

Summary of integrative structure determination of Invariant surface glycoprotein 65 of Trypanosoma brucei gambiense (PDB ID: 9A3G, PDB-Dev ID: PDBDEV_00000201)

1. Model Composition	
Entry composition	Invariant surface glycoprotein 65: chain(s) A (420 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 3DEM volume, EMDB: EMD-14707 - Mass Spectrometry data, PRIDE: PXD033606 - Experimental model, PDB: 7ZGJ - De Novo model, Not available - De Novo model, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 7
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 2 unique EM3DRestraint: SSM and convolution-based shape searches using Phenix Dock-in-map, Real-space refinement using Phenix, manual refinements using Coot (where applicable) - 1 unique CrossLinkRestraint: CYS, 3 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 29.23 - Ramachandran outliers: 52 - Sidechain outliers: 25
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
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. Name	AlphaFold model prediction
2. Name	Modelling
3. Name	Refinement
Software	<ul style="list-style-type: none">- AlphaFold2 (version Not available)- Coot (version Not available)- Phenix (version Not available)