

EXECUTIVE SUMMARY

- Analysis of 999 Au₂₀ cluster structures
- Best structure identified: 350.xyz
- Best energy: -1557.209460 eV
- Energy is 2.07σ below mean
- 3 structure families identified

DETAILED ENERGY STATISTICS

Mean energy: -1551.249569 eV

Standard deviation: 2.874059 eV

Variance: 8.260214 eV²

Skewness: 1.152175 (positively skewed)

Energy range: 26.301097 eV

Average energy gap (top 50): 0.036140 eV

TOP 10 ELITE STRUCTURES

Rank | Structure | Energy (eV) | ΔE (eV) | Bonds | Shape

1	350.xyz	-1557.209460	0.000000	60	tetrahedron (highly symmetric)
2	351.xyz	-1557.196241	0.013219	60	tetrahedron (highly symmetric)
3	804.xyz	-1556.299794	0.909666	61	icosahedron-like (moderately symmetric)
4	316.xyz	-1555.942377	1.267083	54	star shape (oblate)
5	952.xyz	-1555.942376	1.267084	54	star shape (oblate)

6 | 918.xyz | -1555.942374 | 1.267086 | 54 | star shape (oblate)

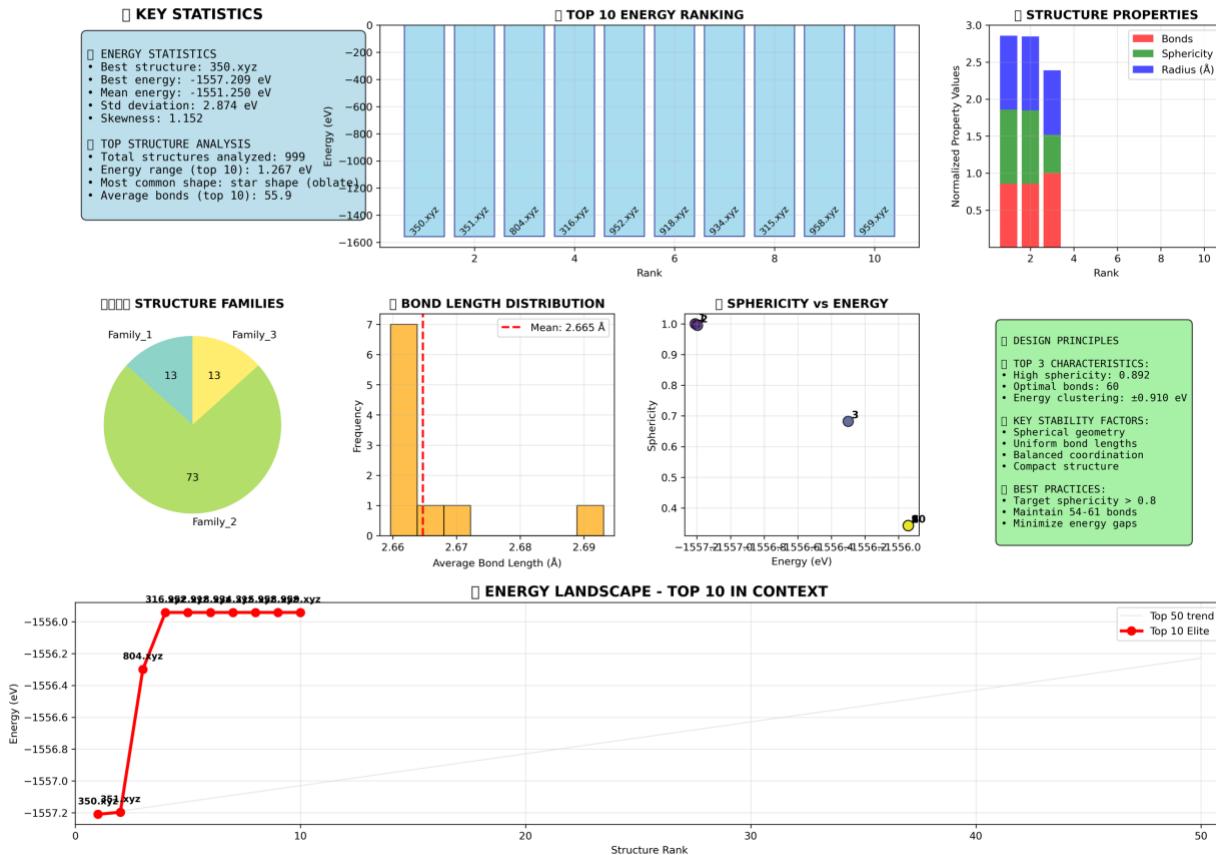
7 | 934.xyz | -1555.942374 | 1.267086 | 54 | star shape (oblate)

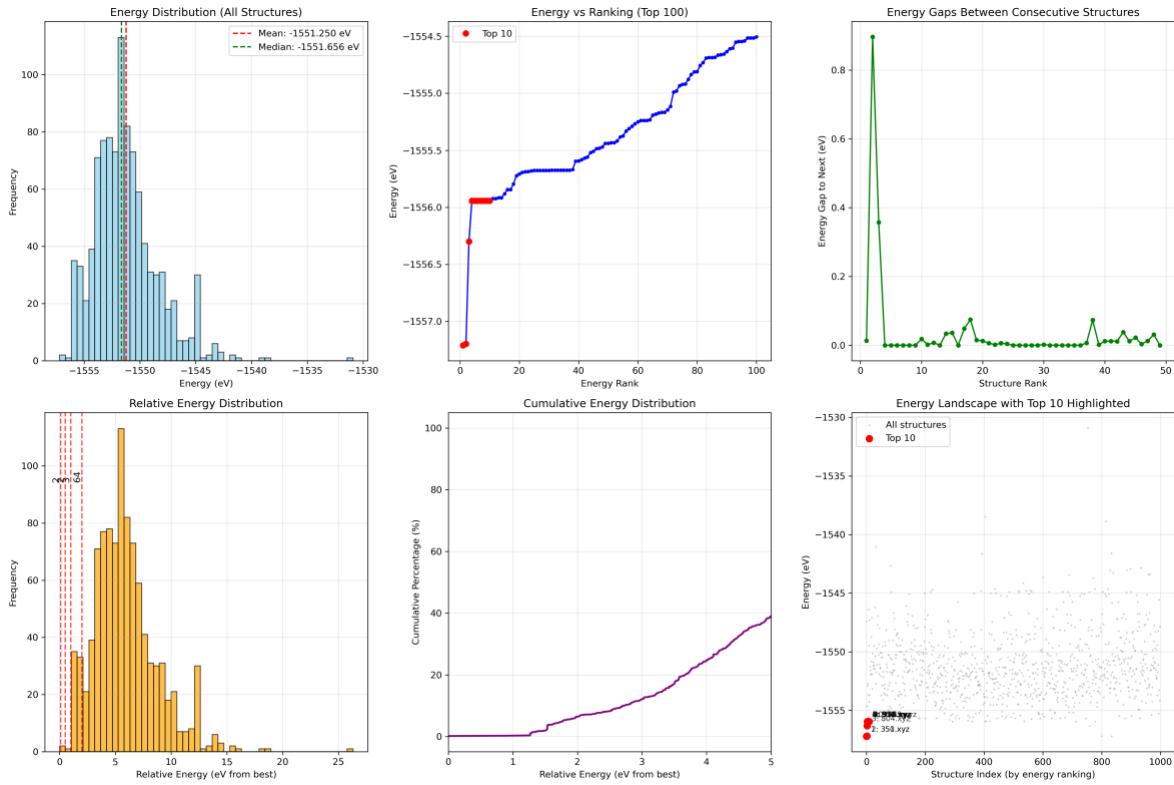
8 | 315.xyz | -1555.942373 | 1.267087 | 54 | star shape (oblate)

9 | 958.xyz | -1555.942367 | 1.267093 | 54 | star shape (oblate)

10 | 959.xyz | -1555.942366 | 1.267094 | 54 | star shape (oblate)

□ TASK 2: COMPREHENSIVE Au₂₀ STRUCTURE ANALYSIS DASHBOARD
Statistical Analysis • Structure Families • Top 10 Elite Ranking • Design Principles





TOP 10 ELITE Au_{20} STRUCTURES - ENERGY RANKING
Atom size \propto coordination number | Gold spheres = Au atoms | Gray lines = bonds

