NON CONFIDENTIAL EVIDENCE REPORT

LINUR Conditional Fe S4 Reconstruction Report

Max Planck 9TA4 and 9TA6 regression comparison

4 September 2026

Purpose

This report tests whether the sealed LINUR molecular layers can advance the previously admitted Fe S4 topology to an absolute bond scale and complete local coordinates without using the Max Planck structures as forward inputs.

Topology	Scale	Coordinates	Energy
PASS	**PASS**	**FAIL**	**PENDING**

The two structures were opened in earlier work and are regression references, not a new blind validation.

Executive result

Conclusion. The conditional bond scale passed both frozen regression gates, but the ideal tetrahedral coordinates did not pass the complete local coordinate gate. The missing information is the protein environment that distorts the local Fe S4 centre.

The forward calculation used one independently published ferric tetrathiolate bond scale, the sealed four-coordinate topology and symmetry-derived branch angles. It used no 9TA4 or 9TA6 coordinates, diffraction data, bond lengths, angles or target-specific corrections.

Stage	Status	Evidence meaning
S0 Local topology	PASS	Derived regular tetrahedral coordination at 109.471 degrees; previously admitted.
S1 Bond scale	PASS CONDITIONAL	2.284 plus or minus 0.002 angstrom from an independent synthetic ferric tetrathiolate calibration.
S2 Local coordinates	FAIL	Aligned RMSD 0.1684 and 0.1661 angstrom; both exceed the frozen 0.15 angstrom gate.
S3 Energy and Hessian	NOT RUN	A lawful target-independent molecular coupling model has not yet been supplied.
S4 Conformers	NOT RUN	Continuous conformational completeness and environment coupling remain unresolved.
S5 Protein fold	NOT AUTHORIZED	A local five-atom motif is not a complete protein-fold prediction.

Evidence vocabulary

Term	Meaning in this report
Derived	A consequence of the sealed symmetry topology.
Calibrated	Absolute scale supplied by an independent published reference.
Reconstructed	Coordinates assembled from declared topology, scale and branch inputs.
Measured	The experimental regression structures used only after the prediction was frozen.

Frozen inputs and forward calculation

The forward input was intentionally narrow:

- Connectivity: one Fe centre joined to four thiolate S sites.
- Topology: the sealed N equals 4 centered regular-simplex branch.
- Scale: 2.284 plus or minus 0.002 angstrom from a distinct 1990 synthetic ferric tetrathiolate complex.
- Orientation: symmetry-derived torsions of plus and minus two pi over three.
- Target-specific fitted parameters: zero.

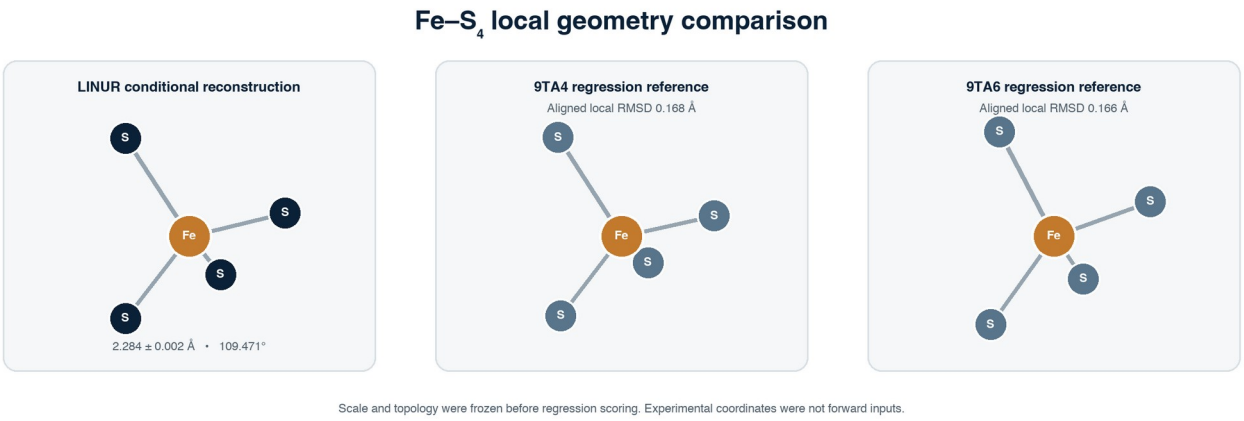

Figure 1 Conditional ideal geometry and aligned regression references

Numerical certificate

The R5BR XV coordinate constructor placed all five atoms and passed its CPU float64 plus complex128 recheck. The maximum relative build-bond residual was 1.13e-16. That certificate proves internal numerical consistency only; it does not convert the calibrated scale into a first-principles bond-length prediction.

Regression comparison

The bond-scale result passed. The stricter complete-coordinate result did not.

Structure	Bond MAE Å	Max bond error Å	Local RMSD Å	Outcome
9TA4	0.0218	0.0364	0.1684	Scale pass Coordinates fail
9TA6	0.0330	0.0688	0.1661	Scale pass Coordinates fail

Why the coordinate gate failed

A regular tetrahedron captures the dominant local coordination but not the unequal Fe S distances and angular distortions created by cysteine side-chain geometry, backbone hydrogen bonding, oxidation state and solvent conditions. Those effects are visible in both regression structures and account for the residual coordinate error.

Next reusable capability

The next operator should couple the Fe S4 centre to its protein environment using only predeclared chemistry and conditions. It must be built target-blind, tested on more than one independent system, and frozen before a genuinely unopened structure is scored. The current failure is retained as the baseline; it must not be erased by a target patch.

R5BR XW independently sealed this as a no-go rather than fabricating a correction. Its missing interfaces are oxidation-dependent metal-thiolate interaction; atom-typed cysteine and backbone mechanics; nonbonded electrostatics, dispersion and exclusions; directional hydrogen bonding; solvent free energy; a bounded continuous conformer solver; and dimensionful energy couplings with provenance and uncertainty.

Public claim boundary

Permitted claim. Given connectivity, a sealed tetrahedral topology and one independent ferric tetrathiolate scale, LINUR reconstructed the dominant local Fe S4 geometry with zero target-specific fits. Bond-length MAE was 0.0218 to 0.0330 angstrom on two regression structures.

Do not claim. The Engine derived absolute SI scale without measurement, reproduced the complete Max Planck structures exactly, predicted a full protein fold, replaced X-ray crystallography, or established new blind validation.

Source and receipts

Independent scale source: Gebhard and colleagues, Journal of the American Chemical Society 112, 2217 to 2231, DOI 10.1021/ja00 162a023. Frozen coordinate result SHA-256 66fc41d4bc702fbd8042a5acc1c5eb1a849d6c7fdc747 709b8ef045a751ca824. R5BR XW ZIP SHA-256 8ad78a5b78d4405b6bdf6bd9c7172bff5066e96 496 324d374ae0eb18b020ea36.