```
output.txt
test results_nic
    hierarchical
        MenW hierarchical average
          — RMSD-matrix.png
           clusters-hierarchical.txt
           - dendrogram-clustering-average-W.png
            results-hierarchical.txt
           scatterplot-hierarchical.png
         MenW hierarchical complete
           RMSD-matrix.png
            clusters-hierarchical.txt
           dendrogram-clustering-complete-W.png
            results-hierarchical.txt
           scatterplot-hierarchical.png
        MenW_hierarchical_single
           RMSD-matrix.png
           clusters-hierarchical.txt
           - dendrogram-clustering-single-W.png
           scatterplot-hierarchical.png
         MenW hierarchical ward
           - RMSD-matrix.png
           clusters-hierarchical.txt
           dendrogram-clustering-ward-W.png
            results-hierarchical.txt
          — scatterplot-hierarchical.png
         MenY_hierarchical_average
          — RMSD-matrix.png
           clusters-hierarchical.txt
            - dendrogram-clustering-average-Y.png
            results-hierarchical.txt
           scatterplot-hierarchical.png
         MenY hierarchical complete
           – RMSD-matrix.png
           clusters-hierarchical.txt
           dendrogram-clustering-complete-Y.png
           - results-hierarchical.txt
           scatterplot-hierarchical.png
        MenY hierarchical single
           - RMSD-matrix.png
           clusters-hierarchical.txt
           dendrogram-clustering-single-Y.png
           - results-hierarchical.txt
            scatterplot-hierarchical.png
         MenY_hierarchical_ward
            - RMSD-matrix.png
            clusters-hierarchical.txt
           dendrogram-clustering-ward-Y.png
            results-hierarchical.txt
            scatterplot-hierarchical.png
         dendograms
            - dendrogram-clustering-average-W.png
           dendrogram-clustering-average-Y.png
```

```
dendrogram-clustering-complete-W.png
        dendrogram-clustering-complete-Y.png
        dendrogram-clustering-single-W.png
        dendrogram-clustering-ward-W.png
        dendrogram-clustering-ward-Y.png
qt
   MenW(1.5)
      – RMSD-matrix.png
       clusters-qt.txt
      - results-qt.txt
       rmsd-vs-frame.png
      scatterplot-qt.pnq
   MenW(2.5)
     — RMSD-matrix.png
       - clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      — scatterplot-qt.png
   MenW(3.5)
      RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      scatterplot-qt.png
   MenW(4.5)
      - RMSD-matrix.png
      clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      scatterplot-qt.png
   MenY(1.5)
      - RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      scatterplot-qt.png
   MenY(2.5)
      – RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
       - rmsd-vs-frame.png
      - scatterplot-qt.pnq
   MenY(3.5)
     — RMSD-matrix.png
       clusters-qt.txt
      - results-qt.txt
       - rmsd-vs-frame.png
      scatterplot-qt.png
   MenY(4.5)
      - RMSD-matrix.png
      - clusters-qt.txt
      results-qt.txt
       rmsd-vs-frame.png
      scatterplot-qt.pnq
```

```
S3RUY(2.5)
       - RMSD-matrix.png
        clusters-qt.txt
      - results-qt.txt
       rmsd-vs-frame.png
      scatterplot-qt.png
    S3RUY(3.5)
      — RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
       - rmsd-vs-frame.png
      — scatterplot-qt.png
    S3RUY(4.5)
     — RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
     — scatterplot-qt.png
    S6RU6(6.5)
      RMSD-matrix.png
      — clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      scatterplot-qt.png
    S6RU6(7)
      - RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      scatterplot-qt.png
    S6RU6(7.5)
      RMSD-matrix.png
      clusters-qt.txt
      - results-qt.txt
       - rmsd-vs-frame.png
      scatterplot-qt.png
atvector
  - MenW(1.5)
      - RMSD-matrix.png
      - clusters-qtvector.txt
      - results-qtvector.txt
      - rmsd-vs-frame.png
      scatterplot-qtvector.png
   MenW(2.5)
      - RMSD-matrix.png
      clusters-qtvector.txt
      - results-qtvector.txt
      - rmsd-vs-frame.png
      scatterplot-qtvector.png
   MenW(3.5)
     — RMSD-matrix.png
      clusters-qtvector.txt
      results-qtvector.txt
      - rmsd-vs-frame.png
```

```
scatterplot-qtvector.png
MenW(4.5)
 — RMSD-matrix.png
  clusters-qtvector.txt
  - results-qtvector.txt
  - rmsd-vs-frame.png
  scatterplot-qtvector.pnq
MenY(1.5)
  RMSD-matrix.png
  clusters-qtvector.txt
 — results-qtvector txt
   - rmsd-vs-frame.png
  — scatterplot-qtvector.png
MenY(2.5)
 RMSD-matrix.pngclusters-qtvector.txt
 — results-qtvector.txt
   - rmsd-vs-frame.png
 — scatterplot-qtvector.png
MenY(3.5)
 — RMSD-matrix.png
  clusters-qtvector.txt
 — results-qtvector.txt
   - rmsd-vs-frame.png
 — scatterplot-qtvector.png
MenY(4.5)
  — RMSD-matrix.png
  — clusters-qtvector.txt
 — results-qtvector.txt
  - rmsd-vs-frame.png
   scatterplot-qtvector.png
S3RUY(2.5)
  – RMSD-matrix.png
  – clusters-qtvector.txt
  — results-qtvector.txt
  - rmsd-vs-frame.png
 — scatterplot-qtvector.png
S3RUY(3.5)
  RMSD-matrix.png
  clusters-qtvector.txt
 — results-qtvector.txt
   - rmsd-vs-frame.png
  scatterplot-qtvector.png
S3RUY(4.5)
  — RMSD-matrix.png
  clusters-qtvector.txt
  - results-qtvector.txt
   - rmsd-vs-frame.png
 — scatterplot-qtvector.png
S6RU6(6.5)
 — RMSD-matrix.png
  clusters-qtvector.txt
   results-qtvector.txt
  - rmsd-vs-frame.png
```

```
S6RU6(7)

RMSD-matrix.png

clusters-qtvector.txt

results-qtvector.txt

rmsd-vs-frame.png
scatterplot-qtvector.png

S6RU6(7.5)

RMSD-matrix.png
clusters-qtvector.txt
results-qtvector.txt

results-qtvector.txt
scatterplot-qtvector.png
scatterplot-qtvector.png
```

41 directories, 187 files