

## EXECUTIVE SUMMARY

- Analysis of 999 Au<sub>20</sub> 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 eV<sup>2</sup>

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
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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)

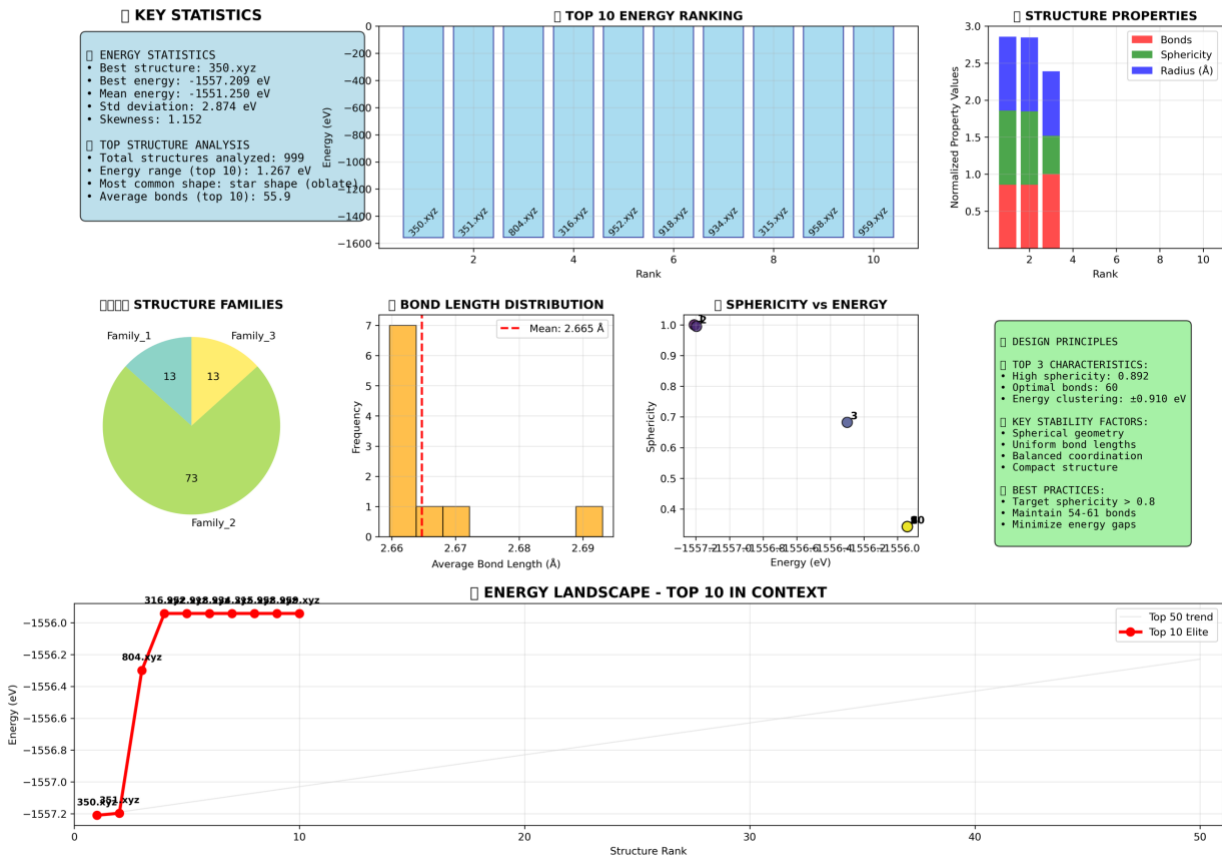
8 | 315.xyz | -1555.942373 | 1.267087 | 54 | star shape (oblate)

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

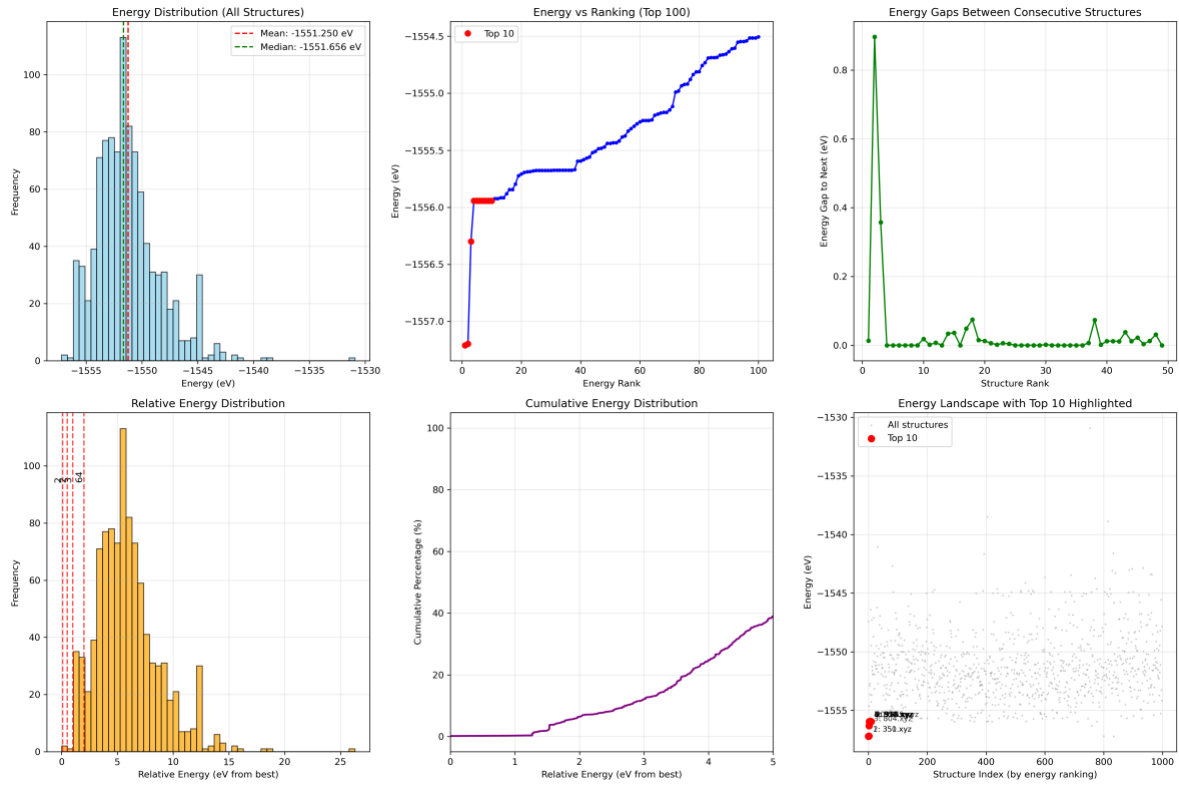
10 | 959.xyz | -1555.942366 | 1.267094 | 54 | star shape (oblate)

TASK 2: COMPREHENSIVE Au<sub>20</sub> STRUCTURE ANALYSIS DASHBOARD

Statistical Analysis • Structure Families • Top 10 Elite Ranking • Design Principles



ENERGY LANDSCAPE - TOP 10 IN CONTEXT



**TOP 10 ELITE Au<sub>20</sub> STRUCTURES - ENERGY RANKING**  
**Atom size  $\propto$  coordination number | Gold spheres = Au atoms | Gray lines = bonds**

