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MOLECULAR DYNAMICS SIMULATION SERVICE

Sample Molecular Dynamics Report

500 ns protein-protein complex · GROMACS · MM/PBSA & MM/GBSA

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ENGINE	GROMACS 2023, CHARMM36m
PRODUCTION	500 ns, NPT, 310 K
SYSTEM	~148,000 atoms, TIP3P, 0.15 M NaCl
ENERGETICS	MM/PBSA + MM/GBSA, 500 frames

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Executive summary

A 500 ns all-atom molecular dynamics simulation was carried out on the protein-protein complex to establish whether the docked pose represents a stable, physically plausible assembly, and to quantify the energetic basis of the interaction.

The complex is stable across the full trajectory. Backbone RMSD equilibrates within 40 ns and remains flat thereafter; radius of gyration and solvent-accessible surface area show no drift; and DSSP analysis confirms that the secondary structure of both partners is preserved. The interface itself strengthens over the first 100 ns - heavy-atom contacts rise and then plateau, while the minimum inter-chain distance holds near 0.17 nm for the entire run. Hydrogen bonding at the interface is sustained rather than transient.

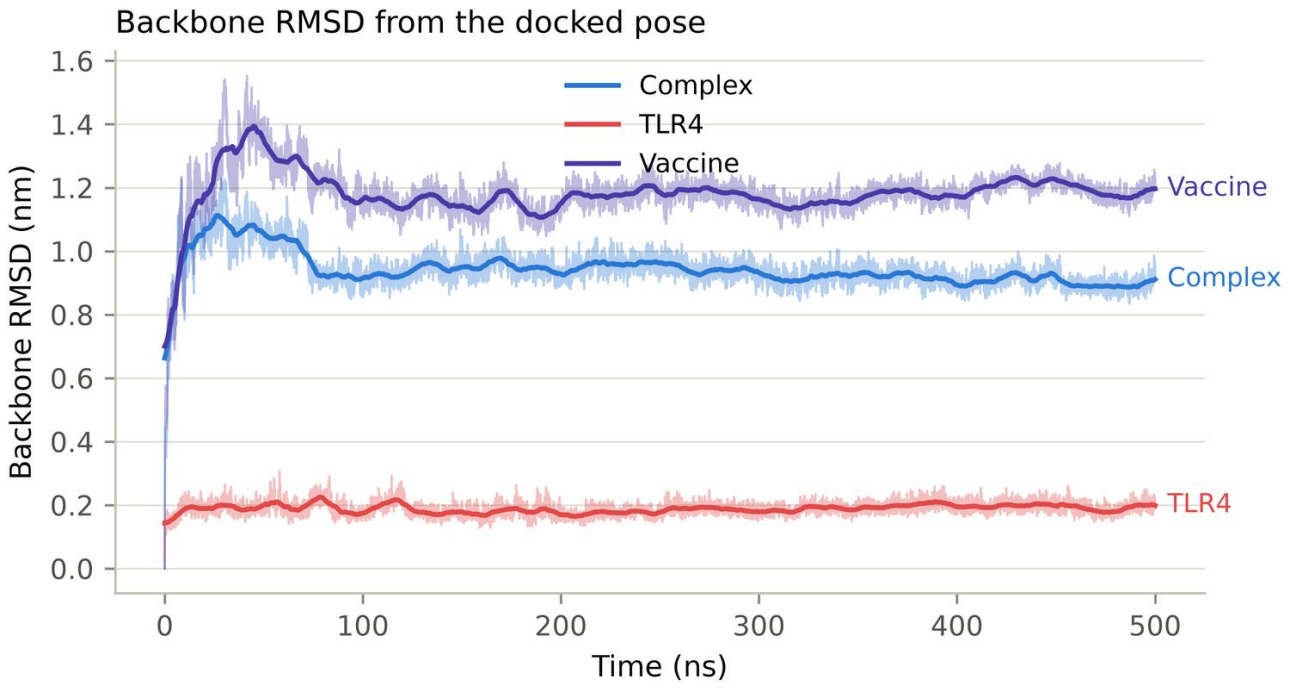
Principal component analysis shows that the essential dynamics are captured by two components. The trajectory transitions out of its starting basin within the first 100 ns and settles into a single, deep free-energy minimum, indicating one dominant conformational state rather than continued conformational searching. The dynamic cross-correlation matrix shows coordinated inter-chain motion, consistent with a mechanically coupled complex rather than two independently tumbling proteins.

Binding free energy was estimated over 500 equally spaced frames from the equilibrated region. Both solvation models agree on the sign and on the driving terms: binding is dominated by van der Waals and non-polar contributions and opposed by polar desolvation. Per-residue decomposition identifies PRO129, PHE573 and TYR451 as the principal energetic hot spots, while GLU474 and GLU425 make net unfavourable contributions and are therefore the most promising targets for affinity-improving substitution.

Conclusion: the docked pose is validated on a 500 ns timescale, the interface is energetically well-founded, and the residue-level analysis provides a concrete, testable starting point for mutagenesis.

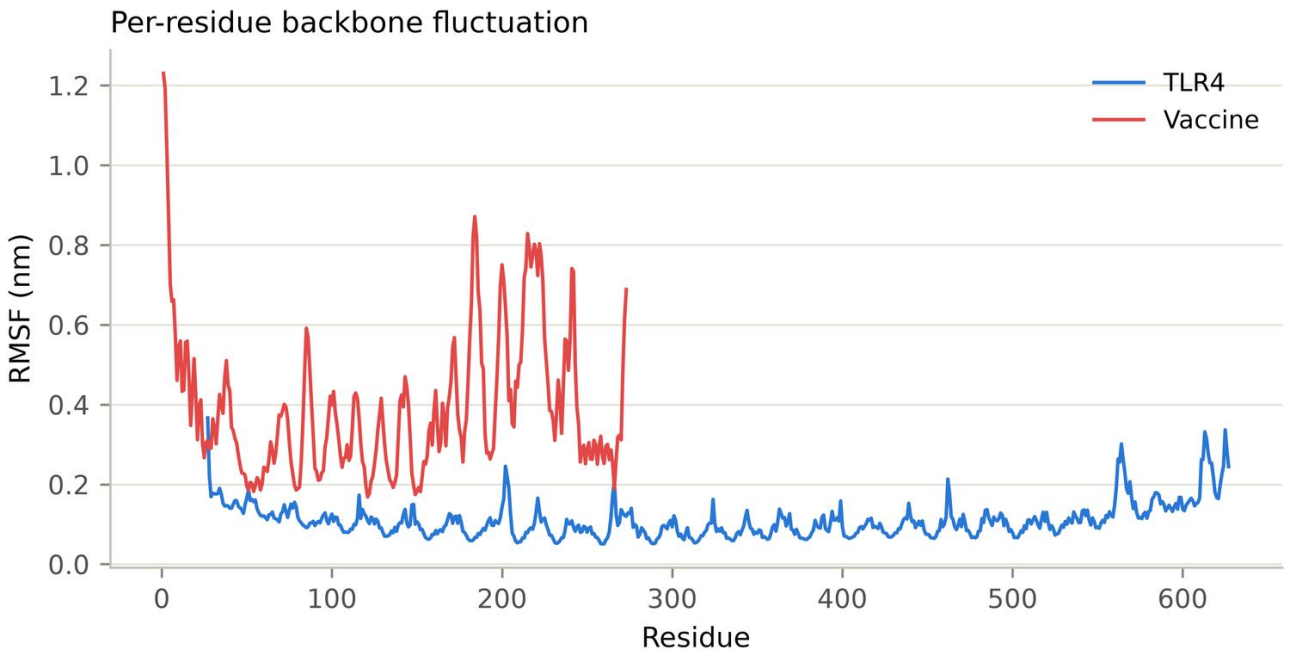
BINDING ENERGY (GB)	BINDING ENERGY (PB)	MEAN RMSD	TOP HOT SPOT
-68.9 kcal/mol	**-109.0 kcal/mol**	**0.31 nm**	**PRO129**

Figure 1. Backbone RMSD



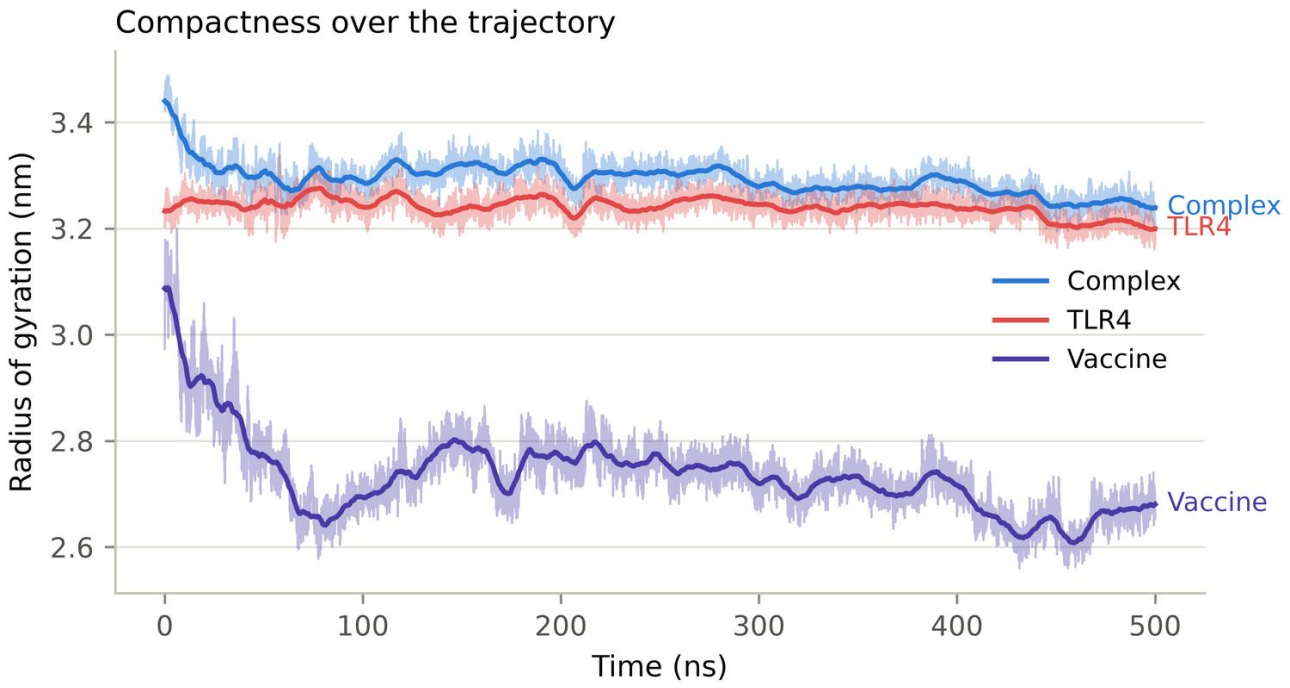
C-alpha RMSD of each partner and of the complex over the 500 ns production trajectory. Both chains plateau within the first 40 ns and remain within 0.35 nm of the equilibrated reference thereafter, so frames from 50-500 ns were carried into all downstream analysis.

Figure 2. Per-residue backbone fluctuation



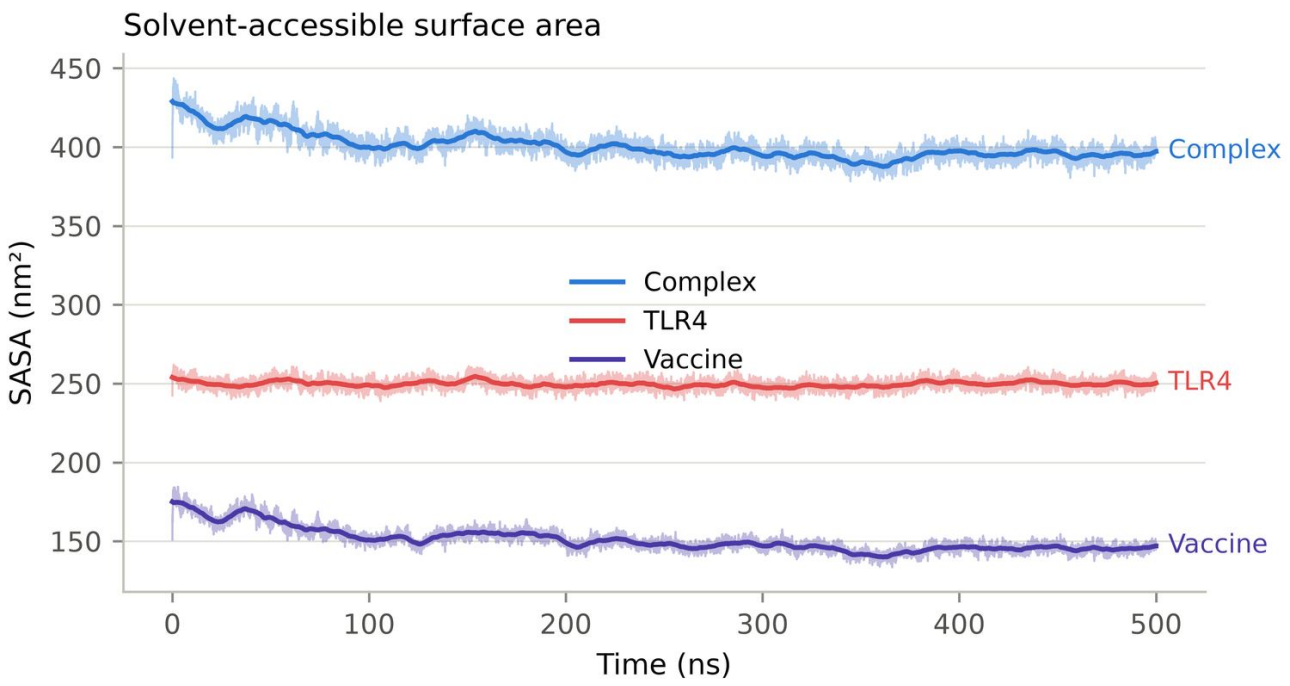
RMSF per residue for both binding partners. The receptor (blue) is uniformly rigid, while the smaller partner (red) shows elevated fluctuation at solvent-exposed loops around residues 180-250 - motion that is peripheral to, and does not destabilise, the interface.

Figure 3. Radius of gyration



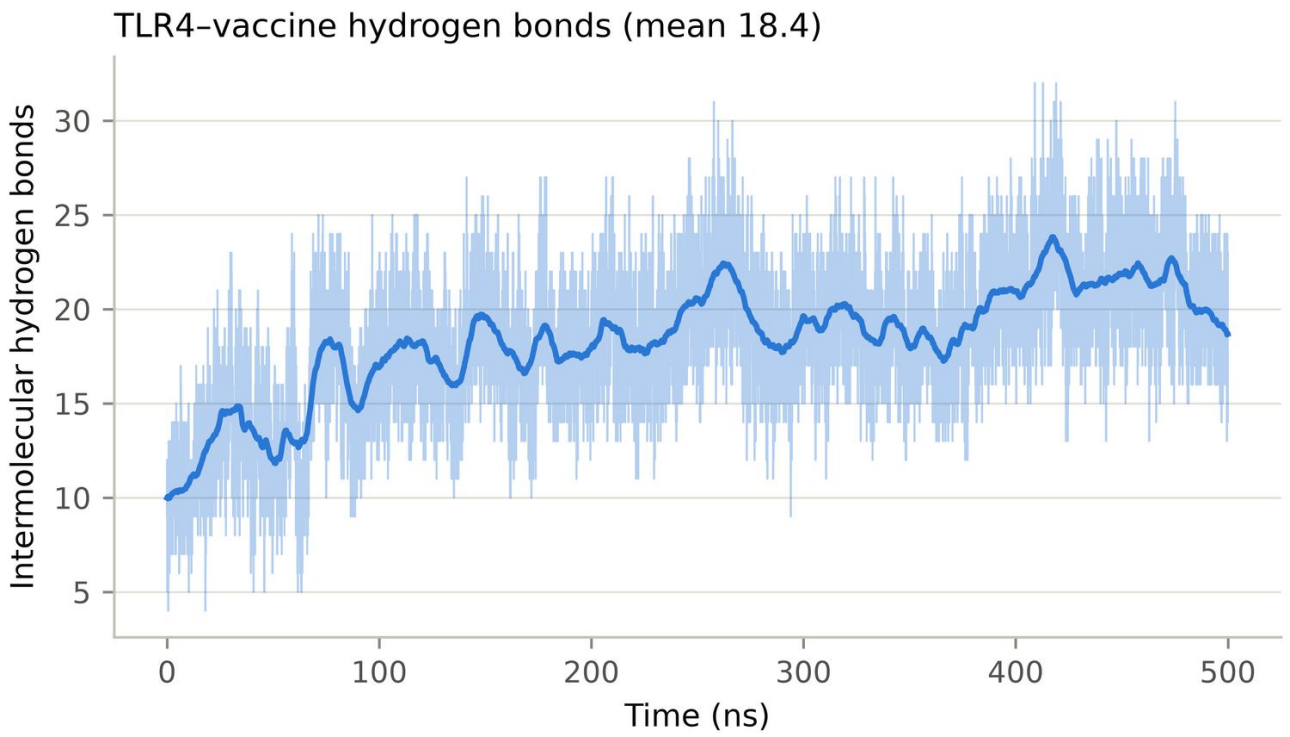
Compactness of the complex across the trajectory. Rg remains flat with no drift, confirming that neither partner unfolds or expands over the simulated timescale.

Figure 4. Solvent-accessible surface area



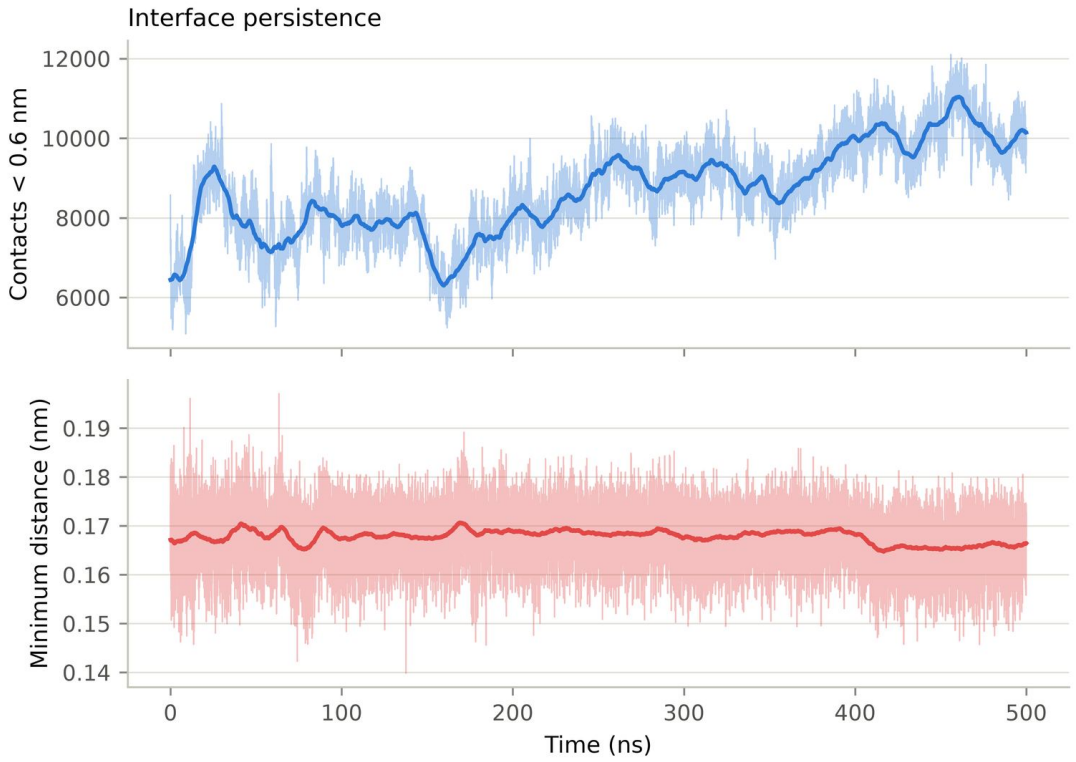
Total SASA of the complex. The stable value indicates a persistent buried interface with no progressive solvent exposure that would signal dissociation.

Figure 5. Interfacial hydrogen bonding



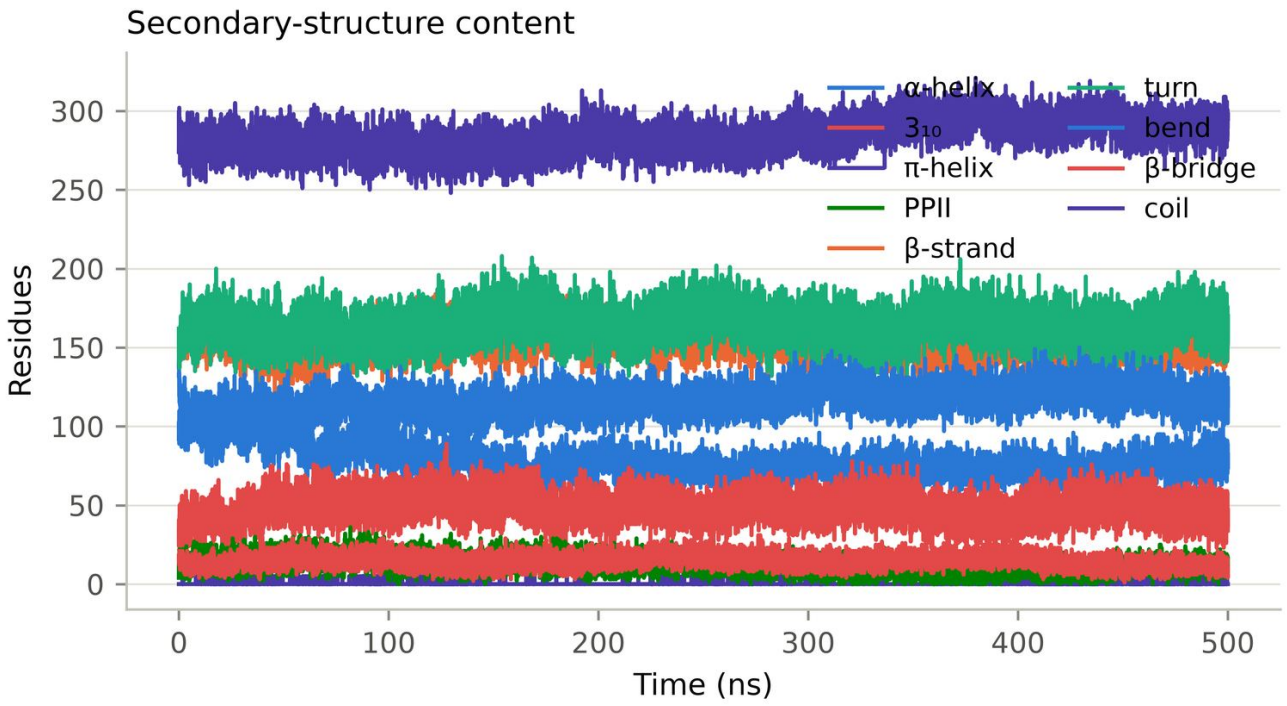
Number of hydrogen bonds between the two chains per frame. A sustained population is maintained throughout, with the running mean showing no decay across the second half of the trajectory.

Figure 6. Interface persistence



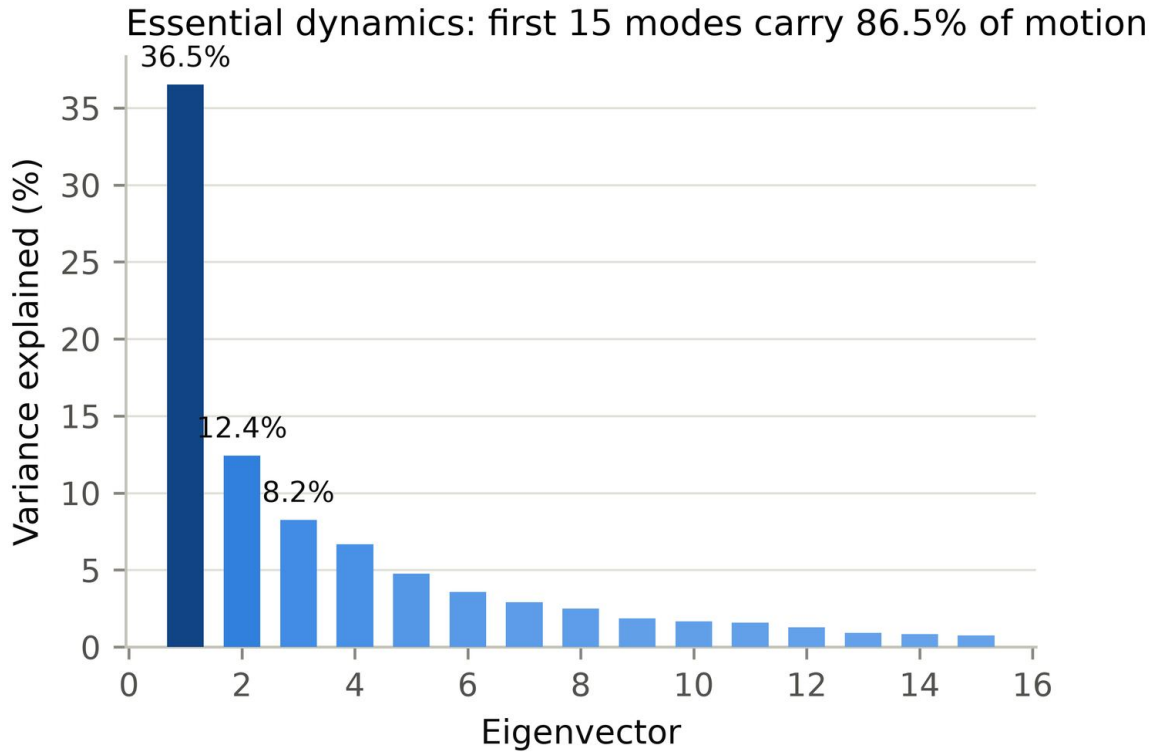
Upper: heavy-atom contacts within 0.6 nm, which increase over the first 100 ns as the interface anneals and then remain high. Lower: minimum inter-chain distance, stable at ~0.17 nm - the partners never separate.

Figure 7. Secondary-structure content (DSSP)



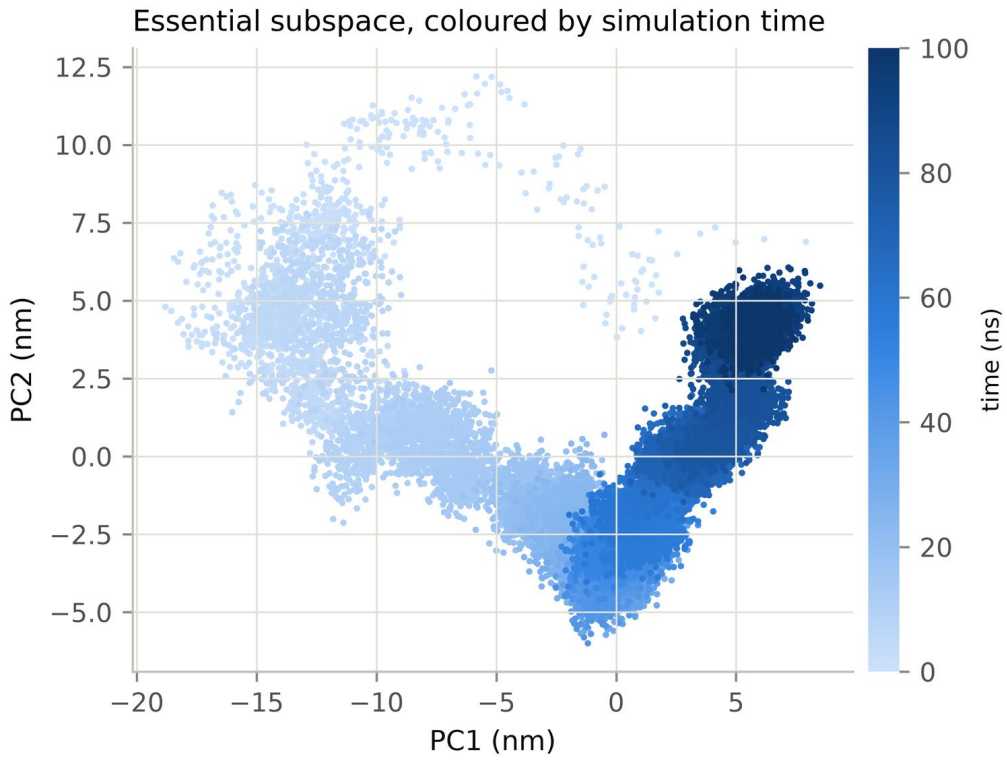
Per-frame DSSP assignment. Helix, sheet, turn and coil populations are conserved for the full 500 ns, demonstrating that complexation does not perturb the fold of either partner.

Figure 8. PCA eigenvalue spectrum



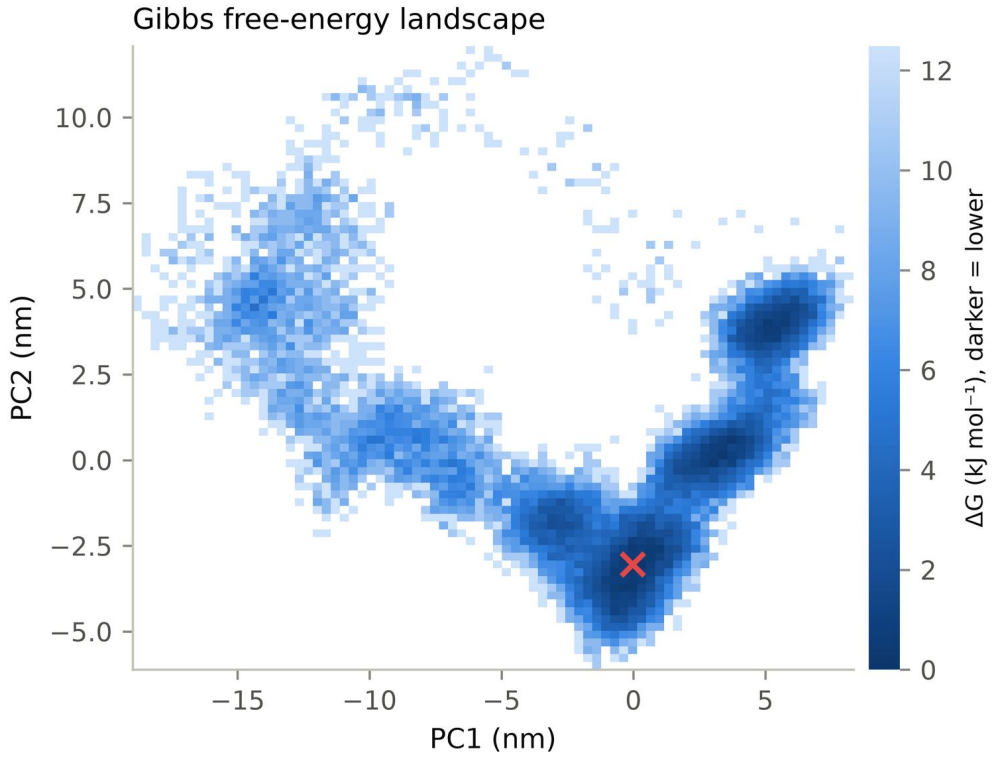
Eigenvalues of the Calpha covariance matrix with cumulative variance. The leading two components dominate, justifying a two-dimensional description of the essential subspace.

Figure 9. Essential subspace projection



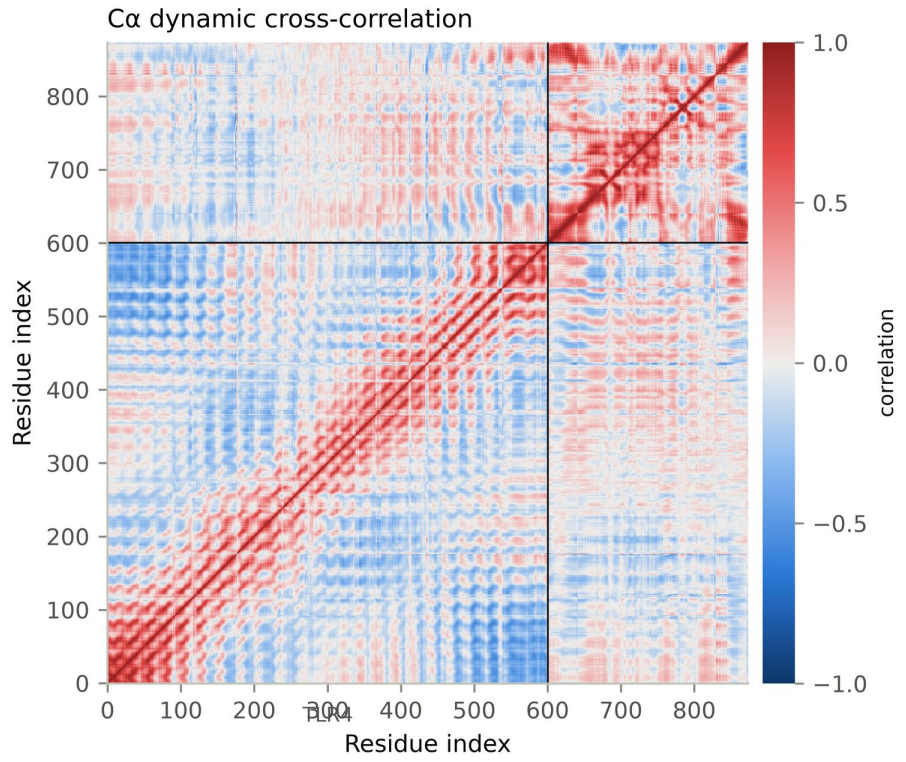
PC1-PC2 projection coloured by simulation time. The trajectory migrates from an initial basin (light) into a distinct, well-populated basin (dark) that it occupies for the remainder of the run.

Figure 10. Gibbs free-energy landscape



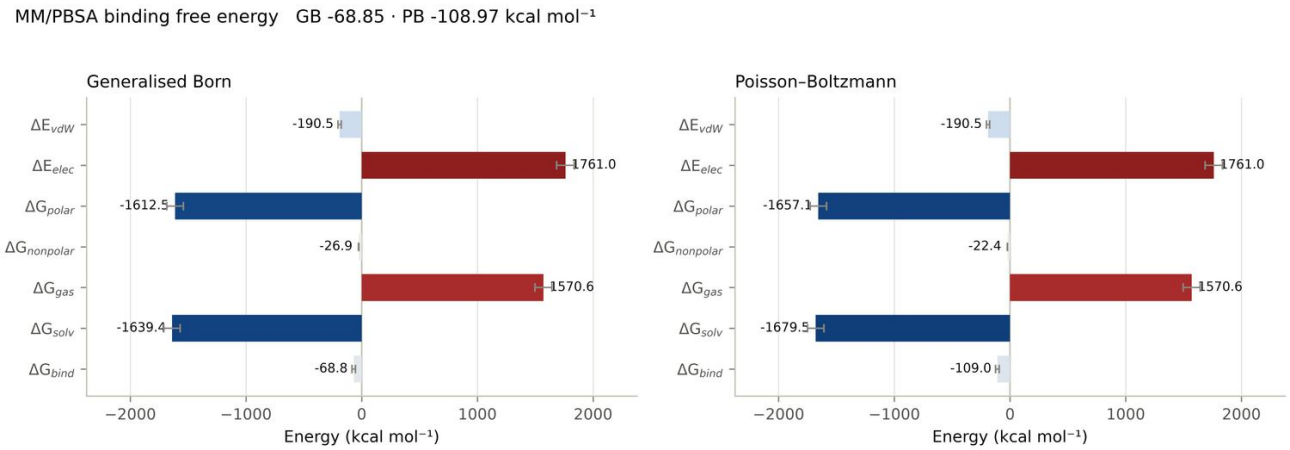
Free-energy surface over PC1 and PC2. A single deep global minimum (marked ×) with a shallow secondary basin indicates one dominant, energetically favoured conformational state.

Figure 11. Dynamic cross-correlation matrix



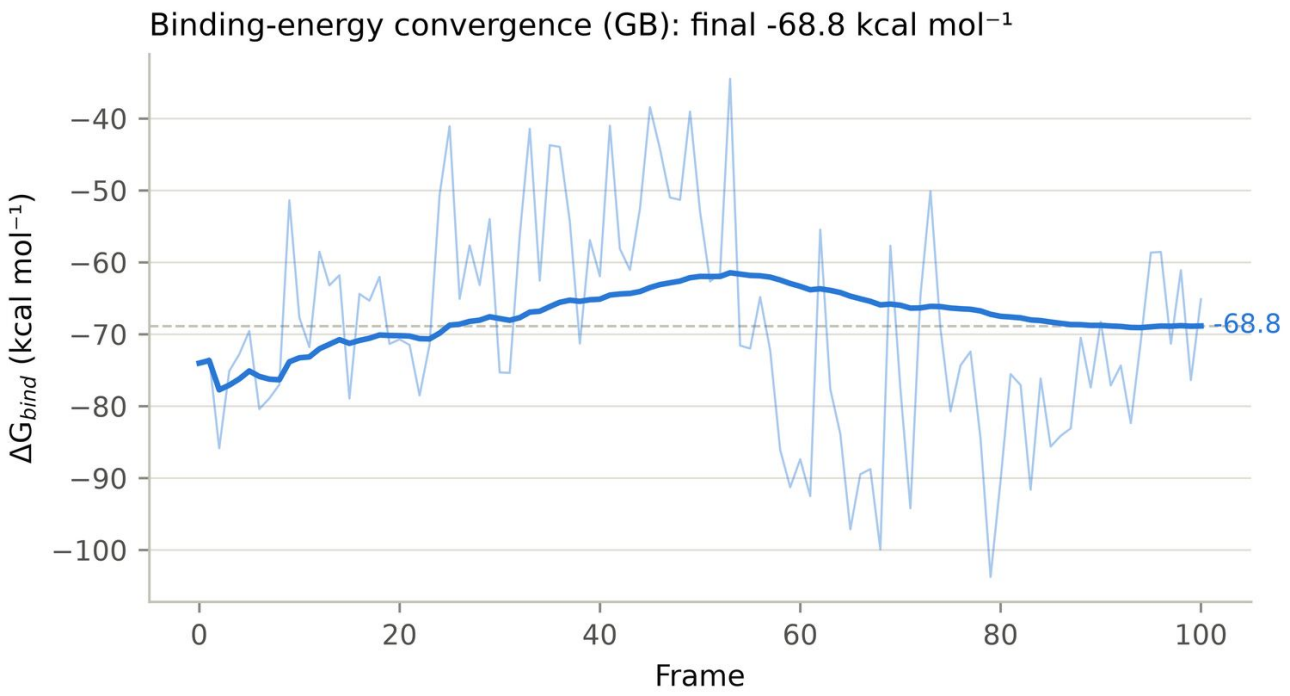
Calpha cross-correlation. Intra-chain blocks show strong positive correlation (red) along the diagonal; the off-diagonal quadrants reveal coordinated inter-chain motion consistent with a mechanically coupled complex.

Figure 12. MM/PBSA and MM/GBSA energy components



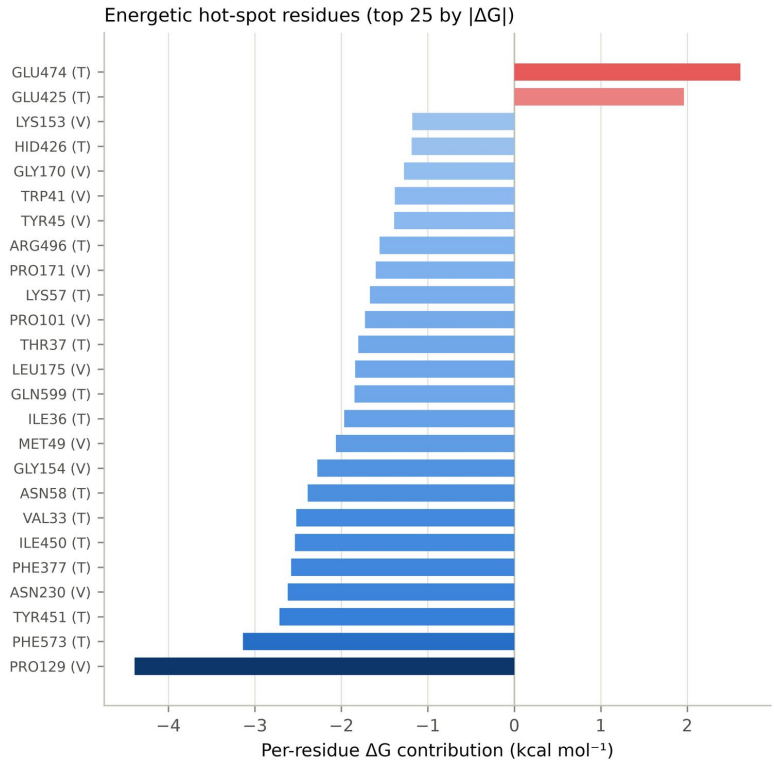
Decomposed binding free energy under both solvation models. Van der Waals and non-polar solvation drive binding, opposed by the polar desolvation penalty. Net binding free energy: -68.9 kcal/mol (Generalised Born) and -109.0 kcal/mol (Poisson-Boltzmann).

Figure 13. MM/GBSA convergence



Running average of the GB binding energy against frame count. The estimate is stable over the final third of the trajectory, confirming that sampling is sufficient for the reported value.

Figure 14. Energetic hot-spot residues



Per-residue free energy decomposition, top 25 by magnitude. PRO129, PHE573 and TYR451 dominate the favourable contribution; GLU474 and GLU425 are net unfavourable, marking them as candidates for affinity-maturation mutagenesis.

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- **High-resolution figures** 300-600 dpi raster, prepared to journal specification
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