

Summary of integrative structure determination of Integrative structure of Gaussia Luciferase "open" and "closed" structural states from NMR data (PDB ID: 9A8V | pdb_00009a8v)

1. Model Composition	
1.1. Entry composition	Luciferase: chain(s) A (168 residues)
1.2. Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, BMRB: 36385 - NMR data, Zenodo: 10.5281/zenodo.13831427 - NMR data, Zenodo: 10.5281/zenodo.13831427 - NMR data, Zenodo: 10.5281/zenodo.13831427 - NMR data, Zenodo: 10.5281/zenodo.13831427
2. Representation	
2.1. Number of representations	1
2.2. Scale	Atomic
2.3. Number of rigid and flexible segments	0, 1
3. Restraints	
3.1. Physical principles	Information about physical principles was not provided
3.2. Experimental data	
4. Validation	
4.2. Number of ensembles	0
4.3. Number of models in ensembles	Not applicable
4.4. Number of deposited models	10
4.5. Model precision	Not available
4.6. Data quality	Data quality has not been assessed
4.7. Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 5.87-12.92 - Ramachandran outliers: 1-15 - Sidechain outliers: 1-9
4.8. Fit to data used for modeling	Fit of model to information used to compute it has not been determined
4.9. Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. 5.1. Method name	modeling

<u>5.3. Method description</u>	AFsample modeling calculations were carried out using modified version of AlphaFold v2.2.0. AFsample calculations, which use six different settings with network dropouts to create conformational heterogeneity, were carried out to generate ~6000 models
2. <u>5.1. Method name</u>	modeling
<u>5.3. Method description</u>	A modified version of AlphaFold v2.2.0 used by AFsample. AF2 was trained using the PDB database of 2018-04-30 and did not include any NMR structures in the training data.
<u>5.5. Software</u>	<ul style="list-style-type: none"> - <u>Protein Structure Validation Software</u> (version 2.0) - <u>DoubleRecall</u> (version 1.0) - <u>RPF server</u> (version ASDP ver 1.0) - <u>AISAR</u> (version 1.0) - <u>AFsample</u> (version Not available) - <u>AlphaFold2</u> (version 2.2.0) - <u>RCI</u> (version Not available)