.add_cartoon(color="lightgrey")
view.add_ball_and_stick(selection="protein", color="grey")
view
```

Structure exists: '.\pdb1zg4.ent'
The file was downloaded to: .\pdb1zg4.ent
Renamed to: 1zg4.pdb
The structure was successfully loaded from: 1zg4.pdb
NGLWidget()

```
In [34]: # قائمة الحفظ الأمينية الحرجة (AA positions)
critical_aas = [44, 66, 104, 130, 166, 237, 238]

for aa in critical_aas:
    view.add_ball_and_stick(
        selection=f"resi {aa} and protein",
        color="lightnavy",
        radius=1.8
    )

view.background = "black" # و "black"
view.parameters = {
    "clipNear": 0.1,
    "clipFar": 1000,
    "lightIntensity": 1.0
}

view.download_image(
    filename="mutations_on_structure.png",
    factor=3
)
```

```
In [35]: import os
from IPython.display import Image, display
view
```

```
NGLWidget(background='black', n_components=1, picked={'atom1': {'index': 18, 'residueIndex': 2, 'resname': 'GL...'}}
```

import os import webbrowser

1) Parameters

```
pdb_id = "1zg4" critical_residues = [44, 66, 104, 130, 166, 237, 238] file_name = "mutations_viewer.html"
```

2) Build the HTML content

```
html = f"""
```

TEM-1 β-lactamase Mutational Mapping

```
Critical residues highlighted: {'join(map(str, critical_residues))}
```

```
.....
```

3) Write the HTML to disk

```
with open(file_name, "w", encoding="utf-8") as f: f.write(html) print(f" ✅ Written interactive viewer to {file_name}")
```

4) Open the file in the default web browser (usually Chrome)

```
path = os.path.abspath(file_name) webbrowser.open_new_tab(f"file:///{{path}}")
```

```
In [33]: view.clear_representations()

view.add_cartoon(color="lightgrey")           # cartoon
view.add_ball_and_stick(color="lightnavy", sele="resi 44-50")
view.add_ribbon(color="navy")                  # ribbon
view.add_licorice(color="green")              # licorice
view.add_line(color="gray")                   # line
view.add_point(color="black")                # point

view.parameters = {"clipNear":0.5, "clipFar":300}
view
```

NGLWidget(n_components=1, picked={'atom1': {'index': 18, 'residueIndex': 2, 'resname': 'GLU', 'x': 6.738999843...

```
In [31]: import os, webbrowser

# 1) PARAMETERS
pdb_id = "1zg4"
critical_residues = [44, 66, 104, 130, 166, 237, 238]
html_file = "mutations_structure.html"

# 2) BUILD THE HTML
html = f"""<!DOCTYPE html>
<html>
<head>
<meta charset="utf-8">
<title>TEM-1 β-lactamase 3D Viewer</title>
<script src="https://cdn.jsdelivr.net/npm/ngl@latest/dist/ngl.js"></script>
<style>
body {{ margin:0; font-family:sans-serif; background:#f0f0f0 }}
#header {{ padding:12px; background:#333; color:#fff }}
#header h1 {{ margin:0; font-size:1.4em }}
#header p {{ margin:4px 0 0; font-size:.95em }}
#viewport {{ width:100vw; height:calc(100vh - 60px) }}
</style>
</head>
<body>
```

```
<div id="header">
    <h1>TEM-1 Mutational Mapping</h1>
    <p>Highlighted residues: {', '.join(map(str, critical_residues))}</p>
</div>
<div id="viewport"></div>
<script>
    const stage = new NGL.Stage("viewport");
    stage.loadFile("rcsb:///{pdb_id}").then(o => {{
        o.addRepresentation("cartoon", {{ color: "lightgrey" }});
        o.addRepresentation("surface", {{color:"lightblue", opacity:0.3}});
        o.addRepresentation("ball+stick", {{{
            sele: "' or '.join(':'+str(r) for r in critical_residues)'",
            color: "crimson",
            radius: 1.4
        }}});
        stage.autoView();
    }});
</script>
</body>
</html>
"""

# 3) WRITE TO DISK
with open(html_file, "w", encoding="utf-8") as f:
    f.write(html)
print("✅ Written standalone HTML to", html_file)

# 4) OPEN IN BROWSER
path = os.path.abspath(html_file)
webbrowser.open(f"file:///path")
```

✅ Written standalone HTML to mutations_structure.html

Out[31]: True

In []: