NON CONFIDENTIAL EVIDENCE REPORT

LINUR Rubredoxin Molecular Topology Evidence Report

Coordinate blind transfer and reduced protein response reconstruction

4 September 2026

Purpose

This report separates what LINUR has derived, what transfers to external structures, what works only through a reduced physical adapter, what failed, and what remains blocked by unavailable data. The central result is a zero-fit local coordination-topology transfer across sixteen newly opened structures; it is not a claim of complete protein folding or X-ray electron-density reconstruction.

Valid external structures	Target-specific fits	Median angular MAE	Median topology energy
16 of 16	0	4.97 deg	0.0481

The 30OH and 30OR atomic coordinates were not publicly retrievable when this report was prepared.

Executive evidence summary

The strongest result is local rather than global. The sealed N=4 coordination operator predicts the regular-tetrahedral minimum from connectivity alone. It transferred to every eligible site in a newly opened sixteen-structure Zn-S4 rubredoxin panel. By contrast, a fixed protein elastic network driven only by Fe-S expansion explained little of the measured dose response, and the earlier sequence-to-fold calculation did not recover the complete fold.

Workstream	Outcome	Evidence class	Public meaning
9TA4 and 9TA6 Fe-S4 topology	PASS	Derived topology with post-freeze measured comparison	Strong local molecular geometry result
Sixteen-structure Zn-S4 panel	PASS	Coordinate-blind external transfer	The local topology generalizes without target fitting
Fe-S bond scale	PASS within 0.10 A gate	Reduced empirical UFF adapter	Useful scale estimate, not Engine-derived SI length
Dose-response elastic network	WEAK	Calibrated reduced reconstruction	One local expansion is insufficient for the full response
Complete protein fold	FAIL	Target-free forward model scored after freeze	Do not market as a folding result
30OH and 30OR comparison	PENDING	Frozen coordinate-blind protocol	Predictions preserved until coordinates are public

Evidence vocabulary

Derived means obtained from the stated mathematical operator. Reduced means a compact physical or empirical adapter is used and remains visible. Calibrated means one or more measured quantities fix parameters. Predicted is reserved for a frozen forward result before its target is opened. Measured refers to the deposited experimental structure. These categories are complementary; they are not interchangeable.

Frozen local coordination model

For four neighbours around one centre, R5BR-XS minimizes the normalized orientation functional

$$U4 = \sum_{i<j} [n_i \cdot n_j + 1/3]^2$$

The global minimum is zero when every pair of unit bond directions has dot product −1/3. This gives the regular-tetrahedral angle 109.47122 063 449 069 degrees. The result uses connectivity and orientation only; it contains no bond length, chemical energy scale, temperature, oxidation state or diffraction data.

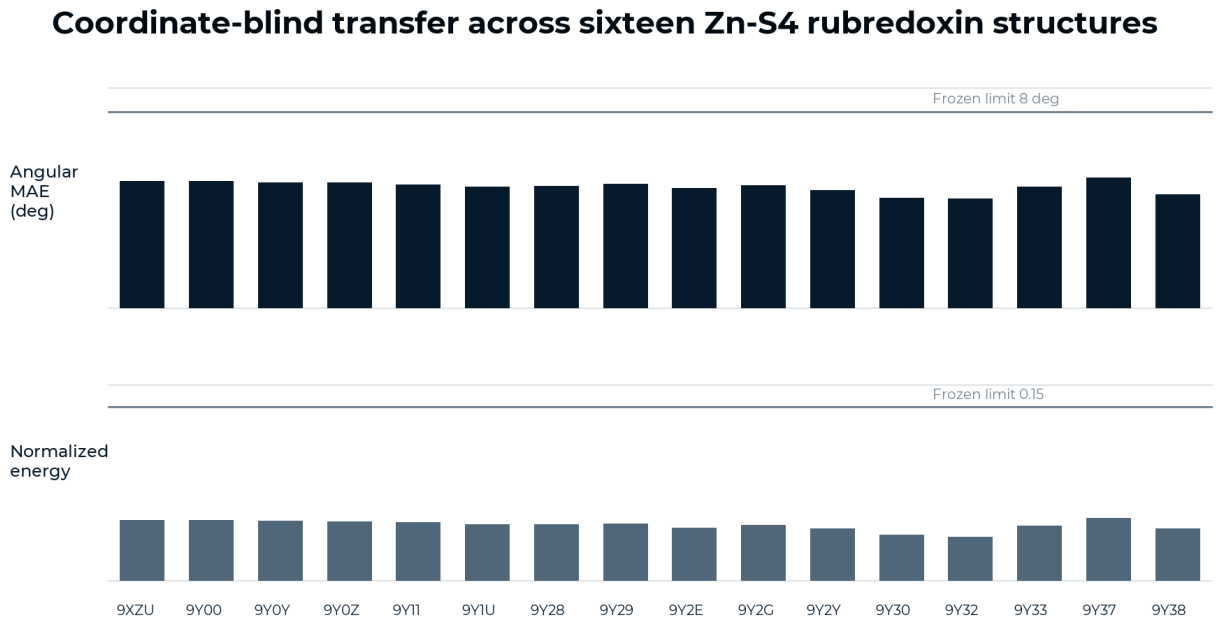
Input	Used by the operator	Excluded from the prediction
Connectivity	One centre and four equivalent neighbours	Atomic coordinates
Geometry variable	Four unit bond directions	Measured bond lengths
Objective	Nonnegative pair-orientation sum of squares	Target-specific coefficients
Output	Ideal angle and normalized topology energy	Absolute SI energy and full protein fold

Earlier blind local comparison

Before accessing the held-out coordinates, the model predicted 109.4712206 degrees. Against the 9TA4 and 9TA6 Fe-S4 sites, the angular MAE was 5.8312 and 5.6825 degrees. The earlier Coulomb-like normalized energy excesses were 0.2930% and 0.2715%, respectively. Those historical numbers remain preserved; the present R5BR-XS energy is a different sum-of-squares quantity and must not be conflated with them.

External sixteen structure transfer

The exact PDB list, topology equation, eligibility rule and panel limits were hashed before coordinate download. All sixteen entries were eligible. Each contains a Zn-S4 centre; therefore this panel tests the scale-free four-coordinate geometry across structures and experimental conditions, not Fe-specific radial physics.



All entries remained below both frozen panel limits. No entry was removed after scoring.

Metric	Frozen limit	Observed panel result	Status
Valid entries	At least 12	16 of 16	PASS
Entry angular MAE	Median <= 8 deg	Median 4.9680 deg; range 4.4316-5.3013	PASS
Normalized U4	Median <= 0.15	Median 0.04808; range 0.03752-0.05345	PASS
Target-specific fits	0	0	PASS

Bond scale and complete fold remain separate

Reduced Fe-S radial estimate

The previous technical package used a general UFF Fe3+2/S_3+2 bond rule to obtain 2.2805 676 413 A before scoring 1YK4. The measured Fe-S bond MAE was 0.019488 A and RMSE was 0.027461 A, passing the predeclared 0.10 A gate. This is a useful reduced empirical result, but the absolute length is not derived from R5BR-XS or from Engine 3 absolute SI physics.

Whole fold negative result

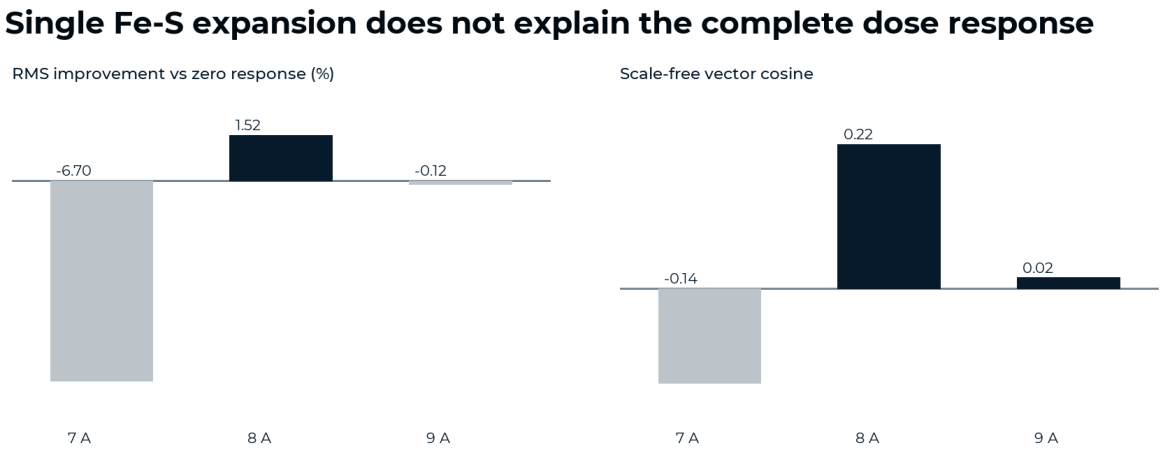
Adding explicit Fe and sulfur pseudo-sites sharply improved the local sulfur topology, reducing the topology excess from 0.247243 to 0.002600, a 98.95% reduction. It did not solve the protein fold. C-alpha RMSD improved only from 9.520497 to 9.061602 A, contact F1 worsened from 0.224719 to 0.209302, and the optimizer did not satisfy its convergence condition. The complete-fold conjunction therefore failed.

Quantity	Baseline	With local Fe-S topology	Interpretation
Sulfur topology excess	0.247243	0.002600	Strong local improvement
C-alpha RMSD	9.520497 A	9.061602 A	Small global improvement
Contact F1	0.224719	0.209302	Global contact map worsened
Complete-fold gate	Not passed	Not passed	Preserved negative result

Public language: LINUR predicts dominant local coordination topology. Do not state that LINUR folded this protein in 0.23 seconds.

Reduced dose response reconstruction

A frozen anisotropic elastic network was built from the measured low-dose 9TA4 coordinates. The only drive was an equal outward Fe-S rest-length change. Three contact cutoffs were declared in advance and all were retained. A second lane used exactly one high-dose scalar, the 0.0365749 A change in the mean Fe-S distance, to set amplitude. No C-alpha displacement was fitted.



Only the 8 A network improved the zero-response RMS, and the gain was just 1.52%.

Cutoff	Vector cosine	RMS change vs zero	Conclusion
7 A	−0.1437	−6.70%	Worse than zero
8 A	0.2189	+1.52%	Weak improvement
9 A	0.0162	−0.12%	Worse than zero

Interpretation: the local Fe-S expansion is real, but a single central expansion does not determine the complete protein-wide displacement field. A defensible next operator must add anisotropic bond weakening, side-chain coupling, occupancy/disorder or explicit dose dynamics before any general radiation-response claim.

Connection to the 0.43 Angstrom article

The 2026 Acta Crystallographica D study “Towards routine accurate electron-density studies of biological macromolecules” reports a 0.43 A rubredoxin data set and compares independent-atom and transferable-aspherical-atom refinements. The published article reports Rwork/Rfree values of 6.82/7.25% for IAM and 6.51/6.93% for TAAM.

Crucially for LINUR, the paper did not assign aspherical factors to the Fe-S4 centre because the required atom types were unavailable in the MATTS databank. Residual density remained around that site, and the authors identified its detailed electronic structure as future quantum-mechanical work. That makes Fe-S4 a legitimate future challenge, but the present topology agreement is not an electron-density solution.

Frozen 30OH and 30OR continuation

Before any coordinate request, LINUR froze the 109.4712206 degree and U4 = 0 predictions, a reduced Fe-S radial estimate, and explicit topology gates for PDB 30OH and 30OR. Public RCSB and PDBe coordinate requests returned no retrievable entries on 4 September 2026. The comparison is therefore paused without altering the frozen predictions.

Required next datum	Permitted use	Still prohibited
Public 30OH and 30OR coordinates	Score frozen local angles and reduced scale	Retuning the topology after inspection
Reflections or map coefficients	Independent scattering comparison after a frozen readout exists	Calling a rendered deposited map a LINUR prediction
Engine geometry-to-scattering operator	Prospective field-to-observable benchmark	Equating normalized topology with electron density

Evidence boundary and next work

Status	What can be said	What cannot be said
Validated	The N=4 local topology transferred to 16 of 16 newly opened Zn-S4 structures with median angular MAE 4.97 deg and zero target fits.	This alone predicts neither scale nor a complete molecule.
Reduced	A general UFF adapter estimated Fe-S scale accurately in the earlier 1YK4 comparison.	The absolute bond length is not yet Engine-derived.
Negative	One Fe-S expansion plus a fixed elastic network barely improved the complete dose response; the whole-fold model failed.	These results must not be marketed as successful protein folding or dynamics.
Pending	The 30OH/30OR protocol is frozen and ready to score when public coordinates become retrievable.	No Max Planck coordinate or electron-density result exists yet.

Recommended development sequence

- Score the unchanged 30OH and 30OR local predictions when the deposited coordinates become public.
- Derive a bond-scale operator tied to the Engine action and physical SI interface, then test it without UFF.
- Build a target-blind anisotropic damage operator and require transfer across more than one protein or dose series.
- Only after a field-to-scattering readout is frozen should LINUR compare calculated structure factors, held-out reflections and maps.

Primary sources

Paknia E et al. Towards routine accurate electron-density studies of biological macromolecules. Acta Cryst D 82 (2026) 1044-1055. DOI 10.1107/S2059798326007448.

Bourenkov G et al. Radiation damage in sub-Angstrom resolution macromolecular crystallography: a low-dose study. Acta Cryst D 82 (2026) 484-491. DOI 10.1107/S205979832600269X. PDB 9TA4 and 9TA6.

Some Like It Hot - Structural Changes in Extremophile Rubredoxin at 120 C. Angew Chem Int Ed (2026). DOI 10.1002/anie.202520302. PDB entries listed in the frozen protocol.

Machine-readable results, prefreeze hashes, scripts and detached verification receipts are stored in the accompanying LINUR evidence packages.